BISON Users Manual

BISON Release 1.2

J. D. Hales

K. A. Gamble

B. W. Spencer

S. R. Novascone

G. Pastore

W. Liu

D. S. Stafford

R. L. Williamson

D. M. Perez

R. J. Gardner



NOTICE

This information was prepared as an account of work sponsored by an agency of the U.S. Government. Neither the U.S. Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for any third party's use, or the results of such use, of any information, apparatus, product, or process disclosed herein, or represents that its use by such third party would not infringe privately owned rights. The views expressed herein are not necessarily those of the U.S. Nuclear Regulatory Commission.

BISON Users Manual

J. D. Hales
K. A. Gamble
B. W. Spencer
S. R. Novascone
G. Pastore
W. Liu
D. S. Stafford
R. L. Williamson
D. M. Perez
R. J. Gardner

September 2015

Idaho National Laboratory
Fuel Modeling and Simulation Department
Idaho Falls, Idaho 83415

Prepared for the
U.S. Department of Energy
Office of Nuclear Energy
Under U.S. Department of Energy-Idaho Operations Office
Contract DE-AC07-99ID13727

BISON Users Manual

¹J. D. Hales
¹K. A. Gamble
¹B. W. Spencer
¹S. R. Novascone
¹G. Pastore
²W. Liu
¹D. S. Stafford
¹R. L. Williamson
¹D. M. Perez
¹R. J. Gardner

¹Idaho National Laboratory ²ANATECH, Inc.

Fuel Modeling and Simulation Idaho National Laboratory P.O. Box 1625 Idaho Falls, ID 83415-3840

September 2015

Contents

1	Introduction	7				
2	Running BISON 2.1 Checking Out the Code	8				
	2.1 Checking Out the Code	8				
	2.1.2 External Users	9				
	2.2 Updating BISON	10				
	2.3 Executing BISON	11				
	2.4 Getting Started	11				
	2.4.1 Input to BISON	11				
	2.4.2 Post Processing	12				
	2.4.3 Graphical User Interface	12				
	1					
3	Overview	13				
	3.1 Basic Syntax	13				
	3.2 BISON Syntax Page	14				
	3.3 Units	14				
	3.4 High-Level Description of a BISON Simulation	14				
4	Global Parameters	16				
5	Problem	17				
6	Mesh	18				
7	Variables 2					
8	AuxVariables	22				
9	Functions	23				
•	9.1 Composite	23				
	9.2 ParsedFunction	23				
	9.3 PiecewiseBilinear	24				
	9.4 PiecewiseConstant	24				
	9.5 PiecewiseLinear	25				
10) Boundary Conditions	27				
_	10.1 BulkCoolantBC	27				
	10.2 ConvectiveFluxBC	28				

	10.3	10.3 ConvectiveFluxFunction						28						
10.4 CoolantChannel					 	29								
	10.5	Dirichl	et					 	 				 	32
		10.5.1	DirichletBC					 	 				 	32
			PresetBC											33
		10.5.3	FunctionDirichletBC					 	 				 	33
		10.5.4	FunctionPresetBC .					 	 				 	33
	10.6		skHeatFlux											33
		-	genPickup											34
			Pressure											35
	10.9	Pressur	e					 	 		 		 	36
11	Cont													38
	11.1	Mecha	nical Contact					 	 				 	38
	11.2	Therma	al Contact					 	 				 	39
		11.2.1	GapHeatTransfer					 	 				 	39
		11.2.2	GapHeatTransferLWR					 	 				 	41
		_												
12	_	Kernels												45
	12.1		rnels for Output											45
			MaterialRealAux											45
			MaterialTensorAux .											46
	12.2		rnels for Specifying Fig											46
			FissionRateAux											46
			FissionRateAuxLWR											47
			FissionRateFromPowe	•										48
	12.3		AuxKernels											48
			Al2O3Aux											48
			BurnupAux											49
			FastNeutronFluenceA											49
			FastNeutronFluxAux											49
			GrainRadiusAux											50
			OxideAux											50
		12.3.7	PelletIdAux					 	 				 	51
40	_													
13	Burn	lup												52
14	Kern	els												55
• •	-		ius Diffusion					 						55
			orce											55
		•	/											56
		•	onduction											56
			onduction Time Deriva											56
			ource											57
	1.0	110m D			•			 	 	•	 •	•	 	51

	14.7	Isotrop	ic Diffusion
			n Heat Source
	14.9	SolidM	echanics
	14.10)Thermo	o-diffusion (Soret effect, thermophoresis)
	14.11	TimeDe	erivative
15	-		nation in the cladding 61
			he CladdingHydrides Action (the easy way) 61
	15.2		ndividual kernels and materials (the hard way)
			HydridePrecipitationRate
			HydrogenSource and HydrideSource
			HydrogenTimeDerivative
			HydrogenDiffusivity
		15.2.5	Other things needed for modeling hydrides without the CladdingHy-
			drides Action
16	Mate	riale	66
10			al Models
	10.1		HeatConductionMaterial
			ThermalCladMaterial
			ThermalFeCrAl
			ThermalFuel
			ThermalFastMOX
			ThermalFuelMaterial
			ThermalUPuZr
			ThermalU3Si2
	16.2		Inchmare 3312 70 Iechanics Models 71
	10.2		CreepFastMOXModel
			CreepPyC
			CreepSiC
			CreepU10Mo
			CreepUO2
			CreepUPuZr
			Elastic
			FailureCladding
			IrradiationGrowthZr4
			MechFeCrAl
			MechMaterial
			MechZry
			OxidationCladding
			RelocationUO2
			ThermalIrradiationCreepZr4
			PyCIrradiationStrain
			VSwellingFeCrAl
		10.4.1/	**************************************

