BISON Users Manual

BISON Release 1.3

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1 Introduction

BISON [1] is a finite element-based nuclear fuel performance code applicable to a variety of fuel forms including light water reactor fuel rods, TRISO particle fuel [2], and metallic rod [3] and plate fuel. It solves the fully-coupled equations of thermomechanics and species diffusion, for 1D spherically symmetric, 2D axisymmetric or 3D geometries. Fuel models are included to describe temperature and burnup dependent thermal properties, fission product swelling, densification, thermal and irradiation creep, fracture, and fission gas production and release. Plasticity, irradiation growth, and thermal and irradiation creep models are implemented for clad materials. Models are also available to simulate gap heat transfer, mechanical contact, and the evolution of the gap/plenum pressure with plenum volume, gas temperature, and fission gas addition. BI-SON is based on the MOOSE framework [4] and can therefore efficiently solve problems using standard workstations or very large high-performance computers.

Two input files are required as input when running BISON. One is a mesh file. While MOOSE supports several file formats, the ExodusII [5] format is the one used almost exclusively in BISON. This file commonly has "e" as its file extension. The mesh file may be generated using CUBIT [6] or another meshing tool. A further option is a meshing script bundled with BISON. This script, dependent on CUBIT and suitable for LWR fuel rod meshes, is the subject of Chapter 26.

The second file is a text file. This file commonly has "i" as its extension and contains a description of the variables, equations, boundary conditions, and material models associated with an analysis. The structure of the text input file is the main focus of this document.

2 Running BISON

2.1 Checking Out the Code

BISON uses GitLab for code management and distribution. Detailed instructions for checking out, building and contributing to the code can be found in the BISON Workshop slides located in the BISON repository (bison/docs/workshop) or https://bison.inl.gov.

2.2 Executing BISON

When first starting out with BISON, it is recommended to start from an example problem similar to the problem that you are trying to solve. Multiple examples can be found at bison/examples/ and bison/assessment/. It may be worth running the example problems to see how the code works and modifying input parameters to see how the run time, results and convergence behavior change.

To demonstrate running BISON, consider the inputSmeared.i example problem.

```
cd ~/projects/bison/examples/2D-RZ_rodlet_10pellets
# To run with one processor
~/projects/bison/bison-opt -i inputSmeared.i
# To run in parallel (4 processors)
mpiexec -n 4 ../../bison-opt -i inputSmeared.i
```

2.3 Getting Started

2.3.1 Input to BISON

Before running any problem, the power function, axial profile, mesh, and any functions needed for boundary conditions need to be generated.

Typically, a PiecewiseLinear function is used together with an external data file to specify a complex power history. This file has time and power specified in columns or rows, with the first row (or column) being the time (seconds) and the second row (or column) being power (W/m). Any data file that is used as input to BISON must be in Windows comma separated values (csv) format. Looking at inputSmeared.i, the power history is specified as:

```
[./power_history]
  type = PiecewiseLinear
  data_file = powerhistory.csv
  format = rows
  scale_factor = 1.0
```

```
[../]
```

The axial power profile, if present, is input as a PiecewiseBilinearFile. The axial peaking factors are input as a table within the file, with the top row being the axial location from the bottom of the rod and the left column as time. The axial peaking factors used for the example problem inputSmeared.i for the first three axial locations is as follows:

```
9.44E-03, 1.54E-02, 2.13E-02

0.00E+00, 0.00E+00, 0.00E+00, 0.00E+00

1.00E+00, 5.37E-01, 8.68E-01, 1.01E+00

1.50E+08, 5.37E-01, 8.68E-01, 1.01E+00
```

The mesh can either be generated with the mesh script described in Chapter 26, or if you do not have CUBIT, you can generate a simple 2D-RZ axisymmetric mesh with smeared solid fuel pellets (single fuel column) with the SmearedPelletMesh within BISON. To generate the mesh similar to the one used in the example problem inputSmeared.i, the mesh block would look like:

```
type = SmearedPelletMesh
   clad_mesh_density = customize
   pellet_mesh_density = customize
   ny_p = 80 # Total number of axial elements in fuel
   nx p = 11 # Number of radial elements in fuel
   nx_c = 5 # Number of elements through thickness of clad
   ny_cu = 3 # Number of axial element of upper clad gap
   ny_c = 80 \# Number of axial elements of clad wall
  ny_cl = 3 # Number of axial elements of lower clad cap
   clad\_thickness = 5.6e-4
   pellet outer radius = 0.0041
  clad_bot_qap_height = 1.0e-3
   pellet_quantity = 10
   pellet_height = 0.01186
   plenum_fuel_ratio = 0.045 # or use clad_top_gap_height = 3.0e-3
   clad_gap_width = 8e-5
   top\_bot\_clad\_height = 2.24e-3
   elem_type = QUAD8
   displacements = 'disp_x disp_y'
   patch\_size = 1000
[]
```

2.3.2 Post Processing

BISON typically writes solution data to an ExodusII file. Data may also be written in other formats, a simple comma separated file giving global data being the most common.

Several options exist for viewing ExodusII results files. These include commercial as well as open-source tools. One good choice is Paraview, which is open-source.

Paraview is available on a variety of platforms. It is capable of displaying node and element data in several ways. It will also produce line plots of global data or data from a particular node

or element. A complete description of Paraview is not possible here, but a quick overview of using Paraview with BISON results is available in the BISON workshop material.

2.3.3 Graphical User Interface

It is worth noting that a graphical user interface (GUI) exists for all MOOSE-based applications. This GUI is named Peacock. Information about Peacock and how to set it up for use may be found on the MOOSE wiki page.

Peacock may be used to generate a text input file. It is also capable of submitting the analysis. Finally, it provides basic post processing capabilities.

3 Overview

3.1 Basic Syntax

The input file used by BISON is broken into sections or blocks identified with square brackets. The type of input block is placed in the opening brackets, and empty brackets mark the end of the block.

Each block may have subblocks, which may in turn have subblocks. The Functions block, for example, will have multiple subblocks, each corresponding to a specific function. The line commands in the Functions subblocks will describe the function details.

subblocks are opened and closed as

```
[./subblock_name]
cline commands>
[../]
```

Note that the name given in the subblocks must be unique when compared with all other subblocks in the current block.

Line commands are given as key/value pairs with an equal sign between them. They specify parameters to be used by the object being described. The key is a string (no whitespace), and the value may be a string, an integer, a real number, or a list of strings, integers, or real numbers. Lists are given in single quotes and are separated by whitespace.

Often subblocks will include a type line command. This line command specifies the particular type of object being described. The object type indicates which line commands are appropriate for describing the object. BISON will give an error message if a line command is given that does not apply for the current object type. An error message will also be given if a line command is repeated within the current block or if a line command is unused during the initial setup of the simulation.

In this document, line commands are shown with the keyword, an equal sign, and, in angle brackets, the value. If a default value exists for that line command, it is shown in parentheses.

In the initial description of a block, line commands common to all subblocks will be described. Those line commands are then omitted from the description of the subblocks but are nonetheless valid line commands for those subblocks.

The name of a subblock ([./<name>]) is most often arbitrary. However, the names of subblocks of Variables, AuxVariables, and Postprocessors define the names used for those entities.

3.2 BISON Syntax Page

A complete listing of all input syntax options in MOOSE is available on the MOOSE Documentation page. See the section on Input File Documentation. Note also that you can run ./bison-opt --dump to get a list of valid input options for BISON.

3.3 Units

Because BISON uses several empirical models, BISON input expects SI units. This simplifies model input by eliminating the possibility of one set of units for one model and another set of units for a different model. Any needed unit conversions are done inside BISON.

3.4 High-Level Description of a BISON Simulation

The primary purpose of BISON is to solve coupled systems of partial differential equations (PDEs), where the equations represent important physics related to engineering scale nuclear fuel behavior. Fuel simulations typically consist of solving the following energy, momentum, and mass (or species) conservation equations,

$$\rho C_p \frac{\partial T}{\partial t} + \nabla \cdot \mathbf{q} - e_f \dot{F} = 0, \tag{3.1}$$

$$\nabla \cdot \mathbf{\sigma} + \rho \mathbf{f} = 0. \tag{3.2}$$

$$\frac{\partial C}{\partial t} + \nabla \cdot \mathbf{J} + \lambda C - S = 0, \tag{3.3}$$

In Equation 3.1, T, ρ and C_p are the temperature, density and specific heat, respectively, e_f is the energy released in a single fission event, and \dot{F} is the volumetric fission rate.

Momentum conservation (Equation 3.2) is prescribed assuming static equilibrium at each time increment where σ is the Cauchy stress tensor and \mathbf{f} is the body force per unit mass (e.g. gravity). The displacement field u, which is the primary solution variable, is connected to the stress field via the strain, through a constitutive relation.

In the equation for species conservation (3.3) C, λ , and S are the concentration, radioactive decay constant, and source rate of a given species, respectively.

Often, fuels performance problems are limited to thermomechanics, where only Equations 3.1 and 3.2 are solved.

Each term in Equations 3.1 - 3.3 (time derivatives, divergence, source, sinks, etc.) are referred to as kernels and are discussed in greater detail in Chapter 14.

These equations are solved simultaneously using the finite element method (FEM) and JFNK approach [7] on a discretized domain. The domain (also referred to as a mesh) may represent uranium dioxide fuel pellets and zirconium clad in a light water reactor (LWR) simulation. Blocks, side sets, and node sets are defined on the mesh such that material models and boundary

conditions can be assigned to different parts of the model. Details regarding the mesh, material models, and boundary conditions can be found in chapters 6, 16, and 10 respectively.

Kernels, boundary conditions, and material models may require supporting information and calculations. This is achieved through the use of Functions and AuxKernels, which are detailed in chapters 9 and 12. For example, a function can be used to define power and time value pairs, which would inform the source term in the energy equation (Equation 3.1). An AuxKernel could be used to define fission rate or burnup, which could be used to inform material models that are dependent on those values. AuxKernels can also be used for writing information, such as stress components, to the output file.

Execution on the analysis is described in the Executioner block. Line commands describe time stepping details and solver options. See Chapter 19 for details.

MOOSE Postprocessors compute a single scalar value at each timestep. These can be minimums, maximums, averages, volumes, or any other scalar quantity. One example of the use of Postprocessors in BISON is computing the gas volume of an LWR rod. The gas volume changes timestep to timestep, but since it is a single scalar quantity, a Postprocessor computes this value. Chapter 18 gives examples.

The following sections delve deeper into the topics mentioned here. The format basically follows that of a typical BISON LWR input file and provides details for each section. Required parameters have **Required** included in their description throughout the document.

4 Global Parameters

The GlobalParams block specifies parameters that are available, as appropriate, in any other block or subblock in the input file. For example, imagine a subblock that accepts a line command with the keyword value. If the subblock has a line command for value, that line command will be used regardless of what is in GlobalParams. However, if the line command is missing in the subblock but defined in GlobalParams, the subblock will use the parameter defined in GlobalParams. In the example below, the line commands order = FIRST and family = LAGRANGE will be available in all blocks and subblocks in the remainder of the input file.

```
[GlobalParams]
order = FIRST
family = LAGRANGE
[]
```

5 Problem

The Problem block is typically only used to indicate that a model should run as axisymmetric (RZ) or spherically symmetric (RSPHERICAL). If the model is 3D, the Problem block may be omitted.

```
[Problem]
  coord_type = <string>
[]
```

There are two advanced cases that require a [Problem] block to be included in the input file. These cases are a known as ReferenceResidualProblem and FrictionalContactProblem. When using either of these types there are many required additions throughout the input file. Therefore ReferenceResidualProblem and FrictionalContactProblem are discussed in Chapters 24 and 25 respectively.

6 Mesh

The Mesh block's purpose is to give details about the finite element mesh to be used. Typically meshes for BISON simulations are created using the mesh generation tool Cubit (known as Trelis for non-DOE users). For simulations of LWR fuel there is a mesh script found in bison/tools/UO2/. The details of the mesh script are provided in Chapter 26.

```
file = <string>
displacements = <string list>
patch_size = <integer> (40)
```

file

Required. This is the mesh file name. BISON uses ExodusII mesh files.

displacements

List of the displacement variables. This line must be given if the analysis is to use contact or nonlinear geometry. Typically 'disp_x disp_y' for an axisymmetric analysis.

patch_size

Number of nearby elements to consider as possible contacting surfaces. The value for the patch size depends upon whether Dirac or Constraint based contact is used. For Dirac a typical value is 1000. For Constraint it is ideal to choose a small enough patch size that encompasses all possible contacting surfaces to reduce memory requirements. For example, if the fuel moves up the clad 8 nodes make the patch size 20. This will allow the contact search to use 10 nodes above and 10 nodes belows the point at which the fuel comes into contact with the clad.

For users that do not have access to Cubit or Trelis but want to simulate LWR fuel there is a SmearedPelletMesh type that can be used to generate a mesh for modeling a smeared column of fuel (i.e. no dishes and or chamfers). The structure of the SmearedPelletMesh block is outlined below:

```
[Mesh]
   type = SmearedPelletMesh
   clad_mesh_density = <string> (medium)
   pellet_mesh_density = <string> (medium)
   ny_p = \langle integer \rangle (24)
   nx_p = \langle integer \rangle (8)
   nx_c = \langle integer \rangle (2)
   ny_cu = \langle integer \rangle (1)
   ny_c = \langle integer \rangle (24)
   ny_cl = \langle integer \rangle (1)
```

```
bx_p = <real> (1)
  clad_thickness = <real> (0.00041)
  pellet_outer_radius = <real> (0.0041)
  clad_bot_gap_height = <real> (0.00127)
  pellet_quantity = <real> (2)
  elem_type = <string> (QUAD4)
  displacements = <string list>
   patch_size = <integer> (4)
[]
```

Clad_mesh_density Mesh density of the clad. Choices are coarse, medium, fine or custom. Default is medium. Mesh density of the fuel pellets. Choices are coarse, medium, fine or custom. Default is medium. Number of finite elements in a fuel pellet in the axial direction. Number of finite elements in a fuel pellet in the radial direction. Number of finite elements through the thickness of the cladding in the radial direction of the upper plug. Number of finite elements through the thickness of the cladding in the axial direction of the upper plug. Number of finite elements axially through the cladding. Number of finite elements through the thickness of the cladding in the axial direction of the lower plug. bx_p The amount to grow (or shrink) the fuel elements in the radial direction. Range is 0.5 to 2.0. clad_thickness pellet_outer_radius clad_bot_gap_height Gap between bottom of pellet stack and the inside bottom surface of the cladding. Pellet_height The height of the pellet. Ratio of the axial gas height to the fuel height inside the cladding. Either plenum_fuel_ratio or clad_top_gap_height must be specified but not both. clad_gap_width Gap between top of pellet and inside top surface of cladding. Either plenum_fuel_ratio or clad_top_gap_height must be specified but not both. clad_gap_width Thickness of top and bottom cladding walls.	type	SmearedPelletMesh
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ny_cu Number of finite elements through the thickness of the cladding in the axial direction of the upper plug. ny_c Number of finite elements axially through the cladding. ny_cl Number of finite elements through the thickness of the cladding in the axial direction of the lower plug. bx_p The amount to grow (or shrink) the fuel elements in the radial direction. Range is 0.5 to 2.0. clad_thickness The cladding thickness. pellet_outer_radius The outer radius of the pellet. clad_bot_gap_height Gap between bottom of pellet stack and the inside bottom surface of the cladding. pellet_quantity Number of pellets to be included. pellet_height The height of the pellet. plenum_fuel_ratio Ratio of the axial gas height to the fuel height inside the cladding. Either plenum_fuel_ratio or clad_top_gap_height must be specified but not both. clad_gap_width Gap between outer radius of pellet and inside surface of cladding.	nx_p	Number of finite elements in a fuel pellet in the radial direction.
ny_c Number of finite elements axially through the cladding. ny_cl Number of finite elements through the thickness of the cladding in the axial direction of the lower plug. bx_p The amount to grow (or shrink) the fuel elements in the radial direction. Range is 0.5 to 2.0. clad_thickness The cladding thickness. pellet_outer_radius The outer radius of the pellet. clad_bot_gap_height Gap between bottom of pellet stack and the inside bottom surface of the cladding. pellet_quantity Number of pellets to be included. pellet_height The height of the pellet. plenum_fuel_ratio Ratio of the axial gas height to the fuel height inside the cladding. Either plenum_fuel_ratio or clad_top_gap_height must be specified but not both. clad_gap_width Gap between outer radius of pellet and inside surface of cladding. Clad_gap_width Gap between outer radius of pellet and inside surface of cladding.	nx_c	· · · · · · · · · · · · · · · · · · ·
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Either plenum_fuel_ratio or clad_top_gap_height must be specified but not both. clad_top_gap_height Gap between top of pellet and inside top surface of cladding. Either plenum_fuel_ratio or clad_top_gap_height must be specified but not both. clad_gap_width Gap between outer radius of pellet and inside surface of cladding.	pellet_height	The height of the pellet.
plenum_fuel_ratio or clad_top_gap_height must be specified but not both. clad_gap_width Gap between outer radius of pellet and inside surface of cladding.	plenum_fuel_ratio	Either plenum_fuel_ratio or clad_top_gap_height must be
• • • • • • • • • • • • • • • • • • • •	clad_top_gap_height	plenum_fuel_ratio or clad_top_gap_height must be specified
ton bot clad height. Thickness of ton and bottom cladding walls	clad_gap_width	Gap between outer radius of pellet and inside surface of cladding.
top 250 telegate Timekness of top and bottom cladding wans.	top_bot_clad_height	Thickness of top and bottom cladding walls.

elem_type

Type of finite element. Default is QUAD4. For second-order meshes use QUAD8.

displacements

List of the displacement variables. This line must be given if the analysis is to use contact or nonlinear geometry. Typically 'disp_x disp_y' for an axisymmetric analysis.

patch_size

Number of nearby elements to consider as possible contacting surfaces. The value for the patch size depends upon whether Dirac or Constraint based contact is used. For Dirac a typical value is 1000. For Constraint it is ideal to choose a small enough patch size that encompasses all possible contacting surfaces to reduce memory requirements. For example, if the fuel moves up the clad 8 nodes make the patch size 20. This will allow the contact search to use 10 nodes above and 10 nodes belows the point at which the fuel comes into contact with the clad.

7 Variables

The Variables block is where all of the primary solution variables are identified. The name of each variable is taken as the name of the subblocks. Primary solution variables often include temperature (usually named temp) and displacement (usually named disp_x, disp_y, and disp_z).

```
[Variables]
  [./var1]
    order = <string>
    family = <string>
  [../]
  [./var2]
    order = <string>
    family = <string>
    initial_condition = <real>
    scaling = <real> (1)
  [../]
[]
```

order The order of the variable. Typical values are FIRST and SECOND.

family The finite element shape function family. A typical value is

LAGRANGE.

initial_condition Optional initial value to be assigned to the variable. Zero is assigned

if this line is not present.

scaling Amount to scale the variable during the solution process. This scal-

ing affects only the residual and preconditioning steps and not the final solution values. This line command is sometimes helpful when solving coupled systems where one variable's residual is orders of

magnitude different that the other variables' residuals.

8 AuxVariables

The AuxVariables block is where all of the auxiliary variables are identified. The name of each variable is taken as the name of the subblocks. Auxiliary variables are used for quantities such as fast neutron flux, element-averaged stresses, and other output variables.

```
[AuxVariables]
  [./var1]
    order = <string>
    family = <string>
  [../]
  [./var2]
    order = <string>
    family = <string>
    initial_condition = <real>
  [../]
[]
```

order The order of the variable. Typical values are CONSTANT, FIRST, and SECOND.

family The finite element shape function family. Typical values are

MONOMIAL and LAGRANGE.

initial_condition Optional initial value to be assigned to the variable. Zero is assigned

if this line is not present.

9 Functions

9.1 Composite

The Composite function takes an arbitrary set of functions, provided in the functions parameter, evaluates each of them at the appropriate time and position, and multiplies them together. The function can optionally be multiplied by a scale factor, which specified using the scale_factor parameter.

```
[./composite]
  type = CompositeFunction
  functions = <string list>
  scale_factor = <real> (1.0)
[../]
```

type CompositeFunction

functions List of functions to be multiplied together.

scale_factor Scale factor to be applied to resulting function. Default is 1.

9.2 ParsedFunction

The ParsedFunction function takes a mathematical expression in value. The expression can be a function of time (t) or coordinate (x, y, or z). The expression can include common mathematical functions. Examples include '4e4+1e2*t', 'sqrt(x*x+y*y+z*z)', and 'if($t<=1.0, 0.1*t, (1.0+0.1)*\cos(pi/2*(t-1.0)) - 1.0$)'. Constant variables may be used in the expression if they have been declared with vars and defined with vals. Further information can be found at http://warp.povusers.org/FunctionParser/.

```
[./parsedfunction]
  type = ParsedFunction
  value = <string>
  vals = <real list>
  vars = <string list>
[../]
```

type ParsedFunction

value Required. String describing the function.

vals Values to be associated with variables in vars.

vars Variable names to be associated with values in vals.

9.3 PiecewiseBilinear

The PiecewiseBilinear function reads a csv file and interpolates values based on the data in the file. The interpolation is based on x-y pairs. If axis is given, time is used as the y index. Either xaxis or yaxis or both may be given. Time is used as the other index if one of them is not given. If radius is given, xaxis and yaxis are used to orient a cylindrical coordinate system, and the x-y pair used in the query will be the radial coordinate and time.

```
[./piecewiselinear]
  type = PiecewiseBilinear
  data_file = <string>
  axis = <0, 1, or 2 for x, y, or z>
  xaxis = <0, 1, or 2 for x, y, or z>
  yaxis = <0, 1, or 2 for x, y, or z>
  yaxis = <0, 1, or 2 for x, y, or z>
  scale_factor = <real> (1.0)
  radial = <bool> (false)
[../]
```

type PiecewiseBilinear
data_file File holding your csv data.

axis Coordinate direction to use in the function evaluation.

xaxis Coordinate direction used for x-axis data.

yaxis Coordinate direction used for y-axis data.

scale_factor Scale factor to be applied to resulting function. Default is 1.

radial Set to true if interpolation should be done along a radius rather than along a specific axis. Requires xaxis and yaxis.

9.4 PiecewiseConstant

The PiecewiseConstant function defines the data using a set of x-y data pairs. Instead of linearly interpolating between the values, however, the PiecewiseConstant function is constant when the abscissa is between the values provided by the user. The direction parameter controls whether the function takes the value of the abscissa of the user-provided point to the right or left of the value at which the function is evaluated.

```
[./piecewiseconstant]
  type = PiecewiseConstant
  x = <real list>
  y = <real list>
  xy_data = <real list>
  data_file = <string>
  format = <string> (rows)
  scale_factor = <real> (1.0)
  axis = <0, 1, or 2 for x, y, or z>
  directon = <string> (left)
```

type	PiecewiseConstant
X	List of x values for x-y data.
У	List of y values for x-y data.
xy_data	List of pairs of x-y data points.
data_file	Name of an file containing x-y data.
format	Format of x-y data in external file.
scale_factor	Scale factor to be applied to resulting function. Default is 1.
axis	Coordinate direction to use in the function evaluation. If not present, time is used as the function input.

9.5 PiecewiseLinear

The PiecewiseLinear function performs linear interpolations between user-provied pairs of x-y data. The x-y data can be provided in three ways. The first way is through a combination of the x and y paramaters, which are lists of the x and y coordinates of the data points that make up the function. The second way is in the xy_data parameter, which is a list of pairs of x-y data that make up the points of the function. This allows for the function data to be specified in columns by inserting line breaks after each x-y data point. Finally, the x-y data can be provided in an external file containing comma-separated values. The file name is provided in data_file, and the data can be provided in either rows (default) or columns, as specified in the format parameter.

By default, the x-data corresponds to time, but this can be changed to correspond to x, y, or z coordinate with the axis line. If the function is queried outside of its range of x data, it returns the y value associated with the closest x data point.

```
[./piecewiselinear]
  type = PiecewiseLinear
  x = <real list>
  y = <real list>
  xy_data = <real list>
  data_file = <string> (rows)
  format = <string>
  scale_factor = <real> (1.0)
  axis = <0, 1, or 2 for x, y, or z>
[../]
```

```
type PiecewiseLinear
x List of x values for x-y data.
y List of y values for x-y data.
xy_data List of pairs of x-y data points.
```

data_file Name of an file containing x-y data. format Format of x-y data in external file.

 ${\tt scale_factor} \quad \textbf{Scale factor to be applied to resulting function. Default is 1.}$

axis Coordinate direction to use in the function evaluation. If not present, time

is used as the function input.

10 Boundary Conditions

The BCs block is for specifying various types of boundary conditions.

```
[BCs]
  [./name]
   type = <BC type>
   boundary = <string list>
   ...
  [../]
[]
```

type Type of boundary condition.

boundary List of boundaries (side sets). Either boundary numbers or names.

10.1 BulkCoolantBC

The BulkCoolantBC boundary condition determines the heat transfer from a boundary based upon a bulk coolant temperature and coolant heat tansfer coefficient.

```
[./bulkcoolantBC]
  type = BulkCoolantBC
  variable = <variable>
  boundary = <string list>
  bulk_temperature = <real> (800)
  heat_transfer_coefficient = <real> (2000)
[../]
```

type BulkCoolantBC

variable Required. Primary variable associated with this boundary

condition.

boundary Required. List of boundary names or ids where this bound-

ary condition will apply.

bulk_temperature The bulk coolant temperature.

heat_transfer_coefficient The heat transfer coefficient of the coolant.

