Material
& Structure
Analysis Suite

Z-set

Materials manual
Version 9.1

Z-set software is distributed by

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Contents

Chapter 1

Introduction

What's in this manual

Description:
This Z-mat user-commands handbook covers the command syntax and some of the details for the different files related to use of Z-mat. This includes the material behaviors, utilities and extra programs, and interfaces to the different FEA codes which Z-mat works with.

For users who are interested only in the Z-mat interface to another FEA solver the primary source of information will be in the **Examples/Training** and this **Z-mat User commands** manual. There is supplementary information in the other books however, such as user development, and model theory. The Zmaster program has increasingly expanded its capabilities, and will continue to explore new interfaces with other software products, The Post computations section in the **Z-set** manual also has information on making batch post computations of imported results from various codes.

Handbook Summary:
The following list summarizes the documentation for all of Z-set. As part of our 8.2/8.3 developments, greatly expanding the software documentation is one of our primary goals.

The list below is sorted in what we feel would be an appropriate sequence for the normal user, starting with installation and reviewing capabilities, to creating input files and eventually scripting and developing add-ons to the software.

Release Notes/Zmaster The basic overview of the software, installation instructions, and documentation for the graphical user interface Zmaster on all platforms. The Zmaster manual also now covers all the base reference chapters such as environment variables, user parameters, function reference, command line programs, etc.

Examples/Training This book is essentially the "getting started" documentation for the software. The book describes Z-mat, simulation, optimization, material models, and the FEA code use. The examples cover setup of complete models, and are meant to demonstrate the capabilities with relatively simple examples.

Z-mat User commands This summarizes the command file formats and capabilities of the Z-mat interface, simulation, optimization and material files for all of Z-mat and Z-set.

Z-set User commands This summarizes the command file formats for the FEA related capabilities including meshing, FEA solution, post processing, etc.

Developer A guide to the user-extensible features of the software, including scripting, ZebFront material model development, making plugins, and the C++ programming API.

Plugins A guide to add-on features available.

Theory Theory manual covering formulations (under development).

Conventions

This page summarizes the conventions used for the Z-set input files. An overview of the general command syntax (command hierarchies) is given in the beginning of the *Examples/Training* manual.

- Running of Z-set modules generally requires that a "problem name" be given. Most input and output data files are based on this name with a variety of suffixes attached. Henceforth, *problem* will often be used to indicate the problem name given while running the commands.

- The characters `%` and `#` indicate that the rest of the line is a comment. For example:
  ```
  ***load % external problem loading
  ```

- There are no abbreviations allowed in the use of keywords. All keywords and command names must be written entirely.

- The admissible characters for the names of user variables are: `a-z, A-Z, ", +, -, *, ., =, /, _, ), (, \, ~`

- The text entry is *always* case-sensitive.

- The use of braces `[ ]` in the syntax descriptions indicates an option with a default definition.

- All parameter values used in the input files and described as "real" in the syntax descriptions must have a decimal point. All standard specifications of floating point values are accepted. Two examples of real values are: `3.0  4.2e-5`

- The use of parenthesis `()` indicates data input of real values in vector form. An example is: `(0.1 0.2 1.0)`. In most cases the size of such vectors must be compatible with the overall problem dimension.

The symbol indicates a section where the calculation is sensitive to input data or format.

Introduction to Z-mat

Starting with version 7.2 of Zebulon (approx 1997), the program has been modularized into components relating to finite element methods, and components for material simulation and optimization. These later programs are grouped into Z-mat which, while of course is natively implemented with all of Z-set, also includes interfaces to other codes. One of the more interesting aspects of this is to be able to use Z-set material behaviors as an "extension set" to codes which support user materials such as ABAQUS/Standard, ABAQUS/Explicit, ANSYS, LS-Dyna, MARC, and Cosmos/M.

The Z-mat product is thus mainly a library of material behavior routines (constitutive equations) which can be interfaced with FEA software, and its supporting utilities. In contrast with other FEA software products however, Z-set and Z-mat are built on C++ with a strong object-oriented design, and many utility programming classes for advanced tensorial mathematics. Such advanced program design techniques have enabled the software to be enormously extensible, on many different levels of sophistication.

In developing extensions to Z-mat, a user can make new behaviors using the many abstract "building bricks" to create a modular, flexible model based on *fundamentals.* For final use, we then let the different implemented "bricks" define the specifics. That is to say, the user always chooses the final model form (e.g specific evolution or state equations) in the input file, after development is finished. In that way, each model is really a "model class" or framework within which a user has a high degree of flexibility. One can also add to the "types" available for these building bricks. This not only lets one work on a smaller specific aspect, but allows extending the capabilities of *every model* using that particular "abstract" type. In this book, examples of the general behavior frameworks are the subject of the chapters *Material Models* (page 10.2) *Secondary Models* (page 11.2) and *Other Models* (page 12.2). The material "bricks" are described in the *Material Components* chapter beginning on page 13.2.

In addition to the material behaviors, and the development kit, the Z-mat product also ships with a number of additional programs bundled. One such program is the ZebFront pre-processing language which greatly aids the development of user models. Others which are optionally included are the *Simulation* module and the *Optimization* module. These two combine to make a very powerful material coefficient identification tool[1]. One can efficiently simulate and identify using the exact same model code as is used in the finite element code. This will virtually eliminate an extra testing/verification step, and ensures compatibility of behavior between the different stages of material modeling. The optimization works efficiently on multiple experimental/simulation data sets, and can even be used in conjunction with structural calculations.

Finally with versions 8.3 and greater, Z-mat has been expanded to include more "method level" capabilities, such as pre and post processing of results, along with other analysis add ons such as cycle skipping and user elements. It is our hope that Z-mat will grow to be a large-scale CAE complimentary product for commercial and academic users.

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[1] although they are general purpose and can be used with subjects that have nothing to do with materials, or finite elements

System Requirements

Z-mat is an integral part of Z-set, and therefore is implemented on all the Z-set platforms [2] Floating licenses allow the user to employ model simulation and coefficient calibration on desktop systems, while the Z-mat interface can be used on different platform servers optimized for large FEA runs. Also, all file formats used by Z-set and Z-mat are platform independent, including the reading of externally created binary files such as the abaqus `.fil` or ansys `.rst` files. Specifics outlined below relate to the interfaces with the Z-mat available solvers.

External interfaces are, at the time of this writing, available for ABAQUS 6.3-6.4, MARC, Ansys version 7.x, LS-Dyna 970, and COSMOS/M 2.7. Machine platforms for ABAQUS include Solaris (32 bit), IRIX (64 bit), HP-UX 11, HP-UX 11/Itanium, AIX 5, OSF1, Linux i86, Linux Itanium, and windows (NT4/2000/XP). The COSMOS interface is available on windows platforms only. Z-mat for Ansys is available on Windows, SunOS (64-bit), and IRIX64. Z-mat for MARC is available on 64 bit IRIX only at this time.

Some of the platforms have limitations due to the methods of the different solvers. Information on these is described in the different Z-mat chapters. Normally we find the interface for ABAQUS the most robust, with Ansys next, then Cosmos followed by MARC.

The library is compiled as a dynamic shared object which can be linked to other programs. The library is entirely programmed in C++, but only a system linker (`ld`) is required for basic use of the program. Again, some specifics relating to the different platforms are relevant. In particular for Ansys and Cosmos the user needs to compile a custom executable because we are not allowed to distribute a pre-linked Z-mat executable. To have user routines attached to the basic library (plug-ins), a C++ compiler is necessary. Which C++ to use is determined by the requirements of the interfacing code (e.g. ABAQUS), and one should seek information from that vendor for compatibility. For use with Z-set only a `g++` version is available for all platforms. All Win32 platforms use Microsoft Visual C++.

On SGI systems the development foundation package may be required on older systems. This package is supplied with all the MIPSpro compilers, or can be purchased separately. The package is required for the system libraries and linker which are not supplied with the standard system. The C++ compiler is required only for user additions to the package. Also, the software is currently compiled on IRIX 6.5, which will generate an undefined symbol error for earlier systems. A workaround is now available, so if you need that please contact your distributor.

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[2]The development of Z-mat interfaces requires of course operating copies of the mating code at our site for development and maintenance. It is frequently possible for additional platforms to be added per request (possibly with a supplemental charge). Please inquire to your vendor regarding any additional such desired ports.

Material Frameworks

One thing which needs mentioning right away with regards to the Z-mat documentation is that the material models are in general not documented with respect to the type of material, but rather the model framework. Each framework can be considered an assembly of different user-created "building blocks" which then finalize the full model definition.

The commands for configuring Z-mat can be classified as follows:

- **Controls and context** are commands which adjust the specific numerical run (Note: for Zebulon runs these controls are defined in the Z-set users manual, so this section does not apply). These are all ***-level commands in the Z-mat control file (filename depends on specific interface chosen).

- **Framework** This part is determined basically by a selection of a ***behavior *model-type* pair. All sub-commands after the behavior declaration will be context-sensitive.

- **Components**

Chapter 2

Z-mat General Commands

Z-mat interfaces

The current version of Z-mat (Z-mat 8.3) supports the following interfaces.

- Z-mat ABAQUS Both ABAQUS/Standard and ABAQUS/Explicit are supported. With ABAQUS there are perhaps the most comprehensive set of features due primarily to the very robust user capability within ABAQUS. In this regard, Z-mat is constantly looking for additional paths of interface, and with the 8.3 version we have added significant ODB input and output functions, and also UEL interfacing for all the Zebulon element formulations.

- Z-mat ANSYS The Zansys interface has improved immensely in terms of stability and robustness due to the new ability for ANSYS to load shared libraries dynamically.

- Z-mat MSC-Marc Marc fully supports Z-mat material models, and there is an interface for results files reading.

- Z-mat SAMCEF SAMCEF is supported by the Transvalor group in France only.

- Z-mat LS-DYNA The LS-DYNA fully supports the user materials numbers 41 and 42 currently. The remaining material numbers are left for the user to optionally select. The Z-mesh, Z-post, and Zmaster codes allow for inputting of the k file as well as the d3plot results files. There is currently no output to the LS-DYNA formats.

- Cosmos/M Cosmos is no longer supported because of lacking customer demand. This port could potentially be re-activated upon request.

Later in the manual these interfaces are discussed in detail.

Interface files

The Z-mat interface file exists as a medium to configure the interface, translation, and provide extra convergence parameters for the local integration. This interface effectively duplicates the controls which exist in the Zebulon FEA input file.

All the different Z-mat platforms (target FEA systems) use the same basic controls described in this chapter. Some certain commands may however have functionality specific to one or some of the codes due to limitations or special features available in the user interfaces. These differences will be noted in the description section for each command.

Note that the interface file name itself is very dependent on the particular solver which is being interfaced to. For example, with ABAQUS materials are assigned character names, and that name will be the same ASCII filename to be opened by Z-mat. On other solvers such as ANSYS only a material number is given as an identifier, and in that case a convention of naming the file as: 100+material number+".txt" (for example 105.txt for material id 5). Please double-check in the different chapters specific to each solver for further information.

Syntax:
The following commands are available in the Z-mat interface file. Reading of the commands will stop when a ***return command or the end of file is reached.

```
***automatic_time
***behavior
***debug
***external_storage
***material
***parameter
***save_energies
***skip_cycle
***state_var_engineering_shear
***state_var_no_change
***state_var_real_shear
***suppress_temperature
***symmetrize_tgmat
***verbose
***plane_stress_modifier
***zero_dt_for_first_dt
```

These commands and their options are the subject of the rest of this chapter. Some of the commands are simply switches and thus do not have any sub-commands. These simple commands will be discussed in the following.

***state_var_no_change** This command indicates that the user does not require changing the Z-mat internal format of shear variables to a real measure. Shear components output are multiplied by a factor $\sqrt{2}$ from the actual tensor component (t12 in the output is $\sqrt{2}t_{12}$).

***state_var_engineering_shear**   Transform shear variables to be output with an additional factor of $\sqrt{2}$. (e.g. $\gamma_{12} = 2\epsilon_{12}$). **This is now the default**.

***state_var_real_shear**   Divide the $\sqrt{2}$ term out of the shear components so the output is the real component of the tensor.

***suppress_temperature**   Eliminate the setup for temperature as a parameter. This optimizes slightly the computations so constant coefficients may be assumed.

***symmetrize_tgmat**   Make an extra step to symmetrize the material tangent returned from the Z-set behavior.

***verbose**   verbose message outputs.

***plane_stress_modifier**   This command may be used to de-activate the automatic detection of the plane stress condition and allows the use of an explicitly defined `plane_stress` modifier of the behavior instead. Note that automatic plane stress treatment is not implemented for all behaviors, and that in the case of anisothermal loadings convergence may be very slow, In those two cases the `plane_stress` modifier method should be preferred.

***zero_dt_for_first_dt**   use a zero Δt for the pre-step test (with zero strain increment). This pre-step is used by ABAQUS to get the initial tangent modulus. Time-dependent materials may be non-linear if the time step is > 0 even with zero strain increment, because of stress relaxation under fixed displacement.

The Z-mat material file:
The Z-mat material file is the input which determines which constitutive model from the available models in Z-mat to use, and then specifies the particular coefficients accordingly. This file is the same as input for Zebulon, and for the Z-sim. The input format is the subject of chapters 4 and 5.

Note:
By default, the input file name for the material file is the same as the Z-mat interface file, so the behavior definition can follow the Z-mat interface commands.

. . . continued

Example:
The following small material file is a simple example of Z-mat use (taken from the ABAQUS interface tests which puts together some of these concepts. Many more examples will of course be given in the different code-specific chapters and around the discussion of each sub-command.

```
***suppress_doing_first
***state_var_no_change
***suppress_temperature
***material
  *integration theta_method_a 1.0 1.e-10 1500
  *initialize_variable
     epcum  0.43
     X11    7.529e-03
     X22   -1.065e-02
     X33    3.118e-03

***behavior gen_evp
**elasticity isotropic
  young 2.1e5
  poisson 0.3
 **potential gen_evp ep
  *flow plasticity
  *criterion mises
  *isotropic nonlinear
    R0 200.
    Q  2000.0
    b  0.26
  *kinematic nonlinear X
    C  25500.0
    D  81.
***return
```

***automatic_time

Description:
This command is used to give parameters controlling the time stepping based on the convergence and gross change in material variables. Variables which control the time step may be taken from the `FLUX` or `VINT` data members.

Note:
This automatic time-stepping controls the *global* convergence stepping, which means that if there is a local divergence or violation of a limit variable, the current increment will be thrown away and the global solution time step reduced. One can use the `auto_step` beahvior modifier to control local-only automatic time stepping (see page 14.7). This command depends on the capabilities of the FEA solver used. ABAQUS allows the material to control the next time step to be used, while Cosmos and Ansys only allow the material to sub-cut the time step by 2.

Syntax:
The syntax for the automatic time stepping control is the following:

```
***automatic_time
[ *security factor ]
[ *divergence div ]
  *limit var1 val1 [ ... varN valN ]
```

where the following parameters are used:

factor   real value giving the maximum time increase factor for a well converged time step. The value must be greater than one.

div   dividing factor for a diverging increment. The global solution step will be re-run with a time step smaller than the rejected one by this factor.

var1   a character name of a variable of the problem. This can be from the `FLUX`, or `VINT` variables. If the name is the base name of a tensorial or vector set of variables, the limit will be placed on all the components of that variable (e.g. if `sig` is given all the stress components will be used).

val1   real value for the limit of the last-given variable name. Limit names/values must be given in pairs.

Example:
Here is a small typical use for viscoplasticity type problems. The time step will be limited both in the increment of viscoplastic strain (`evcum` to changes less than 0.1% and stress component changes to less that 15 MPa. All components of the stress tensor will be checked to be within the limits.

```
***automatic_time
  *limit
     evcum    1.e-3
     sig      15.
  *divergence 2.0
  *security   1.2
```

***behavior

Description:

This command is more fully described in the chapter *Material Models* and *Material Components*. This command lets the user include in-line a material definition in the Z-mat interface file. If this command is not used, the material file will be sought using the `*file` or `*standard` sub-commands of `***material`.

Be aware of the following items when defining a Z-mat behavior.

- Behavior definitions have the "external parameter" value `temperature` available always for coefficient definitions, thermal strains, and similar coefficient taking material objects. With ABAQUS, additional field variables can be defined using the field options.

- One may use the Lagrangian modifiers described on page 14.4 to transform the behavior into finite strain when the conditions for calculating the deformation gradient in a UMAT have been met (see ABAQUS user manual 25.2.26[1]).

- For use with ABAQUS/Explicit one must add the material modifier `explicit`.

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[1]from version 5.6 handbook

***debug

Description:
This command indicates that debug output will be included during the run. This is primarily for user-defined functions and behavior models using the `prn` set of C++ functions. The command will also print out the active list of auto-load keywords so one may verify if a particular function is loaded with the Z-mat/ABAQUS link.

Output from the debug statements will be in a file named `OUT` located in the given directory (full path). If no path is given, and the library is unable to determine the problem directory, the full path of the output file is `/tmp/OUT`. This path sometimes helps to get around the problem copying to a scratch directory by ABAQUS.

Syntax:

```
***debug [ path ]
[ *local_debug ele gp ]
[ *flags flags ]
[ *limit_debug_time st end ]
```
---

where *path* is the path to use for storing the `OUT` debug file.

*local_debug   localize the debug output to a given element number and a given Gauss point number.

*flags   Set flags for the internal int *DeBuG*. This is used control what gets printed. One can use the `prn2` to make certain debug selections. See the developer manual for more information.

*limit_debug_time   Limit the time for debug output. Give the start and end time for debug output in the solution time scale.

Example:
The following example is taken from material input file `e3danis` located in test database directory $Z-mat/umat\_v61$.

```
***debug
***material
  *integration runge_kutta 1.e-3 1.e-3
```

***external_storage

Description:

This option is used to specify that the state variable storage is to be made in a separate file instead of using the FEA solver's internal database. The command currently works with the ABAQUS and ANSYS interfaces.

With this command, there is no limit to the number of state variables which can be used in a Z-mat model. In some cases we find that the codes efficiency can be improved as well by using external storage, because of the buffering and relief from some copying operations.

Syntax:

```
***external_storage
 *buffer_size sz
 *file db-tmp-file
 *full_path db-tmp-file
 *vars list
```

*buffer_size   The buffer size determines the file buffering given in number of integration points. This means that only every *sz* integration points will the storage be serialized to disk.

*file   Specifies the external file to be used for the storage. This file name is relative to the current working directory.

*full_path   Specifies a fully qualifies filename for the external storage. Note that ABAQUS copies your input problem to a temporary directory, so do not use relative path names for this one.

*vars   Specifies the variables which will be made available for output. Zpreload can be used to determine the variable naming which is required here (the Zebulon type names, not `sdv##`. In the screen or log output the `sdv`-type naming will be printed, for example:

```
done with material file reading...

** real state variables
   sdv(1)          epcum
   sdv(2)          epi22
```

Example:

The following lines are an excerpt from a Z-mat material input file `doghri_st`, which demonstrates the usage of the `external_storage` keyword. The material file can be found in the test database in $/Z - mat/umat\_v61$.

```
***external_storage
   *file oo.store
   *vars epi22 epcum
   *buffer_size 5000
```

***material

Description:

This command marks the definition of the materials in a structure to be studied. The behavior of each material is defined in a file with special syntax (see the chapter *Material Behavior*). The purpose of this command is therefore to define the material file names, associate these files to different element sets, and specify other global applications on top of a material model such as rotation of material coordinates or give local integration methods.

Syntax:

```
***material
[ *file file ]
[ *standard std-file ]
[ *integration    ]
[ *rotation       ]
[ *initialize_variable ]
```

The sub-commands for ***material pertain to the behavior defined in the current material file only. Note that the function of this command is somewhat different than the equivalently named command used in the Z-set .inp file.

A last comment: **Always Verify Your Materials**. The behaviors supplied in the Z-mat library are compatible with the simulation program, so there is no excuse to not validate the material behavior with a given set of coefficients.

*integration

Description:

This option determines the local integration method for a material behavior.

Syntax:

---

*integration *method params*

The allowable methods are summarized in the table below:

CODE	DESCRIPTION
runge_kutta	explicit Runge-Kutta integration with automatic time stepping based on integration error
theta_method_a	implicit generalized midpoint integration; this method normally supplies the best tangent matrix
theta_auto_a	automatic time stepping in the implicit θ-method

runge_kutta The Runge-Kutta method implements a second order explicit integration with automatic time stepping. Variables are normalized to allow varied variable magnitudes in "stiff" sets of equations. The method takes two real parameters. These are the convergence criteria followed by a minimum value for normalization. Standard RK error calculation for each integrated variable will be normalized by either the increment of the variable or this second parameter, whichever is greater. the resulting error is compared with the first parameter.

The Runge-Kutta integration with the `gen_evp` material behavior provides a tangent matrix in models with a single inelastic deformation. This matrix is however not consistent with the integration scheme, and thus yields less than optimal global convergence. The explicit integration also performs poorly in heavily time-dependent problems such as viscoplasticity. However, some complex models are only implemented with this method.

theta_method_a The θ-A method is the standard integration for the majority of material laws requiring integration.

$$x(t + \Delta t) - x(t) = \dot{x}\left(t + \theta\Delta t\right)\Delta t$$

This method requires 3 parameters to describe the convergence. These are first the θ value (real) followed by the residual required for convergence (real) and the maximum number of local iterations in the integration (integer).

The value for θ must be greater than zero and less than one. It is **strongly** advised to use theta values of 1 for time independent (plastic) materials, and $1/2$ for time dependent (viscoplastic) problems. Time independent plasticity will normally show strong oscillations about the solution for values of θ less than 1.

Reasonable values of convergence range from 10^{-6} to 10^{-10}. Values which are too large usually lead to poor global convergence. Too small values will not converge due to numerical roundoff (10^{-12} is about the limit). Convergence will rarely take more than 25 iterations, and should not take more than 50. If this is the case, there may be some

error in the integration (make a bug report), or the material parameters are excessive (damage laws may provoke this). If the local iterations are greater than 50 it is probably better to reduce the global iterations or use automatic time stepping (global or local).

The default integration is dependent on the material law used. Most behaviors modeling plastic or viscoplastic materials use a default of the θ-method with $theta = 1.0$, $eta = 1.e\text{-}9$ and $max\_iteration = 200$.

Example:

```
% plasticity or large deformation
*integration theta_method_a 1.0 1.e-9 50

% difficult viscoplastic case
*integration theta_method_a 0.5 1.e-6 100

% complex law
*integration runge_kutta 1.e-3 1.e-3
```

*rotation

Description:
This material option is used to change a coordinate systems by rotation. It is used here to simplify specification of some materials (anisotropy, etc), but the syntax is general. Other applications using the rotation object include specification of grain orientations for polycrystals (see page 13.79).

There are currently two methods for specifying a rotation. These are by vectors of the rotated coordinate axes in the global coordinate system, and by Euler angles (used for crystal orientation for example). The first case is displayed in the following figure:
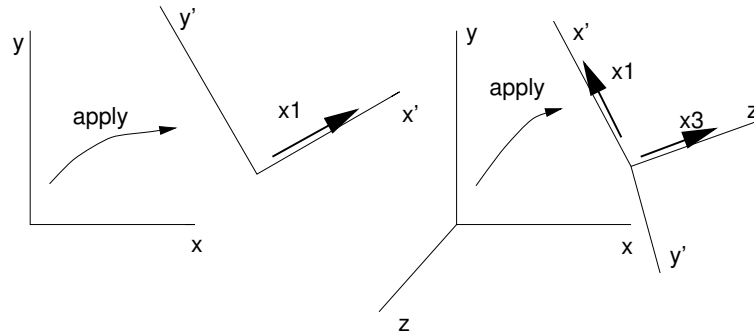
For the material rotation of this section, the material gradient will be rotated (rotation is applied) before being integrated by the material behavior. For small deformation mechanics, this would be a rotation of the strain tensor.

$$\epsilon'_{tot} = \mathbf{R}^T \epsilon_{tot} \mathbf{R}$$

The material behavior then solves for the flux in terms of the new gradient, which is $\epsilon'_{tot} \rightarrow \sigma'$ for the mechanical problem. Afterwards the flux is rotated to the global coordinates again:

$$\sigma = \mathbf{R} \sigma' \mathbf{R}^T$$

Rotation by giving Euler angles is similar. The significance of the three angles is given in the following figure:
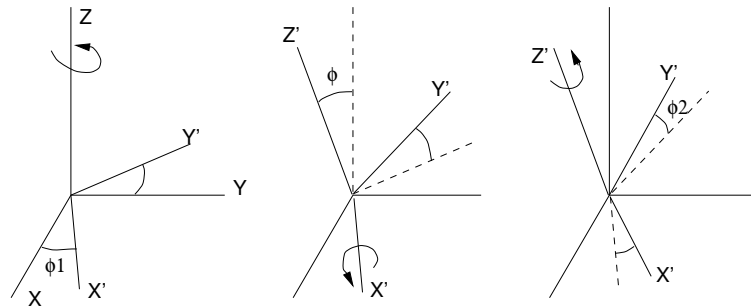
. . . continued

Syntax:

For rotations specified using coordinate axes:

```
*rotation
[ x1 x* y* [z*] ]
[ x2 x* y* [z*] ]
[ x3 x* y* [z*] ]
```

The arguments `x1, x2, x3` indicate the components of direction vectors for the transformed coordinate frame. Exactly one direction is required in 2D problems, and two directions are required in 3D. The order of definition is not important. The local coordinate system may be assembled with any of the geometrical axes. The input vectors will also be normalized by the program to automatically make unit vectors.

Using the notation here that *t1* is the first direction vector defined, and *t2* is the second (for 3D problems), direction vectors of the coordinate system are defined as follows: The first vector is collinear to *t1*. The second vector is a vector in the plane defined by *t1,t2* and is perpendicular to *t1*. The third direction will always be calculated using the vector product of the first two vectors. The *t* vectors will replaced by those given by you using the `x1`, `x2`, `x3` choices.

For rotations specified using Euler angles:

```
*rotation   φ₁  φ  φ₂
```

*initialize_variable

Description:

This command is used to give initial values to the variables of a material. Currently, only constant (uniform) values are allowed. This command is used in the place of the initializing commands in ABAQUS.

Syntax:

The syntax for the automatic time stepping control is the following:

```
***initialize_variable
  var1  val1
  ...
  varN  valN
```

The syntax is free format, except for the fact that variable name and initial values must be given in pairs. The definable parameters are:

var_i a character name of a variable of the problem. This can be from the FLUX, or VINT variables. Each component of a tensorial or vector variable must be initialized separately.

var_i real value for the limit of the last-given variable name.

Example:

This is an example for the problem 4022301 of ABAQUS. The input file is the following (this is for a custom behavior integrating the same Ziegler model as in ABAQUS:

```
***material
  *integration theta_method_a 1.0 1.e-7 1500
  *initialize_variable
    epcum  0.43
    X11  128.0
    X22 -181.0
    X33   53.0
***behavior ziegler_test
   ...
***return
```

***parameter

Description:
This command controls the translation of ABAQUS field variables to Z-mat external parameters which can be used in coefficient dependancies. Remember that the `temperature` parameter is always active in Z-mat.

Syntax:

```
 ***parameter
[ **ambient_temperature val ]
[ **field_variable var-name location ]
[  **initial_value val ]
```

ambient_temperature sets the ambient temperature used as T_0. This is important for thermal strain calculations (see page 13.112). In the event that this command is not used, an additional state variable is added with fixed value of the temperature at the beginning of the problem (if there are dependancies on temperature in the behavior that is). It is probably desirable to use this command therefore if the initial temperature field is constant.

field_variable add a new field variable to the problem, with index *location* in the list of fields defined within the ABAQUS problem. This index starts with 1.

*initial_value optional command with a similar meaning as **ambient_temperature has for temperature.

Example:
The following example illustrates the use of `parameter` keyword. It is an excerpt of file `ts1` located in test database in $Z - mat/umat\_v61$.

```
***parameter
  **ambient_temperature 125.0
  **field_variable humidity 2
  **initial_value 0.25
```

***save_energies

Description:
This command indicates stores the elastic energy for output. The command is a bit simplistic, but extracts from the material the variable `eel` and returns

$$\mathtt{sse} = \frac{1}{2}\boldsymbol{\sigma} : \boldsymbol{\epsilon}_{el}$$

if $\boldsymbol{\epsilon}_{el}$ does not exist in the material (not normally the case for standard materials, but possible) an error will occur, and the option should be removed.

***skip_cycle

Description:

The `***skip_cycle` command is used to give cyclic based extrapolation of the material state to allow skipped cycles for structures loaded with many cycles.

Syntax:

```
***skip_cycle
  *check_with_component list-of-components
  *file sdv-file
```

Zmaster interfaces

Description:

Many of the different Z-mat platforms have integrated functionality for their mesh input and results files within the other Z-set products including the Zmaster GUI program. This software is what NW Numerics uses exclusively for validation and problem processing for all the different interfaces. Generally the Z-mat user could be interested in the following:

- Opening results files for visualization and rendering. The following simple commands are examples:

  ```
  Zmaster -odb my_calculation.odb
  Zmaster my_calculation.fil
  Zmaster ansys_calc.rst
  ```

- The 8.3.6 version includes the Simulation GUI interface for setting up and working with material simulation and fitting work.

- Mesh files can be imported and saved to different formats with sets and other boundary condition data preserved.

- Many of the Z-mat validation test cases use a post processing step to extract X-Y data in an automated manner. Zmaster can be used to plot general ASCII file data using the Plot button:

  ```
  Zmaster doghri.test
  ```

More detail on the file format translators and use of Zmaster is given in the **Release Notes / Zmaster** handbook.

Chapter 3

Z-mat ABAQUS

Z-mat ABAQUS interface

Description:
The commands described in this chapter are used to enable a Z-mat material model for use within ABAQUS[1].

Syntax:
Z-mat jobs are launched via the `Zmat` command line script only.

    % `Zmat` [*opts*] *problem* ↩

The command syntax for `Zmat` is given in more detail in the **Release Notes & Zmaster handbook**, including discussion of all the command line switches used to control the specifics of the Z-mat launch.

The script will initially launch ABAQUS, and then be called again by the ABAQUS preprocessor in compile and link mode. By default the launch submits the job to the ABAQUS queue, and therefore the script exits rapidly (even though the job continues in the background). To see the status of the calculation, look at the *problem*.`log` file (e.g. `tail -f myprob.log`), or run with the `-fg` switch.

ABAQUS Input:
The definition of a material for the Z-mat behaviors always uses an external file to establish the model components and coefficients. Z-mat never uses the material parameters defined in the ABAQUS `.inp` file. This is because the Z-set coefficient definitions are much more flexible in their definitions, and are integral to the actual structuring of the material model to be used. Global dependencies are established using the temperature parameter, or other global field variables.

Other commands are available in addition to the behavior definition which control the local integration method (implicit mid-point, Runge-Kutta explicit, etc), variable initializations, automatic time stepping parameters depending on the maximum allowable variable increments, and the local rotations.

Linking summary:
The Z-mat library is delivered as a dynamic shared object which can be linked to other programs. The library is entirely programmed in C++, but only a system linker (`ld`) is required for basic use of the program. The `Zmat` script prepares the proper link command in place of using the C++ or Fortran command lines. On Windows platforms no development software is necessary at all.

To have user routines attached to the basic library, a C++ compiler will be necessary, as a second add-on shared library must be prepared[2]. Since the standardization of C++, the compiler requirements are greatly reduced from what was previously the case. In most systems

---

[1]The Z-mat interface is also known as Z-aba or ZeBaBa in some older circles. The Z-mat name is however the official product name and symbolizes an approach which is a step beyond classical single code UMAT solutions, and one which is tied to the extensive Z-set software.

[2]actually there is no limit to the number of plugins which can be used. There is a specific naming convention for Z-mat plugins however. For unix systems the user-library should begin with `libZmat` and on windows the DLL should start with `zmat`.

Z-mat plugins can be made which whatever C++ compiler is convenient. Normally the user would be best advised to use the most modern version possible. The general compiler level requirements specified by ABAQUS, Inc will most likely not be absolutely necessary, though we validate that those compilers do in fact work so they can be used as a guideline.

User plugins will always be compiled and linked before running ABAQUS, and the end-user will therefore not need any additional development tools in the same manner as running Z-mat without the plugins.

Current status

Since the initial releases, many improvements have been made for the ABAQUS interface of Z-mat. Some issues still remain however.

Some of the additions with this version include:

- Continuing streamlining and performance improvements. The distributed domain solvers in ABAQUS at versions 6.5 and above are well supported and are proven to give decent scalability with Z-mat.

- Support for ABAQUS/Explicit is complete.

- Improved automatic time stepping.

- Improvements in the simulation/optimization tools, including support for finite strain problems.

- Compatibility with the rest of Z-set, making one installation for sites with Z-set and Z-mat.

- External disk storage for state variables. This allows models with thousands of state variables.

- Finite strain has been improved, including now the addition of hyperelastic and Hyper-viscoelastic models.

- Direct reading of the `.fil` format is greatly improved. Abaqus ODB files can also be read and written by Zpost/Zmaster and Zebulon. This data file interface is without question the most robust of all the Z-mat interfaces.

- All the Z-mat test cases use Z-post.

- Support for all Abaqus 6.x versions.

- Zebulon elements can be used as a UEL with output to an ODB file or other Zebulon supported output. This includes full state variable name and typing information.

- Optional post processing step to translate all the Z-mat `SDV#` variable names to be the proper named and typed variable in a new ODB file.

Site definition

There are a number of site definition files which must be configured to make the Z-mat program additions work with ABAQUS. These will most likely be configured by NW Numerics during the installation.

The location of the `abaqus` executable to use is adjustable. There are two possibilities for defining the path. The first is to edit the file `$Z7PATH/lib/Zmat/ABAQUS_ROOT` and make an entry for the machine name (the name given via `hostname`) and the path to the ABAQUS installation directory. The second method is to define the environment variable `ABAQUS_ROOT` to point to the abaqus directory.

When launching the script will automatically link the Z-mat library and all plugins with the `libZmat` (unix) or `zmat` (win32 DLL) prefixes found in the standard search path (see the Zmaster/release manual reference section on search paths).

Unix configuration:
The most important issue for the Z-mat programs to work is the definition of an environment variable `Z7PATH` to point to the root directory of the Z-mat distribution (see release notes). The next important thing is to source the `$Z7PATH/lib/Z7_cshrc` file to set up additional environment variables. These two definitions can be put in a users `.cshrc` file for the C-shell.

The second most important environment variable is the `Z7MACHINE` variable. All the scripts which access binary executables use the `Z7MACHINE` variable to determine where and which binary to run. By default (if the variable is not set before sourcing the `$Z7PATH/lib/Z7_cshrc` file) the machine type will be set as `setenv Z7MACHINE 'uname'`. Sometimes this is not sufficient to distinguish an architecture, so the user may add additional machine types. Additional architectures may be defined for different machines in the `$Z7PATH/lib/MACHINE_TYPES` file. This file is also used to define different compilers to be used. The Release Notes/Zmaster manual has more information in the Configuration chapter.

Windows configuration:
Aside from specifying the `ABAQUS_ROOT` position, no special work is needed for running Zmat on windows platforms. Only a command line interface is available however.

Interface files

The fact that Z-mat is developed for use in Z-set (Zebulon FEA) natively, and that the interface with codes like ABAQUS is based on a Fortran subroutine implies that a certain amount of translation back and forth is required. Also, there are additional inputs required to control Z-mat outside of ABAQUS. The following figure outlines The interaction of different programs, and the use of input files.
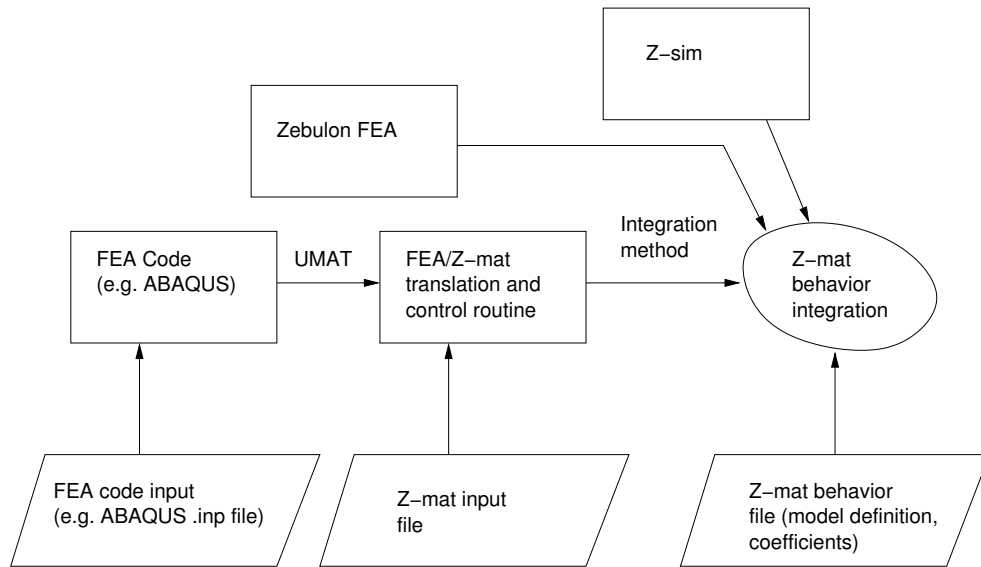
The ABAQUS `.inp` file:
The use of an externally defined material behavior in ABAQUS requires a number of special entries to be made in the ABAQUS `.inp` file. Some of these entries are superfluous given the structure of the Z-mat library, but are nevertheless required to satisfy ABAQUS's *umat* interface. The entries are:

- `*MATERIAL`   command to define the different materials of the problem. The name given to this command (using `*NAME=`) will be the name of an external file containing a Z-mat behavior definition (see previous section).

- `*DEPVAR`   command which establishes the storage per integration point for the material variables. This value must be greater or equal (best case) of the size determined by Z-mat for the behavior. There is no way except for user intervention to size this value, so the line must be included. If the value is too small for the behavior, an error message is printed in the `.log` file, and the calculation terminates.

- `*USER MATERIAL`   this defines that there is a user behavior. As as parameter to this command, one **must** give a `CONSTANTS` option, **with at least one** coefficient. This coefficient is **not** used in the Z-mat behavior however.

ABAQUS commands for initializing the state variables, giving a material orientation, and material coefficients are not used with Z-mat. There are instead alternatives which may be defined in the separate Z-mat material file (see the commands starting at page 2.10).

Output variables

All the material variables should be available for output in ABAQUS calculations if the `**external_storage` option is not used. This should include the `GRAD`, `FLUX`, `VINT` and `VAUX` variables as shown with the `Zpreload` utility. The variables will all be stored as `SDV` variables. *Caution*

There are some tricky spots which remain in the Z-mat output which may not be obvious to the new user. These are summarized below:

- The shear components of *symmetric tensional* variables are natively stored with a factor of $\sqrt{2}$, which is removed by default at each exit of the z-mat routine. This operation takes up some CPU however, so it can be suppressed by using the `***state_var_shear_alter` command. Also the default transformation for state variables is to change them to the real tensorial shear component. Engineering output is available by using the `***state_var_engineering_shear` option. This is true for variables in the integrated vector and the auxiliary variables (`VINT` and `VAUX` variables). The `GRAD` and `FLUX` variables always have the factor removed however.

- The integrated and auxiliary variables (`VINT` and `VAUX`) are stored sequentially in the vector prefixed `sdv` in ABAQUS.

- For mechanical problems, the stress variable is named `S` and the strain `E` with all behavior as in ABAQUS standard.

- Some extra variables such as the energy output variables are not yet calculated.

Extra files

The compilation and linking of `UMAT` routines (Z-mat included) are controlled by parameters in the `abaqus_v6.env` file (located in the `Site` directory of the ABAQUS distribution.

    Alterations must therefore exist in the active `abaqus_v6.env` file to link with the Z-mat library. An `abaqus_v6.env` to do this is supplied in the `$Z7PATH/lib/Zmat/` directories. There is a default `abaqus_v6.env` file, and the option to have specific files for different machines (example files exist and it should be obvious how to manipulate these). The `abaqus_v6.env` file which is needed will be copied into the calculation directory in order to be the first read configuration file, and can thus be verified by looking at that file after an execution (possibly add comments to make the env file creation clearer).

    The user can add configuration options in their customized personal files also. The standard `abaqus_v6.env` file *will not* be used in this case, replacing that with the file named `zebaba_v6.env` (replaced only for Zmat jobs). The Zmat program will search first in a users home directory, followed by the local execution directory.

    The environment file shipped in the Z-mat for HP-UX is for example:

```
link_sl="Zmat -link_v6 /usr/ccs/lbin/ld64 -b -ashared_archive +k +n
     +FPD +vnocompatwarnings +pd L +pi D +s -c%E +h%U -o %U %F %A %B %L
     -lpthread -lcps -lcl"

compile_cpp="Zmat -compile_v6"
compile_fortran="Zmat -compile_v6"
```

In the standard Z-mat validation tests in the directory `test/Z-mat/umat_v61` we have the custom file `zebaba_v6.env` with the following:

```
ask_delete=OFF
split_dat=ON
```

For personal files one may wish to remove the `ask_delete` parameter.

User additions

Extensions to Z-mat:
User functions and classes may be added to the Z-mat library without limit. This is one of the advantages of working with Z-mat, as a site can create a library of user functionality in combination with Z-mat, and use it repeated without distributing the source files for each problem run. Also, the user classes will be automatically available to the simulation and optimization methods, creating a coherent extensible modeling environment.

In order to make user-additions to Z-mat, a custom shared library must be compiled and installed into the proper location with the proper name. For running Z-mat with other ABAQUS, the shared library must be named `libZmat*.so` where `*` is replaced by a user designated character filename. On HP-UX systems the suffix is `.sa` and on AIX it is `.a`. Files fitting the above wildcard name will be automatically loaded using the system `dlopen` command (or equivalent). The search path is:

- the current working directory.

- the path pointed to by the environment variable `ZEBU_PATH`

- the default binary location `$Z7PATH/PUBLIC/lib-$Z7MACHINE`

More detail about the compiling process is given in the developer handbook, and there is always a pre-configured user-project in the installation directory `$Z7PATH/User-project` .

ABAQUS user routines:
The Z-mat package uses the ABAQUS UMAT function to interface with that FEA solver. This does not prevent one from programming extra user routines to run along with Z-mat. If the user routines are unrelated to the material (such as user loads or MPCs), an extra Fortran file can simply be appended to the Z-mat interface by using the `Zmat` option `-uf`. An example is provided in the +$Z7PATHtest/Z-mat/UMAT+ directory as problem `4020201`. The execution is for example:

```
Zmat -fg -uf mpc.f 4020201
```

which will link in the user routines in `mpc.f`.

The user can override the default UMAT interface as well, by modifying the file +$Z7PATHlib/Zmat/mech-sd.c+ and using the `-UF` command switch.

Example

This is an example material file which can be used with Z-mat. Note that all input is **case sensitive**!

This example has the material definition in the file `e3danis`. The following lines are the material related entries for the ABAQUS `.inp` input file:

```
*MATERIAL,NAME=e3danis
*DEPVAR
   20
*USER MATERIAL,CONSTANTS=1
0.0
*SOLID SECTION,MATERIAL=e3danis,ELSET=A1
```

Note that this syntax is very sensitive to positions, and connectivity. Commands are not case sensitive, but filenames may be. The command `*DEPVAR` allocates in ABAQUS storage for the material variables at each Gauss point. There is no way to dimension this quantity from the *UMAT* routine, so the user is obliged to enter the correct number corresponding to the material model used. Information concerning this quantity will be printed to the `.log` file generated by the ABAQUS output.

```
***material
  *integration runge_kutta 1.e-3 1.e-3
***behavior gen_evp
 **thermal_strain isotropic
    alpha  temperature
      2.0e-06    -0.1
      1.0e-06   1000.1
**elasticity isotropic
    young 200000.
    poisson 0.25
**potential gen_evp ev
   *criterion mises
   *flow norton
     n 4.0
     K 500.
   *kinematic nonlinear % x1
     C 10000.0
     D 100.0
   *isotropic constant
     R0 100.e+00
***return
```

For this material file, the output of the Zpreload program shows the material variables and their associated ABAQUS output variables.

```
=============================================
Flux Name:
```

```
sig11   sig22   sig33   sig12   sig23
sig31

Grad Name:
  eto11   eto22   eto33   eto12   eto23
  eto31

var_int Name:
  eel11(sdv1) eel22(sdv2) eel33(sdv3) eel12(sdv4) eel23(sdv5)
  eel31(sdv6)
  evcum(sdv7)
  al111(sdv8) al122(sdv9) al133(sdv10) al112(sdv11) al123(sdv12)
  al131(sdv13)

var_aux Name:
  evi11(sdv14) evi22(sdv15) evi33(sdv16) evi12(sdv17) evi23(sdv18)
  evi31(sdv19)
===========================================
```

Post calculations

Description:

With version 8.3 all the Z-set post computations can be used with ABAQUS results files, and are in fact used for each of the Z-mat validation examples. It is sufficient to use the `***data_source` selection to choose an import format for the results files. The post processing environment contains a large number of very convenient curve extraction routines which can be used to automate analysis post processing. There are also a large number of both *global* and *local* post computations which can be applied for failure analysis etc. The post computations are now part of the Z-mat bundle.

Example:

An example from the Z-mat tests follows, generating an ASCII datafile with the stress strain behavior as computed at node 2345 of the structure. Note that some *mesher* operations can be included in the post computation as well to generate nsets for example which were not included in the abaqus model during the pre-processing stage.

```
****post_processing
   ***data_source fil
    **open doghri.fil

   ***global_post_processing
    **file node
    **output_number 1-999
    **nset ALL_NODE
    **process curve doghri.test
     *precision 4
     *node 2345    eto11 sig11
****return
```

Note:

For Zansys the capability and input is quite the same thing, except that the file format should be `***data_source rst` and the problems `.rst` file should be placed in the open input.

Chapter 4

Z-mat ANSYS

Zansys ANSYS interface

Description:
The Zansys functionality mirrors very much the same principals as in the Z-mat for ABAQUS port, and so we refer the user to that documentation as well. This section provides a getting started guide to Zansys.

Syntax:
% `Zansys` [*opts*] *problem* ↩

Getting started:
Perform a standard installation of Z-set, including the binaries and shared files. The install location will henceforth be referred to as the `Z7PATH`. The launch procedures for Zansys will also need to be able to locate the ansys

Note:
In versions prior to 8.3.6 it was necessary to perform a user build and link process in order to generate a user executable of ansys. The newer versions interface with `ANSYS` via shared libraries, and henceforth the user needs to do nothing special for the interface to work. There are some test cases in the `%Z7PATH%\test\Zansys\INP` directory. The Z-mat material files are named `10#.txt` where `#` is the material number selected in the test using ansys commands such as:

```
TB,USER,4,0,0
TB,STATE,4,,40
MPCHG,4,1
```

which would set the Z-mat material for element group 1 to be read in the file `104.txt`. Currently all the commands listed in the Z-mat handbook for the ABAQUS interface are supported with ANSYS as well, except the use of multiple field variables. Temperature is available as a parameter, and can be set using commands like:

```
BFUNIF,TEMP,523.0
```

The name `TEMP` will be re-mapped to `temperature` in the Z-mat files. To try the test cases, do for example:

```
z:
cd %Z7PATH%\test\Zansys\INP
Zansys plast3
```

which launches the ansys GUI from which the input file can be loaded:

```
/INPUT,plast3,inp
```

Elements and output
Z-mat for ansys must be run using the 18x class elements. In order to get output for the state variables in the Z-mat material model, an additional command must be issued to get the variables stored to the output database, such as:

```
OUTRES,SVAR,ALL,
```

To plot the variable one can use the command:

```
PLESOL,SVAR5,1
```

Note:
With user materials in ANSYS the solver is by default set to not extrapolate integration point stresses to the nodal points. In fact ANSYS only does this extrapolation by default for linear materials, while most other codes assume that a least-squares fit extrapolation method should be done in all cases. In order to activate extrapolation the following lines can be used before the SOLVE command is issued:

```
ERESX,YES
```

With the Z-set RST file reader direct integration point visualization is supported, so unfortunately there is no refined solution for this issue.

Chapter 5

Z-mat MSC-Marc

Z-mat MSC-Marc interface

Description:
The command described in this chapter allows to use a Z-mat behavior within a MSC-Marc analysis. The interface with the Z-mat library is implemented by means of the `uvscpl` Marc user subroutine. The choice of `uvscpl` to build the interface, against other candidate subroutines available to implement user materials, has been motivated by its flexibility. Note however that Zmarc capabilities are by no means restricted to time-dependent creep behaviors.

Syntax:
`% Zmarc -j` *problem* [*run_marc options*] ↩

where *problem*`.dat` is the name of an MSC-Marc input data file.

The `Zmarc` script is a simple copy of the standard `run_marc` script, where commands needed to link automatically the Z-mat package to build a custom `marc` executable have been added. Therefore, standard options of the `run_marc` procedure are also available with the `Zmarc` command.

MSC-Marc Input:
The definition of a material for the Z-mat behaviors always uses an external file to establish the model components and coefficients. Z-mat never uses the material parameters defined in the Marc `.dat` file.

In the current implementation the definition of the Zmat behavior should be given in a file named *problem*`.zebulon`.

Several additions to a standard Marc `.dat` file are necessary to activate the use of Zmat. Some of them cannot be accessed by means of the Mentat graphical interface and should be done directly in the `.dat` file. Those commands are listed hereafter:

- Parameters section

  - The `state vars` command should be added to specify the number of material variables needed by the Zmat behavior. The `Zpreload` utility can be used to compute the number of variables required. In any case, Zmat outputs to the `.log` file the correspondence between the Marc user state variables and Zmat the behavior components. If not enough state variables are available for the behavior the analysis is stopped. Otherwise a warning is printed if more variables than necessary have been specified.

    `state vars,20,20,`

  - The creep procedure should be activated by means of the `creep` command, even if no creep effects are involved in the analysis. This is needed by Marc, because the `uvscpl` user subroutine can only be used within the creep algorithm.

    `creep,0,0,1`

- Model definition section

- The `visco plas` parameter of the `isotropic` or `orthotropic` command must be selected, to activate the use of material integration by means of the `uvscpl` user subroutine. Note that either `isotropic` or `orthotropic` materials can be selected indifferently, since values of the material coefficients given as arguments of these commands are ignored by Zmat, that reads the material definition in a separate *problem*.`zebulon` file.

```
isotropic
,
1,visco plas,isotropic,0,0,0,0,material1,
2.E+4,3.E-1,8.E-6,2.E-5,0.0,0.0,0.0,0.0,
1 to 1000
```

- To benefit from the consistent tangent matrix calculated by most Zmat behaviors, and accelerate the convergence of the global equilibrium iterations, the full newton-raphson algorithm should be selected by setting the 6th parameter of the `control` command to 1.

```
control
1000,10,2,0,0,1,1,0,1,0,
0.001,0.,0.1E-8,0.,0.1,0.,0.1E-4,1.E-12,
```

- Output of material variables to the Marc results file

  The `post` command allows to select which material variable should be stored in the results files. In this case the element codes that should be given as argument of the `post` command, is a negative integer value such as `-varid`, where `varid` is the number of the user variable required for output.

```
post
14,16,17,0,0,19,20,0,1,0,
   301
   461
   311
   391
-30,,d1
-31,,d2
-32,,d3
```

The above command adds user variables `30`, `31` and `32` to the `.t16` result file. The corresponding values will then be accessed by the graphical post-processor of Mentat. Within Mentat the names given to those state variables will be respectively `d1`, `d2` and `d3`, as defined by the `post` command.

Note that this output capability makes use of the user subroutine `plotv` to interpret correctly the user element codes. An appropriate `plotv` code is provided in the Zmarc package. However, this means that the user cannot redefine this particular user subroutine for its own purpose.

- History definition section

The use of the `auto step` procedure for adaptative load step control is strongly advised. Moreover, starting with Marc2003, `auto load` doens't seem to handle anymore user material implemented with the `uvscpl` subroutine. Also, as described in the next section, the `enhanced scheme` of this procedure can be used to provide Marc some feedback about local integration results obtained in the Zmat library. This option should then be activated as well by setting the 9th parameter of the second data block to 1.

```
auto step
0.02,0.4,,,0.0001,0.1,100,6,1,
,10,0,,,,,,,,,2,
```

Automatic time-stepping and Zmat local integration:

For complex material behaviors and/or large strain increments, non-convergence may occur during integration of the behavior equations by Zmat. Without a proper procedure, such local divergence will cause either premature convergence (especially in the case of anisothermal analysis under purely thermal loadings), or run-away newton iterations until the specified maximum number of recycles is reached and increment cutback eventually occurs.

Unfortunately there is nothing available in `uvscpl` (as in other user material subroutines) to signal a local divergence back to Marc and force an immediate increment cutback.

However, the enhanced scheme of the `auto step` command, that allows to specify user criteria to control the step-size, may be used to implement some kind of emergency procedure. The input data necessary to implement this mechanism from the `.dat` file is not trivial, and is described hereafter:

- activate the enhanced scheme of the `auto step` procedure by setting to 1 the 9th parameter of the second data block,

- choose to use user criteria as *limits* (versus *targets*) by setting to 0 the third parameter of the third data block,

- add a criterion on a Zmat variable, that will cause increment cutback in case of its violation during local integration. To select a particular user state variable, a code such as *13x100 + state variable id* should be used as first argument of the fourth data block.

```
auto step
0.02,0.4,,,0.0001,0.1,100,6,1,0
,10,0,,,1.2,,,,,,2,
1330,cmc
10.,0.01
```

In the above example, the user criterion used to monitor convergence is defined on user state variable number 30 (element code `1330`). The criterion defines that this variable at any integration point of the element set named `cmc`, should not increase of a value of more than `10.0` (defined in the fifth data-block) over an increment. If the increase of the variable exceeds the limit value specified, the `auto step` procedure will discard the load increment, and the step size will be cut back accordingly.

More precisely, denoting by Δt the current step size, Δv the maximum variation of variable v found by local integration during the current increment cycle, and v_{max} the limit value specified, if $\Delta v > v_{max}$ a new icrement will be attempted with a lower step size calculated as:

$$\Delta t \; \frac{v_{max}}{\Delta v}$$

.