	16.2.18 VSwellingUO2 16.2.19 VSwellingUPuZr 16.2.20 ZrPhase 16.3 Mass Diffusion Models 16.4 Other Models 16.4.1 Arrhenius Material Property 16.4.2 Density	91 92 93 93 94 94
17	Fission Gas Models	96
	17.1 Sifgrs	96
	17.2 ForMas	98
	17.3 FgrUPuZr	99
18	Postprocessors	100
	18.1 DecayHeatFunction	100
	18.2 ElementIntegralPower	101
	18.3 Elemental Variable Value	101
	18.4 Fission Gas Postprocessors	102
	18.5 InternalVolume	103
	18.6 MaterialTimeStep	103
	18.7 NodalVariableValue	103
	18.8 NumNonlinearIterations	104
	18.9 PlotFunction	104
	18.10SideAverageValue	105
	18.11SideFluxIntegral	105105
	18.12TimestepSize	103
19	Solution Execution and Time Stepping 19.1 Timestepping 19.1.1 Direct Time Step Control with Constant Time Step 19.1.2 Direct Time Step Control with Varying Time Step Size 19.1.3 Adaptive Time Stepping 19.2 PETSc Options 19.2.1 Constraint Contact 19.2.2 Dirac Contact 19.3 Quadrature	106 107 107 108 108 110 110 111
20	Outputs20.1 Basic Input File Syntax	112 112 112 113 114 114
	20.0 Typicai Dioott Damipic	114

21	Dampers	116
	21.1 MaxIncrement	116
22	Restart and Recover	117
	22.1 Definitions	117
	22.2 Simple Restart (Variable initialization)	117
	22.3 Enabling Checkpoints	118
	22.4 Advanced Restart	119
	22.5 Reloading Data	119
	22.6 Recover	119
23	UserObjects	120
	23.1 FuelPinGeometry	120
	23.2 PelletBrittleZone	120
	23.3 SolutionUserObject	121
24	Reference Residual Problem	123
25	Frictional Contact Problem	124
26	Mesh Script	126
	26.1 Overview	126
	26.1.1 Run the Main Script	126
	26.1.2 Mesh Architecture	126
	26.2 Input File Review	126
	26.2.1 Pellet Type	126
	26.2.2 Pellet Collection	128
	26.2.3 Stack Options	129
	26.2.4 Clad	129
	26.2.5 Meshing Parameters	130
	26.3 Output File Review	132
	26.4 Things to Know	132
	26.4.1 Main Script	132
	26.4.2 Error Messages	133
Bik	bliography	134

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. BISON 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 is now hosted on GitLab and the process of checking out the code has significantly changed since SVN. The instructions for checking out the code is different depending upon whether you are an internal (INL onsite user) or external user. These instructions are only for checking out and running the code. If you plan to contribute to BISON detailed instructions for contributing can be found on the idaholab/bison wiki page on GitLab.

2.1.1 Internal Users

The first step is to obtain an INL High Performance Computing (HPC) account. Once HPC access has been granted go to the GitLab website (https://hpcgitlab.inl.gov/) and login with your HPC username and password on the LDAP tab shown in Figure 2.1.

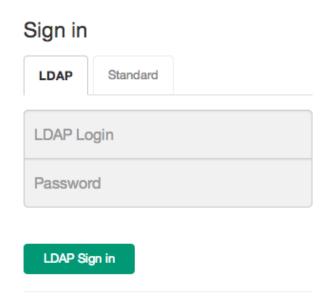


Figure 2.1: GitLab login screen.

Once logged in and access has been granted to the idaholab/bison repository the following steps are required for the initial checkout of the code:

First add an SSH key to your GitLab profile. To do so execute the code below in a terminal. and copy-paste the key to the 'My SSH Keys' section under the 'SSH' tab in your user profile on GitLab.

```
ssh-keygen -t rsa -C "your_email" cat ~/.ssh/id_rsa.pub
```

Then copy-paste the key to the 'My SSH Keys' section under the 'SSH' tab in your user profile on GitLab. Next clone the BISON GitLab repository.

```
cd ~/projects/
git clone git@hpcgitlab.inl.gov:idaholab/bison.git
```

Next initialize the MOOSE submodule:

```
cd ~/projects/bison/
git submodule update --init
```

It is necessary to build libMesh before building any application:

```
cd ~/projects/bison/moose/scripts
./update_and_rebuild_libmesh.sh
```

Once libMesh has compiled successfully, you may now compile BISON:

```
cd ~/projects/bison/
make (add -jn to run on multiple "n" processors)
```

Once BISON has compiled successfully, it is recommended to run the tests to make sure the version of the code you have is running correctly.

```
cd ~/projects/bison/
./run_test (add -jn to run "n" jobs at one time)
```

2.1.2 External Users

For external users there are a few additional steps to checking out the code. First request an HPC account. This can be requested at the HPC registration page (https://secure.inl.gov/caims/). Once an HPC account has been generated an ssh tunnel will need to be set up to access GitLab. Add the following lines to your /.ssh/config file. Replace <USERNAME> with the username for your HPC account.

```
User <USERNAME>
ProxyCommand nc -x localhost:5555 %h %p

#Forward license servers, webpages, and source control
Host hpclogin hpclogin.inl.gov
User <USERNAME>
HostName hpclogin.inl.gov
LocalForward 8080 hpcweb:80
LocalForward 4443 hpcsc:443
```

Next create a tunnel into the HPC environment and leave it tunning while you require access to GitLab. If you close this window, you close the connection:

```
ssh -D 5555 username@hpclogin.inl.gov
```

Then you have to adjust your socks proxy settings for your web browser to reflect the following settings localhost:5555

If you do not know how to do that, look up **Change socks proxy settings for <insert the name of your web browser here**> on google.com or some other search engine. Once that is complete you can login to the GitLab website. The rest of the steps for checking out the code are the same as for internal users.