10.2 ConvectiveFluxBC

The ConvectiveFluxBC boundary condition determines the value on a boundary based upon the initial and final values, the flux through the boundary and the duration of exposure..

```
[./convectivefluxBC]
  type = ConvectiveFluxBC
  variable = <variable>
  boundary = <string list>
  initial = <real> (500)
  final = <real> (500)
  rate = <real> (7500)
[../]
```

```
type ConvectiveFluxBC
variable Required. Primary variable associated with this boundary condition.
boundary Required. List of boundary names or ids where this boundary condition will apply.
initial The initial value of the variable on the boundary.
final The final value of the variable on the boundary.
The flux of the variable through the boundary.
```

10.3 ConvectiveFluxFunction

The ConvectiveFluxFunction boundary condition determines the value on a boundary based upon the heat transfer coefficient of the fluid on the outside of boundary and far-field temperature.

```
[./convectivefluxFunction]
  type = ConvectiveFluxFunction
  variable = <variable>
  boundary = <string list>
  T_infinity= <string>
  coefficient = <real>
  coefficient_function = <string>
[../]
```

type ConvectiveFluxFunction

Required. Primary variable associated with this boundary condition.

boundary Required. List of boundary names or ids where this boundary condition will apply.

T_infinity Required. The name of the function describing the far-field temperature.

coefficient Required. The heat transfer coefficient of the fluid in contact

with the boundary. If coefficient_function is provided this coefficient multiplies the function.

coefficient_function Function describing the heat transfer coefficient.

10.4 CoolantChannel

The effect of the coolant on the heat transfer at the exterior cladding surface can be modeled using the CoolantChannel feature. This feature appears in the input file in its own block (i.e., not inside the BCs block).

The presence of some input parameters causes others to be ignored. The following describes the input parameter precedence.

If heat_transfer_coefficient is given, its value will be assigned to the given boundary. All other parameters related to the heat transfer coefficient calculation are ignored.

Enthalpy is taken as <code>coupledEnthalpy</code> if present. Otherwise, heat flux is calculated based on <code>linear_heat_rate</code>, specification of <code>number_axial_zone</code>, and specification of heat_flux, in highest precedence order. The integrated heat flux is computed based on the same precedence. As an example, if <code>number_axial_zone</code> and <code>heat_flux</code> are specified, <code>heat_flux</code> will be ignored. These are used as inputs to the heat transfer coefficient correlations.

The coolant_material is water by default. It can be instead set to sodium, and a heat transfer correlation for liquid sodium is used. With sodium coolant, calculations for phase change are disabled. By default, the subchannel geometry is set to triangular if the user selects sodium coolant, but this can be changed to a square channel if desired.

```
[CoolantChannel]
 [./coolantchannel]
   boundary = <string list>
   variable = <string>
   axial_power_profile = <string>
   blockage_ratio = <real> (0)
   chf_correlation_type=<int> (4)
   compute_enthalpy =<bool> (true)
   cond_metal = <real>
   cond_oxide = <real>
   coolant_material = <string>
   coupledEnthalpy = <string>
   direction = <string>
   direction2 = <string>
   flooding_rate = <real>
   flooding time = <real>
   flow_area = <real>
   fuel_stack_length = <real>
   fuel_stack_bottom = <real>
   heat_flux = <string>
   heat_transfer_coefficient = <string or real>
   heat_transfer_mode = <string> (0)
```

```
heated_diameter = <real>
   heated_perimeter = <real>
   htc_correlation_type = <string>
   hydraulic_diameter = <real>
    initial_power = <real>
   initial_temperature = <real>
   inlet_massflux = <string or real>
   inlet_pressure = <string or real>
   inlet_temperature = <string or real>
   input_Tchf = <real> (0)
   input_Tmin = <real> (0)
   input_rewetting_htc = <real> (1.0e5)
   linear_heat_rate = <string>
   model_post_chf = <bool> (true)
   number_axial_zone = <integer> (0)
   number_lateral_zone = <integer> (1)
   oxide_thickness = <string>
   oxide_model = <string> (zirconia)
   pbr = <real>
   reflooding_model = <int> (1)
   rod_diameter = <real> (0.01)
   rod_pitch = \langle real \rangle (0.0126)
   specified_height = <real> (0)
   subchannel_geometry = <string>
  [../]
[]
```

boundary Required. List of boundaries. Typically only one boundary id is given. variable Required. Name of variable associated with this BC. Typically temp. axial_power_profile Function name for function describing axial power factors. blockage_ratio Flow blockage ratio used in FLECHT correlations. chf_correlation_type CHF correlatons. one of 1 for EPRI, 2 for GE, 3 for Zuber, and 4 for BIASI. compute_enthalpy option to turn on /off the enthalpy calculation. cond_metal Conductivity of the metal. Used if oxide_model is user. cond_oxide Conductivity of the oxide. Used if oxide_model is user. coolant_material Water or sodium. Defaults to water. coupledEnthalpy Variable name. If given, enthalpy is taken from this variable directly instead of being calculated. direction One of x, y, or z. Coordinate direction associated with fluid flow. Default is y.

direction2 One of x, y, or z. Coordinate direction associated with lat-

eral dimension of model. Default is x. This input is used

for plate geometry.

flooding_rate Inlet fooding rate.

flooding_time The starting time of flooding.

flow_area Flow area. If used, must be used with heated_diameter,

heated_perimeter, and hydraulic_diameter. If used,

rod_diameter and rod_pitch will be ignored.

fuel_stack_bottom The axial position of the fuel stack bottom.

heat_flux Function name for function describing the heat flux at the

cladding surface.

transfer coefficient or a real value to be assigned as the heat transfer coefficient. If present, other parameters controlling the heat transfer coefficient calculation will be ignored.

heat_transfer_mode One of 0 (automatic), 1 (natural convection), 2 (forced liq-

uid convection), 3 (subcooled boiling), 4 (saturated boiling), 5 (transition boiling), 6 (film boiling), and 7 (single

phase vapor).

heated_diameter Heated diameter. If used, must be used with flow_area,

heated_perimeter, and hydraulic_diameter. If used,

rod_diameter and rod_pitch will be ignored.

heated_perimeter Heated perimeter. If used, must be used with flow_area,

heated_diameter, and hydraulic_diameter. If used,

rod_diameter and rod_pitch will be ignored.

htc_correlation_type One of 1 (Thom), 2 (Jens Lottes), 3(Chen) or 4 (Shrock-

Grossman) for pre-CHF correlations;

or 1 (McDonough-Milich-King) and 2 (modified Condie-

Bengtson) for transition boiling correlations;

or 1 (Groenveld) and 2 (Dougall-Rohsenow) for film boil-

ing correlations.

heated_perimeter, and heated_diameter. If used,

rod_diameter and rod_pitch will be ignored.

initial_power Initial peak power (kW/m).

inlet_massflux Either a function name for a function describing the inlet

mass flux or a real value to be assigned as the inlet mass

flux.

inlet_pressure Either a function name for a function describing the inlet

pressure or a real value to be assigned as the inlet pressure.

inlet_temperature Either a function name for a function describing the inlet

temperature or a real value to be assigned as the inlet tem-

perature.

input_Tchf Input temperature at critical heat flux.

input_Tmin Input rewetting temperature.

 ${\tt linear_heat_rate} \qquad \qquad {\tt Function \, name \, for \, a \, function \, describing \, the \, linear \, heat \, rate.}$

number_axial_zone Number of axial divisions along the cladding to be used in

integrating the heat flux.

in integrating the heat flux. This input is used for plate

geometry.

model_post_chf Option to turn on or off post-CHF calculations.

 $oxide_thickness \qquad \qquad Name\ of\ \texttt{AuxVariable}\ representing\ the\ oxide\ thickness.\ If$

not given, the calculated heat transfer coefficient will not

account for an oxide layer.

oxide_model One of zirconia, alumina, or user.

reflooding_model Model options for modeling reflooding: either 0

 $old correlation \ or \ 1 \ new We sting house correlation \ .$

rod_diameter Diameter of the fuel rod.

rod_pitch Pitch or spacing between fuel rods.

specified_height The input to compute reflooding heat transfer at a specified

axial location; used for testing purpose only.

subchannel_geometry Geometry of the pin array: either square or triangular. If

not specified, the geometry is square if the coolant is water

or triangular if the coolant is sodium.

10.5 Dirichlet

10.5.1 DirichletBC

```
[./dirichletbc]
  type = DirichletBC
  variable = <variable>
  boundary = <string list>
  value = <real>
[../]
```

type DirichletBC

variable Required. Primary variable associated with this boundary condition.

boundary Required. List of boundary names or ids where this boundary condition will

apply.

value Required. Value to be assigned.

10.5.2 PresetBC

The PresetBC takes the same inputs as DirichletBC and also acts as a Dirichlet boundary condition. However, the implementation is slightly different. PresetBC causes the value of the boundary condition to be applied before the solve begins where DirichletBC enforces the boundary condition as the solve progresses. In certain situations, one is better than another.

10.5.3 FunctionDirichletBC

```
[./functiondirichletbc]
  type = FunctionDirichletBC
  variable = <variable>
  boundary = <string list>
  function = <string>
[../]
```

type FunctionDirichletBC

variable Required. Primary variable associated with this boundary condition.

boundary Required. List of boundary names or ids where this boundary condition will

apply.

function Required. Function that will give the value to be applied by this boundary

condition.

10.5.4 FunctionPresetBC

The FunctionPresetBC takes the same inputs as FunctionDirichletBC and also acts as a Dirichlet boundary condition. However, the implementation is slightly different. FunctionPresetBC causes the value of the boundary condition to be applied before the solve begins where FunctionDirichletBC enforces the boundary condition as the solve progresses. In certain situations, one is better than another.

10.6 DryCaskHeatFlux

The DryCaskHeatFlux BC is used to model the heat flux from a rod in the center of a fuel assembly, stored inside a dry cask storage system (DCSS). The flux includes radiative and conductive effects inside the assembly and conductive/convective effects from the assembly to ambient.

```
[./decay_heat_in_dcss]
  type = DryCaskHeatFlux
  variable = <variable>
  boundary = <string list>
  bwr_or_pwr = <string>
  fill_gas = <string>
  ambient_temperature = <real>
  cask_effective_htc = <real>
  start_time = <real>
  drying_duration = <real>
[../]
```

Required. Primary variable associated with this boundary condition.

boundary Required. List of boundaries where this BC will apply.

bwr_or_pwr Required. Whether to use a typical geometry from a BWR or a PWR assembly.

fill_gas Required. helium, nitrogen, or vacuum.

ambient_temperature Temperature outside the cask.

cask_effective_htc Required. Effective heat transfer coefficient from assembly to am-

cask_effective_htc Required. Effective heat transfer coefficient from ass bient (W/K).

DryCaskHeatFlux

 $\label{eq:thm:bc} \text{Start_time} \qquad \qquad \text{The time when this BC will begin.}$

drying_duration If drying (vacuum) is desired, it will be applied immediately after

the start_time. After drying in vacuum, the calculation switches

from vacuum fill gas to fill_gas specified by the user.

10.7 HydrogenPickup

type

The HydrogenPickup BC is used to model the flux of hydrogen into the clad that is caused by oxide growth. The flux is approximated as a constant fraction of the hydrogen liberated by oxide growth at the interface between the coolant water and the clad.

Note that this BC must be coupled to a variable that gives the thickness of the oxide over time, such as with the OxideAux kernel. For this to work properly, OxideAux must be set to update on updates to the residual; *it will not work if the OxideAux is set to update on time steps*.

```
[./hydrogen_pickup]
  type = HydrogenPickup
  variable = <variable>
  boundary = <string list>
  oxide_thickness = <variable>
  pickup_fraction = <real> (0.15)
  clad_thickness = <real> (660e-6)
```

```
fuel_pin_geometry = <string>
[../]
```

type	HydrogenPickup
variable	Required . Primary variable associated with this boundary condition.
boundary	Required . List of boundary names or ids where this boundary condition will apply.
oxide_thickness	Required . The coupled variable that gives the oxide thickness on the boundary.
pickup_fraction	The fractional amount of hydrogen liberated by the oxide growth that is absorbed into the clad.
clad_thickness	The initial thickness of the clad; only needed if fuel_pin_geometry is not specified.
fuel_pin_geometry	Name of the FuelPinGeometry object (see 23.1).

10.8 PlenumPressure

The PlenumPressure block is used to specify internal rod pressure as a function of temperature, cavity volume, and moles of gas.

The PlenumPressure boundary condition uses two levels of nesting within the BCs block. This allows the pressure to be applied properly in all coordinate directions although it is specified one time only.

The volume and pressure specified in the plenum pressure block along with the initial condition specified in the temperature variable block are used to calculate the initial moles. The initial moles are then used to update the plenum pressure throughout the simulation. It is worth noting to make sure the initial temperature is set to the temperature of the gas when fabricated, usually room temperature (293 K).

The postprocessors coupled to the plenum pressure boundary condition (gas volume and rod interior temperature) need to be executed at each residual such that the plenum pressure is calculated for that specific timestep. If calculated at each timestep, the calculation uses volume and temperature from the previous step to calculate the plenum pressure for the current step, causing a lag in the plenum pressure used and reported for that timestep.

```
[./PlenumPressure]
  [./plenumpressure]
  boundary = <string list>
  initial_pressure = <real> (0)
  initial_temperature = <real>
  startup_time = <real> (0)
  R = <real>
  output_initial_moles = <string>
  temperature = <string>
  volume = <string>
```

```
material_input = <string list>
  output = <string>
  refab_time = <real list>
  refab_pressure = <real list>
  refab_volume = <real list>
  refab_type = <integer list>
[../]
```

boundary Required. List of boundary names or ids where this boundary

condition will apply.

initial_pressure The initial pressure in the plenum.

initial_temperature The initial temperature of the plenum. If not given, will use the

initial value from the Postprocessor given by temperature.

 ${\tt startup_time} \qquad \qquad {\tt The \ amount \ of \ time \ during \ which \ the \ pressure \ will \ ramp \ from}$

zero to its true value.

R Required. The universal gas constant. In BISON, SI units are

used, and R should be 8.3143.

temperature Required. The name of the Postprocessor holding the average

temperature value.

volume Required. The name of the Postprocessor holding the internal

volume.

material_input The name of the Postprocessors that hold the amount of mate-

rial injected into the plenum.

output If given, the name to use for reporting the plenum pressure value.

If not given, the block name will be used.

refab_time The time(s) at which the plenum pressure must be reinitialized

(likely due to fuel rod refabrication).

refab_pressure The pressure of fill gas at refabrication. Number of values must

match number in refab_time.

number in refab_time.

refab_volume The gas volume at refabrication. Number of values must match

number in refab_time.

10.9 Pressure

The Pressure boundary condition uses two levels of nesting within the BCs block. This allows the pressure to be applied properly in all coordinate directions although it is specified one time only.

```
[./Pressure]
  [./pressure]
   boundary = <string list>
   factor = <real> (1)
   function = <string>
  [../]
[../]
```

boundary **Required**. List of boundary names or ids where this boundary condition will apply.

factor Magnitude of pressure to be applied. If function is also given, factor is multiplied by the output of the function and then applied as the pressure.

function Function that will give the value to be applied by this boundary condition.

11 Contact

Finite element contact enforces constraints between surfaces in the mesh. Mechanical contact prevents penetration and develops contact forces. Thermal contact transfers heat between the surfaces. In BISON there are currently two systems to choose from for mechanical contact: Dirac and Constraint. Constaint based contact is recommended for two-dimensional problems and Dirac for three-dimensional problems. Constraint contact is more robust but due to the patch size requirement specified in the Mesh block constraint contact uses too much memory on 3D problems. Depending upon the contact formalism chosen the solver options to be used change. The details of the solver parameters recommended for Dirac and Constraint contact formalisms are provided in Section 19.2.

11.1 Mechanical Contact

```
[Contact]
  [./contact]
   disp_x = <variable>
   disp_y = <variable>
   disp_z = <variable>
   formulation = <string> (DEFAULT)
   friction_coefficient = <real> (0)
   master = <string>
   model = <string> (frictionless)
   normal_smoothing_distance = <real>
   normal_smoothing_method = <string> (edge_based)
   order = <string> (FIRST)
   penalty = \langle real \rangle (1e8)
   normalize_penalty = <bool> (false)
   slave = <string>
   system = <string> (Dirac)
   tangential_tolerance = <real>
   tension_release = <real> (0)
  [../]
[]
```

disp_x

Required. Variable name for displacement variable in x direction. Typically $disp_x$.

disp_y

Variable name for displacement variable in y direction. Typically disp_y.

disp_z Variable name for displacement variable in z direction.

Typically disp_z.

formulation One of DEFAULT, KINEMATIC, or PENALTY. DE-

FAULT is KINEMATIC.

friction_coefficient The friction coefficient.

master **Required.** The boundary id for the master surface.

model One of frictionless, glued, or coulomb.

normal_smoothing_distance Distance from face edge in parametric coordinates over

which to smooth the contact normal. 0.1 is a reasonable

value.

nodal_normal_based, must also have a NodalNormals

block.

order The order of the variable. Typical values are FIRST and

SECOND.

penalty The penalty stiffness value to be used in the constraint.

normalize_penalty Whether to normalize the penalty stiffness by the nodal area

of the slave node.

slave **Required**. The boundary id for the slave surface.

system The system to use for constraint enforcement. Options are

Dirac (DiracKernel) or Constraint. The default system is

Dirac.

tangential_tolerance Tangential distance to extend edges of contact surfaces.

tension_release Tension release threshold. A node will not be released if

its tensile load is below this value. If negative, no tension

release will occur.

In LWR fuel analysis, the cladding surface is typically the master surface, and the fuel surface is the slave surface. It is good practice to make the master surface the coarser of the two.

The robustness and accuracy of the mechanical contact algorithm is strongly dependent on the penalty parameter. If the parameter is too small, inaccurate solutions are more likely. If the parameter is too large, the solver may struggle.

The DEFAULT option uses an enforcement algorithm that moves the internal forces at a slave node to the master face. The distance between the slave node and the master face is penalized. The PENALTY algorithm is the traditional penalty enforcement technique.

11.2 Thermal Contact

11.2.1 GapHeatTransfer

[ThermalContact]
[./thermalcontact]

```
type = GapHeatTransfer
   cylinder_axis_point_1 = <RealVectorValue>
   cylinder_axis_point_2 = <RealVectorValue>
   disp_x = <variable>
   disp_y = <variable>
   disp_z = <variable>
   emissivity_1 = \langle real \rangle (0)
   emissivity_2 = <real> (0)
   gap_conductivity = <real> (1)
   gap_conductivity_function = <string>
   gap_conductivity_function_variable = <string>
   gap_geometry_type = <MooseEnum>
   master = <string>
   min_gap = \langle real \rangle (1e-6)
   max_gap = \langle real \rangle (1e6)
   normal_smoothing_distance = <real>
   normal_smoothing_method = <string> (edge_based)
   order = <string> (FIRST)
   quadrature = <bool> (false)
   slave = <string>
   sphere_origin = <RealVectorValue>
   stefan_boltzmann = <real> (5.669e-8)
   tangential_tolerance = <real>
   variable = <string>
 [../]
[]
```

type	GapHeatTransfer
cylinder_axis_point_1	Start point for defining cylindrical axis
cylinder_axis_point_2	End point for defining cylindrical axis
disp_x	Variable name for displacement variable in x direction. Typically disp_x. Optional.
disp_y	Variable name for displacement variable in y direction. Typically disp_y. Optional.
disp_z	Variable name for displacement variable in z direction. Typically disp_z. Optional.
emissivity_1	The emissivity of the fuel surface.
emissivity_2	The emissivity of the cladding surface.
gap_conductivity	The thermal conductivity of the gap material.
<pre>gap_conductivity_function</pre>	Thermal conductivity of the gap material as a function. Multiplied by gap_conductivity.
<pre>gap_conductivity_function_variable</pre>	Variable to be used in thermal_conductivity_function in place of time.

gap_geometry_type Gap calculation type. Choices are: PLATE

CYLINDER SPHERE

master Required. The boundary id for the master sur-

face.

min_gap
The minimum permissible gap size.
max_gap
The maximum permissible gap size.

nates over which to smooth the contact normal.

0.1 is a reasonable value.

 ${\tt normal_smoothing_method} \qquad \qquad {\tt One \ of \ edge_based \ or \ nodal_normal_based}.$

If nodal_normal_based, must also have a

NodalNormals block.

order The order of the variable. Typical values are

FIRST and SECOND.

quadrature Whether or not to use quadrature point-based

gap heat transfer.

slave Required. The boundary id for the slave sur-

face.

sphere_origin Origin for sphere geometry
stefan_boltzmann The Stefan-Boltzmann constant.

tangential_tolerance Tangential distance to extend edges of contact

surfaces.

variable **Required**. The temperature variable name.

The quadrature option is recommended with second-order meshes. Also note that the type of conductance used depends on the value of the <code>gap_geometry_type</code> parameter (PLATE, CYLINDER, or SPHERE). An example of how to use this can be found in moose/modules/combined/tests/gap_heat_transfer_htonly/.

11.2.2 GapHeatTransferLWR

GapHeatTransferLWR differs from GapHeatTransfer in that the gap conductivity is computed based on the gases in the gap. To this may also be added the effect of solid-solid conduction. The gas in the gap may be flushed in a refabrication step. (See also PlenumPressure (10.8).) Also note that parameters gap_geometry_type, cylinder_axis_1 and 2, and sphere_origin can be used in the this block.

```
[ThermalContact]
[./thermalcontact]
  type = GapHeatTransferLWR
  contact_coef = <real> (10)
  contact_pressure = <string>
  disp_x = <variable>
  disp_y = <variable>
```

```
disp_z = <variable>
    emissivity_1 = \langle real \rangle (0)
    emissivity_2 = \langle real \rangle (0)
    external_pressure = <real> (0)
    initial_gas_fractions = <real list> (1 0 0 0 0 0 0 0 0)
    initial_moles = <string>
    gas_released = <string list>
    gas_released_fractions = <real list> (0 0 0.153 0.847 0 0 0 0 0)
    jump_distance_fuel = <real> (0)
    jump_distance_clad = <real> (0)
    jump_distance_model = <string> (DIRECT)
    master = <string>
    meyer_hardness <real> (0.68e9)
    min_gap = \langle real \rangle (1e-6)
    max_gap = \langle real \rangle (1e6)
    normal_smoothing_distance = <real>
    normal_smoothing_method = <string> (edge_based)
    order = <string> (FIRST)
    quadrature = <bool> (false)
   refab_gas_fractions = <real list>
   refab_time = <real list>
   refab_type = <integer list>
   roughness_fuel = <real> (1e-6)
   roughness_clad = <real> (1e-6)
   roughness_coef = <real> (1.5)
   interaction_layer = <integer> (0)
   slave = <string>
    stefan_boltzmann = \langle real \rangle (5.669e-8)
    tangential_tolerance = <real>
    variable = <string>
  [../]
[]
```

type	GapHeatTransferLWR
contact_coef	The leading coefficient on the solid-solid conduction relation $(1/\sqrt{m})$.
contact_pressure	The contact pressure variable. Typically contact_pressure.
disp_x	Variable name for displacement variable in x direction. Typically disp_x. Optional.
disp_y	Variable name for displacement variable in y direction. Typically disp_y. Optional.
disp_z	Variable name for displacement variable in z direction. Typically disp_z. Optional.
emissivity_1	The emissivity of the fuel surface.

emissivity_2 The emissivity of the cladding surface.

external_pressure The external (gas) pressure.

gon, krypton, xenon, hydrogen, nitrogen, oxygen, carbon

monoxide, carbon dioxide, water vapor).

initial_moles The Postprocessor that will give the initial moles of gas.

gas_released List of one or more Postprocessors that give the gas re-

leased.

gon, krypton, xenon, hydrogen, nitrogen, oxygen, carbon monoxide, carbon dioxide, and water vapor. One set of fractions for each Postprocessor listed in gas_released.

jump_distance_fuel The temperature jump distance of the fuel.

jump_distance_clad The temperature jump distance of the clad.

jump_distance_model One of DIRECT (specify distances directly) or KENNARD

(jump distances computed based on gas properties).

master The boundary id for the master surface.

meyer_hardness The Meyer hardness of the softer material (Pa).

min_gap The minimum permissible gap size.
max_gap The maximum permissible gap size.

normal_smoothing_distance Distance from face edge in parametric coordinates over

which to smooth the contact normal. 0.1 is a reasonable

value.

nodal_normal_based, must also have a NodalNormals

block

order The order of the variable. Typical values are FIRST and

SECOND.

plenum_pressure The name of the plenum pressure Postprocessor.

quadrature Whether or not to use quadrature point-based gap heat

transfer.

refab_gas_fractions The fractions of constituent gases at refabrication (helium,

argon, krypton, xenon, hydrogen, nitrogen, oxygen, carbon

monoxide, carbon dioxide, water vapor).

refab_time The time(s) at which refabrication occurs. If multiple times

are given, multiple sets of refab_gas_fractions and mul-

tiple refab_types must be given.

refab_type One of 0 (instantaneous reset, evolving gas fraction there-

after) or 1 (instantaneous reset, constant gas fraction there-

after).

roughness_fuel The roughness of the fuel surface.

roughness_clad The roughness of the cladding surface.

roughness_coef The coefficient for the roughness summation.

interaction_layer One of 0 (fuel-cladding chemical interaction layer not con-

sidered) and 1 (interaction layer considered).

The boundary id for the slave surface.

stefan_boltzmann The Stefan-Boltzmann constant.

tangential_tolerance Tangential distance to extend edges of contact surfaces.

variable **Required**. The temperature variable name.

12 AuxKernels

AuxKernels are used to compute values for AuxVariables. They often compute quantities based on functions, solution variables, and material properties. AuxKernels can apply to blocks or boundaries. If not block or boundary is specified, the AuxKernel applies to the entire model.

```
[AuxKernels]
  [./name]
   type = <AuxKernel type>
   block = <string list>
   boundary = <string list>
   ...
  [../]
[]
```

type Type of auxiliary kernel.

block List of blocks. Either block numbers or names.

boundary List of boundaries (side sets). Either boundary numbers or names.

