

# Truchas Reference Manual

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# Contents

Co	ontents	iii
1	Introduction         1.1 Invoking Truchas	1 1 2 2 3 3 4 4 4
2	ALTMESH Namelist  Overview  Components  Altmesh_Coordinate_Scale_Factor  Altmesh_File  Grid_Transfer_File  Partitioner  Partition_File  First_Partition	5 5 5 5 6 6 6 7
3	BC Namelist Overview Components BC_Name BC_Variable BC_Type BC_Type BC_Value Bounding_Box Conic_Constant Conic_Tolerance Conic_X Conic_XX Conic_XY Conic_XY	9 9 9 10 10 10 11 11 11 11 12 12

	Conic_Y	12
	Conic_YY	12
	Conic_YZ	13
	Conic_Z	13
	Conic_ZZ	13
	Mesh_Surface	13
		13
		13
4	BODY Namelist	<b>5</b>
	Overview	15
	Components	15
	axis	16
		16
	height	16
		16
		16
		- ° 16
	<del>_</del>	17
	1	17
		17 17
	_ 0	17 17
	<u>—</u> 1	17
		18
	I	18
	I	18
	<u>—1</u>	10 19
	velocity	ГЭ
5		21
	Overview	21
	Fig. 1. The state of the state	21
	Abs_Conc_Tol	22
	Abs_Enthalpy_Tol	22
	Abs_Temp_Tol	23
	Cond_Vfrac_Threshold	23
	Hypre_AMG_Debug	24
	Hypre_AMG_Logging_Level	24
	Hypre_AMG_Print_Level	24
	Max_NLK_Itr	24
	Max_NLK_Vec	25
		25
	_ :-	25
		26
	<del></del>	26
	<del></del>	- ° 26
	· · · · · · · · · · · · · · · · · · ·	-0 26

	PC_SSOR_Sweeps	26
	Rel_Conc_Tol	27
	Rel_Enthalpy_Tol	27
	Rel_Temp_Tol	27
	Residual_Atol	28
	Residual_Rtol	28
	Stepping Method	28
	Verbose_Stepping	28
	Void_Temperature	29
6	DS SOURCE Namelist	31
Ü	Components	31
	Equation	31
	Cell_Set_IDs	31
	Source Constant	32
	Source_Function	32
	Source_1 uncolon	02
7	ELECTROMAGNETICS Namelist	33
	Overview	33
	Components	33
	CG_Stopping_Tolerance	34
	EM_Domain_Type	34
	Graphics_Output	34
	Material_Change_Threshold	35
	Maximum_CG_Iterations	35
	Maximum_Source_Cycles	35
	Num_Etasq	36
	Output_Level	36
	Source_Frequency	36
	Source_Times	37
	SS_Stopping_Tolerance	37
	Steps_Per_Cycle	37
	Symmetry_Axis	38
	Uniform_Source	38
8	ENCLOSURE_RADIATION Namelist	39
	Overview	39
	Components	39
	Name	39
	Enclosure_File	39
	Coord_Scale_Factor	40
	Ambient_Constant	40
	Ambient Function	40
	Error_Tolerance	40
	toolpath	41
	Precon Method	41
	Precon Iter	41

	Precon_Coupling_Method	41
	Skip_Geometry_Check	41
9	ENCLOSURE_SURFACE Namelist	43
	Overview	43
	Components	43
	Name	43
	Enclosure_Name	43
	Face Block IDs	43
	Emissivity_Constant	44
		44
	Emissivity_Function	44
<b>10</b>	EVAPORATION Namelist (Experimental)	45
	Overview	45
	Components	45
	Face_Set_IDs	45
	Prefactor	45
	Temp_Exponent	46
	Activation_Energy	46
11		47 47
	Overview	
	Components	47
	inviscid	48
	courant_number	48
	viscous_number	48
	viscous_implicitness	48
	track_interfaces	49
	material_priority	49
	vol_track_subcycles	49
	nested_dissection	49
	vol_frac_cutoff	50
	fischer_dim	50
	fluid frac threshold	50
	min face fraction	50
	void_collapse	50
	void_collapse_relaxation	50
<b>12</b>	<del>-</del>	<b>53</b>
	Overview	53
	Components	54
	name	54
	face_set_ids	54
	type	54
	pressure	55
	pressure_func	55
	velocity	55

	velocity_func	55
	dsigma	55
	inflow_material	55
		56
<b>13</b>	FLOW_PRESSURE_SOLVER and FLOW_VISCOUS_SOLVER Namelists 5	7
	Overview	57
	krylov_method	57
	krylov_dim	57
	conv_rate_tol	58
	abs_tol	58
	rel_tol	58
	max_ds_iter	58
		58
	print level 5	58
<b>14</b>	FUNCTION Namelist 6	31
	Overview	31
	Components	32
	Name	62
	Type	32
	Library_Path	32
	Library Symbol	33
	Parameters	33
		33
	·	33
		33
	·	34
		- 34
		34
		34
	_ 1	35
		35
	_ 1_	35
	_ 1_	36
		,0
<b>15</b>	INDUCTION_COIL Namelist 6	67
	<del>-</del>	37
		38
	•	58
		58
		38
		38
		, 38