2.2 Updating BISON

If it has been some time since you have checked out the code an update will be required to gain access to the new features within BISON. The following instructions apply to both internal and external users to update the code. Note that external users must have their ssh tunnel set up prior to proceeding. First update BISON:

```
cd ~/projects/bison/
git pull
```

Then update the MOOSE submodule:

```
cd ~/projects/bison/
git submodule update
```

Next rebuild libMesh:

```
cd ~/projects/bison/moose/scripts/
./update_and_rebuild_libmesh.sh
```

And finally recompile BISON:

```
cd ~/projects/bison/
make (add -jn to run on multiple "n" processors)
```

2.3 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 input Smeared.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
```

2.4 Getting Started

2.4.1 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:

```
[Mesh]
  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_gap_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
[]
```

2.4.2 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.

2.4.3 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]
     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.

```
[Mesh]
  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 = <integer> (24)
  nx_p = <integer> (8)
  nx_c = <integer> (2)
  ny_cu = <integer> (1)
  ny_c = <integer> (24)
  ny_cl = <integer> (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)
```

SmearedPelletMesh type Mesh density of the clad. Choices are coarse, medium, fine or clad_mesh_density custom. Default is medium. Mesh density of the fuel pellets. Choices are coarse, medium, fine pellet_mesh_density or custom. Default is medium. Number of finite elements in a fuel pellet in the axial direction. ny_p Number of finite elements in a fuel pellet in the radial direction. nx_p Number of finite elements through the thickness of the cladding in nx_c the radial direction. Number of finite elements through the thickness of the cladding in ny_cu the axial direction of the upper plug. Number of finite elements axially through the cladding. ny_c Number of finite elements through the thickness of the cladding in ny_cl the axial direction of the lower plug. The cladding thickness. clad_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. Gap between top of pellet and inside top surface of cladding. Either clad_top_gap_height plenum_fuel_ratio or clad_top_gap_height must be specified but not both. Gap between outer radius of pellet and inside surface of cladding. clad_gap_width top_bot_clad_height Thickness of top and bottom cladding walls. Type of finite element. Default is QUAD4. For second-order elem_type meshes use QUAD8.

displacements

patch_size

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.

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, $(1.0+0.1)*\cos(\text{pi}/2*(t-1.0))$ - 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>
  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
Х	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.

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.

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.

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
variable	Required. Primary variable associated with this boundary condi-
	tion.
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 tem-
	perature.

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 <code>example</code>, 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>
 [../]
[]
```

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

direction 2 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.

hydraulic_diameter Hydraulic diameter. If used, must be used with flow_area,

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.

linear_heat_rate 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.

number_lateral_zone Number of lateral divisions along the cladding to be used

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 Name of 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

oldcorrelation or 1 newWestinghousecorrelation.

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>
[../]
```

type DryCaskHeatFlux variable Required. Primary variable associated with this boundary condi-**Required**. List of boundaries where this BC will apply. boundary **Required**. Whether to use a typical geometry from a BWR or a bwr_or_pwr PWR assembly. Required. helium, nitrogen, or vacuum. fill_gas ambient_temperature Temperature outside the cask. cask_effective_htc Required. Effective heat transfer coefficient from assembly to ambient (W/K). start_time The time when this BC will begin. If drying (vacuum) is desired, it will be applied immediately after drying_duration the start_time. After drying in vacuum, the calculation switches

10.7 HydrogenPickup

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.

from vacuum fill gas to fill_gas specified by the user.

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>
[../]
```

Required. List of boundary names or ids where this boundary boundary condition will apply. The initial pressure in the plenum. initial_pressure The initial temperature of the plenum. If not given, will use the initial_temperature initial value from the Postprocessor given by temperature. startup_time The amount of time during which the pressure will ramp from zero to its true value. Required. The universal gas constant. In BISON, SI units are R used, and R should be 8.3143. If given, the name to use to report the initial moles of gas. output_initial_moles **Required**. The name of the Postprocessor holding the average temperature temperature value. **Required**. The name of the Postprocessor holding the internal volume volume. The name of the Postprocessors that hold the amount of matematerial_input rial injected into the plenum. If given, the name to use for reporting the plenum pressure value. output If not given, the block name will be used. The time(s) at which the plenum pressure must be reinitialized refab_time (likely due to fuel rod refabrication). The pressure of fill gas at refabrication. Number of values must refab_pressure match number in refab_time. The temperature at refabrication. Number of values must match refab_temperature number in refab_time. The gas volume at refabrication. Number of values must match refab_volume 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

disp_y

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

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.

normal_smoothing_method 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.

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
    disp_x = <variable>
    disp_y = <variable>
    disp_z = <variable>
    emissivity_1 = \langle real \rangle (0)
    emissivity_2 = \langle real \rangle (0)
    gap_conductivity = <real> (1)
    gap_conductivity_function = <string>
    gap_conductivity_function_variable = <string>
    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>
    stefan_boltzmann = \langle real \rangle (5.669e-8)
    tangential_tolerance = <real>
    variable = <string>
  [../]
[]
```

type	GapHeatTransfer
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.
gap_conductivity_function	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.
master	Required . The boundary id for the master surface.
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.
normal_smoothing_method	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
quadrature	FIRST and SECOND. Whether or not to use quadrature point-based gap heat transfer.
slave	Required . 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.

The quadrature option is recommended with second-order meshes. Also note that the type of conductance used depends on the value of the coord type parameter (XYZ (default), RZ, or RSPHERICAL), which is defined in the Problem block.

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).)