12.1 AuxKernels for Output

12.1.1 EutecticThicknessFCCI

The EutecticThicknessFCCI AuxKernel is used to calculated the eutectic penetration thickness when the temperature is above the eutectic melting point for Fuel-Clad Chemical Interaction of metal fuels with cladding. The boundary temperature is required. The rate of penetration is added to the variable tracking the penetration thickness for each time step. The penetration thickness may only grow or remain the same.

```
[./eutecticthicknessfcci]
  type = EutecticThicknessFCCI
  boundary = <string list>
  variable = <variable>
  temperature = <variable>
  eutectic_melt = <real> (988.15)
  unit_factor = <real> (1.0)
[../]
```

type EutecticThicknessFCCI

boundary Required. Boundary where the eutectic penetration thickness is calcu-

lated.

variable **Required**. Name of AuxVariable that holds the penetration thickness

value.

temperature Required. Name of Variable that holds the temperature value.

eutectic_melt Temperature at which the eutectic melts.

unit_factor Factor multiplying the rate which may be used to change the units from

meters per second.

12.1.2 MaterialRealAux

The MaterialRealAux AuxKernel is used to output material properties. Typically, the Aux-Variable computed by MaterialTensorAux will be an element-level, constant variable. The computed value will be the volume-averaged quantity over the element.

```
[./materialrealaux]
  type = MaterialRealAux
  property = <material property>
  variable = <variable>
[../]
```

type MaterialRealAux

property Required. Name of material property.

variable Required. Name of AuxVariable that will hold result.

12.1.3 MaterialTensorAux

The MaterialTensorAux AuxKernel is used to output quantities related to second-order tensors used as material properties. Stress and strain are common examples of these tensors. The AuxKernel allows output of specific tensor entries or quantities computed from the entire tensor. Typically, the AuxVariable computed by MaterialTensorAux will be an element-level, constant variable. By default, the computed value will be the volume-averaged quantity over the element. If the parameter qp_select is set to the value of an integration point number (0, 1, ..., n), the computed valued will be the value at that integration point.

```
[./materialtensoraux]
  type = MaterialTensorAux
  tensor = <material property tensor>
  variable = <variable>
  index = <integer>
  quantity = <string>
  point1 = <vector> (0, 0, 0)
  point2 = <vector> (0, 1, 0)
  qp_select = <integer> (0, 1, ..., n)
[../]
```

type MaterialTensorAux

tensor Required. Name of second-order tensor material property. A typical second-

order tensor material property is stress.

variable Required. Name of AuxVariable that will hold result.

index Index into tensor, from 0 to 5 (xx, yy, zz, xy, yz, zx). Either index or quantity

must be specified.

quantity One of VonMises, PlasticStrainMag, Hydrostatic, Hoop, Radial,

Axial, MaxPrincipal, MedPrincipal, MinPrincipal, FirstInvariant, SecondInvariant, ThirdInvariant, or TriAxiality. Either index or

quantity must be specified.

12.1.4 ThicknessLayerFCCI

The ThicknessLayerFCCI AuxKernel is used to calculated the interaction layer thickness during Fuel-Clad Chemical Interaction for metal fuels. The mass flux through the boundary is required from a postprocessor. The change in thickness layer is then applied to the variable storing the thickness layer on the boundary. The boundary may be an internal boundary. The growth of the interaction layer assumes the same sign as the normal mass flux. Negative thickness values correspond to negative flux values with respect to the boundary normal. If the boundary normal is in the same direction as the mass flux, the thickness layer would be positive as well. The GapHeatTransfer thermal contact model may be used to provide gap species diffusion to calculate mass flux across gap sections.

```
[./thicknesslayerfcci]
  type = ThicknessLayerFCCI
  boundary = <string list>
  variable = <variable>
  postproc_flux = <string>
  initial_contact_time = <real> (0)
  method = <integer>
  layer_density = <real> (7700)
  layer_mol_weight = <real> (1.215)
  solubility_species = <variable>
  solubility_fuel = <real> (0)
[../]
```

type ThicknessLayerFCCI

boundary Required. Boundary where the interaction layer thickness is cal-

culated.

variable Required. Name of AuxVariable that holds the thickness layer

value.

postproc_flux Required. Name of the Postprocessor computing the mass flux

through the boundary.

initial_contact_time The thickness layer is only calculated after this time value has

passed.

method Required. 1 for the correlation with density and molecular

weight. 2 for the correlation with solubility limits.

layer_density *Method 1*. Interaction layer density.

layer_mol_density *Method 1*. Interaction layer molecular weight.

solubility_species *Method 2.* Name of Variable for solubility fractions.

solubility_fuel *Method 2*. Solubility limit in the fuel.

12.2 AuxKernels for Specifying Fission Rate

Note that these AuxKernels are not needed if the Burnup block (see Chapter 13) is present.

12.2.1 FissionRateAux

The FissionRateAux AuxKernel simply sets the value of a variable that stores the fission rate (fissions/m³/s) to either a constant value or a value prescribed by a function. If both function and value are provided, value is used as a scaling factor on the function.

```
[./fissionrateaux]
  type = FissionRateAux
  variable = <string>
  block = <string list>
  function = <string>
  value = <real>
  variable = <string>
[../]
```

type FissionRateAux

variable Required. Name of AuxVariable that will hold fission rate. Typically

fission_rate.

value Value of fission rate. If function is present, value is multiplied by the function

value.

function Function describing the fission rate.

12.2.2 FissionRateAuxLWR

FissionRateAuxLWR is designed to calculate fission rate given rod averaged linear power and pellet dimensions.

```
[./fissionrateauxlwr)
  type = FissionRateAuxLWR
  value = <real> (1)
  rod_ave_lin_pow= <string>
```

```
axial_power_profile = <string>
pellet_diameter = <real>
pellet_inner_diameter = <real> (0)
fuel_volume_ratio = <real> (1)
energy_per_fission = <real> (3.28451e-11)
variable = <string>
[../]
```

value Fission rate if rod_ave_lin_pow is not present. Scale factor if

rod_ave_lin_pow is given.

variable Required. Name of AuxVariable that will hold fission rate.

Typically fission_rate.

rod_ave_lin_pow Function describing rod averaged linear power. This power is

the total power, the power from the volumetric fission rate times

the volume of fuel times the energy per fission.

axial_power_profile Function describing axial power profile.

pellet_diameter Required. The diameter of the fuel.

The inner diameter of the fuel.

fuel_volume_ratio Reduction factor for deviation from right circular cylinder fuel.

The ratio of actual volume to right circular cylinder volume.

energy_per_fission The energy released per fission in J/fission.

12.2.3 FissionRateFromPowerDensity

Like FissionRateAux, the FissionRateFromPowerDensity AuxKernel sets the fission rate based on a function and a scaling factor. This AuxKernel is intended to be used specifically in the case where the input function defines the power density (in W/m^3). The power density is divided by user-provided constant that defines the energy per fission (J/fission) to provide the fission rate in (fissions/ m^3/s).

```
[./fissionratefrompowerdensity]
  type = FissionRateFromPowerDensity
  variable = <string>
  block = <string list>
  function = <string>
  energy_per_fission = <real>
[../]
```

type FissionRateAux

variable Required. Name of AuxVariable that will hold fission rate. Typi-

cally fission_rate.

function **Required**. Function describing the power density in W/m³.

energy_per_fission Required. Energy released per fission in J/fission.

12.3 Other AuxKernels

12.3.1 Al2O3Aux

```
[./al2o3aux]
  type = Al2o3Aux
  variable = <string>
  function = <string>
  model = <string> (function)
  temp = <string>
[../]
```

type Al203Aux

variable **Required**. Variable name corresponding to the Al2O3 thickness. function Function describing the Al2O3 thickness as a function of time.

model One of function or griess. The griess option invokes a correlation appropriate for

plate fuel.

temp Variable name for temperature variable. Typically temp.

12.3.2 BurnupAux

BurnupAux computes burnup given the fission rate. Note that this AuxKernel is not needed if the Burnup block (see Chapter 13) is present.

```
[./burnupaux]
  type = BurnupAux
  fission_rate = <string>
  density = <real>
  molecular_weight = <real> (0.270)
[../]
```

type BurnupAux

variable Required. Variable name corresponding to the burnup. Typically

burnup.

fission_rate Required. Variable name corresponding to the fission rate. Typically

fission_rate.

density Required. The initial fuel density.

molecular_weight The molecular weight.

12.3.3 FastNeutronFluenceAux

```
[./fastneutronfluenceaux]
type = FastNeutronFluenceAux
```

```
variable = <string>
  fast_neutron_flux = <string>
[../]
```

type FastNeutronFluenceAux

variable Required. Variable name corresponding to the fast neutron fluence.

Typically fast_neutron_fluence.

fast_neutron_flux Required. Variable name corresponding to the fast neutron flux. Typ-

ically fast_neutron_flux.

12.3.4 FastNeutronFluxAux

```
[./fastneutronfluxaux]
  type = FastNeutronFluxAux
  variable = <string>
  rod_ave_lin_pow = <string>
  axial_power_profile = <string>
  factor = <real>
  function = <string>
  q_variable = <string>
[../]
```

type FastNeutronFluxAux

variable Required. Variable name corresponding to the fast neutron flux.

Typically fast_neutron_flux.

rod_ave_lin_pow Function describing rod averaged linear power. This power is the

total power, the power from the volumetric fission rate times the

volume of fuel times the energy per fission.

axial_power_profile Function describing axial power profile.

factor The fast neutron flux if function, rod_ave_lin_pow, or

q_variable is not given. Otherwise, a scale factor. Recommended

scale factor value is $3e13 (n/(m^2-s)/(W/m))$.

 $\begin{array}{ll} \hbox{function} & \hbox{Function that describes the fast neutron flux.} \\ \hbox{q_variable} & \hbox{Variable holding linear heat rate in pellet in W/m.} \end{array}$

Only one of function, rod_ave_lin_pow, and q_variable may be given.

12.3.5 GrainRadiusAux

The GrainRadiusAux model is a simple empirical model for calculating grain growth. This can be used with the Sifgrs model (17.1).

```
[./grainradiusaux]
```

```
type = GrainRadiusAux
variable = <string>
temp = <string>
[../]
```

type GrainRadiusAux

variable **Required**. Variable name corresponding to the fuel grain radius. temp **Required**. Variable name for temperature variable. Typically temp.

12.3.6 OxideAux

```
[./oxideaux]
  type = OxideAux
  variable = <string>
  fast_neutron_flux = <string>
  lithium_concentration = <real> (0)
  model_option = <int> (1)
  oxide_scale_factor = <real> (1)
  tin_content = <real> (1.38)
  temperature = <string>
  use_coolant_channel = <bool> (false)
  start_time = <real> (0)
  end_time = <real> (inf)
```

type OxideAux

variable Required. Variable name corresponding to the zirconia thick-

ness.

fast_neutron_flux Variable name corresponding to the fast neutron flux. Typically

fast_neutron_flux.

lithium_concentration Lithium concentration in ppm.

model_option If 1, uses the EPRI KWU CE model. Otherwise, uses the EPRI

SLI model.

oxide_scale_factor Scale factor applied to the rate of oxide growth.

tin_content Tin content in wt%.

temperature Required. Variable name for temperature variable. Typically

temp.

coolant channel model.

start_time Start the oxide growth at a specific time.

end_time End the oxide growth at a specific time, for example in dry stor-

age.

12.3.7 FeCrAlOxideAux

```
[./fecraloxideaux]
  type = FeCrAlOxideAux
  variable = <string>
  parabolic_rate_constant = <real> (784.0)
  activation_energy = <real> (41373.7)
  oxide_scale_factor = <real> (1)
  temperature = <string>
  start_time = <real> (0)
  end_time = <real> (inf)
[../]
```

type FeCrAlOxideAux Required. Variable name corresponding to the oxide thickvariable The constant preceding the exponential term in the parabolic parabolic_rate_constant rate equation. Needs to be entered in units of kg²/m⁴-s. The activation energy for oxidation divided by the ideal gas acitivation_energy constant. Entered in units of K. Scale factor applied to the rate of oxide growth. oxide_scale_factor Required. Variable name for temperature variable. Typically temperature start_time Start the oxide growth at a specific time. End the oxide growth at a specific time, for example in dry end_time

12.3.8 PelletIdAux

PelletIdAux is used to compute a pellet number. It may be used with a discrete pellet or smeared fuel column mesh.

storage.

```
[./pelletidaux]
  type = PelletIdAux
  variable = <string>
  a_lower = <real>
  a_upper = <real>
  number_pellets = <integer>
[../]
```

type PelletIdAux
variable Required. AuxVariable name corresponding to the Pellet ID.
allower Required. The lower axial coordinate of the fuel stack.

a_upper Required. The upper axial coordinate of the fuel stack.

number_pellets Required. Number of fuel pellets.

13 Burnup

The Burnup block computes fission rate and burnup for LWR fuel including the radial power factor. It is not appropriate for other fuel configurations. Use of the Burnup block will cause BISON to create and populate burnup, fission_rate, and optionally other AuxVariables.

The radial power factor calculation is performed on a secondary numerical grid, created internally by BISON. This is the reason for the num_radial and num_axial line commands. Once the fission rate, burnup, and other quantities are computed on this secondary grid, they are mapped back to the finite element mesh.

```
[Burnup]
 [./burnup]
    block = <string list>
    rpf_active = <bool> (true)
    fuel_type = <string> (UO2)
    reactor_type = <string> (LWR)
    include_gadolinia = <bool> (false)
    rod_ave_linear_power = <string>
    axial_power_profile = <string>
    num_radial = <integer>
    num_axial = <integer>
    fuel_pin_geometry = <string>
    a_lower = <real>
    a_upper = <real>
    fuel_inner_radius = <real> (0)
    fuel_outer_radius = <real> (0.0041)
    fuel_volume_ratio = <real> (1)
    density = <real>
    energy_per_fission = <real> (3.28451e-11)
    p1 = \langle real \rangle (3.45)
    i_{enrich} = \langle real \ list \rangle (0.05, 0.95, 0, 0, 0, 0)
    wtfract_gadolinia = <real>
    sigma_c = \langle real \ list \rangle (9.7, 0.78, 58.6, 100, 50, 80)
    sigma_f = \langle real \ list \rangle \ (41.5, 0, 105, 0.584, 120, 0.458)
    sigma_a_thermal = <real list> (359.68, 1.56, 1207.5,
                                         193.5, 1095.24, 11.11)
    N235 = \langle string \rangle
    N238 = \langle string \rangle
    N239 = \langle string \rangle
    N240 = \langle string \rangle
    N241 = \langle string \rangle
    N242 = \langle string \rangle
    N155 = \langle string \rangle
```

```
N157 = <string>
    RPF = <string>
[../]
```

block Required. List of fuel blocks. Either block numbers or names.

rpf_active Flag for turning calculation of radial power factor on.

fuel_type Fuel type. One of UO2 or U3Si2. Will set defaults for sigma_f and

sigma_c in conjunction with the reactor type.

reactor_type Reactor type. One of LWR or HWR. Will set default values for p1,

 $\verb|sigma_f|, and \verb|sigma_c| if those are not otherwise specified.$

include_gadolinia Flag for turning on calculation of gadolinia (Gd₂O₃) effects.

rod_ave_lin_pow Function describing rod averaged linear power. This power is the

total power, the power from the volumetric fission rate times the

volume of fuel times the energy per fission.

axial_power_profile Function describing axial power profile.

num_radial Number of radial divisions in secondary grid used to compute ra-

dial power profile.

num_axial Number of axial divisions in secondary grid used to compute radial

power profile.

fuel_pin_geometry Name of the FuelPinGeometry object (see 23.1).

a_lower Required if fuel_pin_geometry is not specified. The lower axial

coordinate of the fuel stack.

a_upper Required if fuel_pin_geometry is not specified. The upper axial

coordinate of the fuel stack.

fuel_inner_radius The inner radius of the fuel.

fuel_outer_radius The outer radius of the fuel.

fuel_volume_ratio Reduction factor for deviation from right circular cylinder fuel. The

ratio of actual volume to right circular cylinder volume.

density Required. The initial fuel density.

energy_per_fission The energy released per fission in J/fission.

Distribution function coefficient p1. If not given, will take default

value based on reactor_type.

i_enrich The initial enrichment for the six isotopes.

tion of Gd₂O₃.

sigma_c The capture cross sections for the considered isotopes (6 by default,

 $8\ if\ \mbox{include_gadolinia=true}).$ If not given, will take default

value based on reactor_type.

sigma_f	The fission cross sections for the considered isotopes (6 by default, 8 if include_gadolinia=true). If not given, will take default value based on reactor_type.
sigma_a_thermal	The thermal absorption cross sections for the considered isotopes (6 by default, 8 if include_gadolinia=true).
N235	Indicates that the output of the concentration of U-235 is required. Typically N235.
N238	Indicates that the output of the concentration of U-238 is required. Typically N238.
N239	Indicates that the output of the concentration of Pu-239 is required. Typically N239.
N240	Indicates that the output of the concentration of Pu-240 is required. Typically N240.
N241	Indicates that the output of the concentration of Pu-241 is required. Typically N241.
N242	Indicates that the output of the concentration of Pu-242 is required. Typically N242.
N155	Indicates that the output of the concentration of Gd-155 is required. Typically N155. Use only with include_gadolinia=true.
N157	Indicates that the output of the concentration of Gd-157 is required. Typically N157. Use only with include_gadolinia=true.
RPF	Indicates that the output of the radial power factor is required. Typically RPF.

14 Kernels

Kernels are used to evaluate integrals associated with a given term in a PDE. They often compute quantities based on functions, solution variables, auxiliary variables, and material properties. All Kernels act on blocks. If no block is specified, the Kernel will act on the entire model.

```
[Kernels]
  [./name]
  type = <kernel type>
  block = <string list>
    ...
  [../]
[]
```

type Type of kernel.

block List of blocks. Either block numbers or names.

14.1 Arrhenius Diffusion

Kernel for applying an Arrhenius diffusion term. If present, an ArrheniusDiffusionCoef material model must also be present.

```
[./arrheniusdiffusion]
  type = ArrheniusDiffusion
  variable = <variable>
[../]
```

type ArrheniusDiffusion

variable Required. Variable associated with this volume integral.

14.2 BodyForce

Kernel for applying an arbitrary body force to the model.

```
[./bodyforce]
  type = BodyForce
  variable = <variable>
  value = <real> (0)
```

```
function = <string> (1)
[../]
```

type BodyForce

variable Required. Variable associated with this volume integral.

value Constant included in volume integral. Multiplied by the value of function if

present.

function Function to be multiplied by value and used in the volume integral.

14.3 Gravity

Gravity may be applied to the model with this kernel. The required density is computed and provided internally given inputs in the Materials block.

```
[./gravity]
  type = Gravity
  variable = <variable>
  value = <real> (0)
[../]
```

type Gravity

variable Required. Variable name corresponding to the displacement direction in which

the gravity load should be applied.

value Acceleration of gravity. Typically -9.81 (m/s²).

14.4 Heat Conduction

Kernel for diffusion of heat or divergence of heat flux.

```
[./heatconduction]
  type = HeatConduction
  variable = <variable>
[../]
```

type HeatConduction

variable Required. Variable name corresponding to the heat conduction equation. Typi-

cally temp.

14.5 Heat Conduction Time Derivative

Kernel for $\rho C_p \partial T / \partial t$ term of the heat equation.

```
[./heatconductiontimederivative]
  type = HeatConductionTimeDerivative
  variable = <variable>
[../]
```

type HeatConductionTimeDerivative

variable Required. Variable name corresponding to the heat conduction equation. Typi-

cally temp.

14.6 Heat Source

The HeatSource kernel applies a volumetric heat source to specified blocks within the model. Built on the BodyForce kernel's code, the HeatSource kernel provides a more relevant name for easier input-file specification.

```
[./heatsource]
  type = HeatSource
  variable = <variable>
  value = <real> (1)
  function = <string> (1)
  block = <string list>
[../]
```

type HeatSource

variable Required. The variable associated with the heat source.

value Value of the heat source; will be multiplied by the optional function.

function The function describing the volumetric heat source.

block The list of block id's (SubdomainID) to which the heat source will be applied.

14.7 Isotropic Diffusion

IsotropicDiffusion is just like ArrheniusDiffusion except that it takes an arbitrary material property and uses it as the diffusivity. For example, it could be coupled to the material property ArrheniusDiffusionCoef using the material property "arrhenius_diffusion_coef" or to ArrheniusMaterialProperty using any name for the diffusivity.

```
[./diffusion]
  type = IsotropicDiffusion
  variable = <variable>
  diffusivity_property = <string> (diffusivity)
[../]
```

type IsotropicDiffusion

variable **Required**. Variable associated with this volume integral. diffusivity_property The name of the material property to be used as the diffusivity.

14.8 Neutron Heat Source

Kernel for the volumetric heat source associated with fission.

```
[./neutronheatsource]
  type = NeutronHeatSource
  variable = <variable>
  burnup_function = <string>
  fission_rate = <variable>
  decay_heat_function = <string>
  fuel_pin_geometry = <string>
  outer_diameter = <real>
  inner_diameter = <real>
[../]
```

type NeutronHeatSource

variable Required. Variable name corresponding to the heat conduction

equation. Typically temp.

burnup_function Name of the Burnup sub-block, if any (typically burnup). May

not be used with fission_rate. Use of burnup_function is pre-

ferred.

fission_rate Variable name corresponding to the fission rate. Typically

fission_rate.

decay_heat_function Name of the postprocessor giving the decay heat curve. Typically

supplied for LOCA simulations.

fuel_pin_geometry Name of the FuelPinGeometry object (see 23.1).

outer_diameter Outer diameter of the cold fuel pellets if fuel_pin_geometry is

not specified.

inner_diameter Inner diameter of the cold fuel pellets if fuel_pin_geometry is not

specified.

area Cross-sectional area of the cold fuel pellets if fuel_pin_geometry

or the diameters are not specified.

14.9 SolidMechanics

The SolidMechanics block specifies inputs for the divergence of stress as part of the equations of solid mechanics. The divergence of stress is a Kernel in MOOSE nomenclature. The

SolidMechanics block informs MOOSE of the divergence kernels but is not placed inside the Kernels block in the input file.

```
[SolidMechanics]
  [./solidmechanics]
    disp_x = <variable>
    disp_y = <variable>
    disp_z = <variable>
    disp_r = <variable>
    temp = <variable>
    [../]
[]
```

- disp_x Variable name for displacement variable in x direction. Typically disp_x.
- disp_y Variable name for displacement variable in y direction. Typically disp_y.
- disp_z Variable name for displacement variable in z direction. Typically disp_z for 3D and disp_y for axisymmetric models.
- disp_r Variable name for displacement variable in radial direction for axisymmetric or spherically symmetric cases. Typically disp_x.
- temp Variable name for temperature variable. Necessary for thermal expansion. Typically temp.

14.10 Thermo-diffusion (Soret effect, thermophoresis)

ThermoDiffusion is used to model mass flux of the form

$$J = -\frac{DQC}{RT^2}\nabla T \tag{14.1}$$

where D is the mass diffusivity (property name is "mass_diffusivity"), Q is the heat of transport, C is the concentration, R is the gas constant, and T is the temperature.

```
[./soret_diffusion]
  type = ThermoDiffusion
  variable = <variable>
  temp = <variable>
  gas_constant = <real> (8.31446)
[../]
```

type ThermoDiffusion

variable Required. Variable associated with this volume integral.

temp Required. Coupled temperature variable.

gas_constant Universal gas constant.

14.11 TimeDerivative

Kernel for applying a time rate of change term $(\partial u/\partial t)$ to the model.

```
[./timederivative]
  type = TimeDerivative
  variable = <variable>
[../]
```

type TimeDerivative

variable Required. Variable associated with this volume integral.

15 Hydride formation in the cladding

Modeling the evolution of hydrides in the cladding requires two variables to track concentration of the hydrogen in solution and the hydrogen as hydride, kernels that act as source/sink terms for the concentration variables, kernels for Fickian and thermal diffusion of the hydrogen, a kernel for the time derivative of hydrogen, and a set of material models that calculate precipitation and dissolution rates, and the heat of transport and diffusivity of hydrogen. In addition, if hydrogen pickup is of interest, a corrosion model and pickup boundary condition must be added. However, there is also an Action that sets up everything except for the two variables and the hydrogen pickup; we cover the variables and the Action first.

15.1 Using the CladdingHydrides Action (the easy way)

The two concentration variables track the hydrogen in solid solution (commonly referred to as C_{ss}) and the equivalent concentration of hydrogen bound in the precipitated hydrides (commonly referred to as C_p). These concentrations are usually specified in ppm by weight. Since the hydride may have a steep gradient, monomials are helpful to keep the concentration positive. Also note below the large scalings that are useful for speeding convergence.

```
[Variables]
  [./hydrogen_in_solution_ppm]
    scaling = 1e12
    block = 'clad'
  [../]
  [./hydrogen_as_hydride_ppm]
    order = CONSTANT
    family = MONOMIAL
    scaling = 1e12
    block = 'clad'
  [../]
[]
```

The CladdingHydrides Action adds Fick's Law, the Soret effect, a precipitation/dissolution sink/source term, and a specialized time derivative for soluble hydrogen. It also adds a precipitation/dissolution source/sink term and a time derivative for hydrogen as hydride. These kernels require a few specialized material models for the actual precipitation/dissolution rate, the mass diffusivity of hydrogen in the matrix, and the heat of transport for hydrogen; these are also added by the Action. Thus, if you use this Action and have the variables listed above, then you only need to add a hydrogen pickup boundary condition (see 10.7) to get the complete hydride model for the cladding.

```
[CladdingHydrides]
  [./some_name]
   block = <list of blocks>
   temperature = <string>
    hydrogen_in_solution_ppm = <string>
    hydrogen_as_hydride_ppm = <string>
    hydride_clamp = <real> (1)
    diffusivity_frequency_factor = <real> (0.8e-7)
    diffusivity_activation_energy = <real> (33306)
    heat_of_transport = <real> (25121)
  [../]
[]
```

List of blocks where the hydride model is to be applied block (the cladding blocks). Required. Name of the temperature variable. temperature Required. Name of the variable for hydrogen in soluhydrogen_in_solution_ppm tion (wt.ppm). Required. Name of the variable for hydrogen as hyhydrogen_as_hydride_ppm drides (wt.ppm). The limiting value of the volume fraction of hydrides. hydride_clamp This is used to control creation of a thick hydride rim. Must be in [0,1]. diffusivity_frequency_factor The Arrhenius coefficient for hydrogen mass diffusivity in the cladding. The Arrhenius activation energy for hydrogen mass diffusivity_activation_energy diffusivity in the cladding. The heat of transport for dissolved hydrogen in the heat_of_transport cladding.