Additional commands may then be used in the Zmat *problem*.`zebulon` file, to control increment cut-back in case of local divergence. Those commands are the following ones:

`***divergence_variable 30 20.`

The above command select variable 30 to monitor local convergence, and specify that in the event of divergence a Δv value of `20.` should be sent back to Marc (ie. two times the v_{max} limit value defined in the `auto step` command). Hence the effect will be to force a division by 2 of the global step size in the event of local divergence.

When using this scheme, care must be taken to carefully select the v_{max} limit value. Typically the value should exceed likely variations for the variable selected, and the `***divergence_variable` increment value set accordingly to produce an increment cut-back of the required size.

Example:

The following listing summarizes the options needed in a `visco.dat` Marc input file when using the Zmarc interface.

```
title visco
$ parameters section
...
state var,19,19
creep,0,0,1
end
$ model definition section
...
isotropic
,
1,visco plas,isotropic,0,0,0,0,material1,
20000.,0.3,8.E-6,2.E-5,0.0,0.0,0.0,0.0,
all_element
...
post
14,16,17,0,0,19,20,0,1,0,
301,
311,
-7,,evcum
...
control
100,10,2,0,0,1,1,0,1,0,
0.001,0.,0.1E-8,0.,0.1,0.,0.1E-4,1.E-12,
```

```
$ history definition section
auto step
0.02,0.4,,,0.0001,0.1,100,6,1,
,10,0,,,,,,,,,2,
1308,all_element
10.,0.01
...
```

The Zmat behavior is defined in a separate `visco.zebulon` file included hereafter. The cooresponding model is a typical Chaboche viscoplasticity model. Note that the value of the young's modulus will indeed be 150000. as defined in the Zmat file, and that the value of 20000. given after the `isotropic` command of the `.dat` file has no impact whatsoever on the results.

```
***material
*integration theta_method_a 1. 1.e-9 100
***divergence_variable 8 20.
***behavior gen_evp
  **elasticity
   young 150000.
   poisson 0.3
  **potential gen_evp ev
   *criterion mises
   *flow norton
     n 7.
     K 1200.
   *kinematic nonlinear
     C 126000.
     D 380.
   *isotropic constant
     R0 10.
***return
```

Using the Zpreload utility on the above material file would produce the following output:

```
$ Zpreload visco.zebulon

Reading behavior in file: visco.zebulon

===========================================
Flux Name:
  sig11   sig22   sig33   sig12   sig23
  sig31

Grad Name:
  eto11   eto22   eto33   eto12   eto23
  eto31
```

```
var_int Name:
  eel11(sdv1) eel22(sdv2) eel33(sdv3) eel12(sdv4) eel23(sdv5)
  eel31(sdv6)
  evcum(sdv7)
  al111(sdv8) al122(sdv9) al133(sdv10) al112(sdv11) al123(sdv12)
  al131(sdv13)
var_aux Name:
  evi11(sdv14) evi22(sdv15) evi33(sdv16) evi12(sdv17) evi23(sdv18)
  evi31(sdv19)
==========================================
done with material file reading...

Temperature not needed...
...
```

This allows to select the number of state variables needed by the behavior (19 variables in the example) that should be given as argument of the **state var** command. State variable number 7 is the cumulated plastic strain (named **evcum**) for this particular Zmat behavior. This material variable will be stored in the Marc results file using the appropriate **post elem var** code (-7 in this case). This variable is also used to monitor local divergence (**1308** code to define the user criterion used in the **auto step** procedure), and a corresponding *****divergence_variable** is included in the Zmat file to control the increment cut-back in case of local divergence. Note that Marc always use the first state variable to store the temperature, such that the state variable id given by Zpreload must be incremented by one to select the proper material variable.

Finally, note that this shift in the state variable id, is automatically taken into account for the **post** command (the shift is done in the **plotv** user subroutine included in the Zmarc release).

Chapter 6

Z-mat SAMCEF

Z-mat SAMCEF interface

Description:
The command described in this chapter allows to use a Z-mat behavior within a SAMCEF-MECANO analysis. The interface makes use of the `OVMAXX` user subroutine that allows to implement user-defined behavior within SAMCEF.

Syntax:
% Zsamcef *problem* ←↩
    where *problem*`.dat` is the name of a SAMCEF input data file.

The `Zsamcef` script activates a non-standard MECANO executable with name:
    `$Z7PATH/Zsamcef/mecano_zmat_$Z7MACHINE`
Please verify that this file is indeed included in your Zset distribution.

    A new user module (module `"mecano_zmat"` associated to module Id `"zm"`) should be declared in the SAMCEF environment by means of the `samrc.ini` configuration file.
    The `samrc.ini` file in the user home directory is automatically updated by the `Zsamcef` script with the command required to declare this new user module:

    `module*zm.me: mecano_zmat $Z7PATH/Zsamcef/mecano_zmat_$Z7MACHINE`

    Note that a MECANO calculation with a Z-mat behavior can alternatively be launched by the following standard SAMCEF command, that chains the `bacon` mesher with the `mecano_zmat` user module:
% samcef ba,zm *problem* n 1 ←↩

MECANO Input:
The main Z-mat modification needed in a standard MECANO input file concerns the `.MAT` command used to define material properties.
    Syntax is the following, where the `BEHA` parameter that usually allows to specify the name of a standard MECANO material behavior is replaced by a `ROUTIN` parameter followed by the name of the Zmat material file :

```
.MAT NOM "MATERIAU"
      ROUTIN "zmat_fname"
!     Elastic parameters definition is needed
!     but values are not meaningful
      YT 10.
      NT 0.3
!     For anisothermal problems thermal expansion
!     coef A should be set to 0. and defined
!     in the Z-mat file by means of a **thermal_strain object
      A  0.
```

    where `zmat_fname` is the name of a Z-mat material file. Note that:

- definition of some elastic properties (coefficients `YT` and `NT`) is required in the SAMCEF input file. However, values given for those coefficients have no incidence on the results, since the actual definition of the elasticity coefficients is given in the Z-mat material file

- for anisothermal problems the value of the thermal expansion coefficient needed to calculate thermal strains should be given in the Z-mat file, and it is safer to set the `A` coefficient to zero in the SAMCEF input file.

Z-mat interface file:

Most of the commands are common to the various Z-mat interfaces and are described in the Z-mat interface file section (page 2.3). However, some commands are not supported by the SAMCEF interface, while others are specific to this port. Hence, the various commands allowed in the `Zsamcef` interface file are summarized hereafter. Only options that are indeed specific to SAMCEF will be described in detail.

Syntax:

```
[ ***debug ]
[   *local_debug ip  ]
[ ***automatic_time ]
[   *limit name1 vmax1 ]
...
[   *limit namei vmaxi ]
[ ***save_tensor tname  ]
[ ***save_scalar sname  ]
[ ***needs_temperature ]
  ***material
[   *file fname  ]
[   *integration ...         ]
[   *rotation ...            ]
[   *initialize_variable ... ]
[   *dim dim ]
  ***behavior
    ...
  ***return
```

debug   This command indicates that debug output will be generated during MECANO execution. Output will be stored in a file named "fname.msg", where "fname" is the name of the Z-mat interface file.

*local_debug *ip*

This subcommand restricts debug output to the integration point number *ip* given as argument. *ip* is an integration point counter managed internally by Zsamcef, incremented during the loop on the elements and resetted to zero at the beginning of each newton global iteration. Note that the `OVMAXX` SAMCEF user subroutine doesn't provide any information on the element/integration point number that could allow a more meaningful selection mechanism. By default debug output will be generated for all integration

point of the FE mesh, which will result in huge ouput files and may dramatically slow down the calculation.

***automatic_time   This command may be used in conjunction with the SAMCEF automatic time step procedure based upon material integration error. To enable this option the following parameters must be given as arguments of the `.SUB` command in the SAMCEF input file:

```
.SUB ...
 VISC 1  ! activates material automatic time step
 PRCV 1. ! material allowable error. note that default value
         ! of 0.1 is not compatible with the Z-mat mechanism
 SREF 1. ! material ref norm (default value)
...
```

*limit *namei   vmaxi*

This command indicates that, during a loading increment, the increase of the *namei* material variable should not be greater than a given value of *vmaxi*. Several `*limit` commands acting on different material variables may be added if necessary. The material error returned by Z-mat to SAMCEF will be calculated as follows:

$$ERRLOC = \max_i \left\{ \frac{\Delta v_i}{vmax_i} \right\}$$

where Δv_i is the increase of variable number i, and the max is taken over all material variables v_i specified by a `*limit` command. This `ERRLOC` value will then be compared by SAMCEF to the `PRCV` parameter of the `.SUB` command in order to estimate the appropriate time step size. Note that `PRCV` should always be set to 1.0 in this particular context.

***save_tensor *tname*

***save_scalar *sname*

Output of user-behavior material variables to the SAMCEF results files is restricted to one tensor and/or scalar only. Corresponding FAC codes are `1399` and `1499` that should be requested by an appropriate `.SAI` command in the SAMCEF input file:

```
.SAI ...
 ARCHIVE ALL_ELEMENTS STYPE 1399 ! user scalar
                             1499 ! user tensor
...
```

The `***save_tensor` and `***save_scalar` commands then allow to specify which Z-mat variable will be saved in the results files.

***needs_temperature   Z-mat automatically detects that the temperature should be stored in the state variables when a material coefficient dependence on this parameter is defined in the behavior. However, if all material coefficients are constant, temperature is

removed from the state vars management to cut down storage requirements. In this case the thermal strains calculated by the **thermal_strain object will always be zero.

The ***needs_temperature command may then be used to force storage of the temperature and allow thermal strain calculation even if no coefficients are temperature-dependent.

material   As decribed in the Interface file section (page 2.10), this bloc of commands is used to set integration methods parameter (command *integration), define local axis for the calculation of material quantities (command *rotation), initialize material variables, etc... A different file may also be specified that will contain the actual behavior definition (behavior commands) by using the *file command. This allows to separate the interface commands, that may be specific to the FEA code, and the material coefficients. Default is to look for the ***behavior definition in the interface file.

*dimension *dim*

Second order tensors passed in by SAMCEF as arguments of the user-material subroutine OVMAXX always have 6 components (storage of a 3D symmetric second order tensor in a vector), regardless of the problem dimension. Theorically, the particular kinematic hypothesis used in the calculation (3D, axisymetric, plane strain, plane stress ...), can be known at the level of the OVMAXX routine by means of the IHYP argument.

Unfortunately, in the current SAMCEF version (SAMCEF v10.1), this argument is not correctly initialized during the loading phase of the Z-mat behavior. Therefore, by default, all Z-mat objects will be initialized with a 3D size. A *dimension 2 command may then be used to bypass this problem and cut-down material state variables storage requirements for 2D problems.

Note also that for the same reason, it is currently necessary to add an explicit plane_stress modifier to the behavior, or a **plane_stress switch in the gen_evp assembly, in order to properly take into account the plane stress hypothesis.

Chapter 7

Z-mat Cosmos

Z-mat Cosmos/M interface

Description:
Currently we are not providing any implicit interface for Z-mat with Cosmos. Users are encouraged to contact the distributor if they require a separate interface for Cosmos. Unfortunately demand for this port has been extremely limited.

Like many of the older style interfaces, the user interface for Cosmos/M required compilation of a custom executable and therefore requires specifically the compiler and development environment recommended by SRAC. The build scripts are still supplied with Z-mat distributions, and it is very likely a user could modify that for current versions of Cosmos. The last supported Cosmos release was 2.8.

Chapter 8

Z-mat LS-Dyna

Zlsdyna LS-Dyna interface

Description:
The Zlsdyna port applies to the user material facility within the explicit dynamics code LS-Dyna. Implicit integration modes are not supported for this interface, so the port is strictly explicit and therefore somewhat different from the other codes.

The user is referred to the LS-Dyna documentation sections under the `*MAT` chapter of the user commands manual for topic `*MAT_USER_DEFINED_MATERIAL_MODELS`, and also to information included in the Appendix A of the 970 user manual.

Syntax:
% `Zlsdyna` [*opts*] *problem* ↩

Compatibility:
The Zlsdyna interface is tested at the time of writing with LS Dyna 970 which requires building a custom executable from the development kit. The interface has been tested with both single process and MPP versions of LS-Dyna. Unfortunately because of licensing restrictions NW Numerics is unable to re-distribute modified binaries of LS-Dyna, so the compilation obligation falls on the end user. In some cases NW Numerics has been able to assist in this compilation process, so please inquire with the distributor.

This procedure imposes the following very strict requirements:

- Precisely the same compiler as defined by LSTC must be available and used for the build process.

- The development kit must be obtained from LSTC. There are different development kits for the single and MPI based distributed domain solver.

- Check with NW Numerics on our testing level with the platform chosen. Because of the many different computer/distribution levels possible there is likely some configuration work to be done.

Note: With LS Dyna 971 MPP versions there will be a more robust "plug-in" style interface will be implemented similar to `ABAQUS` and `ANSYS`. In that case the Zlsdyna installation and version tracking will become a negligible effort. All aspects of the user launch process will remain the same however.

Getting started:
Perform a standard installation of Z-set, including the binaries and shared files. The install location will henceforth be referred to as the `Z7PATH`. In the user-compiled case the LS-Dyna executable will be located in a common library directory. With the shared library method used with 971 it will be necessary to specify the location of the LS-Dyna executable via the `Z7_DYNA_ROOT` environment variable.

There are some test cases in the `Zlsdyna/` directories in the validation test database. For `LS-Dyna` the Z-mat interface file name is standardized to be `umat41` or `umat42`. Note that because of the need to have an automated testing environment with all the LS-Dyna validation cases in the same directory, the testing program copies a Z-mat interface file *prob*`.zmat` to

umat41 where *prob* is the basename of the *prob*.k input before running Zlsdyna. In fact this behavior is a convenienace option of the Zlsdyna command, with the -auto switch. One can equivalently set the environment variable Z7_DYNA_AUTOCOPY to be equal to yes.

Input file change:
Like all the other Z-mat interfaces, there are some lines in the user's input deck (the .k file) which must be changed to indicate that a user-material is being used, and to specify the amount of state variable storage. The following is an example:

```
*MAT_USER_DEFINED_MATERIAL_MODELS
$       mid        ro        mt       lmc       nhv     iorth     ibulk        ig
          1     8.930        41         2        40         0         1         2
$     ivect     ifail  ithermal
          0         0         0
$        p1        p2
        1.3     0.433
```

The **mt** data entry specifies the user routine to use, and the **nhv** entry specifies the number of state variables required.

Zmaster interface:

The **d3plot** results files can be read via Zmaster directly as an alternate choice for post processing, though the standard LS-Dyna prepost is quite a nice environment and there may not be so much reason to do this. Because there is no default suffix an added switch **-d3d** is needed to indicate an LS Dyna file. When a numbered series of **d3plot** files is to be read only the 1st file (unnumbered) should be specified on the command line.

```
Zmaster -d3d d3plot
```

Either the Zmaster **Mesh**, **Plot**, or **Results** buttons can be used.

Zpost interface:
Probably more interesting than running in Zmaster for commercial users is the ability to do post processing or results file translations. The following is an example for extracting time displacement data at a node in a batch task (execute with **Zrun -pp**):

```
****post_processing
   ***data_source d3plot
    **open d3plot

   ***global_post_processing
    **file node
    **output_number 1-999
    **nset ALL_NODE
    **process curve control_energy.bar-impact.test
     *precision 3
     *node    1333  U3

****return
```

Chapter 9

Behavior functionality

Introduction to Behaviors

Material behaviors in Z-mat use by far the most dynamic and object oriented input of all the Z-set modules. This is because behaviors are a set of constitutive equations which get built from fundamental "building bricks" of sub-models. There is widespread re-use of all these "bricks" between different behavior models. It is therefore necessary to adjust our input syntax (or at least documentation of it) to allow for more flexibility.

<u>Classes</u>:

The most important concept for this chapter is the notion of a *class* of permissible options, of which the user will choose one or more *objects* from that class in the material definition.

A class is an abstract notion of basic functionality, and will henceforth be denoted by the following convention: `EXAMPLE_CLASS` indicating that an object of type `EXAMPLE_CLASS` is permitted. In the handbook, one will find another section with heading `EXAMPLE_CLASS` which describes the different types allowable for the class.

An example is an `ELASTICITY` *class* which handles the calculation of stress from a strain, usually employing a 4th order tensor of various modulus coefficients. Because of this very general function, many behavior models allow for an `ELASTICITY` instance. In turn, the elasticity class has many possible types which one can select to fill in an elasticity object (isotropic, orthotropic, etc).

```
**elasticity <ELASTICITY>
```

The keyword `**elasticity` used here is in fact specific to the behavior model. While we frequently see the same keyword indicating classes between behaviors, this is not necessarily so. The function of each sub-command will be described in the discussion of the behavior model itself. What defines the syntax which follows this line is the `ELASTICITY` notation, indicating an elasticity matrix should be input. Again, the use should then go to the `ELASTICITY` section of the handbook, and investigate the possible models for this option.

Many behavior models also include the possibility of multiple instances of certain keywords. These possibilities will be described in the section of the containing class (behavior is a "material piece" class, but there are many others which can contain sub-pieces themselves). The standard notation for multiple instances of a class is to include three dots following the data entry line:

```
*kinematic <KINEMATIC>
   ...
```

This means that the material at this location can take *any* number of `*kinematic` entries, in any order, and with no restriction on type.

<u>Example</u>:

An example file follows, which is of a simple elasto-viscoplastic model with non-linear isotropic hardening, and two kinematic hardening components. Note that the behavior has taken two objects, an elasticity matrix and a "potential" (dissipation potential with an inelastic deformation associated to it). The material behavior is `gen_evp` which stands for generalized

elasto-viscoplastic (see page 10.12). The potential has in turn taken on a number of sub-objects: criterion, flow, kinematics and an isotropic hardening. This behavior actually allows for more than one **potential instance, so very complex behaviors are possible.

```
***behavior gen_evp
 **elasticity isotropic
       young 260000.
       poisson 0.3
 **potential associated ev
   *criterion mises
   *flow norton
       n  7.0
       K  400.
   *kinematic linear
       C  15000.0
   *kinematic nonlinear
       C  6000.0
       D  100.0
   *isotropic nonlinear
       R0 130.0
       Q  20.0
       b  500.0
 ***return
```

Another important thing to notice here is the coefficient C is entered after each *kinematic entry. These coefficients are distinct in the behavior because they *belong* strictly to the kinematic objects. This totally illuminates the possible conflicts inherent with hard-coding the model to have for example C1 and C2.

Grad-Flux

The compatibility of material behaviors with the element is determined dynamically based on their gradient (or primal) and flux (dual) variables. These can also be thought of as the material input-output combination. These variables are also *observable* state variables and observable associated forces. Some of the primal-dual variable combinations in Z-mat are as follows[1]:

CODE	DESCRIPTION
`eto – sig`	small deformation ϵ–$\boldsymbol{\sigma}$
`F – sig`	updated Lagrangian large-strain $\mathbf{F}$–$\boldsymbol{\sigma}$
`dT – q`	thermal analysis
`dC – J`	diffusion analysis

The process relative to element integration is shown schematically below. Non-linear finite element analysis consists of a loop over all elements in order to fabricate the global DOF residual vector (and possibly fabricate the stiffness if needed). In turn, there is a loop within the element over the integration points in order to numerically integrate the elements volume integrals. At each integration point, the new increment in primal variable is calculated using the increment of degrees of freedom, and their derivatives (this is where *grad* comes from), and this is passed to the material behavior with the current value of state variables.

---
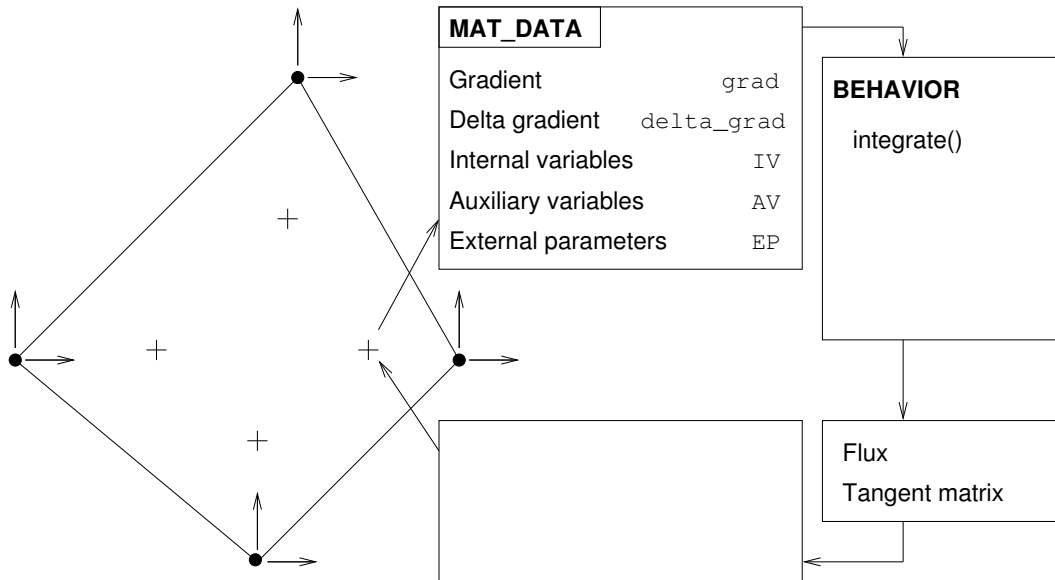
[1] Z-mat used for other codes such as ABAQUS establish a similar relationship, where the *UMAT* interface adjusts itself according to the material primal-dual couple

Material variables

As introduced in the previous section, material behaviors in Z-mat are dynamically "created" by the user through the assemblage of material sub-objects. The example given of a `gen_evp` behavior on page 9.3 was certainly structured this way. Of interest to the user is what variables are contained in the model, and what is available for output [2].

Principally all material *objects* (behaviors and their sub-component classes) have the possibility of the following variables:

grad   is the gradient or primal observable input variable.

flux   is the flux or dual output variable. Normally thermodynamically conjugate with the grad.

var-int   integrated state variables. These define the current state of the material, and are the subject of the integration method. Normally the more var-int variables, the higher the cost of local integration.

var-aux   auxiliary variables; normally used for output, or maintaining state information on a total basis (secondary to var-int).

ext-param   External parameters. These are imposed using `***parameter` statements in Zebulon, or with field variables in other codes.

coefs   material coefficients. Can depend on any of the above! Note however that the integration method or implementation restrictions can limit such dependence.

Each variable is assigned a name, but unlike other codes where the relationship between model options is hard-coded, the naming scheme is not known *a priori*. Much of the final naming is up to the user. The example on the next page demonstrates how the names are constructed.

Variable attributes:
When asking for specific output of the material variables, some additional attributes are available. These are summarized as follows:

CODE	DESCRIPTION
scal`::fabs`	absolute value of scalar
tens`::mises`	von Mises equivalent of tensor
tens`::trace`	Trace of tensor
tens`::p1`	Principal eigen values of tensor; also `::p2` and `::p3`
vec`::eq`	Equivalent of vector

---

[2]Because of the dynamic nature of the object construction, it is often difficult to strictly define the names of all the stored variables ahead of time. Users are thus **strongly** advised to observe the stored variables by using the `-v` command line switch or `**verbose` output option.

An example of accessing these secondary variables in a Zebulon output statement follows:

```
***output
 **component sig::mises sig::p1 sig::p2 sig::p3
             sig11 sig22 sig33 sig12
             eto11 eto22 eto33 eto12
```

Example:
Taking the `gen_evp` material file example given previously (page 9.3), and running it with verbose set (on by default in Z-mat for ABAQUS, or with a `-v` switch running in Zebulon or Z-sim) gives the following output:

```
===========================================
Flux Name:
  sig11  sig22  sig33  sig12
Grad Name:
  eto11  eto22  eto33  eto12
var_int Name:
  eel11  eel22  eel33  eel12
  evcum
  al111  al122  al133  al112
  al211  al222  al233  al212
var_aux Name:
  evi11  evi22  evi33  evi12
Default Output:
  eto11  eto22  eto33  eto12
  sig11  sig22  sig33  sig12
  evcum
  evi11  evi22  evi33  evi12
===========================================
```

In fact what happens here is the behavior is put together by the different "bricks," with each brick naming its own variables. Note that the potential line input was `**potential associated ev` and that the last key `ev` was used as a pre-fix for that potentials variables. Thus one has `evcum` for the plasticity (viscoplasticity in this case) multiplier, and `evi##` as components of the inelastic strain tensor. The variable construction in this model can be represented as shown below:
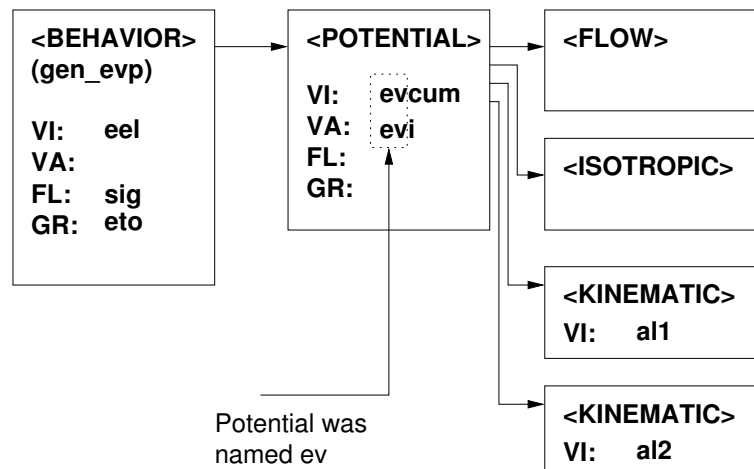
Naming conventions:

The dynamic nature of the material assembly notwithstanding, some conventions are given in the documentation and reflected in the default naming of variables. A small summary table of some common names follows.

CODE	DESCRIPTION
eto	total strain
ETO	"material strain" for finite strain. This is the integration of the corotational strain measure – not the logarithmic strain, etc.
sig	Cauchy stress
eel	elastic strain
eth	thermal strain
evcum	cumulated, monotonically increasing scalar measure of viscoplastic strain. Actually the integration of the viscoplastic multiplier.
epcum	cumulated plasticity equivalent of evcum. The naming difference is usually only symbolic.
f	porosity for porous materials.

Material file

The material and global-scope coefficients to be used are defined in a separate file henceforth described as the material file. The material file is a standard ASCII text file of form similar to the main input file. Most instances where a material filename needs to be specified allows an optional integer value for the instance of behavior in that file, the default instance being the first. So, when a material file is opened, the program will search for the n-th occurrence of the keyword ***behavior, skipping all other data contained before. Frequently for example and verification problems, the material file is given in the same physical file as the referring input file for compactness and file management purposes[3].

Regardless of how or where the material file is located, the material file is a separate entity from the other input commands, with an independent command hierarchy starting at the ***-level. The general structure of this file is the following:

```
***behavior BEHAVIOR [ modifiers ]
 **functions
   list of function declarations
   ...
 **behavior sub-procedures
   ...
 **coefficient
   coefficient_name COEFFICIENT
   ...
 **save_coefficients
   coef-names
 **plane_stress
***return
```

***behavior begins the definition of a material law. The options which follow are of course specific to each material model.

**coefficient indicates the definition of intrinsic coefficients which are not specific to material laws[4]. These coefficients are applicable to all the material models. The allowable global coefficients are summarized below:

CODE	DESCRIPTION
masvol	volumetric mass of the material
capacity	volumetric heat capacity (ρC_p)

---

[3]Note that we frequently find this the advisable approach for production runs as well, as it avoids confusion or possible version conflicts when numerous runs are to be made.

[4]Older definitions with the ***coefficient command outside the ***behavior and ***return commands are no longer allowed.

Units should be coherent within the problem definition. For example, if using SI system, `masvol` is in $kg \cdot m^{-3}$ and `capacity` in $J \cdot m^{-3} \cdot K^{-1}$, but if using the (mm,MPa,s) unit system, `masvol` is in $ton \cdot mm^{-3}$ and `capacity` in $J \cdot mm^{-3} \cdot K^{-1}$.

**plane_stress   indicates that a plane stress behavior is to be used ($\sigma_{33} = 0$). This is not available with all material behaviors. Zébulon plane stress must not use this option.

**save_coefficients   list coefficient names which are to be saved as output variables. New var-aux variables are created, and therefore increase the total storage for each material integration point. This option is extremely useful when the variation of coefficients is important, such as in coupled problems.

Example:
Another example of material file input follows, showing some tabular coefficient input:

```
***behavior linear_elastic
  **elasticity isotropic
    young temperature humidity
        200000.e0  100.    0.
        100000.0    "      1.
        100000.0   200.    0.
         50000.0    "      1.
    poisson 0.3
  **thermal_strain
    alpha temperature
        1.e-6   0.
        1.e-6   1000.
    ref_temperature 0.0
 **coefficient
    masvol 7.e-9
***return
```

<BEHAVIOR>

<BEHAVIOR>

Description:
This class of objects provides the basic building block for material models. Each object type tries to cover as broad a range of behavior as possible, using the idea of sub-model objects to increase the possible combinations.

Syntax:

***behavior BEHAVIOR   [*modifier*]
 **-*level commands*
 **coefficient
    coefficient list
***lagrange_modifier *type*

We have broken the behavior models up into three classifications reflecting the following three chapters of this book. The first is for models which make up significant *frameworks* for treating broad ranges of characteristics, the details of which are fixed by selecting from a broad range of options and sub-components. The second group of models are "secondary models" in that they are coded in a specific fashion, usually as a prototype stage on their way to being incorporated into the general class materials. The third "Other" classification is for material models fitting a particular application which in general is not suitable for Z-mat interfaces with standard mechanical codes (e.g. debonding or spring behaviors specific to Zebulon).

Finite Strain:
The behaviors are normally defined using small strain assumptions. These models may be transformed to finite deformations / rotations using one of the behavior modifiers described on page 14.2. The hyper_elastic behavior models are however formulated specially with total Lagrangian assumptions and must therefore be used with the appropriate total Lagrangian elements.

Chapter 10

Material Models

***behavior linear elastic

Description:

This behavior class provides classical linear elastic behavior with optional thermal deformation. The behavior understands two "blocks" from which it is defined.

Syntax:

```
***behavior linear_elastic [ modifier ]
 **elasticity ELASTICTY
[ **thermal_strain THERMAL STRAIN ]
```

By default there is no thermal dilatation in the model.

Example:

Two examples of linear elastic behavior follow:

```
***behavior linear_elastic
**elasticity isotropic
    young 200000.
    poisson 0.30
***return


***behavior linear_elastic
  **thermal_strain anisotropic
    codila1  1.0e-06
    codila2  2.0e-06
    codila3  3.0e-06
  **elasticity orthotropic
      y1111 350000.
      y2222 280000.
      y3333 280000.
      y1122 150000.
      y2233 120000.
      y3311 150000.
      y1212 180000.
      y2323 180000.
      y3131 180000.
  ***return
```

***behavior damage_elasticity

Description:

This is a simple behavior for elastic energy based damage. It is duplicated by the `gen_evp` `**damage` option with type `*elastic`. This behavior is given as an example of a simple user model programmed without ZebFront. The source is available in the developer handbook.

$$\boldsymbol{\sigma} = (1 - D)\mathbf{D}_{el} : (\boldsymbol{\epsilon}_{to} - zeth)$$

$$\bar{Y} = \frac{1}{2}\boldsymbol{\epsilon}_{el} : \mathbf{D}_{el} : \boldsymbol{\epsilon}_{el}$$

$$D = \alpha \left[\max \sqrt{\bar{Y}} - \sqrt{Y_0} \right]$$

Syntax:

```
***behavior damage_elasticity
 **elasticity <ELASTICITY>
 **YO    COEFFICIENT
 **alpha COEFFICIENT
```

Stored Variables:

The grad variable is the gradient of temperature, and the flux is the heat flux.

prefix	size	description	default
eto	T-2	total (small deformation) strain	yes
sig	T-2	Cauchy stress	yes
y_max	S	$\bar{Y}$	no
damage	S	damage D	yes

Example:

```
***behavior damage_elasticity
 **elasticity isotropic
    young 200000.
    poisson 0.0
 **YO    20.0
 **alpha  0.001
***return
```

***behavior hyper_elastic

Description:

This behavior handles all (simply) hyperelastic material laws. For cases of hyper-viscoelastic or hyper-viscoplastic models please see those corresponding behaviors. Note that the syntax for hyperelasticity in Z-mat has changed significantly with the 8.3 release, and the (un-mixed) hyperelastic laws are now available for use with the different Z-mat interfaces. All the previous individual behaviors for each potential form have been deprecated, though a compatibility syntax is still provided.

The hyperelastic potential is defined by a material component for this task, which is shared between the other laws employing such a potential. There are several main classes of hyperelastic "rules" which can be inserted in this behavior depending on their assumptions and integrated rules. The following type are allowed:

- default HYPERELASTIC_LAW objects.

- isotropic HYPERELASTIC_LAW objects which are somewhat more specific and where certain properties of the potential tangent can be made.

Syntax:

```
 ***behavior hyper_elastic
[ **thermal_strain <THERMAL_STRAIN> ]
[ **hyperelasticity <HYPERELASTIC_LAW> ]
[ **isotropic_hyperelasticity <ISOTROPIC_HYPERELASTIC_LAW> ]
[ **model_coef ]
     ...
```

Example:

```
***behavior hyper_elastic
  **hyperelasticity arruda_boyce
  **model_coef
    mu      0.893
    lambda 9.0
    K0      10000.0
***return
```

***behavior linear_viscoelastic

Description:
This behavior defines a generalized linear viscoelastic Maxwell model. The model defines the stress, $\boldsymbol{\sigma}$, to the strain $\boldsymbol{\epsilon}$ by the following relation:

$$\boldsymbol{\sigma}(t) = \int_0^t 2G(t-\tau)\dot{\mathbf{e}}(\tau)\,d\tau + \mathbf{1}\int_0^t K(t-\tau)\operatorname{Trace}\dot{\boldsymbol{\epsilon}}\,d\tau$$

with $\mathbf{e}$ the deviator of the strain tensor $\boldsymbol{\epsilon}$. The terms G and K are relaxation functions defined by Prony series:

$$
\begin{aligned}
\mathrm{G}(\tau) &= G_\infty - (G_\infty - G_0)\Psi_1(\tau) & \Psi_1(\tau) = \sum_{i=1}^{i=n_\alpha} \omega_i \exp(-\tau/\tau_i) \\
\mathrm{K}(\tau) &= K_\infty - (K_\infty - K_0)\Psi_2(\tau) & \Psi_2(\tau) = \sum_{i=1}^{i=n_\beta} \omega_i \exp(-\tau/\tau_i)
\end{aligned}
\tag{1}
$$

G_0 and G_∞ are shear modulus coefficients

K_0 and K_∞ are bulk modulus coefficients

Remark:
The sum of the coefficients ω for modulus terms must equal one.

The implementation of the model is in differential form with the internal variables $\boldsymbol{\alpha}$ and β. The state equations are written in the following form:

$$\boldsymbol{\sigma} = \sum_{i=1}^{i=n_\alpha} \mathbf{X}_i + \sum_{i=1}^{i=n_\beta} \mathbf{Y}_i + 2G_\infty \mathbf{e} + K_\infty \operatorname{Trace}\boldsymbol{\epsilon}\mathbf{1}$$

with

$$
\begin{aligned}
\mathbf{X}_i &= -2(G_\infty - G_0)\omega_i(\mathbf{e} - \boldsymbol{\alpha}_i) & 1 \le i \le n_\alpha \\
\mathbf{Y}_i &= -3(K_\infty - K_0)\omega_i(\operatorname{Trace}(\boldsymbol{\epsilon})/3 - \beta_i)\mathbf{1} & 1 \le i \le n_\beta
\end{aligned}
\tag{2}
$$

The evolution equations for the internal variables are:

$$
\begin{aligned}
\dot{\boldsymbol{\alpha}}_i &= \tfrac{1}{\tau_i}(\mathbf{e} - \boldsymbol{\alpha}_i) & 1 \le i \le n_\alpha \\
\dot{\beta} &= \tfrac{1}{\tau_i}(\operatorname{Trace}\underset{\sim}{\epsilon}/3 - \beta_i) & 1 \le i \le n_\beta
\end{aligned}
\tag{3}
$$

It is necessary to define a single time the coefficients K_0, K_∞, G_0 and G_∞ using the key words **K0, **K_inf, **G0 and **G_inf respectively. One may then define an arbitrary number of the variables $\boldsymbol{\alpha}$ and β using the key words omega and tau. omega is a constant coefficient.

Syntax:
The syntax for this behavior model is the following:

```
   **K0           COEFFICIENT
   **K_inf        COEFFICIENT
   **G0           COEFFICIENT
   **G_inf        COEFFICIENT
   **shear        ...
   **volumic      ...
```

Options **shear** represent the shear mechanisms and are defined by the following form:

```
**shear
    tau   COEFFICIENT
    omega COEFFICIENT
```

where the coefficient `tau` corresponds to the material constant τ and `omega` to ω as in equation 1.

Similarly, the option *volumic* represents the volumetric mechanisms using the same coefficient / material constant naming:

```
**volumic
    tau   COEFFICIENT
    omega COEFFICIENT
```

Stored Variables:

The internal variables stored for this model are the total strain (code `etoxx`), the tensorial variables α_i (code `alpha#xx`) and the β_i variables (code `beta#`).

prefix	size	description	default
eto	T-2	total (small deformation) strain	yes
sig	T-2	Cauchy stress	yes
alpha#	T-2	$\boldsymbol{\alpha}$ variable	no
beta#	S	β variable	no

The code names will replace the `#` symbol with the sequential number of that variable type as given by the order of declaration, and the *xx* symbols will be replaced with the tensorial components. The default saving of variables in the output files are only `eto` and `sig`. Specify other saved variables in the `.inp` file.

Example:

```
***behavior linear_viscoelastic
**K0    42261.904761
**K_inf 13500.0
**G0    29098.360655
**G_inf 0.
**shear
   tau   0.4321660
   omega 0.2324006
**shear
   tau   9.070154
```

```
   omega 0.1891879
**shear
   tau    27.61690
   omega 0.2665674
**shear
   tau    102.8596
   omega 0.3118441
**volumic
   tau   0.1000000E-01
   omega 0.29800651
**volumic
   tau    0.3096638
   omega 0.8500050E-01
**volumic
   tau    0.2696395
   omega 0.4522469E-01
**volumic
   tau    6.517014
   omega 0.5717688
***return
```

***behavior viscoelastic_spectral

Description:

This behavior defines a spectral viscoelastic model. The model defines the stress, $\boldsymbol{\sigma}$, to the strain $\boldsymbol{\epsilon}$ by the following differential equations system:

$$\sigma = C_0(T) : (\epsilon - \epsilon_a - \epsilon_{th})$$

$$\epsilon_{th} = \alpha(T - T_0)$$

$$\dot{\epsilon}_a = g(\sigma) \sum_{i=1}^{i=n_t} \dot{X}_i$$

$$\dot{X}_i = \frac{1}{\tau_i}(\mu_i(T) * g(\sigma)C_R^{-1}(T) : \sigma - X_i)$$

C_0 is the elastic matrix. Note that S_0 used latter is defined by : $S_0 = C_0^{-1}$.

$g(\sigma)$ is the viscous non linear function

τ_i and μ_i define the spectrum. Each mechanism X_i is associated with a relaxation time τ_i weighted by μ_i. The whole strain family (X_i) describes a gaussian continuous spectrum.

Note:

For the moment, the thermal strains are not taken into account.

Syntax:

The material file structure for the `viscoelastic_spectral` model consists of an elasticity object, the definition of spectrum, of the viscous_effects tensor and of the assymptote. The syntax for this behavior model is the following:
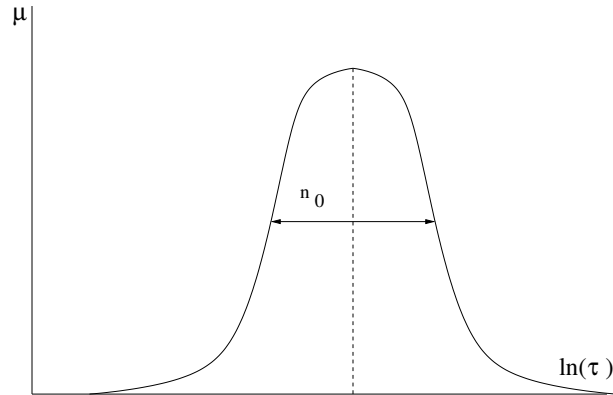
```
***behavior viscoelastic_spectral [ modifier ]
   **elasticity            <ELASTICITY>
   **spectrum              ...
   **viscous_effects       ...
   **reversible_asymptote  ...
```

Options **spectrum represent the spectrum which defined μ_i and τ_i (see next figure).

$$\mu_i = \frac{1}{n_o * \pi} exp(-(\frac{i - n_c}{n_0})^2)$$

The spectrum is defined by the following form:

```
**spectrum
   [*limit   double]
   [*n1  double]
   [*n2  double]
   *nt interger
   *nc COEFFICIENT
   *n0 COEFFICIENT
```

See the figure for the meaning of nt, nc and n0. n1 and n2 can be read in the material file (*n1 and *n2) or calculated such as $\mu(n1) > limit$ and $\mu(n2) < limit$.

Note:

By default `limit` is equal to 1.e-4 and `nt` to 30.

The option *viscous_effects defined the viscous effects tensor C_R.

```
**viscous_effects
   *lrt   COEFFICIENT
   *lrc   COEFFICIENT
```

C_R is defined such as :

for i equal 1 to 3 :

$$C_R(i, i) = lrt * S_0(i, i)$$

for i equal 4 to 6 :

$$C_R(i, i) = lrc * S_0(i, i)$$

and if $i \neq j$ for i and j equal 1 to 3 (isotropic condition):

$$C_R(i, j) = lrn * S_0(i, j)$$

with $lrn = (lrt * S_0(1, 1) - lrc * S_0(2, 2))/S_0(1, 2)$.

Finally the option *reversible_asymptote is used to define the non linear funtion $g(\sigma)$.

```
**reversible_asymptote
   *beta   COEFFICIENT/
   *p   COEFFICIENT/
```

$$g(\sigma) = 1 + beta(\sqrt{(\sigma : C_R^{-1} : \sigma)})^p$$

Remark:

beta=0 is equivalent to a classical linear assymptote.

Note:

Another definition of the asymptote (**plastic_asymptote**) is also implemented but not documented here because still under development.

Stored Variables:

The internal variables stored for this model are the total strain (code **etoxx**), the tensorial variables X_i (code **kip#xx**).

prefix	size	description	default
eto	T-2	total (small deformation) strain	yes
sig	T-2	Cauchy stress	yes
eel	T-2	elastic strain	yes
ean	T-2	anelastic strain	yes
kip#	T-2	X_i variable	no

The code names will replace the **#** symbol with a sequential number from 1. to nt.

The default saving of variables in the output files are only those marked by yes in the previous table.

Example:

```
***behavior viscoelastic_spectral
  **elasticity isotropic
    young 2800.
    poisson 0.3
  **spectrum
         *n1 -30.
         *n2  30.
         *nt  50
         *nc  7.
         *n0  3.
  **viscous_effects
         *lrt 0.6
         *lrc 0.6
  **reversible_asymptote
         *beta 1.
         *p    1.
***return
```

***behavior hyperviscoelastic

Description:
This behavior is a general Hyper-viscoelastic form with both shear and volumetric recovery components. The model is based on the discussions from Simo and Hughs [Simo98]. The model uses the same hyperelastic potential components as in the `hyper_elastic` behavior. Also *any number* of shear and volumetric terms can be added to the model.

Syntax:

```
 ***behavior hyperviscoelastic
[ **thermal_strain <THERMAL_STRAIN> ]
[ **hyperelasticity <HYPERELASTIC_LAW> ]
[ **hyperelasticity <ISOTROPIC_HYPERELASTIC_LAW> ]
[ **model_coefficients  ]
    ...
     possible **-level commands for hyper law
```

Example:
The following example comes from the validation tests. More examples can be found in `test/Viscoelastic_test/INP`

```
***behavior hyperviscoelastic
  **hyperelasticity logarithmic
  **elasticity isotropic
    young   2.8125
    poisson 0.40625
  **shear
     tau   1.0
     omega  0.4
  **shear
     tau   10.0
     omega  0.4
  **volumic
     tau   3.
     omega  0.5
***return
```

***behavior gen_evp

Description:
This material model is a generalized implementation of elastic, elastic-plastic or viscoplastic, and multi potential constitutive equations. The model is constructed entirely using object "bricks." For the moment, the model will be constructed using an elasticity object, a number of "potentials" and interactions between the potentials. Potentials represent inelastic dissipations which describe the evolution of independent inelastic deformation mechanisms. Hardening mechanisms are modeled with objects within the individual potentials (type of hardening depending on the type of potential) and are thus not yet specified. This behavior is essentially a manager of sub-model objects, and will be discussed in general terms about the permissible variables.

The model's internal variables are determined by the sub-objects which have been selected by the user. The general storage form includes variables which are "global" to the material laws, and therefore form relations with the imposed (observable) variables or apply to all the potentials. Each potential may additionally contain "parameter" variables which do not have associated forces, and "hardening" variables which do have associated forces. The distinction concerns the form of interaction which is possible. The total variables may therefore be envisioned as:

$$[\boldsymbol{\epsilon}_{el} \ldots][\mathbf{p}_1 \mathbf{h}_1][\mathbf{p}_2 \mathbf{h}_2] \ldots [\mathbf{p}_n \mathbf{h}_n]$$

where the first bracketed term represents the "global" model variables and each additional represents the potential mechanisms chosen. The first term is noted to assume a linear elastic small deformation law[1]. Again, the $\mathbf{p}_i$ and $\mathbf{h}_i$ variables are defined by the chosen potentials.

The model additionally stores auxiliary variables used as secondary output data. These variables take the following form:

$$[\ldots][\boldsymbol{\epsilon}_1 \ldots][\boldsymbol{\epsilon}_2 \ldots] \ldots [\boldsymbol{\epsilon}_n \ldots]$$

The first bracketed term is again for the "global" auxiliary variables and the following bracketed terms indicates each potential's variables. In the event of more than one potential, the first total inelastic strain, $\boldsymbol{\epsilon}_{in} = \sum \boldsymbol{\epsilon}_i$ will be stored in addition to each inelastic deformation component.

If interactions are present, the hardening variable evolutions will take the form:

$$\dot{\mathbf{h}}_i = \dot{\lambda}_i \ \mathbf{m}_i(\boldsymbol{\sigma}, \ v_i, \ \mathbf{H}_i) - \dot{\boldsymbol{\omega}}_i(\mathbf{H}_i)$$

where $\dot{\lambda}_i$ is the plasticity or viscoplasticity multiplier for the i-th potential, v_i is the cumulated inelastic strain equivalent, and $\mathbf{H}_i$ are the associated forces for the potential i. Note that the evolution equations will normally only be written in terms of the associated force and thus one can immediately extend these models to include state coupling[2].

State coupling is given through symmetric interaction matrices $\mathbf{M}$:

$$\mathbf{H}_i = \mathbf{M}_{ij} \ \mathbf{h}_j$$

---

[1]extensions which change the $\boldsymbol{\epsilon}_{el}$ variable will be given in the next release of ZéBuLoN
[2]exceptions are available

Syntax:

The material file structure for the `gen_evp` model consists of an elasticity object, an optional thermal strain object, an optional arbitrary number of potentials (without restriction on types), and a number of optional interaction objects:

```
***behavior gen_evp [ modifier ]
  **elasticity        <ELASTICITY>
[ **global_output                         ]
[ **damage            <DAMAGE>            ]
[ **localization      <LOCALIZATION>      ]
[ **global_function   <GLOBAL_FUNCTION>   ]
[ **thermal_strain    <THERMAL_STRAIN>    ]
[ **conductivity      <CONDUCTIVITY>      ]
[ **potential         <POTENTIAL>  [name] ]
    ...
[ **interaction       <INTERACTION>       ]
    ...
```

The compatibility of objects with the other objects, and with the integration method will be investigated during the running of the problem. Because of the dynamic nature of these models however, it is often difficult to make any verification as to the physical meaning of a particular model combination. It is therefore strongly advised to observe the material behavior on a single element. This allows experimentation of the integration method and selection of the output variables without performing costly full scale calculations.

Multi-potential models are primarily used for cases of time independent plasticity in combination with viscoplastic deformation, or to assemble multiple crystalline deformation systems. By default, there is no thermal strain, no inelastic deformation or any interactions.

The optional names (`name`) given after each potential type are used as a means to specify individual potentials (for interactions), and in construction of the output variable names. Normally, it is advised to use `ep` for a plastic potential's name, and `ev` for a viscoplastic one.

Unless the option **global_output** is given, the internal variables are stored in their local material frame instead of the global one.

Stored Variables:

The stored variables for this model are the following:

prefix	size	description	default
eto	T-2	total (small deformation) strain	yes
sig	T-2	Cauchy stress	yes
eel	T-2	elastic strain	no
ein	T-2	total inelastic strain tensor	yes
e*nm*i	T-2	potential named *nm* inelastic strain tensor	yes

The variable `ein` is only stored in the event of multiple potentials. The separate inelastic strain tensors for each potential, and their hardening variable names will be given for each separate potential type.

Because the behavior does not know any specifics of the potentials or the user supplied names, and the applications of the same potential object may differ according to the rest of the behavior options, the variable names are vaguely specified at this moment. Name

verifications are strongly advised with the `-v` command line switch or using the `**verbose` output option.

Example:
The first example is for a viscoplastic behavior with two kinematic hardening variables and a Von Mises criterion (see the following sections for the sub-model syntax):

```
***behavior gen_evp
 **elasticity isotropic
    young 200000.
    poisson 0.30
 **potential gen_evp ev
  *criterion mises
  *flow norton
       n  7.0
       K  400.
  *kinematic nonlinear
       C  15000.0
       D  300.0
  *kinematic nonlinear
       C  6000.0
       D  100.0
  *isotropic constant
       R0 130.0
 ***return
```

Different cases using this behavior are described more fully in the example handbook.

This behavior is designed to work normally with all the integration methods, and gives the best tangent matrix possible for a given model. The use of specialized options may however limit the use to a certain integration, or otherwise. The user of this behavior is therefore advised to try the `theta_method` method integration on a volume element, and adjust solution parameters according to the messages output if any[3].

---

[3]This process will be automated for the best combination in later versions of the code

***behavior reduced_plastic

Description:
The reduced plastic behavior is an alternate formulation of the `gen_evp` behavior which provides a much more efficient implicit integration. The behavior reduces the integration variables to a single tensor and a scalar per deformation potential. Because the integration must assume certain forms for the potentials and hardening variables, this behavior uses a sub-set of the `gen_evp` options. In particular, there is no possibility for state interactions, and the number of potentials implemented is reduced. Domain modifying options such as damage or localization is nor currently implemented in this framework either.

Thermal deformations, variable coefficients, all the elasticity models, all the flow laws, and the majority of kinematic hardening models are implemented. There is no limitation on the number or mixing of kinematic models which are entered per potential, as long as they support the reduced integration. Note that certain laws break distinctly the reduced integration and are not implemented (i.e. Ziegler).

There is currently a limitation that the isotropic hardening be a function of the cumulated multiplier. This means that the internal variable versions of isotropic model are not supported. Note that non-macro potential models such as the mono-crystals are not implemented.

Syntax:

```
***behavior reduced_plastic [ modifier ]
  **elasticity      <ELASTICITY>
[ **thermal_strain <THERMAL_STRAIN>    ]
[ **potential       <POTENTIAL>  [name] ]
     ...
```

Stored Variables:

The stored variables for this model are the following:

prefix	size	description	default
eto	T-2	total (small deformation) strain	yes
sig	T-2	Cauchy stress	yes
eel	T-2	elastic strain	no
ein	T-2	total inelastic strain tensor	yes

The variable `ein` is only stored in the event of multiple potentials. The separate inelastic strain tensors for each potential, and their hardening variable names will be given for each separate potential type.

This behavior must be used with a θ-method of type A.

Example:
An example the input for which can be found in $/test/Kinematic/MAT/..$ is given below.

```
***behavior reduced_plastic
 **elasticity isotropic
      young 185000.
      poisson 0.3
 **potential gen_evp ev
```

```
    *store_all
    *flow norton
        K   .05
        n   2.0
    *kinematic nonlinear_with_crit
        C       600000.
        D       1000.
        omega 0.50
        m1      1.
        m2      1.
        eta   1.e-12
    *isotropic constant
        R0 400.
***return
```

***behavior porous_plastic

Description:
This material model is used for damage and densification of porous materials for which the flow rule is associated[4]. The model will be fabricated based on an assemblage of various objects to model the elasticity, criterion, flow, and various hardening (isotropic and kinematic) and nucleation options. The model supports multiple potentials, viscoplasticity, anisotropy, and combined isotropic and kinematic hardening. Many other features are also available for modifying the behavior including models for nucleation of porosity, fine tuning the numerical implementation, and studying the onset of bifurcation instabilities.

Please note that the kinematic hardening for porous plasticity is fundamentally different from what is used for non-porous unified viscoplastic models such as in `gen_evp` [BessXX]. The purpose of kinematic hardening is also not so much to simulate cyclic behavior, but rather to provide control of the yield surface curvature.

Many porous plastic analysis problems involve finite strain. Please refer to the documentation for `<MODIFIER>` at page 14.4 for the specifics of different corotational finite strain methods. Note that frequently we use the `no_J` option where the $\det(\mathbf{F})$ volumetric adjustment of the Cauchy stress is ignored. The reason to do this is because the volumetric change effects on the stress are essentially resolved by the porous potentials.