```
[ThermalContact]
  [./thermalcontact]
    type = GapHeatTransferLWR
    contact\_coef = \langle real \rangle (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 = \langle real \ list \rangle (1 0 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 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.
initial_gas_fractions	The initial fractions of constituent gases (helium, argon, 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 released.

gas_released_fractions The fraction of released gas that is assigned to helium, ar-

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.

normal_smoothing_method One of edge_based or nodal_normal_based. If

 $nodal_normal_based, \ must \ also \ have \ a \ {\tt NodalNormals}$

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).

slave The boundary id for the slave surface.

stefan_boltzmann The Stefan-Boltzmann constant.

tangential_tolerance
variable

Tangential distance to extend edges of contact surfaces.

 $\boldsymbol{Required}.$ 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 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.

12.1.2 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)
[../]
```

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.

12.2 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.

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/m³). The power density is divided by user-provided constant that defines the energy per fission (J/fission) to provide the fission rate in (fissions/m³/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 $3e13 (n/(m^2-s)/(W/m))$.

function Function that describes the fast neutron flux.
q_variable Variable holding linear heat rate in pellet in W/m.

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 PelletIdAux

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

```
[./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.

a_lower 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

block

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>
    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)
    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> (sum of sigma_c and sigma_f)
    reactor_type = <string> (LWR)
    N235 = \langle string \rangle
    N238 = \langle string \rangle
    N238 = \langle string \rangle
    N240 = \langle string \rangle
    N241 = \langle string \rangle
    N242 = \langle string \rangle
    RPF = <string>
  [../]
[]
```

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

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.

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

value based on reactor_type.

i_enrich The initial enrichment for the six isotopes.

sigma_c The capture cross sections for the six isotopes. If not given, will

take default value based on reactor_type.

sigma_f The fission cross sections for the six isotopes. If not given, will

take default value based on reactor_type.

sigma_a_thermal The absorption (thermal) cross sections for the six isotopes.

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

sigma_f, and sigma_c if those are not otherwise specified.

N235 Indicates that the output of the concentration of N235 is required.

Typically N235.

N238 Indicates that the output of the concentration of N238 is required.

Typically N238.

N239 Indicates that the output of the concentration of N239 is required.

Typically N239.

N240 Indicates that the output of the concentration of N240 is required.

Typically N240.

N241 Indicates that the output of the concentration of N241 is required.

Typically N241.

N242	Indicates that the output of the concentration of N242 is required. Typically N242.
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>
[../]
```

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

NeutronHeatSource type variable **Required**. Variable name corresponding to the heat conduction equation. Typically temp. Name of the Burnup sub-block, if any (typically burnup). May burnup_function not be used with fission_rate. Use of burnup_function is preferred. fission_rate Variable name corresponding to the fission rate. **Typically** fission_rate. Name of the postprocessor giving the decay heat curve. Typically decay_heat_function supplied for LOCA simulations. fuel_pin_geometry Name of the FuelPinGeometry object (see 23.1). Outer diameter of the cold fuel pellets if fuel_pin_geometry is outer_diameter not specified. inner_diameter Inner diameter of the cold fuel pellets if fuel_pin_geometry is not specified. Cross-sectional area of the cold fuel pellets if fuel_pin_geometry area

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

or the diameters are not specified.

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.

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)
[../]
```

block List of blocks where the hydride model is to be applied (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). 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 Arrhenius coefficient for hydrogen mass diffusivdiffusivity_frequency_factor ity 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 modelblock 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 Thermal conductivity Postprocessor for the z direction.

thermal_conductivity_temperature_function Function describing

Function describing thermal conductivity 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 and Resistalloy International Fecralloy.

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

type ThermalFeCrAl

block List of blocks this material applies to.

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

FECRALLOY

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 ThermalFuelMaterial

The ThermalFuelMaterial model computes specific heat and thermal conductivity for a variety of exotic fuel materials. The choices are ThermalU, ThermalU10Mo, ThermalU3Si2. 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.

density Required. Density, assumed constant.

16.1.7 ThermalUPuZr

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.

```
[./thermalUPuZr]
  type = ThermalUPuZr
  block = <string list>
  temp = <string>
  porosity = <string>
  porosity_material = <bool> (false)
  pu_weight = <real>
  zr_weight = <real>
[../]
```

type ThermalUPuZr

block List of blocks this material applies to.

temp Name of temperature variable. Typically temp.

porosity Name of porosity variable. Typically porosity. Optional.

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

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

pu_weight Required. The weight fraction of plutonium in the fuel. Given as a

decimal (e.g., 0.2)

zr_weight Required. The weight fraction of zirconium in the fuel. Given as a

decimal (e.g., 0.15)

16.1.8 ThermalU3Si2

The ThermalU3Si2 model computes the specific heat and thermal conductivity for U_3Si_2 fuel. Two models are available for both thermal conductivity and specific heat. The details of these models can be found in the theory manual.

```
[./thermalU3Si2]
  type = ThermalU3Si2
  block = <string list>
  temp = <string>
  specific_heat_model = <string> (WHITE)
  thermal_conductivity_model = <string> (WHITE)
[../]
```

type ThermalU3Si2

block List of blocks this material applies to.

temp Name of temperature variable. Typically temp.

porosity Name of porosity variable. Typically porosity. Op-

tional.

specific_heat_model 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 and SHIMIZU.

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>
[../]
```

CreepFastMOXModel type Absolute convergence tolerance for subabsolute_tolerance newtion iteration creeprate_scalef scaling factor for creep rate fission_rate Coupled fission rate fraction_of_temp_outside_model_bounds Fraction of temperature limit outside of model bounds grain_size grain size in micro meters Maximum creep strain increment allowed max_creep_increment by accuracy time step criterion

max_its Maximum number of sub-newton iterations

output The reporting postprocessor to use for the

max_iterations value

output_iteration_info Set true to output sub-newton iteration in-

formation

output_iteration_info_on_error Set true to output sub-newton iteration in-

formation when a step fails

output_properties List of material properties, from this ma-

terial, to output (outputs must also be de-

fined 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 sub-

newtion iteration

stress_free_temperature The stress-free temperature. If not speci-

fied, the initial temperature is used.