15.2 Using individual kernels and materials (the hard way)

15.2.1 HydridePrecipitationRate

A single material is used to calculate the precipitation or dissolution rate. This is not a material property *per se*; it is just used this way for convenience.

```
[Materials]
[./precip_rate]
  type = HydridePrecipitationRate
  block = <string>
  temp = <variable>
  hydrogen_in_solution_ppm = <variable>
```

```
hydrogen_as_hydride_ppm = <variable>
hydride_clamp = <real> (1)
[../]
[]
```

type HydridePrecipitationRate

block The volume associated with this material. temp Required. Coupled temperature variable.

hydrogen_in_solution_ppm Required. Coupled C_{ss} in wt.ppm. hydrogen_as_hydride_ppm Required. Coupled C_p in wt.ppm.

hydride_clamp The limiting value of the volume fraction of hydrides. This

is used to control creation of a thick hydride rim. Must be in

[0,1].

The clamping feature is used to limit the amount of hydride that forms by precipitation. If the hydride concentration exceeds the clamp value, the local rate of hydride precipitation will drop to zero even if there is local over saturation of hydrogen in solid solution.

15.2.2 HydrogenSource and HydrideSource

Finally, we just need to add two source kernels: one for C_{ss} and one for C_p . The kernel is a source if precipitation increases the concentration or a sink if precipitation decreases the concentration (i.e. precipitation is a sink for hydrogen in solid solution). For convenience, these are split into HydrogenSource and HydrideSource so that the user does not have to keep track of the sign on the source term.

```
[Kernels]
[./hydride_source]
  type = HydrideSource
  variable = <variable>
[../]
[]
```

type HydrideSource

variable Required. The concentration of hydrogen in one of the phases.

HydrogenSource has the same form as HydrideSource (only the type changes).

15.2.3 HydrogenTimeDerivative

Due to the special treatment of the hydrogen in solution (a volume fraction term appears in the time derivative), we need a special kernel for this term. It needs to couple into the hydride variable as well.

```
[Kernels]
[./hydrogen_dHdt]
  type = HydrogenTimeDerivative
  variable = <variable>
  hydrogen_as_hydride_ppm = <string>
[../]
[]
```

type HydrogenTimeDerivative

variable Required. The concentration of hydrogen in solution (wt.ppm).

hydrogen_as_hydride_ppm Required. The concentration of hydrogen as hydrides (wt.ppm).

hydride_clamp The limiting value of the volume fraction of hydrides. This is used to control creation of a thick hydride rim. Must be in [0,1].

15.2.4 HydrogenDiffusivity

Similarly to HydrogenTimeDerivative, the diffusion term for the hydrogen in solution must also account for the phase fraction of alloy that is available for diffusion.

```
[Materials]
[./hydrogen_diffusivity]
    type = HydrogenDiffusivity
    frequency_factor = <real>
    activation_energy = <real>
    temp = <string>
    property_name = <string>( 'mass_diffusivity')
    hydrogen_as_hydride_ppm = <string>
    hydride_clamp = <real> (1)
[../]
[]
```

type HydrogenDiffusivity
frequency_factor Arrhenius frequency factor.
activation_energy Arrhenius activation energy.

temp Required. The coupled temperature.

property_name The named property that will be declared by this material.
hydrogen_as_hydride_ppm Required. The concentration of hydrogen as hydrides (wt.ppm).

hydride_clamp

The limiting value of the volume fraction of hydrides. This is used to control creation of a thick hydride rim. Must be in [0,1].

15.2.5 Other things needed for modeling hydrides without the CladdingHydrides Action

The kernels and materials for simulating the transport of the hydrogen in solution are generic kernels and are not covered here; see 14.7 for mass diffusion and 14.10 for the Soret effect. These two kernels require material properties for mass diffusivity (use <code>HydrogenDiffusivity</code>) and heat of transport of hydrogen (use <code>GenericConstantMaterial</code> and name the property "heat_of_transport") in the alloy. Also not shown here is the flux boundary condition for hydrogen pickup at the oxide interface (see 10.7).

16 Materials

The Materials block is for specifying material properties and models.

```
[Materials]
[./name]
  type = <material type>
  block = <string list>
   ...
[../]
[]
```

type Type of material model

block List of blocks. Either block numbers or names.

16.1 Thermal Models

16.1.1 HeatConductionMaterial

HeatConductionMaterial is a general-purpose material model for heat conduction. It sets the thermal conductivity and specific heat at integration points.

```
[./heatconductionmaterial]
  type = HeatConductionMaterial
  thermal_conductivity = <real>
  thermal_conductivity_x = <string>
  thermal_conductivity_y = <string>
  thermal_conductivity_z = <string>
  thermal_conductivity_temperature_function = <string>
  specific_heat = <real>
  specific_heat_temperature_function = <string>
[../]
```

type HeatConductionMaterial
thermal_conductivity Thermal conductivity.
thermal_conductivity_x Thermal conductivity Postprocessor
for the x direction.
thermal_conductivity_y Thermal conductivity Postprocessor
for the y direction.

 $thermal_conductivity_z \\ \hspace*{1.5cm} Thermal\ conductivity\ \texttt{Postprocessor} \\$

for the z direction.

tivity as a function of temperature.

specific_heat Specific heat.

specific_heat_temperature_function Function describing specific heat as a

function of temperature.

16.1.2 ThermalCladMaterial

The ThermalCladMaterial model computes the specific heat and thermal conductivity for a variety of exotic cladding materials. The choices are Thermal316, ThermalAlloy33, ThermalD9, ThermalHT9, ThermalIrradiationCreepHT9, ThermalMo, and ThermalNa. The details of these models are described in the Theory Manual. Examples of their use can be found in /bison/tests/thermalTests/, /bison/tests/thermalD9/, /bison/tests/thermalNa/, and /bison/tests/thermalHT9/.

```
[./thermalCladMaterial]
  type = Thermal < string >
  block = < string list >
  temp = < string >
[../]
```

type Thermal<string>, where <string> is the fuel material type (eg. HT9)

block List of blocks this material applies to.

temp Name of temperature variable. Typically temp.

16.1.3 ThermalFeCrAl

The ThermalFeCrAl model computes the specific heat and thermal conductivity for a variety of FeCrAl cladding alloys. The alloys to choose from are Special Metals Incoloy MA956, Plansee PM2000, Kanthal APMT, Resistalloy International Fecralloy and ORNL's C35M.

```
[./thermalFeCrAl]
  type = ThermalFeCrAl
  block = <string list>
  material = <string> (APMT)
  temp = <string>
[../]
```

type ThermalFeCrAl

block List of blocks this material applies to.

material Name of the chosen FeCrAl alloy. Choices are MA956, PM2000, APMT, FE-

CRALLOY or C35M

16.1.4 ThermalFuel

The ThermalFuel model computes specific heat and thermal conductivity for oxide fuel. A number of correlations are available.

```
[./thermalfuel]
  type = ThermalFuel
  temp = <string>
  burnup_function = <string>
  burnup = <string>
  porosity = <string>
  initial_porosity = <real> (0.05)
  oxy_to_metal_ratio = <real> (2.0)
  Pu_content = <real> (0.0)
  Gd_content = <real> (0.0)
  model = < 0, 1, 2, 3, 4, or 5 for
        Duriez, Amaya, Fink-Lucuta, Halden, NFIR, or Modified NFIR >
[../]
```

type ThermalFuel

temp Name of temperature variable. Typically temp.

burnup_function Name of the Burnup sub-block, if any (typically burnup). May not

be used with the burnup line command. Use of burnup_function

is preferred.

burnup Name of burnup variable. Typically burnup.

porosity Name of porosity variable. Typically porosity. Optional.

oxy_to_metal_ratio Ratio of oxygen atoms to metal atoms.

Pu_content Weight fraction of Pu in MOX fuel (typically 0.07).

Gd_content Weight fraction of Gd in fuel.

model Required. The chosen thermal conductivity model.

16.1.5 ThermalFastMOX

The ThermalFastMOX model computes the thermal conductivity for fast MOX fuel. Currently a single correlation is available from Inoue and used by Karahan. Details are provided in the theory manual. The specific heat capacity is treated as a constant value for now.

```
[./thermalfastmox]
  type = ThermalFastMOX
  temp = <string>
  burnup_function = <string>
```

```
burnup = <string>
porosity = <string>
initial_porosity = <real> (0.05)
oxy_to_metal_ratio = <real> (2.0)
[../]
```

type ThermalFastMOX

temp Name of temperature variable. Typically temp.

burnup_function Name of the Burnup sub-block, if any (typically burnup). May not

be used with the burnup line command. Use of burnup_function

is preferred.

burnup Name of burnup variable. Typically burnup.

porosity Name of porosity variable. Typically porosity. Optional.

oxy_to_metal_ratio Ratio of oxygen atoms to metal atoms.

16.1.6 ThermalMAMOX

The ThermaMAMOX model computes the thermal conductivity for minor actinide, Np- and Ambearing, fast MOX fuel (MA-MOX). This model is based on the correlation found here [8]. The correlation takes in to account the oxygen to metal ratio of the fuel, the Am quantity and the Np quantity present. The specific heat capacity is treated as a constant value.

```
[./thermalMAMOX]
  type = ThermalMAMOX
  temp = <string>
  burnup_function = <string>
  burnup = <string>
  porosity = <string>
  initial_porosity = <real> (0.05)
  oxy_to_metal_ratio = <real> (2.0)
[../]
```

type ThermalFastMOX

temp Name of temperature variable. Typically temp.

burnup_function Name of the Burnup sub-block, if any (typically burnup). May not

be used with the burnup line command. Use of burnup_function

is preferred.

burnup Name of burnup variable. Typically burnup.

porosity Name of porosity variable. Typically porosity. Optional.

oxy_to_metal_ratio Ratio of oxygen atoms to metal atoms.

16.1.7 ThermalFuelMaterial

The ThermalFuelMaterial model computes specific heat and thermal conductivity for a variety of exotic fuel materials. The choices are ThermalU, ThermalU10Mo, ThermalU3Si5UN. The details of these models are described in the Theory Manual. Examples of their use can be found in /bison/tests/thermalTests/.

```
[./thermalFuelMaterial]
  type = Thermal<string>
  block = <string list>
  temp = <string>
  porosity = <string>
  density = <real>
[../]
```

```
type Thermal<string>, where <string> is the fuel material type (eg. U10Mo)
block List of blocks this material applies to.
temp Name of temperature variable. Typically temp.
porosity Name of porosity variable. Typically porosity. Optional.
```

Required. Density, assumed constant.

16.1.8 ThermalUPuZr

density

The ThermalUPuZr model computes the specific heat and thermal conductivity for any alloy of U-Pu-Zr metal fuel. If porosity and porosity_material are both defined an error will result. The user has the choice of not supplying any porosity, supplying a variable for porosity or couple to a material that calculates the porosity.

In addition, a user can specify molar (X_i) or weight fraction (w_i) . It is important to note that molar fraction can be coupled to a variable, while weight fraction remains constant.

```
[./thermalUPuZr]
  type = ThermalUPuZr
  block = <string list>
  temp = <string>
  porosity = <string>
  porosity_material = <bool> (false)
  X_Pu = \langle string \rangle
  X_Zr = \langle string \rangle
  pu_weight = <real>
  zr_weight = <real>
  thcond model = <string> (billone)
  spheat_model = <string> (karahan)
  A_U = \langle real \rangle (0.2380289)
  A_Pu = < real > (0.244)
  A_Zr = \langle real \rangle (0.091224)
  k_{scalar} = \langle real \rangle (1.0)
```

porosity_factor = <real></real>	(2.5)
[/]	

ThermalUPuZr type

List of blocks this material applies to. block

Name of temperature variable. Typically temp. temp

Name of porosity variable. Typically porosity. Optional. porosity

porosity_material A flag indicating whether porosity is being calculated by a material

property (e.g., VSwellingUPuZr). Optional.

Name of the molar fraction of plutonium variable. Typically X_Pu. X_Pu Name of the molar fraction of zirconium variable. Typically X_Zr. X_Zr The weight fraction of plutonium in the fuel. This value remains pu_weight

constant. Given as a decimal (e.g., 0.2).

zr_weight The weight fraction of zirconium in the fuel. This value remains

constant. Given as a decimal (e.g., 0.15).

 A_U Molar mass of uranium in [kg/mol]. Molar mass of plutonium in [kg/mol]. A_Pu A_Zr Molar mass of zirconium in [kg/mol].

Multiplication factor multiplied against the thermal conductivity. k_scalar

Factor used when calculating porosity correction). porosity_factor

16.1.9 ThermalSilicideFuel

The ThermalSilicideFuel model computes the specific heat and thermal conductivity for different phases of uranium silicide fuel including pure silicon, pure uranium metal, U₃Si₂, U₃Si, and U₃Si₅. Three models are available for thermal conductivity and two models for specific heat. The details of these models can be found in the theory manual.

```
[./thermalSilicideFuel]
 type = ThermalSilicideFuel
 block = <string list>
 temp = <string>
 silicon_mole_fraction = <real> (0.4)
 specific_heat_model = <string> (WHITE)
 thermal_conductivity_model = <string> (WHITE)
[../]
```

type ThermalSilicideFuel

List of blocks this material applies to. block

Name of temperature variable. Typically temp. temp

silicon_mole_fraction The mole fraction of silicon in the fuel. For example for

U₃Si₂ this parameter would be 0.4

 ${\tt specific_heat_model} \qquad \qquad {\tt Name~of~the~model~to~be~used~to~compute~the~specific~heat.}$

Default is WHITE. Options are WHITE and IAEA.

thermal_conductivity_model Name of the model to be used to compute the thermal

conductivity. Default is WHITE. Options are WHITE,

SHIMIZU, and ZHANG.

16.2 Solid Mechanics Models

16.2.1 CreepFastMOXModel

CreepFastMOXModel is used to model the creep behavior of fast MOX.

```
[./creepfastmox]
 type = CreepFastMOXModel
 absolute_tolerance = <real>
 creeprate_scalef = <real>
 fission_rate = <string>
 fraction_of_temp_outside_model_bounds = <real>
 grain_size = <real>
 max_creep_increment = <real>
 max_its = \langle int \rangle
 output = <string>
 output_iteration_info = <bool>
 output_iteration_info_on_error = <bool>
 output_properties = <string>
 outputs = <string>
 relative_tolerance = <real>
 stress_free_temperature = <real>
 temp = <string>
 thermal_expansion = <real>
 thermal expansion coefficient = <real>
 thermal_expansion_function = <string>
  thermal_expansion_function_type = <string>
 thermal_expansion_reference_temperature = <real>
  use_displaced_mesh = <bool>
[../]
```

type CreepFastMOXModel

absolute_tolerance Absolute convergence tolerance for sub-

newtion iteration

creeprate_scalef scaling factor for creep rate

fission_rate Coupled fission rate

 $fraction_of_temp_outside_model_bounds \qquad \quad Fraction \ of \ temperature \ limit \ outside \ of$

model bounds

grain size in micro meters grain_size Maximum creep strain increment allowed max_creep_increment by accuracy time step criterion Maximum number of sub-newton itera max_its The reporting postprocessor to use for the output max_iterations value Set true to output sub-newton iteration inoutput_iteration_info formation output_iteration_info_on_error Set true to output sub-newton iteration information when a step fails output_properties List of material properties, from this material, to output (outputs must also be defined to an output type) outputs Vector of output names were you would like to restrict the output of variables(s) associated with this object relative_tolerance Relative convergence tolerance for subnewtion iteration stress_free_temperature The stress-free temperature. If not specified, the initial temperature is used. Coupled Temperature temp The thermal expansion coefficient thermal_expansion thermal_expansion_function Thermal expansion coefficient as a function of temperature thermal_expansion_function_type Type of thermal expansion function. Choices are: instantaneous mean thermal_expansion_reference_temperature Reference temperature for mean thermal expansion function

16.2.2 CreepPyC

CreepPyC is used to model the creep behavior of pyrolytic carbon.

```
[./creeppyc]
  type = CreepPyC
  disp_x = <string>
  disp_y = <string>
  disp_z = <string>
  disp_r = <string>
  temp = <string>
  flux = <string>
  density = <real>
```

```
youngs_modulus = <real>
poissons_ratio = <real>
thermal_expansion = <real> (0)
stress_free_temperature = <real>
[../]
```

type	CreepPyC
disp_x	Variable name for displacement variable in x direction. Typically disp_x.
disp_y	Variable name for displacement variable in y direction. Typically disp_y.
disp_z	Variable name for displacement variable in z direction. Typically disp_z for 3D and disp_y for axisymmetric models.
disp_r	Variable name for displacement variable in radial direction for axisymmetric or spherically symmetric cases. Typically disp_x.
temp	Name of temperature variable. Typically temp.
flux	Required . Variable name corresponding to the fast neutron flux. Typically fast_neutron_flux.
density	Required. The initial material density.
thermal_expansion	Coefficient of thermal expansion.
stress_free_temperature	The stress-free temperature. If not specified, the initial temperature is used.

16.2.3 CreepSiC

```
[./creepsic]
  type = CreepSiC
  disp_x = <string>
  disp_y = <string>
  disp_z = <string>
  temp = <string>
  temp = <string>
  fast_neutron_flux = <string>
  k_function = <string>
  youngs_modulus = <real>
  poissons_ratio = <real>
  thermal_expansion = <real> (0)
  stress_free_temperature = <real>
[../]
```

type CreepSiC

disp_x	Variable name for displacement variable in x direction. Typically ${\tt disp_x}$.
disp_y	Variable name for displacement variable in y direction. Typically ${\tt disp_y}$.
disp_z	Variable name for displacement variable in z direction. Typically ${\tt disp_z}$ for 3D and ${\tt disp_y}$ for axisymmetric models.
disp_r	Variable name for displacement variable in radial direction for axisymmetric or spherically symmetric cases. Typically disp_x.
temp	Name of temperature variable. Typically temp.
fast_neutron_flux	Variable name corresponding to the fast neutron flux. Typically fast_neutron_flux.
k_function	Required . Function that takes temperature as input and gives the K coefficient as output.
youngs_modulus	Young's modulus.
poissons_ratio	Poisson's ratio.
thermal_expansion	Coefficient of thermal expansion.
stress_free_temperature	The stress-free temperature. If not specified, the initial temperature is used.

CreepSiC is used to model the creep behavior of silicon carbide. The relation is

$$\dot{\varepsilon}_{cr} = K \sigma \phi. \tag{16.1}$$

16.2.4 CreepU10Mo

 ${\tt CreepU10Mo}\ is\ used\ to\ model\ the\ thermal\ and\ irradiation\ creep\ behavior\ of\ U-10Mo\ fast\ reactor\ fuel.$

```
[./creepu10mo]
  type = CreepU10Mo
  disp_x = <string>
  disp_y = <string>
  disp_z = <string>
  disp_r = <string>
  temp = <string>
  fission_rate = <string>
  youngs_modulus = <real>
  poissons_ratio = <real>
  thermal_expansion = <real> (0)
  stress_free_temperature = <real>
[../]
```

type CreepU10Mo

Variable name for displacement variable in x direction. Typidisp_x cally disp_x. Variable name for displacement variable in y direction. Typidisp_y cally disp_y. Variable name for displacement variable in z direction. Typidisp_z cally disp_z for 3D and disp_y for axisymmetric models. Variable name for displacement variable in radial direction disp_r for axisymmetric or spherically symmetric cases. Typically disp_x. Name of temperature variable. Typically temp. temp Variable name corresponding to the fast neutron flux. Typifission_rate cally fission_rate. Young's modulus. youngs_modulus poissons_ratio Poisson's ratio. Coefficient of thermal expansion. thermal_expansion stress_free_temperature The stress-free temperature. If not specified, the initial temperature is used.

16.2.5 CreepUO2

The CreepU02 is used to model the creep behavior of UO_2 .

```
[./creepuo2]
 type = CreepUO2
 disp x = \langle string \rangle
 disp_y = <string>
 disp_z = <string>
 disp_r = <string>
 temp = <string>
 burnup_function = <string>
 fission_rate = <string>
 density = <real>
 youngs_modulus = <real>
 poissons_ratio = <real>
 thermal_expansion = <real> (0)
 grain_radius = <real> (10e-6)
 oxy_to_metal_ratio = <real> (2)
 relative_tolerance = <real> (1e-4)
 absolute_tolerance = <real> (1e-20)
 max_its = \langle integer \rangle (10)
 output_iteration_info = <true or false> (false)
 stress_free_temperature = <real>
 matpro_youngs_modulus = <true or false> (false)
 matpro_poissons_ratio = <true or false> (false)
 matpro_thermal_expansion = <true or false> (false)
```

```
burnup = <string>
  isotropic_cracking = <true or false> (false)
  rod_ave_lin_pow = <string>
[../]
```

CreepUO2 type Variable name for displacement variable in x direction. Typdisp_x ically disp_x. disp_y Variable name for displacement variable in y direction. Typically disp_y. Variable name for displacement variable in z direction. Typdisp_z ically disp_z for 3D and disp_y for axisymmetric models. Variable name for displacement variable in radial direction disp_r for axisymmetric or spherically symmetric cases. Typically disp_x. Name of temperature variable. Typically temp. temp burnup_function Name of the Burnup sub-block, if any (typically burnup). May not be used with fission_rate. of burnup_function is preferred. fission_rate Variable name corresponding to the fission rate. Typically fission_rate. density **Required**. The initial fuel density. youngs_modulus Young's modulus. poissons_ratio Poisson's ratio. thermal_expansion Coefficient of thermal expansion. grain_radius Fuel grain radius. oxy_to_metal_ratio Oxygen to metal ratio. relative_tolerance Relative convergence tolerance for material model iterations. absolute_tolerance Absolute convergence tolerance for material model iterations. Maximum number of material model convergence iterations. max_its Whether to output material model convergence information. output_iteration_info stress_free_temperature The stress-free temperature. If not specified, the initial temperature is used. matpro_youngs_modulus Set to true to use correlations for Young's modulus from MATPRO [9]. Set to true to use correlations for Poisson's modulus from matpro_poissons_ratio MATPRO [9]. matpro_thermal_expansion Set to true to use correlations for coefficient of thermal expansion from MATPRO [9].

burnup Name of burnup variable. Only required if using MATPRO correlations. Typically burnup.

isotropic_cracking Set to true to use isotropic cracking model.

Name of linear power function. Only required if isotropic_cracking = true.

16.2.6 HotPressingUO2

rod_ave_lin_pow

```
[./hotpressinguo2]
 type = HotPressingUO2
 disp_x = <string>
 disp_y = <string>
 disp_z = <string>
 disp_r = <string>
 temp = <string>
 fission_rate = <string>
 youngs_modulus = <real>
 poissons_ratio = <real>
 thermal_expansion = <real> (0)
 grain_radius = <real> (10e-6)
 oxy_to_metal_ratio = <real> (2)
 relative_tolerance = <real> (1e-4)
 absolute_tolerance = <real> (1e-20)
 max_its = \langle integer \rangle (10)
 output_iteration_info = <true or false> (false)
 stress_free_temperature = <real>
 matpro_youngs_modulus = <true or false> (false)
 matpro_poissons_ratio = <true or false> (false)
 matpro_thermal_expansion = <true or false> (false)
 burnup = <string>
 abs\_error = \langle real \rangle (1.0e-6)
 compute_pressure = <true or false> (true)
 debug_output = <true or false> (false)
 has_hotpressing_plasticity = <true or false> (false)
 hotpressing_alpha = <real> (0)
 hotpressing_nu = <real> (0)
 input_hardening_modulus = <real> (0)
 input_hotpressing = <true or false> (false)
 input_yield_stress = <real> (0)
 max_iteration = \langle integer \rangle (1000)
 model_hotpressing = <true or false> (true)
 rel\_error = \langle real \rangle (0.001)
 use_flow_rule = <true or false> (true)
[../]
```

type

HotPressingUO2

disp_x Variable name for displacement variable in x direction.

Typically disp_x.

disp_y Variable name for displacement variable in y direction.

Typically disp_y.

disp_z Variable name for displacement variable in z direction.

Typically disp_z for 3D and disp_y for axisymmetric

models.

disp_r Variable name for displacement variable in radial direc-

tion for axisymmetric or spherically symmetric cases.