A common theme in porous plasticity is that a matrix stress $\sigma_\star$ is solved for based on the macroscopic nominal stress $\boldsymbol{\sigma}$, current plastic strain p, and current porosity f.
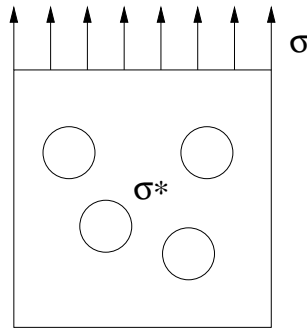
The means of localizing to the effective matrix stress is therefore given by a potential function ϕ which must always be satisfied:

$$\phi(\boldsymbol{\sigma}, f, \sigma_\star) = 0$$

Since the matrix stress $\sigma_\star$ is the "real material," porous plasticity uses the measure $\sigma_\star - R$ as the overstress condition with R being the current isotropic yield radius. The general porous viscoplastic material is therefore described by the following plastic multiplier:

$$\dot{p} = \dot{v}(\sigma_\star - R)$$

with $\dot{v}$ being any of the Z-mat flow laws given under `<FLOW>` (see page 13.43). The evolution of plastic strain is found via an equivalence of plastic work between the matrix stress/plastic

---

[4]This behavior is programmed only for the θ-method. No plane stress is available. The coefficients can depend on porosity, notably of which is the f^* for the Gurson potential.

strain and the macroscopic stress and strain (of the composite porous medium):

$$(1-f)\sigma_\star \dot{p} = \dot{\underset{\sim}{\epsilon}}_p : \underset{\sim}{\sigma} = (1-f)\dot{\lambda}\frac{\partial \sigma_\star}{\partial \underset{\sim}{\sigma}} : \underset{\sim}{\sigma}$$

The evolution of porosity is given via conservation of mass given that the plastic strain has a volumetric part due to the pore growth or compaction:

$$\dot{f} = (1-f)\,\mathrm{Trace}\,\dot{\underset{\sim}{\epsilon}}_p$$

In the case of multiple criterions Hp and Hf are used to specify interaction between potential so that:

$$
\begin{aligned}
p_e^i &= \sum_j H_p^{ij}(p^j) \\
f^i &= \sum_j H_f^{ij}(f_g^j + f_n^j) \\
f_t^i &= \sum_j H_f^{ij}(f_g^j + f_n^j + f_{ncl}^j)
\end{aligned}
$$

. . . continued

Syntax:
The whole-behavior keyword summary is given below:

```
***behavior porous_plastic [modifier]
    **thermal_strain        <THERMAL_STRAIN>
    **elasticity            <ELASTICITY>
    **porous_potential      [name]
     *porous_criterion      <POROUS_CRITERION>
     *flow                  <FLOW>
     *isotropic_hardening   <ISOTROPIC>
     *strain_nucleation     <STRAIN_NUCLEATION>
     *kinematic             <POROUS_KINEMATIC>
     *shear_anisotropy      <CRITERION>
    **porous_potential      ...
    **Hf                    <SMATRIX>
    **Hp                    <SMATRIX>
    **broken_behavior       <ELASTICITY>
    **adiabatic_heating
    **no_C_trick
    **save_D
    **save_L
    **bifurcation_D
    **bifurcation_L
    **perturbation
    **additional_var_aux
```

The following sub-options control the global behavior operation, while the rest of the specific model will be determined by the dynamic components chosen, most important of which is the porous potential.

additional_var_aux allows requesting that additional auxiliary variables be added to the model output. These can be chosen from `triax`, `p1`, `p2`, `p3`. These variables are closely coupled to the behavior so can be used for additional coefficient dependencies.

adiabatic_heating includes adiabatic heating via plastic work, and temperature is included as a state variable named `T`.

broken_behavior is used to enter an elasticity matrix to be used as the behavior after failure has been reached. The measure of "breaking" is determined by the models potentials (there could be different criteria for several potentials together).

Hf Coupling term for porosity given above. The matrix is read in as a series of real (floating point) values to fill the matrix. Note these are not general coefficients, but fixed values. The matrix is read $H_f^{11}, H_f^{12}, \ldots, H_f^{1N}, H_f^{21}, \ldots, H_f^{NN}$ with N the number of porous potentials.

Hp Interaction matrix for plastic strain influence between potentials. The matrix is read $H_p^{11}, H_p^{12}, \ldots, H_p^{1N}, H_p^{21}, \ldots, H_p^{NN}$ with N the number of porous potentials.

porous_potential   define a potential which is part of the model. This command is detailed separately on page 10.22. Any number of potentials (greater than or equal to 1) can be entered with repeated uses of this command.

Stored Variables:

The stored variables for this model are the following:

prefix	size	description	default
eto	T-2	Total (small deformation) strain	yes
sig	T-2	Cauchy stress	yes
eel	T-2	Elastic strain	no
broken	S	if broken	yes
seq	S	effective flow stress $\boldsymbol{\sigma}_*$	yes
p	S	equivalent plastic strain	yes
fg	S	growth porosity	yes
fn	S	nucleation porosity	yes
fncl	S	effective crack like nucleation porosity	yes
f	S	void volume fraction $f_g + f_n$	yes
ft	S	total effective porosity $f_g + f_n + f_{ncl}$	yes
pe	S	effective plastic strain	yes
Xmic	T-2	microscopic back stress	no
Xmac	T-2	macroscopic back stress	no
alpha	T-2	kinematic hardening internal variable	no
X	T-2	sum of all macroscopic back stresses	no

Example:

As discussed above, the porous plastic material behavior is a very broad code, and encompasses many options and features. The following is a simple "whole" example to give an indication of overall syntax. The user will please refer to the different applicable porous potentials for further examples and details.

```
***behavior porous_plastic lagrange_rotate_no_J
 **elasticity isotropic
    young 210000.  poisson 0.3
 **porous_potential
   *porous_criterion gurson
       fs = f
       q1 1.5
       q2 1.
   *shear_anisotropy mises
   *isotropic_hardening constant
       R0      T
       200.  -50.
       200.    0.
       150.  100.
       100.  500.
   *flow norton K .01 n 5.
 **adiabatic_heating .9
 **coefficient
    capacity 3.6
***return
```

**porous_potential

Description:

 *porous_criterion

 *shear_anisotropy

 *flow

 *isotropic

 *strain_nucleation

 *kinematic

***behavior mechanical_step_phase

Description:
This behavior is given to model materials which undergo a a phase change

Syntax:

```
***behavior mechanical_step_phase
  **integer_steps
  **parameter phase_id
  **phase Oxide 0
   *file step.mat 2
   *rotation <rot definition>
  **phase Alu 1 *file Alu.mat
 **return
```

Example:

```
***behavior mechanical_step_phase
  **integer_steps              % specify integer step values to be used
  **parameter phase_id         % the parameter defining the step phases
  **phase Oxide 0              % use this phase if phase_id = 0 (int value)
   *file step.mat 2            % This file, 2nd ***behavior instance
   *rotation <rot definition>  % a possible rotation defintion
  **phase Alu 1 *file Alu.mat  % use mat defined in Alu.mat for phase_id = 1
 **return
```

***behavior umat

Description:
This behavior is used to run a UMAT function within Z-set. It can be used to run Z-mat using the ABAQUS interface within Zebulon, or can be used to run a "real" Fortran UMAT within Z-set, which is perhaps very useful to be able to run the UMAT within the simulation module.

Syntax:

```
***behavior umat
  **constants num-coef
  **finite_strain
  **skip_param
  **cmname mat-name
  **umat_file fname
  **depvar num-sdv
  **model_coef
    C##   value
```

Example:
The following example shows a umat material definition, which is linked in fact to the Z-mat file on the right. By default (in the absence of a **umat_file** definition) the umat behavior uses a Z-mat one.

```
***behavior umat              ***suppress_temperature
 **cmname visc3_zmat.mat      ***material
 **depvar 2                     *file visc3_zmat.mat
 **coefficient                  *integration theta_method_a 0.5 1.e-9 120
  masvol 8.1e-9                 ***external_storage
***return                         *file oo.store
                                  *vars
                                    evi22 evcum
                                  *buffer_size 3

                              ***behavior gen_evp
                               **elasticity isotropic
                                    young 260000.
                                    poisson 0.3
                               **potential gen_evp ev
                                 *criterion mises
                                 *flow norton
                                    n  7.0
                                    K  400.
                                 *kinematic nonlinear  x1
                                    C  30000.0
                                    D  500.0
                                 *isotropic constant
```

```
            R0 130.0
***return
```

Chapter 11

Secondary Models

***behavior aging

Description:
This behavior is a viscoplastic model intended for modeling the thermally activated aging behavior of aluminum for applications such as cast Al cylinder heads in TMF loading. The model includes classical combined nonlinear isotropic-kinematic hardening (only 2 kinematic terms are now allowed). The model is programmed for both Runge-Kutta and theta-method implicit integration, and for both general FEA and simulation modes.

The model has a standard additive strain decomposition with elastic, viscoplastic and thermal strain parts.

$$\dot{\boldsymbol{\epsilon}}_{\text{el}} = \dot{\boldsymbol{\epsilon}}_{to} - \dot{\boldsymbol{\epsilon}}_{th} - \dot{\boldsymbol{\epsilon}}_{vp}$$

The stress is computed from linear elasticity depending on the elastic matrix component selected:

$$\boldsymbol{\sigma} = \mathbf{D}_{el} : \boldsymbol{\epsilon}_{el}$$

There is an integrated aging parameter ζ which will cause aging effects on the hardening. This parameter evolves from 0 (unaged) to 1 (fully aged) with a saturating nonlinear form.

$$\dot{\zeta} = \left\langle \frac{\zeta_\infty - \zeta}{\tau} \right\rangle$$

and the coefficient τ is the time constant for saturation of the aging. We expect that the two coefficients ζ_∞ and τ are functions of temperature to be able to handle overheating effects.

The hardening parameters are computed with aging effects as follows:

$$\begin{aligned}
\mathbf{X}_1 &= \tfrac{2}{3}C_1\boldsymbol{\alpha}_1 \\
\mathbf{X}_2 &= (1-\zeta)\tfrac{2}{3}C_2\boldsymbol{\alpha}_2 \\
\text{R} &= R_0 + Q(1 - e^{-b\lambda}) + (1-\zeta)R_0^*
\end{aligned}$$

The remainder of the model is classical viscoplasticity:

$$\begin{aligned}
\text{f} &= J(\mathbf{s} - \mathbf{X}_1 - \mathbf{X}_2) - R \qquad \mathbf{n}\frac{\partial f}{\partial \boldsymbol{\sigma}} \\
\dot{\lambda} &= \left\langle \frac{f}{K} \right\rangle^n \\
\dot{\boldsymbol{\epsilon}}_{\text{vp}} &= \dot{\lambda}\mathbf{n} \\
\dot{\boldsymbol{\alpha}}_{\text{i}} &= \dot{\lambda}\left[\mathbf{n} - \tfrac{3}{2}\tfrac{D_i}{C_i}\mathbf{X}_i\right]
\end{aligned}$$

Note the aging effects are in the recall term for $\mathbf{X}_2$.

Syntax:

The basic input syntax here is:

```
***behavior aging_theta
[ **elasticity      <ELASTICITY> ]
[ **thermal_strain <THERMAL_STRAIN> ]
  **model_coef
      ...
```

The following coefficients are available:

K,n viscoplastic Norton law coefficients for $\dot{\lambda} = \langle f/K \rangle^n$

C1,D1 nonlinear Armstrong-Frederick kinematic hardening. **C1** is the kinematic modulus and **D1** is the saturation rate. The saturation back stress is occurs at $C1/D1$.

C2,D2 nonlinear kinematic coefficients which have the aging effects applied to them.

R0, Q, b nonlinear isotropic hardening (or softening with $Q < 0$) having the same meaning as the **nonlinear** isotropic model.

R0_star isotropic aging effect on the yield radius.

Tau,a_inf the two aging variable coefficients.

alpha optional thermal strain expansion coefficient.

Stored Variables:

The following variables are stored with this model:

prefix	size	description	default
eto	T-2	total strain	yes
sig	T-2	Cauchy stress	yes
eel	T-2	elastic strain tensor	yes
evi	T-2	viscoplastic strain tensor	yes
eme	T-2	mechanical strain tensor	yes
evcum	S	cumulated viscoplastic strain magnitude	yes
age	S	aging variable	yes
alpha(i)	T-2	kinematic back strain, i=1,2	yes

Note:

Early releases of this model misspell the model name as **ageing**

Example:

There is an example file in the test database directory **ZebFront_test/INP** named **aging*.inp**

These tests are normally deprecated compared to the equivalent but more general capability in the tests **Simulator_test/INP aging_tmf***.

***behavior aniso_damage

Description:

This model implements an anisotropic damage model for fibrous ceramic composites[1]. The damage is described by a number of scalar and tensorial variables as input by the user. The effect of closure strains and non-symmetric tension-compression behavior is handled as well.

The stress is calculated using the following definition of effective modulus:

$$\boldsymbol{\sigma} = \mathbf{C}_0 : \boldsymbol{\epsilon} - \sum \mathbf{C}^{\mathit{eff}} : (\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_c)$$

where $\mathbf{C}_0$ is the undamaged elasticity tensor, $\mathbf{C}^{\mathit{eff}}$ is the damage modification of the elasticity, and $\boldsymbol{\epsilon}_c$ is a user loadable closure strain. Each scalar and tensorial variable will contribute a term to the summation of $\mathbf{C}^{\mathit{eff}}$.

Syntax:

```
   ***behavior aniso_damage [modifier ]
    **C0 ELASTICITY
 [ **thermal_strain THERMAL_STRAIN ]
 [ **damage   ANISOTROPIC_DAMAGE]
 [ **closure ]
 [    t1  ...  t6 ]
 [ **scalar_interaction (full | identity)  ]
```

Stored Variables:

prefix	size	description	default
eto	T-2	strain tensor	yes
sig	T-2	Cauchy stress	yes
d(i)	S	scalar damage variables	yes
D	T-2	tensor damage variable	yes

Example:

The following example shows the input format for a material with two scalar variables:

```
***behavior aniso_damage
  **closure 1.e-3 1.e-3 1.e-3  .5e-3 .5e-3 .5e-3   % 11 22 33 12 23 31
  **c0 orthotropic
    c11       2.5662e11
    c22       2.5662e11
    c33       2.6887e11
    c12       6.0439e10
    c13       8.2435e10
    c23       8.2435e10
    c44       8.5e9
    c55       8.5e9
    c66       8.5e9

  **damage scalar
    *eta 1.0
```

---

[1]the model is coded in `Aniso_damage.z` in the source dir `zZfrontBehavior`

```
   *n          (1. 0. 0.)
   *K_coeffs  1. 0. 0. 0. 0. 0. 0.7 0.0 0.7
   *g g1
       Y0         1.69e4
       Yc         1.6e5
       delta_c   0.6
 **damage scalar
   *n          (0. 1. 0.)
   *K_coeffs  0. 1. 0. 0. 0. 0. 0.7 0.7 0.0
   *g g1
       delta_c 0.6
       Y0 1.69e4
       Yc 1.6e5
 **damage scalar
   *n          (0. 0. 1.)
   *K_coeffs  0. 0. 1. 0. 0. 0. 0.0 0.7 0.7
   *g g1
       delta_c   0.6
       Y0         1.69e4
       Yc         1.6e5

 **damage  elastic_tensorial
   *Q  diagonal   Q1  1.0
   *Qd diagonal   Qd1 1.0
   *K_coeffs     1. 1. 1. 0.7 0.7 0.7 0.5 0.5 0.5
   *g g1
       delta_c   0.6
       Y0         0.0
       Yc         1.6e5
***return
```

***behavior becker_needleman

Description:
This model is a direct implementation of the viscoplastic porous damage model given by R. Becker and A. Needleman "Effect of Yield Surface Curvature on Necking and Failure in Porous Plastic Solids," *J. Appl. Mech.* v53, 491-498 (1986).

$$\mathbf{B} = \boldsymbol{\sigma} - \mathbf{X} \qquad \mathbf{B}' = \mathbf{U} : \mathbf{B}$$

$$\phi = \frac{3}{2}\frac{\mathbf{B}' : \mathbf{B}'}{\sigma_F^2} + 2q_1 f^* \cosh\left[\frac{q_2 \mathbf{B} : \mathbf{1}}{2\sigma_F}\right] - 1 - q_1 f^{*2} \qquad \mathbf{n} = \frac{\partial \phi}{\partial \boldsymbol{\sigma}}$$

Where f^* is a modification of the porosity f[2] so that if $f < f_c$ $f^* = f$ and otherwise $f^* = f_c + ((1/q_1 - f_c)/(f_f - f_c)) * (f - f_c)$

$$\Delta\lambda = \frac{(1-f)\sigma_F \Delta p}{\mathbf{B} : \mathbf{n}}$$

$$\rho = \frac{(1-b)}{1 - b + bg(p)}[\mathbf{B} : \mathbf{n}]^{-1}\left[\frac{g'(p)(\mathbf{B} : \mathbf{n})^2}{(1-f)\sigma_F} + (1-f)(1-g(p))\frac{\partial \phi}{\partial f}(\mathbf{1} : \mathbf{n})\right]$$

Rate equations

$$\dot{\boldsymbol{\epsilon}}_{\text{el}} = \dot{\boldsymbol{\epsilon}}_{to} - \dot{\lambda}\mathbf{n} - \dot{\boldsymbol{\epsilon}}_{th}$$

$$\dot{p} = \epsilon_o\left[\frac{\sigma_F}{(1-b)\sigma_o + b\sigma_o g(p)}\right]^{1/m}$$

$$\dot{f} = \dot{\lambda}(1-f)(\mathbf{1} : \mathbf{n})$$

$$\dot{\boldsymbol{\alpha}} = \dot{\lambda}\rho\mathbf{B}$$

Syntax:

---

[2]In the `porous_plastic` behavior f^* is calculated from f using the coefficient mechanism

```
   ***behavior becker_needleman modifier
     **elasticity <ELASTICITY>
  [ **thermal_strain <THERMAL_STRAIN>
     **model_coef
        coefs
```

q1, q2, f_c, f_f, e_dot0, b, sig0, m, eps0, C

Example:

Here is an example using coefficients from the original paper.

```
***behavior becker_needleman
 **elasticity isotropic
      young   1865.67
      poisson 0.3
 **model_coef
      q1      2.38
      q2      0.748
      eps0    0.0125
      e_dot0  1.e-3  % same as loading rate
      sig0    1.0
      b       1.0    % 1==isotropic, 0==kinematic
      f_c     0.15
      f_f     0.25
      m       0.02 % 0.002
      C       1.
***return
```

***behavior cast_iron

Description:
This behavior is a combined damage-viscoplasticity model to simulate the nonlinear and fatigue behavior of cast iron materials. It allows significant flexibility in terms of the combination of damage and plastic mechanisms, hardening models, and driving force for damage.

This model uses a scalar damage variable which is the summation of a brittle mode based on maximum principal stress values, and a fatigue damage model like that described by [Lema85b]. The total effective damage at any time is a sum of brittle (d_b) and fatigue (d_f) damage contributions:

$$d = d_b + d_f$$

The scalar damage value is however applied to an anisotropic closure treatment utilizing 2 separate closure/opening criteria. The use of a scalar variable is an approximation assuming close to cyclically proportional strain paths. The closure point is based on a strain criterion which shifts into compression as damage accumulates, and the opening criterion is a sole function of the principle stress being positive. Both terms are smoothed using an interpolation function with adjustable width. Note that the opening and closing combined with the general difficulties of damage based models can lead to convergence difficulties. The damage effects here are not really meant for predicting true failure, but rather are needed to predict the LCF hysteresis loops. Other methods of cast iron modeling are available using the `cast_iron` yield criterion and non-symmetric kinematic hardening model.

Syntax:
The basic input syntax accepts a number of sub-objects: thermal_strain, elasticity, criterion, flow and isotropic hardening and can be represented as shown below:

```
   ***behavior cast_iron
 [ **thermal_strain <THERMAL_STRAIN> ]
 [ **elasticity     <ELASTICITY> ]
 [ **flow           <FLOW> ]
 [ **criterion      <CRITERION> ]
 [ **isotropic      <ISOTROPIC_HARDENING> ]
   **model_coef
      ...
```

With the specific model's coefficients (**model_coef**) available:

Q1,D1 nonlinear Armstrong-Frederick kinematic hardening. **Q1** is the saturation stress level and **D1** is the saturation rate. Any number of these terms may be added, but both coefficients must be entered always, and the numbering is sequential from 1 to N.

dmax,dmax_b,dmax_f damage limits preventing total failure (**dmax_b** and **dmax_f** allow to control brittle and fatigue damage limits independently).

e_0, e, E Brittle mode damage equation takes the following form:

$$d_b = \left(\frac{\sqrt{<s_1>^2 + <s_2>^2 + <s_3>^2} - e_0}{E} \right)^e$$

delta_e, delta_s Controls for the width of closure in strain dimensions (δ_e of 0.004 recommended as a start) and damage "opening" in stress dimensions (δ_s of 25 recommended). The interpolation functions used for the closure and opening which allows for smooth transitioning between damage active and damage closure are:

opening:

$$h_i(\sigma) = \frac{1}{2}\left[1 + tanh\left(\frac{-4\sigma_i}{\delta_s}\right)\right]$$

closure:

$$h_i(\epsilon) = \frac{1}{2}\left[1 + tanh\left(\frac{-4(\epsilon_i + \delta_d \times (d + \delta_{d0}))}{\delta_e}\right)\right]$$

delta_d0 Initial shift in the strain damage closing effect

delta_d Shift parameter for progressively compressive closure as damage increases. The closure point is $\delta_d \times (d + \delta_{d0})$

a, b, A, r Simple cumulated plastic strain fatigue mode damage:

$$\chi(\underset{\sim}{\sigma}) = \alpha J_0 + \beta J_1 + (1 - \alpha - \beta)J_2$$

$$\dot{d}_f = \left(\frac{\chi}{A}\right)^r \dot{p}$$

where p is the cumulated plastic strain

Stored Variables:

prefix	size	description	default
eto	T-2	total strain	yes
sig	T-2	Cauchy stress	yes
eel	T-2	elastic strain	yes
eps_me	T-2	mechanical strain	yes
eps_th	T-2	thermal strain	yes
evi	T-2	viscoplastic strain	yes
evcum	S	inelastic strain equivalent	yes
d_f	S	fatigue damage	yes
d_b	S	brittle damage	yes
Dsum	S	total effective damage	yes
alpha(i)	T-2	kinematic hardening variable	yes

Example:
The following is a short example material file for gray iron.

```
***behavior cast_iron
 **elasticity isotropic
    young   130000.
    poisson 0.26
 **flow norton
```

```
    K   400.
    n   4.
 **criterion mises
 **isotropic constant
    R0   150.
 **model_coef
   % kinematic hardening
    Q1 300.0
    D1 80.
   % brittle damage
    e    1.0  % exponent
    e_0 2.0  % criterion
    E   1000. % approx critical stress
   % progressive closure
    delta_d   0.006 % shift in strain closure according to d
    delta_e   0.008 % width of strain transition
   % damage limits
    dmax   0.25
    dmax_b 0.25
***return
```

***behavior cast_iron_brittle

Description:
This model is a simplified version of the more general `cast_iron` model, as it implements brittle damage mechanism only. The implementation of the model has been revisited to improve local and global convergences. The same manner as `cast_iron` model, this behavior is a combined damage-viscoplasticity model to simulate the nonlinear and fatigue behavior of cast iron materials. It allows significant flexibility in terms of the combination of damage, viscoplastic mechanisms and hardening models.

This model uses a scalar damage variable which is brittle mode damage (d_b) based on maximum principal stress values, like that described by [Lema85b].

The scalar damage value is applied to an anisotropic closure treatment utilizing 2 separate closure/opening criteria. The use of a scalar variable is an approximation assuming close to cyclically proportional strain paths. The closure point is based on a strain criterion which shifts into compression as damage accumulates, and the opening criterion is a sole function of the principle stress being positive. Both terms are smoothed using an interpolation function with adjustable width. Note that the opening and closing combined with the general difficulties of damage based models can lead to convergence difficulties. The damage effects here are not really meant for predicting true failure, but rather are needed to predict the LCF hysteresis loops.

Syntax:
The basic input syntax accepts a number of sub-objects: thermal_strain, elasticity, criterion, flow and isotropic hardening and can be represented as shown below:

```
   ***behavior cast_iron_brittle
 [ **thermal_strain <THERMAL_STRAIN> ]
 [ **elasticity     <ELASTICITY> ]
 [ **flow           <FLOW> ]
 [ **criterion      <CRITERION> ]
 [ **isotropic      <ISOTROPIC_HARDENING> ]
   **model_coef
      ...
```

With the specific model's coefficients (`**model_coef`) available:

Q1,D1,M1,m1   nonlinear Armstrong-Frederick kinematic hardening with the possibility to activate static recovery mechanism. `Q1` is the saturation stress level and `D1` is the saturation rate. The coefficients `M1` and `m1` are the standard Norton-like static recovery coefficients. Any number of these terms may be added, but both coefficients must be entered always, and the numbering is sequential from 1 to N.

dmax   damage limit preventing total failure.

e_0, e, E   Brittle mode damage equation takes the following form:

$$d_b = \left(\frac{\sqrt{< s_1 >^2 + < s_2 >^2 + < s_3 >^2} - e_0}{E} \right)^e$$

delta_e, delta_s Controls for the width of closure in strain dimensions (δ_e of 0.004 recommended as a start) and damage "opening" in stress dimensions (δ_s of 25 recommended). The interpolation functions used for the closure and opening which allows for smooth transitioning between damage active and damage closure are:

opening:

$$h_i(\sigma) = \frac{1}{2}\left[1 + tanh\left(\frac{-4\sigma_i}{\delta_s}\right)\right]$$

closure:

$$h_i(\epsilon) = \frac{1}{2}\left[1 + tanh\left(\frac{-4(\epsilon_i + \delta_d \times (d + \delta_{d0}))}{\delta_e}\right)\right]$$

delta_d0 Initial shift in the strain damage closing effect

delta_d Shift parameter for progressively compressive closure as damage increases. The closure point is $\delta_d \times (d + \delta_{d0})$

d_b_ini Initial damage convenient for identification purposes

Stored Variables:

prefix	size	description	default
eto	T-2	total strain	yes
sig	T-2	Cauchy stress	yes
eel	T-2	elastic strain	yes
eps_me	T-2	mechanical strain	yes
eps_th	T-2	thermal strain	yes
evi	T-2	viscoplastic strain	yes
evcum	S	inelastic strain equivalent	yes
d_b	S	brittle damage	yes
Dsum	S	total effective damage	yes
alpha(i)	T-2	kinematic hardening variable	yes

Example:
The following is a short example material file for gray iron.

```
***behavior cast_iron_brittle
 **elasticity isotropic
     young   130000.
     poisson 0.26
 **flow norton
     K   400.
     n   4.
 **criterion mises
 **isotropic constant
     R0   150.
 **model_coef
   % kinematic hardening
```

```
      Q1 300.0
      D1 80.
   % brittle damage
      e    1.0  % exponent
      e_0 2.0  % criterion
      E   1000. % approx critical stress
   % progressive closure
      delta_d   0.006 % shift in strain closure according to d
      delta_e   0.008 % width of strain transition
   % damage limit
      dmax    0.25
***return
```

***behavior bodner_partom

Description:

This behavior is an implementation of the classical model due to Bodner and Partom. The model is viscoplastic and incorporates scalar and tensorial hardening variables. There is no initial yield radius thereby allowing inelastic deformation at very low stress levels over long periods of time. The state and evolution equations are the following:

$$Z = Z_i + Z_0 + \boldsymbol{\beta} : \mathbf{u} \qquad \mathbf{u} = \boldsymbol{\sigma}/\sqrt{\boldsymbol{\sigma} : \boldsymbol{\sigma}}$$

$$D_{p_2} = D_0^2 \exp\left[-\left(\frac{Z^2}{3J_2}\right)^n\right]$$

$$\dot{\boldsymbol{\epsilon}}_{vi} = \sqrt{\lambda_2}\mathbf{S} \qquad \mathbf{S} = \mathbf{U} : \boldsymbol{\sigma} \qquad \lambda_2 = D_{p_2}/J_2 \qquad J_2 = \tfrac{1}{2}\mathbf{S} : \mathbf{S}$$

$$W_p = \boldsymbol{\sigma} : \dot{\boldsymbol{\epsilon}}_{vi} = \sqrt{\lambda_2}\mathbf{S} : \boldsymbol{\sigma}$$

$$\begin{aligned}
\dot{\boldsymbol{\epsilon}}_{\text{el}} &= \dot{\boldsymbol{\epsilon}}_{to} - \dot{\boldsymbol{\epsilon}}_{vi} \\
\dot{Z}_i &= m_1(Z_1 - Z_i - Z_0)W_p \\
\dot{\boldsymbol{\beta}} &= m_2(Z_3\mathbf{u} - \boldsymbol{\beta})W_p
\end{aligned}$$

$$(1)$$

Syntax:

```
   ***behavior bodner_partom
 [ **thermal_strain <THERMAL_STRAIN> ]
 [ **elasticity     <ELASTICITY> ]
   **model_coef
```

Coefficient names are `n, Z0, Z2, D0, Z1, Z3, m1, m2, A1, A2, r1, r2`

Stored Variables:

prefix	size	description	default
eto	T-2	total strain	yes
sig	T-2	Cauchy stress	yes
evi	T-2	inelastic strain tensor	yes
Zi	S	isotropic drag stress	yes
beta	T-2	kinematic variable	yes
p	S	inelastic strain equivalent	yes
Ztot	S	Sum of Z parts	yes

Example:

The following is a simple example of the Bodner-partom material using room temperature coefs for HASTELLOY-X as given by Rowley and Thornton *J. Eng. Mat. Tech.* **118**, 19-27 (1996).

```
***behavior bodner_partom
 **elasticity isotropic
   young  196.6e3
   poisson 0.33
 **model_coef
   n   1.0
   Z0  1860.
   Z2  1860.
   D0  10000.0
   Z1  2390.
   Z3  603.
   m1  0.139
   m2  3.49
   A1  1.0e-9
   A2  1.0e-9
   r1  1.
   r2  1.
***return
```

***behavior finite_strain_crystal

Description:
This behavior is a simple implementation of a finite strain formulation of a single crystal[3]
This behavior is included as an example of ZebFront programming, and the source can be found in the developers manual. This model only allows one crystal orientation to be input, and works for Runge-Kutta integration only.

This model works with the assumption of multiplicative plasticity, where the deformation gradient $\mathbf{F}$ is broken into an elastic part $\mathbf{F}_e$ and a plastic part $\mathbf{F}_p$.

$$\mathbf{F}_e = \mathbf{F}\mathbf{F}_p^{-1};$$

The elastic deformation gradient is separated into a rotation component and a stress component.

$$\mathbf{F}_e = \mathbf{R}_e\mathbf{U}_e$$

and the stress is calculated using the logarithmic strain measure from the elastic stretch.

$$\boldsymbol{\sigma} = \mathbf{D}_{el} : \log(\mathbf{F}_e)$$

There is a yield criterion for each slip system.

$$f_i = \mathbf{m}_i : \boldsymbol{\sigma} - C\alpha_i - R(g_i)$$

which is used to calculate the evolution.

$$\dot{\mathbf{F}}_p = \sum_i \dot{v}(f_i)\mathbf{m}_i\mathbf{F}_p$$

γ_i is the integration of $\dot{v}(f_i)$.

$$\dot{\alpha}_i = \dot{\gamma}_i\mathrm{sign}(\mathbf{m}_i : \boldsymbol{\sigma} - C\alpha_i) - D * \alpha_i * \dot{\gamma}_i$$

---

[3]Only Runge-Kutta integration is implemented.

Syntax:

```
***behavior finite_strain_crystal
 **elasticity  <ELASTICITY>
 **flow        <FLOW>
 **isotropic   <ISOTROPIC_HARDENING>
 **orientation <CRYSTAL_ORIENTATION>
 **model_coef
  C COEFFICIENT
  D COEFFICIENT
```

Stored Variables:

prefix	size	description	default
F	UT-2	deformation gradient	yes
sig	T-2	total Cauchy stress	yes
Fp	UT-2	plastic deformation gradient	yes
gamma#	V	resolved shear strains	yes
alpha#	V	back strains on slip system	yes
crss#	V	current resolved shear stress	yes

<div align="center">

***behavior matmod

</div>

Description:
This model is an implementation of the MATMOD equations due to Miller [Mill76]. The model accounts for isotropic/kinematic hardening and presents a particular form of temperature dependence in the material coefficients.

$$\dot{\boldsymbol{\epsilon}}_{in} = B\theta' \left\{ \sinh \left[Af_1 \left(\frac{J(\boldsymbol{\sigma} - \mathbf{R})}{D} \right)^{3/2} \right] \right\}^n \frac{3}{2} \frac{\mathbf{s} - \mathbf{R}}{J(\boldsymbol{\sigma} - \mathbf{R})}$$

$$\begin{aligned} \theta' &= \exp \left\{ \left[-\frac{Q}{0.6kT_m} \right] \left[\ln \left(\frac{0.6T_m}{T} \right) + 1 \right] \right\} \qquad \text{for } T \leq 0.6T_m \\ \theta' &= \exp -Q/kT) \qquad \text{for } T \geq 0.6T_m \end{aligned}$$

$$(2)$$

$$\dot{\mathbf{R}} = H_1 (\dot{\boldsymbol{\epsilon}}_{in} - B\theta' [\sinh(A_1|\mathbf{R}|)]^n) \frac{\mathbf{R}}{|\mathbf{R}|}$$

$$\dot{D} = H_2 |\dot{\boldsymbol{\epsilon}}_{in}| \left[C_2 + |\mathbf{R}| - (A_2/A_1)D^3 \right] - H_2 C_2 B\theta' \left[\sinh(A_2 D^3) \right]^n$$

Syntax:

```
   ***behavior matmod
 [ **thermal_strain <THERMAL_STRAIN> ]
 [ **elasticity     <ELASTICITY> ]
   **model_coef
```

Stored Variables:

prefix	size	description	default
eto	T-2	total strain	yes
sig	T-2	Cauchy stress	yes
ein	T-2	inelastic strain tensor	yes
D	S	isotropic drag stress	yes
R	T-2	kinematic rest stress	yes

Example:
The following is a simple example of the MATMOD material corresponding to the material in Miller's original paper:

```
%
%  As given by Mill76 (Tests matmod#)
%
***behavior matmod
```

```
 **elasticity
    young    temperature
     1.93e5  23.0
     1.55e5  538.0
    poisson 0.3
***model_coef
    A1   0.108     % MPa^-1
    A2   2.27e-7   % MPa^-1
    B    1.e15     % sec^-1
    C2   0.69      % MPa
    H1   1930      % MPa
    H2   100       %
    n    5.8       %
    Q    91000.0   % cal/mol
    Tm   1800.0    % Degree K
***return
```

***behavior matmod_z

Description:
This model is an implementation of the MATMOD-Z equations due to Miller [Mill76]. The model accounts for isotropic/kinematic hardening and presents a particular form of temperature dependence in the material coefficients.

Syntax:

```
    ***behavior matmod
  [ **thermal_strain <THERMAL_STRAIN> ]
    **model_coef
```

Stored Variables:

prefix	size	description	default
eto	T-2	total strain	yes
sig	T-2	Cauchy stress	yes
lam_vp,	S	plastic multipliers	yes
lam_ir			
R	S		yes
Fdef	S		yes
Fsol	S		yes
evp	T-2	viscoplastic strain	yes
eir	T-2	irradiation strain	yes

Example:
The following is a simple example of the MATMOD-Z material corresponding to the material in Miller's original paper:

```
%
% Zircaloy model from Oldsberg, Miller and Lucas STP 681 (1978).
%
***behavior matmod_z
**model_coef
E function 9.65e4 - (9.65e4-5.51e4)*(temperature-300.0)/700.0;
poisson 0.3
F 0.5
G 0.25
H 0.75
A 500.0
A1 3240.0
A2 1.78e8
A4 8.89e-13
B 5.0e12
C1 0.143
C2 1.0e-10
Fsa -1.815e-7
```

```
Fsb 4.99e-8
Fsm2 2.32e-7
Fsm3 3.25e-6
H1 0.0070 % dR
H2 6.64e-4 % dFdef
H3 2.0e-26 % dFdef irr
k 1.9859
kp 91.0
kq 3.0
n 4.5
p 0.5
Qs 60000.0
Q4 8400.0
Tt 930.0
Z2 1.0e23
Z3 1.0e12
beta2 6.0
beta3 3.0
% phi = flux
phi 0.0
```

***behavior memory

Description:
This behavior is a ZebFront implementation of a strain range memory isotropic hardening model described by Lemaitre and Chaboche [Lema91]. The model has 2 non-linear kinematic hardening components (coefficients `C1`, `D1`, `C2`, and `D2`), and a Norton type flow law (coefficients `K` and `n`).

$$
\begin{aligned}
Q &= Q_0 + (Q_{sat} - Q_0)\exp(-2\mu q) \\
R &= R_0 + bQr
\end{aligned}
\tag{3}
$$

$$
\begin{aligned}
\mathbf{n}^* &= \tfrac{1}{2}(\boldsymbol{\epsilon}_{vi} - \mathbf{z})/J(\boldsymbol{\epsilon}_{vi} - \mathbf{z}) \\
\eta &= \mathbf{n} : \mathbf{n}^* \\
\dot{q} &= \eta\dot{\lambda}
\end{aligned}
\tag{4}
$$

$$
\dot{r} = \dot{\lambda}\left[1 - (R - R_0)/Q\right]
$$

$$
\dot{\mathbf{z}} = 2(\mathbf{n}^* : \boldsymbol{\epsilon}_{vi})\mathbf{n}^*
$$

Syntax:

```
***behavior memory
 **elasticity <ELASTICITY>
 **model_coef
    coefs
```

Example:

```
***behavior memory
 **elasticity isotropic
      young 260000.
      poisson 0.3
 **model_coef
      n      7.0
      K      100.
      C1     30000.0
      D1     80.
      C2     100000.
      D2     1200.
      R0     150.0
      b      150.
      Q0     400.
      Qsat -350.
      mu     100.
***return
```

***behavior non_associated

Description:

The `non_associated` behavior is a ZebFront behavior used as an example for non-associated deformation with kinematic hardening variables, which can have deviatoric and spherical components[4]. The source for this model can be found in the developer manual.

The model uses elasticity, criterion, flow, and isotropic classes. An interesting use of this model is with a non-associated criterion such as `linear_drucker_prager`. There is however no such requirement, so the model could be used with von Mises as well.

Any number of kinematic hardening variables are possible. For kinematic i, the back stress $\mathbf{X}$ is calculated as follows:

$$
\begin{aligned}
\mathrm{X}_{s_i} &= C_{s_i}\alpha_{s_i} \\
\mathbf{X}_{d_i} &= C_{d_i}\boldsymbol{\alpha}_{d_i} \\
\mathbf{X}_i &= \mathbf{X}_{d_i} + \boldsymbol{\delta}X_{s_i}
\end{aligned}
\tag{5}
$$

Noting that different back stress moduli are available for the two components.

The evolution of back stress is also separated in two components:

$$
\dot{\alpha}_{s_i} = \dot{\lambda}\left[\mathrm{Tr}(\mathbf{n}) - \frac{D_{s_i}}{C_{s_i}}X_{s_i}\right]
$$

$$
\dot{\boldsymbol{\alpha}}_{d_i} = \dot{\lambda}\left[\mathbf{n}' - \frac{D_{d_i}}{C_{d_i}}\mathbf{X}_{d_i}\right]
$$

Note here that $\mathbf{n}$ is the criterions *normal* and not $\frac{\partial f}{\partial \boldsymbol{\sigma}}$.

Syntax:

The syntax is in standard ZebFront format, with a number of standard sub-classes.

```
***behavior non_associated
 **elasticity   <ELASTICITY>
 **flow         <FLOW>
 **isotropic    <ISOTROPIC_HARDENING>
 **criterion    <CRITERION>
 **model_coef
  Cd1 COEFFICIENT
  Cs1 COEFFICIENT
  Dd1 COEFFICIENT
  Ds1 COEFFICIENT
     ..
```

---

[4]there is only a Runge-Kutta implementation in Z8.0 – this model will be implemented in **gen_evp** in Z8.1

Stored Variables:

prefix	size	description	default
F	UT-2	deformation gradient	yes
sig	T-2	total Cauchy stress	yes
Fp	UT-2	plastic deformation gradient	yes
gamma#	V	resolved shear strains	yes
alpha#	V	back strains on slip system	yes
crss#	V	current resolved shear stress	yes

Example:

```
***behavior drucker_prager
 **elasticity isotropic
     young    2.25
     poisson 0.125
 **isotropic constant
     R0      0.0011547
 **flow norton
     K 1.e-6
     n 2.
 **criterion linear_drucker_prager
  friction_angle 20.0
  dilatation_angle 20.0
  K        .9
 **model_coef
     Cd1 1.e-1
     Dd1 0.0
     Cs1 1.e-1
     Ds1 0.0
***return
```

***behavior rousselier_poly

Description:
This behavior is a model developed within the self-consistent polycrystalline framework intended for taking into account various mechanisms. The framework of physically based polycrystalline metal plasticity has intrinsic advantages in describing the anisotropy and distortion of the yield surface, as well as realistic anisotropic hardening. It enables the prediction of complex behaviors in multi-axial and multi-path loadings.

The mathematical framework of polycrystalline plasticity is developed within a reduced texture methodology (RTM) in order to dramatically increase the computational efficiency while keeping the physically-based constitutive equations (Rousselier et al., 2009, 2010, 2012; Luo and Rousselier, 2014). The RTM can make use of any polycrystalline plasticity model with a very small number of crystallographic orientations. These orientations are determined from mechanical experiments through inverse optimization, in place of crystallographic measurements (EBSD).

In order to model ductile fracture, macroscopic void nucleation and growth models have been reformulated in the polycrystalline framework. Various models are introduced at the slip system scale: nucleation and growth models of a second population of very small voids, the Coulomb fracture model, dynamic strain aging model (DSA) and texture evolution.

Syntax:
The basic input syntax here is:

```
***behavior rousselier_poly [modifier ]
  **elasticity <ELASTICITY>
    ...
  **elasticity0 <ELASTICITY>              #broken behaviour young, poisson
    ...
  **grain_number ...                      #define grain number
  **system_type  fcc | bcc                #choose crystal structure
  **orientation_file filename             #load grain orientation file
  **system_file filename                  #load slip system file
  **back_stress_file_[...] filename       #load back stresses file
[ **hardening                             #define hardening law
   *isotropic <ISOTROPIC_HARDENING>
   *matrix_h_[fcc | bcc]
    ...
  **hardening
   *isotropic <ISOTROPIC_HARDENING>
   *matrix_h_[fcc | bcc]
    ...                            ]
[  **beta_rule scalar | cs_dt | ct_dt    #choose beta rule type
   ...                            ]
  **use_MC                                #Mohr-coulomb
  **use_Rdamage                           #Rousselier damage model
    ...
  **model_coef
    coefs
```

A phenomenological Norton-like viscoplastic model (Cailletaud, 1992) is used for the constitutive equations of each slip system. The hardening term r_s in each slip system is described by:

$$r_s = R_0 + Q_1 \sum_{t=1}^{M} H_1^{st}[1 - \exp(-b_1 v_t)] + Q_2 \sum_{t=1}^{M} H_2^{st}[1 - \exp(-b_2 v_t)]$$

where H_1 and H_2 are constant hardening matrices modeling the interactions between the slip systems. With two matrices, the self and latent hardening rates of the slip systems evolve with deformation. For BCC materials, we need to provide h_0 and h_1. For FCC materials, h_0, h_1, h_2, h_3, h_4, h_5 need to be specified.

Example:
For BCC materials:

```
   **hardening
    *isotropic nonlinear
     Q  69.9
     b  23.2
    *matrix_h_bcc
     h0 1.0
     h1 0.1
   **hardening
    *isotropic nonlinear
     Q  49.7
     b   2.6
    *matrix_h_bcc
     h0 1.0
     h1 0.1
```

In each 'grain' g of volume fraction f_g, the stress $\boldsymbol{\sigma}_g$ and strain $\boldsymbol{\epsilon}_{to} = \boldsymbol{\epsilon}_{el} + \boldsymbol{\epsilon}_{vp}$ are assumed to be homogeneous. The macroscopic stress and strain are defined as spatial averages of the N grains. To establish a unique relationship between the stresses at the macroscopic and microscopic scale, the so-called β-rule (Cailletaud, 1992; Sai et al., 2006) is adopted here.

$$\boldsymbol{\sigma}_g = \boldsymbol{\Sigma} + C(\boldsymbol{\beta} - \boldsymbol{\beta}_g) \quad \text{with} \quad \boldsymbol{\beta} = \sum_{g=1}^{N} f_g \boldsymbol{\beta}_g$$

$$\dot{\boldsymbol{\beta}}_g = \dot{\boldsymbol{\epsilon}}_{vpg} - \mathbf{D} : \boldsymbol{\beta}_g \|\dot{\boldsymbol{\epsilon}}_{vpg}\| \quad \text{where} \quad \|\dot{\boldsymbol{\epsilon}}_{vpg}\| = \sqrt{\frac{2}{3} \dot{\boldsymbol{\epsilon}}_{vpg} : \dot{\boldsymbol{\epsilon}}_{vpg}}$$

where C is a scalar. The fourth order tensor $\mathbf{D}$ is proposed by Sai et al. (2006) for anisotropic materials. With the Voigt notation, $\mathbf{D}$ has 10 independent elements for orthotropic materials. The current module offers 3 types of β-rule by choosing different key words: scalar, cs_dt and ct_dt. 'scalar' is used when C and D are both scalars. 'cs_dt' is used when C is a scalar and $\mathbf{D}$ is a tensor. 'ct_dt' is used when $\mathbf{C}$ and $\mathbf{D}$ are both tensors.

Example:
For cs_dt β-rule:

```
        **beta_rule cs_dt
         *C  5.4e+04
         *Dtensor
          gr11          100.0
          gr21          0.0
          gr22          100.0
          gr23          0.0
          gr31          0.0
          gr32          0.0
          gr33          100.0
          gr44          100.0
          gr55          100.0
          gr66          100.0
```

Other models such as macroscopic Rousselier damage model, secondary void nucleation, Coulomb fracture model and dynamic strain aging model (DSA) etc. can be activated using the key words **use_[...] defined before **model_coef. The associated parameters can then be defined after **model_coef.

Macroscopic porous plasticity:
Porous plasticity is coupled with polycrystalline plasticity. The aggregate contains voids with variable volume fraction f. The volume fractions of the matrix grains are $(1 - f)f_g$. The following plastic potential is used:

$$F(\frac{\boldsymbol{\sigma}}{1-f}) = \frac{\sigma_{eq}}{1-f} - \left(\sum_{g=1}^{N} f_g \boldsymbol{\sigma}_g \right) + D_1 f \sigma_1 \exp\left(\frac{\sigma_m^*}{(1-f)\sigma 1} \right)$$

where $\sigma_m^* = \alpha_L \boldsymbol{\sigma}_{LL} + \alpha_T \boldsymbol{\sigma}_{TT} + \alpha_N \boldsymbol{\sigma}_{NN}$ with $\alpha_L + \alpha_T + \alpha_N = 1$. For isotropic void growth, $\alpha_L = \alpha_T = \alpha_N = 1/3$. In the current version, the void volume fraction rate $\dot{f}$ is the sum of a first term due to the mass conservation law and a second term for void nucleation. The nucleation term involves 3 parameters $f_N, \sigma_N, \epsilon_N$ (Chu and Needleman, 1980). It is worth noting the material is considered as 'broken' when the void volume fraction exceeds an ultimate value f_u.

Example:

```
        **use_Rdamage
        **model_coef
          f0,D1,s1,aL,aT,aN,fN,eN,sN,fu
```

Porous plasticity at the slip system:
A second population of very small voids that nucleate and grow in shear band can be considered in the current model. These voids can contribute to void coalescence of the larger voids with the so-called 'void sheet mechanism'. An additional void volume fraction variable f_s is considered for each slip system. The contribution of all grains is added to F.

$$F(\frac{\boldsymbol{\sigma}}{1-f}) = \frac{\sigma_{eq}}{1-f} - \left(\sum_{g=1}^{N} f_g \boldsymbol{\sigma}_g \right) + D_1 \left(f + \sum_{g=1}^{N} f_g \left(\sum_{s=1}^{M} f_s \right)_g \right) \sigma_1 \exp\left(\frac{\sigma_m^*}{(1-f)\sigma 1} \right)$$

The void fraction rate could take a similar form to the macroscopic one.

Example:

```
      **use_void_meso
      **model_coef
        f02,D12,t12,fN2,eN2,sN2
```

Coulomb fracture model:
The Coulomb fracture model can be used to simulate the transgranular shear fracture without voids. This mechanism is observed in some metals. To integrate this phenomenon, an additional slip rate $\dot{\gamma}_s^C$ is introduced, so that the total slip rate is $\dot{\gamma}^{tot} = \dot{\gamma}_s + \dot{\gamma}_s^C$.

Example:

```
      **use_MC
      **model_coef
        c3,r3,Q3,b3,p3,gvC
```

Dynamic strain ageing model:
Dynamic strain ageing is the pinning of dislocations by solute atoms that diffuse during straining. The so-called KEMC model is added to the hardening equation of each slip system.

Example:

```
      **use_DSA
      **model_coef
        P1,P2,aP,omP,nP,ta0
```

Available coefficients:
In summary, the following coefficients are available:

R0   yield radius in the nonlinear isotropic hardening term at slip system scale.

K,n   viscoplastic Norton law coefficients for $\dot{\lambda} = \langle f/K \rangle^n$.

c,d   nonlinear Armstrong-Frederick kinematic hardening.

a00,a90,ash,ap45,an45   initial back stresses coefficients.

f0,D1,s1,aL,aT,aN,fN,eN,sN,fu   Damage (**use_Rdamage).

f02,D12,t12,fN2,eN2,sN2   Secondary voids (**use_void_meso).

c3,r3,Q3,b3,p3,gvC   Mohr Coulomb model (**use_MC).

P1,P2,aP,omP,nP,ta0   DSA model (**use_DSA).

Note:
There is an example file in the test database directory ZebFront_test/INP named *.inp
    The support document is...

***behavior visco_aniso_damage

Description:

This model implements a model of viscoplasticity with fully anisotropic coefficients and damage. The model accepts a number of mixed damage components based on scalar or tensorial variables, and any number of kinematic variables. The later must be chosen from a sub-set of the KINEMATIC objects described later in this chapter. The compatible models are indicated in the later section.

Syntax:

```
    ***behavior visco_aniso_damage [modifier ]
  [ **thermal_strain THERMAL_STRAIN
    **C0        ELASTICITY
    **H0        COEFFICIENT_MATRIX
    **flow      FLOW
    **isotropic ISOTROPIC
    **kinematic KINEMATIC
        ...
  [ **effective_stress   ]
  [ **effective_operator ]
  [ **damage    ANISOTROPIC_DAMAGE
        ...
  [ **closure ]
  [    t11 t22 t33 t12 t23 t31   ]
  [ **scalar_interaction (full | identity)  ]
```

Stored Variables:

prefix	size	description	default
eto	T-2	strain tensor	yes
sig	T-2	Cauchy stress	yes
delta(i)	S	scalar damage variables	yes
d	T-2	tensor damage variable	yes
Y	T-2	driving force for tensorial damage	yes
evi	T-2	inelastic strain tensor	yes
evcum	S	inelastic strain equivalent	yes
alpha(i)	T-2	kinematic hardening variable	yes

Example:

```
***behavior visco_aniso_damage
 **effective_stress
 **C0 orthotropic
    c11  154844.0
    c22  154844.0
    c33  203236.0
    c12  54844.0
```

```
   c23  49357.0
   c31  49357.0
   c44  50000.0 % 0.5(b11-b12)
   c55  50000.0
   c66  50000.0
 **H0 orthotropic
   c11 0.5
   c22 0.5
   c33 0.15
   c12 -0.3
   c23 -0.1
   c31 -0.1
   c44 0.4
   c55 0.35
   c66 0.35
 **flow norton
   n  12.0
   K  250.0
 **isotropic nonlinear
   R0  240.0
   Q   -70.0
   b   180.0
 **kinematic nonlinear X1
  *C orthotropic
   c11  15000.00  c12 0.0 c23 0.0 c31 0.0
   c22  15000.00
   c33  50000.00
   c44   7500.00 % 0.5(b11-b12)
   c55   7500.00
   c66   7500.00
 **kinematic nonlinear X2
  *C orthotropic
   c11  30000.00  c12 0.0 c23 0.0 c31 0.0
   c22  30000.00
   c33 100000.00
   c44  15000.00 % 0.5(b11-b12)
   c55  15000.00
   c66  15000.00
  *D diagonal 180.0
***return
```

Chapter 12

Other Models

***behavior coefficient_diffusion

Description:
Diffusion behavior which uses the COEFFICIENT to model variations in D with respect to the concentration.

$$\vec{J} = D(C)\nabla C$$

Syntax:

```
***behavior coefficient_diffusion
    D COEFFICIENT
```

Stored Variables:

prefix	size	description	default
dC	V	gradient of concentration	yes
J	V	flux of concentration	yes
C	S	the concentration	yes

Example:

```
***behavior coefficient_diffusion
    D             C
    5.50339E-22  -1000.
     5.50339E-22     0.
     4.02370E-20     0.29
     8.39143E-20     0.40
     1.02221E-18     0.55
     2.56706E-18     0.59
     2.56706E-18     0.66
     2.56706E-18  1000.

***return
```

***behavior needleman_debonding

Description:
This behavior[1] is used for the special problem of interface debonding. See the command
`**create_interface_elements` (and similar) in the Z-set user manual on how to insert
cohesive elements in the mesh. The Needleman model[2] is described through a scalar variable
λ which characterizes the relative crack opening:

$$\lambda = \sqrt{\left(\frac{\langle u_N \rangle}{\delta_N}\right)^2 + \left(\frac{\|\vec{u}_T\|}{\delta_T}\right)^2}, \tag{1}$$

where $\langle x \rangle = x$ if $x > 0$ and $\langle x \rangle = 0$ if $x \leq 0$. With respect to the interface normal $\vec{n}$,
$\vec{u}_N = (\vec{u} \cdot \vec{n})\,\vec{n} \equiv u_N \vec{n}$ and $\vec{u}_T \equiv \vec{u} - \vec{u}_N$ denote, respectively, the normal and shear opening
displacements and δ_N and δ_T the corresponding maximum allowable values of their norms.
The damage variable λ_{max}, which is the maximum value of λ reached up until the current
instant, increases from 0 (no damage) to 1 (for a broken element). The normal and shear
components of the cohesive traction $\vec{T}$, i.e. $\vec{T}_N = \left(\vec{T} \cdot \vec{n}\right)\vec{n} \equiv T_N \vec{n}$ and $\vec{T}_T = \vec{T} - \vec{T}_N$, are
defined by

$$T_N = \frac{u_N}{\delta_N} F\left(\lambda_{max}\right), \quad \vec{T}_T = \alpha \frac{\vec{u}_T}{\delta_T} F\left(\lambda_{max}\right), \quad F\left(\lambda\right) = \frac{27}{4}\sigma_{max}\left(1 - \lambda\right)^2, \tag{2}$$

with α a constant representing the relative magnitude of $\|\vec{T}_T\|$ with respect to T_N, and σ_{max}
the maximum stress allowable by the element. For the compressive case, where $u_N < 0$, the
normal component of the traction is modified to

$$T_N = \alpha_c \frac{u_N}{\delta_N} F(0), \tag{3}$$

with α_c a penalization factor. In the literature, α_c usually is at least 10α. Figure 1 illustrates
the typical response of the cohesive zone model under specific loads, for the parameters as
given in the example.