temp Coupled Temperature

thermal_expansion The thermal expansion coefficient

thermal_expansion_function Thermal expansion coefficient as a func-

tion of temperature

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>
  temp = <string>
  flux = <string>
  density = <real>
  youngs_modulus = <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>
  fast_neutron_flux = <string>
  k_function = <string>
  youngs_modulus = <real>
  poissons_ratio = <real>
  thermal_expansion = <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 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.

cally 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 tem-

perature 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

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_r = <string>
  temp = <string>
  fission_rate = <string>
  youngs_modulus = <real>
  poissons_ratio = <real>
  thermal_expansion = <real>
[../]
```

type CreepU10Mo

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.

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. thermal_expansion Coefficient of thermal expansion. The stress-free temperature. If not specified, the initial temstress_free_temperature perature is used.

16.2.5 CreepUO2

The CreepU02 is used to model the creep behavior of UO₂.

```
[./creepuo2]
  type = CreepUO2
  disp_x = <string>
  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 = \langle real \rangle (0)
  grain radius = \langle real \rangle (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>
[../]
```

type CreepUO2

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

ically disp_x.

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

ically disp_y.

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

ically 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.

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.

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 itera-

tions.

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.

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

MATPRO [8].

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

MATPRO [8].

matpro_thermal_expansion Set to true to use correlations for coefficient of thermal ex-

pansion from MATPRO [8].

burnup Name of burnup variable. Only required if using MATPRO

correlations. Typically burnup.

16.2.6 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]
  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>
  thermal_expansion = <real> (0)
  stress_free_temperature = <real>
[../]
```

type	CreepUPuZr
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.
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. Typically 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 temperature is used.

16.2.7 Elastic

The Elastic model is a simple hypo-elastic model.

```
[./elastic]
  type = Elastic
  disp_x = <string>
  disp_y = <string>
  disp_z = <string>
  temp = <string>
  youngs_modulus = <real>
  poissons_ratio = <real>
  thermal_expansion = <real>
[../]
```

type	Elastic
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.
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.

16.2.8 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 16.2.13). 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 overstress. 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. Name of the auxiliary variable for the volume fraction of Zr β fract_beta_phase phase, calculated by the model ZrPhase (Section 16.2.20). 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 16.2.13).

16.2.9 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)
[../]
```

type IrradiationGrowthZr4

fa	ast_neutron_fluence	Name	of	fast	neutron	fluence	variable.	Typically
		fast_n	eutr	con_fl	uence.			
Αç	g	Materia	ıl coı	nstant	that depend	ds on the c	ladding me	talurgical state.
n	g	Materia	ıl coı	nstant	that depend	ds on the c	ladding me	talurgical state.

16.2.10 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>
  scale_factor_A = \langle real \rangle (1.0)
  scale_factor_Q = <real> (1.0)
  scale_factor_n = \langle real \rangle (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.
disp_x	Variable name for displacement variable in x direction. Typically \mathtt{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.			
fast_neutron_flux	Name of the fast flux variable. Typically fast_neutron_flux.			
youngs_modulus	Young's modulus.			
poissons_ratio	Poisson's ratio.			
material	Name of chosen FeCrAl alloy. Choices are MA956, PM2000, APMT, FECRALLOY.			
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.			
scale_factor_youngs	Scale factor to be applied to the Young's modulus.			
scale_factor_nu	Scale factor to be applied to the Poisson's ratio.			
model_thermal_expansion	Whether to calcluate 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.			
model_irradiation_creep	Whether or not to model irradiation creep.			
stress_free_temperature	The stress-free temperature. If not specified, the initial temperature is used.			

16.2.11 MechMaterial

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, and MechSS316. These materials are typically used as cladding materials. Examples of their use can be found in /bison/tests/HT9 and /bison/tests/mechTests/.

```
[./mechMaterial]
  type = Mech<string>
  block = <string list>
  disp_x = <string>
  disp_y = <string>
  disp_z = <string>
  disp_z = <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 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.
youngs_modulus	Young's modulus.
poissons_ratio	Poisson's ratio.

16.2.12 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 18.6).

```
[./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 = <real> (1.e-03)
creeprate_scalef = <real> (1.)
[../]
```

type MechZry

Typically fast_neutron_flux.

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.

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

material_type

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

temp_standard_creep_end

The upper limit of temperature where the standard 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 allowed by the time step control.

Scale factor applied to the creep rate (for sensitivity

studies).

16.2.12.1 CombinedCreepPlasticity

creeprate_scalef

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>
[../]
```

CombinedCreepPlasticity type Relative convergence tolerance for combined subrelative_tolerance model iterations. Absolute convergence tolerance for combined subabsolute_tolerance model iterations. Maximum number of submodel convergence iteramax_its tions. Whether to output submodel convergence informaoutput_iteration_info Whether to output submodel convergence informaoutput_iteration_info_on_error tion if an error occurs. submodels Name of submodels used for combined creep and plasticity.

16.2.12.2 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 = <real> (1.e-03)
   creeprate_scalef = <real> (1.)
[../]
```

type	CreepZryModel
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.
cold_work_factor	Cold work factor.
oxygen_concentration	Oxygen concentration in ppm.
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.

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. Whether to model primary creep. model_primary_creep Whether to model steady state thermal creep. model_thermal_creep model_thermal_creep_loca Whether to model thermal creep considering a specific correlation at LOCA temperatures. Cladding material type. SRA(or 0), RXA(or 1), or material_type PRXA(or 2). The upper limit of temperature where the standard temp_standard_creep_end thermal creep model no longer applies. The lower limit of temperature where the loca thermal temp_loca_creep_begin creep model begins to apply. The maximum increment of effective creep strain almax_creep_increment lowed by the time step control. Scale factor applied to the creep rate (for sensitivity creeprate_scalef studies).