Typically disp_x.

temp Name of temperature variable. Typically temp.

fission_rate Variable name corresponding to the fission rate. Typically

fission_rate.

youngs_modulus Young's modulus. poissons_ratio Poisson's ratio.

thermal_expansion Coefficient of thermal expansion.

grain_radius Fuel grain radius.

oxy_to_metal_ratio Oxygen to metal ratio.

relative_tolerance Relative convergence tolerance for material model itera-

tions.

absolute_tolerance Absolute convergence tolerance for material model itera-

tions.

max_its Maximum number of material model convergence itera-

tions.

output_iteration_info Whether to output material model convergence informa-

tion.

stress_free_temperature The stress-free temperature. If not specified, the initial

temperature is used.

matpro_youngs_modulus Set to true to use correlations for Young's modulus from

MATPRO [9].

matpro_poissons_ratio Set to true to use correlations for Poisson's modulus from

MATPRO [9].

expansion from MATPRO [9].

burnup Name of burnup variable. Only required if using MAT-

PRO correlations. Typically burnup.

abs_error Absolute error in the sub-newton iteration loop to com-

pute trial pressure.

compute_pressure Set to true to compute trial pressure.

debug_output Set to true to output debug information.

has_hotpressing_plasticity Set to true to turn on instantaneous plasticity model.

hotpressing_alpha Parameter alpha in the hot-pressing model.
hotpressing_nu Parameter nu in the hot-pressing model.

input_hardening_modulus Hardening modulus in a linear hardening model for UO2.

input_hotpressing Set true to input hot-pressing parameters.

input_yield_stress Yield stress of UO₂.

max_iteration Maximum iteration number in the sub-newton interation

loop to compute trial pressure.

model_hotpressing Set true to model hot-pressing of UO_2 .

rel_error Relative error in the sub-newton interation loop to com-

pute trial pressure.

use_flow_rule Use modified flow rule for modeling hot-pressing plastic-

ity.

The HotPressingUO2 is used to model the stress induced densification of UO₂.

16.2.7 CreepUPuZr

CreepUPuZr is used to model the thermal and irradiation creep behavior of U-Pu-Zr fast reactor fuel. If porosity and porosity_material are both defined an error will result. The user has the choice of not supplying any porosity, supplying a variable for porosity or couple to a material that calculates the porosity.

CreepUPuZr can also be used to calculate the open pore compression strain increment (hot pressing strain), due to the closing of open pores. The hydrostatic_stress must be set to include the hot pressing strain in the model, and the plenum_pressure should also be defined to correctly calculate the hot pressing strain.

```
[./creepupuzr]
  type = CreepUPuZr
  disp_x = <string>
  disp_y = <string>
  disp_z = <string>
  disp_r = <string>
  temp = <string>
  porosity = <string>
  porosity_material = <bool> (false)
  fission_rate = <string>
  youngs_modulus = <real>
  poissons_ratio = <real>
  hydrostatic_stress = <string>
  plenum_pressure = <string>
  gamma_transition = <real> (923)
```

```
thermal_expansion = <real> (0)
stress_free_temperature = <real>
[../]
```

type	CreepUPuZr
disp_x	Variable name for displacement variable in x direction. Typi-
	cally disp_x.
disp_y	Variable name for displacement variable in y direction. Typi-
	cally disp_y.
disp_z	Variable name for displacement variable in z direction. Typi-
	cally disp_z for 3D and disp_y for axisymmetric models.
disp_r	Variable name for displacement variable in radial direction
	for axisymmetric or spherically symmetric cases. Typically
	disp_x.
temp	Name of temperature variable. Typically temp.
porosity	Variable name corresponding to the porosity. Typically
	porosity.
porosity_material	A flag indicating whether porosity is being calculated by a
	material property (e.g., VSwellingUPuZr). Optional.
fission_rate	Variable name corresponding to the fast neutron flux. Typi-
	cally fission_rate.
youngs_modulus	Young's modulus.
poissons_ratio	Poisson's ratio.
hydrostatic_stress	Variable name for the hydrostatic (mean) stress value. Typi-
	cally hydrostatic_stress.
plenum_pressure	The postprocessor name for the plenum pressure. Typically
	plenum_pressure.
gamma_transition	Gamma phase transition temperature, in Kelvin.
thermal_expansion	Coefficient of thermal expansion.
stress_free_temperature	The stress-free temperature. If not specified, the initial tem-
	perature is used.

16.2.8 Elastic

The Elastic model is a simple hypo-elastic model.

```
[./elastic]
  type = Elastic
  disp_x = <string>
  disp_y = <string>
  disp_z = <string>
  disp_r = <string>
```

```
temp = <string>
youngs_modulus = <real>
poissons_ratio = <real>
thermal_expansion = <real> (0)
stress_free_temperature = <real>
[../]
```

type Elastic Variable name for displacement variable in x direction. Typidisp_x cally disp_x. Variable name for displacement variable in y direction. Typidisp_y cally disp_y. Variable name for displacement variable in z direction. Typidisp_z cally disp_z for 3D and disp_y for axisymmetric models. disp_r Variable name for displacement variable in radial direction for axisymmetric or spherically symmetric cases. Typically Name of temperature variable. Typically temp. temp Young's modulus. youngs_modulus Poisson's ratio. poissons_ratio Coefficient of thermal expansion. thermal_expansion The stress-free temperature. If not specified, the initial temstress_free_temperature perature is used.

16.2.9 FeCrAIPlasticity

The IsoPlasticityFeCrAl model is a model used to model the instantaneous isotropic plasticity of FeCrAl cladding. A yield stress function as a function of temperature is automatically set based upon data in the literature. See the Theory Manual for details.

```
[./fecral_plasticity]
  type = IsoPlasticityFeCrAl
  relative_tolerance = <real> (1e-5)
  absolute_tolerance = <real> (1e-20)
  max_its = <integer> (30)
  output_iteration_info = <bool> (false)
  output_iteration_info_on_error = <bool> (false)
  hardening_constant = <real>
  hardening_function = <string>
  yield_stress = <real>
[../]
```

type

IsoPlasticityFeCrAl

relative_tolerance Relative convergence tolerance for sub-newton itera-

tions.

absolute_tolerance Absolute convergence tolerance for sub-newton itera-

tions.

max_its Maximum number of sub-newton convergence itera-

tions.

output_iteration_info Whether to output sub-newton convergence informa-

tion

output_iteration_info_on_error Whether to output material model convergence infor-

mation if an error occurs.

hardening_function True stress as a function of plastic strain.

yield stress as a function of temperature inherent to

the model.

16.2.10 FailureFeCrAl

FailureFeCrAl models the failure of FeCrAl cladding. The hoop stress is compared against the ultimate tensile strength (UTS) which is determined as a function of temperature based upon data in the literature. See the Theory Manual for details.

```
[./failure_fecral]
   type = FailureFeCrAl
   block = <string list>
   boundary = <string list>
   temperature = <string>
   hoop_stress = <string>
[../]
```

type FailureFeCrAl

block Required. Only required if boundary not supplied. Block ids for which

failure of elements will be calculated. Material property failed becomes

1.0 when failure of that element has occurred.

boundary Required. Only required if block not supplied. Boundary ids for which

failure of side surfaces will be calculated. Material property failed.

temp Required. Name of temperature variable. Typically temp.

hoop_stress Required. Name of the hoop stress aux variable. Typically hoop_stress.

16.2.11 FailureCladding

FailureCladding is the model for Zircaloy-4 cladding failure due to burst during a LOCA accident.

```
[./failurecladding]
  type = FailureCladding
  boundary = <string list>
  criterion = <integer> (2)
  hoop_stress = <string>
  eff_strain_rate_creep = <string>
  eff_strain_rate_plast = <string>
  temperature = temperature
  fract_beta_phase = <string>
  fract_oxygen_gain = <string>
[../]
```

FailureCladding type boundary Required. Waterside cladding boundary. The model in the current version is applied to the boundary because it is coupled to the waterside oxidation model (Section 16.2.19). Choice of the failure criterion. One of 0 (overstress), 1 (plascriterion tic instability) or 2 (combined overstress and plastic instability). criterion = 2 is recommended. hoop_stress Name of hoop stress auxiliary variable. For evaluating over-Name of the auxiliary variable for the effective strain rate due to eff_strain_rate_creep creep. For evaluating plastic instability. Name of the auxiliary variable for the effective strain rate due to eff_strain_rate_plast plasticity. For evaluating plastic instability. temperature Name of temperature variable. For evaluating overstress. fract_beta_phase Name of the auxiliary variable for the volume fraction of Zr β phase, calculated by the model ZrPhase (Section 16.2.28). Name of the auxiliary variable for the gained weight fraction fract_oxygen_gain of oxygen in the cladding, calculated by the model Oxidation-Cladding (Section 16.2.19).

16.2.12 FailureCladHT9

FailureCladHT9 is the model for HT9 cladding failure during both long and short transients. Long transient failure is traditionally predicted with the Cumulative Damage Fraction (CDF) method. Short transients track cavity growth along grain boundaries with a Constrained Cavity Growth (CCG) with Diffusion and Creep with Sliding (D&CS) mechanism.

```
[./failurecladht9]
  type = FailureCladHT9
  block = <string list>
  boundary = <string list>
```

```
transient = <boolean>
temperature = temperature
hoop_stress = hoop_stress
boltzmann = \langle real \rangle (1.3806488e-23)
q_val = \langle real \rangle (6.44336e5)
avogadro_num = \langle real \rangle (6.0221409e23)
a_{initial} = \langle real \rangle (7.0e-08)
atomic_volume = <real> (1.18e-29)
b = \langle real \rangle (3.5e-06)
boundary_diffusivity = <real> (1.1e-12)
boundary_free_energy = <real> (0.85)
creep_n_power = \langle real \rangle (5.0)
eff_strain_rate_creep = <string>
hydrostatic_stress = <string>
surface_free_energy = <real> (2.1)
von_mises_stress = <string>
```

type FailureCladHT9

block Required. Only required if boundary not supplied. Block ids

for which failure of elements will be calculated. Material property failed becomes 1.0 when failure of that element has oc-

curred.

boundary Required. Only required if block not supplied. Boundary ids

for which failure of side surfaces will be calculated. Material property failed becomes 1.0 when failure of that side surface

has occurred.

transient Required. CCG with D&CS activated with true. CDF activated

with false.

temperature Required. Name of temperature variable.

hoop_stress Required. Name of variable containing the hoop stress.

boltzmann Boltzmann constant. Used for both CCG and CDF.

boltzmann Boltzmann constant. Used for both CCG and CDF. q_val CDF. Q value for data collapse to the Dorn parameter.

avogadro_num CDF. Avogadro's number.

a_initial *CCG*. Initial cavity radius. Cannot be equal to zero.

b CCG. Distance from cavity center to midplane between cavities.

2b is the distance between periodic cavity centers.

boundary_free_energy *CCG*. Grain boundary diffusivity.

**CCG. Grain boundary free energy.

creep_n_power CCG. Exponent power n for a material obeying a creep power

law.

eff_strain_rate_creep CCG. Variable containing the effective creep strain rate value.

16.2.13 IrradiationGrowthZr4

The IrradiationGrowthZr4 model incorporates anisotropic volumetric swelling to track axial elongation in Zr4 cladding.

```
[./irradiationgrowthzr4]
  type = IrradiationGrowthZr4
  fast_neutron_fluence = <string>
  Ag = <real> (3e-20)
  ng = <real> (0.794)
[../]
```

16.2.14 MechFeCrAl

The MechFeCrAl model computes the elastic moduli, coefficient of thermal expansion, and thermal creep of a variety of FeCrAl alloys being considered for accident tolerant cladding.

```
[./mechFeCrAl]
 type = MechFeCrAl
 block = <string list>
 disp_x = <string>
 disp_y = <string>
 disp_z = <string>
 disp_r = <string>
 temp = <string>
 fast_neutron_flux = <string>
 youngs_modulus = <real>
 poissons_ratio = <real>
 material = <string> (APMT)
 scale_factor_A = <real> (1.0)
 scale_factor_Q = <real> (1.0)
 scale_factor_n = <real> (1.0)
 scale_factor_alpha = <real> (1.0)
 scale_factor_cte = <real> (1.0)
 scale_factor_youngs = <real> (1.0)
 scale_factor_nu = <real> (1.0)
```

```
model_thermal_expansion = <bool> (true)
model_elastic_modulus = <bool> (false)
model_thermal_creep = <bool> (true)
model_irradiation_creep = <bool> (true)
stress_free_temperature = <real>
[../]
```

type MechFeCrAl. block The list of blocks this material applies to. Variable name for displacement variable in x direction. Typidisp_x cally disp_x. disp_y Variable name for displacement variable in y direction. Typically disp_y. Variable name for displacement variable in z direction. Typidisp_z cally disp_z for 3D and disp_y for axisymmetric models. disp_r Variable name for displacement variable in radial direction for axisymmetric or spherically symmetric cases. Typically disp_x. Name of temperature variable. Typically temp. temp Name of the fast flux variable. Typically fast_neutron_flux fast_neutron_flux. Young's modulus. youngs_modulus Poisson's ratio. poissons_ratio Name of chosen FeCrAl alloy. Choices are MA956, PM2000, material APMT, FECRALLOY, C35M. Scale factor to be applied to the creep prefactor. scale_factor_A scale_factor_0 Scale factor to be applied to the creep activation energy. scale_factor_n Scale factor to be applied to the creep stress exponent. Scale factor to be applied to the temperature coefficient. scale_factor_alpha scale_factor_cte Scale factor to be applied to the thermal expansion coefficient. Scale factor to be applied to the Young's modulus. scale_factor_youngs scale_factor_nu Scale factor to be applied to the Poisson's ratio. model_thermal_expansion Whether to calculate the thermal expansion coefficient as a function of temperature. model_elastic_modulus Whether to calculate temperature dependent elastic moduli. model_thermal_creep Whether or not to model thermal creep. Whether or not to model irradiation creep. model_irradiation_creep stress_free_temperature The stress-free temperature. If not specified, the initial temperature is used.

16.2.14.1 MechFeCrAlModel

The MechFeCrAlModel model is the default constitutive model used in MechFeCrAl. This model is used as a separate block in the input file when it is specified as one of the submodels in CombinedCreepPlasticity model.

```
[./MechFeCrAlModel]
   type = MechFeCrAlModel
   material = <string> (APMT)
   temp = <string>
   fast_neutron_flux = <string>
   scale_factor_A = <real> (1.0)
   scale_factor_Q = <real> (1.0)
   scale_factor_n = <real> (1.0)
   scale_factor_alpha = <real> (1.0)
   scale_factor_cte = <real> (1.0)
   scale_factor_irrad = <real> (1.0)
   creep_coefficient = <real> (2.89e-36)
   stress\_exponent = \langle real \rangle (5.5)
   activation_energy = <real> (29709)
   model_thermal_expansion = <bool> (true)
   model_thermal_creep = <bool> (true)
   model_irradiation_creep = <bool> (true)
   relative_tolerance = <real> (1e-5)
   absolute_tolerance = <real> (1e-20)
   max_its = \langle integer \rangle (10)
   output_iteration_info = <bool> (false)
   output_iteration_info_on_error = <bool> (false)
   max_creep_increment = <real> (1.e-03)
   stress_free_temperature = <real>
[../]
```

type	MechFeCrAlModel
material	Name of chosen FeCrAl alloy. Choices are MA956, PM2000, APMT, FECRALLOY, C35M.
temp	Name of temperature variable. Typically temp.
fast_neutron_flux	Variable name corresponding to the fast neutron flux. Typically fast_neutron_flux.
scale_factor_A	Scale factor to be applied to the creep prefactor.
scale_factor_Q	Scale factor to be applied to the creep activation energy.
scale_factor_n	Scale factor to be applied to the creep stress exponent.
scale_factor_alpha	Scale factor to be applied to the temperature coefficient.
scale_factor_cte	Scale factor to be applied to the thermal expansion coefficient.

Whether to model thermal creep. model_thermal_creep creep_coefficient Pre-exponential coefficient in the thermal creep correlation. The default value is for C35M. stress_exponent Exponent applied to the stress in the thermal creep correlation. The default value is for C35M. Activation energy for thermal creep. The default activation_energy value is for C35M. model_irradiation_creep Whether to model irradiation-induced creep. Whether to calculate the thermal expansion coeffimodel_thermal_expansion cient as a function of temperature. relative_tolerance Relative convergence tolerance for material model iterations. absolute_tolerance Absolute convergence tolerance for material model iterations. max_its Maximum number of material model convergence iterations. output_iteration_info Whether to output material model convergence information. output_iteration_info_on_error Whether to output material model convergence infor-

Scale factor to be applied to the irradiation creep.

16.2.15 MechMaterial

max_creep_increment

scale_factor_irrad

The MechMaterial model computes the elastic moduli and thermal expansion a variety of materials. The MechMaterial is used to describe a variety of materials that have the same form in the input file. The choices are MechAlloy33, MechHT9, MechMo, MechSS316 and MechU3Si5UN. These materials are typically used as cladding materials. Examples of their use can be found in /bison/tests/HT9 and /bison/tests/mechTests/.

mation if an error occurs.

lowed by the time step control.

The maximum increment of effective creep strain al-

```
[./mechMaterial]
  type = Mech < string >
  block = < string | list >
  disp_x = < string >
  disp_y = < string >
  disp_z = < string >
  disp_z = < string >
  temp = < string >
  temp = < string >
  youngs_modulus = < real >
  poissons_ratio = < real >
[../]
```

type	Mech <string>. Where <string> represents the particular material to be used (e.g. HT9).</string></string>
block	The list of blocks this material applies to.
disp_x	Variable name for displacement variable in x direction. Typically ${\tt disp_x}$.
disp_y	$\label{thm:continuous} \mbox{Variable name for displacement variable in y direction. Typically $\tt disp_y.}$
disp_z	Variable name for displacement variable in z direction. Typically ${\tt disp_z}$ for 3D and ${\tt disp_y}$ for axisymmetric models.
disp_r	Variable name for displacement variable in radial direction for axisymmetric or spherically symmetric cases. Typically disp_x.
temp	Name of temperature variable. Typically temp.
youngs_modulus	Young's modulus.
poissons_ratio	Poisson's ratio.

16.2.16 MechMAMOX

The MechMAMOX model computes the thermal expansion of minor actinide doped mixed oxide fast fuel (MA-MOX). The Young's modulus and Poisson's ratios are set default to 249.3e9 Pa and 0.317, respectively, but can be changed in the input file if desired. This model was built based on the correlation found here [10] and is good for oxygen to metal ratios of 2.00, 1.99, 1.98 and 1.97. Oxygen to metal ratio is a required parameter. The correlation describes a mean thermal expansion coefficient with a reference temperature of 300 K. porosity can either be coupled or defined as a function in the input file.

```
[./mechMAMOX]
  type = MechMAMOX
  block = <string list>
  disp_x = <string>
  disp_y = <string>
  disp_z = <string>
  temp = <string>
  temp = <string>
  oxy_to_metal_ratio = <string> (required)
  porosity = <string>
  youngs_modulus = <real>
  poissons_ratio = <real>
[../]
```

type	MechMAMOX.	
block	The list of blocks this material applies to.	
disp_x	Variable name for displacement variable in x direction. disp_x.	Typically
disp_y	Variable name for displacement variable in y direction. disp_y.	Typically

Variable name for displacement variable in z direction. Typically disp_z disp_z for 3D and disp_y for axisymmetric models. Variable name for displacement variable in radial direction for axdisp_r isymmetric or spherically symmetric cases. Typically disp_x. Name of temperature variable. Typically temp. temp The oxygen to metal ratio of the fuel, this can be 2.00, 1.99, 1.98 or oxy_to_metal_ratio 1.97 only and will error with anything else. Variable name corresponding to the porosity. Typically porosity. porosity Young's modulus. youngs_modulus Poisson's ratio. poissons_ratio

16.2.17 MechUPuZr

MechUPuZr is used to calculate mechanical properties and thermal expansion, as well to model thermal and irradiation creep behavior of U-Pu-Zr fast reactor fuel. If porosity and porosity_material are both defined an error will result. The user has the choice of not supplying any porosity, supplying a variable for porosity or couple to a material that calculates the porosity.

```
[./mechupuzr]
 type = MechUPuZr
 disp_x = <string>
 disp_y = <string>
 disp_z = <string>
 disp_r = <string>
 temp = <string>
 X_Pu = \langle string \rangle
 X_Zr = \langle string \rangle
  porosity = <string>
  porosity_material = <bool> (false)
 fission_rate = <string>
 youngs_modulus = <real>
 poissons_ratio = <real>
 thermal_expansion = <real> (0)
 stress_free_temperature = <real>
 model_creep = <bool> (true)
 calc_youngs = <bool> (true)
 calc_poissons = <bool> (true)
 model_swelling = <bool> (false)
  name_swelling_model = <string> (VSwellingUPuZr)
 LTE_scalar = <real> (1.0)
 A_U = \langle real \rangle (0.2380289)
 A_Pu = < real > (0.244)
 A_Zr = \langle real \rangle (0.091224)
[../]
```

type MechUPuZr

disp_x Variable name for displacement variable in x direction. Typi-

cally disp_x.

disp_y Variable name for displacement variable in y direction. Typi-

cally disp_y.

disp_z Variable name for displacement variable in z direction. Typi-

cally disp_z for 3D and disp_y for axisymmetric models.

disp_r Variable name for displacement variable in radial direction

for axisymmetric or spherically symmetric cases. Typically

disp_x.

temp Name of temperature variable. Typically temp.

X_Pu Name of plutonium molar fraction variable. Typically X_Pu.

X_Zr Name of zirconium molar fraction variable. Typically X_Zr.

porosity Variable name corresponding to the porosity. Typically

porosity.

porosity_material A flag indicating whether porosity is being calculated by a

material property (e.g., VSwellingUPuZr). Optional.

fission_rate Variable name corresponding to the fast neutron flux. Typi-

cally fission_rate.

youngs_modulus Young's modulus.
poissons_ratio Poisson's ratio.

thermal_expansion Coefficient of thermal expansion.

stress_free_temperature The stress-free temperature. If not specified, the initial tem-

perature is used.

model_creep Flag to model creep using CreepUPuZrModel.

calc_youngs Flag to calculate Young's Modulus as a function of molar frac-

tions, temperature, and porosity.

calc_poissons Flag to calculate Poisson's Ratio as a function of molar frac-

tions, and temperature.

model_swelling Flag to model swelling.

name_swelling_model Material name for swelling model.

LTE_scalar Multiplier multiplied against the calculated linear expansion

coefficient. Use 0 to turn thermal expansion off.

A_U Uranium molar mass.
A_Pu Plutonium molar mass.
A_Zr Zirconium molar mass.

16.2.18 MechZry

The MechZry model includes the options to model primary, thermal, and irradiation-induced creep. Modeling of creep under LOCA conditions is available. Also, it is possible to turn on irradiation growth. If irradiation growth is turned on, do not include the IrradiationGrowthZr4 model. Finally, an accuracy-controlling time step criterion is implemented, which can be applied through the MaterialTimeStep postprocessor (Section 18.7).

```
[./mechzry]
 type = MechZry
 fast_neutron_flux = <string>
 fast_neutron_fluence = <string>
 initial_fast_fluence = <real> (0.0)
 cold_work_factor = <real> (0.01)
 constitutive_model = <string>
 oxygen_concentration = <real> (0.0)
 relative_tolerance = <real> (1e-4)
 absolute_tolerance = <real> (1e-20)
 max_its = \langle integer \rangle (10)
 output_iteration_info = <bool> (false)
 output_iteration_info_on_error = <bool> (false)
 model_irradiation_creep = <bool> (true)
 model_primary_creep = <bool> (true)
 model_thermal_creep = <bool> (true)
 model_thermal_creep_loca = <bool> (false)
 model_irradiation_growth = <bool> (true)
 growth_direction = <integer>
 model_thermal_expansion = <bool> (true)
 model_elastic_modulus = <bool> (false)
 stress_free_temperature = <real>
 material_type = <string>(SRA) or <integer>(0)
 temp_standard_creep_end = <real> (700.)
 temp_loca_creep_begin = <real> (900.)
 max\_creep\_increment = \langle real \rangle (1.e-03)
 creeprate_scalef = <real> (1.)
 constitutive_model = <string>
 scale_factor = <real> (1.0)
[../]
```

type	MechZry
fast_neutron_flux	Variable name corresponding to the fast neutron flux. Typically fast_neutron_flux.
fast_neutron_fluence	Name of fast neutron fluence variable. Typically fast_neutron_fluence.
initial_fast_fluence	The initial fast neutron fluence.
constitutive_model	Name of constitutive model.
cold_work_factor	Cold work factor.

oxygen_concentration Oxygen concentration in ppm.

relative_tolerance Relative convergence tolerance for material model it-

erations.

absolute_tolerance Absolute convergence tolerance for material model it-

erations.

max_its Maximum number of material model convergence it-

erations.

output_iteration_info Whether to output material model convergence infor-

mation.

output_iteration_info_on_error Whether to output material model convergence infor-

mation if an error occurs.

model_irradiation_creep Whether to model irradiation-induced creep.

model_primary_creep Whether to model primary creep.

model_thermal_creep Whether to model steady state thermal creep.

model_thermal_creep_loca Whether to model thermal creep considering a spe-

cific correlation at LOCA temperatures.

model_irradiation_growth Whether to model irradiation growth.

growth_direction The direction in which irradiation growth is applied.

Typically 1 (axial direction).

model_thermal_expansion Whether to use MATPRO model for thermal expan-

sion.

model_elastic_modulus Whether to calculate temperature-dependent elastic

moduli.

stress_free_temperature The stress-free temperature. If not specified, the ini-

tial temperature is used.

material_type Cladding material type. SRA(or 0), RXA(or 1),

PRXA(or 2), ZIRLO(or 3).

thermal creep model no longer applies.

temp_loca_creep_begin The lower limit of temperature where the loca thermal

creep model begins to apply.

max_creep_increment The maximum increment of effective creep strain al-

lowed by the time step control.

creeprate_scalef Scale factor applied to the creep rate (for sensitivity

studies).

constitutive_model By default (when the constitutive model parameter is

not given in input file) CreepZryModel constitutive model is used else the constitutive model specified by

the user is used.