Syntax:

```
    ***behavior needleman_debonding
        sigmax    σmax
        deltan    δn
        deltat    δt
        alpha     α
        alphac    αc
        [no_penetration]
```

... *continued*

---

[1]this behavior is Z-set specific, and therefore does not apply for Z-mat for other codes

[2]Needleman A., "A continuum model for void nucleation by inclusion debonding", J. of Applied Mechanics,
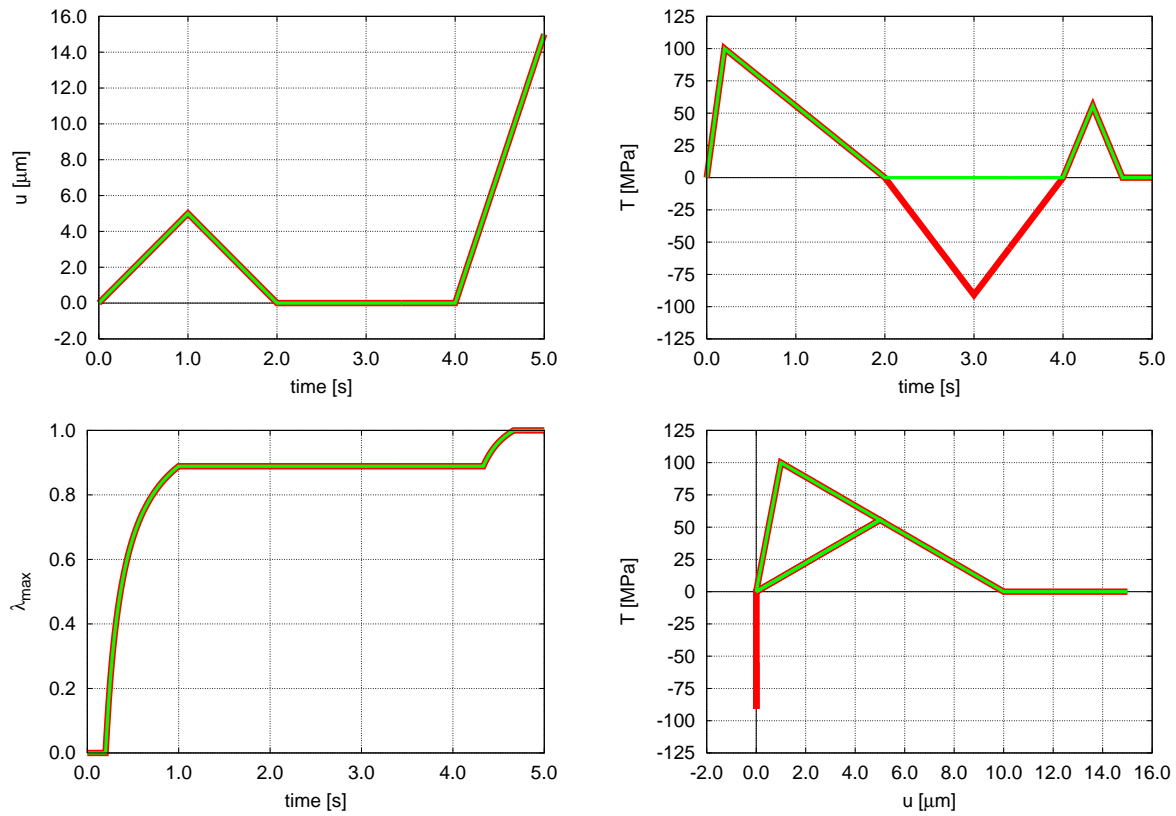**54** (1987), pp. 525-531.
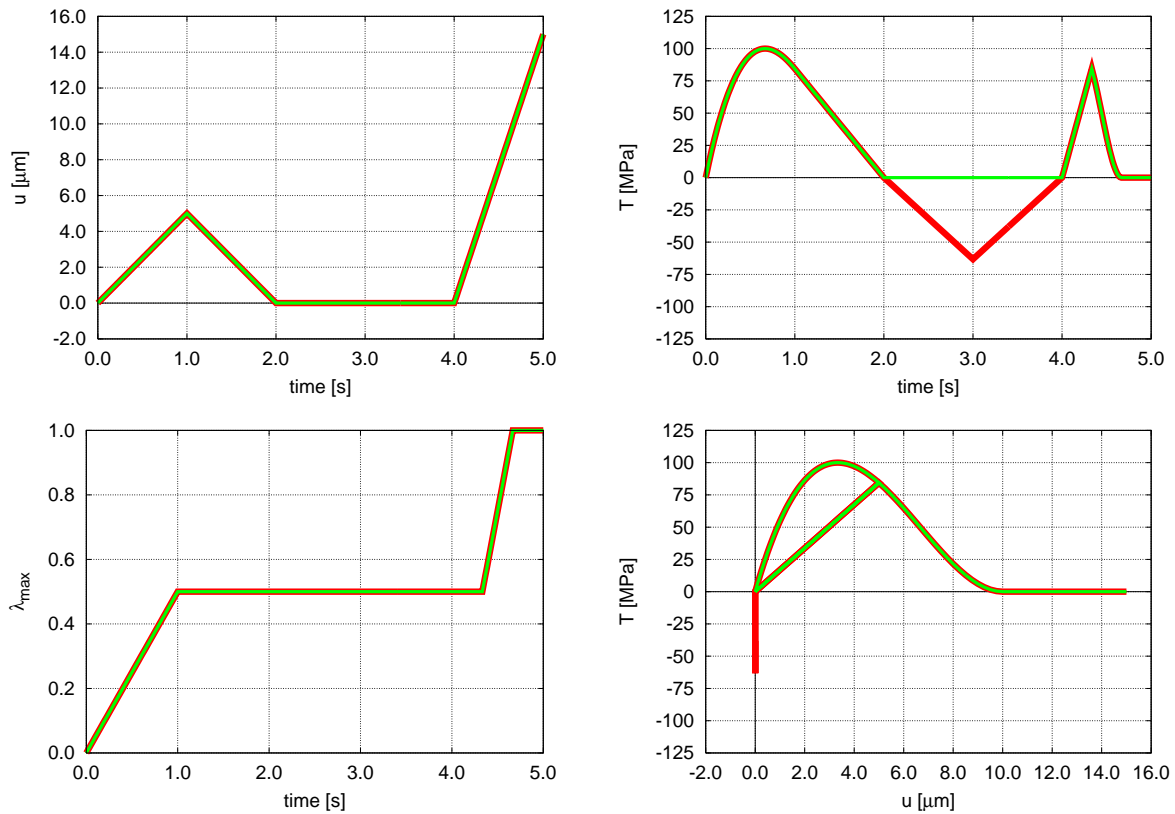
Figure 1: Example in two dimensions of the evolution of the cohesive traction as a function of the opening displacement, for two different loading cases: $u_N(t)$ with $u_T(t) = 0$ (thick red curves), and $u_T(t)$ with $u_N(t) = 0$ (thin green curves). Top left: applied load $u(t)$. Note: for $2 \leq t \leq 4$ s, the applied loading becomes negative (but the response u_N remains 0 because of an implicit non-penetration condition). Top right: response $T(t)$. Bottom left: $\lambda_{max}(t)$. Bottom right: $u(t)$ vs $T(t)$.

If `no_penetration` is specified, a *broken* element continues to prevent penetration.

Example:

```
***behavior needleman_debonding
   sigmax  100.
   deltan    1.e-5
   deltat    1.e-5
   alpha     1.
   alphac    1.e3
***return
```

***behavior crisfield_debonding

Description:
This behavior[3] is used for the special problem of interface debonding. See the command
`**create_interface_elements` (and similar) in the Z-set user manual on how to insert
cohesive elements in the mesh. The Crisfield model[4] is described through a scalar variable λ,
which characterizes the relative crack opening:

$$\lambda = \frac{1}{\eta} \frac{\langle \kappa \rangle}{1 + \langle \kappa \rangle}, \quad \kappa = \sqrt{\left(\frac{\langle u_N \rangle}{u_{0N}}\right)^2 + \left(\frac{\|\vec{u}_T\|}{u_{0T}}\right)^2} - 1, \quad \eta = 1 - \frac{u_{0N}}{\delta_N} = 1 - \frac{u_{0T}}{\delta_T}, \tag{4}$$

where $\langle x \rangle = x$ if $x > 0$ and $\langle x \rangle = 0$ if $x \leq 0$. With respect to the interface normal $\vec{n}$,
$\vec{u}_N = (\vec{u} \cdot \vec{n})\,\vec{n} \equiv u_N \vec{n}$ and $\vec{u}_T \equiv \vec{u} - \vec{u_N}$ denote, respectively, the normal and shear opening
displacements and δ_N and δ_T the corresponding maximum allowable values of their norms.
The parameters u_{0N} and u_{0T} denote, respectively, the opening displacements corresponding
to the maximum cohesive traction of the normal and shear components. The damage variable
λ_{max}, which is the maximum value of λ reached up until the current instant, increases from 0
(no damage) to 1 (for a broken element). In this model the ratios $\frac{u_{0N}}{\delta_N}$ and $\frac{u_{0T}}{\delta_T}$ have to be the
same. The normal and shear components of the cohesive traction $\vec{T}$, i.e. $\vec{T}_N = \left(\vec{T} \cdot \vec{n}\right)\vec{n} \equiv$
$T_N \vec{n}$ and $\vec{T}_T = \vec{T} - \vec{T}_N$, are defined by:

$$T_N = \frac{u_N}{u_{0N}} F(\lambda_{max}), \quad \vec{T}_T = \alpha \frac{\vec{u}_T}{u_{0T}} F(\lambda_{max}), \quad F(\lambda) = \sigma_{max}\left(1 - \lambda\right), \tag{5}$$

with α a constant representing the relative magnitude of $\|\vec{T}_T\|$ with respect to T_N, and σ_{max}
the maximum stress allowable by the element. For the compressive case, where $u_N < 0$, the
normal component of the traction is modified to

$$T_N = \alpha_c \frac{u_N}{u_{0N}} F(0), \tag{6}$$

with α_c a penalization factor. In the literature, α_c usually is at least 10α. Figure 5 illustrates
the typical response of the cohesive zone model under specific loads, for the parameters as
given in the example.

Syntax:

```
    ***behavior crisfield_debonding
        sigmax    σ_max
        u0n       U_0N
        u0t       U_0T
        deltan    δ_n
        deltat    δ_t
        alpha     α
        alphac    α_c
```

... continued

---

[3]this behavior is Z-set specific, and therefore does not apply for Z-mat for other codes
[4]Alfano G. and Crisfield M. A., "Finite element interface models for the delamination analysis of laminated
composites: mechanical and computational issues.", Int. J. Numer. Meth. Engng. **50** (2001), 1701-1736.
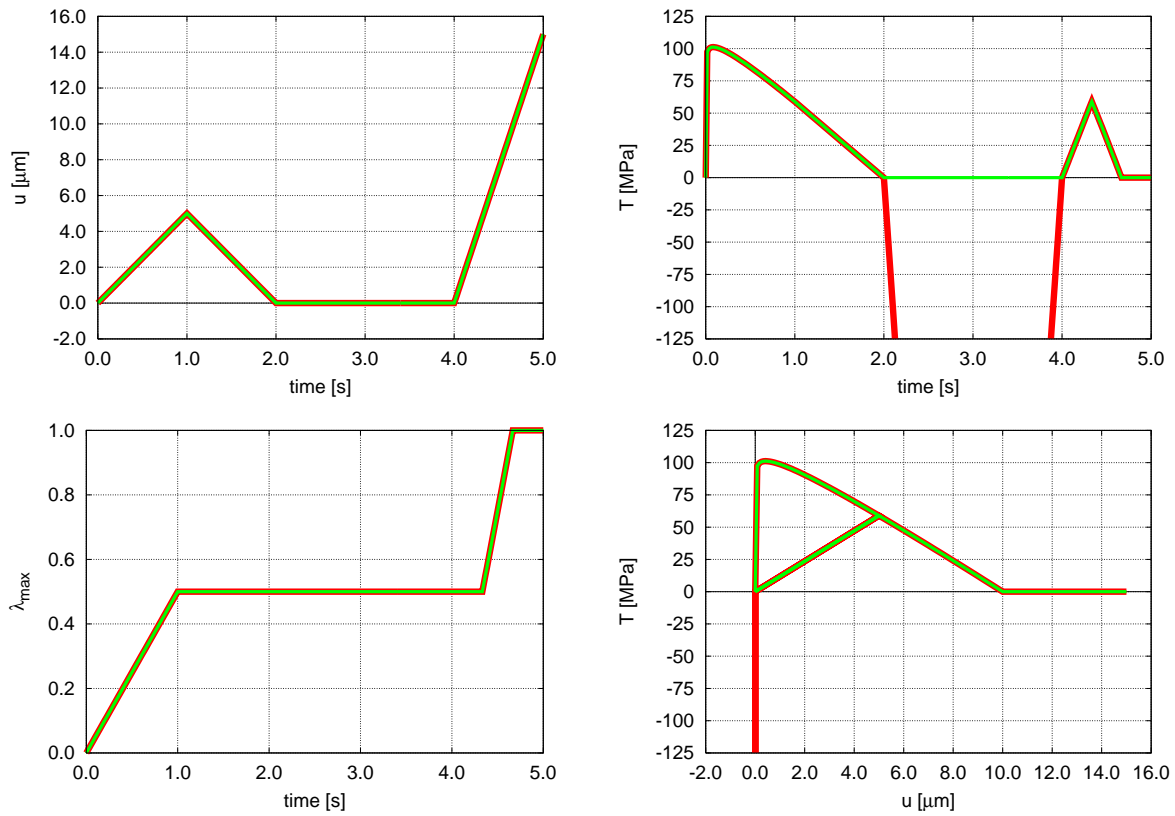
Figure 2: Example in two dimensions of the evolution of the cohesive traction as a function of the opening displacement, for two different loading cases: $u_N(t)$ with $u_T(t) = 0$ (thick red curves), and $u_T(t)$ with $u_N(t) = 0$ (thin green curves). Top left: applied load $u(t)$. Note: for $2 \leq t \leq 4$ s, the applied loading becomes negative (but the response u_N remains 0 because of an implicit non-penetration condition). Top right: response $T(t)$. Bottom left: $\lambda_{max}(t)$. Bottom right: $u(t)$ vs $T(t)$.

Example:

```
***behavior crisfield_debonding
   sigmax  100.
   u0n        1.e-6
   u0t        1.e-6
   deltan     1.e-5
   deltat     1.e-5
   alpha      1.
   alphac     1.e3
***return
```

***behavior chaboche_debonding

Description:
This behavior[5] is used for the special problem of interface debonding. See the command
create_interface_elements (and similar) in the Z-set user manual on how to insert
cohesive elements in the mesh. The Chaboche model[6] is described through a scalar variable
λ which characterizes the relative crack opening:

$$\lambda = \sqrt{\left(\frac{\langle u_N \rangle}{\delta_N}\right)^2 + \left(\frac{\|\vec{u}_T\|}{\delta_T}\right)^2}, \tag{7}$$

where $\langle x \rangle = x$ if $x > 0$ and $\langle x \rangle = 0$ if $x \leq 0$. With respect to the interface normal $\vec{n}$,
$u_N = (\vec{u} \cdot \vec{n})\,\vec{n} \equiv u_N \vec{n}$ and $\vec{u}_T \equiv \vec{u} - \vec{u}_N$ denote, respectively, the normal and shear opening
displacements and δ_N and δ_T the corresponding maximum allowable values of their norms.
The damage variable λ_{max}, which is the maximum value of λ reached up until the current
instant, increases from 0 (no damage) to 1 (for a broken element). The normal and shear
components of the cohesive traction $\vec{T}$, i.e. $\vec{T}_N = \left(\vec{T} \cdot \vec{n}\right)\vec{n} \equiv T_N \vec{n}$ and $\vec{T}_T = \vec{T} - \vec{T}_N$, are
defined by:

$$T_N = \frac{u_N}{\delta_N} F\left(\lambda_{max}\right), \quad \vec{T}_T = \alpha \frac{\vec{u}_T}{\delta_T} F\left(\lambda_{max}\right), \quad F\left(\lambda\right) = \frac{27}{4} K \sigma_{max} \lambda^{\frac{1}{n}-1}\left(1 - \lambda\right) \tag{8}$$

with α a constant representing the relative magnitude of $\|\vec{T}_T\|$ with respect to T_N, σ_{max} the
maximum stress allowable by the element and K and n model parameters. When $\lambda <$ 1.e-8,
the finite values of the cohesive traction and the consistent matrix are guaranteed by the
parameters df_0 and dfdl_0. For the compressive case, where $u_N < 0$, the normal component
is modified to

$$T_N = \alpha_c \frac{u_N}{\delta_N} F(0), \tag{9}$$

with α_c a penalization factor. In the literature, α_c usually is at least 10α. Figures 3 illustrates
the typical response of the cohesive zone model under specific loads, with the parameters as
given in the example.

Syntax:

```
***behavior chaboche_debonding
    sigmax    σmax
    deltan    δn
    deltat    δt
    alpha     α
    alphac    αc
    n         n
    K         K
    df_0      value
    dfdl_0    value
```

... *continued*

---

[5] this behavior is Z-set specific, and therefore does not apply for Z-mat for other codes
[6] Caliez M., "Approche locale pour la simulation de l'écaillage des barrières thermiques EBPVD", Ph.D.
thesis, Ecole Nationale Supérieure des Mines de Paris, 2001

Figure 3: Example in two dimensions of the evolution of the cohesive traction as a function of the opening displacement, for two different loading cases: $u_N(t)$ with $u_T(t) = 0$ (thick red curves), and $u_T(t)$ with $u_N(t) = 0$ (thin green curves). Top left: applied load $u(t)$. Note: for $2 \leq t \leq 4$ s, the applied loading becomes negative (but the response u_N remains 0 because of an implicit non-penetration condition). Top right: response $T(t)$. Bottom left: $\lambda_{max}(t)$. Bottom right: $u(t)$ vs $T(t)$.

Example:

```
***behavior chaboche_debonding
   sigmax        100.
   deltan          1.e-5
   deltat          1.e-5
   alpha         1.
   alphac          1.e3
   n              22.6
   K               0.18
   df_0     44260000.
   dfdl_0          0.
***return
```

***behavior generalized_debonding

<u>Description</u>:
This behavior[7] is used for the special problem of interface debonding. See the command `**create_interface_elements` (and similar) in the Z-set user manual on how to insert cohesive elements in the mesh. The Generalized model[8] is based on the consideration of the characterization of interfacial properties and permits to use three different shapes for the cohesive law (bi-linear, tri-linear and trapezoidal). This model is described through a scalar variable λ, which characterizes the relative crack opening:

$$\lambda = \left(1 - \frac{\langle \delta - \delta^* \rangle}{(\delta - \delta^*)}\right) \langle \delta - \delta_0 \rangle \left(\frac{\delta^* - \alpha_\sigma \delta_0}{\delta(\delta^* - \delta_0)}\right) + \left(\frac{\langle \delta - \delta^* \rangle}{(\delta - \delta^*)}\right) \left(1 + \frac{\alpha_\sigma \delta_0 \langle \delta_f - \delta \rangle}{\delta(\delta^* - \delta_f)}\right), \quad (10)$$

where $\langle x \rangle = x$ if $x > 0$ and $\langle x \rangle = 0$ if $x \leq 0$. The parameter δ is the relative displacement defined as

$$\delta = \sqrt{\langle u_N \rangle^2 + \|\vec{u}_T\|^2}. \quad (11)$$

With respect to the interface normal $\vec{n}$, $\vec{u}_N = u_N \vec{n}$ and $\vec{u}_T \equiv \vec{u} - \vec{u_N}$ denote, respectively, the normal and shear opening displacements. The parameters δ_0 and δ_f are respectively the relative displacement associated with the interfacial strength τ_0 and the one attained when the energy release rate is equal to the fracture toughness G_C. It should be noted that the evolution of τ_0 (resp. G_C), as a function of the mixed-mode ratio, is defined by the stress criterion (resp. the propagation law). Finally, the parameter δ^* is associated with the stress τ^* attained at the end of the first part of the damage process (Figure 4). These both parameters depend on the shape of the cohesive law which is defined using two shape parameters : α_σ and α_δ determined by

$$\alpha_\sigma = \frac{\tau^*}{\tau_0}, \quad \alpha_\delta = \frac{(\delta^* - \delta_0)}{(\delta_f - \delta_0)}. \quad (12)$$
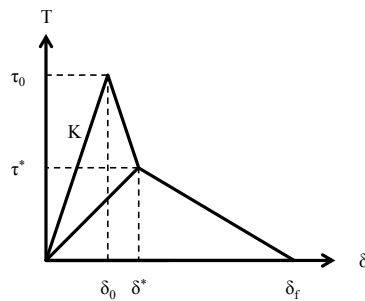
Figure 4: Shape of the tri-linear model for a constant mixed-mode ratio in the (δ, T) plane .

The damage variable λ_{max}, which is the maximum value of λ reached up until the current instant, increases from 0 (no damage) to 1 (for a broken element). The normal and shear

---

[7]this behavior is Z-set specific, and therefore does not apply for Z-mat for other codes

[8]Vandellos T., Huchette C. and Carrere N., "Proposition of a framework for the development of a cohesive zone model adapted to Carbon-Fiber Reinforced Plastic laminated composites.", Comp. Struct. **105** (2013), 199-206.

components of the cohesive traction $\vec{T}$, i.e. $\vec{T}_N = \left(\vec{T} \cdot \vec{n} \right) \vec{n} \equiv T_N \vec{n}$ and $\vec{T}_T = \vec{T} - \vec{T}_N$, are defined by:

$$T_N = K u_N \left(1 - \lambda \right), \quad \vec{T}_T = K \vec{u}_T \left(1 - \lambda \right), \tag{13}$$

where K is the interfacial stiffness. For the compressive case, where $u_N < 0$, the normal component of the traction is modified to

$$T_N \quad = \quad \alpha_c K u_N, \tag{14}$$

with α_c a penalization factor. Figure 5 illustrates the typical response of the cohesive zone model under specific loads, for the parameters as given in the example.

<u>Remarks:</u>

- the parameter α_δ is not required with the bi-linear shape;

- the parameter α_σ has to be defined only with the tri-linear law;

- two stress criteria (*puissance* and *reinforcement*) and three propagation laws (*puissance*, *benzeggagh* and *vandellos*) are available;

- the option `*turon` is required for applying the modification proposed by Turon[9].

... *continued*

---

[9]Turon A., Camanho P.P., Costa J. and Renart J., "Accurate simulation of delamination growth under mixed-mode loading using cohesive elements: Definition of interlaminar strengths and elastic stiffness.", Comp. Struct. **92** (2010), 1857-1864.

Syntax:

```
***behavior generalized_cohesive_zone
  *strength
   Zt            Zt
   Sc            Sc
  *toughness
   G1c           G_IC
   G2c           G_IIC
  *stiffness
   K             K
   alphac        α_c
  *propagation   propagation law (puissance or benzeggagh or vandellos)
   n             n
  *initiation    stress criterion (puissance or reinforcement)
  *softening     shape of the cohesive law (bi_linear or tri_linear or trapezoidal)
   alpha_delta   α_δ
   alpha_sigma   α_σ
  *turon         (optional)
```

The `*strength` entries are Zt and Sc. The `*toughness` entries are G_{IC} and G_{IIC}. The `*stiffness` entries are K and α_c. The `*propagation` law is *propagation law (puissance or benzeggagh or vandellos)* with n. The `*initiation` is *stress criterion (puissance or reinforcement)*. The `*softening` is *shape of the cohesive law (bi_linear or tri_linear or trapezoidal)* with α_δ and α_σ. The `*turon` is *(optional)*.

Example:

```
***behavior generalized_cohesive_zone
  *strength
   Zt      100.
   Sc      100.
  *toughness
   G1c       0.0005
   G2c       0.0005
  *stiffness
   K           1.e8
   alphac    1.e3
  *propagation benzeggagh
   n 1.142
  *initiation puissance
  *softening tri_linear
   alpha_delta 0.4
   alpha_sigma 0.8
 ***return
```

. . . continued
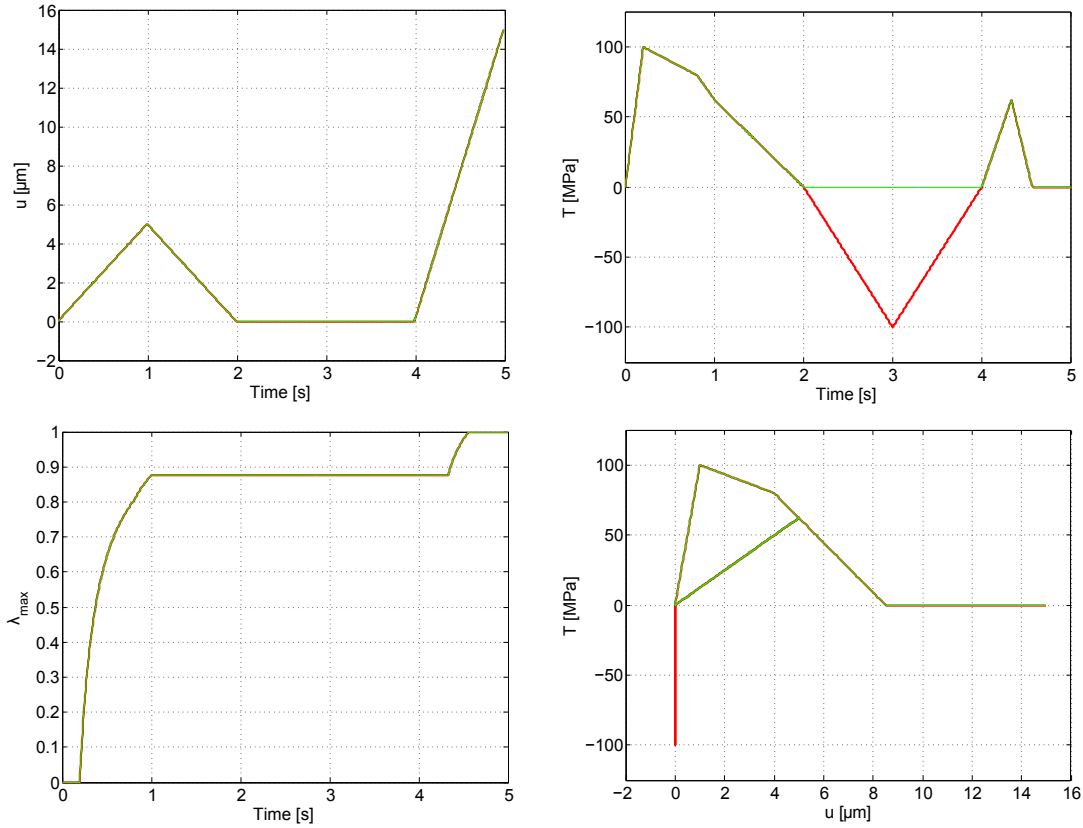
Figure 5: Example in two dimensions of the evolution of the cohesive traction as a function of the opening displacement, for two different loading cases: $u_N(t)$ with $u_T(t) = 0$ (thick red curves), and $u_T(t)$ with $u_N(t) = 0$ (thin green curves). Top left: applied load $u(t)$. Note: for $2 \leq t \leq 4$ s, the applied loading becomes negative (but the response u_N remains 0 because of an implicit non-penetration condition). Top right: response $T(t)$. Bottom left: $\lambda_{max}(t)$. Bottom right: $u(t)$ vs $T(t)$.

***behavior diffusion

Description:
Diffusion behavior is analogous to the stationary thermal behaviors.

$$\vec{J} = \mathbf{D}\nabla C$$

Syntax:

```
***behavior diffusion
 **inter_phase_diffusion val
 **phase
    D COEFFICIENT
    comp_max val
    comp_min val
```

Stored Variables:

prefix	size	description	default
dC	V	gradient of concentration	yes
J	V	flux of concentration	yes
C	S	the concentration	yes
phase	S	phase id (in input order)	yes
Deff	S	effective D at point	yes

Example:

```
***behavior diffusion
  **inter_phase_diffusion 8.e-10
  **phase oxide
     D 1.e-7
     comp_min 1200.0
  **phase metal
     D 5.e-9
     comp_max 400.
***return
```

***behavior linear_spring

Description:
 This behavior class is used to specify linear response for spring or truss elements (element formulation `linear_spring` or `spr`).

$$F = \mathbf{k}U$$

Where F is the spring tension, and U is the axial displacement of the spring. Note that $\mathbf{k}$ can vary with any external parameter, but not in relation to U.

Syntax:

```
***behavior linear_spring
   k coef
```

By default there is no thermal dilatation in the model.

Example:
A simple spring definition:

```
***behavior linear_spring
  k 1.e4
***return
```

***behavior thermal

Description:
This is the basic thermal behavior. The conductivity is determined using a `CONDUCTIVITY` object. Transient thermal problems require that a coefficient `capacity` be defined as well (global behavior coefficient, see page 9.8).

The behavior calculates the heat flux from the gradient in temperature:

$$\vec{q} = \mathbf{k}\nabla T$$

The enthalpy term is

$$dH = \int_{T0}^{T} C_p(\tau)d\tau$$

where the integration will be carried out numerically if the heat capacity depends on the temperature.

Syntax:

```
***behavior thermal
 **conductivity CONDUCTIVITY
 **coefficient
    capacity val
```

Note that capacity and the coefficients in the conductivity object can be a variable coefficients (e.g. tables, functions, etc) of the `temperature` variable. This gives the model the possibility of including considerable non-linear effects.

Stored Variables:
The grad variable is the gradient of temperature, and the flux is the heat flux.

prefix	size	description	default
dT	V	gradient of temperature	yes
q	V	heat flux	yes
temperature	S	the temperature at the Gauss point	yes

Example:
Two examples of thermal behavior follow:

```
***behavior thermal
 **conductivity isotropic
   k   48.822
 **coefficient
   capacity 4.8168e6
***return

***behavior thermal
**conductivity isotropic
k temperature
0.1    0.0
0.6    500.0
***return
```

***behavior variable_friction

Description:
This behavior[10] is used to specify a variable friction in certain contact models (see the command ***contact **zone *variable_friction in the Z-set user manual). The behavior specifies a friction coefficient μ that may depend on the current total relative sliding u_s of the contact surfaces, and/or the cumulative relative sliding u_{cum}. This is analogous to the role played by the current inelastic deformation and the cumulative plastic deformation in isotropic and kinematic hardening in conventional material models. The analogy is as follows: the total friction coefficient μ is written as $\mu = \mu_0 + \mu_R(u_{cum}) + \mu_X(u_{cum}, u_s)$, where μ_0 plays the role analogous to the elastic limit, μ_R to the isotropic hardening and μ_X to the kinematic hardening.

Syntax:

```
***behavior variable_friction

  *isotropic constant | linear | nonlinear
   fric1 μ0
[  fric3 Q ]
[  b1     b1 ]
[  betai  βi ]

[ *kinematic linear | nonlinear ]
[  fric2 C ]
[  b      b ]
[  betak  βk ]
```

Possible choices are:

*isotropic constant   takes one parameter μ_0.

*isotropic linear   takes two parameters μ_0 and Q to give $\mu_R = Qu_{cum}$.

*isotropic nonlinear   takes four parameters μ_0, Q, b_1 and β_i to give $\mu_R = Q\left(1. - \exp[-(b_1 u_{cum})^{\beta_i}]\right)$.

*kinematic linear   takes one parameter C to give $\mu_X = C|u_s|$.

*kinematic nonlinear   takes three parameters C, b and β_k, to give $\mu_X = C\left(1. - \exp[-(bu_{cum})^{\beta_k}]\right)\frac{|u_s|}{u_{max}}$. Here u_{max} is...

Currently, the behavior parameters cannot depend on any external parameter (such as temperature). Also note that not all contact models support a variable friction coefficient. If so, it is indicated in the description of each contact model.

Example:

---

[10]this behavior is Z-set specific, and therefore does not apply for Z-mat for other codes

```
***behavior variable_friction
  *kinematic nonlinear
  fric2 3.
  b 4.e-2
  betak 1.8
  *isotropic nonlinear
  fric1 0.18
  fric3 3.
  b1 5.e-2
***return
```

Chapter 13

Material Components

<ANISOTROPIC_DAMAGE>

<ANISOTROPIC_DAMAGE>

Description:

These behavior objects are specific to the elastic and viscoplastic anisotropic damage models. They allow different types of damage variable to be used easily, and in combination. All the coefficients and functions entered here are local to the each damage object, and must therefore be input for all applicable objects even if the coefficients have the same meaning.

Syntax:

```
**damage  [ type ]
[ *use_e_bar          ]
[ *dont_use_e_bar     ]
[ *eta   <COEFFICIENT> ] % default 1.0
[ *K_coeffs   V₁ V₂ V₃ V₄ V₅ V₆ V₇ V₈ ]
[ *g      <G_FUNCTION> ]
```

---

where *type* may be from the following types:

CODE	DESCRIPTION
scalar	scalar variables with fixed direction
elastic_tensorial	tensorial variable
rate_tensorial	tensorial variable

*use_e_bar   Makes the calculation of Y or $\mathbf{Y}$ use the $\bar{\boldsymbol{\epsilon}}$ tensor in place of $\boldsymbol{\epsilon}_{el}$.

*dont_use_e_bar   use $\boldsymbol{\epsilon}_{el}$ to calculate Y or $\mathbf{Y}$ in place of $\bar{\boldsymbol{\epsilon}}$. This option is currently the default.

*K_coeffs   coefficients are entered to construct the tensor $\mathbf{K}$ use the compliance matrix $(\mathbf{S} = \mathbf{D}_{el}^{-1})$ and are as follows:

$$\mathbf{H}_0 = \begin{bmatrix} S_{11}V_1 & S_{12}V_4 & S_{13}V_5 & & & \\ & S_{22}V_2 & S_{23}V_6 & & & \\ & & S_{33}V_3 & & & \\ & & & S_{44}V_7 & & \\ & sym & & & S_{55}V_8 & \\ & & & & & S_{66}V_9 \end{bmatrix}$$

note that the tensors are stored as

$$[S_1 \ldots S_6] = [S_{11} \quad S_{22} \quad S_{33} \quad S_{12} \quad S_{23} \quad S_{31}]$$

$$\mathbf{K} = \mathbf{D}_{el} : \mathbf{H}_0 : \mathbf{D}_{el}$$

The factors for V are entered in order after the ***K_coeffs** keyword is entered. See the behavior descriptions for examples.

<ANISOTROPIC_DAMAGE>

*K matrix form for the **K**. This input is entered as an `ELASTICITY` object.

Only one definition for the matrix $\mathbf{K}_i^0$ may be given with the `K_coeffs` or `K`. The coefficients correspond directly to the associate terms marked with a subscript i.

<ANISOTROPIC_DAMAGE>

<ANISOTROPIC_DAMAGE> scalar

Description:

Each scalar damage variable is defined using a "damage direction" input by the user, $\vec{n}_i$, and an effective fourth order "damage effects" tensor $\mathbf{K}_i^0$. The modulus modification induced by a scalar damage variable i is the following:

$$\mathbf{C}_i^{eff} = \delta_i(\mathbf{K}_i^0 - \eta_i h(-\bar{\epsilon}_i)\mathbf{N}_i : \mathbf{K}_i^0 : \mathbf{N}_i)$$

where δ_i is the scalar internal damage variable. The above uses the following terms to measure the degree of opening strain:

$$
\begin{aligned}
\bar{\epsilon}_i &= (\vec{n}_i \otimes \vec{n}_i) : (\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_c) \\
\mathbf{N}_i &= (\vec{n}_i \otimes \vec{n}_i) \otimes (\vec{n}_i \otimes \vec{n}_i)
\end{aligned}
\tag{1}
$$

The material coefficient η is used to describe the influence of closing on the damage softening.

```
**damage scalar
    std options
[ *n    <VECTOR> ]      % orientation
```

n   the directions of the axes of damage for the isotropic variables entered as a vector.

Example:

Please see the examples in the anisotropic behaviors `aniso_damage` and `visco_aniso_damage`.

<ANISOTROPIC_DAMAGE>

<ANISOTROPIC_DAMAGE> elastic_tensorial

Description:

This model using a 2nd order tensorial damage variable is calculated as follows:

$$\mathbf{C}_j^{eff} = \mathbf{D}_j : \mathbf{K}_j^0 - \sum_{n=0}^{3} \eta_j h(-\bar{\epsilon}_n) \mathbf{P}_n : (\mathbf{D}_j : \mathbf{K}_j^0) : \mathbf{P}_n)$$

where the summation over n is over the three principal directions of the strain tensor, and $\mathbf{D}_j$ is a fourth order tensor constructed based on the second order damage variable $\mathbf{d}_j$. This will use the following calculations based on the principal strain eigenvectors $\vec{p}_n$:

$$\begin{aligned}
\bar{\epsilon}_n &= (\vec{p}_n \otimes \vec{p}_n) : (\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_c) \\
\mathbf{P}_n &= (\vec{p}_n \otimes \vec{p}_n) \otimes (\vec{p}_n \otimes \vec{p}_n)
\end{aligned} \tag{2}$$

and the fourth order tensors $\mathbf{D}_j$ are constructed their tensorial variables as:

$$\mathbf{D}_j = (\alpha - \beta)(\mathbf{1} \otimes \mathbf{d}_j)_s + \tfrac{\beta}{2}\left((\mathbf{1}\overline{\otimes}\mathbf{d})_s + \mathbf{1}\underline{\otimes}\mathbf{d})_s\right)$$

<COEFFICIENT>

<COEFFICIENT>

Description:
Coefficient objects are used to enter the values for material coefficients. Each behavior object may have any number of coefficients to parameterize the models for different materials. The coefficients are themselves behavior objects however, and therefore have a standard format for entry. Coefficients also provide the means to add external parameter or local material variable dependencies.

Creating user-dependency on the internal variables may however significantly alter the material model, and invalidate integration methods. The only sure use for arbitrary dependencies on the integrated variables is with Runge-Kutta integration, and a time-dependent flow law. The tangent matrix may also be altered by these dependencies. Coefficients which are a function of the external parameters are however robustly implemented, and are valid for all integration methods.

Syntax:
Supposing that a material model coefficient C is required, a syntax similar to the following will be given:

```
    C COEFFICIENT
```
---

where the term `COEFFICIENT` is to be replaced with a coefficient definition. The replacement syntax using the coefficient objects is given below:

```
    C  [ type ]
    parameters
```

CODE	DESCRIPTION
equivalence	coefficient which is the value of a variable
=	same as equivalence
function	coefficient which is a function of variables (see chapter *Functions*)
equivalence	coefficient which is the value of variables
step_wise	step-wise tabular values
default	tabular description in terms of variables

Example:
The first example is for a tabular coefficient. This example has an equivalent stress, `sigeq`, as a function of the cumulated flow, and the temperature. Note any number of variables may be given. If the parameter values are out of range from what is given in the table, and error will result.

```
  sigeq epcum temperature
  400.0  0.0     20.0
  350.0   "     120.0
  290.0   "     200.0
```

<COEFFICIENT>

```
450.0   0.002   20.0
410.0     "     120.0.
330.0     "     200.0
500.0   0.01    20.0
460.0     "     120.0
400.0     "     200.0
```

The second example uses functions to describe the coefficient value. Function syntax is described more fully in the *Functions* chapter. Note parameter names must be on the same line as the `function` declaration.

```
young function 230. + 1.e-2*temperature + temperature^2.0;
```

The last example assumes a parameter is calculated in the material law called `Bpa1v`. This example will set the coefficient value to the value of that parameter at all times.

```
*kinematic nonlinear
    A1  40.0
    Bp  = Bpa1v
```

<COEFFICIENT_MATRIX>

<COEFFICIENT_MATRIX>

Description:
This object is used to enter coefficients for a desired form of 4th order coefficient matrix. The use of these matrices is often as an elasticity matrix, so we sometimes refer to the object as `ELASTICITY`.

Syntax:
These objects take a list of coefficient declarations after the type keyword is given. There are no explicit restrictions on the types of coefficients or their dependencies. The different types (keywords) available are the following:

CODE	DESCRIPTION
diagonal	1 or *dim* coefficients
isotropic	2 coefficients
cubic	3 coefficients
transverse	5 coefficients
orthotropic	9 coefficients
anisotropic	21 coefficients

The default type depends on its application. For elasticity objects this is `isotropic`. The `anisotropic` model represents the most general elasticity model. Coefficient names follow the same convention to describe components of the coefficient matrix. This sets the coefficient name for a component C_{ijkl} to `Cijkl`. For example, a component y_{1212} is named `y1212`.

When using elasticity objects, special care has to be taken with respect to the nomenclature of the components. When representing a tensor of elasticity in 6×6 form, the Voigt convention is assumed, but with one important difference: the order of storage is

$$11 \rightarrow 1,\ 22 \rightarrow 2,\ 33 \rightarrow 3,\ 12 \rightarrow 4,\ 23 \rightarrow 5,\ 31 \rightarrow 6 \text{ (Zebulon)}$$

instead of the usual

$$11 \rightarrow 1,\ 22 \rightarrow 2,\ 33 \rightarrow 3,\ 23 \rightarrow 4,\ 31 \rightarrow 5,\ 12 \rightarrow 6 \text{ (Voigt)}$$

For instance, a Voigt coefficient c_{66} becomes `c44` or `y1212` in Zmat/Zebulon.

The matrix forms are given below:

isotropic The isotropic model allows several methods of entering the coefficients for convenience. The primary method gives the Young's modulus (E) and Poisson coefficient (ν) which correspond to the names `young` and `poisson` respectively.

$$D_{ij} = \frac{E}{1+\nu} + \frac{\nu E}{(1-2\nu)(1+\nu)}\delta_{ij}$$

An alternate definition defines the shear modulus (G or μ) and the bulk modulus (K or κ). These correspond to the coefficient names `G` or `mu`, and `K` or `kappa`.

<COEFFICIENT_MATRIX>

transverse Transverse isotropy has two directions which are equivalent. There are two ways to specify transverse elasticity parameters.

Elasticity modules

Direction 1 is the longitudinal one and directions 2 and 3 are the two transverse ones. The elasticity is specified with 5 classical parameters : *El*, *Et*, *nult*, *nutt* and *Glt*. They define the Hooke relation such as :

$$
\begin{pmatrix}
\varepsilon_{11} \\
\varepsilon_{22} \\
\varepsilon_{33} \\
\varepsilon_{23} \\
\varepsilon_{13} \\
\varepsilon_{12}
\end{pmatrix}
=
\begin{pmatrix}
\frac{1}{El} & \frac{-nult}{Et} & \frac{-nult}{Et} & 0 & 0 & 0 \\
 & \frac{1}{Et} & \frac{-nutt}{Et} & 0 & 0 & 0 \\
 & & \frac{1}{Et} & 0 & 0 & 0 \\
 & & & \frac{1+nutt}{Et} & 0 & 0 \\
 & \text{sym} & & & \frac{1}{2Glt} & 0 \\
 & & & & & \frac{1}{2Glt}
\end{pmatrix}
\begin{pmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{33} \\
\sigma_{23} \\
\sigma_{13} \\
\sigma_{12}
\end{pmatrix}
$$

An old parameter named *glt* (instead of *Glt*) is defined as :

$$\sigma_{12} = glt\,\varepsilon_{12}$$

whereas *Glt* is defined as :

$$\sigma_{12} = 2\,Glt\,\varepsilon_{12}$$

This old parameter is still available for compatibility with old data sets.

Matrix coefficients

The program allows the user to specify which terms in the elastic matrix will be set equal, with a tag input after the `transverse` keyword. It is best to explain this syntax through an example:

$$
D =
\begin{pmatrix}
c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\
 & c_{11} & c_{13} & 0 & 0 & 0 \\
 & & c_{33} & 0 & 0 & 0 \\
 & & & \frac{1}{2}(c_{11} - c_{12}) & 0 & 0 \\
 & \text{sym} & & & c_{55} & 0 \\
 & & & & & c_{55}
\end{pmatrix}
$$

which is created by `**elasticity transverse` and the coefficients `c11`, `c12`, `c13`, `c33` and `c55` (or the corresponding `y1111` etc.).

For the moment it is only possible to work with `c11` and `c22` equal instead of, for instance, equal `c22` and `c33`.

The following relations are also given for reference in the case of $c_{11} = c_{22}$:

$$
\begin{aligned}
c_{11} &= \frac{(1 - n\nu_{zx}^2)E_x}{AB} \\
c_{12} &= \frac{(\nu_{xy} + n\nu_{zx}^2)E_x}{AB} \\
c_{13} &= \frac{\nu_{zx}E_x}{B}
\end{aligned}
$$

<COEFFICIENT_MATRIX>

$$
\begin{aligned}
c_{33} &= \frac{(1 - \nu_{xy})E_z}{B} \\
c_{44} &= \tfrac{1}{2}(C_{11} - C_{12}) \\
c_{55} &= C_{66} = G_{xy} = G_{xz} \\
c_{xy} &= \frac{E_x}{2(1 + \nu_{xy})} \\
n &= E_x/E_z \qquad A = 1 + \nu_{xy} \qquad B = 1 - \nu_{xy} - 2n\nu_{zx}^2
\end{aligned}
$$

cubic

$$
D = \begin{pmatrix}
y_{1111} & y_{1122} & y_{1122} & 0 & 0 & 0 \\
 & y_{1111} & y_{1122} & 0 & 0 & 0 \\
 & & y_{1111} & 0 & 0 & 0 \\
 & & & y_{1212} & 0 & 0 \\
 & \text{sym} & & & y_{1212} & 0 \\
 & & & & & y_{1212}
\end{pmatrix}
$$

orthotropic

$$
D = \begin{pmatrix}
y_{1111} & y_{1122} & y_{3311} & 0 & 0 & 0 \\
 & y_{2222} & y_{2233} & 0 & 0 & 0 \\
 & & y_{3333} & 0 & 0 & 0 \\
 & & & y_{1212} & 0 & 0 \\
 & \text{sym} & & & y_{2323} & 0 \\
 & & & & & y_{3131}
\end{pmatrix}
$$

An alternative naming uses `c11`, `c22`, `c33`, `c44`, `c55`, `c66`, `c12`, `c13`, and `c23` (or their symmetric counterparts).

anisotropic

$$
D = \begin{pmatrix}
y_{1111} & y_{1122} & y_{1133} & y_{1112} & y_{1123} & y_{1131} \\
 & y_{2222} & y_{2233} & y_{2212} & y_{2223} & y_{2231} \\
 & & y_{3333} & y_{3312} & y_{3323} & y_{3331} \\
 & & & y_{1212} & y_{1223} & y_{1231} \\
 & \text{sym} & & & y_{2323} & y_{2331} \\
 & & & & & y_{3131}
\end{pmatrix}
$$

Example:

```
**elasticity isotropic
   young   200000.
   poisson 0.3

**elasticity cubic
   y1111 162321.0
   y1122  78075.0
```

<COEFFICIENT_MATRIX>

```
   y1212 110615.0

**elasticity
   young     T
     200000. 0.
     200000. 1000.
   poisson  0.3

**elasticity transverse
   El      115000.
   Et        8500.
   Glt       4500.
   nult        0.32
   nutt        0.40
```

Description:
Thermal conductivity is available in istropic and anisotropic forms. Conductivity acts much like the elasticity matrix does in mechanical problems, except the thermal behavior accounts for direct coefficient variations with respect to the temperature.

$$\vec{q} = \mathbf{k}\nabla T$$

Syntax:

    **conductivity *type*

       ...

The following forms are available:

`isotropic`

$$\mathbf{k} = \begin{bmatrix} k & 0 & 0 \\ 0 & k & 0 \\ 0 & 0 & k \end{bmatrix}$$

where `k` is the only coefficient.

`anisotropic`

$$\mathbf{k} = \begin{bmatrix} k1 & 0 & 0 \\ 0 & k2 & 0 \\ 0 & 0 & k3 \end{bmatrix}$$

where the coefficients `k1`, `k2`, and `k3` are to be entered.

<CRITERION>

<CRITERION>

Description:
The criterion object is used for specifying the calculation of an equivalent stress to be used in plasticity and viscoplasticity behavior models (for each potential in a `gen_evp` material). The criterion may also be used for determining the flow direction and in hardening evolution models depending on the application.

Syntax:
The syntax to specify a criterion object will consist of giving the keyword for a particular criterion desired, followed by a list of appropriate coefficients which are dependent on the model chosen. The possible criterion types are:

CODE	DESCRIPTION
mises	classical von Mises criterion
2M1C	criterion 2M1C (only for potential `mises_2m1c`)
hill	Hill criterion
ratio	classical criterion useful as viscoplastic overstress function
karafillis_boyce	Karafillis Boyce criterion
full_hill	Hill criterion
tensile_mises	acts as von Mises criterion
nouailhas	macroscopic model developed by ONERA
modified_nouailhas	modified nouailhas model
linear_drucker_prager	non-associated drucker-prager criterion
anisotropic	classical energy equivalent form due to von Mises
cast_iron	criterion which provides asymmetric tension/compression
bron	modes anisotropic behavior in the criterion and flow direction
unsym	non-symmetric deviatoric / hydrostatic criterion
tresca	Tresca criterion

Some expressions which will be used are:

$$J_2(\hat{\boldsymbol{\sigma}}) = \sqrt{\frac{3}{2}\hat{\mathbf{s}} : \hat{\mathbf{s}}} \qquad s_{ij} = \sigma_{ij} - \frac{1}{3}\ \sigma_{ii}\delta_{ij}$$

where $\hat{\boldsymbol{\sigma}}$ is the effective stress which may be displaced by a kinematic back stress:

$$\hat{\boldsymbol{\sigma}} = \boldsymbol{\sigma} - \sum \mathbf{X}$$

The true form of this stress will be determined by the potential.

Stored Variables:
Criterion objects are not allowed to have any variables.

<CRITERION>

<CRITERION> anisotropic

Description:
This criterion is the classical energy equivalent form due to von Mises. Here the effective stress is calculated based on the J_2 stress invariant:

$$f_{cr} = \sqrt{\tfrac{3}{2}(\mathbf{s} - \mathbf{X}) : \mathbf{M} : (\mathbf{s} - \mathbf{X})} - R$$

where $\mathbf{s}$ is the deviatoric component of stress.

> **<cmd>** `anisotropic` *matrix-type*
> *coefficients*

The input *matrix-type* indicates one of the `COEFFICIENT_MATRIX` type keywords, and the coefficients will depend on the matrix chosen (e.g. `diagonal`, `orthotropic`, etc).

Example:
brief example using the anisotropic criterion is:

```
*criterion anisotropic orthotropic
   c11 .44667    c22 .58     c33  .666
   c44 0.        c55 1.7     c66  0.
   c12 -.18      c23 -.4     c31 -.26667
```

The `*criterion` command indicates the application of the created criterion object in the higher-level, so can generally be different depending on the application.

<CRITERION>

<CRITERION> bron

Description:

The Bron criterion allows modeling of anisotropic behavior in the criterion and flow directions.

The proposed yield function is defined by an equivalent stress:

$$\bar{\sigma} = \left(\alpha(\bar{\sigma}^1)^a + (1 - \alpha)(\bar{\sigma}^2)^a \right)^{1/a}$$

$$\bar{\sigma}^k = \left(\psi^k \right)^{1/b^k}$$

$$\psi^1 = \frac{1}{2} \left(\left| S_2^1 - S_3^1 \right|^{b^1} + \left| S_3^1 - S_1^1 \right|^{b^1} + \left| S_1^1 - S_2^1 \right|^{b^1} \right)$$

$$\psi^2 = \frac{3^{b^2}}{2^{b^2} + 2} \left(\left| S_1^2 \right|^{b^2} + \left| S_2^2 \right|^{b^2} + \left| S_3^2 \right|^{b^2} \right)$$

where $S_{i=1-3}^k$ are the principal values of a modified stress deviator $\underset{\sim}{\mathbf{s}}^k$ defined as follows:

$$\underset{\sim}{\mathbf{s}}^k = \underset{\sim}{\mathbf{L}}^k : \underset{\sim}{\sigma}$$

$$\underset{\approx}{\mathbf{L}}^k = \begin{pmatrix} (c_2^k + c_3^k)/3 & -c_3^k/3 & -c_2^k/3 & 0 & 0 & 0 \\ -c_3^k/3 & (c_3^k + c_1^k)/3 & -c_1^k/3 & 0 & 0 & 0 \\ -c_2^k/3 & -c_1^k/3 & (c_1^k + c_2^k)/3 & 0 & 0 & 0 \\ 0 & 0 & 0 & c_4^k & 0 & 0 \\ 0 & 0 & 0 & 0 & c_5^k & 0 \\ 0 & 0 & 0 & 0 & 0 & c_6^k \end{pmatrix}$$

a, b^1, b^2 and α are four material parameters that influence the shape of the yield surface but not its anisotropy which is only controlled by $c_{i=1-6}^{k=1-2}$. Thereby, the yield function has 16 parameters. To ensure convexity and derivability the following conditions are required: $a \geq 1$ and $b^k \geq 2$. No restriction applies to the c_i^k coefficients; in particular they can be negative. The particular case where $\underset{\sim}{\mathbf{L}}^1 = \underset{\sim}{\mathbf{L}}^2$ and $a = b^1 = b^2$ corresponds to the yield function of Karafillis and Boyce (1993) and the case where $\alpha = 1$ corresponds to the yield function of Barlat et al. (1991). Finally, when $\alpha = 1$ and $c_i^1 = 1$, it amounts to von Mises yield function if $b^1 = 2$ or 4 and to Tresca yield function if $b^1 = 1$ or $+\infty$. If $c_i^k = 1$, the resulting yield function is isotropic as it only depends on the eigenvalues of $\underset{\sim}{\sigma}$.

Example:

```
**porous_potential
  *porous_criterion modified_rousselier ...
  *isotropic function ...
  *flow plasticity
  *shear_anisotropy bron
    a 2.2 alpha 0.60
    b1 10.3
    c11 0.58 c12 1.35 c13 1.14 c14 1.23 c15 1.35 c16 1.57
    b2 13.1
    c21 2.07 c22 0.20 c23 0.33 c24 0.85 c25 1.31 c26 0.59
```

<CRITERION>

<CRITERION> cast_iron

Description:
This criterion provides assymetric tension/compression behavior which is suggested for cast iron modeling [Hjel94,Jose95]. In general this model would be used with behavior `gen_evp` potential `gen_evp2` and includes one or more `non_symmetric` kinematic hardening terms (and possibly others as well).