16.2.12.3 IsotropicPlasticity

The IsotropicPlasticity model is a model used to model the instantaneous plasticity of Zry cladding. It is used as one of the submodels in 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

relative_tolerance

Relative convergence tolerance for sub-newton iterations.

absolute_tolerance

Absolute convergence tolerance for sub-newton iterations.

max_its

Maximum number of sub-newton convergence iterations.

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.

16.2.13 OxidationCladding

The OxidationCladding 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 Required. Waterside cladding boundary.
clad_inner_radius Required. Inner cladding radius (m).
clad_outer_radius 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 (Leis-

tikov) or 1 (Cathcart-Pawel). In both cases, the model uses the

Prater-Courtright correlation above 1900 K.

temp **Required**. Name of temperature variable. Typically temp.

fast_neutron_flux Variable name corresponding to the fast neutron flux. Typically

fast_neutron_flux.

the coolant channel model.

oxygen_wtfract_initial As-fabricated oxygen weight fraction in cladding.

oxidation_scalef

Scale factor applied to the oxide scale thickness (for sensitivity studies).

16.2.14 RelocationUO2

The RelocationUO2 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 = \langle string \rangle
 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)
[../]
```

type	RelocationUO2	
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.	
fuel_pin_geometry	Name of the FuelPinGeometry object (see 23.1).	
diameter	Required if fuel_pin_geometry is not specified . As fabricated cold diameter of pellet in meters.	
q	Function describing linear heat rate in pellet in W/m.	
q_variable	Variable holding linear heat rate in pellet in W/m.	
gap	Required if fuel_pin_geometry is not specified . As fabricated cold diametral gap in m.	
burnup_relocation_stop	Burnup at which relocation strain stops in FIMA.	
relocation_activation1	First activation linear power in W/m. The linear power at which relocation turns on.	
relocation_activation2	Second activation linear power in W/m. The linear power at 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.

16.2.15 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 = \langle string \rangle
  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 = \langle real \rangle (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 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.

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.

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.

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

perature is used.

burnup Name of burnup variable. Typically burnup.

16.2.16 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.

16.2.17 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.

16.2.18 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.

Whether to save the solid swelling as a material property (solid_swell).

Save_densification

Whether to save the densification as a material property (densification).

Gas_swelling_type

Either SIFGRS to use the gas swelling computed by the Sifgrs 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).

16.2.19 VSwellingUPuZr

The VSwellingUPuZr model computes a volumetric strain to account for solid and gaseous swelling for U-Pu-Zr metal fuel systems.

```
[./vswelling_upuzr]
  type = VSwellingUPuZr
  temp = <string>
  fission_rate = <string>
  hydrostatic_stress = <string>
  fabrication_porosity = <real> (0.0)
[../]
```

type VSwellingUPuZr

 $\label{eq:local_norm} \mbox{Name of temperature variable. Typically temp.}$

fission_rate Name of fission rate variable. Typically fission_rate.

hydrostatic_stress Name of hydrostatic stress variable. Typically

 $\verb|hydrostatic_stress|.$

fabrication_porosity The as-fabricated porosity

Note that solid swelling and gaseous swelling are always 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.

16.2.20 ZrPhase

The 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>
[../]
```

type ArrheniusDiffusionCoef

dl First coefficient (m²/2).

dl_function Function to be multiplied by dl.

dl_function_variable Variable to be used when evaluating dl_function. If not given, time will be used.

d2 Second coefficient $(m^2/2)$.

```
q1 First activation energy (J/mol).
q2 Second activation energy (J/mol).
gas_constant Universal gas constant (J/mol/K).
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 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>
  disp_r = <string>
  density = <real>
[../]
```

```
type Density
```

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

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

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

 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 = <real> (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>
 diff_coeff_option = <integer> (3)
 res_param_option = <integer> (0)
 transient_option = <integer> (0)
 rod_ave_lin_power = <string>
  axial_power_profile = <string>
 temperature_scalef = <real> (1.)
 grainradius_scalef = <real> (1.)
 igdiffcoeff_scalef = <real> (1.)
 resolutionp_scalef = <real> (1.)
  gbdiffcoeff_scalef = <real> (1.)
[../]
```