16.2.18.1 CombinedCreepPlasticity

The CombinedCreepPlasticity model is used when it is specified as the constitutive_model in MechZry. CombintedCreepPlasticity models the deformation under both creep and instanteous plasticity. Submodels need to be specified in the input to model creep and instantaneous plasticity of Zry cladding.

```
[./CombinedCreepPlasticity]
    type = CombinedCreepPlasticity
    relative_tolerance = <real> (1e-5)
    absolute_tolerance = <real> (1e-5)
    max_its = <integer> (30)
    output_iteration_info = <bool> (false)
    output_iteration_info_on_error = <bool> (false)
    submodels = <string>
[../]
```

type	CombinedCreepPlasticity
relative_tolerance	Relative convergence tolerance for combined submodel iterations.
absolute_tolerance	Absolute convergence tolerance for combined submodel iterations.
max_its	Maximum number of submodel convergence iterations.
output_iteration_info	Whether to output submodel convergence information.
output_iteration_info_on_error	Whether to output submodel convergence information if an error occurs.
submodels	Name of submodels used for combined creep and plasticity.

16.2.18.2 CreepZryModel

The <code>CreepZryModel</code> model is the default constitutive model used in MechZry. Therefore, the interface is similar to the <code>MechZry</code> except for the options and paramters to model elastic modulus, thermal expansion, and irradiation growth. This model is used as a separate block in the input file when it is specified as one of the submodels in <code>CombinedCreepPlasticity</code> model.

```
[./CreepZryModel]
    type = CreepZryModel
    fast_neutron_flux = <string>
    fast_neutron_fluence = <string>
```

```
initial_fast_fluence = <real>
   cold_work_factor = <real> (0.01)
   oxygen_concentration = <real> (0.0)
   relative_tolerance = <real> (1e-5)
   absolute_tolerance = <real> (1e-20)
   max_its = \langle integer \rangle (30)
   output_iteration_info = <bool> (false)
   output_iteration_info_on_error = <bool> (false)
   model_irradiation_creep = <bool> (true)
   model_primary_creep = <bool> (true)
   model_thermal_creep = <bool> (true)
   model_thermal_creep_loca = <bool> (false)
   material_type = <string>(SRA) or <integer>(0)
   temp_standard_creep_end = <real> (700.)
   temp_loca_creep_begin = <real> (900.)
   max\_creep\_increment = \langle real \rangle (1.e-03)
   creeprate_scalef = <real> (1.)
[../]
```

CreepZryModel type fast_neutron_flux Variable name corresponding to the fast neutron flux. Typically fast_neutron_flux. Name of fast neutron fluence variable. Typically fast_neutron_fluence fast_neutron_fluence. initial_fast_fluence The initial fast neutron fluence. cold_work_factor Cold work factor. oxygen_concentration Oxygen concentration in ppm. Relative convergence tolerance for material model itrelative_tolerance Absolute convergence tolerance for material model itabsolute_tolerance erations. max_its Maximum number of material model convergence iterations. Whether to output material model convergence inforoutput_iteration_info mation. Whether to output material model convergence inforoutput_iteration_info_on_error mation if an error occurs. model_irradiation_creep Whether to model irradiation-induced creep. model_primary_creep Whether to model primary creep. model_thermal_creep Whether to model steady state thermal creep. model_thermal_creep_loca Whether to model thermal creep considering a specific correlation at LOCA temperatures.

material_type Cladding material type. SRA(or 0), RXA(or 1), PRXA(or 2), or ZIRLO(or 3).

thermal creep model no longer applies.

temp_loca_creep_begin The lower limit of temperature where the loca thermal

creep model begins to apply.

max_creep_increment The maximum increment of effective creep strain al-

lowed by the time step control.

creeprate_scalef Scale factor applied to the creep rate (for sensitivity

studies).

16.2.18.3 IsotropicPlasticity

The ${\tt IsotropicPlasticity}$ model is a model used to model the instantaneous plasticity of ${\tt Zry}$ cladding. It is used as one of the submodels in ${\tt CombinedCreepPlasticity}$ model.

```
[./IsotropicPlasticity]
  type = IsotropicPlasticity
  relative_tolerance = <real> (1e-5)
  absolute_tolerance = <real> (1e-20)
  max_its = <integer> (30)
  output_iteration_info = <bool> (false)
  output_iteration_info_on_error = <bool> (false)
  hardening_constant = <real>
  hardening_function = <string>
  yield_stress = <real>
[../]
```

type IsotropicPlasticity

relative_tolerance Relative convergence tolerance for sub-newton itera-

tions.

absolute_tolerance Absolute convergence tolerance for sub-newton itera-

tions.

max_its Maximum number of sub-newton convergence itera-

tions.

output_iteration_info Whether to output sub-newton convergence informa-

tion.

output_iteration_info_on_error Whether to output material model convergence infor-

mation if an error occurs.

hardening_function True stress as a function of plastic strain.

yield_stress Input initial yeild stress.

16.2.18.4 ZryPlasticity

The <code>ZryPlasticity</code> model is used to model the instantaneous plasticity of the Zry cladding. The stress vs total strain curve after yield follows a power law hardening. The yield stress and hardening curve is calculated based on the fast neutron fluence, fast neutron flux, temperature and cold work factor. This model is used in conjunction with MechZry. The Young's modulus and Poisson's ratio are evaluated by MechZry (using the MATPRO CELMOD subroutine) as a function of fast neutron fluence, temperature, cold work factor and oxygen concentration. So model_elastic_modulus in MechZry model should be set to true and all the other modeling parameters like model_thermal_expansion, model_primary_creep, e.t.c, should be set to false.

A scale factor can be applied to scale down the Young's modulus, yield stress and hardening modulus. The yield stress and hardening modulus are scaled in ZryPlasticity and the Young's modulus is scaled in MechZry.

```
[./ZryPlasticity]
 type = ZryPlasticity
 relative_tolerance = <real> (1e-5)
 absolute_tolerance = <real> (1e-20)
 max_its = \langle integer \rangle (30)
 output_iteration_info = <bool> (false)
 output_iteration_info_on_error = <bool> (false)
 fast_neutron_flux = <string>
 fast_neutron_fluence = <string>
 temp = <string>
 cold_work_factor = <real> (0.0)
 Ziracloy_type = <unsigned int> (4)
 use_matpro = <bool> (false)
 scale_factor = <real> (1.0)
 initial_fast_fluence = <real> (0.0)
  strain_rate = <real>
[../]
```

type	ZryPlasticity
relative_tolerance	Relative convergence tolerance for sub-newton itera-
	tions.
absolute_tolerance	Absolute convergence tolerance for sub-newton itera-
	tions.
max_its	Maximum number of sub-newton convergence itera-
	tions.
output_iteration_info	Whether to output sub-newton convergence informa-
	tion.
output_iteration_info_on_error	Whether to output material model convergence infor-
	mation if an error occurs.
fast_neutron_flux	Variable name corresponding to the fast neutron flux.
	Typically fast_neutron_flux.

fast_neutron_fluence.

temp Name of the temperature variable.

cold_work_factor Cold work factor.

Ziracloy_type Type of Ziracloy used - 2 or 4.

use_matpro Parameters for the power law hardening model (K.n

and m) will be modeled using the expression in MAT-PRO if this is set to true. A fixed strain rate of 1e-3 is

used with this model.

scale_factor Yield stress and Hardening modulus are scaled down

by this parameter.

initial_fast_fluence The initial value of fast fluence variable.

strain_rate Fixes strain rate to the value provided. Works only

with the default model (use_matpro = false). When use_matpro is set to true, the strain rate is automati-

cally set to 1e-3.

16.2.19 OxidationCladding

The <code>OxidationCladding</code> model incorporates correlations for Zircaloy cladding oxidation through metal-water reactions. Described processes include outer oxide scale thickness growth and oxygen mass gain. The model is to be applied to the cladding waterside boundary.

```
[./oxidationcladding]
  type = OxidationCladding
  boundary = <string list>
  clad_inner_radius = <real>
  clad_outer_radius = <real>
  normtemp_model = 0
  hightemp_model = <integer> (0)
  temperature = <string>
  fast_neutron_flux = <string>
  use_coolant_channel = <bool> (false)
  oxygen_wtfract_initial = <real> (0.0012)
  oxidation_scalef = <real> (1.)
[../]
```

type OxidationCladding

boundary

clad_inner_radius

clad_outer_radius

Required. Waterside cladding boundary.

Required. Inner cladding radius (m).

Required. Outer cladding radius (m).

normtemp_model Selection of the normal operating temperatures correlation.

Only 0 (EPRI/KWU/C-E) is considered at this time.

hightemp_model Selection of the high temperatures correlation. One of 0 (Leistikov) or 1 (Cathcart-Pawel). In both cases, the model uses the Prater-Courtright correlation above 1900 K. Required. Name of temperature variable. Typically temp. temp Variable name corresponding to the fast neutron flux. Typically fast_neutron_flux fast_neutron_flux. If true, the model will adjust the surface temperature based on use_coolant_channel the coolant channel model. As-fabricated oxygen weight fraction in cladding. oxygen_wtfract_initial Scale factor applied to the oxide scale thickness (for sensitivity oxidation_scalef studies).

16.2.20 RelocationUO2

q

The Relocation UO2 model accounts for cracking and relocation of fuel pellet fragments in the radial direction. This model is necessary for accurate modeling of LWR fuel. Only one of q and q_variable may be given.

```
[./relocationuo2]
 type = RelocationUO2
 burnup_function = <string>
 burnup = <string>
 fuel_pin_geometry = <string>
 diameter = <real>
 q = <string>
 q_variable = <string>
 gap = <real>
 burnup_relocation_stop = <real>
 relocation_activation1 = <real> (19685.039)
 relocation_activation2 = <real> (45931.759)
 relocation_activation3 = <real> (32808.399)
 axial_axis = <0, 1, or 2 for x, y, or z>
 model = <ESCORE_modified, ESCORE, or GAPCON> (ESCORE_modified)
[../]
```

burnup_function

Name of the Burnup sub-block, if any (typically burnup).

May not be used with the burnup line command. Use of burnup_function is preferred.

burnup

Name of burnup variable. Typically burnup.

Name of the FuelPinGeometry object (see 23.1).

Required if fuel_pin_geometry is not specified. As fabricated cold diameter of pellet in meters.

Function describing linear heat rate in pellet in W/m.

Variable holding linear heat rate in pellet in W/m. q_variable Required if fuel_pin_geometry is not specified. As fabricated gap cold diametral gap in m. Burnup at which relocation strain stops in FIMA. burnup_relocation_stop First activation linear power in W/m. The linear power at relocation_activation1 which relocation turns on. Second activation linear power in W/m. The linear power at relocation_activation2 which relocation transitions from the initial regime to the secondary regime. relocation_activation3 Third activation linear power in W/m. The linear power offset in the secondary regime. axial_axis Coordinate axis of the axial direction of the fuel stack. model Which relocation correlation to use.

16.2.21 ThermallrradiationCreepZr4

The ThermalIrradiationCreepZr4 is used for Zr4 cladding in LWR simulations. It includes fits for the temperature, irradiation, and stress effects on cladding creep.

```
[./thermalirradiationcreepzr4]
 type = ThermalIrradiationCreepZr4
 disp_x = <string>
 disp_y = <string>
 disp_z = <string>
 disp_r = <string>
 temp = <string>
 a\_coeff = \langle real \rangle (3.14e24)
 n_{exponent} = \langle real \rangle (5)
 activation\_energy = \langle real \rangle (2.7e5)
 gas\_constant = \langle real \rangle (8.3143)
 fast_neutron_flux = <string>
 c0\_coef = < real > (9.881e-28)
 c1\_coef = \langle real \rangle (0.85)
 c2\_coef = \langle real \rangle (1)
 youngs_modulus = <real>
 poissons_ratio = <real>
 thermal_expansion = <real> (0)
 relative_tolerance = <real> (1e-4)
 absolute_tolerance = <real> (1e-20)
 max_its = \langle integer \rangle (10)
 output_iteration_info = <true or false> (false)
  stress_free_temperature = <real>
[../]
```

type

ThermalIrradiationCreepZr4

disp_x Variable name for displacement variable in x dire	ction. Typi-
--	--------------

cally disp_x.

disp_y Variable name for displacement variable in y direction. Typi-

cally disp_y.

disp_z Variable name for displacement variable in z direction. Typi-

cally disp_z for 3D and disp_y for axisymmetric models.

disp_r Variable name for displacement variable in radial direction

for axisymmetric or spherically symmetric cases. Typically

disp_x.

temp Name of temperature variable. Typically temp.

a_coef The leading coefficient in the thermal creep term.

n_exponent The exponent in the thermal creep term.

activation_energy The activation energy.
gas_constant The universal gas constant.

fast_neutron_flux Variable name corresponding to the fast neutron flux. Typi-

cally fast_neutron_flux.

c0_coef The leading coefficient in the irradiation creep term.

c1_exponent The exponent on the irradiation creep fast neutron flux term.

c2_exponent The exponent on the irradiation creep stress term.

youngs_modulus Young's modulus.
poissons_ratio Poisson's ratio.

thermal_expansion Coefficient of thermal expansion.

relative_tolerance Relative convergence tolerance for material model iterations.

absolute_tolerance Absolute convergence tolerance for material model iterations.

max_its Maximum number of material model convergence iterations.

output_iteration_info Whether to output material model convergence information.

stress_free_temperature The stress-free temperature. If not specified, the initial tem-

perature is used.

burnup Name of burnup variable. Typically burnup.

16.2.22 PyClrradiationStrain

The PycIrradiationStrain model tracks the irradiation-induced strain in pyrolytic carbon. The strain is isotropic for the buffer type and differs in the radial and tangential directions for the dense type.

```
[./pycirradiationstrain]
  type = PyCIrradiationStrain
  fluence = <string>
  pyc_type = <string> (buffer)
```

```
[.../]
```

type PyCIrradiationrStrain

fluence Required. Variable name corresponding to the fast neutron fluence. Typically

fast_neutron_fluence.

pyc_type One of buffer or dense.

16.2.23 VSwellingFeCrAl

The VSwellingFeCrAl model computes a volumetric strain to account for irradiation induced swelling of FeCrAl alloys used for cladding.

```
[./vswelling_fecral]
  type = VSwellingFeCrAl
  fast_neutron_fluence = <string>
  swelling_scalef = <real> (1.0)
[../]
```

type VSwellingFeCrAl

fast_neutron_fluence The name of the variable for the fast neutron fluence.

swelling_scalef A scaling factor to be applied to the swelling creep strain.

16.2.24 VSwellingUO2

The VSwellingUO2 model computes a volumetric strain to account for solid and gaseous swelling and for densification. VSwellingUO2 also computes porosity (fabrication_porosity, gaseous_porosity, and sintering_porosity).

```
[./vswellinguo2]
  type = VSwellingUo2
  temp = <string>
  burnup_function = <string>
  burnup = <string>
  density = <real>
  total_densification = <real> (0.01)
  complete_burnup = <real> (5)
  initial_porosity = <real> (0.05)
  save_solid_swell = <bool> (false)
  save_densification = <bool> (false)
  gas_swelling_type = <string> (SIFGRS)
[../]
```

type VSwellingUO2

temp Name of temperature variable. Typically temp.

burnup_function Name of the Burnup sub-block, if any (typically burnup). May not be used with the burnup line command. Use of burnup_function is preferred.

burnup Name of burnup variable. Typically burnup.

density **Required**. Initial fuel density.

total_densification The densification that will occur given as a fraction of theoretical

density.

complete_burnup The burnup at which densification is complete (MWd/kgU).

initial_porosity The initial fuel porosity.

save_solid_swell Whether to save the solid swelling as a material property

(solid_swell).

save_densification Whether to save the densification as a material property (densifica-

tion).

model or MATPRO to use MATPRO's empirical model. IMPORTANT: if using SIFGRS, the following line must be place in the block defining the solid mechanics material model for the fuel (e.g., CreepUO2 or Elastic) so that the models run in the correct

order: "dep_matl_props = deltav_v0_bd"

Note that the total swelling will be stored as a material property (named total_swell) if both save_solid_swell and save_densification are true. Solid swelling is saved as solid_swell, and densification is saved as densification. The total swelling includes solid swelling, densification, and gaseous swelling. Gaseous swelling is always stored as a material property (named gas_swell).

16.2.25 VSwellingU3Si2

The VSwellingU3Si2 model computes a volumetric strain to account for solid and gaseous swelling and densification In U_3Si_2 fuel.

```
[./vswellingu3si2]
  type = VSwellingU3si2
  temp = <string>
  burnup_function = <string>
  burnup = <string>
  total_densification = <real> (0.01)
  complete_burnup = <real> (5)
  save_solid_swell = <bool> (false)
  save_densification = <bool> (false)
  save_gas_swell = <bool> (false)
[../]
```

type

VSwellingU3Si2

temp Name of temperature variable. Typically temp.

burnup_function Name of the Burnup sub-block, if any (typically burnup). May not

be used with the burnup line command. Use of burnup_function

is preferred.

burnup Name of burnup variable. Typically burnup.

total_densification The densification that will occur given as a fraction of theoretical

density.

complete_burnup The burnup at which densification is complete (MWd/kgU).

save_solid_swell Whether to save the solid swelling as a material property

(solid_swelling).

save_densification Whether to save the densification as a material property (densifica-

tion).

save_gas_swell Whether to save the gaseous swelling as a material property

(gaseous_swelling).

Note that the total swelling will be stored as a material property (named total_swell) if save_solid_swell, save_gas_swell, and save_densification are true. Solid swelling is saved as solid_swelling, gaseous swelling is saved as gaseous_swelling, and densification is saved as densification. The total swelling includes solid swelling, densification, and gaseous swelling.

16.2.26 VSwellingU3Si5UN

The VSwellingU3Si5UN model computes a volumetric strain to account for solid and gaseous swelling and for densification.

```
[./vswellingU3Si5UN]
  type = VSwellingU3Si5UN
  temp = <string>
  burnup_function = <string>
  burnup = <string>
  density = <real>
  initial_porosity = <real> (0.05)
[../]
```

type VSwellingU3Si5UN

temp Name of temperature variable. Typically temp.

burnup_function Name of the Burnup sub-block, if any (typically burnup). May not

be used with the burnup line command. Use of burnup_function is

preferred.

burnup Name of burnup variable. Typically burnup.

density **Required**. Initial fuel density. initial_porosity The initial fuel porosity.

16.2.27 VSwellingUPuZr

The VSwellingUPuZr model computes a volumetric strain to account for solid and gaseous swelling and for open pore compression in U-Pu-Zr metal fuel systems. The solid swelling and gaseous swelling are optionally saved as a material property, named solid_swell and gas_swell, respectively. Also, porosity (as-fabricated + gas swelling porosity) is available as a material property. The compressive strain increment due to open pore compression (hot pressing) is computed in CreepUPuZrModel and passed to VSwellingUPuZr as the material property open_pore_compression.

The dilatational components of the strain increment tensor can be scaled in this model with a user-defined input parameter called the anisotropic_strain_scaling vector. The default value of this parameter is '1 1 1', where these components are of type Real in C++ parlance. Those components can be changed, but are limited such that the sum of the components divided by 3 must equal 1 and the components can only be positive and less than or equal to 3. For example, taking the total amount of strain and applying it all in the first component of the strain increment tensor can be done by setting anisotropic_strain_scaling to '3 0 0'. This ensures that the total amount of strain is preserved.

To include the open core compression strain in VSwellingUPuZr, the hydrostatic_stress and plenum_pressure must be defined in the CreepUPuZr block.

```
[./vswelling_upuzr]
  type = VSwellingUPuZr
  anisotropic_strain_scaling = <three component vector> (1.0 1.0 1.0)
  temp = <string>
  fission_rate = <string>
  fabrication_porosity = <real> (0.0)
  hydrostatic_stress = <string>
  hot_pressing_strain_increment = <string>
  plenum_pressure = <string>
  save_gas_swell = <bool> (false)
  save_solid_swell = <bool> (false)
[../]
```

type

anisotropic_strain_scaling

The scale factor applied to each component of the dilatational strain computed in this model. When defining these scale factors ensure that total strain is preserved.

temp

Name of temperature variable. Typically temp.

fission_rate

Name of fission rate variable. Typically fission_rate.

fabrication_porosity

The as-fabricated porosity

hydrostatic_stress The name of hydrostatic stress variable. Typically

hydrostatic_stress.

hot_pressing_strain_increment The name of variable storing increment of strain

due to compression of the open pores. Typically

open_pore_compression

plenum_pressure The postprocessor name for the plenum pressure. Typ-

ically plenum_pressure.

save_gas_swell A flag indicating whether the gaseous swelling should

be saved in a material property.

save_solid_swell A flag indicating whether the solid swelling should be

saved in a material property.

16.2.28 ZrPhase

The ${\tt ZrPhase}$ model computes the volume fraction of β phase for Zr-based cladding materials as a function of temperature and time.

```
[./zrphase]
  type = ZrPhase
  block = <string list>
  temperature = <string>
  numerical_method = <integer>
[../]
```

type ZrPhase

block List of blocks this material model applies to.

temperature Required. Name of temperature variable. Typically temp.

numerical_method Choice of numerical method to solve the differential equation for the

phase transformation rate. One of 1 (implicit Euler method) or 2 (sec-

ond order Adams-Moulton method - AM2).

16.3 Mass Diffusion Models

This material computes a two-term Arrhenius diffusion coefficient of the form

$$d = d_1 \exp\left(\frac{-q_1}{RT}\right) + d_2 \exp\left(\frac{-q_2}{RT}\right). \tag{16.2}$$

```
[./arrheniusdiffusioncoef]
  type = ArrheniusDiffusionCoef
  d1 = <real> (5.6e-8)
  d1_function = <string>
  d1_function_variable = <string>
  d2 = <real> (5.2e-4)
```

```
q1 = <real> (2.09e5)
q2 = <real> (3.62e5)
gas_constant = <real> (8.3143)
temp = <string>
[../]
```

ArrheniusDiffusionCoef type First coefficient (m²/2). d1 d1_function Function to be multiplied by d1. Variable to be used when evaluating dl_function. If not given, d1_function_variable time will be used. Second coefficient $(m^2/2)$. d2 First activation energy (J/mol). q1 Second activation energy (J/mol). q2 Universal gas constant (J/mol/K). gas_constant temp Name of temperature variable. Typically temp.

16.4 Other Models

16.4.1 Arrhenius Material Property

Arrhenius Material Property is used to declare an arbitrary material property D that has the form $D=Ae^{-Q/RT}$, where A is the frequency factor, Q is the activation energy, R is the gas constant, and T is the temperature.

```
[./some_property]
  type = ArrheniusMaterialProperty
  frequency_factor = <real>
  activation_energy = <real>
  gas_constant = <real> (8.314)
  temp = <variable>
  property_name = <string>
[../]
```

type ArrheniusMaterialProperty

frequency_factor The coefficient in front of the exponential.

activation_energy The activation energy.

gas_constant The universal gas constant.

temp Coupled temperature variable.

property_name The name for this property.

16.4.2 Density

The Density model creates a material property named density. If coupled to displacement variables, the model adjusts density based on deformation.

```
[./density]
  type = Density
  disp_x = <string>
  disp_y = <string>
  disp_z = <string>
  disp_r = <string>
  density = <real>
[../]
```

```
type Density

disp_x Variable name for displacement variable in x direction. Typically disp_x.

disp_y Variable name for displacement variable in y direction. Typically disp_y.

disp_z Variable name for displacement variable in z direction. Typically disp_z for 3D and disp_y for axisymmetric models.

disp_r Variable name for displacement variable in radial direction for axisymmetric or spherically symmetric cases. Typically disp_x.

density Required. Density.
```

17 Fission Gas Models

Fission gas production and release modeling plays a vital role in fuel performance analysis. Fission gas affects swelling, porosity, thermal conductivity, gap conductivity, and rod internal pressure. The Sifgrs model is recommended.