You can have either isotropic hardening scaling both the compressive and tensile behavior (with a given ratio relating them), or use isotropic hardening in only the tensile, or only the compressive with extra coefficients given for the non-hardening one. Probably the calling application requires that an R be given, so defining both Rt and Rc is not allowed.

R_c	$= \texttt{ratio } R$	$R_t = R$	if `ratio` is entered
R_c	$= \texttt{Rc}$	$R_t = R$	if `Rc` is entered
R_c	$= R$	$R_t = \texttt{Rt}$	if `Rt` is entered

The different tension and compression yield values R_c and R_t are applied to two distinct different yield functions as follows.

$$F_1 = \left[\tfrac{3}{2}\mathbf{s} : \mathbf{s} + \mathrm{Tr}(\boldsymbol{\sigma})(R_c - R_t)\right]^{1/2} - (R_c R_t)^{1/2}$$
$$F_2 = \left[\tfrac{3}{2}\mathbf{s} : \mathbf{s}\right]^{1/2} - R_c$$

The transition from the tension yield F_1 to the compression yield F_2 is determined if the trace of the effective stress $\boldsymbol{\sigma} - \sum \mathbf{X}$ is less than $-R_c$. See the section for the `non_symmetric` direct kinematic model on page 13.40 for a demonstration of the model's effect.

Syntax:
The basic input syntax here is:

```
 *criterion cast_iron
[  ratio  value ]
[  Rc     value ]
[  Rt     value ]
[  associated 0 | 1 ]
```

Only one choice of `ratio` `Rc` or `Rt` may be given as discribed above. If the `associated` is set to 1, the F_1 yield function will be used all the time. The default is associated behavior.

Example:

```
 *criterion cast_iron
   ratio 3.
   associated 1
```

<CRITERION>

<CRITERION> hill

Description:

The Hill criterion allows modeling of anisotropic behavior in the criterion and flow directions.

$$f_{cr} = \left[\frac{3}{2} \hat{\boldsymbol{\sigma}} : \mathbf{M}_{hill} : \hat{\boldsymbol{\sigma}} \right]^{1/2} - R$$

where $\mathbf{M}_{hill}$ is a diagonal matrix of independent coefficients. These coefficients are named `hill1` ... `hillN` with N being 4 for two dimensional problems, and 6 for three dimensional. There is no problem giving the complete 6 coefficients in a 2D problem however.

Example:

```
**potential gen_evp ev
  *flow norton
   n   4.0
   K   500.
  *criterion hill
   hill1 1.
   hill2 2.
   hill3 3.
   hill4 1.2
   hill5 1.7
   hill6 0.8
...
```

<CRITERION>

<CRITERION> karafillis_boyce

Description:
Also known as the K-B criterion, the karafillis-boyce criterion was developed in 1993 at MIT. This criterion is constructed by mixing two yield functions ϕ_1 and ϕ_2. As shown in the equations below ϕ_1 represents a yield locus located between the Von Mises yield locus and the Tresca yield locus and ϕ_2 varies from von Mises to a theoretical upper bound as m changes from 2 to ∞.

$$\phi = (1 - c)\,\phi_1 + c\phi_2 = 2Y^m$$

where

$$\phi_1 \quad = |S_1 - S_2|^m + |S_2 - S_3|^m + |S_3 - S_1|^m$$
$$\phi_2 \quad = \frac{3^m}{2^m - 1 + 1}\left(|S_1|^m + |S_2|^m + |S_3|^m\right)$$

and S_i are the principal values of the isotropic plasticity equivalent(IPE) stress tensor as defined below, Y is the average yield stress in uniaxial tension, and L is a fourth order tensorial operator which introduces material anisotropy.

$$\mathbf{S} = \mathbf{L}\,(\boldsymbol{\sigma} - \mathbf{B})$$

Syntax:
The basic input sytax here is:

```
*criterion karafillis_boyce
```
coefficients c1, c2, c3 c4, c5, c6.

Example:

```
*criterion karafillis_boyce
    m  2.0
    c  0.0
    c1 1.0
    c2 1.0
    c3 1.0
    c4 1.0
    c5 1.0
    c6 1.0
```

<CRITERION>

<CRITERION> linear_drucker_prager

Description:
This criterion is a non-associated criterion (flow direction is not the same as the normal to the yield surface $\frac{\partial f}{\partial \boldsymbol{\sigma}}$. It is commonly used for soils and plastics.

β friction angle (general coef)

ψ dilatation angle (general coef)

K ratio of triaxial yield in tension to triaxial yield in compression. $0.778 \leq K \leq 1$

$$
\begin{aligned}
\mathbf{S} \quad &= \mathbf{U} : \boldsymbol{\sigma} = \boldsymbol{\sigma} + p\mathbf{1} \\
p \quad &= -\tfrac{1}{3}\mathbf{1} : \boldsymbol{\sigma} \\
q \quad &= \left[\tfrac{3}{2}\mathbf{S} : \mathbf{S}\right]^{1/2} \\
r^3 \quad &= \left[\tfrac{9}{2}\mathbf{S} \cdot \mathbf{S} : \mathbf{S}\right]
\end{aligned}
\tag{3}
$$

$$
t \quad = \frac{q}{2}\left[1 + \frac{1}{K} - \left(1 - \frac{1}{K}\right)\frac{r^3}{q^3}\right]
$$

$$
f \quad = t - p\tan\beta - d
$$

$$
\begin{aligned}
d \quad &= \left(1 - \tfrac{1}{3}\tan\beta\right)\sigma_c && \sigma_c \text{ is the compressive yield} \\
d \quad &= \left(1 + \tfrac{1}{3}\tan\beta\right)\sigma_t && \sigma_t \text{ is the tensile yield} \\
d \quad &= d \equiv \frac{\sqrt{3}}{2}\tau(1 + K^{-1}) && \tau = \text{shear yield (cohesion)}
\end{aligned}
\tag{4}
$$

$$
g \quad = t - p\tan\psi
$$

$$
\mathbf{n} \quad = \frac{1}{c}\frac{\partial g}{\partial \boldsymbol{\sigma}}
$$

$$
\begin{aligned}
c \quad &= 1 - \tfrac{1}{3}\tan\psi && \text{defined in compression yield} \\
c \quad &= \frac{1}{K}\left(1 + \tfrac{1}{3}\tan\psi\right) && \text{defined in tension yield} \\
c \quad &= \left[\frac{5}{2} + \frac{5}{2K^2} - \frac{4}{K}\right]^{1/2} && \text{defined in pure shear (cohesion)}
\end{aligned}
$$

<CRITERION>

$$(5)$$

Note:

Since this criterion is not associated, it should only be used with behaviors and criterion which accept a different criterion function from normal definition.

Syntax:

The criterion takes a few options and parameters. The following assumes that the criterion is selected with a **criterion command as in gen_evp behaviors.

```
    **criterion linear_drucker_prager
     friction_angle   COEFFICIENT
     dilatation_angle COEFFICIENT
     K                COEFFICIENT
   [ use_sigma_c ]
   [ use_sigma_t ]
   [ use_cohesion ]
```

Example:

```
 **criterion linear_drucker_prager
  friction_angle 20.0
  dilatation_angle 20.0
  K        .9
```

<CRITERION>

<CRITERION> mises

Description:
This criterion is the classical energy equivalent form due to von Mises. Here the effective stress is calculated based on the J_2 stress invariant:

$$f_{cr} = \left[\frac{3}{2}\hat{\boldsymbol{\sigma}} : \hat{\boldsymbol{\sigma}}\right]^{0.5} - R$$

$$\mathbf{n} = \frac{3}{2}\frac{\hat{\boldsymbol{\sigma}}}{f_{cr}}$$

Example:

```
**potential gen_evp ev
  *flow plasticity
  *criterion mises
  *isotropic constant R0 300.
```

<CRITERION>

<CRITERION> modified_nouailhas

Description:

This criterion modifies the `nouailhas` model above by basing the calculation of the I's on the actual tensors $\boldsymbol{\sigma} - \mathbf{X}$ in place of the deviator, and includes an extra term:

$$f_{cr} = \left\{ \left(\left[\tfrac{3}{2}(I_1 + 2a_2 I_2 + 2a_4 I_4) \right]^2 + 3a_8 I_8 \right)^3 - (a_6 I_6)^4 \right\}^{1/12} - R$$

$I_1 = S_{11}^2 + S_{22}^2 + S_{33}^2$

$I_2 = S_{11} S_{22} + S_{22} S_{33} + S_{33} S_{11};$

$I_4 = S_{12}^2 + S_{23}^2 + S_{31}^2$

$I_6 = S_{12} * S_{23} * S_{31}$

$I_8 = S_{12}^4 + S_{23}^4 + S_{31}^4$

with

$$\mathbf{S} = \boldsymbol{\sigma} - \mathbf{X}$$

This criterion is fully implemented, such that it will work with any normal `gen_evp` or `reduced_plastic` potential, with any otherwise valid integration. In 2D, the 23 and 31 terms are taken as zero.

<CRITERION>

<CRITERION> nouailhas

Description:
This criterion is a macroscopic model developed by ONERA for simulating anisotropic deformation of single crystals. The model does not accurately represent the individual slip system deformations, or their interactions, but could be useful for efficiently modeling the basic anisotropic behavior of a single crystal.

The criterion is written:

$$f_{cr} = \left\{ \left(\left[\tfrac{3}{2}(I'_1 + 2a_4 I'_4) \right]^2 + 3a_8 I'_8 \right)^3 - (a_6 I'_6)^4 \right\}^{1/12} - R$$

$$I_1 = S_{11}^2 + S_{22}^2 + S_{33}^2$$

$$I_2 = S_{11}S_{22} + S_{22}S_{33} + S_{33}S_{11};$$

$$I_4 = S_{12}^2 + S_{23}^2 + S_{31}^2$$

$$I_8 = S_{12}^4 + S_{23}^4 + S_{31}^4$$

with

$$\mathbf{S} = \boldsymbol{\sigma}' - \mathbf{X}'$$

The criterion is associated:

$$\mathbf{n} = \frac{\partial f}{\partial I_1}\frac{\partial I_1}{\partial \boldsymbol{\sigma}} + \frac{\partial f}{\partial I_2}\frac{\partial I_2}{\partial \boldsymbol{\sigma}} + \frac{\partial f}{\partial I_4}\frac{\partial I_4}{\partial \boldsymbol{\sigma}} + \frac{\partial f}{\partial I_8}\frac{\partial I_8}{\partial \boldsymbol{\sigma}}$$

This criterion is fully implemented, such that it will work with any normal `gen_evp` or `reduced_plastic` potential, with any otherwise valid integration. In 2D, the 23 and 31 terms are taken as zero.

<CRITERION>

<CRITERION> ratio

Description:
This is a classical type criterion which may be useful for some users seeking compatibility with other programs. Its usefulness is as a viscoplastic overstress function (i.e. when $f > 0$).

$$f_{cr} = \frac{J(\hat{\boldsymbol{\sigma}})}{R} - L$$

Note that R is a radius measure passed in by the controlling behavior or potential object, and would normally be an isotropic hardening function. The effective stress $\hat{\boldsymbol{\sigma}}$ is likewise determined by the behavior and can include back stress influences, etc.

Syntax:
The model accepts a single optional coefficient for L (named L) in order to allow the user the option of having simply a ratio of f over R, which could be used to apply the isotropic hardening law as a viscosity hardening. The default value of L is 1, and the user should note that only values of 1 and 0 make sense.

Example:
The following example is from `rate_crit02.inp` in `test/Volume_test/INP`.

```
  ***behavior gen_evp
  **elasticity isotropic
       young 2.e9
       poisson 0.4
  **potential gen_evp ev
     *criterion ratio
       L    1.0
     *flow norton
       A  1000.
       n  2.
     *isotropic by_point
       sigeq  evcum
       60.e6  0.
       1.e8   2.
       1.e8   200.
  ***return
```

`<CRITERION> tensile_mises`

Description:
This is a criterion which acts as a von Mises yield if the trace of the effective stress (e.g. $\boldsymbol{\sigma} - \sum \mathbf{X}_i$) is greater than zero. If it is less than zero, the criterion will never yield.

$$
\begin{aligned}
f_{cr} &= \left[\frac{3}{2} \hat{\boldsymbol{\sigma}} : \hat{\boldsymbol{\sigma}} \right]^{0.5} - R & Tr(\boldsymbol{\sigma}) \geq 0 \\
f_{cr} &= 0 & otherwise
\end{aligned}
$$

$$(6)$$

`<CRITERION> tresca`

Description:
The plasticity threshold in Tresca criterion is linked to the maximum shear stress and is given by:

$$\frac{1}{2} \max_{i \neq j} \left(|\sigma_i - \sigma_j| \right)$$

The complete equation of the criterion can be written as:

$$f = \max_{i \neq j} \left(|\sigma_i - \sigma_j| \right) - \sigma_s = 0$$

<CRITERION>

<CRITERION> unsym

Description:
This criterion models the equivalent stress and deformation with deviatoric and hydrostatic terms. The criterion is written:

$$f_{cr} = (1 - a)\sigma_{eq} + a\,\texttt{Tr}(\boldsymbol{\sigma}) - R$$

This criterion accepts a single coefficient `a` which must be input on a separate line from the `unsym` token. This criterion is also non-associated where the flow normal is written:

$$\mathbf{n} = \frac{3}{2}\frac{\boldsymbol{\sigma}' - \mathbf{X}}{J_2(\boldsymbol{\sigma} - \mathbf{X})}$$

with the $\mathbf{X}$ term being the summation of back stresses. Often this criterion is used in conjunction with the `ziegler` kinematic hardening options [Croi92], but this is not necessarily so.

<CRITERION> 2M1C

Description:

For this case, the criterion is calculated in two parts using the following form:

$$f_{cr} = \sqrt{f_1^2 + f_2^2} - R \qquad f_i = J_2(A_i\boldsymbol{\sigma} - \mathbf{X}_i)$$

The coefficients `ga1` and `ga2` exist in order to define the localization parameters A_i.

<CRYSTAL_KINEMATIC>

<CRYSTAL_KINEMATIC>

Description:
Because the crystal potential models takes into account the strains on the individual slip planes, kinematic hardening represents a linear measure of a slip offset distance X_i, or backstress, on the slip line. As described in the `<POTENTIAL> crystal` section (see page 13.98), the yield criterion on each slip plane i is of the form $|\tau_i - \sum_j X_i^j| - r_i$, where τ_i is the resolved shear stress on slip plane i and r_i is the sum of all isotropic hardenings on that slip plane.

The internal variables α_i, to which the backstresses are associated, are thus *scalar* and distinct from the *tensorial* kinematic hardening laws in the macroscopic potentials. They are related to the backstresses X_i through $X_i = \texttt{x0} + \texttt{C}\alpha_i$ with `x0` and `C` parameters having the dimensions of a stress. Trick: a large *negative* offset `x0` might be used to model unidirectional slip, provided that the same *positive* offset is added to the corresponding isotropic hardening.

These hardening laws will apply uniquely for the monocrystal potentials. Permissible crystalline kinematic types are with their additional parameters are

`linear`	$\dot{\alpha}_i = \dot{\gamma}$
`nonlinear`	$\dot{\alpha}_i = \dot{\gamma} - \texttt{D} X_i \left\|\dot{\gamma}\right\| / \texttt{C}$
`nonlinear_phi`	$\dot{\alpha}_i = \dot{\gamma}\phi(v_i) - \texttt{D}\left(X_i - \texttt{Xbar}\right)\left\|\dot{\gamma}\right\|/\texttt{C}$ with $\phi(v_i) = (1 - \texttt{phi}) + \texttt{phi}\ e^{-\texttt{delta}\ v_i}$

<CRYSTAL_ORIENTATION>

<CRYSTAL_ORIENTATION>

Description:

This class is used to load in particular crystal slip systems into `gen_evp` crystal potentials (see page 13.98), or in seperate crystal behaviors. The crystal orientation will define the number of slip systems in the model, as well as the number of independent interaction parameters between these slip systems.

The default orientations are as follows. For cubic crystals the (1 0 0)-axis is oriented horizontally to the right (along the zebulon x-axis), (0 1 0) vertically upwards (along the Zebulon y-axis) and (0 0 1) out of the paper towards the reader (along the Zebulon z-axis). For hexagonal crystals, the directions in the basal plane are depicted in the following figure (after [Tome and Kocks 1985]), and the c-axis coincides with the Z-set z-axis.

$$\beta = [\bar{1}2\bar{1}0] \qquad y = [01\bar{1}0]$$

$$\alpha = [2\bar{1}\bar{1}0] \qquad x = [2\bar{1}\bar{1}0]$$

$$\gamma = [\bar{1}\bar{1}20]$$
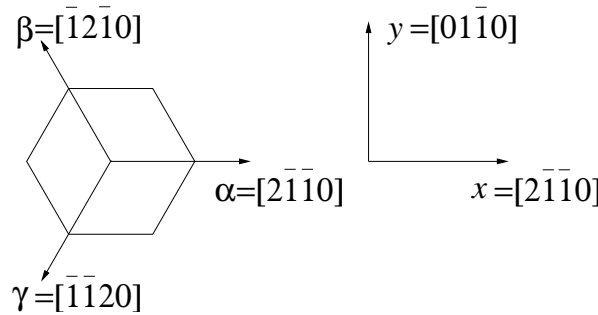
The crystal orientation will provide the localization tensors for the different slip systems i in a crystal:

$$\tau_i = \mathbf{m}_i : \boldsymbol{\sigma}$$

with τ_i the resolved shear stress on slip system i and $\boldsymbol{\sigma}$ the 'macroscopic' stress tensor. For each slip system i in the particular crystal set, the second order Schmid tensor $\mathbf{m}_i$ is defined as follows:

$$\mathbf{m}_i = \frac{1}{2} \left[\vec{n}_i \otimes \vec{\ell}_i \right],$$

with $\vec{n}_i$ the normal of slip plane i, and $\vec{\ell}_i$ the corresponding slip direction.

Syntax:

```
<creating-command> type
[ *interaction h-coefs ]
[ *c_over_a ]   c-a value
```

In absence of the `*interaction` command, only self-hardening is taken into account (i.e. `h1=1.` and the other coefficients are `0.`). For some hexagonal crystals the ratio of the length of the c-axis to the length of the a-axis is needed.

... *continued*

<CRYSTAL_ORIENTATION>

The following crystal systems are available:

cubic This orientation is for the 6 FCC cubic systems with up to 3 hardening coefficients.

```
( 0 0 1)[-1 1 0 ]
( 0 0 1)[ 1 1 0 ]
( 1 0 0)[ 0 1 1 ]
( 1 0 0)[ 0-1 1 ]
( 0 1 0)[-1 0 1 ]
( 0 1 0)[ 1 0 1 ]
```

octahedral This type of crystal is used for the 12 FCC octahedral slip systems, with up to 6 hardening coefficients.

```
( 1  1  1 )[-1  0  1 ]
( 1  1  1 )[ 0 -1  1 ]
( 1  1  1 )[-1  1  0 ]
( 1 -1  1 )[-1  0  1 ]
( 1 -1  1 )[ 0  1  1 ]
( 1 -1  1 )[ 1  1  0 ]
(-1  1  1 )[ 0 -1  1 ]
(-1  1  1 )[ 1  1  0 ]
(-1  1  1 )[ 1  0  1 ]
( 1  1 -1 )[-1  1  0 ]
( 1  1 -1 )[ 1  0  1 ]
( 1  1 -1 )[ 0  1  1 ]
```

basal 3 HCP basal slip systems with 2 hardening coefficients.

```
( 1 -2  1  0 )[ 0  0  0  1 ]
( 2 -1 -1  0 )[ 0  0  0  1 ]
( 1  1 -2  0 )[ 0  0  0  1 ]
```

prismatic 3 HCP second-order prismatic systems with 2 hardening coefficients.

```
( 1  0 -1  0 )[ 1 -2  1  0 ]
( 0  1 -1  0 )[ 2 -1 -1  0 ]
(-1  1  0  0 )[ 1  1 -2  0 ]
```

pyramidal0 6 pyramidal systems - requires **c_over_a** to be entered.

```
( 1  0 -1  1 )[ 1 -2  1  0 ]
( 0  1 -1  1 )[ 2 -1 -1  0 ]
(-1  1  0  1 )[ 1  1 -2  0 ]
(-1  0  1  1 )[ 1 -2  1  0 ]
( 0 -1  1  1 )[ 2 -1 -1  0 ]
( 1 -1  0  1 )[ 1  1 -2  0 ]
```

. . . continued

<CRYSTAL_ORIENTATION>

pyramidal1   12 additional pyramidal systems - requires **c_over_a** to be entered.

```
( 1   0 -1   1 )[ 2 -1 -1 -3 ]
( 1   0 -1   1 )[ 1   1 -2 -3 ]
( 0   1 -1   1 )[ 1   1 -2 -3 ]
( 0   1 -1   1 )[-1   2 -1 -3 ]
(-1   1   0   1 )[-1   2 -1 -3 ]
(-1   1   0   1 )[-2   1   1 -3 ]
(-1   0   1   1 )[-2   1   1 -3 ]
(-1   0   1   1 )[-1 -1   2 -3 ]
( 0 -1   1   1 )[-1 -1   2 -3 ]
( 0 -1   1   1 )[ 1 -2   1 -3 ]
( 1 -1   0   1 )[ 1 -2   1 -3 ]
( 1 -1   0   1 )[ 2 -1 -1 -3 ]
```

pyramidalPi1

```
( 1   0 -1   1 )[ 1 -2   1   0 ]
( 0   1 -1   1 )[ 2 -1 -1   0 ]
(-1   1   0   1 )[ 1   1 -2   0 ]
(-1   0   1   1 )[ 1 -2   1   0 ]
( 0 -1   1   1 )[ 2 -1 -1   0 ]
( 1 -1   0   1 )[ 1   1 -2   0 ]
```

pyramidalPi2

```
(-1   2 -1   2 )[-1   2 -1 -3 ]
( 2 -1 -1   2 )[ 2 -1 -1 -3 ]
( 1   1 -2   2 )[ 1   1 -2 -3 ]
( 1 -2   1   2 )[ 1 -2   1 -3 ]
(-2   1   1   2 )[-2   1   1 -3 ]
(-1 -1   2   2 )[-1 -1   2 -3 ]
```

twinning   6 twinning systems in hexagonal crystals - requires **c_over_a** to be entered.

```
( 1   0 -1 -1 )[ 1   0 -1   2 ]
( 0   1 -1 -1 )[ 0   1 -1   2 ]
(-1   1   0 -1 )[-1   1   0   2 ]
(-1   0   1 -1 )[-1   0   1   2 ]
( 0 -1   1 -1 )[ 0 -1   1   2 ]
( 1 -1   0 -1 )[ 1 -1   0   2 ]
```

. . . continued

<CRYSTAL_ORIENTATION>

bcc112   12 additional slip systems for bcc crystals. These also apply to Shockley partial
         dislocations in fcc crystals.

```
( 2   1   1 )[-1   1   1 ]
( 1   2   1 )[ 1 -1   1 ]
( 1   1   2 )[ 1   1 -1 ]
(-2   1   1 )[ 1   1   1 ]
( 1 -2   1 )[ 1   1   1 ]
( 1   1 -2 )[ 1   1   1 ]
( 2 -1   1 )[ 1   1 -1 ]
( 1   2 -1 )[-1   1   1 ]
(-1   1   2 )[ 1 -1   1 ]
( 2   1 -1 )[ 1 -1   1 ]
(-1   2   1 )[ 1   1 -1 ]
(-1   2 -1 )[-1   1   1 ]
```

climb_cfc   4 climb directions on octahedral planes:

```
( 1   1   1 )[ 1   1   1 ]
( 1 -1   1 )[ 1 -1   1 ]
(-1   1   1 )[-1   1   1 ]
( 1   1 -1 )[ 1   1 -1 ]
```

climb_cubic   3 climb directions on cubic planes:

```
( 1   0   0 )[ 1   0   0 ]
( 0   1   0 )[ 0   1   0 ]
( 0   0   1 )[ 0   0   1 ]
```

climb_cubic1   The first of the cubic climb directions:

```
( 1   0   0 )[ 1   0   0 ]
```

climb_cubic2   The second of the cubic climb directions:

```
( 0   1   0 )[ 0   1   0 ]
```

climb_cubic3   The third of the cubic climb directions:

```
( 0   0   1 )[ 0   0   1 ]
```

plane   Enter in a single slip system. The first system in octahedral could be entered in as:

```
**potential plane ( 1.   1.   1. ) (-1. 0.   1. )
```

<DAMAGE>

<DAMAGE>

Description:
This object class permits addition of damage mechanisms to a behavior assembly of type `gen_evp`. These models are of the type "continuum damage mechanics" (CDM), and thus provide interaction through alteration of the elasticity modulus with damage and calculation of plasticity with the use of an effective stress.

Damage models may be used in the `gen_evp` behavior with and without inelastic deformation potentials. The coupling with inelastic deformations and their hardening variables is discussed below.

Syntax:
The damage mechanisms are added through the use of a token `**damage` input *after* the `**elasticity` declaration. The general syntax is:

```
    **damage  dama_type
[   *elastic ]
[   *plastic ]
[   *creep ]
[   *coupling type ]
```

There is a restriction currently that the `*damage` statement must come *after* the `*elasticity` statement in the behavior.

The number of coefficients for each option depends of course on on the particular damage model selected. The currently implemented types are summarized below:

CODE	DESCRIPTION
`*elastic`	elastic damage
`*anisotropic_elastic`	anisotropic elastic damage with scalar and tensorial variables
`*plastic`	plasticity damage which depends on the rate of inelastic deformation
`*creep`	time dependent damage
fatigue	*cyclic damage*

`*elastic`   The coefficients here are: `B0` et `alpha`. The damage is calculated directly at a given time as:

$$\bar{Y} = \frac{1}{2}\boldsymbol{\epsilon}_{el} : \mathbf{D}_{el} : \boldsymbol{\epsilon}_{el}$$

$$Y_{\max}^{t+\Delta t} = \max(\bar{Y}, Y_{max}^t)$$

$$d = \begin{array}{ll} \alpha\,(Y_{max}^{1/2} - Y_o^{1/2}) & Y_{max} > Y_o \\ 0 & Y_{max} \leq Y_o \end{array}$$

<DAMAGE>

*plastic This model integrates the damage as a function of the inelastic strain equivalent in the following manner:

$$\dot{d} = \dot{p}_i \, (Y/\texttt{S0})^{\texttt{s0}}$$

For the i-th component of inelastic deformation. Note that $\dot{p}$ is calculated as:

$$\dot{p}_i = \left[\tfrac{2}{3}\dot{\boldsymbol{\epsilon}}_i : deps_i \right]^{1/2}$$

*creep Classical viscoplastic damage using the Hayhurst stress function. The damage is calculated as:

$$\chi(\boldsymbol{\sigma}) = \alpha J_0 + \beta J_1 + (1 - \alpha - \beta) J_2$$

The rate of damage production will be calculated as:

$$\dot{d} = \left\langle \frac{\chi(\boldsymbol{\sigma})}{A} \right\rangle^r (1 - d)^{-k}$$

with J_0 the maximum principle stress, J_1 the trace of the stress tensor, and J_2 the second invariant of the deviator $(\tfrac{3}{2}\mathbf{s} : \mathbf{s})^{1/2}$.

<u>Coupling with plasticity</u>:
Applying simply the damage mechanisms to a `gen_evp` plasticity model will only couple the stress calculation in the potentials and modify the elastic modulus. For the hardening mechanisms to be coupled to the damage rate, several additional changes must be made to the syntax.

Addition of one or more plasticity potentials to a behavior with damage causes the following equations to be used for the inelastic strain rate:

$$\begin{aligned}
\tilde{\boldsymbol{\sigma}} &= \mathbf{D}_{el} : \boldsymbol{\epsilon}_{el} \\
\boldsymbol{\sigma} &= (1 - d)\tilde{\boldsymbol{\sigma}} \\
\dot{\boldsymbol{\epsilon}}_{\text{to}} &= \dot{\boldsymbol{\epsilon}}_{el} + (1 - d)^{-1}\dot{\lambda}\mathbf{n} \\
\dot{\mathbf{h}} &= \dot{\lambda}\mathbf{m} - \dot{\boldsymbol{\omega}}
\end{aligned}$$

The default situation interfacing damage to the potential only involves use of the effective stress in the place of the actual (weakened) stress. This leads to the following set of evolution equations:

$$\begin{aligned}
\text{f} &= f(\tilde{\boldsymbol{\sigma}}, \mathbf{H}, p) \\
\dot{\lambda} &= \dot{\lambda}(f, p) \\
\mathbf{n} &= \frac{\partial f}{\partial \boldsymbol{\sigma}} = \frac{\partial f}{\partial \tilde{\boldsymbol{\sigma}}}\frac{\partial \tilde{\boldsymbol{\sigma}}}{\partial \boldsymbol{\sigma}} \\
\mathbf{m} &= \frac{\partial \phi(\tilde{\boldsymbol{\sigma}}, \mathbf{H}, p)}{\partial \mathbf{H}}
\end{aligned}$$

from which it is noted that the hardening forces $\mathbf{H}$ are related to the internal (strain analogue) variables $\mathbf{h}$ by the same linear relationship:

$$\mathbf{H}_i = \mathbf{M}_{ij}\mathbf{h}_j$$

<DAMAGE>

Example:

```
***behavior gen_evp
 **elasticity isotropic
      young 260000.
      poisson 0.3
 **damage isotropic
  *creep
      alpha  0.75
      beta   0.0
      A      3000.
      r      5.3
      k      15.
  *coupling damage_hardening
 **potential gen_evp ev
  *var_coefs
  *flow alt_norton
      n      7.0
      K      2070.
      K2     1600.0
      K3     19.0
  *kinematic nonlinear
      C      inv_one_minus dv 15000.0
      D      300.0
  *kinematic nonlinear
      C      inv_one_minus dv 6000.0
      D      100.0
  *isotropic constant
      R0     130.
***return
```

<DIRECT_KINEMATIC>

<DIRECT_KINEMATIC>

Description:
This object defines a class of kinematic hardening (tensorial back stresses) which can have a more general state variable form, and possibly nonlinear relationship between the integrated strains and the associated stresses. In the `gen_evp` behavior framework, these models must be used with the following potentials only:

CODE	DESCRIPTION
gen_evp2	Generalized viscoplastic potential 13.104

The kinematic models all support static recovery, and possibly have more than a 1-1 relation between the integrated variable size and the kinematic back stress size (forcibly the active tensor size for given problem dimension).

Syntax:
The syntax consists of specifying the type of kinematic object, supplying an optional name on the same line, and giving the appropriate coefficient definitions on the following lines. This is summarized below where the keyword specifying a DIRECT_KINEMATIC object is assumed to be *kinematic:

> *kinematic *type* [*name*]
>   *coefficients*

Example:
A duplication of the classical Armstrong Frederick kinematic class is implemented for verification and testing purposes (Normally using the `nonlinear` KINEMATIC type is the model to choose). An example use of that class is:

```
*kinematic armstrong_frederick
   C    40000.
   D    500.
```

<DIRECT_KINEMATIC>

<DIRECT_KINEMATIC> asaro

Description:
This kinematic hardening model provides nonlinear modulus behavior forming a hysteresis loop with slight S shape. Normally this kinematic type would be combined with other linear and nonlinear hardenings to fine tune cyclic behavior.

$$\alpha_{\text{eq}} = \left[\tfrac{3}{2}\boldsymbol{\alpha} : \boldsymbol{\alpha}\right]^{1/2}$$

$$\mathbf{X}_{\text{i}} = \frac{C\ \tanh(D\,\alpha_{eq})}{D\,\alpha_{eq}}\boldsymbol{\alpha}_i$$

$$\dot{\boldsymbol{\alpha}}_{\text{i}} = \dot{\lambda}\mathbf{n}$$

Syntax:
The basic input syntax here is:

```
    *kinematic asaro  name
[  C        coef-value ]
[  D        coef-value ]
[  M        coef-value ]
[  m        coef-value ]
```

. . . continued

<DIRECT_KINEMATIC>

Example:

The following example shows the use of this kinematic model in combination with a number of other kinematic hardenings, with the separate terms plotted below.

```
***behavior gen_evp
 **elasticity isotropic
   young 69000.00
   poisson 0.3
 **potential gen_evp2 ev
  *store_all
  *criterion mises
  *isotropic nonlinear
    R0 340.0
    b  900.0
    Q -210.0
  *kinematic nonlinear 1_
    C  187500.
    D  1250.0
  *kinematic armstrong_frederick 2_
    C  11250.0
    D  150.0
  *kinematic linear    3_
    C  1000.0
  *kinematic asaro     4_
    C  56250.0
    D  750.0
***return
```

<DIRECT_KINEMATIC>
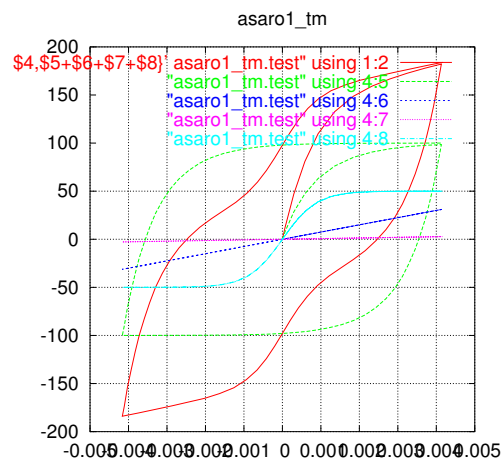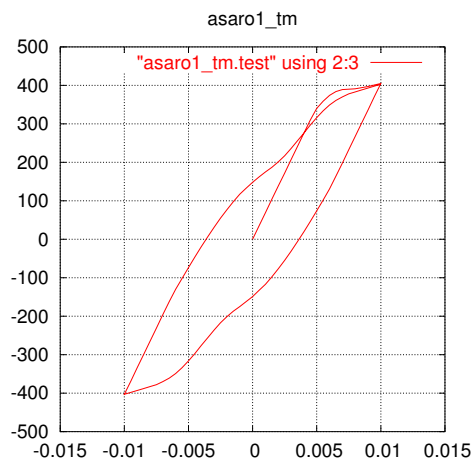
<DIRECT_KINEMATIC> non_symmetric

Description:
This kinematic hardening model provides asymmetric behavior between tension and compression as recommended for cast iron materials [Hjel94,Jose95].

This model takes the tensile coefficients for computing $\mathbf{X}_i$ if the trace of the actual stress $\mathbf{1} : \boldsymbol{\sigma}$ is greater than the `I1_trans` value. The evolution is therefore:

$$\dot{\boldsymbol{\alpha}}_i \quad = \dot{\lambda} \left[\mathbf{n} - \frac{3}{2} \frac{D^*}{C^*} \mathbf{X}_i \right] \qquad \text{if } \texttt{use\_alpha} \text{ is set}$$

$$\dot{\mathbf{X}}_i \quad = C^* \dot{\lambda} \left[\mathbf{n} - \frac{3}{2} \frac{D^*}{C^*} \mathbf{X}_i \right] \qquad \text{if } \texttt{use\_x} \text{ is set}$$

where the coefficients C^* and D^* are either C_t, D_t or C_c, D_c depending on the above check on the stress. Note that in the `use_x` case the evolution **is not** the complete derivative where the terms involving the change in C^* with temperature are not taken into account.

Syntax:
The basic input syntax here is:

```
   *kinematic non_symmetric
[  I1_trans coef-value ]
[  Ct      coef-value ]
[  Cc      coef-value ]
[  Dc      coef-value ]
[  Dc      coef-value ]
[  M       coef-value ]
[  m       coef-value ]
[  use_x | use_alpha]
```

Only one choice of `use_x` or `use_alpha` can be used (default is `use_x`). The default value of `I1_trans` is 0. The coefficients `M` and `m` are the standard Norton-like static recovery coefficients.

. . . continued

<DIRECT_KINEMATIC>

Example:

The following example shows the use of this kinematic model in combination with the `cast_iron` yield criterion.

```
***behavior gen_evp
 **elasticity isotropic
   young 126000.
   poisson 0.265
 **potential gen_evp2 ev
   *criterion cast_iron
     ratio 3.
     associated 1
   *kinematic non_symmetric  x1
       I1_trans 50.
       Ct 300000.0
       Dt    5000.0
       Cc  30000.0
       Dc     500.0
   *isotropic constant
       R0 100.0
***return
```

<ELASTICITY>

<ELASTICITY>
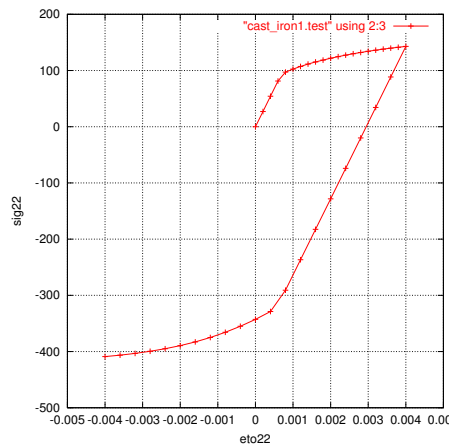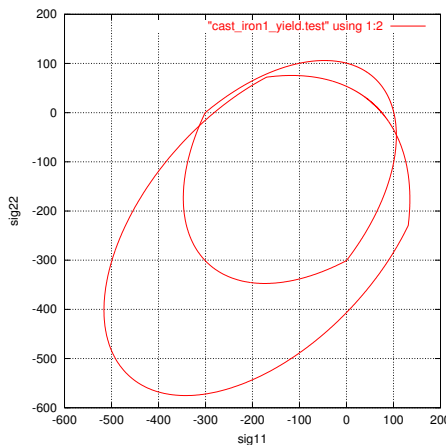
Description:
An `ELASTICITY` behavior object is actually just an alias for `COEFFICIENT_MATRIX` (see page 13.8). The class is frequently defined in the behavior descriptions however to further accentuate its task in the scheme of the constitutive relation. Virtually every location where this keyword is used, a hypoelastic relation is employed:

$$\boldsymbol{\sigma} = \mathbf{D}_{el} : \boldsymbol{\epsilon}_{el}$$

Noting however that the total internal strain $\boldsymbol{\epsilon}_{el}$ may be calculated in some manner which extends it from the normal limitations of hypoelasticity (e.g. the finite strain material transformations).

The matrix $\mathbf{D}_{el}$ is the elasticity matrix defined by the `ELASTICITY` class, and can take many forms, and vary according to any external parameter.

Description:

This object class defines the model for inelastic flow in plastic and viscoplastic models and potentials.

Syntax:

The syntax to specify a flow object will consist of giving the keyword for a particular flow desired, followed by a list of appropriate coefficients which are dependent on the model chosen. The flow type may be chosen among the following laws:

CODE	DESCRIPTION
norton	Norton power law
hyperbolic	hyperbolic sin function applied to power law of overstress
strain_hardening	Norton type viscoplastic rate with hardening
gsell	viscoplastic model for some polymers
modified_visco	viscoplastic rate using strain hardening or softening
sellars_tegart	Coupled with hardening to study variable strain rate
function	A function in terms of overstress and cumulated plastic strain
abq_strain_hardening	flow class available through ABAQUS
norton_exp	exponential (saturating) Norton law
double_norton	two term Norton law
flow_sum	summation of Norton terms
flow_sum_inv	summation of inverse Norton rates
inv_exp	viscoplastic according to $\dot{\epsilon} = A \exp\left((p - p_0)/\alpha\sigma^n\right)$
interface_control	interface reaction flow
plasticity	time independent plasticity
use_global_function	uses a function defined elsewhere
exponential_crystal	physically based exponential flow law esp. useful for crystal deformation

The default type of flow is `plasticity`.

norton This law corresponds to the classical Norton creep power law. The coefficients are chosen to normalize the stress term, and then apply the exponent:

$$\dot{\lambda} = < f/K >^n$$

with f positive. The coefficients K and n must be non-zero.

<FLOW>

norton_exp This flow provides a limit stress approximating creep at low stress levels and plasticity at high stresses:

$$\dot{\lambda} = < f/K >^n \exp(\alpha < f/K >^{n+1})$$

which uses the coefficient names: K, n, and alpha.

double_norton This model is a two term variation of the Norton law in order to model changes in flow mechanisms over a wide stress range:

$$\dot{\lambda} = < f/K >^{n_1} + < f/K_2 >^{n_2}$$

with the required coefficients K, n1, K2, n2.

plasticity This flow type indicates time-independent plasticity ($f = 0$). The use of **plasticity** may limit integration to implicit only in the case of some complex models. There are no coefficients.

inv_exp This law provides an exponential dependence on the inverse of the effective over-stress: $\dot{\lambda} = A \exp\left(-\frac{p+p_0}{\alpha\sigma^n}\right)$ with the coefficients n, A alpha, and p0, where p0 is optional (default 0).

interface_control This flow rule is expressed:

$$\dot{\lambda} = \frac{1}{d^2} \frac{k_1\sigma}{1 + \frac{k_2}{d\sigma^m}}$$

with the coefficients k1, k2, m, d. d represents a grain size.

flow_sum_inv This model is similar to the `flow_sum` rule, but sums the inverse of the different flow rules:

$$\dot{\lambda} = \left[\sum_i \frac{1}{\dot{\lambda}_i} \right]^{1/2}$$

where the $\dot{\lambda}_i$ terms are given by the various sub-laws (different than `sum_flow` and `flow_sum_inv`).

exponential_crystal This law is a physically based flow law for crystalline slip which can be used with the **crystal POTENTIAL** models (actually it can be used anywhere viscoplasticity is allowed).

$$\dot{\gamma} = \texttt{gamma0} \exp\left[-\texttt{F0\_RT} \left[1 - \left\langle \frac{f}{K} \right\rangle^{\texttt{n1}} \right]^{\texttt{n2}} \right]$$

Note that the terms for this equation may be composed of function coefficient types in the event that a functional form is desired. For example: `F0_RT function 6.8e4/(1.9868*temperature);`

strain_hardening This flow law is a Norton type viscoplastic rate with a hardening effect.

$$\dot{\lambda} = \left\langle \frac{f}{K} \right\rangle^n (v + v_0)^m$$

The flow law accepts coefficients K, n, m, and v_0. Because when $v = 0$ there will be no flow rate in the absence of v_0 (and therefore v will never become anything other than null), the coefficient should have a non-zero value (but possibly very small).

<FLOW>

<FLOW> function

Description:
This flow law is defined by a function which can be in terms of overstress f and cumulated plastic strain p.

Syntax:
The flow law will accept coefficients depending on the function. For example the above flow law will accept K, n, p as coefficients.

Example:
A function such as a Norton law combined with cumulative plastic strain could be of interest:

$$\dot{\lambda} = \left\langle \frac{f}{K} \right\rangle^n (1 - e^p)$$

This would result in the following syntax:

```
*flow function
  K 120.0
  n 5.0
  p 10.e-3
```

<FLOW>

<FLOW> gsell

Description:
This is a viscoplastic model appropriate for some polymer materials. It includes some hardening behavior using the cumulated viscoplastic multiplier v.

$$\dot{\lambda} = \left\langle \frac{f}{K \left(1 - e^{-wv}\right) e^{hv^n}} \right\rangle^{m_1}$$

Note that at $v = 0$ the term $1 - e^{-wv}$ in the denominator will become zero, setting the denominator to zero (infinite initial strain rate). To alleviate this numerical difficulty, the term is modified to be $1 - e^{-w(v+e_0)}$

Example:
A simple example of purely viscoplastic material follows. Because the yield radius R0 is zero, the material is always flowing. The use of elasticity in this case is also a pseudo-elasticity, attempting to model a purely viscous material in a displacement based FEA model. The higher the modulus, the more ϵ_{in} approaches $\epsilon_{to} - \epsilon_{th}$.

```
***behavior gen_evp
 **elasticity isotropic
      young 100000.
      poisson 0.48
 **potential gen_evp ev
  *isotropic constant
      R0 0.0
  *flow gsell
      e0   1.e-5
      K    40.0
      w    65.
      h    0.75
      n    1.75
      m    0.08
***return
```

<FLOW>

<FLOW> hyperbolic

Description:
For this law, the hyperbolic sin function is applied to the power law of overstress, and in turn taken to a second power. The flow is written:

$$\dot{\lambda} = \texttt{eps0}\left[\sinh < f/\texttt{K} >^{\texttt{n}}\right]^{\texttt{m}}$$

with f positive. The coefficient K must be non-zero, and the coefficients n and m default to one.

The flow law is fully implemented for Runge-Kutta or the standard theta method. It cannot presently be applied to the reduced integration.

Because the sinh can "blow up" with large values of f/K a cutoff limit on that ratio is applied. This can be user-adjusted by entering a real value for cutoff in the law's coefficient section. The default value is 10.0 which would result in an unrealistically high strain rate for this type of model.

Syntax:
The flow law accepts coefficients eps0, K, n, and m as outlined above.

Example:
A simple example follows:

```
*flow hyperbolic
    K    22.3
    m    1.44
    eps0 .202e-8
    cutoff 8.
```

<FLOW>

<FLOW> modified_visco

Description:
This flow law is a Norton type viscoplastic rate, using a strain hardening or softening viscocity term.

Let the following terms be defined:

$$d_1 = \left\langle \frac{f}{K} \right\rangle^n \qquad\qquad K = K_0 + Q(1 - e^{-bv})$$

With which the flow law is written:

$$\dot{\lambda} = d_1 \exp\left[\alpha d_1 \frac{f}{K}\right]$$

Syntax:
The flow law accepts coefficients K0, Q, b, n and alpha.

Note:
There is another version of this flow called **norton_hardening** which reduces to:

$$\dot{\lambda} = \left\langle \frac{f}{K_0 + K(1 - e^{-bv})} \right\rangle^n$$

<FLOW>

<FLOW> sellars_tegart

Description:

This is a flow rule given by C M Sellars and W J Tegart in 1969 as a proposed rate equation for hot forming conditions. The use of a hyperbolic sine function allows for increasing overstress at low strain rates, which is followed by essentially a saturation level of overstress. Another way of describing the model is viscous at low overstress levels followed by essentially rate independent behavior for high stresses. Normally this behavior would be combined with hardening (viscoplasticity) and not taken as a pure viscous creep law.

The rule is given as:

$$\dot{\lambda} = \epsilon_0 \left[\sinh \left\langle \frac{f}{\sigma_0} \right\rangle \right]^m$$

Note that the Z-mat formulation utilizes a ratio of the overstress by a normalizing flow stress σ_0. Once the overstress becomes of the order of the flow stress this law will make the transition to rate independence.

Many uses of this equation include explicitly the activation energy term to scale the flow viscosity according to thermally activated mechanisms. In Z-mat the activation term should be entered in using the coefficient mechanism (either as tables or functions) for the value of `de0`.

Syntax:

The flow law accepts coefficients `de0`, `m`, `sigma0`

Example:

An example input using the coefficient mechanism to add thermal activation is given below:

```
*flow sellars_tegart
  de0    function  0.202e-2*exp(-401.0/(8.3144e-3*(temperature+273.0)));
  sigma0 120.0
  m      1.44
```

`<FLOW>` sum

Description:

This law provides a summation of different flow rates $\dot{\lambda} = \sum_i \dot{\lambda}_i$ where the $\dot{\lambda}_i$ are the rates given by other flow objects (other than `sum_flow` or `flow_sum_inv`).

Syntax:

The syntax is the following:

```
*flow flow_sum
    <FLOW>
    <FLOW>
```

Similar kind of syntax applies to `flow_sum_inv` law also.

Example:

A simple example is given below which uses the Norton law as one of the flow rule.

```
***behavior gen_evp
**elasticity isotropic
    young 260000.
    poisson 0.3
**potential gen_evp ev
 *criterion mises
 *flow flow_sum
    norton
    K 140.0
    n  5.0
 *isotropic constant
    R0 130.0
```

<HYPERELASTIC_LAW>

<HYPERELASTIC_LAW>

Description:
This object class defines the model for hyperelasticity in hyperelastic, hyper_viscoelastic and hyperelastic viscoplastic models and potentials.

Syntax:
The syntax to specify a hyperelasticity object will consist of giving the keyword for a particular hyperelasticity model desired, followed by a list of appropriate coefficients which are dependent on the model chosen. The hyperelasticity type may be chosen among the following laws:

CODE	DESCRIPTION
st_venant_kirchhoff	St Venant-Kirchhoff hyperelastic material
modified_sv_kirchhoff	Modified St Venant-Kirchhoff hyperelastic model
ristinmaa	Wallin-Ristinmaa hyperelastic model
arruda_boyce	Arruda-Boyce hyperelastic model
mooney	Mooney hyperelastic model
ogden	Odgen hyperelastic model
van_der_waals	Van der Waals hyperelastic model
fung	Anisotropic hyperelastic model

The structure of the object is summarized below:

```
***behavior   [hyper_elastic] or [finite_strain_plasticity]
 **hyperelasticity <HYPERELASTIC_LAW>
 **model_coef
    ...
[ **pull_back]
```

Stored Variables:
The stored variables for this object include the Green-Lagrange total strain tensor, the Cauchy stress tensor, and the strain energy density W. As an auxiliary output variable, the Piola-Kirchhoff stress tensor:

$$\mathbf{S} = \frac{\partial W}{\partial \mathbf{E}}$$

is stored but not saved during the calculation. The post-processor prefixes used for these variables are the following:

prefix	size	description	default
eto	T-2	Green-Lagrange strain	yes
sig	T-2	Cauchy stress	yes
welas	S	strain energy density	yes

...continued

<HYPERELASTIC_LAW>

If the option **pull_back is given, the Piola-Kirchhoff stress tensor is requested as output[1].

Compatible elements:
This object class is programmed to be used with all versions of the total Lagrangian elements (element types starting with total_lagrangian) and the updated Lagrangian elements (element types starting with updated_lagrangian). The behavior must therefore be used in conjunction with a declaration of these elements in the .inp file (see ***mesh under ****calcul).

---

[1]Only for the ****simulate calculation definition.

<HYPERELASTICITY>

<HYPERELASTICITY> st_venant_kirchhoff

Description:

The St. Venant-Kirchhoff model is a simple hyperelastic model, which is defined by a strain energy W as

$$W(E) = \frac{\lambda}{2}(trace\ E)^2 + \mu E : E$$

where λ and μ are Lamé coefficients and E is the Green-Lagrange strain tensor. The second Piola-Kirchhoff stress tensor can be obtained as

$$S = \frac{dW}{dE} = \lambda(trace\ E)I + 2\mu E \quad or \quad S = C : E$$

where I is the identity tensor of order 2 and C is the elasticity tensor defined as

$$C_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$$

This model has some inconvenients, especially in compression loading conditions (fig. 1). Let's consider the following loading

$$\begin{pmatrix} F_{11} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

the value of Cauchy stress component σ_{11} tends to zero as F_{11} approaches 0 and it goes through a minimum at $F_{11} = \sqrt{1/3}$.

Syntax:

```
***behavior hyper_elastic
 **hyperelasticity st_venant_kirchhoff
  *elasticity isotropic
    young COEFFICIENT
    poisson COEFFICIENT
```

Example:
The following is a simple example of the hyperelastic Saint Venant-Kirchhoff model.

```
***behavior hyper_elastic
 **hyperelasticity st_venant_kirchhoff
  *elasticity isotropic
    mu              80000.
    lambda         121000.
***return
```

<HYPERELASTICITY>

<HYPERELASTICITY> modified_sv_kirchhoff

Description:

This hyperelastic model is a modified St Venant-Kirchhoff model [Hjel05], which is defined by the following strain energy W:

$$W(E) = \frac{\lambda}{2}(\log J)^2 + \mu\ tr(E^2)$$

where λ and μ are Lamé coefficients in the infinitesimal elasticity theory, E is the Green-Lagrange strain tensor and $J = det\ F$. The second Piola-Kirchhoff stress tensor can be obtained as

$$S = \frac{dW}{dE} = \lambda \log(J)C^{-1} + 2\mu E$$

where C is the right Cauchy-Green deformation tensor. This model overcomes the limits of St Venant-kirchhoff ones.
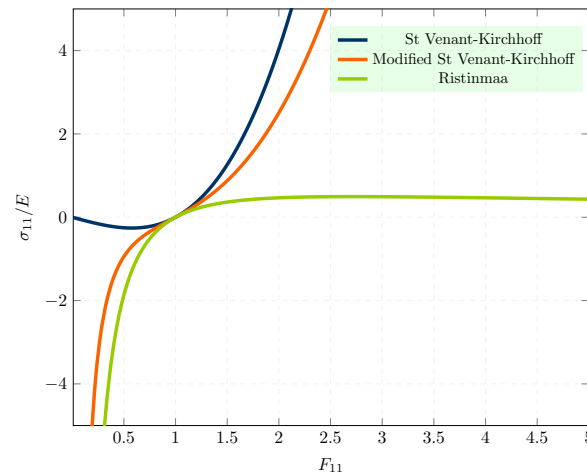
Figure 1: Some hyperelastic materials response under extension/compression

Syntax:

```
***behavior hyper_elastic
 **hyperelasticity modified_sv_kirchhoff
  *elasticity
    young COEFFICIENT
    poisson COEFFICIENT
```

Example:

The user can supply either (λ, μ) or (E, ν).

```
***behavior hyper_elastic
 **hyperelasticity modified_sv_kirchhoff
  *elasticity
    mu            80000.
    lambda        121000.
***return
```

<div align="center">

\<HYPERELASTICITY\> ristinmaa
</div>

Description:

This hyperelastic model is a modified St Venant-Kirchhoff model proposed by [wall05], which is defined by a strain energy W as

$$W(E) = \frac{K}{2}(\log J)^2 + \mu \ (\log U)^{dev} : (\log U)^{dev}$$

where the material parameters K and μ correspond in the limit of small strains to the bulk and the shear modulus, respectively, $(\log U)^{dev}$ is the deviatoric part of the logarithm of the Hencky strain tensor $U = C^{1/2}$ and $J = det\ F$. The second Piola-Kirchhoff stress tensor can be obtained as

$$S = \frac{dW}{dE} = \lambda \log(J) C^{-1} + 2\mu \log(U) C^{-1}$$

where C is the right Cauchy-Green deformation tensor.