```
type Sifgrs
initial_porosity Initial fuel porosity (/).
```

A constant value for fuel grain radius (m). Ignored if grain_radius_const grain_radius is given. A constant value for hydrostatic stress (Pa). Ignored if hydrostatic_stress_const

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

gbs_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.

burnup Name of burnup variable. Typically burnup.

Name of the Burnup sub-block, if any (typically burnup_function

> May not be used with fission_rate. burnup).

of burnup_function is preferred.

Variable name for hydrostatic stress. **Typically** hydrostatic_stress

hydrostatic_stress.

Name of the auxiliary variable for pellet id. pellet_id **Typically**

pellet_id. Used if ath_model = true.

The name of the UserObject that computes the width of the pellet_brittle_zone

brittle zone in the fuel pellet. Used if ath_model = true.

Choice of the intra-granular diffusion coefficient. One of 0 diff_coeff_option

> (Turnbull et al. [9] with purely irradiation-dependent term not considered), 1 (Andersson et al. [10]), 2 (Turnbull et al. [11]), or 3 (Turnbull et al. [11] with purely irradiation-

dependent term not considered).

Choice of the intra-granular resolution parameter. One of 0 res_param_option

> (heterogeneous model [12]) or 1 (compromise between the heterogeneous and the homogeneous models, see [13] - for

sensitivity studies).

To consider the burst release effect during transients, set transient_option

equal to 2.

Function describing rod averaged linear power. rod_ave_lin_pow

Function describing axial power profile. axial_power_profile

Scale factor applied to temperature (for sensitivity studies). temperature_scalef

grainradius_scalef

Scale factor applied to grain radius (for sensitivity studies).

Scale factor applied to intra-granular diffusion coefficient (for sensitivity studies).

resolutionp_scalef

Scale factor applied to intra-granular resolution parameter (for sensitivity studies).

gbdiffcoeff_scalef

Scale factor applied to grain-boundary diffusion coefficient (for sensitivity studies).

17.2 ForMas

external_pressure_function

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

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

ForMas type Initial fuel grain radius. grain_radius Resolution rate from intergranular bubbles (1/s). resolution_rate resolution_depth Resolution layer depth. bubble_radius Grain boundary bubble radius. bubble_shape_factor Non-spherical bubble shape factor. Bubble surface tension (J/m²). surface_tension fractional_coverage Fractional coverage of grain boundary at saturation. external_pressure Constant external hydrostatic pressure. The name of the plenum pressure Postprocessor. plenum_pressure

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

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>
  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.

outputs Vector of output names where you would like to restrict trhe outrputr 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 Elemental Variable Value

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

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

to 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 postprocessors 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 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.

18.6 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 16.2.12). 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

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

18.7 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.

18.8 NumNonlinearIterations

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

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

type NumNonlinearIterations

18.9 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.

18.10 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.

18.11 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.

18.12 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 = \langle real \rangle
 end_time = <real>
 num_steps = <integer>
 dtmax = <real>
 dtmin = <real>
 [TimeStepper]
   #TimeStepper commands
 [\ldots/]
```

Required. Several available. Typically Transient. type solve_type One of PJFNK (preconditioned JFNK), JFNK (JFNK), NEWTON (Newton), or SolveFD (Jacobian computed by finite differenceserial only, slow). PETSc flags. petsc_options petsc_options_iname Names of PETSc name/value pairs. Values of PETSc name/value pairs. petsc_options_value line_search Line search type. Typically none. l_max_its Maximum number of linear iterations per solve. 1_tol 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.		
	TT1 1 0.1		

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 TimeStepper block. There are a number of types of TimeStepper 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 ConstantDT type of 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 FunctionDTtime_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.

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.

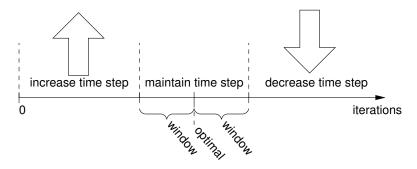


Figure 19.1: Criteria used to determine adaptive time step size

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 Outputs 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
 [../]
 [./exodus_3]
                           # create a second [Exodus II][1] output
                           # 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.

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.

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

type PelletBrittleZone Variable name for pellet id. Typically pellet_id. pellet_id temp Name of temperature variable. Typically temp. Required if fuel_pin_geometry is not specified. The outer radius of pellet_radius a_lower Required if fuel_pin_geometry is not specified. The lower axial coordinate 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 = \langle string \rangle
  disp_y = <string>
  residual_x = <string>
  residual_y = <string>
  diag_stiff_x = <string>
  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>
[../]
```

type

frictionalContactProblem

Required. The friction coefficient applied between the interacting surfaces.

master

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 <code>FrictionalContactProblem</code> work. In addition references to saved variables as in the <code>ReferenceResidualProblem</code> case is also required. If you would like to use <code>FrictionalContactProblem</code> please contact a BISON developer for assistance. The implementation and robustness of <code>FrictionalContactProblem</code> 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/UO2/. 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).

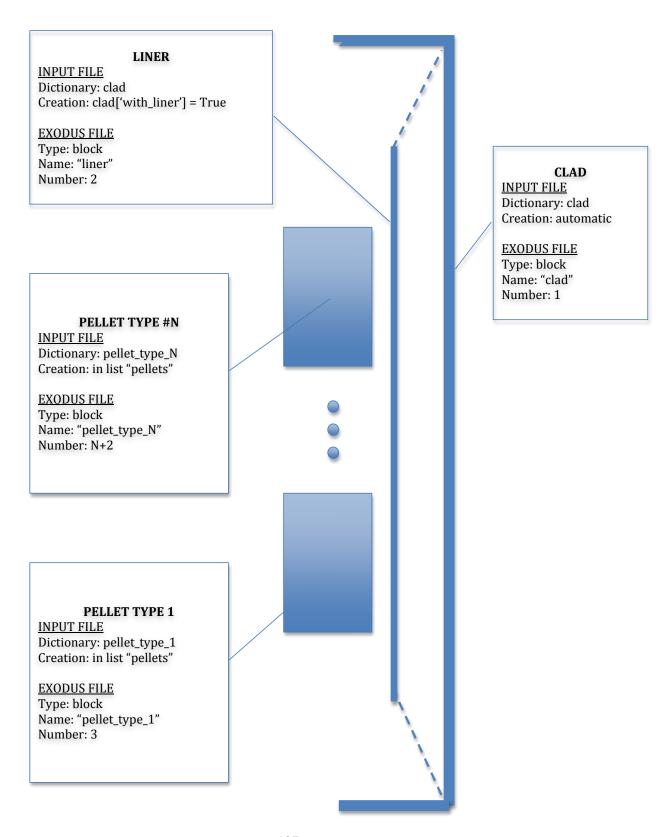


Figure 26.1: Overview of the architecture of a fuel rod.