17.1 Sifgrs

Sifgrs is the recommended fission gas model. It computes both fission gas release and fuel gaseous swelling.

```
[./sifgrs]
 type = Sifgrs
 initial\_porosity = \langle real \rangle (0.05)
 grain_radius_const = <real> (5.e-06)
 hydrostatic_stress_const = <real> (0.)
 saturation_coverage = <real> (0.5)
 ath_model = <bool> (false)
 gbs_model = <bool> (false)
 hbs model = <bool> (false)
 grain_radius = <string>
 temp = <string>
 fission_rate = <string>
 burnup = <string>
 burnup_function = <string>
 hydrostatic_stress = <string>
 pellet_id = <string>
 pellet_brittle_zone = <string>
 eff_diff_coeff_option = <integer> (0)
 diff_coeff_option = <integer> (3)
 res_param_option = <integer> (0)
 trap_param_option = <integer> (0)
 iq_fully_coupled = <integer> (0)
 ig_bubble_model = <integer> (0)
 ig_diff_algorithm = <integer> (0)
 transient_option = <integer> (0)
 rod_ave_lin_power = <string>
 axial_power_profile = <string>
 temperature_scalef = <real> (1.)
 grainradius_scalef = <real> (1.)
 effdiffcoeff_scalef = <real> (1.)
 igdiffcoeff_scalef = <real> (1.)
  resolutionp_scalef = <real> (1.)
```

```
trappingp_scalef = <real> (1.)
gbdiffcoeff_scalef = <real> (1.)
[../]
```

Sifgrs type Initial fuel porosity (/). initial_porosity A constant value for fuel grain radius (m). grain_radius_const Ignored if grain_radius is given. hydrostatic_stress_const A constant value for hydrostatic stress (Pa). Ignored if hydrostatic_stress is given. Initial value of fractional grain boundary bubble coverage at saturation_coverage saturation (/). Whether to consider athermal (recoil and knockout) gas reath_model qbs_model Whether to consider the grain boundary sweeping effect. hbs_model Whether to consider intra-granular gas depletion in the high burnup structure (HBS). Name of the auxiliary variable for grain radius, calculated by grain_radius GrainRadiusAux (Section 12.3.5). Typically grain_radius. Variable name for temperature variable. Typically temp. temp fission_rate Variable name corresponding to the fission rate. Typically fission_rate. Name of burnup variable. Typically burnup. burnup Name of the Burnup sub-block, if any (typically burnup_function burnup). May not be used with fission_rate. Use of burnup_function is preferred. hydrostatic_stress Variable name for hydrostatic stress. **Typically** hydrostatic_stress. Name of the auxiliary variable for pellet id. Typically pellet_id pellet_id. Used if ath_model = true. pellet_brittle_zone The name of the UserObject that computes the width of the brittle zone in the fuel pellet. Used if ath_model = true. Choice of the intra-granular effective diffusion coefficient. eff_diff_coeff_option One of 0 (based on Speight formulation [11]), or 1 (correlation from [12]). Choice of the intra-granular diffusion coefficient. One of 0 diff_coeff_option (Turnbull et al. [13] with purely irradiation-dependent term not considered), 1 (Andersson et al. [14]), 2 (Turnbull et al. [15]), or 3 (Turnbull et al. [15] with purely irradiation-

dependent term not considered).

res_param_option	Choice of the intra-granular resolution parameter. One of 0 (heterogeneous model [16]), 1 (homogeneous model from [17]), or 2 (reference value for sensitivity analysis as in [18]).
trap_param_option	Choice of the intra-granular trapping parameter. Only the option 0 (based on [19]) is currently available.
ig_fully_coupled	Not currently available.
ig_bubble_model	Choice of the intra-granular bubble model. One of 0 (empirical model from [16]), or 1 (constant values from [20]).
ig_diff_algorithm	Choice of the algorithm to solve the intra-granular diffusion equation. One of 0 (algorithm from [21]), or 1 (more recent and accurate algorithm PolyPole-1 [22]).
transient_option	To consider the burst release effect during transients, set equal to 2.
rod_ave_lin_pow	Function describing rod averaged linear power.
axial_power_profile	Function describing axial power profile.
temperature_scalef	Scale factor applied to temperature (for sensitivity studies).
grainradius_scalef	Scale factor applied to grain radius (for sensitivity studies).
effdiffcoeff_scalef	Scale factor applied to intra-granular effective diffusion coefficient (for sensitivity studies).
igdiffcoeff_scalef	Scale factor applied to intra-granular atomic diffusion coefficient (for sensitivity studies).
resolutionp_scalef	Scale factor applied to intra-granular resolution parameter (for sensitivity studies).
trappingp_scalef	Scale factor applied to intra-granular trapping parameter (for sensitivity studies).
gbdiffcoeff_scalef	Scale factor applied to grain-boundary diffusion coefficient (for sensitivity studies).

17.2 ForMas

The ForMas model is maintained but not actively developed. The Sifgrs model is recommended.

```
[./formas]
  type = ForMas
  grain_radius = <real> (10e-6)
  resolution_rate = <real> (1e-7)
  resolution_depth = <real> (1e-8)
  bubble_radius = <real> (5e-7)
  bubble_shape_factor = <real> (0.287)
```

```
surface_tension = <real> (0.626)
fractional_coverage = <real> (0.5)
external_pressure = <real> (10e6)
plenum_pressure = <string>
external_pressure_function = <string>
release_fraction = <real> (0)
fractional_yield = <real> (0.3017)
calibration_factor = <real> (1)
[../]
```

type ForMas

grain_radius Initial fuel grain radius.

resolution_rate Resolution rate from intergranular bubbles (1/s).

resolution_depth Resolution layer depth.

bubble_radius Grain boundary bubble radius.

bubble_shape_factor Non-spherical bubble shape factor.

surface_tension Bubble surface tension (J/m²).

fractional_coverage Fractional coverage of grain boundary at saturation.

external_pressure Constant external hydrostatic pressure.

plenum_pressure The name of the plenum pressure Postprocessor.

external_pressure_function Function describing the external pressure.

release_fraction Fraction of boundary and resolved gas released at satura-

tion.

fractional_yield Fractional yield of fission gas atoms per fission.

calibration_factor Calibration factor to be multiplied by gas saturation den-

sity.

17.3 FgrUPuZr

 ${\tt FgrUPuZr} \ is \ a \ fission \ gas \ release \ model \ for \ UPuZr \ metal \ fuel.$

```
[./upuzr_fission_gas_release]
  type = FgrUPuZr
  fission_rate = <string>
  fractional_yield = <real> (0.3017)
[../]
```

type FgrUPuZr

fission_rate Coupled Fission Rate

fractional_yield Fractional yield of fission gas atoms per fission.

18 Postprocessors

MOOSE Postprocessors compute a single scalar value at each timestep. These can be minimums, maximums, averages, volumes, or any other scalar quantity. One example of the use of Postprocessors in BISON is computing the gas volume of an LWR rod. The gas volume changes timestep to timestep, but since it is a single scalar quantity, a Postprocessor computes this value.

```
[Postprocessors]
[./name]
   type = <postprocessor type>
   block = <string list>
   boundary = <string list>
   execute_on = <string list>
   outputs = <string>
   ...
[../]
[]
```

type Type of postprocessor

block List of blocks. Either block numbers or names.

boundary List of boundaries (side sets). Either boundary numbers or names.

execute_on Set to (nonlinear—linear—timestep_end—timestep_begin) to execute at that moment.

outputs Vector of output names where you would like to restrict the output of variable(s) associated with the postprocessor.

Most Postprocessors act on either boundaries or blocks. If no block or boundary is specified, the Postprocessor will act on the entire model. There are a few Postprocessors that act on specific nodes or elements within the finite element mesh.

18.1 DecayHeatFunction

DecayHeatFunction computes the value of the decay heat function. The value is zero prior to the specified time_at_shutdown. This postprocessor is typically used for Loss of Coolant Accident simulations.

```
[./decayheatfunction]
  type = DecayHeatFunction
  energy_per_fission = <real> (3.28451e-11)
```

```
neutron_capture_factor = <real> (1)
  time_at_shutdown = <real> (1e10)
[../]
```

type DecayHeatFunction

energy_per_fission The energy released per fission in J/fission.

neutron_capture_factor The neutron capture factor used to account for the effect of neu-

tron capture in fission products.

time_at_shutdown The time the reactor is shutdown and decay heat begins to take

effect.

18.2 ElementIntegralPower

ElementIntegralPower computes the power in the supplied block given the fission rate variable and energy per fission.

```
[./elementintegralpower]
  type = ElementIntegralPower
  burnup_function = <string>
  fission_rate = <string>
  energy_per_fission = <real> (3.28451e-11)
  variable = <string>
[../]
```

type ElementIntegralPower

burnup_function Name of the Burnup sub-block, if any (typically burnup). May not

be used with fission_rate. Use of burnup_function is preferred.

fission_rate Variable name corresponding to the fission rate. Typically

fission_rate.

energy_per_fission The energy released per fission in J/fission.

variable The variable name this Postprocessor applies to. Typically temp.

18.3 ElementalVariableValue

In some cases it may be of interest to output an elemental variable value (e.g., stress) at a particular location in the model. This is accomplished by using the ElementalVariableValue postprocessor.

```
[./elementalvariablevalue]
type = ElementalVariableValue
elementid = <string>
variable = <string>
[../]
```

type ElementalVariableValue

element id Required. The global element id from the mesh to which this postprocessor is

o be applied.

variable Required. The variable whose value is output to this postprocessor for the

given element.

18.4 Fission Gas Postprocessors

When using the Sifgrs fission gas release model there are four postprocessors that are used to report the fission gas that is produced in moles (ElementIntegralFisGasGeneratedSifgrs), fission gas within the grains (ElementIntegralFisGasGrainSifgrs), fission gas on the grain boundary (ElementIntegralFisGasBoundarySifgrs), and the fission gas released to the plenum in moles (ElementIntegralFisGasReleasedSifgrs). The details of including these postprocessors in the input file is outlined below:

```
[./fis_gas_produced]
 type = ElementIntegralFisGasGeneratedSifgrs
 variable = <string>
 block = <string list>
[./fis_gas_grain]
 type = ElementIntegralFisGasGrainSifgrs
 variable = <string>
 block = <string list>
[../]
[./fis_gas_boundary]
 type = ElementIntegralFisGasBoundarySifgrs
 variable = <string>
 block = <string list>
[./fis_gas_released]
 type = ElementIntegralFisGasReleasedSifgrs
 variable = <string>
 block = <string list>
[../]
```

type The type of postprocessor

variable Required. The variable the postprocessor applies to. For these fission gas post-

processors the variable is typically temp.

block The blocks the postprocessor applies to. For nuclear fuel simulations fission gas

calculations apply to the fuel/pellet block.

18.5 IFBAHeProduction

IFBAHeProduction computes the Helium gas production as a result of an IFBA layer applied to the surface of a fuel rod.

```
[./he_prod]
  type = IFBAHeProduction
  zrb2_load = <real>
  b10_load = <real>
  ifba_len = <real>
  b10_enrich = <real>
  zrb2_rel_dens = <real>
  zrb2_thk = <real>
  fuel_out_rad = <real>
  model = <string>
  u235_enrich = <real>
  burnup = <string>
  rod_ave_lin_pow = <string>
[../]
```

type	IFBAHeProduction	
zrb2_load	ZrB ₂ loading of IFBA layer (kg/m).	
	(Cannot be used with b10_load)	
b10_load	B-10 loading of IFBA layer (kg/m).	
	(Cannot be used with zrb2_load)	
ifba_len	Required . The length of the IFBA layer (m).	
b10_enrich	Required . B-10 enrichment in atomic percent (fraction).	
zrb2_rel_dens	ZrB ₂ relative density (fraction).	
	(Cannot be used with either zrb2_thk or fuel_out_rad)	
zrb2_thk	ZrB_2 layer thickness (m). Must also specify fuel_out_rad.	
	(Cannot be used with zrb2_dens)	
fuel_out_rad	Outer radius of fuel (m). Must also specify zrb2_thk.	
	(Cannot be used with zrb2_dens)	
model	Specifies which equation to use for Helium generation (string).	
	burnup = Burnup based equation, frapcon = FRAPCON equation.	
u235_enrich	U-235 enrichment of the fuel in atomic percent (fraction).	
	(Only used with model = burnup)	
burnup	Postprocessor providing the average burnup.	
	(Only used with model = burnup, typically average_burnup)	
ifba_rod_pct	Percentage of IFBA rods in a fuel assembly (fraction).	
	(Only used with model = frapcon)	

```
rod_ave_lin_pow Postprocessor providing the rod linear power.

(Only used with model = frapcon, typically power_history)
```

18.6 InternalVolume

InternalVolume computes the volume of an enclosed space. The entire boundary of the enclosed space must be represented by the given side set. If the given side set points outward, InternalVolume will report a negative volume.

```
[./internalvolume}
  type = InternalVolume
  scale_factor = <real> (1)
  addition = <addition> (0)
[../]
```

type InternalVolume

scale_factor Scale factor to be applied to the internal volume calculation.

addition Number to be added to internal volume calculation. This addition is not

scaled.

18.7 MaterialTimeStep

MaterialTimeStep allows one to apply physics-based time step criteria implemented in material models. For this purpose, this postprocessor takes the overall minimum across the domain of the time steps provided by (one or more) material models. At this time, a creep rate based time step criterion is available in MechZry (Section 16.2.18). MaterialTimeStep will retrieve the time step length, which MechZry computes at each mesh point, and return the minimum. This time step can then be used by a time stepper such as PostprocessorDT. MaterialTimeStep can be extended to consider multiple material model time step criteria as they become available.

```
[./materialtimestep]
  type = MaterialTimeStep
  variable = <string>
[../]
```

type MaterialTimeStep

ariable **Required**. The variable whose value is output to this postprocessor.

18.8 NodalVariableValue

In order to obtain the value of a nodal variable at a particular location (i.e., temperature and displacement) a NodalVariableValue postprocessor is used. For example, this postprocessor

is useful for obtaining the centerline temperature at the location of a thermocouple to compare against experimental data.

```
[./nodalvariablevalue]
  type = NodalVariableValue
  elementid = <string>
  scale_factor = <real>
  variable = <string>
[../]
```

type NodalVariableValue

nodeid **Required**. The global node id from the mesh to which this postprocessor is

to be applied.

scale_factor A scalar value to be multiplied by the value of the variable.

variable Required. The variable whose value is output to this postprocessor for the

given node.

18.9 NumNonlinearIterations

NumNonlinearIterations reports the number of nonlinear iterations in the just-completed solve.

```
[./numnonlineariters]
type = NumNonlinearIterations
[../]
```

type NumNonlinearIterations

18.10 PlenumTemperature

PlenumTemperature gives an estimate of the temperature of the gas in the plenum. This is done by computing a volume weighted average temperature using gap sizes between surfaces. A typical use is to pair a set of fuel surfaces (inner_surfaces) with a corresponding set of cladding surfaces (outer_surfaces). Another possible use is to pair the inner radius of the cladding (inner_surfaces) with the outer radius of the fuel (outer_surfaces). It is also possible to pair up surfaces automatically for a discrete pellet mesh using the num_pellets option.

```
[PlenumTemperature]
  [./plenumtemperature]
  boundary = <string list>
  inner_surfaces = <string list>
  outer_surfaces = <string list>
  inner_radius_surfaces = <string list>
  temp = <string>
```

```
num_pellets = <integer>
  order = <string> (FIRST)
[.../]
```

boundary Required. List of boundaries (side sets). Either boundary num-

bers or names. The calculation of the temperature will occur

along these boundaries.

inner_surfaces List of boundaries. Will be paired with outer_surfaces to de-

termine the temperature on the opposite surface.

outer_surfaces List of boundaries. Will be paired with inner_surfaces.

inner_radius_surfaces List of boundaries. These are typically fuel surfaces along the

inner radius of annular fuel pellets.

temp Required. Variable name for temperature. Typically temp.

num_pellets Number of discrete pellets in the model. Cannot be

sed with inner_surfaces, outer_surfaces, and

inner_radius_surfaces.

order The order of the variables used. Typical values are FIRST and

SECOND.

18.11 PlotFunction

PlotFunction gives the value of the supplied function at the current time, optionally scaled with scale_factor.

```
[./plotfunction]
  type = PlotFunction
  function = <string>
  scale_factor = <real> (1)
[../]
```

type PlotFunction

function Required. The function to evaluate.

scale_factor Scale factor to be applied to the function value.

18.12 SideAverageValue

SideAverageValue computes the area- or volume-weighted average of the named variable. It may be used, for example, to calculate the average temperature over a side set.

```
[./sideaveragevalue]
  type = SideAverageValue
```

```
variable = <string>
[../]
```

type SideAverageValue

variable Required. The variable this Postprocessor acts on.

18.13 SideFluxIntegral

SideFluxIntegral computes the integral of the flux over the given boundary.

```
[./sidefluxintegral]
  type = SideFluxIntegral
  variable = <string>
  diffusivity = <string>
[../]
```

type SideFluxIntegral

variable Required. Variable to be used in the flux calculation.

diffusivity **Required**. The diffusivity material property to be used in the calculation.

18.14 TimestepSize

TimestepSize reports the timestep size.

```
[./dt]
type = TimestepSize
[../]
```

type TimestepSize

19 Solution Execution and Time Stepping

The Executioner block describes how the simulation will be executed. It includes commands to control the solver behavior and time stepping. Time stepping is controlled by a combination of commands in the Executioner block, and the TimeStepper block nested within the Executioner block.

```
[Executioner]
 type = <string>
 solve_type = <string>
 petsc_options = <string list>
 petsc_options_iname = <string list>
 petsc_options_value = <string list>
 line_search = <string>
 l_max_its = <integer>
 l_tol = <real>
 nl_max_its = <integer>
 nl_rel_tol = <real>
 nl_abs_tol = <real>
 start_time = <real>
 dt = <real>
 end_time = <real>
 num_steps = <integer>
 dtmax = <real>
 dtmin = <real>
 [TimeStepper]
   #TimeStepper commands
```

type **Required**. Several available. Typically Transient.

solve_type One of PJFNK (preconditioned JFNK), JFNK (JFNK), NEWTON

(Newton), or SolveFD (Jacobian computed by finite difference-

serial only, slow).

petsc_options PETSc flags.

petsc_options_iname Names of PETSc name/value pairs.

petsc_options_value Values of PETSc name/value pairs.

Line_search type. Typically none.

1_max_its Maximum number of linear iterations per solve.

1_to1 Linear solve tolerance.

nl_max_its Maximum number of nonlinear iterations per solve.

nl_rel_tol	Nonlinear relative tolerance.
nl_rel_abs	Nonlinear absolute tolerance.
start_time	The start time of the analysis.
end_time	The end time of the analysis.
num_steps	The maximum number of time steps.
dtmax	The maximum allowed timestep size.
dtmin	The minimum allowed timestep size.

Several Executioner types exist, although the Transient type is typically the appropriate one to use for transient BISON analyses. For each type, specific options are available. To see the complete set of possibilities, follow the Input Syntax link on the BISON wiki page.

Similarly, many PETSc options exist. Please see the online PETSc documentation for details. Given the many possibilities in the Executioner block, it may be helpful to review examples in the BISON tests, examples, and assessment directories.

19.1 Timestepping

The method used to calculate the size of the time steps taken by BISON is controlled by the <code>TimeStepper</code> block. There are a number of types of <code>TimeStepper</code> available. Three of the types most commonly used with BISON are described here. These permit the time step to be controlled directly by providing either a single fixed time step to take throughout the analysis, by providing the time step as a function of time, or by using adaptive timestepping algorithm can be used to modify the time step based on the difficulty of the iterative solution, as quantified by the numbers of linear and nonlinear iterations required to drive the residual below the tolerance required for convergence.

19.1.1 Direct Time Step Control with Constant Time Step

The ${\tt ConstantDT}$ type of ${\tt TimeStepper}$ simply takes a constant time step size throughout the analysis.

```
[TimeStepper]
  type = ConstantDT
  dt = <real>
[../]
```

type ConstantDT

dt **Required**. The initial timestep size.

ConstantDT begins the analysis taking the step specified by the user with the dt parameter. If the solver fails to obtain a converged solution for a given step, the executioner cuts back the step size and attempts to advance the time from the previous step using a smaller time step. The time step is cut back by multiplying the time step by 0.5.

If the solution with the cut-back time step is still un-successful, it is repeatedly cut back until a successful solution is obtained. The user can specify a minimum time step through the dtmin parameter in the Executioner block. If the time step must be cut back below the minimum size without obtaining a solution, BISON exits with an error. If the time step is cut back using ConstantDT, that cut-back step size will be used for the remainder of the the analysis.

19.1.2 Direct Time Step Control with Varying Time Step Size

If the FunctionDT type of TimeStepper is used, BISON takes time steps that vary over time according to a user-defined function.

```
[TimeStepper]
  type = FunctionDT
  time_t = <real list>
  time_dt = <real list>
[../]
```

```
type FunctionDT
```

time_t The abscissas of a piecewise linear function for timestep size.

time_dt The ordinates of a piecewise linear function for timestep size.

The time step is controlled by a piecewise linear function defined using the time_t and time_dt parameters. A vector of time steps is provided using the time_dt parameter. An accompanying vector of corresponding times is specified using the time_t parameter. These two vectors are used to form a time step vs. time function. The time step for a given step is computed by linearly interpolating between the pairs of values provided in the vectors.

The same procedure that is used with ConstantDT is used to cut back the time step from the user-specified value if a failed solution occurs.

19.1.3 Adaptive Time Stepping

The IterationAdaptiveDT type of TimeStepper provides a means to adapt the time step size based on the difficulty of the solution.

```
[TimeStepper]
  type = IterationAdaptiveDT
  dt = <real>
  optimal_iterations = <integer>
  iteration_window = <integer> (0.2*optimal_iterations)
  linear_iteration_ratio = <integer> (25)
  growth_factor = <real>
  cutback_factor = <real>
  timestep_limiting_function = <string>
  max_function_change = <real>
  force_step_every_function_point = <bool> (false)
[../]
```

dt **Required**. The initial timestep size.

optimal_iterations The target number of nonlinear iterations for adap-

tive timestepping.

iteration_window The size of the nonlinear iteration window for adap-

tive timestepping.

linear_iteration_ratio The ratio of linear to nonlinear iterations to deter-

mine target linear iterations and window for adaptive

timestepping.

growth_factor Factor by which timestep is grown if needed.

cutback_factor Factor by which timestep is cut back if needed.

timestep_limiting_function Function used to control the timestep.

max_function_change Maximum change in the function over a time step.

 $\hbox{force_step_every_function_point} \quad \hbox{Controls whether a step is forced at every point in}$

the function.

IterationAdaptiveDT grows or shrinks the time step based on the number of iterations taken to obtain a converged solution in the last converged step. The required optimal_iterations parameter controls the number of nonlinear iterations per time step that provides optimal solution efficiency. If more iterations than that are required to obatin a converged solution, the time step may be too large, resulting in undue solution difficulty, while if fewer iterations are required, it may be possible to take larger time steps to obtain a solution more quickly.

A second parameter, iteration_window, is used to control the size of the region in which the time step is held constant. As shown in Figure 19.1, if the number of nonlinear iterations for convergence is lower than (optimal_iterations—iteration_window), the time step is increased, while if more than (optimal_iterations+iteration_window), iterations are required, the time step is decreased. The iteration_window parameter is optional. If it is not specified, it defaults to 1/5 the value specified for optimal_iterations.

The decision on whether to grow or shrink the time step is based both on the number of non-linear iterations and the number of linear iterations. The parameters mentioned above are used to control the optimal iterations and window for nonlinear iterations. The same criterion is applied to the linear iterations. Another parameter, linear_iteration_ratio, which defaults to 25, is used to control the optimal iterations and window for the linear iterations. These are calculated by multiplying linear_iteration_ratio by optimal_iterations and iteration_window, respectively.

To grow the time step, the growth criterion must be met for both the linear iterations and non-linear iterations. If the time step shrinkage criterion is reached for either the linear or nonlinear iterations, the time step is decreased. To control the time step size only based on the number of nonlinear iterations, set linear_iteration_ratio to a large number.

If the time step is to be increased or decreased, that is done using the factors specified with the growth_factor and cutback_factor, respectively. If a solution fails to converge when adaptive time stepping is active, a new attempt is made using a smaller time step in the same manner as with the fixed time step methods. The maximum and minimum time steps can be optionally

specified in the Executioner block using the dtmax and dtmin parameters, respectively.

In addition to controlling the time step based on the iteration count, IterationAdaptiveDT also has an option to limit the time step based on the behavior of a time-dependent function, optionall specified by providing the function name in timestep_limiting_function. This is typically a function that is used to drive boundary conditions of the model. The step is cut back if the change in the function from the previous step exceeds the value specified in max_function_change. This allows the step size to be changed to limit the change in the boundary conditions applied to the model over a step. In addition to that limit, the boolean parameter force_step_every_function_point can be set to true to force a time step at every point in a PiecewiseLinear function.

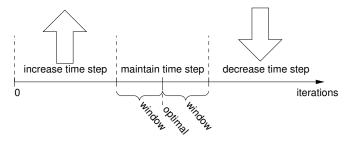


Figure 19.1: Criteria used to determine adaptive time step size

19.2 PETSc Options

The amount of PETSc options to choose as solver parameters is vast and cannot be covered in detailed here. This section provides the recommended PETSc options depending upon whether Dirac or Constraint based contact is used. The values for the petsc_options_value can change depending on the particular problem being analyzed. For specialized problems where these standard options do not work the user is encouraged to consult the PETSc User's Manual or contact the bison-users mailing list.

19.2.1 Constraint Contact

The recommended PETSc options for use with Constraint based contact are given below:

19.2.2 Dirac Contact

The recommended PETSc options for use with Dirac based contact are given below:

19.3 Quadrature

When using higher order meshes (e.g. second) it is recommended to use quadrature = true in the thermal contact block. When this parameter is set the order of the quadrature can be specified using a [./Quadrature] subblock within the [Executioner] block as follows:

```
[./Quadrature]
  type = <string>
  element_order = <string>
  order = <string>
  side_order = <string>
[../]
```

type The type of quadrature used. Default is Gauss.

order Order of quadrature used.

side_order Order of quadrature used on the sides.

The recommended [./Quadrature] block when using second-order meshes is the following:

```
[./Quadrature]
order = FIFTH
side_order = SEVENTH
[../]
```

20 Outputs

The Outputs block lists parameters that control the frequency and type of results files produced. It is possible to create multiple output objects each outputting at different interals, or different variables, or varying file types. The Outputs system is vary complex and enables a large amount of customization. This section will highlight different capabilities of the system. At the end of the this section an example of a typical Outputs block for BISON assessment cases will be presented.