Syntax:

```
***behavior hyper_elastic
 **hyperelasticity ristinmaa
  *elasticity
    young COEFFICIENT
    poisson COEFFICIENT
```

Example:

The following is a simple example of Ristinmaa model. The user can supply either (λ, μ) or (E, ν).

```
***behavior hyper_elastic
 **hyperelasticity ristinmaa
  *elasticity
    mu            80000.
    lambda        121000.
***return
```

<HYPERELASTICITY>

<HYPERELASTICITY> arruda_boyce

Description:

This physically-based model, proposed by Arruda and Boyce [Arru93], consists in a chain model with a distribution of chains upon eight directions corresponding to the vertices of a cube inscribed in a unit sphere. The implemented model includes an additional coefficient for compressibility treatment. The coefficients for the hyperelastic law are declared under **hyperelasticity arruda_boyce.

Hyperelastic behavior here defines the strain energy density with the following form:

$$W(I_1, I_3) = \quad \mathtt{nK}\theta[\tfrac{1}{2}(I_1 - 3) + \tfrac{1}{20N}(I_1^2 - 9)] + \tfrac{11}{1050N^2}(I_1^3 - 27)] + \tfrac{19}{7000N^3}(I_1^4 - 81)] + \\ \tfrac{519}{673750N^4}(I_1^5 - 243)] + \tfrac{\mathtt{K0}}{2}[(I_3^2 - 1)/2 - \mathtt{log}(I_3)] \tag{7}$$

with I_1 and I_3 the first and third invariants of the Green-Lagrange strain tensor. $\mathtt{nK}\theta$, N and K0 are the three material coefficients. K0 represents the Bulk modulus, while mu = nkθ is the material modulus, it corresponds to the slope of the stress-strain curve during loading, and $\sqrt{lambda}$ = N is the number of connected rigid-links in a chain.

This model of strain energy presents a good agreement with experimental data for equibiaxial extension.

Syntax:

```
**hyperelasticity arruda_boyce
**model_coef
   mu COEFFICIENT
   lambda COEFFICIENT
   K0 COEFFICIENT
```

Example:
The following is a simple example of the hyperelastic Arruda-Boyce model[2]:

```
***behavior hyper_elastic
 **hyperelasticity arruda_boyce
 **model_coef
    mu          2.1
    lambda      3.0
    K0       10000.
***return
```

---

[2]The model parameters have been taken from [Berg98]

<HYPERELASTICITY>

<HYPERELASTICITY> mooney

Description:

This model implements a two coefficient Mooney-Rivlin hyperelastic behavior [Moon40] including an additional coefficient for compressibility treatment. The coefficients for the hyperelastic law are declared under **hyperelasticity mooney**.

Hyperelastic behavior here defines the strain energy density with the following form:

$$W(I_1, I_2, I_3) = \texttt{C10}(I_1 - 1) + \texttt{C01}(I_2 - 1) + \frac{\texttt{K0}}{2}[(I_3^2 - 1)/2 - \texttt{log}(I_3)] \tag{8}$$

with I_1, I_2, and, I_3 the first, second, and third invariants of the Green-Lagrange strain tensor. C10, C01 and K0 are the three material coefficients. K0 represents the Bulk modulus, while C10 and C01 have the dimension of stress.

This model of strain energy is classically used for very large strain problems.

Syntax:

```
    **hyperelasticity mooney
    **model_coef
      C10 COEFFICIENT
      C01 COEFFICIENT
      K0 COEFFICIENT
```

Example:
The following is a simple example of the hyperelastic Mooney model[3]:

```
***behavior hyper_elastic
 **hyperelasticity mooney
 **model_coef
    C10              0.7
    C01              0.1
    K0            1000.
***return
```

---

[3]The model parameters have been taken from [Lion97]

<HYPERELASTICITY>

<HYPERELASTICITY> ogden

Description:

This model implements the Ogden's phenomenological theory of elasticity [Ogde84] including an additional coefficient for compressibility treatment. The strain energy density is written in terms of generalized strain. The coefficients for the hyperelastic law are declared under **hyperelasticity ogden.

Hyperelastic behavior here defines the strain energy density with the following form:

$$W(\lambda_1, \lambda_2, \lambda_3, I_3) = \sum_{n=1}^{N} \frac{\mu_n}{\alpha_n} (\lambda_1^{\alpha_n} + \lambda_2^{\alpha_n} + \lambda_3^{\alpha_n} - 3) + \frac{\texttt{K0}}{2}[(I_3^2 - 1)/2 - \texttt{log}(I_3)] \tag{9}$$

where the material parameters $(\mu_n, \alpha_n)_{n=1,N}$ should fulfilled the following stability condition:

$$\mu_n \alpha_n > 0 \quad \forall n = 1, N \tag{10}$$

with λ_1, λ_2, and, λ_3 the three generalized stretches and I_3 the third invariant of the Green-Lagrange strain tensor. μ_n, α_n and K0 are the three material coefficients. K0 represents the Bulk modulus, while μ_n and α_n are material constants.

This model is possibly the most extended model after Mooney-Rivlin model. Even if the determination of material parameters leads to some difficulties, this model is one of the most widely used for large strain problems.

Syntax:

```
**hyperelasticity ogden
**model_coef
 *term
  mu COEFFICIENT
  alpha COEFFICIENT
  K0 COEFFICIENT
 *term
  mu COEFFICIENT
  ...
```

. . . continued

<HYPERELASTICITY>

Example:
The following is a simple example of the hyperelastic Ogden model[4]:

```
***behavior hyper_elastic
 **hyperelasticity ogden
 **model_coef
  *term
   mu         0.63
   alpha      1.3
   K0      10000.
  *term
   mu         1.2e-3
   alpha      5.0
  *term
   mu        -1.e-2
   alpha     -2.0
***return
```

---

[4]The model parameters have been taken from [Trel44]

<HYPERELASTICITY>

<div style="text-align:center"><HYPERELASTICITY> van_der_waals</div>

Description:

This hyperelastic model, taking into account the van der Waals forces, is based in the works of Kilian et al.[Kili81]. The implemented model includes an additional coefficient for compressibility treatment. The coefficients for the hyperelastic law are declared under ****hyperelasticity van_der_waals**.

Hyperelastic behavior here defines the strain energy density with the following form:

$$W(I_1, I_2, I_3) = \mu[-(\lambda_m^2 - 3)(\ln(1 - \Theta) + \Theta) - \tfrac{2}{3}a(\tfrac{\tilde{I}-3}{2})^{\frac{3}{2}}] + \frac{\texttt{K0}}{2}[(I_3^2 - 1)/2 - \texttt{log}(I_3)] \tag{11}$$

where

$$\Theta = \sqrt{(\tilde{I} - 3)/(\lambda_m^2 - 3)} \tag{12}$$

$$\tilde{I} = (1 - \beta)I_1 + \beta I_2 \tag{13}$$

with I_1, I_2, and, I_3 the first, second, and third invariants of the Green-Lagrange strain tensor. μ, λ_m, a and β are the four material coefficients. μ is the initial shear modulus; λ_m is the locking stretch; a is a global interaction parameter and β has no physical meaning, conferring an empirical nature to this model. K0 represents the Bulk modulus.

Syntax:

```
**hyperelasticity van_der_waals
**model_coef
   mu COEFFICIENT
   lambda_m COEFFICIENT
   a COEFFICIENT
   beta COEFFICIENT
   K0 COEFFICIENT
```

Example:

The following is a simple example of the hyperelastic van der Waals model[5]:

```
***behavior hyper_elastic
 **hyperelasticity mooney
 **model_coef
    mu            0.434
    lambda_m     10.24
    a             0.32
    beta          0.958
    K0         1000.
***return
```

---

[5]The model parameters have been taken from [Kili86]

<HYPERELASTICITY>

<HYPERELASTICITY> fung

Description:

This model implements a Fung-type anisotropic hyperelastic behavior [Fung79] including an additional coefficient for compressibility treatment. The coefficients for the hyperelastic law are declared under ****hyperelasticity fung**.

Hyperelastic behavior here defines the strain energy density with the following form:

$$W(I_3) = \frac{c}{2}(\exp Q - 1) + \frac{K0}{2}[(I_3^2 - 1)/2 - \log(I_3)] \tag{14}$$

where

$$Q = \tilde{a}_4 \times \frac{F_b^T F_b - I}{2} \tag{15}$$

$$F_b = \frac{F}{J^{1/3}} \tag{16}$$

with $I_3 = J^2$ the third invariant of the Green-Lagrange strain tensor and I the unity tensor. c, $\tilde{a}_4$ and K0 are the three material coefficients. K0 represents the Bulk modulus, while c is a material constant. $\tilde{a}_4$ is the 4th order tensor of orientation.

This model of strain energy is classically used for very large strain biomechanics-related problems.

Syntax:

```
**hyperelasticity fung
**model_coef
  c COEFFICIENT
  K0 COEFFICIENT
 *b orthortropic
  y1111 COEFFICIENT
  y1122 COEFFICIENT
  y2222 COEFFICIENT
  y1133 COEFFICIENT
  y2233 COEFFICIENT
  y3333 COEFFICIENT
  y2323 COEFFICIENT
  y3131 COEFFICIENT
  y1212 COEFFICIENT
```

. . . continued

<HYPERELASTICITY>

Example:
The following is a simple example of the hyperelastic Fung-type model[6]:

```
***behavior hyper_elastic
 **hyperelasticity fung
 **model_coef
    c              26.95e-1
   K0          1000.
   *b orthotropic
   y1111          0.0089
   y1122          0.0193
   y2222          0.4180
   y1133          0.0295
   y2233          0.0749
   y3333          0.9925
   y2323          0.5
   y3131          0.5
   y1212          0.5
***return
```

---

[6]The model parameters have been taken from [Fung93]

<ISOTROPIC_HYPERELASTIC_LAW>

<ISOTROPIC_HYPERELASTIC_LAW>

Description:
This object class defines the model for isotropic hyperelasticity in hyperelastic and hyper_viscoelastic models and potentials.

Syntax:
The syntax to specify an isotropic hyperelasticity object will consist of giving the keyword for a particular hyperelasticity model desired, followed by a list of appropriate coefficients which are dependent on the model chosen. The hyperelasticity type may be chosen among the following laws:

CODE	DESCRIPTION
arruda_boyce	Arruda-Boyce hyperelastic model
mooney	Mooney hyperelastic model
rivlin	Rivlin hyperelastic model
neo_hookean	Neo-Hookean law
hookean_log	Logarithmic Hookean law

The structure of the object is summarized below:

```
  ***behavior  hyper_elastic
   **isotropic_hyperelasticity <HYPERELASTIC_LAW>
   **model_coef
     ...
 [ **pull_back]
```

Stored Variables:
The stored variables for this object include the Green-Lagrange total strain tensor, the Cauchy stress tensor, and the strain energy density W. As an auxiliary output variable, the Piola-Kirchhoff stress tensor:

$$\mathbf{S} = \frac{\partial W}{\partial \mathbf{E}}$$

is stored but not saved during the calculation. The post-processor prefixes used for these variables are the following:

prefix	size	description	default
eto	T-2	Green-Lagrange strain	yes
sig	T-2	Cauchy stress	yes
welas	S	strain energy density	yes

If the option **pull_back is given, the Piola-Kirchhoff stress tensor is requested as output[7].

---

[7]Only for the ****simulate calculation definition.

<ISOTROPIC_HYPERELASTICITY>

<ISOTROPIC_HYPERELASTICITY> arruda_boyce

Description:

This physically-based model, proposed by Arruda and Boyce [Arru93], consists in a chain model with a distribution of chains upon eight directions corresponding to the vertices of a cube inscribed in a unit sphere. The implemented model includes an additional coefficient for compressibility treatment. The coefficients for the hyperelastic law are declared under **isotropic_hyperelasticity arruda_boyce.

Hyperelastic behavior here defines the strain energy density with the following form:

$$W(I_1, I_3) = \quad \text{nK}\theta[\tfrac{1}{2}(I_1 - 3) + \tfrac{1}{20N}(I_1^2 - 9)] + \tfrac{11}{1050N^2}(I_1^3 - 27)] + \tfrac{19}{7000N^3}(I_1^4 - 81)] + \tfrac{519}{673750N^4}(I_1^5 - 243)] + \tfrac{\text{K0}}{2}[(I_3^2 - 1)/2 - \text{log}(I_3)] \qquad (17)$$

with I_1 and I_3 the first and third invariants of the Green-Lagrange strain tensor. $\text{nK}\theta$, N and K0 are the three material coefficients. K0 represents the Bulk modulus, while $\text{mu} = \text{nk}\theta$ is the material modulus, it corresponds to the slope of the stress-strain curve during loading, and $\sqrt{lambda}$ = N is the number of connected rigid-links in a chain.

This model of strain energy presents a good agreement with experimental data for equib-iaxial extension.

Syntax:

```
**isotropic_hyperelasticity arruda_boyce
**model_coef
  mu COEFFICIENT
  lambda COEFFICIENT
  K0 COEFFICIENT
```

Example:
The following is a simple example of the hyperelastic Arruda-Boyce model[8]:

```
***behavior hyper_elastic
 **isotropic_hyperelasticity arruda_boyce
 **model_coef
   mu          2.1
   lambda      3.0
   K0       10000.
***return
```

---

[8]The model parameters have been taken from [Berg98]

<ISOTROPIC_HYPERELASTICITY>

<ISOTROPIC_HYPERELASTICITY> mooney

Description:

This model implements a two coefficient Mooney-Rivlin hyperelastic behavior [Moon40] including an additional coefficient for compressibility treatment. The coefficients for the hyperelastic law are declared under **isotropic_hyperelasticity mooney**.

Hyperelastic behavior here defines the strain energy density with the following form:

$$W(I_1, I_2, I_3) = \text{C10}(I_1 - 1) + \text{C01}(I_2 - 1) + \frac{\text{K0}}{2}[(I_3^2 - 1)/2 - \log(I_3)] \tag{18}$$

with I_1, I_2, and, I_3 the first, second, and third invariants of the Green-Lagrange strain tensor. C10, C01 and K0 are the three material coefficients. K0 represents the Bulk modulus, while C10 and C01 have the dimension of stress.

This model of strain energy is classically used for very large strain problems.

Syntax:

```
**isotropic_hyperelasticity mooney
**model_coef
   C10 COEFFICIENT
   C01 COEFFICIENT
   K0 COEFFICIENT
```

Example:
The following is a simple example of the hyperelastic Mooney model[9]:

```
***behavior hyper_elastic
 **isotropic_hyperelasticity mooney
 **model_coef
    C10            0.7
    C01            0.1
    K0          1000.
***return
```

---

[9]The model parameters have been taken from [Lion97]

<ISOTROPIC_HYPERELASTICITY>

<ISOTROPIC_HYPERELASTICITY> rivlin

Description:

This model implements the Rivlin hyperelastic behavior [Rivl51] as a polynomial series of $(I_1 - 3)$ and $(I_2 - 3)$ including an additional coefficient for compressibility treatment. The coefficients for the hyperelastic law are declared under **isotropic_hyperelasticity rivlin**.

Hyperelastic behavior here defines the strain energy density with the following form:

$$W(I_1, I_2, I_3) \;=\; \sum_{i=0,j=0}^{\infty} \mathtt{C_{ij}}(I_1 - 1)^i (I_2 - 1)^j + \frac{\mathtt{K0}}{2}[(I_3^2 - 1)/2 - \log(I_3)] \tag{19}$$

with I_1, I_2, and, I_3 the first, second, and third invariants of the Green-Lagrange strain tensor. $\mathtt{C}_{ij}$ and $\mathtt{K0}$ are material parameters. $\mathtt{K0}$ represents the Bulk modulus, while $\mathtt{C}_{00} = 0$. The series is often truncated to terms of the second or third order.

This model of strain energy is classically used for very large strain problems.

Syntax:

```
**isotropic_hyperelasticity rivlin
**model_coef
  C10 COEFFICIENT
  C01 COEFFICIENT
  C20 COEFFICIENT
  C11 COEFFICIENT
  C02 COEFFICIENT
  ...
  K0 COEFFICIENT
```

. . . continued

<ISOTROPIC_HYPERELASTICITY>

Example:
The following is a simple example of the hyperelastic Rivlin model[10]:

```
***behavior hyper_elastic
 **isotropic_hyperelasticity rivlin
 **model_coef
    C10              0.208
    C01              0.0233
    C20             -0.0024
    C11              0.0
    C02              0.0
    C30              0.0005
    C21              0.0
    C12              0.0
    C03              0.0
    K0            1000.
***return
```

---

[10]The model parameters have been taken from [Trel44]

<ISOTROPIC_HYPERELASTICITY>

<ISOTROPIC_HYPERELASTICITY> neo_hookean

Description:

This model implements the simplest physically based hyperelastic behavior [Trel44], the Neo-Hookean model, including an additional coefficient for compressibility treatment. The coefficients for the hyperelastic law are declared under **isotropic_hyperelasticity neo_hookean**.

Hyperelastic behavior here defines the strain energy density with the following form:

$$W(I_1, I_3) = \tfrac{1}{2}\texttt{nkT}(I_1 - 1) + \frac{\texttt{K0}}{2}[(I_3^2 - 1)/2 - \texttt{log}(I_3)] \tag{20}$$

with I_1 and I_3 the first and third invariants of the Green-Lagrange strain tensor. $\texttt{mu} = \texttt{nkT}$ and K0 are the two material coefficients. K0 represents the Bulk modulus, while nkt is the material Shear modulus.

This model is in good agreement with tensile, simple shear and biaxial tests for deformation lower than 50%.

Syntax:

```
**isotropic_hyperelasticity neo_hookean
**model_coef
   mu COEFFICIENT
   K0 COEFFICIENT
```

Example:
The following is a simple example of the hyperelastic Neo_hookean model[11]:

```
***behavior hyper_elastic
 **isotropic_hyperelasticity neo_hookean
 **model_coef
    mu            0.4
    K0          1000.
***return
```

---

[11]The model parameters have been taken from [Trel44]

<ISOTROPIC_HYPERELASTICITY>

<ISOTROPIC_HYPERELASTICITY> abaqus_neo_hookean

Description:

This model implements the simplest physically based hyperelastic behavior [Trel44], the Neo-Hookean model, including an additional coefficient for compressibility treatment in the same way as ABAQUS - Simulia^{TM}. The coefficients for the hyperelastic law are declared under **isotropic_hyperelasticity abaqus_neo_hookean.

Hyperelastic behavior here defines the strain energy density with the following form:

$$W(I_1, I_3) = \texttt{C10}(I_1 - 1) + \frac{1}{\texttt{D1}}(J - 1)^2 \tag{21}$$

with I_1 and $I_3 = J^2$ the first and third invariants of the Green-Lagrange strain tensor. $\texttt{mu} = \texttt{C10}$ and $\texttt{D}$ are the two material coefficients. $\texttt{K0}$ represents the compressibility modulus, while $\texttt{C10}$ is related with material Shear modulus.

This model is in good agreement with tensile, simple shear and biaxial tests for deformation lower than 50%.

Syntax:

```
**isotropic_hyperelasticity abaqus_neo_hookean
**model_coef
  C10 COEFFICIENT
  D1 COEFFICIENT
```

Example:
The following is a simple example of the hyperelastic Neo_hookean model[12]:

```
***behavior hyper_elastic
**isotropic_hyperelasticity abaqus_neo_hookean
**model_coef
C10            0.2
D1             0.0001
***return
```

---

[12]The model parameters have been taken from [Trel44]

<INTERACTION>

<INTERACTION>

Description:
This option allows addition of various variable interactions in the `gen_evp` behavior object.

Syntax:
The syntax of the interaction types depends on the type of interaction. Generally there will be a specification of the type of interaction and two identifying tokens which define the variables which interact. This structure is summarized below:

interaction *[type] item1 item2*

 ...

where *type* may be from the following types:

CODE	DESCRIPTION
iso	Crystalline isotropic hardening interaction.

`default` In the absence of *type* the default "state" interaction will be implemented as described by [Cont89]. This interaction calculates associated forces including terms of other internal variables. The coupling will be stated by using the (user supplied) name of a potential and the (user supplied) name of hardening mechanisms.

interaction *P1::H P2::H* <COEFFICIENT>

`iso` This interaction will link the isotropic variables of one class of slip systems with another (latent strain coupling) between two mono-crystal potentials. The coupling is written:

$$R_i = R_{o_i} + Q_i \sum_{j=1}^{n} (1 - e^{-bv_j}) h_{ij}$$

syntax for this type of coupling takes the names of the two potentials, and a coefficient definition named **h**:

interaction iso *name1 name2*

 h <COEFFICIENT>

Note: for interactions between slip systems *within one potential* one should use the `SLIP_INTERACTION` class (see page 13.110).

Example:
This is an example of the state-law default coupling to link two kinematic variables in a time-dependent viscoplastic potential and a time-independent plasticity potential.

$$\begin{aligned}
\mathbf{X}_{X1} &= \tfrac{2}{3} C_{X1} \boldsymbol{\alpha}_{X1} + \tfrac{2}{3} C_{int} \boldsymbol{\alpha}_{X2} \\
\mathbf{X}_{X2} &= \tfrac{2}{3} C_{X2} \boldsymbol{\alpha}_{X2} + \tfrac{2}{3} C_{int} \boldsymbol{\alpha}_{X1}
\end{aligned}$$

$$(22)$$

The example material definition for this type of interaction is as follows:

<INTERACTION>

```
***behavior gen_evp
 **elasticity isotropic
   young 170000.0
   poisson 0.30
 **potential gen_evp ev
   *flow norton
       n  1.0
       K  20300.
   *kinematic nonlinear X1
       C  2000.0
       D  50.0
   *isotropic constant
       R0 20.0
 **potential gen_evp ep
   *kinematic nonlinear X2
       C  25000.0
       D  10.0
    *isotropic constant
       R0 850.0
   **interaction ev::X1 ep::X2 25000.0
***return
```

The names `X1` and `X2` were given in order to have readable names for the kinematic variables. In this syntax it is important to notice that a specification `ev::X1` is different than `ev::X1` because the kinematic names are localized within each potential.

<ISOTROPIC>

<ISOTROPIC>

Description:
This object class defines models of isotropic hardening for use in a variety of material behaviors and potentials. Isotropic hardening causes an isotropic expansion or contraction of the yield surface in tensorial stress space. The isotropic hardening may be a function of the simulated multiplier which is normally equal to the cumulated plastic strain equivalent p, or in terms of its own internal variable. The latter must be used for cases of static recovery.

The initial value R_0 for the yield radius is noted here to be the onset of plasticity, and not the engineering yield stress. It may thus be found to be significantly lower than expected.

Syntax:
The syntax to specify a isotropic hardening object will consist of giving the keyword for a particular law desired, followed by a list of appropriate coefficients which are dependent on the model chosen. The possible isotropic laws are the following:

CODE	DESCRIPTION
constant	initial value only (perfect plasticity).
linear	(or iso_linear) linear function of p.
power_law	power law of p.
by_point	hardening defined by a list of experimental points in an external datafile.
iso_table	hardening defined by a table of points.
linear_pp	linear hardening followed by perfect plasticity.
nonlinear	nonlinear, exponentially saturating function of p.
nonlinear_v1	nonlinear with an internal variable and coefs 1.
nonlinear_v2	nonlinear with an internal variable and coefs 2 (equivalent to nonlinear).
nonlinear_bsi	nonlinear with kinematic interaction (for use with the mises_2m1c potential only).
linear_nonlinear	combined linear and nonlinear saturating hardening.
nonlinear_sum	multiple term nonlinear hardening.
nonlinear_double	multiple term nonlinear hardening. This law is rigorously equal to nonlinear_sum, but is retained for backwards compatibility. Although the name suggests that only two terms are allowed, more can be added.
nonlinear_recovery	
function	hardening according to a user-defined function of p.

. . . continued

<ISOTROPIC>

Only the laws with an internal variable may have static recovery and be used in state interactions. Isotropic hardening is available with positive values of the `Q` or `H` parameters (depending on the model), while softening occurs with negative values of these coefficients. The saturation rate coefficients `b` are necessarily positive. All parameters may have the normal dependencies through the `COEFFICIENT` mechanism (see page 13.6).

constant   This gives the radius as a single coefficient `R0`.

linear   (or `iso_linear`) Law with initial radius and a linear evolution depending on the cumulated inelastic strain p (i.e. $R = R0 + Hp$) and using the coefficients `R0` and `H`.

power_law   Gives a power-law evolution according to

$$R = R_0 + K \left(e_0 + p\right)^n$$

with the coefficients `R0`, `K`, `e0`, `n`, and p the cumulated inelastic strain. Negative values for `e0` are set to zero. The case $n < 1$ with $e_0 = 0$ gives an infinite derivative at the onset of inelastic deformation and is therefore not allowed. Use a very small value for `e0` instead.

by_point   Gives the isotropic curve as input by a list of points (see the example). The first column should be `sigeq` and the second the cumulated plastic strain equivalent.

iso_table   Gives the isotropic curve as input by a list of points directly in a table (see example). When the current value of p depasses the last value specified in the table, the isotropic hardening no longer changes, as if the isotropic hardening saturates.

linear_pp   linear hardening with an initial radius `R0` and slope `H` up to `Ru` (i.e. $R = R0 + Hp$ for $R < Ru$), followed by perfect plasticy at $R = Ru$.

nonlinear   This law gives a nonlinear saturating evolution:

$$R = R0 + Q\left(1 - e^{-bp}\right)$$

where the saturation radius will be `R0 + Q` for large p. The law will reach 95% of the saturation value at $p \approx 3.0/b$ so that higher values of `b` give a more rapid saturation.

linear_nonlinear   linear hardening with an initial radius `R0` followed by a combined linear and nonlinear evolution with coefficients `H`, `Q` and `b`, according to

$$R = R0 + Hp + Q\left(1 - e^{-bp}\right).$$

nonlinear_sum   or **nonlinear_double**. This law allows fine tuning of the isotropic hardening by use of multiple-term evolution. For instance, two terms might be combined analogous to short and long term mechanisms. There is no upper limit for the number of terms `N`. The radius is calculated as:

$$R = R_0 + \sum_i^N Q_i \left(1 - e^{-b_i p}\right)$$

with coefficients `R0`, `Q1`, `Q2`, ..., `QN`, and `b1`, `b2`, ..., `bN`.

... *continued*

<ISOTROPIC>

nonlinear_1

$$m_{iso} = 1 - \frac{R - \text{R0}}{\text{Q}}$$

Example:
An example of a three-term nonlinear hardening with a very rapid initial hardening, a very slow hardening (third term) and an intermediate softening (negative Q2). Note: these are not necessarily reasonable values.

```
*isotropic nonlinear_sum
 R0     50.
 Q1     30.  b1  2000.
 Q2    -10.  b2    20.
 Q3     40.  b3     2.
```

The next example shows the use of *isotropic by_point. Between two data points, interpolation is linear.

```
**potential gen_evp ep
 *criterion mises
 *flow plasticity
 *isotropic by_point
  sigeq    epcum
  130.0   0.0000
  140.0   0.0001
  145.0   0.0002
  150.0   0.0004
  160.0   0.0009
  170.0   0.0017
  180.0   0.0028
```

The following gives a point-by-point specification of an isotropic harding. Between two data points, interpolation is linear (as with all Z-set tables). For $p > 0.1$ it uses the values of 0.1 because that was the last specified.

```
*isotropic table
 0.    temperature   % temp table for epcum = 0.
        220.  23.0
        100.  200.
 0.1  temperature   % temp table for epcum = 0.1
        300.  23.0
        120.  200.
```

<KINEMATIC>

<KINEMATIC>

Description:
This object defines the model of kinematic hardening (tensorial back stresses) applicable in behaviors or potential objects in the `gen_evp` behavior. The models generally store an additional tensorial internal variable, and therefore may support static recovery and state coupling without modification. The name of this internal variable will be determined normally by the object to which it belongs (a `POTENTIAL` for example). Kinematic hardening acts as a translation of the yield surface in stress space (often deviatoric).

Syntax:
The syntax consists of specifying the type of kinematic object, supplying an optional name on the same line, and giving the appropriate coefficient definitions on the following lines. This is summarized below where the keyword specifying a `KINEMATIC` object is assumed to be `*kinematic`:

---
*kinematic *type* [*name*]
   coefficients

---

where the possible substitutions for *type* are:

CODE	DESCRIPTION
linear	linear hardening
nonlinear	nonlinear Armstrong-Fredrick hardening with static recovery
nonlinear_ai	same as the `nonlinear` model but using more accurate asymptotic integration
ziegler	nonlinear hardening based on the Euclidean norm I_2
nonlinear_phi	nonlinear with cumulative influence
nonlinear_evrad	nonlinear with reduced ratcheting
nonlinear_with_crit	linear-nonlinear with criterion
aniso_nonlinear	nonlinear model using coefficient matrices for the coefficients

Kinematic models are all formulated in state variable form, where the stored (integrated) variable is analogous to a strain translation in tensorial strain space. The "back stress" component is then calculated using an appropriate modulus. Most of the kinematic models use the convention for calculating the back stress:

$$\mathbf{X} = \frac{2}{3}\mathsf{C}\boldsymbol{\alpha}$$

with $\mathbf{X}$ the back stress and $\boldsymbol{\alpha}$ the internal variable. Material softening through kinematic variables is not thought to be physically reasonable, and so the modulus coefficients `C` should always be positive.

<KINEMATIC>

Evolution of the internal variable is written in the form:

$$\dot{\boldsymbol{\alpha}}_i = \dot{\lambda}\mathbf{m}_{kin}(\boldsymbol{\sigma}, \mathbf{X}, p, \ldots) - \dot{\boldsymbol{\omega}}_{kin}(\mathbf{X})$$

where $\mathbf{m}$ is the "hardening normal" and $\dot{\boldsymbol{\omega}}_{kine}$ a static recovery function.

linear   The linear kinematic hardening has its internal variable evolve with the inelastic strain:

$$\mathbf{m}_{kin} = \mathbf{n}$$

The only coefficient for this model is the `C` modulus (units of stress). The slope in a uniaxial test will be equal to the `C` value.

nonlinear   The nonlinear model evolves much as the isotropic `nonlinear` model does (with a slight change in coefficient meaning). The evolution is the following:

$$\mathbf{m}_{\text{kin}} = \mathbf{n} - \frac{3D}{2C}\mathbf{X}$$
$$\boldsymbol{\omega}_{\text{kin}} = \frac{3}{2}\frac{\mathbf{X}}{J_2(\mathbf{X})}\left\langle \frac{J_2(\mathbf{X})}{M} \right\rangle^m \tag{23}$$

The coefficients are `C` and `D` for the strain evolution, and `M` and `m` for the static recovery term. In the absence of these latter two, there will be no static recovery calculation. The saturation of this model occurs at `C/D` in a uniaxial test at a rate determined by `D`. Increases in `D` yield faster saturating (more nonlinear) behavior.

Static recovery is seen to follow a Norton type formulation in the back stress tensorial space. This kinematic model supports RK, TM, or Reduced TM integrations.

nonlinear_phi   This model installs a kinematic variable with the following evolution:

$$\mathbf{m}_{\text{kin}} = \mathbf{n} - \phi(\lambda)\frac{3D}{2C}\mathbf{X}$$

where the function ϕ is:

$$\phi(\lambda) = \phi_m + (1 - \phi_m)\exp(-\omega\lambda)$$

where the material coefficients ϕ_m and ω are named `phim` and `omega`. Note that ω defines the rapidity of saturation in the non-linear coefficient, and ϕ_m is a factor between zero and one interpolating the `D` coefficient between initial and saturated values. This kinematic model works in RK, TM, or Reduced TM.

nonlinear_evrad   This model limits the ratcheting effect in biaxial conditions by comparing the flow direction with the back stress. Evolution is calculated as follows:

$$\mathbf{m}_{\text{kin}} = \mathbf{n} - \left(\eta\mathbf{1} + \tfrac{2}{3}(1-\eta)\mathbf{n}\otimes\mathbf{n}\right)\frac{3D}{2C}\mathbf{X}$$

The coefficients are defined such that uniaxial response is equivalent to the `nonlinear` model given equivalent coefficients. The coefficient names are `C`, `D`, and `eta`. This model works in RK, TM, or Reduced TM, but has no static recovery.

<KINEMATIC>

ziegler This model describes a back stress with hydrostatic and deviatoric components:

$$\begin{aligned}
\mathbf{m}_{\text{kin}} &= \frac{\boldsymbol{\sigma}-\mathbf{X}}{I_2(\boldsymbol{\sigma}-\mathbf{X})} - \frac{D}{C}\mathbf{X} \\
\boldsymbol{\omega}_{\text{kin}} &= \frac{\mathbf{X}}{I_2(\mathbf{X})}\left\langle\frac{I_2(\mathbf{X})}{M}\right\rangle^{m}
\end{aligned} \tag{24}$$

which takes the coefficients C, D, M and m. In the absence of the latter two, there will be no static recovery. The Ziegler model may not be used with the `reduced_plastic` integration.

nonlinear_with_crit

$$\mathbf{m}_{kin} = \mathbf{n} - \frac{3D}{2C}\phi(\mathbf{X})\mathbf{X}$$

$$\phi(\mathbf{X}) = \left\langle\frac{DJ(\mathbf{X})-\omega}{1-\omega}\right\rangle^{m_1}\frac{1}{DJ(\mathbf{X})^{m_2}}$$

<u>**Example**</u>:

```
*kinematic nonlinear_evrad
    C      40000.
    D      500.
    eta    0.4
```

<KINEMATIC>

<KINEMATIC> aniso_nonlinear

Description:

This kinematic model implements anisotropic coefficients into a `KINEMATIC` behavior object. Note that this model does not include the 1.5 term in the modulus coefficients, so there are none in the evolution. The coefficients are to be entered into `COEFFICIENT_MATRIX` objects (see page 13.8).

$$
\mathbf{m}_{\text{kin}} = \mathbf{n} - \mathbf{D}\mathbf{C}^{-1}\mathbf{X}
$$
$$
\boldsymbol{\omega}_{\text{kin}} = \mathbf{C}^{-1}\xi\mathbf{Q} : \mathbf{X}\left(\frac{\|\mathbf{X}\|_Q}{M}\right)^m
\tag{25}
$$

Any of the coefficients can of course be a function or table of the temperature, or other parameter.

The equivalent term $\|\mathbf{X}\|_Q$ above is calculated as follows:

$$
\|\mathbf{X}\|_Q = [\mathbf{X} : \mathbf{Q} : \mathbf{X}]^{1/2}
$$

Syntax:

```
   **kinematic aniso_nonlinear [name]
     C  <COEFFICIENT_MATRIX>
     D  <COEFFICIENT_MATRIX>
 [   xi <COEFFICIENT>          ] % defines recovery exists
 [   Q  <COEFFICIENT_MATRIX> ] % overrides global
 [   m  <COEFFICIENT>          ] % ditto
 [   M  <COEFFICIENT>          ]
```

Example:

```
  *kinematic aniso_nonlinear  x1
     C  cubic C1111 20000.0 % 30000.0/1.5
              C1122 0.0
              C1212 20000.0
     D  cubic
        D1111 500.
        D1122 0.0
        D1212 500.
```

<LOCALIZATION>

<div align="center">

<LOCALIZATION>

</div>

Description:
This object selects a localization model to be applied to the different potentials of a `gen_evp`
type behavior.

Syntax:
Localization is indicated within a `gen_evp` behavior with an entry of the following type:

**localization *type*

From which the following localization types may be chosen:

CODE	DESCRIPTION
poly	polycrystal (multi-grain) model

poly The polycrystal mode here is a generalized form of that described by Cailletaud and
Pilvin [Cail92, Cail94, Pilv94]. Several potentials of type `crystal` will be assembled to
form a slt/phase/ of the material, which in turn is grouped according to the orientations
and volume fractions of material. The syntax for the model is:

```
  **localization poly
  *model_coefficients
    coefs
[ *grains    ]
[   grain list ]
[ *file file_name ]
```

Example:

```
***behavior gen_evp
 **elasticity isotropic
    young     200000.
    poisson  0.30
  **localization poly
    *grains
      -149.676 15.61819 154.676 1.
      -149.676 15.61819 154.676 1.
      -150.646 33.86400 155.646 0.2
    *model_coefficients
      C  50000.
      D  100.
 **potential octahedral
   *flow norton
       n   25.
       K   50.
   *isotropic nonlinear
       R0   100.
       Q    50.0
       b    50.0
   *kinematic linear
       C    2500.
   *interaction slip
       h1 1.0
       h2 1.0
       h3 1.0
       h4 1.0
       h5 1.0
       h6 1.0
***return
```

<POROUS_CRITERION>

<POROUS_CRITERION>

Description:

This behavior object is used to enter the citerion for a porous plastic material. The description of these models will use the following notation:

CODE	DESCRIPTION
$\boldsymbol{\sigma}$	stress tensor
$\mathbf{s}$	deviatoric stress tensor
J_2	the second invariant of deviatoric stress $\frac{1}{2}\mathbf{s} : \mathbf{s}$
I_1	first invariant of stress Trace $\underset{\sim}{\sigma}$
$\sigma_\star$	current flow stress

Syntax:

The syntax for a porous criterion requires that a type be given, followed by whatever coefficients are allowed for the particular model. As in all of Z-mat, these coefficients are entirely context sensitive.

```
*porous_criterion type
    coefs
```

The available list of porous plastic models are summarized below.

CODE	DESCRIPTION
gurson	model to capture progressive microrupture
elliptic_aniso	generalization of the elliptic criterion for general anisotropy.
elliptic	criterion for densification of material
elliptic_fiber	elliptic criterion for compaction of fibers in a powder matrix.
fkm	NIOT
modified_rousselier	NIOT
rousselier	thermodynamic criterion through free energy
cam_clay	criterion to study the porosity of clay
zhang_niemi	NIOT

The following pages discuss these models in details.

<POROUS_CRITERION>

<POROUS_CRITERION> cam_clay

Description:
This criterion is developed to study the porous behavior of clay. In literature, many modified versions of cam-clay models have been developed recently to study the behavior of partially saturated soils. Zmat currently inlcudes the basic Cam-Clay model.

$$\frac{3J_2}{m^2} + (I_1/3 + p_c)^2 - \sigma_\star^2$$

with p_c and m coefficients named `pc` and `m`.

Syntax:

```
*porous_criterion cam_clay
   coefficients
...
```

Example:
A simple example from a test case is given below

```
*porous_criterion cam_clay
  pc   ft
  100.  0.
  20.   1.
  m     .5
```

<POROUS_CRITERION>

<POROUS_CRITERION> elliptic

Description:

The elliptic criterion is a simple ellipse in P-q plane, and allows a great deal of flexibility in adjusting the pressure sensitivity of plasticity. This model can be used for general densification of problems, such as powder compaction and foam plasticity.

$$3CJ_2 + FI_1^2 - \sigma_\star^2$$

where C and F are the coefficients named C and F.

Because the ratio between the deviatoric and pressure sensitivity is determined by the C and F coefficients, we can get great flexibility by making these coefficients depend on the porosity state variable f. A typical limiting case is that the material should behave in a fully deviatoric way at the fully dense condition (when $f = 0$ then C=1 and D=0), and similarly when the material is fully void there should only be pressure dependence(when $f = 1$ then C=0 and D=1).

Syntax:

```
*porous_criterion elliptic
    coefficients
...
```

Example:

A simple example from a test case is given below

```
*porous_criterion elliptic
 F f
 0.  0.
 5.  1.
 C f
 1. 0.
 11. 1.
```

<POROUS_CRITERION>

<POROUS_CRITERION> elliptic_aniso

Description:

This porous potential allows for a very general anisotropic anisotropic porous plastic material. Anisotropic influence on the direct stress components for the (ordinarily) trace operator for the pressure term are replaced with a coefficient factored trace. Anisotropic effects in the shear term can be implemented with the generally available `*shear_anisotropy` option in the porous plastic material behavior (which replaces the J_2 term with an effective anisotropic measure of the shear criterion).

The potential is therefore:

$$3C\tilde{J}_2^2 + F\tilde{I}_1^2 - \sigma_\star^2$$

where C and F are the coefficients named `C` and `F`, and which can depend notably on the porosity variable `f`. As stated above the $\tilde{J}_2$ will be as supplied by the shear anisotropy (default standard J_2 measure), and the $\tilde{I}$ is calculated by:

$$\tilde{I}_1 = p\,\sigma_{11} + q\,\sigma_{22} + r\,\sigma_{33}$$

and p q and r are coefficients (not depending on state variables).

Syntax:

The syntax follows the typical porous potential format with the 5 coefficients `C`, `F`, `p`, `q`, and `r` to be entered. Again, only `C` and `F` can depend on the porosity.

```
*porous_criterion elliptic
    coefficients
...
```

... continued

<POROUS_CRITERION>

Example:
An example test is in `Sam_test/INP` in the input files `elliptica` and `ellaniso.inp`

```
  ***behavior porous_plastic
    **elasticity orthotropic
      y1111 464.
      y2222 239.
      y3333 239.
      y1212 105.
      y2323 105.
      y3131 105.
      y1122 172.
      y2233 142.
      y3311 172.
    **porous_potential
     *porous_criterion elliptic_aniso
       C 1.
       F          1.839926000000000e-03
       p 1.
       q          2.061266000000000e+01
       r          2.330418000000000e+01
     *shear_anisotropy hill
       hilla           4.172356995000000e-01
       hillb           2.066054000000000e+00
       hillc           1.992586000000000e+00
       hilld 1.
       hillf 1.
       hille 1.
     *flow norton     % pseudo rate independant
       K 0.001 n 10. % plasticity with these coefs
     *isotropic_hardening nonlinear_double
       R0           4.500000000000000e-01
       Q1           3.729991000000000e-01
       b1           3.276424000000000e+02
       Q2           8.166423000000000e+03
       b2 0.001
  ***return
```

<POROUS_CRITERION>

<POROUS_CRITERION> fkm

Description:
This criterion is as developed by Fleck, Kuhn, and McMeeking [Flec92] for metal powder compaction.

$$\frac{6J_2 + \sqrt{27J_2^2 + 4I^2}}{6\alpha}$$

with coefficients f_max, offset and f_s named `fmax`, `offset` and `fs`.

Syntax:

   `*porous_criterion fkm`
     coefficients
 `...`

Example:
A simple example from a test case is given below

```
*porous_criterion fkm
fmax
offset
fs
```

Description:

This criterion was proposed by Gurson and is no doubt a widely accepted model. The model was developed to capture the progressive microrupture through void nucleation and growth. Since then it has been modified in various forms for implementation in a variety of fields, ductile rupture of metals being the most applied one. The model defines the criterion as:

$$\frac{3J_2}{\sigma_\star^2} + 2f^\star q_1 \mathrm{ch}\left(\frac{q_2 I_1}{2\sigma_\star}\right) - (1 + q_1^2 f^{\star 2})$$

where $f^\star$, q_1 q_2 are coefficients of the model. Names for these coefficients are `fs`, `q1` and `q2`. The coefficients q_1 and q_2 have units of stress.

Syntax:

```
*porous_criterion gurson
   coefficients
...
```

prefix	size	description	default
eto	T-2	total strain	yes
sig	T-2	Cauchy stress	yes

Example:

A simple example from a test case is given below

```
*porous_criterion gurson
 q1 1.5
 q2 1.0
 fs = ft
```

<POROUS_CRITERION> rousselier

Description:

The Rousselier model is a thermodynamics model formed by coupling the plasticity and damage through free energy. The criterion is defined as below:

$$\frac{\sqrt{3J_2}}{1-f} + \sigma_1 f D \exp\left(\frac{I_1}{3(1-f)\sigma_1}\right) - \sigma_\star$$

with the coefficients σ_1 and D named `sigma1` and `D`. Although the Rousselier model is very similar to the Gurson model, a major point of difference between the two is that in Rousselier model the damage grows under pure shear and the non zero shear deformation occurs under pure hydrostatic pressure due to the shape of the yield function.

Syntax:

```
*porous_criterion rousselier
   coefficients
...
```

Example:

A simple example from a test case is given below

```
*porous_criterion rousselier
  sigma1  200.
  D       0.85
```

<POROUS_CRITERION>

<POROUS_CRITERION> modified_rousselier

Description:

$$\frac{\sqrt{3J_2}}{1-f} + \sigma_1 f D \exp\left(\frac{q_2 I_1}{3(1-f)\sigma_1}\right) - \sigma_\star$$

where q_2, D and $sigma_1$ are coefficients named `q2`, `D` and `sigma1`.

Syntax:

---

*porous_criterion modified_rousselier
  coefficients

...

Example:
A simple example from a test case is given below

```
*porous_criterion modified_rousselier
  sigma1  200.
  D       0.85
  q2
```

<POROUS_CRITERION>

<POROUS_CRITERION> zhang_niemi

Description:

$$\frac{2J_2 + \frac{I}{3}}{1.5(1 - \chi^2)C_f}$$

The coefficients for the criterion are λ_0, χ_c and f_s named `lambda0`, `chi_c`, `fs`.

Syntax:

```
*porous_criterion zhang_niemi
    coefficients
...
```

Example:
A simple example from a test case is given below

```
*porous_criterion zhang_niemi
lambda0
chi_c
fs
```

<POTENTIAL>

<POTENTIAL>

Description:
The potential object classes define the dissipation potentials within a `gen_evp` behavior assembly. Each potential given describes an inelastic strain mechanism, along with the hardening variables which affect its evolution. We can generally combine an arbitrary number and mix of the potentials in order to create complex behaviors. This combination is however *not* verified for physical compatibility so a particular assembly should be extensively studied under simple volume element loadings.

Syntax:

 **potential *potential_type*   [*name*]

The types and number of sub-options is dependent on the potential type and is thus left to be described with the potential types. The types available are summarized below:

CODE	DESCRIPTION
`gen_evp`	classical plasticity using un-coupled isotropic and kinematic hardening
`non_associated`	need info
`delobelle`	special kinematic hardening evolution with multiple tensor variables
`gen_evp2`	modified `gen_evp` with different hardening variables
`coupled_recovery`	kinematic recovery which couples the back stresses
`associated`	completely associated version of classical plasticity
`z6_gen_evp`	un-associated interactions compatible with Z6
`mises_2m1c`	Complex interaction and criterion 2M1C
memory	`gen_evp` with strain-range memory
`suvic`	SUVIC complex hardening evolutions

If the option *name* is given, the names of the inelastic deformation tensors will be constructed from the names given. By default the names will be generated automatically based on the type and number (by order of definition) of each potential. It is generally advised to use the names `ev` for the first viscoplastic potential and `ep` for the first plastic potential.

<POTENTIAL>

<POTENTIAL> associated

Description:
This potential takes the same form as the `gen_evp` potential described above, but alters the criterion to be associated with the hardening mechanisms input. The criterion form can be written:

$$f = f_{cr}(\mathbf{p},\ \boldsymbol{\sigma} - \Sigma\mathbf{X}_i) + \Omega_i(R) + \Sigma\Omega_i(\mathbf{X}_i)$$

where f_{cr} is the criterion as calculated by the `<CRITERION>` object entered after `*criterion`. There are some additional restrictions with this potential type due to numerical or physical restrictions.

   The resulting behavior includes a nonlinear yield zone radius dependence on the R isotropic variable. A dependence also is introduced with the kinematic hardening variables on the isotropic radius. As the kinematic back stress is increased (through monotonic straining) the yield radius is decreased thereby increasing the Bauschinger type effect (reduced yield on reversal).

Syntax:

The syntax understood by this potential is summarized below:

```
    **potential associated [name]
    [ *flow        <FLOW>              ]
    [ *flow        <RATE_VAR_FLOW>     ]
    [ *criterion   <CRITERION>         ]
    [ *kinematic   <KINEMATIC> [name]  ]
    [ *kinematic   <DIRECT_KINEMATIC> [name] ]
    [ *isotropic   <ISOTROPIC>         ]
    [ *var_coefs                       ]
    [ *store_all                       ]
```

Example:
The example given for the `gen_evp` potential may be run with this potential by only changing the potential name to `associated`.

```
    ***behavior gen_evp
      **elasticity isotropic
         young 260000.
         poisson 0.3
      **potential associated
       *criterion mises
       *flow norton_k_variable
            n  7.0
       *kinematic nonlinear
            A1   15000.0
            Bp      30.0
       *isotropic constant
            R0 130.0
       *K non_linear_recovery
```

<POTENTIAL>

```
            R0   200.
            A      0.0
            Rp     1.0
        *parameters
            A      7.8125e-3
            N      1.0
            vdot0  1.0e-11
            sig0   1.0
            m      1.0
            B01    1.0
            B02    1.0
        ***return
```

<POTENTIAL>

<POTENTIAL> coupled_recovery

This potential provides a slight modification on the `gen_evp` potential in that it couples the back stress effect in recovery. The kinematic variables are the only ones affected in this coupling. The evolution for each kinematic variable j will use the following form:

$$\dot{\mathbf{X}}_j = \dot{\lambda}\mathbf{m}_j(\boldsymbol{\sigma}, \lambda, \mathbf{X}_j) - \dot{\boldsymbol{\omega}}_j(\mathbf{X}) \qquad \mathbf{X} = \sum_i \mathbf{X}_i$$

<POTENTIAL>

<POTENTIAL> delobelle

Description:

Delobelle's potential implements a special form of kinematic hardening evolution using multiple tensorial variables[13]. The implementation is based on the work described in [Delo96].

The class allows any CRITERION, FLOW, object to be used, and uses the ISOTROPIC object in a somewhat different manner than the gen_evp based potentials. There is a limitation on the ISOTROPIC objects which can be used, such that no additional integrated variables are added.

The inelastic flow is controlled using a scalar CRITERION value for the "overstress:"

$$ f = f(\boldsymbol{\sigma} - \mathbf{x}) \qquad\qquad \mathbf{n} = \frac{\partial f}{\partial \boldsymbol{\sigma}} $$

where the function f is selected with the *criterion option below. The tensor $\mathbf{x}$ is the current back stress (not sum of back stresses as in other models).

The scalar flow magnitude $\dot{\lambda}$ is a function defined in terms of f using the *flow option as in other potential models. The inelastic strain rate tensor is also defined as in other models using the normality principle so $\dot{\boldsymbol{\epsilon}}_{in} = \dot{\lambda} : \mathbf{n}$.

The initial hardening slope for kinematic variables follows a flow normal which is modified from the inelastic strain by scalar hardening and a 4th order tensorial orientation matrix:

$$ \mathbf{m} = \tfrac{2}{3}(R(\lambda) + Y_\theta)\mathbf{T}_1 : \mathbf{n} $$

The isotropic function $R(\lambda)$ (λ is the cumulated equivalent inelastic strain) is chosen using the *isotropic option below. Note that only ISOTROPIC objects which have no integrated variables may be used (e.g. no recovery). The $\mathbf{T}_1$ matrix is entered using the *T1 command (required).

The tensorial back stress evolves with the following three coupled state variables:

$$ \dot{\boldsymbol{\alpha}}_2 = \dot{\lambda}\left[\mathbf{m} - \mathbf{T}_2\mathbf{x}_2\right] \qquad\qquad \mathbf{x}_2 = \texttt{p2}\ \boldsymbol{\alpha}_2 $$

$$ \dot{\boldsymbol{\alpha}}_1 = \dot{\lambda}\left[\mathbf{m} - \mathbf{T}_2(\mathbf{x}_1 - \mathbf{x}_2)\right] \qquad\qquad \mathbf{x}_1 = \texttt{p1}\ \boldsymbol{\alpha}_1 $$

$$ \dot{\boldsymbol{\alpha}} = \dot{\lambda}\left[\mathbf{m} - \mathbf{T}_2(\mathbf{x} - \mathbf{x}_1)\right] - \dot{\lambda}_r(g)T_1 : \frac{\partial g}{\partial \mathbf{x}} \qquad \mathbf{x} = \texttt{p}\ \boldsymbol{\alpha} $$

The last term is a static (time based) recovery mechanism in the $\mathbf{x}$ variable. It uses a separate recovery potential (CRITERION) object for g and a flow rate magnitude to find $\dot{\lambda}_r$. These are selected with the *g_function and *recovery_flow options for g and $\dot{\lambda}_r$ respectively. In these evolutions, the matrix $\mathbf{T}_2$ is entered similarly to the $\mathbf{T}_1$ matrix, but using the *T2 command.

An additional isotropic hardening component can be added to handle supplemental hardening in the case of non-radial loading. The variable is integrated using the following evolution:

$$ \dot{Y}_\theta = \dot{\lambda}\left[\texttt{Yt\_inf} f_\theta - Y_\theta\right] \qquad f_\theta = 1 - \texttt{abs}\left[\frac{\mathbf{x}}{g(\mathbf{x})}\frac{\partial h(\dot{\mathbf{x}})}{\partial \dot{\mathbf{x}}}\right] \qquad Y_\theta = \texttt{bt}y_\theta $$

The potential function h is a CRITERION object which can be entered using the optional *h_function command. If it is not entered, the g function will be used.

---

[13]explicit forms of this model are available in the ZebFront files Edf_modif.z and Lma_cwsr.z

<POTENTIAL>

Hardening variables will be stored in the following order:

$$\mathbf{h} = [\boldsymbol{\alpha}_1 \quad \boldsymbol{\alpha}_2 \quad \boldsymbol{\alpha}_3 \quad y_\theta]$$

while y_θ is only included when the coefficient `bt` is given.

Syntax:

The syntax understood by this potential is summarized below:

```
**potential delobelle [name]
[ *flow        <FLOW>          ]
[ *criterion   <CRITERION>     ]
[ *isotropic   <ISOTROPIC>     ]
[ *T1                          ]
[ *T2                          ]
[ *g_function                  ]
[ *recovery_flow               ]
[ *model_coef                  ]
   p p1 p2 bt Yt_inf
[ *h_function                  ]
```

Output:

Internal variables added by a `delobelle` potential instance are the following:

prefix	size	description	default
*pn*vi	T-2	inelastic strain tensor	yes
*pn*cum	S	cumulated value of the $\dot{\lambda}$	yes
*pn*_alpha2	T-2	kinematic strain variable $\boldsymbol{\alpha}_2$	no
*pn*_alpha1	T-2	kinematic strain variable $\boldsymbol{\alpha}_1$	no
*pn*_alpha	T-2	kinematic strain variable $\boldsymbol{\alpha}$	no
yt	S	non-radial hardening variable	no

Note that the program does not normalize the value of $\mathbf{n}$ such that $\mathbf{n} : \mathbf{n} = 1$ which could affect the meaning of the behavior and the influence of the anisotropic coefficients.