```
# 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['merge_pellets'] = True
pellet_stack['higher_order'] = False
pellet_stack['angle'] = 0
```

- 'merge_pellets' Type string. Control type of merging between pellets. Options are: 'yes', 'no', 'point', 'surface'. 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
'yes'	vertex	curve	curve
'no'	not merged	not merged	not merged
'point'	vertex	vertex	curve
'surface'	not merged	curve	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	HEX20

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
```

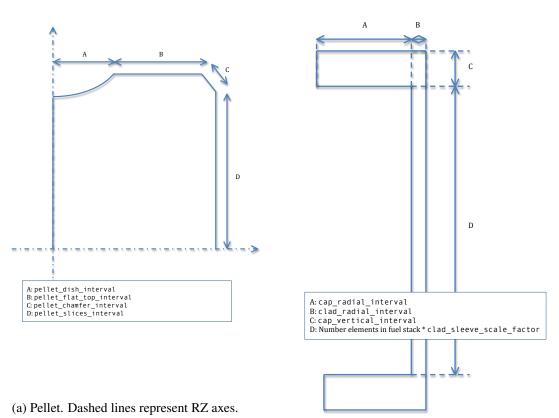
- 'mesh_density' Type *string*. CAUTION: the mesh density of the clad is related to the mesh density of the pellets which use the *same* mesh dictionary as the clad.
- 'gap_width' Type *float*. Radial width of the gap between the fuel and the clad (or the liner).
- 'bot_gap_height' Type float. Axial 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'] = 2
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

Figure 26.2: Mesh parameters



(b) Clad. Represented in RZ.

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.

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.

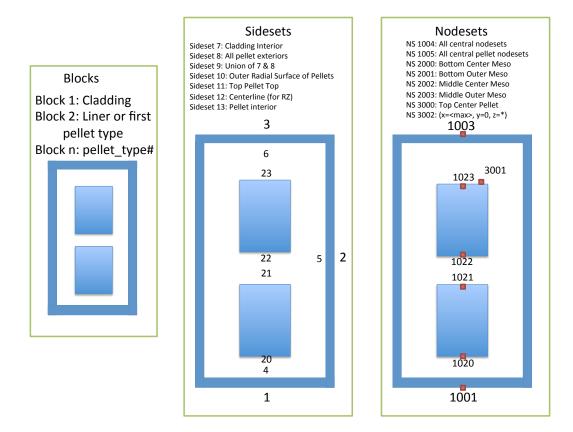


Figure 26.4: Sidesets, nodesets and blocks ids in the exodus file

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.

Bibliography

- [1] R. L. Williamson, J. D. Hales, S. R. Novascone, M. R. Tonks, D. R. Gaston, C. J. Permann, D. Andrs, and R. C. Martineau. Multidimensional multiphysics simulation of nuclear fuel behavior. *J. Nucl. Mater.*, 423:149–163, 2012.
- [2] J. D. Hales, R. L. Williamson, S. R. Novascone, D. M. Perez, B. W. Spencer, and G. Pastore. Multidimensional multiphysics simulation of TRISO particle fuel. *J. Nucl. Mater.*, 443:531–543, November 2013.
- [3] Pavel Medvedev. Fuel performance modeling results for representative FCRD irradiation experiments: Projected deformation in the annular AFC-3A U-10Zr fuel pins and comparison to alternative designs. Technical Report INL/EXT-12-27183 Revision 1, Idaho National Laboratory, 2012.
- [4] D. Gaston, C. Newman, G. Hansen, and D. Lebrun-Grandié. MOOSE: A parallel computational framework for coupled systems of nonlinear equations. *Nucl. Eng. Design*, 239:1768–1778, 2009.
- [5] L. Schoof and V. Yarberry. EXODUS II: A finite element data model. Technical Report SAND92-2137, Sandia National Laboratories, September 1996.
- [6] Sandia National Laboratories. CUBIT: Geometry and mesh generation toolkit. http://cubit.sandia.gov, 2008.
- [7] D. A. Knoll and D. E. Keyes. Jacobian-free Newton-Krylov methods: a survey of approaches and applications. *J. Comput. Phys.*, 193(2):357–397, 2004.
- [8] C. M. Allison, G. A. Berna, R. Chambers, E. W. Coryell, K. L. Davis, D. L. Hagrman, D. T. Hagrman, N. L. Hampton, J. K. Hohorst, R. E. Mason, M. L. McComas, K. A. McNeil, R. L. Miller, C. S. Olsen, G. A. Reymann, and L. J. Siefken. SCDAP/RELAP5/MOD3.1 code manual, volume IV: MATPRO-A library of materials properties for light-water-reactor accident analysis. Technical Report NUREG/CR-6150, EGG-2720, Idaho National Engineering Laboratory, 1993.
- [9] J. A. Turnbull, R.J. White, and C. Wise. The diffusion coefficient for fission gas atoms in uranium dioxide. In *Proceedings of Technical Committee Meeting on Water Reactor Fuel Element Computer Modelling in Steady State, Transient and Accident Conditions*, pages 174–181, Preston, UK, Sept. 18–22, 1988.
- [10] D. A. Andersson, P. Garcia, X. -Y. Liu, G. Pastore, M. Tonks, P. Millett, B. Dorado, D. R. Gaston, D. Andrs, R. L. Williamson, R. C. Martineau, B. P. Uberuaga, and C. R.

- Stanek. Atomistic modeling of intrinsic and radiation-enhanced fission gas (Xe) diffusion in $UO_{2\pm x}$: Implications for nuclear fuel performance modeling. *Journal of Nuclear Materials*, 451:225–242, 2014.
- [11] J. A. Turnbull, C. A. Friskney, J. R. Findlay, F. A. Johnson, and A. J. Walter. The diffusion coefficients of gaseous and volatile species during the irradiation of uranium dioxide. *J. Nucl. Mater.*, 107:168–184, 1982.
- [12] R.J. White and M.O. Tucker. A new fission-gas release model. *J. Nucl. Mater.*, 118:1–38, 1983.
- [13] D. R. Olander and D. Wongsawaeng. Re-solution of fission gas A review: Part I. Intragranular bubbles. *Journal of Nuclear Materials*, 354:94–109, 2006.