20.1 Basic Input File Syntax

To enable output an input file must contain an Output's block. The simplest method for enabling output is to utilize the shortcut syntax as shown below, which enables the Console output (prints to screen) and Exodus output for writing data to a file.

```
[Outputs]
console = true  #output to the screen with default settings
exodus = true  #output to ExodusII file with default settings
[]
```

20.2 Advanced Syntax

To take full advantage of the output system the use of subblocks is required. For example, the input file snippet below is **exactly** equivalent, including the subblock names, to the snippet shown above that utilizes the shortcut syntax.

```
[Outputs]
[./console]
  type = Console  #output to the screen with default settings
[../]
[./exodus]
  type = Exodus  #output to ExodusII file with default settings
[../]
[]
```

However, the subblock syntax allows for increased control over the output and allows for multiple outputs of the same type to be specified. For example, the following creates two Exodus outputs, one outputting the a mesh at every time step including the initial condition the other outputs every 3 time steps without the initial condition. Additionally, performance logging was enabled for Console output.

```
[Outputs]
 [./console]
   type = Console
   perf_log = true
                          # enable performance logging
 [../]
 [./exodus]
   type = Exodus
   output_initial = true # enable the output of the initial
                          # condition for the [ExodusII][1] file
                          # create a second [Exodus II][1] output
 [./exodus_3]
                          # that utilizes a different output interval
   type = Exodus
   file_base = exodus_3 # set the file base
                          # (the extension is automatically applied)
   interval = 3
                          # only output every third step
 [../]
[]
```

20.3 Common Output Parameters

In addition to allowing for short-cut syntax, the Outputs block also supports common parameters. For example, output_initial may be specified outside of individual subblocks, indicating that all subblocks should output the initial condition. If within a subblock the parameter is given a different value, the subblock parameter takes precedence. The input file snippet below demonstrate the usage of a common values as well as the use of multiple output blocks.

```
output_initial = true
                            # set all subblocks to output the
                            # initial condition
 vtk = true
                            # output VTK file with default setting
 [./console]
   type = Console
   perf_log = true
 [../]
 [./exodus]
   type = Exodus
   output_initial = false
                           # this ExodusII files will not contain
                             # the initial condition
 [../]
[]
```

20.4 File Output Names

The default naming scheme for output files utilizes the input file name (e.g., input.i) with a suffix that differs depending on how the output is defined:

- outputs create using the shortcut syntax an "_out" suffix is utilized and
- subblocks use the actual subblock name as the suffix.

For example, if the input file (input.i) contained the following [Outputs] block, two files would be created: input_out.e and input_other.e.

```
[Outputs]
  console = true
  exodus = true  # creates input_out.e
  [./other]  # creates input_other.e
     type = Exodus
     interval = 2
  [../]
[]
```

20.5 Typical BISON Example

Now that some of the basic capabilities of the output system have been outlined, a typical [Outputs] block from a BISON assessment case is presented.

```
[Outputs]
  interval = 1
  output_initial = true
  csv = true
  exodus = true
  color = false
[./console]
    type = Console
    perf_log = true
    linear_residuals = true
    max_rows = 25
[../]
[]
```

interval The interval at which timesteps are output to the solution file. This is a global output parameter since it is not in a subblock.

output_initial Request that the initial condition is output to the solution file. This is a global output parameter since it is not in a subblock.

csv Specify that a csv file be output containing values of all postprocessors.

exodus Specify that an ExodusII file be output.

color Specify that color not be output to the screen for the log. type Specify the type for the subblock. In this case Console. perf_log Specify that the performance log be output to the screen. linear_residuals Specify that the linear residuals be output to the screen.

max_rows The maximum number of postprocessor/scalar values displayed on the

screen during a timestep (set to 0 for unlimited).

21 Dampers

Dampers are used to decrease the attempted change to the solution with each nonlinear step. This can be useful in preventing the solver from changing the solution dramatically from one step to the next. This may prevent, for example, the solver from attempting to evaluate negative temperatures.

The MaxIncrement damper is commonly used.

21.1 MaxIncrement

The MaxIncrement damper limits the change of a variable from one nonlinear step to the next.

```
[Dampers]
[./maxincrement]
  type = MaxIncrement
  max_increment = <real>
  variable = <string>
  [../]
[]
```

type MaxIncrement

max_increment Required. The maximum change in solution variable allowed from one

nonlinear step to the next.

variable Required. Variable that will not be allowed to change beyond

max_increment from nonlinear step to nonlinear step.

22 Restart and Recover

The MOOSE framework provides two ways of continuing a simulation: recover and restart. An example restart problem is located at projects/bison/examples/restart. The instructions below are copied from the MOOSE Wiki.

22.1 Definitions

- Restart: Running a simulation that uses data from a previous simulation. Data in this
 context is very broad, it can mean spatial field data, non-spatial variables or postprocessors, or stateful object data. Usually the previous and new simulations use different input
 files.
- Recover: Resuming an existing simulation either due to a fault or other premature termination.
- **Solution File:** A mesh format containing field data in addition to the mesh (i.e. a normal output file).
- **Checkpoint:** A snapshot of the simulation data including all meshes, solutions, and stateful object data. Typically one checkpoint is stored in several different files.
- N to N: In a restart context, this means the number of processors for the previous and current simulations must match.
- N to M: In a restart context, different numbers of processors may be used for the previous and current simulations.

22.2 Simple Restart (Variable initialization)

- This method is best suited for restarting a simulation when the mesh in the previous simulation exactly matches the mesh in the current simulation and only initial conditions need to be set for one more variables.
- This method requires only a valid Solution File.
- MOOSE supports N to M restart when using this method.

```
# Reading field data from a nodal or elemental field from a
# previous simulation
[Mesh]
 # MOOSE supports reading field data from ExodusII, XDA/XDR, and
 # mesh checkpoint files (.e, .xda, .xdr, .cp)
 file = previous.e
 # This method of restart is only supported on serial meshes
 distribution = serial
[Variables]
 [./nodal]
    family = LAGRANGE
    order = FIRST
    initial_from_file_var = nodal
    initial_from_file_timestep = 10
[]
[AuxVariables]
 [./elemental]
    family = MONOMIAL
    order = CONSTANT
    initial_from_file_var = elemental
    initial_from_file_timestep = 10
  [../]
[]
```

22.3 Enabling Checkpoints

Advanced restart in MOOSE requires checkpoint files. To enable automatic checkpoints using the default options (every time step, and keep last two) in your simulation simply add the following flag to your input file:

```
[Outputs]
checkpoint = true
[]
```

f you need more control over the checkpoint system, you can create a subblock in the input file that will allow you to change the file format, suffix, frequency of output, the number of checkpoint files to keep, etc. For a complete list see the Doxygen page for Checkpoint.

Note: You should always set num_files to at least 2 to minimize the change of ending up with a corrupt restart file.

```
[Outputs]
[./my_checkpoint]
type = Checkpoint
```

```
num_files = 4
  interval = 5
  [../]
[]
```

22.4 Advanced Restart

- This method is best suited for situations when the mesh from the previous simulation and the current simulation match but all variables should be reloaded and all stateful data should be restored.
- Support for modifying some variables is supported such as dt and time_step. By default, MOOSE will automatically use the last values found in the checkpoint files.
- Only N to N restarts are supported using this method.

```
[Mesh]
# Serial number should match corresponding Executioner parameter
file = out_cp/0010_mesh.cpr
# This method of restart is only supported on serial meshes
distribution = serial
[]

[Executioner]
type = Transient

# Note that the suffix is left off in the parameter below.
restart_file_base = out_cp/0010
[]
```

22.5 Reloading Data

It is possible to load and project data onto a different mesh from a solution file usually as an initial condition in a new simulation. MOOSE fully supports this through the use of SolutionUserObject (see Section 23.3).

22.6 Recover

Whenever MOOSE is being run with checkpoints enabled, a simulation that has terminated due to a fault can be recovered simply by using the ——recover CLI flag.

As a supplement to this example, also included is a restart.sh script (bison/examples/restart), which can serve as an example and reference for commands to use when using restart. The purpose of this script is to test the functionality of restart.

23 UserObjects

23.1 FuelPinGeometry

FuelPinGeometry computes the fuel rod outer dimensions, the height, ID, and OD of the fuel stack, and the pellet-clad gap directly from the mesh so that it can be used by other objects such as Burnup, RelocationUO2, and HydrogenPickup. Special attention to the sidesets needs to be made when constructing the mesh. Using the BISON standard sideset convention, FuelPinGeometry uses sideset 8 (Default) to compute the dimensions of the rod. In most of the cases that can be found in the BISON repository sideset 8 only calculates the pellet volume, whereas sideset 9 is used to calculate the plenum gas volume and temperature. The BISON meshing script will assign these sidesets properly if a simple fuel stack configuration is used (ie. solid or annular fuel and cladding only). If insulator pellets are required the current meshing script will include them in sideset 8, thus the pellet volume will be high. The solution is to reassign the sidesets as needed. If a more complex mesh is required, it will have to be built by the user and the user would assign the sidesets. Checking the sidesets before running a simulation is a good practice.

```
[./pin_geometry]
  type = FuelPinGeometry
  clad_inner_wall = <string>( "5" )
  clad_outer_wall = <string>( "2" )
  clad_top = <string>( "3" )
  clad_bottom = <string>( "1" )
  pellet_exteriors = <string>( "8" )
[../]
```

```
type FuelPinGeometry

clad_inner_wall Sideset for inner wall of cladding, not including end caps.

clad_outer_wall Sideset for outer wall of cladding.

clad_top Sideset for top of cladding (top of upper end cap).

clad_bottom Sideset for bottom of cladding (bottom of lower end cap).

pellet_exteriors Sideset for all pellet exteriors.
```

23.2 PelletBrittleZone

PelletBrittleZone computes the brittle zone width on a per-pellet basis.

```
[./pelletbrittlezone]
  type = PelletBrittleZone
  pellet_id = <string>
  temp = <string>
  pellet_radius = <real>
  a_lower = <real>
  a_upper = <real>
  number_pellets = <integer>
  fuel_pin_geometry = <string>
[../]
```

PelletBrittleZone type Variable name for pellet id. Typically pellet_id. pellet_id Name of temperature variable. Typically temp. temp Required if fuel_pin_geometry is not specified. The outer radius of pellet_radius the fuel. Required if fuel_pin_geometry is not specified. The lower axial coa_lower ordinate of the fuel stack. Required if fuel_pin_geometry is not specified. The upper axial coa_upper ordinate of the fuel stack. number_pellets **Required**. Number of fuel pellets. Name of the FuelPinGeometry object (see 23.1). fuel_pin_geometry

23.3 SolutionUserObject

A solution user object reads a variable from a mesh in one simulation to another. In order to use a <code>SolutionUserObject</code> three additional parameters are required, an <code>AuxVariable</code>, a <code>Function</code> and an <code>AuxKernel</code>. The <code>AuxVariable</code> represents the variable to be read by the solution user object. The <code>SolutionUserObject</code> is set up to read the old output file. A <code>SolutionFunction</code> is required to interpolate in time and space the data from the <code>SolutionUserObject</code>. Finally, the <code>FunctionAux</code> is required that will query the function and write the value into the <code>AuxVariable</code>. An example of what additions are required to the input file is shown below:

```
[AuxVariables]
  [./temp]
  [../]
[]

[Functions]
  [./interpolated_temp]
    type = SolutionFunction
    from_variable = 'temp'
    solution = read_thermo_solution
  [../]
```

```
[]
[UserObjects]
[./read_thermo_solution]
    type = SolutionUserObject
    mesh = 'temp_from_another_simulation.e'
    execute_on = 'residual'
    nodal_variables = 'temp'
[../]
[]
[AuxKernels]
[./interp_temp]
    type = FunctionAux
    variable = 'temp'
    function = 'interpolated_temp'
[../]
[]
```

Note that in the SolutionUserObject subblock that the mesh parameter is required.

24 Reference Residual Problem

An advanced scenario that requires the addition of a [Problem] block in the input file is the ReferenceResidualProblem. Reference residual is an alternative way to signify convergence of a timestep. The structure of the [Problem] block for a two-dimensional axisymmetric simulation is as follows:

```
[./referenceresidualproblem]
  coord_type = RZ
  type = ReferenceResidualProblem
  solution_variables = <string list>
  reference_residual_variables = <string list>
  acceptable_iterations = <integer> (0)
  acceptable_multiplier = <integer> (1)
[../]
```

type ReferenceResidualProblem

solution_variables Set of variables to be checked for relative convergences. reference_residual_variables Set of variables that provide reference residuals for the

relative convergence check.

acceptable_iterations Iterations after which convergence to acceptable limits

are accepted.

acceptable_multiplier Multiplier applied to relative tolerance for acceptable

limit.

When using reference residual it is typically acceptable to loosen the relative tolerance for convergence by an order of magnitude. The difficulty in setting up a ReferenceResidualProblem currently is the requirement of creating an AuxVariable for each of the reference residual variables. Then for each Kernel that the corresponding solution variable applies to an additional line is required to save into the reference residual variable. This requires significant changes to the input file. If you would like to try using a ReferenceResidualProblem, please contact one of the BISON developers for more detailed instructions of setting it up.

The implementation of ReferenceResidualProblem is scheduled to be updated within the next year.

25 Frictional Contact Problem

Another advanced use of the [Problem] block is the FrictionalContactProblem. This is used when a user wants to use kinematic (default) enforcement of frictional contact. If a user wants to use the penalty method for frictional contact the friction_coefficient needs to be specified in the [Contact] block and the model parameter set to coulomb. A typical [Problem] block for a two-dimensional axisymmetric case is as follows:

```
[./frictionalcontactproblem]
  coord_type = RZ
  type = FrictionalContactProblem
  friction_coefficient = <real>
  master = <string list>
  slave = <string list>
  slip_factor = <real>
  slip_too_far_factor = <real>
  disp_x = <string>
  disp_y = <string>
  residual_x = <string>
  residual_y = <string>
  diag_stiff_x = \langle string \rangle
  diag_stiff_y = <string>
  inc_slip_x = <string>
  inc_slip_y = <string>
  contact_slip_tolerance_factor = <real> (10)
  target_contact_residual = <real>
  maximum_slip_iterations = <integer> (100)
  minimum_slip_iterations = <integer> (1)
  slip_updates_per_iteration = <integer> (1)
  solution_variables = <string list>
  reference_residual_variables = <string list>
[../]
```

friction_coefficient

Required. The friction coefficient applied between the interacting surfaces.

Required. Number or name IDs of the master surfaces for which slip should be calculated.

Slave

Required. Number or name IDs of the slave surfaces for which slip should be calculated.

slip_factor	Required . The fraction of calculated slip to be applied for each interaction. A value of 1 means the entire amount of calculated slip is applied.
slip_too_far_factor	Required . The fraction of the calculated slip to be applied for each interaction that is in the slipped-too-far-state.
disp_x	Required. Variable name for the x-displacement. Typically $disp_x$.
disp_y	Required . Variable name for the y-displacement. Typically disp_y.
residual_x	Required . Name of auxiliary variable containing the saved x residual.
residual_y	Required . Name of auxiliary variable containing the saved y residual.
diag_stiff_x	Required . Name of auxiliary variable containing the saved x diagonal stiffness.
diag_stiff_y	Required . Name of auxiliary variable containing the saved y diagonal stiffness.
inc_slip_x	Required . Name of auxiliary variable used to store the incremental slip in the x direction.
inc_slip_y	Required . Name of auxiliary variable used to store the incremental slip in the y direction.
contact_slip_tolerance_factor	Multiplier on convergence criteria to determine when to start slipping.
target_contact_residual	Frictional contact residual convergence criterion.
target_relative_contact_residual	Frictional contact relative residual convergence criterion.
maximum_slip_iterations	Maximum number of slip iterations per step.
minimum_slip_iterations	Minimum number of slip iterations per step.
slip_updates_per_iteration	The number of slip updates per contact iteration.
solution_variables	Set of variables to be checked for relative convergences.
reference_residual_variables	Set of variables that provide reference residuals for the relative convergence check.

It can be seen that a significant amount of auxiliary variables are required to be added to the input file to make FrictionalContactProblem work. In addition references to saved variables as in the ReferenceResidualProblem case is also required. If you would like to use FrictionalContactProblem please contact a BISON developer for assistance. The implementation and robustness of FrictionalContactProblem is to be improved in the next year.

26 Mesh Script

26.1 Overview

To ease generation of LWR fuel meshes, a mesh script is available. The script relies on CU-BIT [6].

26.1.1 Run the Main Script

The mesh script is at bison/tools/U02/. The main script (mesh_script.sh) is run from the shell command line. This script invokes the Python meshing script (mesh_script.py) and passes it an input file named mesh_script_input.py by default.

You invoke the script as:

```
> ./mesh_script.sh [-c -d -l] [-p path to mesh_script.py] [-i
    mesh_script_input.py] [-o output file name]
```

The -c flag will cause the script to check whether CUBIT can be loaded. The -d flag results in the deletion of the CUBIT journal file when the script completes. The -1 flag will generate a log file (otherwise messages will go to the terminal). The -p flag, which is rarely used, tells the script where to find the mesh_script.py file. You may supply any mesh script input file with the -i flag. Finally, you may specify the name of the output Exodus file with the -c flag.

The main script generates an exodus file, with QUAD elements in 2D and HEX elements in 3D.

26.1.2 Mesh Architecture

Figure 26.1 provides an overview of the architecture of a fuel rod. A fuel rod is composed of a clad, a stack of pellets, and optionally a liner extruded on the inner surface of the clad. Each component of this architecture corresponds to a different block in the BISON input and mesh files. In the mesh input file, you refer to each block through a specific dictionary to create it. In the Exodus file, blocks are numbered, and a name is provided for each of them.

The pellets contained in a fuel rod can have different geometries. There is a block for each geometry, in the input file as well as in the Exodus file.

26.2 Input File Review

26.2.1 Pellet Type

This dictionary encapsulates a pellet geometry and the quantity of the corresponding pellets. To refer to a parameter, you have to know its key (the quoted string between brackets).

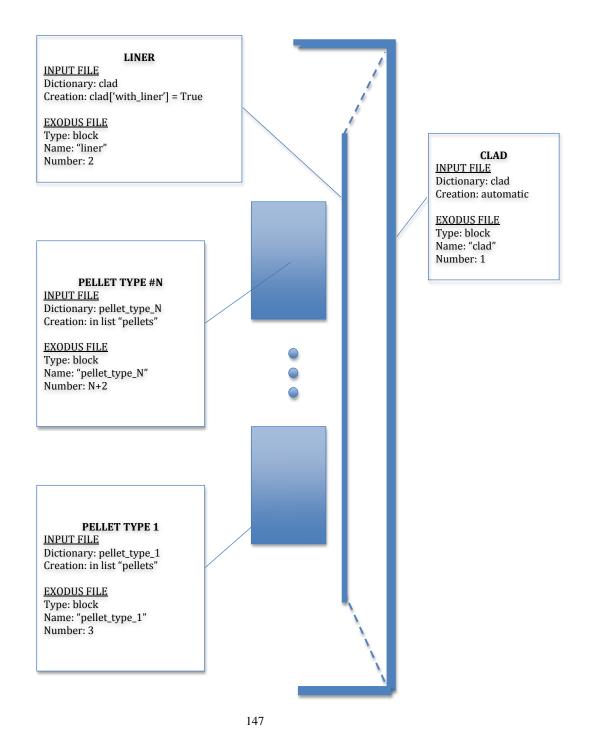


Figure 26.1: Overview of the architecture of a fuel rod.

```
# Pellet Type 1
Pellet1= {}
Pellet1['type'] = 'discrete'
Pellet1['quantity'] = 5
Pellet1['mesh_density'] = 'medium'
Pellet1['outer_radius'] = 0.0041
Pellet1['inner_radius'] = 0
Pellet1['height'] = 2*5.93e-3
Pellet1['dish_spherical_radius'] = 1.01542e-2
Pellet1['dish_depth'] = 3e-4
Pellet1['chamfer_width'] = 5.0e-4
Pellet1['chamfer_height'] = 1.6e-4
```

- 'type' Type *string*. Must be 'discrete' or 'smeared'. From a geometric point of view, a smeared pellet is a rectangle. Two consecutive smeared pellets have their top and bottom surfaces merged.
- 'quantity' Type int. Number of pellets created with this geometry.
- 'mesh_density' Type string.
- 'outer_radius' Type float. Outer radius of the pellet.
- 'inner_radius' Type float. Inner radius of the pellet.
- 'height' Type float. Pellet height.
- 'dish_spherical_radius' Type *float*. Spherical radius of the dishing. Needed only if type is 'discrete'.
- 'dish_depth' Type float. Depth of the dishing. Needed only if type is 'discrete'.
- 'chamfer_width' Type *float*. Radial chamfer length in RZ coordinates. Must be zero for a non-chamfered pellet. Needed only if type is 'discrete'.
- 'chamfer_height' Type float. Axial chamfer length in RZ coordinates. Must be zero for a non-chamfered pellet. Needed only if type is 'discrete'. If either chamfer_width or chamfer_height is zero, both must be zero.

26.2.2 Pellet Collection

```
pellets = [Pellet1, Pellet2, Pellet3]
```

This is a list of the pellets that make up the pellet stack. The geometries are ordered from the bottom to the top of the stack. A pellet type block must be present in this list to be created.

26.2.3 Stack Options

```
# Stack options
pellet_stack = {}
pellet_stack['interface_merge'] = 'point'
pellet_stack['higher_order'] = False
pellet_stack['angle'] = 0
```

- 'interface_merge' Type string. Control type of merging between pellets. Options are: 'point' or 'no'. See Table 26.1 for a complete description. Note that any other string results in pellets that are not merged.
- 'higher_order' Type boolean. Control order of mesh elements. See Table 26.2
- 'angle' Type *int*. Between 0 and 360. Angle of revolution of the pellet stack. If 0, creates a 2D fuel rod. If greater than 0, creates a 3D fuel rod.

	2D discrete	2D smeared	3D discrete
'point'	vertex	curve	curve
'no'	not merged	not merged	not merged

Table 26.1: Merging control. 'Vertex' means that the pellets are merged at their common vertex which is the closest from the centerline. In 2D, 'curve' means that the pellets are merged at their common curve. In 3D, 'curve' means that the pellets are merged at the curve generated by the corresponding merged vertex in 2D RZ geometry.

	False	True
2D	QUAD4	QUAD8
3D	HEX8	HEX27

Table 26.2: Order of generated elements

26.2.4 Clad

```
clad = {}
clad['mesh_density'] = 'medium'
clad['gap_width'] = 8e-5
clad['bot_gap_height'] = 1e-3
clad['top_gap_height'] = 1.67e-3
clad['clad_thickness'] = 5.6e-4
clad['top_bot_clad_height'] = 2.24e-3
clad['plenum_fuel_ratio'] = 0.045
```

```
clad['with_liner'] = False
clad['liner_width'] = 5e-5
```

- 'mesh_density' Type *string*. CAUTION: the mesh density of the clad is related to the mesh density of the pellets which use the *same* mesh dictionary as the clad.
- 'gap_width' Type *float*. Radial width of the gap between the fuel and the clad (or the liner).
- 'bot_gap_height' Type float. Axial gap height between bottom of fuel and the cladding.
- 'top_gap_height' Type *float*. Axial gap height between top of fuel and the cladding. Either this or 'plenum_fuel ratio' must be given.
- 'clad_thickness' Type float. Thickness of the sleeve of the clad.
- 'top_bot_clad_height' Type float. Height of the bottom and of the top of the clad.
- 'plenum_fuel_ratio' Type *float*. Ratio of the axial gas height to the fuel height inside the cladding. Either this or 'top_gap_height' must be given.
- 'with_liner' Type boolean. Whether to include a liner.
- 'liner_width' Type float. Liner width.

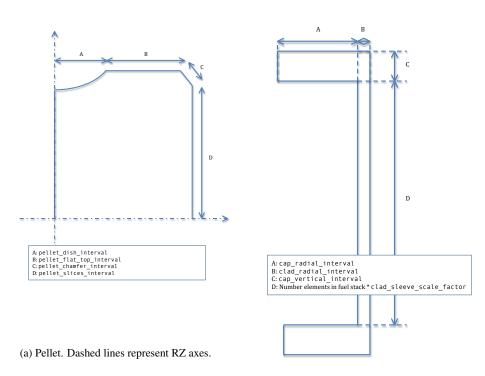
26.2.5 Meshing Parameters

```
# Parameters of mesh density 'coarse'
coarse = {}
coarse['pellet_r_interval'] = 6
coarse['pellet_z_interval'] = 2
coarse['pellet_dish_interval'] = 3
coarse['pellet_flat_top_interval'] = 1
coarse['pellet_chamfer_interval'] = 1
coarse['pellet_slices_interval'] = 4
coarse['clad_radial_interval'] = 3
coarse['clad_sleeve_scale_factor'] = 4
coarse['cap_radial_interval'] = 6
coarse['cap_vertical_interval'] = 3
coarse['pellet_angular_interval'] = 6
coarse['clad_angular_interval'] = 12
```

The user defines a dictionary containing the mesh parameters. The user can specify the name of this dictionary as long as the name is consistent with the names defined in the pellet type blocks for mesh_density. pellet_r_interval and pellet_z_interval are used only with smeared pellet meshes. Figure 26.2 explains other parameters.

The angular intervals are for 3D geometries and correspond to the created arcs of circle. Note that to have a nice mesh, you may want to have the same number of interval on the diameter of the fuel rod and on this arc of circle.

Figure 26.2: Mesh parameters



26.3 Output File Review

Figure 26.1 summarizes names and number of the blocks in the exodus file. Figure 26.4 summarizes the numbering for the sidesets and nodesets.

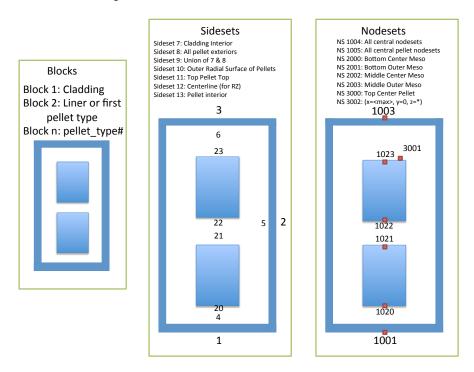


Figure 26.4: Sidesets, nodesets and blocks ids in the exodus file

26.4 Things to Know

26.4.1 Main Script

The main script is written in python v2.5. It is organized in classes: Pellet, PelletStack, Clad, Liner and FuelRod. The link between the input file and the main is assured by three functions. A first function is charged to pick read the input file. A second function checks that the syntax of the input file makes sense for the main script. The third function creates the mesh based on the input file.

26.4.2 Error Messages

AttributeError Caused by a missing class in the input file.

KeyError Often is caused by a wrong key in the input file. The main script should check that the keys entered in the input file are valid and specify which key is not valid if it occurs.

Other errors should be accompanied by a descriptive message. Contact the developers if the error message is not helpful.

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