Compatibility/limitations:

This potential is not valid for the reduced integration behavior. It also does not implement the copy mechanism required for use in the polycrystal. It may not be reasonable to make kinematic state variable coupling, but it should work (in the p coefficients). This model should be valid with the damage mechanics **damage** or other similar `gen_evp` modifiers. Coefficients should not be allowed to vary with VINT or VAUX variables. The use of Y_θ is not exceptionally tested.

Example:

```
***behavior gen_evp
 **elasticity isotropic
     young 80000.0
     poisson 0.32
 **potential delobelle ev
  *flow hyperbolic
```

<POTENTIAL>

```
   K 22.3        m  1.44
   eps0 .202e-8
*isotropic constant
   R0    99.5
*criterion anisotropic orthotropic
   c11 .44667    c22 .58     c33  .666
   c44 0.        c55 1.7     c66 0.
   c12 -.18      c23 -.4     c31 -.26667
*T1 orthotropic
   c11  .1266667 c22  .338   c33  .666
   c44 0.        c55 .66     c66 0.
   c12  .101     c23 -.439   c31 -.2276667
*T2 orthotropic
   c11 .1021667  c22 .3235   c33 .6666666
   c44 0.        c55 1.      c66 0.
   c12 .1205     c23 -.444   c31 -.2226667
*g_function anisotropic orthotropic
   c11 3.346000  c22 3.346   c33 .666
   c44 0.        c55 1.375   c66 0.
   c12 -3.012667 c23 -.333333 c31 -.3333333
*recovery_flow hyperbolic
   K     331.69   n    3.569
   eps0 0.00000019831932773108 % .00354/11900.*2.0/3.0
*model_coef p 11900.0 p1 1656.0 p2 325.5
***return
```

<POTENTIAL>

<POTENTIAL> crystal

Description:
The `crystal` potential type is rather a group of similar potential classes for modeling different monocrystalline slip systems. To construct a single crystal it is normally required to add several different potentials. For instance, a FCC crystal is often constructed with the octahedral and cubic planes modeled in two potentials.

The model includes a localization step, where the stress is resolved into a scalar τ_i acting along the slip direction in the slip plane i (this is the *resolved shear stress*). The localization depends on the precise orientation of slip planes and slip directions, as described in the section <CRYSTAL_ORIENTATION> on page 13.30.

The yield criterion depends on a number of *scalar* kinematic back stress components X_i^j (see page 13.29), which oppose τ_i, and scalar isotropic variables R_i^k modeling the change in resolved shear stress length on plane i. Multiple kinematic components may be specified, but only one isotropic. The other contributions to the isotropic hardening come from latent hardening, i.e. from interactions with other slip systems of the *current* potential (see <SLIP_INTERACTION> on page 13.110), and/or with slip systems of *other* crystal potentials (see <INTERACTION> on page 13.70). The variables are shown schematically below (for the specific case of only one kinematic back stress and all contributions to the isotropic radius contained in R).
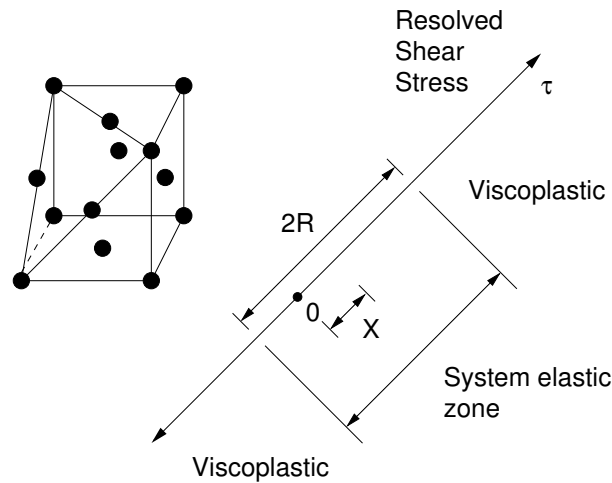
Syntax:
The syntax of each crystalline potential takes the following form:

```
    **potential <CRYSTAL_ORIENTATION> [ name ]
 [ *flow <FLOW>                      ]
 [ *kinematic <CRYSTAL_KINEMATIC>   ]
 [ *isotropic <ISOTROPIC>           ]
 [ *interaction <SLIP_INTERACTION> ]
 [ *rotate <ROTATION>               ]
 [ *store_all                       ]
```

... *continued*

<POTENTIAL>

- The criterion is always: $|\tau_i - x_i| - r_i$ with $x_i = \sum_j X_i^j$ and $r_i = \sum_k R_i^k$, where the term $k = 0$ refers to the isotropic hardening of the current potential (specified with the *isotropic command), and the other terms $k > 0$ reflect the contributions due to SLIP_INTERACTION (see page 13.110), or inter-potential INTERACTION (page 13.70).

- If no *flow command is given, it is assumed to be plasticity (see page 13.43).

- All the ISOTROPIC objects listed later in this manual (page 13.72) which do *not* have an integrated variable may be used for this model (i.e. no static recovery). If no *isotropic command is given, the code will assume *isotropic constant and a value for RO should be given. Only one isotropic hardening object is allowed (but some of these objects contain multiple terms).

- Multiple *kinematic objects may be given.

- Due to the anisotropy of deformation for the single crystals, it is necessary to work in 3D geometries.

- In the absence of SLIP_INTERACTION (see page 13.110), h1=1. and all other values are zero (i.e. only self-hardening).

- The axes with respect to which the slip systems are defined (and thus the slip systems themselves) can be rotated with a *rotation command (see page 2.13 for the correct syntax).

- The *store_all command stores all local associated force variables (such as the resolved shear stresses) as well as the internal hardening variables.

Example:

```
***behavior gen_evp
 **elasticity cubic y1111 162321.0 y1122 78075.0 y1212 110615.0
 **potential octahedral    ev
   *flow norton           K    100.0   n      10.0
   *kinematic nonlinear_phi
                          C   20995.0 D      1105.0
                          phi 0.0      delta 0.0     Xbar   23.8
   *isotropic nonlinear   RO  382.0   Q      7.93    b 2420.0
   *interaction slip      h1  1.0     h2     1.1     h3 1.3
                          h4  1.5     h5     1.7     h6 1.9
 **potential cubic cu
   *flow norton
      K   100.0
      n    10.0
   *kinematic nonlinear_phi
      C   50000.0
      D    1000.0
      phi    0.0
      delta 0.0
      Xbar  -6.0
   *isotropic nonlinear
      RO   382.0
```

<POTENTIAL>

```
      Q     -5.6
      b    2429.0
   *interaction slip
      h1   1.0
      h2   1.2
      h3   1.1
    **interaction iso ev cu
      h    0.2
***return
```

<POTENTIAL>

<POTENTIAL> gen_evp

Description:

The potential object of type `gen_evp` serves as the basic type for classical plasticity and viscoplasticity models with both isotropic variable and an arbitrary number of kinematic hardening variables (c.f. [Lema85]). The potential will accept a wide variety of criterion types, associated and non-associated, as well as a variety of flow rules (plastic and viscoplastic). The dissipation potential for this model is written generally:

$$\Omega_i = f_{cr}(\mathbf{p},\ \boldsymbol{\sigma} - \Sigma\mathbf{X}_i) + \Omega_r(R) + \Sigma\Omega_{\alpha_i}(\mathbf{X}_i)$$

If there are hardening variables, they will be stored in the following order:

$$\mathbf{h} = [\boldsymbol{\alpha}_1\ \ \boldsymbol{\alpha}_2\ \ \dots\ \ \boldsymbol{\alpha}_n\ \ r]$$

where the tensorial variables $\boldsymbol{\alpha}_i$ are the kinematic internal variables (analogue to an offset strain), and r is an internal variable modeling the isotropic expansion or contraction of the yield domain (analogue to an equivalent strain).

Syntax:

The syntax understood by this potential is summarized below:

```
**potential gen_evp [name]
[ *flow        <FLOW>          ]
[ *criterion   <CRITERION>     ]
[ *kinematic   <KINEMATIC> [name] ]
[ *isotropic   <ISOTROPIC>     ]
[ *var_coefs                   ]
[ *store_all                   ]
```

The option `*store_all` is used to make all associated force variables to be stored as well as the internal hardening variables. This allows one to observe directly the effective back stresses or isotropic radius even in the case of coupling.

Other statements may be made about this model:

- The final form of the hardening will be determined by the options `*kinematic` and `*isotropic` which are given by the user. If there is incompatibility with one of the hardening mechanisms with this potential, an error message will be output as the invalid calculation is attempted. Static recovery is allowed in both the isotropic and kinematic variables.

- The type of flow law, $\dot{\lambda}$, and criterion, f, will be determined by the options `*flow` and `*criterion`. Default values for these options are `plasticity` (time independent flow) and `mises` respectively.

- The flow direction is determined by the criterion chosen, which is not necessarily associated.

- The names of the internal variables will be dependent on the choices given by the user. If no name is given for the potential, the potential name (henceforth referred to as *pn* will be "e#" with # being the sequential number of the potential in question (i.e. 1

<POTENTIAL>

for the first potential, etc). In the absence of names for the kinematic variables (kn), default names will be of the form: "pna_#v" with # being the sequential number of the kinematic variable in the potential's kinematic list.

With these comments, the internal variables added by a `gen_evp` potential instance are the following[14]:

prefix	size	description	default
*pn*vi	T-2	inelastic strain tensor	yes
*pn*cum	S	cumulated value of the multiplier $\dot{\lambda}$	yes
kn	T-2	kinematic strain variable	no

Note that the cumulated value of the $\dot{\lambda}$ multiplier is only sometimes equal to the equivalent cumulated inelastic strain (for Von Mises criterion for example, but not for Hill). The current version of the potential does not allow for calculation of the true equivalent for cases where $\int \dot{\lambda} \neq p$.

Example:
An example viscoplastic model with Norton flow, Hill type criterion and kinematic hardening is given here as an example using the `gen_evp` potential. The dissipation potential (flow term only) and criterion may be written as:

$$
\begin{aligned}
\Omega &= [(\boldsymbol{\sigma} - \mathbf{X}) : \mathbf{M} : (\boldsymbol{\sigma} - \mathbf{X})]^{1/2} - R + \tfrac{3D}{2C}\mathbf{X} : \mathbf{X} + (R - R_o)^2/2Q \\
\mathrm{f} &= [(\boldsymbol{\sigma} - \mathbf{X}) : \mathbf{M} : (\boldsymbol{\sigma} - \mathbf{X})]^{1/2} - R
\end{aligned}
\tag{26}
$$

which leads to the evolution rules:

$$
\dot{\boldsymbol{\epsilon}}_{\mathrm{vp}} = \dot{\lambda}\frac{\partial \Omega}{\partial \boldsymbol{\sigma}} = \dot{\lambda}\frac{\partial f}{\partial \boldsymbol{\sigma}} = \dot{\lambda}\frac{2}{3}\frac{\mathbf{M}:(\boldsymbol{\sigma}-\mathbf{X})}{\sigma_{eq}}
\tag{27}
$$

with $\sigma_{eq} = [(\boldsymbol{\sigma} - \mathbf{X}) : \mathbf{M} : (\boldsymbol{\sigma} - \mathbf{X})]^{1/2}$.

```
***behavior gen_evp
 **elasticity isotropic
    young 260000.0
    poisson 0.3
 **potential gen_evp ev
  *flow norton
    n  7.0
    K  400.
  *criterion hill
    hilla 1.      hilld 1.
    hillb 2.      hille 1.
    hillc 3.      hillf 1.
  *kinematic nonlinear  x1
```

---

[14]This of course means in addition to those created by other potentials and the `gen_evp` behavior itself.

<POTENTIAL>

```
   C  30000.0    m  1.0
   D  500.0      M  20000.0
 *isotropic constant
   R0 130.0
***return
```

<POTENTIAL>

<POTENTIAL> gen_evp2

Description:

The `gen_evp2` potential is a modified version of `gen_evp` with different assumptions of hardening and variables. The potential allows use of DIRECT_KINEMATIC objects and RATE_VAR_FLOW laws which can both have arbitrary numbers of integrated variables, and the kinematic law does not limit the calculation of $\mathbf{X}_i$ as a linear modulus function of $\boldsymbol{\alpha}_i$.

Syntax:

The syntax understood by this potential is summarized below:

```
**potential gen_evp [name]
[ *flow        <FLOW>              ]
[ *flow        <RATE_VAR_FLOW>     ]
[ *criterion   <CRITERION>         ]
[ *kinematic   <KINEMATIC> [name] ]
[ *kinematic   <DIRECT_KINEMATIC> [name] ]
[ *isotropic   <ISOTROPIC>         ]
[ *var_coefs                       ]
[ *store_all                       ]
```

Example:

This potential is nominally the same as the original `gen_evp` potential, except for allowing the rate flow type and the direct kinematic types.

```
***behavior gen_evp
 **elasticity isotropic
    young 260000.0
    poisson 0.3
 **potential gen_evp2 ev
  *flow norton
    n  7.0
    K  400.
  *criterion hill
    hilla 1.     hilld 1.
    hillb 2.     hille 1.
    hillc 3.     hillf 1.
  *kinematic armstrong_frederick
    C  30000.0   m  1.0
    D  500.0     M  20000.0
  *isotropic constant
    R0 130.0
 ***return
```

<POTENTIAL>

<POTENTIAL> suvic

Description:
This is the SUVIC model which applies well to ductile rock material such as sodium chloride materials over long term creep loading. There are isotropic and kinematic hardenings with static recovery, as well as evolution in the creep law and changing saturation values for the hardening variables.

$$\dot{\lambda} = A \left\langle \frac{f(\boldsymbol{\sigma} - \mathbf{B}) - R - R_0}{K + K_0} \right\rangle^n$$

$$\dot{\boldsymbol{\epsilon}}_v = \dot{\lambda}\mathbf{n} \qquad \mathbf{n} = \frac{\partial f}{\partial \boldsymbol{\sigma}}$$

$$\dot{\boldsymbol{\alpha}}_i = \dot{\lambda} \left[\mathbf{n} - \frac{\mathbf{B}_i}{B_i'} \right] - \left\langle \frac{J(\mathbf{B}_i) - B_i''}{M_{B_i}} \right\rangle^q$$

$$\dot{r} = \dot{\lambda} \left[1 - \frac{R}{R'} \right] - \left\langle \frac{\|R\| - R''}{M_R} \right\rangle^p$$

$$\dot{k} = \dot{\lambda} \left[1 - \frac{K}{K'} \right] - \left\langle \frac{\|K\| - K''}{M_K} \right\rangle^p$$

$$
\begin{aligned}
\mathbf{B_i} &= A_{1_i}\boldsymbol{\alpha}_i & M_i &= C(A_{1_i}/A_{2_i})^{1/q} \\
\mathrm{R} &= A_3 r & M_r &= C(A_3/A_4)^{1/p} \\
\mathrm{K} &= A_5 k & M_k &= C(A_5/A_6)^{1/u} \\
& \mathrm{B_i'} = B_{i0}' \left[\ln(\dot{\lambda}/v_0) \right]^m \\
& \mathrm{R'} = R_0' \left[\ln(\dot{\lambda}/v_0) \right]^m \\
\mathrm{K'} &= \left[J(\boldsymbol{\sigma}) \ln(\dot{\lambda}/v_0) - B' - R' \right] (\dot{\lambda}/A)^{-1/n}
\end{aligned}
\tag{28}
$$

<POTENTIAL>

Example:

```
***behavior gen_evp
 **elasticity isotropic
      young    18900.
      poisson  0.25
 **potential salt ev
   *criterion mises
   *flow norton_k_variable
      n   4.0
   *kinematic nonlinear   %  short range
      A1 6400.0
      Bp equivalence Bpa0v
   *kinematic nonlinear   % long range
      A1   40.0
      Bp  = Bpa1v
   *isotropic non_linear_recovery
      A    1800.0
      R0      0.0
      Rp  = Rp
    *K non_linear_recovery
       R0    0.04
       A    260.0
       Rp = Kp
   *parameters
      A        6.00e-7
      N        4.0      % must be duplicated!
      vdot0    1.e-13
      sig0     4.63
      R0       1.38
      B01      0.83
      B02      1.25
      m        0.81
***return
```

<POTENTIAL>

<POTENTIAL> 2M1C

Description:
The potential of type `mises_2m1c` exists for the particular case where there are two flow mechanisms which act under a single criterion. This model also allows interaction between the isotropic hardening variable and the kinematic back stresses. The model is particularly useful for accurate modeling of ratcheting phenomenon [Cail95].

$$f = \left[f_1^2 + f_2^2 \right]^{0.5}$$

Syntax:

```
**potential 2M1C [name]
  *criterion    mises_2m1c
    [ A1 <COEFFICIENT> ]
    [ A2 <COEFFICIENT> ]
[ *flow         <FLOW>            ]
[ *kinematic    <KINEMATIC> [name] ]
[ *isotropic    <ISOTROPIC>       ]
[ *coefficient                    ]
    [ C12   <COEFFICIENT>  ]
    [ a     <COEFFICIENT>  ]
    [ beta  <COEFFICIENT>  ]
```

- The model requires giving `mises_2m1c` as a criterion type. This criterion will accept coefficients `A1` and `A2` (scalar) to simulate a localization process in each of the two mechanisms. In this case the stress equivalent terms in the criterion will be calculated as:

$$f_i = J(\mathtt{A}_i \mathbf{s} - \mathbf{X}_{ij}) \quad i = 1, 2$$

with j kinematic hardenings in each mechanism.

- In the event that the isotropic hardening variable is coupled to the kinematic back stress (type `nonlinear_bsi`), the radius will be calculated with kinematic interaction as:

$$R(\boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2) = R_o - \frac{1}{3} kb(\boldsymbol{\alpha}_1 + \boldsymbol{\alpha}_2) : (\boldsymbol{\alpha}_1 + \boldsymbol{\alpha}_2) + Qr$$

A corresponding isotropic interaction is introduced into the kinematic hardening variable:

$$\mathbf{X}_i = \frac{2}{3} [C_{ij}^o + k(1 - br)] \boldsymbol{\alpha}_j \quad i, j = 1, N$$

where i are the mechanisms and j are the kinematic variables in each mechanism.

- The coefficients `a` and `b` indicate that we desire the calculation of the coefficients `C` for the kinematic hardening and `C12` (kinematic interaction) for special forms of the interaction matrix (e.g. zero determinant)

<POTENTIAL>

<POTENTIAL> z6_gen_evp

This potential gives hardening variable evolution in terms of the un-coupled internal state variables and not as a function of the associated forces. The criterion still includes the coupled terms, of course. This type of interaction was given in versions 6 and below. In the case of no interaction this potential is identical to the `gen_evp` potential.

Example:

$$\mathbf{X}_{X1} = \frac{2}{3}C_{X1}\boldsymbol{\alpha}_{X1} + \frac{2}{3}C_{int}\boldsymbol{\alpha}_{X2}$$

$$\mathbf{X}_{X2} = \frac{2}{3}C_{X2}\boldsymbol{\alpha}_{X2} + \frac{2}{3}C_{int}\boldsymbol{\alpha}_{X1}$$

but the evolution of the internal variables has no coupling. The evolution equation for a nonlinear kinematic hardening variable is changed to:

$$\mathbf{m}_{kin} = \mathbf{n} - D\boldsymbol{\alpha}$$

<SINTERING_STRAIN>

<SINTERING_STRAIN>

Description:

The mechanisms of sintering may be represented by a sintering strain ϵ_s.

Syntax:

---

    type
[anisotropic
      a1 COEFFICIENT
      a2 COEFFICIENT
      a3 COEFFICIENT
]
   model_coefficient COEFFICIENT
    ...

The replacements available for *type* are the following

CODE	DESCRIPTION
non_linear	$\dot{f} = -A(f - f_\infty)^n$
	coefficients : A, n, f_∞
	names : `A`, `n`, `f_inf`

The option `anisotropic` allows to enter a non-isotropic strain with the use of the three coefficients `a1`, `a2` and `a3`. The strain is then defined as:

$$\dot{\epsilon}_{11} = a_1 \dot{\epsilon}_s \qquad \dot{\epsilon}_{22} = a_2 \dot{\epsilon}_s \qquad \dot{\epsilon}_{33} = a_3 \dot{\epsilon}_s$$

The following relation must be verified:

$$a_1 + a_2 + a_3 = 3$$

<SLIP_INTERACTION>

<SLIP_INTERACTION>

Description:

The `SLIP_INTERACTION` object is used to model the inter-system hardening of the isotropic variable for single crystal models. In the absence of this option, only self-hardening is taken into account (`h1=1.` and all other interaction parameters equal `0.`). For each crystal potential, the maximum number of interaction parameters is given in the section on `<CRYSTAL_ORIENTATION>` (page 13.30). As an example, the *hardening matrix* describing the inter-system hardening for octahedral slip systems is shown at the end of this section.

Note: hardening between different crystal *potentials* (for instance between cubic and octahedral systems) can be taken into account through the `INTERACTION` object (see page 13.70).

Syntax:

The following models are implemented for slip interaction in single crystals.

CODE	DESCRIPTION
slip	standard Zebulon form.

slip This is the "standard" Zebulon format for full slip interactions described by [Meri91]. The coupled radius R_i' for system i is

$$R_i' = R_0 + \sum_{k=1}^{n} h_{ik} \left(R_k - R_0 \right),$$

where R_k is the radius of slip system k as calculated from the `*isotropic` variable option (e.g. $R_0 + Q(1 - e^{-bv})$).

	Bd	Ba	Bc	Db	Dc	Da	Ab	Ad	Ac	Cb	Ca	Cd			
Bd	h1	h2	h2	h4	h5	h5	h5	h6	h3	h5	h3	h6		Bd	$(111)[\bar{1}01]$
Ba	h2	h1	h2	h5	h3	h6	h4	h5	h5	h5	h6	h3		Ba	$(111)[0\bar{1}1]$
Bc	h2	h2	h1	h5	h6	h3	h5	h3	h6	h4	h5	h5		Bc	$(111)[\bar{1}10]$
Db	h4	h5	h5	h1	h2	h2	h6	h5	h3	h6	h3	h5		Db	$(1\bar{1}1)[\bar{1}01]$
Dc	h5	h3	h6	h2	h1	h2	h3	h5	h6	h5	h5	h4		Dc	$(1\bar{1}1)[011]$
Da	h5	h6	h3	h2	h2	h1	h5	h4	h5	h3	h6	h5		Da	$(1\bar{1}1)[110]$
Ab	h5	h4	h5	h6	h3	h5	h1	h2	h2	h6	h5	h3		Ab	$(\bar{1}11)[0\bar{1}1]$
Ad	h6	h5	h3	h5	h5	h4	h2	h1	h2	h3	h5	h6		Ad	$(\bar{1}11)[110]$
Ac	h3	h5	h6	h3	h6	h5	h2	h2	h1	h5	h4	h5		Ac	$(\bar{1}11)[101]$
Cb	h5	h5	h4	h6	h5	h3	h6	h3	h5	h1	h2	h2		Cb	$(11\bar{1})[\bar{1}10]$
Ca	h3	h6	h5	h3	h5	h6	h5	h5	h4	h2	h1	h2		Ca	$(11\bar{1})[101]$
Cd	h6	h3	h5	h5	h4	h5	h3	h6	h5	h2	h2	h1		Cd	$(11\bar{1})[011]$

<STRAIN_NUCLEATION>

<STRAIN_NUCLEATION>

Description:
This option allows application of different methods from which the nucleation of porosity may occur. **Syntax**:

The nucleation mechanisms are defined as follows:

```
[ crack_like ]
    type
[ yield COEFFICIENT ]
[ porosity_yield COEFFICIENT ]
    model_coefficient COEFFICIENT
        ...
```

crack_like   keyword indicating that the mechanisms of porosity creation takes the form of cracking or "loss of material."

yield   allows to define a value of plastic strain below which there is no nucleation.

porosity_yield   Defines a value for the trace of the stress tensor below which there is no nucleation.

The law of nucleation is given by:

$$\dot{f}_n = A(\ldots)\dot{\lambda}$$

where $\dot{\lambda}$ is the plastic multiplier. The form of the function A is variable according to the type of nucleation chosen. The table below summarizes the possible types of nucleation function:

CODE	DESCRIPTION
constant	$\dot{f}_n = A\dot{\lambda}$
gaussian	$\dot{f}_n = \frac{f_n}{\sqrt{2\pi}s_n} \exp\left(-\frac{1}{2}\left(\frac{(p-\epsilon_n)}{s_n}\right)^2\right)\dot{\lambda}$
exponential	$\dot{f}_n = \frac{B}{\epsilon_0} \exp\left(-\frac{p}{\epsilon_0}\right)\dot{\lambda}$

The corresponding syntaxes are:

```
constant
A COEFFICIENT % A
gaussian
  en  COEFFICIENT  %     εn
  fn  COEFFICIENT  %     fn
  sn  COEFFICIENT  %     σn
exponential
  B   COEFFICIENT  %     B
  e0  COEFFICIENT  %     ε0
```

Where, in the syntax block:
- en corresponds to ϵ_n
- fn corresponds to f_n
- sn corresponds to σ_n
- B corresponds to B
- e0 corresponds to ϵ_0

<THERMAL_STRAIN>

<THERMAL_STRAIN>

Description:
This object is used to define the calculation of a volumetric thermal strain.

Syntax:
The syntax for this object requires only input of the model coefficients (standard form). The types of thermal strain available are the following:

CODE	DESCRIPTION
isotropic	Isotropic thermal dilatation
anisotropic	Anisotropic thermal dilatation

The default type is `isotropic`.

The coefficients for the thermal strains are "secants." That is to say that the thermal deformation ϵ_{th} is given by the relation:

$$\epsilon_{\text{th}_i} = \alpha_i(T, \dots)(T - T_{\text{ref}})$$

where $\alpha_i(T, \dots)$ is the *secant* dilatation coefficient, T is the temperature, and T_{ref} is a reference temperature (zero by default).

NOTE : unexperienced users usually get confused about the exact signification of T_{ref}. Let us consider, to clarify everything, the calculation of the incremental thermal strain at a given time t (it is assumed that the computation starts at $t = 0$ without thermal strain):

$$\Delta\varepsilon_{\text{th}}^{0 \to t} = \alpha(T(t))\,(T(t) - T_{\text{ref}}) - \alpha(T(t = 0))\,(T(t = 0) - T_{\text{ref}})$$

In the previous equation, the dilatation coefficient $\alpha(T)$ is supposed to be measured using T_{ref} as the reference temperature. Do not make any confusion between the initial time, which is the time at the beginning of the computation (usually $t = 0$), and the reference temperature: T_{ref} *is not* related to any particular time; it is just the temperature used as "reference" by the people who did the experiment to *measure* α.

To re-define the reference temperature, a coefficient `ref_temperature`[15] must be input. The method of calculation is schematically shown below:

---
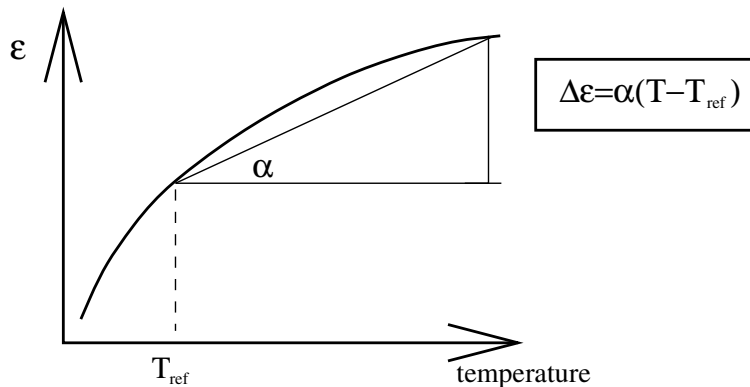
[15]a standard coefficient

<THERMAL_STRAIN>

The coefficients required for the thermal deformation models are given below. All coefficient types and dependencies may be entered for the thermal dilatation coefficients.

isotropic   The isotropic model has only one coefficient for the dilatational secant which is named alpha.

anisotropic   The anisotropic thermal strain object calculates different thermal strains along each axis in the material coordinate frame. The dilatational coefficients names are alpha1, alpha2, and alpha3 to the three material axes.

Example:

```
**thermal_strain isotropic
  alpha      temperature
    10.e-6     25.
    12.e-6    500.
  ref_temperature 100.
```

Chapter 14

Modifiers

<MODIFIER>

<MODIFIER>

Description:
This class is used as a "behavior" wrapper in order to modify the integration method or the formulation in some way. Primarily, these modifiers are used to transform the domain of application for the behavior by providing some translation of the *primal-dual* variable combination, such as is found for corotational large strain modifications.

CODE	DESCRIPTION
lagrange_polar	corotational finite strain equivalent to a Green-Naghdi stress rate formulation (polar decomposition of the deformation gradient)
lagrange_rotate	corotational modification for updated Lagrangian finite strain using an integrated rotation
lagrange_polar_no_J	polar corotational formulation without a density correction
lagrange_rotate_no_J	integrated corotational formulation without a density correction
bifurcation	bifurcation of mechanical solution analysis
auto_step	activates automatic sub-stepping for implicit theta_method_a integration
runge_jacobian	mixed integration method associating explicit (runge_kutta) integration of behavior differential equations with a final Jacobian call (as in theta_method_a) for the computation of the consistent tangent matrix
runge_rollover	replacement of the previous one, that switches to to mixed integration only when the initial theta_method_a integration fails
plane_stress	external wrapper enforcing the plane-stress condition for material behaviors that don't handle this case internally
perturbation	activates calculation of a tangent matrix obtained by perturbation of the loading strain increment tensor

Global convergence may be inhibited by the addition of the finite-strain options, especially corotational frame ones. In this case, it is advised to use small increment steps or automatic time stepping options in the global calculation sequences.

Large deformation methods:
Large deformation formulations in Z-mat are available for the majority of material behaviors[1] based on corotational transformation of the stress-strain problem into an "equivalent material referential." Corotational formulations are implemented because they are applicable to

---

[1]excepting behaviors with explicitly different treatment of finite strain

<MODIFIER>

material models with tensorial internal variables and anisotropic response without modifying the local evolution rules [Lade80]. Description of the models uses the following standard expressions:

$$
\begin{aligned}
\mathbf{L} &= \dot{\mathbf{F}}\mathbf{F}^{-1} \\
\mathbf{D} = \tfrac{1}{2}(\mathbf{L} + \mathbf{L}^T) \qquad \mathbf{\Omega} &= \tfrac{1}{2}(\mathbf{L} - \mathbf{L}^T)
\end{aligned}
\tag{1}
$$

where $\mathbf{F}$ is the deformation gradient and $\mathbf{L}$ the rate of deformation. Both these tensors are non-symmetric. The stretch rate $\mathbf{D}$ and rotation rate $\mathbf{\Omega}$ are symmetric and non-symmetric respectively. These methods require elements of the type `updated_lagrangian` (specified with the option `***mesh` in the `.inp` file).

<MODIFIER> lagrange_polar

The `lagrange_polar` modifier is a corotational formulation for finite strain leading to an equivalent Green-Naghdi stress rate in elastic problems [Gree65, Nagt82]. The stretch rate tensor is transformed into a local strain rate measure through the following expression:

$$\dot{\mathbf{e}} = \mathbf{R}^T \mathbf{D} \mathbf{R}$$

where the rotation tensor $\mathbf{R}$ is found by the polar decomposition of the deformation gradient:

$$\mathbf{F} = \mathbf{R}\mathbf{U}$$

with $\mathbf{R}$ being a pure rotation and $\mathbf{U}$ a pure stretch tensor.

Using the transformed "material" strain rate $\mathbf{e}$, the behavior may be evaluated as in small deformation. An conjugate stress results from the material behavior integration, $\mathbf{S}$ which is transformed to the global Cauchy stress as:

$$\boldsymbol{\sigma} = \det^{-1}(\mathbf{F}) \, \mathbf{R}\,\mathbf{S}\,\mathbf{R}^T$$

<MODIFIER>

<MODIFIER> lagrange_rotate

The `lagrange_rotate` modifier is a corotational finite strain formulation based on an integrated rotation tensor [Lade80]. This method yields an equivalent stress-strain response to a Jaumann-rate formulation but allows tensorial internal variables and anisotropic relations to be used as was in the polar decomposition case [Lade80].

The principle of this method is to always evaluate the material within a local "material" referential. Passing from the global to material referential is made using a rotation tensor in the following relations:

$$
\begin{aligned}
\dot{\mathbf{e}}_{\text{tot}} &= \mathbf{Q}^T \mathbf{D} \mathbf{Q}
\qquad
\begin{aligned}
\dot{\mathbf{Q}} &= \mathbf{\Omega}\mathbf{Q} \qquad \mathbf{Q}_o = \mathbf{1} \\
\boldsymbol{\sigma} &= \mathtt{det}^{-1}(\mathbf{F})\,\mathbf{Q}\,\mathbf{S}\,\mathbf{Q}^T
\end{aligned}
\qquad (\textit{local strain})
\end{aligned}
$$

$$(2)$$

This method requires additional storage at each Gauss point for the non-symmetric rotation tensor, and the local material strain. The name of strain used in the material law is therefore changed to `ETO##` in place of `eto##`. This strain is also observed to be a logarithmic strain.

For the two methods, the nonlinear material tangent $\mathbf{D}_{nl}$ describing the $\partial \Delta \mathbf{S}/\partial \Delta \mathbf{e}$ relationship is modified for the additional large strain non-linearities as follows:

$$
\mathbf{D}'_{nl} = \mathtt{det}^{-1}(\mathbf{F})\,\mathbf{A}\mathbf{D}_{nl}\mathbf{A}^T
\qquad
A_{ijkl} = Q_{ik}Q_{jl}
$$

which relates $\partial \Delta \boldsymbol{\sigma}/\partial \Delta t\mathbf{D}$. The polar decomposition method will of course use $\mathbf{R}$ in the place of $\mathbf{Q}$ in the above.

One may note an improved convergence for conditions where the material behavior calculation of $\mathbf{D}_{nl}$ is best (i.e. implicit θ-method integration with $\theta = 1$). The calculation of the stress is also noted to depend on the determinant of the total value of the deformation gradient ($\mathbf{F}$ from time t_0 to the current time). Nonlinearity in this term (especially in trial solutions during iterations) may limit the convergence of the method.

<MODIFIER>

<MODIFIER> plane_stress

Description:

The `plane_stress` modifier allows any material behavior to be run in plane stress conditions without extra terms being added to the model. This is at the cost of extra local iterations but with the benefit that extremely complex cases can be treated effectively (e.g. multi-mats, runge-kutta models, multi-potential deformations, multiplicative finite strain, etc).

Syntax:
The following options are available after the `**plane_stress_controls` heading.

*skip_first   The code attempts to predict the plane strain effect ahead of time, which in some cases can push the nonlinear computation in the wrong direction. Using this flag prevents that step.

*eps   default from theta method or 10^{-9}

*iter   default from theta method or 200.

Example:
The modifier order is important for this object to be used properly. Some typical examples follow:

```
***behavior gen_evp plane_stress
***behavior gen_evp plane_stress auto_step
***behavior gen_evp lagrange_rotate auto_step plane_stress
```

<MODIFIER>

<MODIFIER> auto_step

Description:

The auto_step modifier applies a "local" method of substepping for any material behavior, in an attempt to pass divergences and improve accuracy without cutting back the global time step.

*divergence *div [num]* takes parameters *div* (real) for the division factor to make when a divergence occurs, and *num* (int) for the maximum number of successive divergences allowed (default 10).

*security *[factor]* set the maximum amount the step can enlarge (e.g. 1.2).

*min_dtime   takes a real value to set the minimum dtime before giving up and calling for a global divergence.

*use_last_tangent   use the last computed tangent matrix instead of averaging the sub-step tangents.

*re_solve   re-solve the step initializing with the sub-step result increment, possibly leading to better global convergence.

*forceit   force sub-stepping, primarily for testing the process.

*limit   takes a list of integrated variable names (VINT) and maximum change values to ensure that any sub-step will not have any greater increment than this one.

*full_step_jacobian   use the resulting computed full-step variable increment to compute a new tangent matrix in place of the averaged sub-step tangents.

Example:

The following is a typical example.

```
***behavior gen_evp auto_step
**elasticity isotropic
   young 170000.0
   poisson 0.30
 **plane_stress
 **potential gen_evp ev
   *flow norton
      n   6.0
      K   800.
   *kinematic nonlinear   X1
      C   3000.0
      D   50.0
   *kinematic nonlinear   X2
      C   3000.0
      D   50.0
   *isotropic constant
      R0  10000.
```

<MODIFIER>

```
***stepping_controls
   *divergence  2. 50
   *min_dtime   1.e-8
   *limit evcum 0.01
***return
```

Note:
For finite strain applications this will only work in the order as in the following example:

```
***behavior gen_evp lagrange_rotate auto_step
```

<div align="center"><MODIFIER> runge_jacobian</div>

Description:

This modifier activates a mixed explicit-implicit integration scheme performed in 2 steps.

(i) integration of the set of material integrated variables V_i using an explicit runge-kutta method:

$$V_i^{t+\Delta t} \;=\; runge\_kutta(t,\ \Delta t,\ \Delta\epsilon,\ V_i^t)$$

with t the time at the beginning of the step, Δt the time increment, and $\Delta\underset{\sim}{\epsilon}$ the strain increment loading.

(ii) once known $V_i^{t+\Delta t}$ calculated during step (i), perform a single implicit iteration to obtain an evaluation of the consistent tangent matrix $\frac{\partial\Delta\sigma}{\partial\Delta\epsilon}$

$$\frac{\partial\Delta\sigma}{\partial\Delta\epsilon} \;=\; calc\_grad\_f(t,\ \Delta t,\ \Delta\epsilon,\ V_i^{t+\Delta t},\ \Delta V_i)$$

where $calc\_grad\_f()$ is the Jacobian calculation function called at each iteration of the implicit `theta_method_a` integration method.

This scheme then combines the benefits of the 2 base local integration methods:

- automatic sub-stepping with error control (`runge_kutta`) efficient for stiff set of differential equations,

- good-quality consistent tangent matrix as provided usually by one-step implicit methods.

and can be used when `theta_method_a` fails to converge, or in replacement of the previously described `auto_step` modifier.

Syntax:

```
    ***material
     *integration runge_kutta ...
    ***behavior   behavior_name   runge_jacobian
 [ ***controls
     *theta   theta  ]
    ***return
```

where the optional command:

theta *theta* allows to specify the θ value used for the tangent-matrix calculation of step (ii). $\theta = 1$ correspond to the fully implicit case (default), while $\theta = 0.5$ may be used to trigger semi-implicit integration.

Example:

```
***behavior gen_evp runge_jacobian
***behavior gen_evp runge_jacobian lagrange_rotate
```

<MODIFIER>

<MODIFIER> runge_rollover

Description:

This definition is an alternative to `runge_jacobian` (see page 14.9), where the mixed scheme described previously is only attempted when a single-step `theta_method_a` implicit integration fails to converge.

Syntax:

```
***material
 *integration theta_method_a ...
***behavior  behavior_name  runge_rollover
[ ***runge_rollover
 *runge  eps   norm  iter nit  min_dtime dtmin  ]
***return
```

where the optional command:

*runge can be used to enter non-default values for the `runge_kutta` integration method parameters (see page 2.11). Default values are *eps=norm=1.e-3*, and no control on the maximum number of runge-kutta steps (*nit=∞*), or the minimum step size during sub-stepping (*dtmin=1.e-19*).

Example:

```
***behavior gen_evp runge_rollover
***behavior gen_evp runge_rollover lagrange_rotate
```

<MODIFIER>

<MODIFIER> perturbation

Description:

This modifier triggers the calculation of a tangent matrix $\left[\dfrac{\partial \Delta \sigma}{\partial \Delta \epsilon}\right]$ obtained by perturbation of each component of the input strain increment tensor $\Delta \epsilon$ (or ΔF for finite-strain models).

This particular scheme may be used for material behaviors that don't implement a proper calculation of a full consistent tangent operator (runge-kutta only ZebFront models for example). In this case, global convergence of FE equilibrium iterations may be greatly improved. However, the increase of global time-step allowed by this option, is somewhat counter-balanced by an increase of local integration cost: for small-strain 3D formulations, one additional integration is needed for each perturbation of the 6 individual components of the symmetric $\Delta \epsilon$ tensor.

Syntax:

```
    ***behavior  behavior_name  perturbation
  [ ***perturbation_controls
    [ *perturb  pert  ]
    [ *symmetrize ]
    [ *one_sided | two_sided ]
  ]
```

where the previous optional command are described hereafter:

*perturb   can be used to set the value of the perturbation parameter
(default value is *pert*=1.e-9)

*symmetrize   this-command activates symmetrization of the tangent operator
(default is no)

*one_sided

*two_sided   those commands control the way the input strain tensor is perturbated to calculate each column of the tangent operator. In the `two_sided` mode (default), two integrations are needed to compute each column of the tangent (perturbation of each ϵ_i component by a value of +/-*pert*), while the `one_sided` option only needs one (perturbation by a value of +*pert* in this case).

Example:

```
***behavior norton perturbation
...
***return
```

<MODIFIER>

<MODIFIER> explicit

Description:

This behavior modifier is used with ABAQUS/Explicit to provide the total integrated corotational strain. One may equally use the `lagrange_polar` and `lagrange_rotate` modifiers, but these duplicate many calculations already done by ABAQUS before entry into VUMAT, and therefore are costly.

<MODIFIER>

<MODIFIER> bifurcation

Description:
This behavior is used to make bifurcation analysis. At each iteration, it find the solution of the following minimization problem :

$$\min_{\vec{n} \in R^3} \left(\vec{n} : \underset{\sim}{\mathbf{C}} : \vec{n} \right)$$

$\underset{\sim}{\mathbf{C}}$ is usually the consistent tangent operator (which means that the solution to the previous problem depends on the time discretization), but may also be the tangent one. The solution vanish to zero when localization occurs. It works with any mechanical behavior, and add the following auxiliary variables :

theta	the first angle of $\vec{n}$
phi	the second angle of $\vec{n}$ (available only in 3D)
det_min	the minimum of the determinant.

Note that the coefficient of the underlying real behavior may depend on these auxiliary variables.

It is possible to specify

```
***bifurcation_controls
  **non_linear_bif
```

to take into account non linear geometry which induces new terms in the minimization, coming from the Jaumann derivative.

Chapter 15

Model Simulation

Model Simulation

Description:
As part of the Z-set package there is a model simulation mode, which can be applied to any differential model as supplied by the user, or used to simulate material behavior for a volume element based on one of the standard behaviors, or a ZebFront behavior (see the developers handbook for a description of the latter). To allow rapid prototyping of models, ZebFront modes are available in either a pure model definition, or (with small additions) to user behaviors defined in this manner.

For mechanical material behaviors, some special functionality is provided. This includes generalized mixed-mode loading, and the visualization of yield surfaces. Note that curve output of a finite element calculation may be obtained using the ****curve** command (in Zebulon), and then fed into the simulator for loading to obtain more detailed output or yield surface visualization.

Syntax:
% Zrun -S *problem* ↵

More Information:
For more information on simulations, please refer to the following manual sections, and example files.

- **Tests** in the directory **$Z7PATH/test/Simulator_test** where there are many examples of input files exercising all the simulator options.

- **Examples** handbook and corresponding example files. There is some information showing basic use (the **Simulation** chapter), and many more examples in the **Material Behaviors** chapter. In fact, most of the behavior outputs are generated with the simulation module.

- **Developer** handbook to see how to make simulation compatible models including ZebFront.

<div align="center">

****simulate

</div>

Description:
This command marks the beginning of a simulator calculation definition. The Z-set program in simulation mode (**-S** switch) will search this command and interpret all the sub-commands until the next ******** level command is reached. More than one simulation block may be included in the input file, which are accessed using the **-N <num>** command line option.

Syntax:
The simulation accepts the following syntax for the problem definition:

> ******simulate**
>   *****test** *test_name*
>   ...
>   *****model**
>   *model definition*
>   *****solver** *solver-type_name*
>   *solver options*
> ******return**

The definition of a *****test** is used to specify particular tests to simulate. The tests will be run through in the order of their appearance, using the default output file prefix of *test_name*. The test *test_name* is required.

In each test, different loading conditions, output, models, etc may be defined. See the following pages for these commands and their syntax.

Options *****model** and *****solver** are available[1] as a means to change the default model definition and the default solver method. It can be a great convenience to define these at the *******-level in simulations where there are many tests of the same material. The command syntax for *****model** is the same as in the *****test** section, as found on page 15.12 as is the command *****solver** found on page 15.14. Note that this includes the *****-level.

Example:
The following is an example of a complete simulation file with a single test definition. See the following pages for descriptions of the individual commands.

```
****simulate
  ***test funny      % define a test name which defines the default output
  **load             % start the loading section
   *segment 100      % 100 outputs per load segment below
            time       sig11 eto22 sig33 eto12 sig23 sig31
            0.0      0.    0.    0.    0.    0.    0.
            1.0      0.    1.e-3 0.    0.    0.    0.
            2.0      0.    1.e-3 0.    .5e-3 0.    0.
            3.0      0.    1.e-3 0.   -.5e-3 0.    0.
            4.0      0.   -1.e-3 0.   -.5e-3 0.    0.
            5.0      0.   -1.e-3 0.    .5e-3 0.    0.
  **model                            % standard model definition with
   *file funny.mat                   % integration, file name, rotation
   *integration runge_kutta 1.e-3    % and other options
```

---

[1]Introduced in 8.2

```
    **yield_surface yield0.test        % make a yield surface output
       *degrees    5.
       *eps        1.e-12
       *component sig22 sig12
       *time       5.0
    **output                           % the default ascii file for output
       time eto22 sig22 eto12 sig12    % is funny.test (from above ***test def).
 ****return
```

***test

Description:

This command marks an individual test condition to simulate. Loadings, output, and model specification will be contained within this option. The output file name will be determined by the test name given after the command. Loadings and outputs may be repeated in the input sequence to create complex cases.

The model definition must be compatible with the solver type chosen. Many simple simulation models are only compatible with the Runge-Kutta integration, with other FEA-specific material models with implicit integration only must be used with the iterative Newton solver. If the model is not compatible, a run-time error message will be issued.

Syntax:

The definition of a test case within the simulation will follow the syntax below:

```
***test     test_name
 **load
 **model type
 **output
 **solver type
 **time_ini
 **time_end
 **var_mat_ini
 **yield_surface
 **error_map
 **constant_parameter
 **simulation_plugin
```

Each of these commands takes at least some extra input. The different sub-commands are all described fully in the following sections. Use of at least one **load** command is required, although multiple entries are possible.

The model must be defined as well, either through the use of a defined default behavior using the ***model** keyword *before* the test instance (see page 15.3. For the explicit solver (more accurate), this may be a simple ZebFront model of type SIMUL_MODEL or a finite element behavior properly modified for the simulation mode[2]. The syntax for a FEM behavior **does not** take a behavior type after the **model** command. The model name will be found in the material file after the command ***behavior**. Specialty simulation models do require the type following **model** in the test definition.

...*continued***Example**:

An example test definition for use with a finite element behavior was given in the previous section (page 15.3). A simulation model (1D simulation only) example follows:

```
****simulate
  ***test relax12
   **time_ini -5.0
   **load
    *file relax12.load 2
```

---

[2]presently (July 1997) all the gen_evp models are implemented as are some ZebFront FEM models; others are in development

```
    **model ddi
      *file relax12.mat
      *integration runge_kutta 2.e-3 2.e-3
    **output time eto sig evcum epcum
****return
```

**constant_parameter

Description:

This option is used to set parameters that are used in the material behavior (temperature for instance). It replaces the `***parameter` bloc in a standard computation, and, as its name suggests, only allows constant parameter values.

Syntax:

---

    constant_parameter *param1 value1 [param2 value2 ...]*

Example:

```
**constant_parameter
  temperature 200.
  depth       60.
```

**error_plot

Description:

This option is used to get error maps for integration algorithms Under non-proportional loading.

Syntax:

The error maps to output are defined in the following manner:

**error_map *output_name*
 *component   *comp1 comp2*
 *direction1 *dir*
 *direction2 *dir*
 *make_contour
 *number   *num*
 *scale   *factor*
 *time   *times*

*component

*direction1

*direction2

*make_contour

*number

*scale

*time

Example:

```
**error_map shear_error.test
 *time      20.    % after loading to the yield surface
 *scale     0.1    % ten percent strain
 *make_contour      % look at with Zmaster shear_error
```

**load

Description:
This command defines a segment of loading for the simulation. The load commands are executed in the order they appear, and there can be any number of loads for the problem. Blocks of loading defined seperately are usefull to change control, or apply cycles in between single segements of loading.

The command looses some coherence in an attempt to give additional options, and due to the fundimental difference in the loading for fem behaviors and the generalized simulator models.

Syntax:
Simulation loading is given with the following syntax:

```
**load [ cycle ]  ncycle
 *rate   var  rate for  dval
 *rate   var  rate stop_at  break_var  dval  dtime
 *segment rate   [num ]
 *segment   [num ]
   loading table
 *file filename  num
```

The `cycle` keyword indicates that the loading is to be repeated a given number of times. This may also be useful in the rate loading case for switching between rates (see example following).

num The number of output points between each given loading segment in the *loading table*.

ncycle The number of times the loading segment will be run in the event of the `cycle` keyword.

loading table a tabular form which describes the loading for the simulation. The table should have `time` as the first column, followed by an appropriate list of imposed variables. For tensor loading with fem behaviors, the size of the behavior (dimension) will be determined from the number of components given. Thus giving 4 variables in small deformation will give 2D behavior, while 6 gives 3D. Note that some models like the crystal potentials require 3D and thus 6 componnets to be given. External parameters are imposed at this level as well, using the prefixed nameing `param:`*var_name*. **Note:** initial values are required.

*rate this option is used for rate loading in the **generalized simulator only** (i.e. not for fem behaviors). The command allows simple rate loading to be defined for a given duration (with the `for` keyword), or with breakpoints which are to be determined (with `stop_at`).

*segment a segment of loading. The optional keyword `rate` indicates that values are in rate form.

*file indicates that the loading table will be given in the external ASCII file with name given by *filename*. The syntax is exactly that desribed by *loading table* above. Note if you use FEM output from a ****curve** option the leading pound sign must be removed from the variable list.

...*continued***Example**:

An example with multiple load segments and cycles follows. Note that the second load segment uses a time variable offset by the ending of the first segment.

```
****simulate
  ***test biaxe
   **load
    *segment time sig11 sig22    sig33 sig12
             0.0  0.0   0.0      0.0   0.0
             1.   0.    100.0    0.    0.0
   **load cycle 4
    *segment
             time sig11 sig22    sig33 eto12
             0.0  0.0   100.0    0.0   0.0
             1.0  0.0   100.0    0.0   0.02
             3.0  0.0   100.0    0.0   -0.02
             4.0  0.0   100.0    0.0   0.0
   **model
     *file biaxe.sim
     *integration runge_kutta 1.e-3 1.e-3
   **output time eto22 sig22 eto12 sig12 evcum
****return
```

The second example imposes an external parameter `temperature` which can be used in the behavior through variable coefficients or a parametric strain definition.

```
****simulate
  ***test genevp_variable_temp
   **load
    *segment time sig11 sig22    sig33 sig12 param:temperature
             0.0  0.0   0.0      0.0   0.0   0.0
             1.0  0.0   210.0    0.    0.0   0.0
             2.0  0.0   210.0    0.    0.0   100.0
   **model
     *file genevp_variable_temp.sim
     *integration runge_kutta 1.e-2
   **output time eto22 epcum sig22 temperature R0 C sig::mises
****return
```

...*continued*Another useful loading employs the rate form to convienantly give a pre-loading, followed by an anternating strain rate:

```
****simulate
  ***test rate_loading
   **load
    *segment 5
       time     sig11  eto22 sig33 sig12
       0.0      0.     0.     0.    0.
       1000.    0.     0.01   0.    0.
   **load cycle 8
    *segment rate 5
       time     sig11 eto22  sig33 sig12
       4.       0.    0.004  0.    0.
```

```
      400.    0.    0.004  0.    0.
   **model
     *file rate_loading.sim
     *integration runge_kutta 5.e-2
   **output time eto22 sig22
****return
```

**model

Description:
This command defines the model to be simulated in the current test.

Syntax:
One specifies the simulation one time per test using the following syntax:

```
**model [ type ]
 *coefficients
     coef list (constant)
 *file   name
 *integration INTEGRATION
 *initial_value
      var_name value
```

If the optional model name *type* is given after the ****model** command, the model will be of the generalized simulation type (not fem compatible). In this case, the model coefficients will be read below the ***coefficients** command, or in a file with the ***coefficients** command in it (terminated with ***return**). Otherwise the ***file** command must be used to specify the external file name with the fem compatible behavior (standard behavior file as described in the chapter "Material File").

*file gives the file name for a *behavior* type model. This can be one of the standard finite element behaviors, or a custom ZebFront behavior. Note that the filename may be the same as the input file name (including the suffix). The file will be scanned for the *****behavior** keyword. We normally suggest putting the behavior definition at the end of the input file. If the material definition is provided in the main simulator input file the command ***this_file** can be used instead of ***file**.

*integration defines the integration method. This command is equivilent to that for a FEM material. Currently only the explicit integration (i.e. Runge-Kutta) methods are supported by the simulator.

*rotation defines a material rotation which will be affected on the gradient/flux combination (for tensorial variables) before and after the loading steps. Note that the rotation defines the transition from global to material as in the finite element method.

*. . . continued***Note**:

In the event of rotation and tensorial integrated variables, the integrated variable values which get output are in the *material* coordiante system. This will change in the future sometime, so tests and examples which depend on that will change.

**output

Description:
This option is used to create an ASCII file with the output values from the simulation. Output is in column format, with a heading of the variable names requested commented with the `#` character.

Several output files may be specified, while the default file name is the problem name (without suffix) appeded with `.test`.

Syntax:
The yield surfaces to output are defined in the following manner:

> **output [*filename* | *variable_list*]
> [*file *filename* *variable_list*]
> [*sido]
> [*precision *digits*]
> [*small *epsilon*]
> [*frequency *options*]
> [*limit_output_var *function*;]

variable_list   a list of variables to be output. The available variables consist of the var-int and var-aux variables listed when the program is run with the `-v` command line switch, and the imposed external parameters.

file   used to specify an output filename.

sido   output compatible with the sidolo program and graphical utilities.

precision   gives the number of significant *digits* (`3` by default) with which the variables are written.

small   specifies a small value *epsilon* (`1.0e-9` by default) below which the (absolute) output value is considered zero. Note: this command is not related to the global parameter `Solver.SmallForTest`, which plays a similar role for the test output of the finite element solver.

frequency   similar to the `***output **frequency` command of the finite element solver (see the Z-set user manual).

limit_output_var   defines a *function* of one or more output variables (or of `time`) which inhibits output if its function value is smaller than 0.5.

Example:

```
**output example.test
   time sig11 sig22 evcum

**output evcum damage

**output
 *file strain.test time eto11 eto22 eto33 eto12
 *file stress.test time sig11 sig22 sig33 sig12
```

**solver

Description:
This command defines the solution method for the simulation. The default solver is an explicit Runge-Kutta method. In some cases, the Runge-Kutta integration may not be available for a material model, or greater efficiency can be achieved with use of the implicit integration. However, use of an implicit solution allows the possibility of divergence. Which approach to use varies greatly with the problem at hand, and some experimentation and experience may be required to find the best choice.

Many of the convergence control options below follow the same syntax as in the Zebulon FEA solver. In fact, the solution parallels very closely the RVE element, but gives improved efficiency and convenience with the other simulation options.

The current solvers available are as follows[3].

CODE	DESCRIPTION
explicit	default explicit solution
newton	iterative solution.

Explicit method:
The solution of mixed loading in the explicit solver requires some additional equations for the model `derivative` function (the function returning rates for all state variables as a function of the current state). This discussion applies primarily to the mechanical solution procedure, while other simulation models would have a similar formulation requirement.

Fundamentally, because the solver needs to support a mixed combination of stress and strain rates, we need to write the complete equation for the rate of change in stress:

$$\dot{\boldsymbol{\sigma}} = \mathbf{D}_{el} : [\dot{\boldsymbol{\epsilon}}_{to} - \dot{\boldsymbol{\epsilon}}_{in} - \dot{\boldsymbol{\epsilon}}_{th} - \ldots] + \dot{\mathbf{D}}_{el} : \boldsymbol{\epsilon}_{el} \tag{1}$$

For rate dependant behaviors, $\dot{\boldsymbol{\epsilon}}_{in}$, $\dot{\boldsymbol{\epsilon}}_{th}$, and $\boldsymbol{\epsilon}_{el}$ are known, while for rate independent behaviors the inelastic strain rate is a function of the total strain rate, normally of the form:

$$\dot{\boldsymbol{\epsilon}}_{in} = \dot{\lambda}\mathbf{n} = \frac{\mathbf{n} : \mathbf{D}_{el} : \dot{\boldsymbol{\epsilon}}_{to}}{\mathbf{n} : \mathbf{D}_{el} : \mathbf{n} + H} \tag{2}$$

This term, while not greatly complicating the solution, may not be handled in the simulation solution for a particular model[4]. In that event a rate dependant flow law must be used, for example using a norton law with very small viscosity to approximate rate independence.

The basic solution proceedure rearranges the mixed equations to first solve for the total strain rates, and then resubstituting them into the basic rate equation to find *dsig*. For example, a 2D solution could take the form:

$$\begin{bmatrix} \dot{\sigma}_1 \\ ? \\ ? \\ \dot{\sigma}_4 \end{bmatrix} = \mathbf{D}_{el} : \begin{bmatrix} ? \\ \dot{\epsilon}_{tot_2} \\ \dot{\epsilon}_{tot_3} \\ ? \end{bmatrix} - \mathbf{D}_{el} : [\dot{\boldsymbol{\epsilon}}_{in} + \dot{\boldsymbol{\epsilon}}_{th}] + \dot{\mathbf{D}}_{el} : \boldsymbol{\epsilon}_{el} \tag{3}$$

---

[3]versions before 8.2 do not allow the `explicit` keyword, it is activated by the absence of a `**solver` entry

[4]starting with 8.2 rate independent plasticity is handled by `gen_evp` and some ZebFront demonstration models

From which the following equation would be extracted:

$$\begin{bmatrix} D_{el_11} & D_{el_14} \\ D_{el_41} & D_{el_44} \end{bmatrix}^{-1} \begin{bmatrix} \dot{\sigma}_1 1 \\ \dot{\sigma}_1 2 \end{bmatrix} = \begin{bmatrix} \dot{\epsilon}_{tot_{11}} \\ \dot{\epsilon}_{tot_{12}} \end{bmatrix} = \tag{4}$$

Syntax:
The solver syntax accepts a number of options which determine the convergence and automatic time stepping controls (primarily applicable to the newton solver). syntax:

```
**solver [ type ]
*algorithm algo-type
*automatic_time
*divergence factor
*iteration iter
*iter_optimal opt-iter
*max_dtime max-time
*min_dtime min-time
*ratio ratio
*security sec
```

*algorithm

*automatic_time

*divergence

*iteration

*iter_optimal

*max_dtime

*min_dtime

*ratio

*security

**yield surface

Description:
This option is used to create an ASCII file with the yield surface data at a load segment start or end time. Any number of yield surfaces may be given for a single test. The output files contain a list of the entire flux variable values for the surface taken in order, followed by the angle.

Syntax:
The yield surfaces to output are defined in the following manner:

```
**yield_surface output_file_name
*time        time0 [ time1 time2 ...  ]
*criterion   num
*potential   num
*component   comp1 comp2
*degrees     degrees
*angles      angle0 [ angle1 angle2 ...  ]
*factor      factor
*eps         eps
*rate      [ rate0 rate1 rate2 ...  ]
*find_offset
*offset      offset values
```

*time A list of one or more real values *time0* [*time1 time2 ...*] to define the time at which the yield surface is evaluated. The times can be any time from 0.0 onward. In the event that multiple times are given, the surface scans will be given in the same file seperated by two blank lines.

*criterion This gives the criterion name which will be used for the surface. They are arbitrary values to match with zero or the rate if given.

*potential A `gen_evp` behavior potential which will be used for the criterion. By default all potentials input will be used to establish the material criteria for flow.

*component Two strain names for the two flux components which are scanned[5]. An example would be to give `sig11 sig12` for the components.

*degrees The sweep angle which will be used for each step in the surface. Note that fineness of the surface depends on this, but also that the sweep center be in the center of the surface. Being close to the surface in one point increases the number of output points because it dominates the "point of view."

*angles Instead of using the sweep angle to define the steps, a list of angles (in degrees) *angle0 angle1 angle2 ...* can be specified. If both ***degrees** and ***angles** are specified, the ***degrees** command will be ignored.

---

[5]unfortunately, gradient values cannot yet be used to scan for strain space yields surfaces, etc.

*factor   A magnitude of the flux gradient which is considered large for the surface. Look in the output file for bad value lines (marked with a comment line). If there are bad values, increase the factor. The default value is 400.

*eps   A positive real value *eps* specifying the degree of convergence in the surface. The actual value depends on the strain rates as specified by the *rate command.

- If neither *eps nor *rate commands are given, then the default value is 1.e-1.
- If no *eps command is given, and the *rate command is given *without* specifying any strain rate, then the default value is 1.e-1.
- If no *eps command is given while the *rate command is given *with* one or more strain rates, then the default value is 1.e-6 times the average of the specified strain rates.
- On the other hand, if the *eps command is given, but the *rate command is not, then the actual value is *eps*.
- If the *eps command is given while the *rate command is given *without* specifying any strain rate, then the actual value is 1.e-12 times *eps*.
- Finally, if the *eps command is given, and if the *rate command specifies one or more strain rates, then the actual value is *eps* times the average of the strain rates.

*rate   Optional rate values for an equipotential surface. If more than one value is given, the surfaces will be placed in the same file with two blank lines between them. The default is zero.

*find_offset   This command is used to find the surface when the current position is outside of it. A large rate value will be used to hopefully expand the surface such that the current position is inside, and an average of that surface will be used to estimate the center. An optional real value following the command sets this large rate factor, while the default is quite arbitrarily 1.0.

*offset   Allows setting the actual offset flux variable (the estimated difference between current position and yield center) in place of the automated method *find_offset (not recommended). Each component of the flux tensor should be specified.

Example:

```
**yield_surface yield_find_offset.test
*degrees    5.0
*factor     1000.0
*find_offset
*time       0.0 50. 200. 500.
*time       1000.
*rate       0.0 1.e-9 1.e-6 1.e-3
```

Chapter 16

Optimization

Introduction

Description:
The version 8.0 of Z-set introduces a generalized optimization module which may be used to identify material coefficients, optimize geometry, etc. The optimizer will modify tokenized parameters in a different user specified ASCII files in order to minimize the combined error of a variety of tests. Each test will generally consist of one or more shell scripts or sub-processes used for "simulation" of the test, and a certain method of comparison with experimental, reference data, or optimal condition. No explicit assumption is made to the nature of simulation method so these simulations may be made using the Z-set programs internally, or by another means. The real strength of this method is one can obtain the best comprehensive approximation to many data sets, even if they are theoretically over-constrained.

The optimizer problem and its solution are defined in an input text file, similar to that for the other main program types. The optimizer uses a template file for definition of the parameters to be modified.

Basic Concepts and Notations:
Optimization problems are formulated in Z-set in the standard form,

$$\text{minimize} \quad \mathcal{F}(x) = \frac{1}{2} \sum_{i=1}^{N} w_i (f(x, t_i) - y(t_i))^2$$

$$= \frac{1}{2} \sum_{i=1}^{N} w_i (f_i(x) - y_i)^2 \tag{1}$$

$$\text{by changing} \quad x \in S$$

$$\text{such that} \quad g_j(x) \leq 0, j = 1, n_g \tag{2}$$

$\mathcal{F}$ is the cost function (scalar), g is a vector of constraints, x are the parameters to be optimized, t_i tags the experiment (experiment number, time, ...), and w_i is the weight associated to experiment i. A variable x (set of parameters) such that $g_j(x) \leq 0$, $j = 1, n_g$ represents a feasible point (vice versa infeasible). Z-set's optimizers are primarily meant for parameter identification of material behaviors. Therefore, the default cost function $\mathcal{F}$ is the least-square distance between experiments and simulations, and constraints g are used to bound and/or to relate parameters with each other. Of course, other general type of optimization problems can be addressed.

There are two main categories of optimization methods, local and global optimizers. Global optimizers seek x^* such that

$$\mathcal{F}(x^*) < \mathcal{F}(x), \ \forall x \in S$$

Local optimizers look for x^* such that

$$\mathcal{F}(x^*) < \mathcal{F}(x), \ \forall x \ \text{ such that} ||x - x^*|| < \epsilon$$

Typically, local methods iterate from a set of variables x in the search space S to another based on information gathered in a neighborhood of x. Zeroth order optimizers use exclusively

the value of $\mathcal{F}$ and g. First order methods additionally use $\mathbf{grad}\mathcal{F}$ and $\mathbf{grad}g$, second order methods hessian$\mathcal{F}$ and hessian$g$ (or an approximation of $\mathbf{grad}$ and hessian). Global optimizers typically rely on pseudo-stochastic transitions in the search space in order to be able to escape local optima (we do not consider optimizers based on enumeration of all possible local optima). Practically, an important difference between global and local optimizers is that global optimizers are slower to converge, but offer greater guarantees on the quality of the solution produced. In many cases, convergence of global optimizers is so slow that a solution cannot be found in a reasonable time.

Optimization methods can also be divided into methods that explicitly handle constraints (2) (SQP) and the others (Levenberg-Marquardt, Simplex, evolutionary algorithm). Penalizing f is a simple way of transforming a constrained optimization problem into an unconstrained optimization problem:

$$\text{minimize} \quad \mathcal{F}_p = \mathcal{F}(x) + \sum_{i=1}^{n_g} p_i \text{max}(0., g_i(x))^\alpha$$

where p is a vector of (positive) penalty parameters. The exponent α is usually taken larger than 1 (typically 2) for gradient based optimization methods (in order to ensure differentiability). The tricky aspect of penalization is in choosing p. If p is to small, the solution to the optimization problem will not satisfy the constraints. On the contrary, if p is taken too large, convergence to the optimum might be difficult. Optimizers that explicitly handle constraints do not require that the user specifies p. Further details on optimization in mechanics can be found in [Gür92].

Four principal optimizers are available in Z-set: Levenberg-Marquardt, simplex, SQP, and an evolutionary algorithm. They span the different categories of optimizers mentioned earlier. A rapid description of their principle can be found in the relevant sections.

Exceution proceedure:
`% Zrun -o` *problem* ↩

****optimize

Description:
This keyword marks the start of an optimization command sequence, which will be terminated by the next ****-level command.

Syntax:
The syntax is as follows:

```
    ****optimize   type
      ***files ...
      ***values ...
      ***shell ...
      ***zrun ...
      ***compare ...
 [  ***enforce ... ]
 [  ***function ... ]
 [  ***convergence ... ]
 [  ***evaluate ...  ]
 [  ***constraint ...  ]
 [  ***linear_constraint ...  ]
    ****return
```

Different optimizer types are available by substituting keywords for *type* from the following:

CODE	DESCRIPTION
nelder_mead	nelder-mead (aka simplex) method (slow but it gets there)
levenberg_marquardt	Levenberg-Marquardt method. (the classic for identification)
augmented_lagrangian	augmented lagrangian dual method for constrained optimization
evolution	evolutionary stochastic method, slow but escapes local minima

Anatomy of an optimization:
All the optimization methods rely on a centralized method of evaluating the error function, and modifying the simulation using the variables being optimized. Error functions will be computed using a weighted sum of reference-simulation comparisons specified using the ***compare commands. The variables of the optimization are specified in the ***values section, and must correspond to one or more entries in the "optimization" files listed in ***files. These optimization files are in fact templates for real files, which alter the simulation result of commands listed in ***shell or ***zrun entries. The optimizer thus constructs new input files for the simulations, with the current optimization variables inserted in the appropriate locations.

The figure below shows a basic diagram of the interaction between the optimizer and any number of sub-simulations which generate the data to be compared with experimental results.
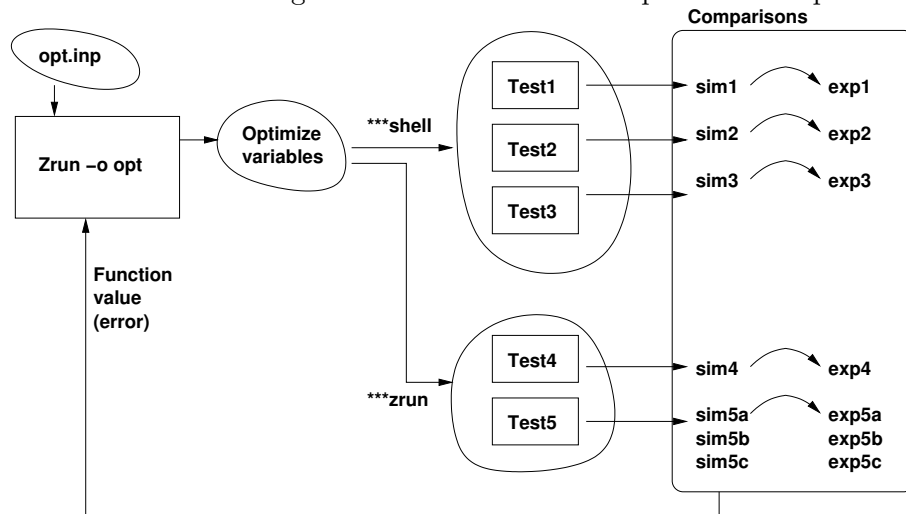
In general (hopefully) the number of simulation-experiment comparisons will lead the problem to be over-constrained. Its the optimizers job then to find the best fit. If certain experiments are "important" the user will employ weights on the comparisons functions to make them more dominant in the function evaluation. Remember that the best, must robust results will be found with many diverse experiment conditions. Repeated experiments which merely provide a slight variation in response should be avoided, while complex experiments with many interacting effects should be emphasized.

Recommendations:
Some comments follow which are purely the personal preferences of the author, but can probably help ahead of time with the management of typical real-life optimization projects. The fact of life is that optimization involves many trials of different models, simulations, and overall rapid iteration towards the solution – both by the code and by the user. Also it is relatively easy to find oneself in a situation where, when lightly "tweaking" some parameters, the last best solution gets lost. It is really important to maintain control of the changes in input files, models, coefficients, etc in order to safeguard against loosing valuable time. Some hints are therefore:

- Use a hierarchical structure for different stages in the analysis, and keep the number of files in each directory very specific to *one task*. That is, if you want to modify the initial values dramatically, or continue from a previous solution, make a new directory, and copy the files before running. A typical directory structure could be:

```
BasicIdentification/
    exp_files/
        ..
    trial1/
        Makefile
        simulation.inp
        levenberg.inp
        simplex.inp
    trial2/
        Makefile
        simulation.inp
        levenberg.inp
        simplex.inp
    continue2/
        Makefile
        simulation.inp
        levenberg.inp
```

  and so on.

- A Makefile can ease the work of cleaning out a lot of secondary files, but more importantly it is a very good way to clean those files without the risk of deleting important files by mistake. I (RF) always set up a makefile more or less as follows:

```
all :

clean :
        Zclean -a
        rm -f *.best
```

  Remember to use tabs for the target lines. to clean the directory one then issues
  `make clean`

- It's helpful to have the experiment (reference) files is a centralized location, as shown above, but instead of using absolute path names use relative ones. In `trial2` for example an experiment file can be accessed[1] as `../exp_files/exp1.dat` In this way the project can be moved without everything breaking. To start a whole new iteration then, one just copies the `BasicIdentification` directory elsewhere and the work starts.

---

[1]this works in Win32 platforms the same

Example:

This example is from `EXAMPLES-MAT/Identify-in738/STEP1`. First is the template file for the material definition `in738.tmpl`:

```
*coefficients
  young    149650.0000
  n        ?n
  K        ?K
  n2       ?n2
  K2       ?K2
  C1       ?C1
  D1       ?D1
  R0       80.0
***return

****optimize levenberg_marquardt
 ***convergence
      perturb 0.06
      lambda0 5.0
      iter    60
 ***zrun Zrun -Q -S simulate
 ***files in738
 ***values
  **auto_init_from_file levenberg.best
      K    700.             min  600.     max  5000.
      n    4.47             min  1.2      max  20.
      K2   500.             min  200.     max  5000.
      n2   35.              min  3.       max  75.
      C1   290.             min  3.0      max  800.
      D1   600.             min   5.      max  5000.
  ***compare
   g_file_file tenx2.test   1 2 ../EXP/tenx2.exp    1 4
   g_file_file tenx3.test   1 2 ../EXP/tenx3.exp    1 4
   g_file_file tx6x2x6.test 1 2 ../EXP/tx6x2x6.exp 1 4
   g_file_file tx6x3x4.test 1 2 ../EXP/tx6x3x4.exp 1 4
   g_file_file cr410.test   1 2 ../EXP/cr410.exp    1 3
   g_file_file frlx3.test   1 2 ../EXP/frlx3.exp    1 4
****return
```

***compare

Description:

The option ***compare constructs the function to be minimized. Four comparisons are possible. It is always possible to indicate a relative weight adding [weight *vweight*] where *vweight* is the relative weight.
The function to the minimized by the optimizer is given by:

$$\mathcal{F} = \sum_i \mathcal{F}_i$$

where $\mathcal{F}_i$ is the function constructed by a ***compare instruction.

Example:

In this example, x and y are function arguments, and a, b, c are optimization variables.

```
****optimize levenberg_marquardt
  ***function f1     ?a*x^2.  +   ?b*x   +   ?c + y;
  ***compare  i_func_file f1 1 2 3 teri.dat
  ***values
       a 1. min -10. max 10.
       b 1. min -10. max 10.
       c 1. min -10. max 10.
  ***convergence
****return
```

Note:
It is recommanded to normalize the functions involved in the optimization ($\mathcal{F}$ and the constraints).

Note:
If one exclusively wishes to minimize a function f subjected to a constraint, one could proceed as follows :
In the "master" file, optimize.inp

```
****optimize <OPTIMIZER>
 ***function f ?a * exp(-1. * ?b);
 ***constraint cos(a - b);
 ***compare  i_func_file  f  1  unreachable_goal.dat
 ***values
    a  1.  min 0.  max 10.
    a  2.  min 2.  max 5.
 ***convergence
    ...
****return
```

where the file *unreachable_goal.dat* contains a lower bound on *f*, for example," 0." here. The optimizer will minimize the distance between the lower bound in the reference file and *f*. Note that if the optimizer is Levenberg-Marquardt, the lower bound should be near the real minimum of the function, otherwise the Levenberg-Marquardt approximation might be poor and convergence impaired.

***compare t_file_file

Description:
This comparison is used to compare two files (names *fname1* et *fname2*) with a time-weighted averaging. Files are "columns" files containing doubles. For each file, one considers a relation $y_i(t)$, $i = 1, 2$ interpolated from columns *y1* and *t1*. To compare two files, one considers the instersection of columns *t1* and *t2*. One defines

$$t_- = \max\left(\min_{t \in t1}, \min_{t \in t2}\right) \qquad t_+ = \min\left(\max_{t \in t1}, \max_{t \in t2}\right)$$

The function to be optimized is given by:

$$\mathcal{F}_i = \frac{1}{2(t_+ - t_-)} \int_{t_-}^{t_+} (y_2(t) - y_1(t))^2 \, dt$$

The optimization variables x should affect one of the two files *fname1* or *fname2*.

Note:
Because of the time weighting of the error, the density of comparison points is not important for the comparison function (although more points will be more accurate). Also, if the time scale of a test changes this method can totally miss important features of the response. For example, if a hold-time loading profile of 10s-300s-10s is applied, the emphasis will be on the response during 300s. Any details of the 10s segments will essentially be lost.

Syntax:

---

  t_file_file *fname1 t1 y1 fname2 t2 y2*
          [**weight** vweight]

**compare g_file_file

Description:

This comparison is a generalized-file-file method, based on point densities. The user therefore has to think about the distribution of comparison points (either in the simulation or reference files) in order to best control the quality of error estimation. Either file (ref or simulation) can have more points, and the points of the *smaller* will be interpolated between points of the *larger* file. This assumes that the larger file will have points who's linear segment will more closely approximate the real curve.

Files must contain continous "column" data of real (floating point format) values. Lines can be commented with `%` or `#`.

The function to be optimized is given by:

$$\mathcal{F}_i = \frac{1}{N} \sum_k^N \left[\frac{y_{s_k} - \bar{y}_k}{|y_{s_{ref_k}}|} \right]^2$$

with $\bar{y}_k$ being the interpolated value from the smaller file, and y_{s_k} the test value from the smaller file. $y_{s_{ref_k}}$ is the points value in the reference file ("experiment" file), which may be an interpolated point if that file was smaller.

Syntax:

> `g_file_file`   *sim-file sx sy exp-file ex ey*
>   [`weight` vweight]

---

sim-file is the simulation file, which the optimization variables x should be changing, *exp-file* is the "reference" which is the goal (should not change during optimization). *sx* and *sy* are the x and y columns of the simulation file, and *ex* and *ey* are the x and y columns of the reference file.

Note:

One is advised to make sure that the x variables are continuously increasing, as a comparison of multi-valued functions or data curves are not allowed. In normal use, time makes a very useful x variable, although a control parameter such as strain could be used as well.

The measure of error may differ quite significantly from the `t_file_file` output, so if it is desired to mix the two types of comparison, use of the weight values will be very useful.

***compare i_file_file

Description:

allows to compare two files (names *fname1* et *fname2*). Files are "columns" files containing doubles. Column *c1* of file *fname1* is compared with column *c2* of file *fname2*. Both files must have the same number of lines. The function to be optimized is given by:

$$\mathcal{F}_i = \frac{1}{2N} \sum_{i=1}^{N} (y_{c2,i} - y_{c1,i})^2$$

where N is the number of lines. The optimization variables x should affect one of the two files *fname1* or *fname2*.

Syntax:

i_file_file *fname1 c1 fname2 c2* [**weight** vweight]

***compare i_func_file

Description:
This comparison is similar to `i_file_file` except that a function will be evaluated for all the x values of the reference file, and the values will be compared directly.

The function to be optimized is given by:

$$\mathcal{F}_i = \frac{1}{2N} \sum_{i=1}^{N} (funame(t_{1,i} \ldots t_{n,i}) - y_i)^2$$

Syntax:
The following syntax is used here:

i_func_file *funame* $t_{i,1}$ ... $t_{i,n}$ *y* *flname*
 [weight vweight]

funame is the name of a function defined under ***function**, *flname* is the name of a "column" file. $t_{i,1} \ldots t_{i,n}$ are the columns id's representing the n arguments of *flname* (other than optimization variables that also can be arguments of the function). y is the column of *flname* representing the function values associated with the n–uplets $(t_{i,1} \ldots t_{i,n})$.

***constraint

Description:
The ***constraint option allows to create constraints that relate the different variables. Constraints are functions that need to be less than or equal to 0. When this option is used, an OPTIMIZER need to be called that can handle constraints (for example, levenberg_marquardt cannot do it).

Syntax:
The syntax is:

```
***constraint FUNCTION [ lambda0 ]
```

where *lambda0* is an optional value for the initial lagrange multiplier associated with the constraint.

Example:

```
***constraint A - b; 0.01
```

In this case, the optimizer will change A and b such that $A - b \leq 0..$

***comparison_constraint

Description:

The ***comparison_constraint option can be used to add constraints that force the solution near some critical points of the reference curves. Note that there may be no solution satisfying the constraint. In this case an appropriate value of the convergence parameter constraint_tol should be used to allow some constraint violation (see the ***convergence options of the corresponding optimization method).

Syntax:

The syntax is:

***comparison_constraint
  s_file_file *xref fname1 t1 y1 fname2 t2 y2* [*lambda0*]

where *xref* is the value along the x coordinate for which a constraint is added to enforce y1(x)=y2(x),

fname1, *fname2* are the names of the two files used in the comparison,

t1, *t2* are the column numbers in files *fname1* and *fname2* that are used to define the x coordinates,

y1, *y2* are the column numbers in files *fname1* and *fname2* that are used to define the y(x) values,

lambda0 is an optional value for the initial lagrange multiplier associated with the constraint.

Example:

```
***comparison_constraint
  s_file_file 55. fat_al2.test 1 3 fat_al2.exp 1 3 0.0001
```

***files

Description:
The `***files` option is used to declare files where the optimization variables are to be replaced during the trial evaluations of the error function. The following diagram shows the function of the template files in order that the the optimizer can alter the execution data for simulations in a general way.
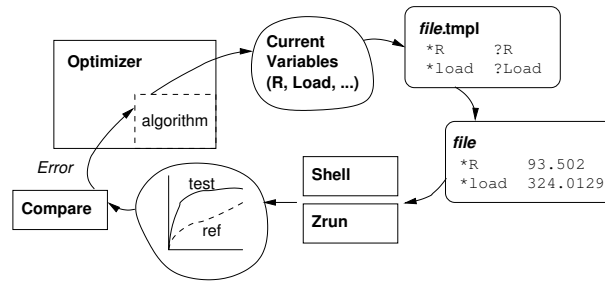
The program detects variables to be optimized in the `.tmpl` suffixed versions of the files by searching for alphanumeric strings with the following format: `?[a-z,A-Z,0-9]*` Thus, the `?` indicates that the parameter is to be optimized, and the following token string is used to reference the variable in the solution. References are needed to give initial values, define constraints on the variables, etc.

If the file exists with the name given with the `***files` command, the initial values will be taken from that file. Otherwise, the `***value` command must be used (see page 16.20). If a variable name is repeatedly found in several files/functions, they are treated to be the same and therefore only one optimization unknown is created. If the initial value file is given, it will be copied to a new file with the suffix `.bak` to save the values.

Syntax:
This command is generally a one-liner, where it only takes the file name bases for optimization files.

```
    ***file f1 ... fn
```
---

where f1...fn are filenames where variables are. The software searches these variables in "template" files named f1.`tmpl` ... fn.`tmpl`. It then creates files f1...fn with the actual values of the variables.

Example:
The following statement declares that file `file1` contains the data to be optimized.

```
    ***files file1
```

where `file1.tmpl` could for example be:

```
***behavior gen_evp
 **elasticity young 260000.  poisson 0.3
 **potential gen_evp ev
   *flow norton
      n  7.0
      K  ?Visco
```

```
  *isotropic constant
      R0 ?RRR
***return
```

The lines `?Visco` and `?RRR` indicate that two variable values are to be substituted in their places during the optimization.

***function

Description:
The ***function is used to declare functions with variables to be optimized. The functions use a similar format for declaring places for optimization variables as in the ***files option. That is, parameters within the function syntax which are named ?[a-z,A-Z,0-9]* are taken to be variables for the optimization algorithm. Initial values and bounds are to be given for each function and file optimization variable using the ***value command (page 16.20).

Syntax:
The syntax is:

***function *name* FUNCTION

where *name* is the name given to the function. If a variable name is repeatedly found in several files/functions, they are treated to be the same and therefore only one optimization unknown is created.

Example:
The horrible function from Ackley.

```
****optimize sqp
  ***function f1 -20. * exp(-0.2*sqrt(0.5*(?x1^2+?x2^2))) -
              exp(0.5*(cos(4.*3.14159265358979*?x1)+
                      cos(4.*3.14159265358979*?x2)))+
                      20.+2.71828182845905;

  ***compare i_func_file f1 1 goal_ackley
  ***values
      x1  -1.1 min -5. max 5.
      x2  -0.5 min -5. max 5.
```

***value

Description:
The `***value` command is used to initialize the variables to be optimized. The initial value of the variables is used to normalize them. It is also possible to indicate min and max values for the variable. Some algorithms need these values (an error message will be given if they are missing).

Variables can conveniantly be taken out of the optimization by using the `fixed` keyword in the variable initialization. All `fixed` variables will still be substituted in the `tmpl` files, but they remain at the given initial value throughout the optimization.

Syntax:
The syntax for variable initialization follows. The sub-commands will be described in the next pages of the manual.

```
    ***value
[ **init_from_file fname ]
[ **auto_init_from_file fname ]
[ **format fmt ]
    vname1   [fixed ] vini1   [min vmin1] [max vmax1] [-log|+log]
      ...
    vnameN   [fixed ] viniN   [min vminN] [max vmaxN] [-log|+log]
```

where *vname* the variable name, *vini* its initial value (also used for scaling) (`double`), *vmin* its min value and *vmax* its max value. Scaling is important, particularly when the variables that are handled are of widely differing magnitudes. Without scaling, matrices used by the optimization algorithms are typically ill-conditionned. Scaling is automatically performed in Z-set using *vname*/*vini* instead of *vname*. It is possible to have different initial and scaling values using the `**init_from_file` command.

`fixed`   fix the value to the initial, and remove the variable from the optimization problem.

`min`   set the minimum allowable value for the variable.

`max`   set the maximum allowable value for the variable.

`+log|-log`   treat variables as being log's of the values to be substituted in the files (the `.tmpl` substitutions)[2]. if `+log` is selected the variables `?` entries in the `.tmpl` file will be substituted not with the variable, but instead e^x. If the option `-log` is chosen the program will use $-e^x$.

Note that the order in which the values are given is not the order in which they are handled (thus printed) by the optimizers. For instance, when reading the results of the `evolution` optimizer, care should be taken not to misinterpret the order of the variables. THE REAL ORDER is given in the ".msg" files, for instance.

Example:

---

[2]this is very useful for variables which span orders of magnitude. A classical example is a creep law of the form $A\sigma^n$ where A much change orders of magnitude in response to small changes in n for similar values of σ. Sometimes a better approach is to re-formulate, for example with $(\sigma/K)^n$

```
    ***values
    **auto_init_from_file levenberg.best
        C1     fixed 200. min  1.e-5 max 1.e6
        f_trans fixed 1.   min  0.3   max 1.1

        m      0.2        min  0.05  max 20.
        M      2.01       min  0.01  max 40.
        f_crit 0.85       min  0.0   max 0.95
```

**auto_init_from_file

Description:

This option is used to conveniantly re-start an optimization from the last best values.

Syntax:

The syntax takes the name of an ascii file which has the format of the *problem*.`best` file. This file is written each time a trial of the function is less than the previous best value.

```
      **auto_init_from_file   file
```

Example:

Supposing the following values entry is given:

```
  ***values
   **auto_init_from_file levenberg.best
      K    700.           min  600.     max  5000.
      n    4.47           min  1.2      max  20.
      K2   500.           min  200.     max  5000.
      n2   35.            min  3.       max  75.
      C1   290.           min  3.0      max  800.
      D1   600.           min  5.       max  5000.
```

An example of the `levenberg.best` file is:

```
# best objective function : 6.050340e-01
# best values :
n 6.101396e+00
K 1.314714e+03
n2 5.967421e+01
K2 5.244540e+02
C1 3.100267e+02
D1 6.302586e+02
```

**init_from_file

Description:
The option **init_from_file filename enables initiating the optimization from the point written in filename. This can be handy in some cases where one does not wish to change the .inp file. The initial values of the design variables are given as real numbers. The order is the order of the variables (cf. note above, this is the order of the .msg and .tra files). When this option is used, the syntax for the rest of the ***value is unchanged. The value that follows the variable name is no longer the starting value (since the starting value is read in filename) but it is used as scaling variable. Therefore, the option **init_from_file filename permits separated initial and reference values.

**format

Description:
The option format controls the output format of the variables declared as `?x` in the .tmpl files. It can be important to output lots of decimals to reduce numerical noise (for example in order to have accurate gradient calculation).

Example:

```
***value A 10. min 1.
 **format %30.15e
 **init_from_file init
         b  2. min 1. max 50.
         c  9.
```

***shell

Description:

The *****shell** option allows to declare external (system) commands to be executed before the evaluation of the function to be optimized. These jobs are done using a posix **system** call. Use the *****zrun** command if the job is a Z-set calculation (using Zrun), because it will not launch a whole new executable.

Example:

```
***shell Zmat -fg test1 >& /dev/null
        abaqus post job=test1 input=test1.jnl >& /dev/null
        awk '{print $3, $4/100.0}' test1.test > result
```

One can also make up a script with the shell commands, for a bit more flexibility:

```
***shell
  ./RUN
```

```
#
# From EXAMPLES-ZBB/Inverse-aba-thermal/Levenberg/RUN
#
#!/bin/sh

Zmat -fg nt4xx28c
PLT nt4xx28c 2>&1 > /dev/null
cat nt4xx28c.test
exit 0
```

***zrun

Description:

The ***zrun option runs a sub-process of Z-set to simulate some part of the model(s) as part of the optimzation comparison scheme. All zrun statements will be run *after* all the ***shell entries.

Example:

Note that for simulation, running with -Q suppresses the screen output of the simulation, so one can watch just the optimization progression.

```
***zrun Zrun -S -Q test1
```

****optimize nelder_mead

Description:
The nelder-mead or simplex method ([Neld65]) is an order 0 local optimizer. The method is numerically simple and robust, but slow for large scale problems. A flow chart of the method is given in the figure hereafter. The simplex method starts with a regular geometric figure called the simplex consisting of $n + 1$ vertices where n is the dimension of the design space. Then, vertices are moved according to their respective values f. There are 3 main steps during a sequential simplex search: the reflection (from the worst point to the best), the expansion (continuation of the displacement towards the best vertex, when reflection improved f), and the contraction of all the vertices towards the simplex gravity center when reflection has failed. In the figure, xh, xl, xs and xm are the highest, lowest, second lowest point, and the gravity center, respectively. fh, fl, and fs are associated cost functions. Typically, $a \approx 1$, $b \approx 2$, et $0 < c < 1$.

This implementation integrates an optional automatic restarting procedure in an attempt to render the algorithm less sensitive to local minima. In this case, the new starting point is automatically evaluated based upon previous results. Optimization constraints are also supported, by means of a basic penalty technique.
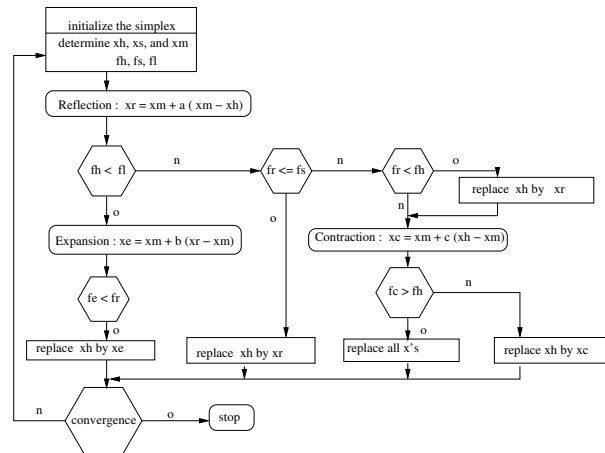
Syntax:
The nelder-mead optimizer has a number of adjustable parameters which can be set in the ***convergence section. These are summarized below.

tolerance   Minimal relative difference between the highest and lowest vertex for convergence. This is exclusive with min. The algorithm stops when the last change in objective function is fractionally smaller than tolerance. It is the default stopping criterion with a value of 1.e-9.

size_optimum   Minimal value of the objective function below which the search stops. This is exclusive with tolerance. It is not the default stopping criterion. Default value is 1.e-5.

size_degeneration   Minimal relative value below which, simplex is considered as degenerate, ie. vertices are no more linearly independent. Default value is 1.e-6.

length   Initial perturbation magnitude as a factor times the initial value. It is the charac-
teristic length scale. It is used to construct the initial simplex from one starting point.
Default value is 1. It is a rather sensitive parameter, and one should play with it if the
simplex does not start the search properly.

iter   Maximum function evaluations before terminating. Default value is 100 .

max_restart   Maximum number of restarts. Default value is 0 (ie. no restart).

reflection   Value of the reflection parameter a (default value is 1.0)

expansion   Value of the expansion parameter b (default value is 2.0)

contraction   Value of the contraction parameter c (default value is 0.5).

lag_mult_step   Step size used to update the penalty parameters associated to the opti-
mization constraint: $if\ g_i > 0.\ \ then\ \ \lambda_i + = step\ .\ g_i$. Default value is 0.01.

constraint_tol   Constraint violation tolerance value, ie. constraints are verified when
$g_i(x) < constraint\_tol$, and the corresponding design point x retained as *feasible*. De-
fault value is 0.001.

****optimize levenberg_marquardt

Description:

This optimizer ([Leve44], [Moré77]) is a robust first order method (uses gradients of the objective function) specially meant for least-square minimization. It does not explicitly handle constraints.

The least-square norm of the distance between simulation and experience can be written,

$$\mathcal{F} = \frac{1}{2}(f(x) - y)^T W (f(x) - y) , \qquad (3)$$

where $f(x)$ is the $(N \times 1)$ vector of simulations, y is the $(N \times 1)$ vector of experiments, and W is the positive diagonal $(N \times N)$ weight matrix. The first and second derivatives of $\mathcal{F}(x)$ are,

$$\texttt{grad}\mathcal{F}(x) = J^T W (f(x) - y) \qquad (4)$$

$$\text{hessian}\mathcal{F}(\S) = J^T W J + \sum_{i=1}^{N} W_{ii}(f_i(x) - y_i)\text{hessian}f_i \qquad (5)$$

$$\qquad (6)$$

where J is the $(n \times N)$ matrix composed of $[\texttt{grad}f_1 \ldots \texttt{grad}f_N]$ (here n is the number of optimization variables). The first fundamental idea in Levenberg-Marquardt is that the last terms of $\text{hessian}\mathcal{F}(\S)$ can be neglected, $\text{hessian}\mathcal{F}(\S) \approx \mathcal{J}^T \mathcal{W} \mathcal{J}$. This is true in particular when the terms $(f_i(x) - y_i)$ are small in comparison to $\text{hessian}f_i$, which stands when the simulation is near the experiments and the largest eigenvalue of $\text{hessian}f_i$ is not too large (if not true, another optimization method, `sqp` for example, should be used). Necessary conditions of optimality state that the gradient of the objective function should vanish at the optimum x^*,

$$\texttt{grad}\mathcal{F}(x^*) = 0 . \qquad (7)$$

Linearization of Equation (7) about the current point x_k yields,

$$\texttt{grad}\mathcal{F}(x_k) + \text{hessian}\mathcal{F}(\S_{\|})(\S_{\|+\infty} - \S_{\|}) = \prime . \qquad (8)$$

The second idea underlying Levenberg-Marquardt is to regularize the approximation of the Hessian of the objective function by adding positive terms on the diagonal, and use this in Equation (8). The regularized approximation to $\text{hessian}\mathcal{F}$ is then strictly positive definite and Equation (8) can always be solved. The fundamental equation used to update optimization variables is,

$$(J_k^T W J_k + \lambda_k I)(x_{k+1} - x_k) = - J_k^T W (f(x_k) - y) . \qquad (9)$$

where λ_k is a scalar positive parameter. The principle of Levenberg-Marquardt algorithm can also be derived from the linearized original optimization problem with a bound on the design variables. This yields an interpretation of λ as Lagrange multiplier associated to the move limit on the design variables. The value of λ can therefore be iteratively adjusted to guarantee that the linearization performed is still valid and that progress in terms of the objective function is made. The Levenberg-Marquardt algorithm proceeds as follows:

Z-set — Non-linear material
& structure analysis suite

1. $k = 0$, $\lambda = \lambda_0$, $x_k = x_0$.

2. Solve (9) for x_{k+1}.

3. If $||\mathbf{grad}\mathcal{F}(x_{k+1})|| < gmin||$ or $\mathcal{F}(x_{k+1}) < fmin$, or number of $\mathcal{F}$ evaluations ¿ $iter$, or $||x_{k+1} - x_k||$ ¡ stepmini, stop.

4. If $\mathcal{F}(x_{k+1}) < \mathcal{F}(x_k)$, $\lambda_{k+1} = \lambda_k/nu$, $k = k + 1$, goto 2.

5. If $\mathcal{F}(x_{k+1}) \geq \mathcal{F}(x_k)$, $\lambda_k = \lambda_k * nu$, goto 2.

Gradients are calculated by finite differences. Min and max bounds on the optimization variables are taken into account by projection into the feasible domain.

Syntax:
The following adjustable parameters are allowed in the ***convergence section.

perturb   Magnitude of the perturbation (in percent of the normalized design variables) used to calculate gradient through finite differences. Default value is 0.5 percent.

lambda0   Initial value of the λ parameter which controls the algorithm. Smaller values when closer to the solution.

lambda_max   Maximal value of lambda. Default is 1.e+07.

iter   Maximum number of function $\mathcal{F}$ evaluations before terminating. Default is 100.

nu   cutting/amplification factor of the lambda parameter on reduced or increased function value. It was originally suggested to have 10 for this parameter (default value). A factor of 4 may be more conservative.

fmin   minimum function value for convergence. Default is 0.0001.

gmin   minimum norm of the gradient of the objective function for convergence. Default is 1.e-8 .

stepmini   minimum step at each iteration. Default is 0.00001. There is a possible false stopping of the optimizer if lambda is taken very large and stepmini very small (because lambda acts as a move limit on the parameter change).

Example:
This following is a complete optimization input using this method:

```
****optimize levenberg_marquardt
 ***files plast.sim
 ***shell
 Zrun -S plast3 2>&1 > /dev/null
 ***values
 cl   1000.  min 200. max 15000.
 cnl 140000.  min 50000. max 200000.
 dnl 100.   min 50.  max 2000.
 r0   260.   min 50.  max 500.
 q    200.   min 20.  max 500.
 b    5.     min 2.   max 20.
```

```
 ***convergence
  perturb 0.005
  lambda0 5
  lambda_max 1.e+08
  iter 100
  nu   5
  fmin  0.00001
  gmin  0.00001
 ***compare
    t_file_file plast3.test 1 3 data_plast3 1 3 weight 1.
****return
```

****optimize evolution

Description:
This section describes indeed the options available for the `evolution` type optimizer engine is used. In that case, an evolutionary (or genetic) algorithm is used for the optimization. Evolution methods search the space of variables using random jumps. Even though such jumps are oriented so as to be more efficient than a completely random search, *evolution* still needs around 1000 calculations of the function to get near the optimum. The advantage of *evolution* is that it can escape local optima in the search space.

A useful application of the evolution method is to generate a starting point for other optimization methods. This is because the evolution method is not sensitive to the convexity of the problem, which permits approaching optimization problems that are numerically ill-conditionned, that diverge, that have discontinuous functions,....

evolution is a steady state genetic algorithm that handles continuous variables. It can handle constraints using a penalization scheme (cf. introduction of the optimization in Z-set, page 16.3). There is a rule of thumb when changing the parameters of *evolution*: some parameters will make the search more random, i.e. more robust but also less efficient, others will increase the speed of convergence, but the probability of getting trapped far from the global optimum simultaneously increases. The tradeoff is clear, and default parameters are supposed to represent a reasonable compromise between randomness and efficiency. Based on its experience, the user may decide to emphasize an aspect or another of **evolution**'s search. `population_size` and `prob_muta` should be increased to increase randomness.

The following files are generated by a run of *evolution*:

`case.evo.log`   contains various data about the convergence of the run.

`case.evo.gnut`   is an executable file that will automatically plot (with gnuplot) the main results found in `case.evo.log` .

`case.evo.best`   contains the best solution found at the end of the run.

`case.evo.gid` contains "good ideas", that is to say good solutions, different from each other, classified in two groups, feasible solutions that satisfy the constraints, and infeasible solutions.

Parameters:
Parameters of *evolution* are given in the `***convergence` section. They may be taken from the following:

`population_size` Sets the population size of the algorithm, i.e., the number of points that are processed by the algorithm. Default value is 50.

`prob_Xover`   Sets the probability of crossover (a number between 0. and 1.). Default value is 0.8 .

`prob_muta`   Sets the probability of mutation (a number between 0. and 1.). Default value is 0.2 .

`max_nb_analyse`   Sets `max_nb_analyse`. The search is stopped after *max_nb_analyse* calculations of the function. Default value is 700.

max_no_progress Sets `max_no_progress` The search is stopped after *max_no_progress* calculations of the function without improvement. Default value is very large, making it inactive.

no_records Sets the number of outputs recorded in the file *case*.evo.log . This is the number of points that will be ploted then with the command *case*.evo.gnut . Default value is 30.

no_feas_pts_res , **no_ifeas_pts_res** *evolution* also collects points that might not be the best overall, but might be the best of their kind. Those points are to be found at the end of the run in the file *case*.evo.gid . They are divided in 2 groups, the feasible and the infeasible points. `no_feas_pts_res` sets the number of feasible points that are collected, and `no_ifeas_pts_res` the number of infeasible points. The algorithm that collects those points make sure that they are different based on a distance metric that can be set with the command `neighborhood_dist`. If two points are separated bby a distance smaller than *neighborhood_dist*, they are considered as being close and only one of them will be kept in *case*.evo.gid . A default value of *neighborhood_dist* is $1/20 \times \sqrt{\sum_{i=0}^{n}(x_{i,max} - xi, min)^2}$.

lag_mult $v_1 \dots v_m$, where m is the number of constraints. It enables to set the lagrange multipliers at the beginning of the runs. Lagrange multipliers apply to each constraint separately, and they are used here as penalties. If a constraint is difficult to satisfy, the corresponding lagrange multiplier should be increased. Lagrange multipliers are automatically changed by the optimizer, and they will eventually represent the real lagrange multipliers after convergence. Default values are 1.

lag_mult_step sets the amount of change of the lagrange multipliers after each evaluation of the function. The lagrange multipliers are updated at each function evaluation according to ,

$$\lambda_i^{k+1} = \lambda_i^k + \texttt{lag\_mult\_step} \times g_i \quad, i = 1, m$$

$$\lambda_i^{k+1} = \max(\lambda_i^{k+1}, 0.)$$

where λ_i^k is the lagrange multiplier of the ith constraint at the kth iteration, and g_i is the value of the ith constraint of the best solution known so far. The larger `lag_mult_step`, the quicker the lagrange multipliers will change. Default value is 0.1 .

****optimize augmented_lagrangian

Description:

This optimizer is a basic implementation of the classic augmented-lagrangian method for constrained optimization. For problems of the form:

$$\begin{cases} Min \ \ f(x) \\ g_i(x) \leq 0 \quad (i = 1, ..., m) \\ x \in \Re^n \end{cases}$$

a dual method is used to find a saddle point of the augmented lagrangian function $\hat{L}(x, \lambda, r)$:

$$\begin{cases} Max_\lambda \ \hat{w}(\lambda, r) \ = \ Max_\lambda \left\{ Min_x \ \hat{L}(x, \lambda, r) \right\} \\ \lambda \in \Re^{m+} \end{cases}$$

where $\hat{L}(x, \lambda, r)$ is defined by:

$$\hat{L}(x, \lambda, r) \ = \ f(x) \ + \ \sum_{i=1}^{m} \lambda_i \ g_i(x) \ + \ r \ \sum_{i=1}^{m} g_i(x)^2$$

with λ_i the lagrange multipliers, and r a penalty parameter that insure the differentiability of the dual function $\hat{w}(\lambda, r)$ near the optimum λ^*.

The penalty parameter r must then be chosen large enough to improve convergence of the dual problem, but not too large because the lagrange function $\hat{L}(x, \lambda, r)$ can become ill-conditioned in this case.

For each value of the lagrange multiplier λ_i the unconstrained problem $Min_x \ \hat{L}(x, \lambda, r)$ is solved by a BFGS method. At each iteration of the BFGS method an economic line-search procedure based upon the Goldstein rule has been implemented.

Syntax:

The following adjustable parameters are allowed in the *****convergence** section.

iter Maximum number of function f evaluations before terminating. Default is 100. Note that this doesn't include function evaluations associated with the line-search procedure.

perturb Magnitude of the perturbation (in percent of the normalized design variables) used to calculate gradient through finite differences. Default value is 0.5 percent.

r0 Value of the penalty parameter r. Default is 1.0.

aug_conv Convergence parameter for dual problem based upon the relative variation of design variables. Default value is 1.e-7.

bfgs_conv Convergence parameter for the inner unconstrained optimization problem based upon the relative variation of design variables. Default value is 1.e-7.

oned_conv Convergence parameter for the line search procedure. Default value is 1.e-7.

gradient_tol Additional convergence parameter for the inner unconstrained problem, based upon the gradient of the lagrangian function. Default value is 1.e-7.

constraint_tol   Constraint violation tolerance value, ie. constraints are verified when $g_i(x) < constraint\_tol$, and the corresponding design point x retained as *feasible*. Default value is 0.001.

****optimize single

Description:
single is not an optimizer, but rather a convenience to test, or re-analyze, a set of optimization parameters. It performs one single calculation of the cost function going through the principal routines of the optimizer. It is particularly meant to be used in conjunction with the ****init_from_file** command to choose a particular initial point. There are no parameters in the convergence section, and the reading of this algorithm will pass by entries there without an error message.

Example:
The following is an example where the variables **cl** ... **b** are read in the ASCII file init. The values 1000 ... 5 are in fact used for scaling only. Only one simulation is performed, and the objective function is calculated.

```
****optimize single
 ***files plast.sim
 ***shell
  Zrun -S -Q plast3 2>&1 > /dev/null
 ***values
  **init_from_file init
  cl  1000.  min 200. max 15000.
  cnl 140000.  min 50000. max 200000.
  dnl 100.   min 50.  max 2000.
  r0  260.   min 50.  max 500.
  q   200.   min 20.  max 500.
  b   5.     min 2.   max 20.
 ***convergence
  delta 0.005
  eps 1.e-08
  iter 100
 ***compare
    t_file_file plast3.test 1 3 data_plast3 1 3 weight 1.
****return
```

Chapter 17

Reference

Functions

Description:
The functions have been generalized in code versions greater than 7.1 to have a natural equation like form, and apply more widely throughout the program. In addition to coefficient definitions, the functions may now be used to define load waveforms, apply to the optimizer, etc. More applications will be added as well.

The functions follow a C-like syntax, and may be defined in terms of pre-defined functions (sin, log, etc) and named parameters of the problem. What parameters are allowed and available depends on application.

Syntax:
Objects which are functions may now be entered using a C-like format. This *must* include a semi-colon at the end of the function definition to terminate the reading of the function. Many operators exist, which have the same meaning and order of selection as in C. Coefficients which are functions still require the keyword `function` to follow the coefficient name, but are otherwise generally given in terms of the relevant parameters.

The following operators are defined in functions:

```
:= == >= <= + - * / ^ > <
```

as are the following functions:

```
triangle floor asinh acosh atanh asin acos atan
cosh sinh tanh ceil sqrt neg abs sqr sin cos tan
exp ln Hx H
```

Pre-defined functions may take complex arguments of other expressions or functions.

triangle   function used to make a sawtooth waveform with period 1 of the parameter.

floor   largest integral value not greater than x.

H   Heaviside function. Equal to 1 for $x > 0$ and 0 otherwise.

Hx   Heaviside of its parameter times its parameter. Equal to x for $x > 0$ and 0 otherwise.

Example:

```
***function load_tab sin(6.28319*time);

***elasticity
   young function 2.e6-100.*temperature -2.*temperature^2.;
   poisson 0.3
```

Environment Variables

The environment variables are used to personalize the Z-set program for individual users, and maintain a self-contained project structure. The function extends as well to manage multi-architecture sites, thereby allowing the transparent use of the program over a diverse network. The currently used environment variables are summarized as:

CODE	DESCRIPTION
Z7PATH	path to the head Z-set's directory structure
Z7_MAX_NB_DOF	number of DOFs above which disk storage is used
Z7_TMP_DIR	path for the temporary files if needed
Z7_LICENSE	path to a license file if not stored in $Z7PATH/lib/Zebulon.License

Z7PATH variable which indicates the location of the Z-set distribution. This variable allows easy switching to different distributions. It also is a cause of much difficulty with users if not configured correctly.

```
cd /usr/local/Z8-Sept-1999
setenv Z7PATH 'pwd'
source lib/Z7_cshrc
```

Z7_MAX_NB_DOF This sets the maximum number of degrees of freedom before the global matrix is stored on disk. Because disk storage is not expensive, it is advisable to set this to a fairly low value (e.g. 5000). One can also use *****file_management** to control the parameter.

Z7_TMP_DIR directory where the temporary files are to be stored. Default is the problem directory. This can also be set with *****file_management**.

Z7_LICENSE fully qualified path to a license file. Extremely useful when there are multiple versions, or for running Zebulon directly off a CD-ROM where one can't put the license file in a read only lib dir.

Example:
In the C-shell, these variables are set using the **setenv** command. The variables may be directly in the user's **.cshrc** file, or in a separate file. For the later case, one may add the line to the **.cshrc** file: **if (-f ~/lib/Z7_vars) source ~/lib/Z7_vars** Examples of variable settings are given below:

```
% cat ~/lib/Z7_vars
setenv Z7_TMP_DIR /home/disk/me/Z7
setenv Z7_MAX_NB_DOF    5000
setenv Z7_PRINTER_COLOR_A3  HPDESKJET
```

Chapter 18

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Chapter 19

Index

Index