16 MATERIAL and PHASE Namelists	71
Overview	71
The MATERIAL Namelist	71
name	71
phases	71
The PHASE Namelist	71
name	71
Property and Attribute Variables	72
17 MESH Namelist	75
Overview	75
Components	75
$\underline{\mathrm{mesh\_file}}  \ldots  \ldots  \ldots  \ldots  \ldots  \ldots  \ldots  \ldots  \ldots $	76
$interface\_side\_sets \ . \ . \ . \ . \ . \ . \ . \ . \ . \ $	76
gap_element_blocks	76
exodus_block_modulus	76
x_axis	77
y_axis	77
z_axis	77
noise_factor	78
coordinate_scale_factor	78
partitioner	78
partition_file	78
first_partition	79
10 WINDDIGG N	0.1
18 NUMERICS Namelist	81
Overview	81
Components	81
Alittle	81
Cutvof	82
Cycle_Max	82
Cycle_Number	82
Discrete_Ops_Type	82
Dt_Constant	83
<u>Dt_Grow</u>	83
Dt_Init	83
Dt_Max	84
Dt_Min	84
t	84
19 OUTPUTS Namelist	85
Overview	85
Components	85
Int_Output_Dt_Multiplier	85
Output_Dt	85
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	86
Probe Output Cycle Multiplier	86

	Short_Output_Dt_Multiplier	86
	Output_Dt_Multiplier	86
	Move_Block_IDs	86
	Move_Toolpath_Name	86
<b>20</b>	PHASE_CHANGE Namelist	87
	Overview	87
	low_temp_phase	87
	high_temp_phase	87
	solidus_temp	87
	liquidus_temp	87
	solid_frac_table	88
	latent_heat	88
<b>21</b>	PHYSICAL_CONSTANTS Namelist	89
	Overview	89
	Components	89
	Absolute_Zero	89
	Stefan_Boltzmann	89
	Vacuum_Permeability	90
	Vacuum_Permittivity	90
<b>22</b>	PHYSICS Namelist	91
	Overview	91
	Components	92
	Materials	92
	Flow	92
	Body_Force_Density	92
	Heat_Transport	93
	Species_Transport	93
	Number_of_Species	93
	Solid_Mechanics	93
	Electromagnetics	93
<b>23</b>	PROBE Namelist	95
	Overview	95
	Components	95
	$\operatorname{coord}\nolimits \ldots \ldots$	95
	coord_scale_factor	96
	data	96
	data file	96
	<del></del>	
	description	96

<b>24</b>	RESTART Namelist	97
	Overview	97
	Components	97
	Ignore_T	97
	Ignore_Dt	97
	Ignore_Joule_Heat	98
	Ignore_Solid_Mechanics	98
<b>25</b>	SIMULATION_CONTROL Namelist (Experimental)	99
	Overview	99
	Components	99
	Phase_Init_Dt	99
	Phase_Init_Dt_Factor	100
	Phase_Start_Times	100
26	SOLID_MECHANICS Namelist	101
	Overview	101
	Components	101
	•	101
	Contact_Norm_Trac	102
	Contact_Penalty	102 $102$
	Displacement_Nonlinear_Solution	$102 \\ 103$
	Solid Mechanics Body Force	103
	Strain Limit	103
	Strain_Limit	103
<b>27</b>	SPECIES_BC Namelist	105
	Overview	105
	Components	105
	name	106
	comp	106
	face_set_ids	106
	type	106
		106
	conc func	107
	flux	107
	flux_func	107
20	THERMAL DC Nomelist	100
40	<del>-</del>	<b>109</b> 109
	Overview	
	Components	110
	name	111
	face_set_ids	111
	type	111
	temp	111
	temp_func	112
	flux	112
	flux func	112

	htc	112
	htc_func	112
	ambient_temp	112
	ambient_temp_func	113
	emissivity	113
	emissivity_func	113
	· —	
<b>29</b>	THERMAL_SOURCE Namelist	115
	Components	115
	name	115
	cell_set_ids	116
	source	116
	source_func	116
	data_file	116
	prefactor	116
	prefactor_func	
	F	
<b>30</b>	TOOLPATH Namelist (Experimental)	117
	Overview	117
	Components	117
	Name	117
	Command_String	117
	Command_File	118
	Start_Time	118
		118
	Time_Scale_Factor	118
	Coord Scale Factor	
	Write Plotfile	119
	Plotfile Dt	
	Partition_Ds	119
		110
31	TURBULENCE Namelist	121
	Overview	121
	Components	121
	Turbulence CMU	121
	Turbulence KE Fraction	121
	Turbulence_Length	122
<b>32</b>	VFUNCTION Namelist	123
	Overview	123
	Components	123
	Name	123
	Type	124
	Tabular_Data	124
	Tabular Dim	194

33 VISCOPLASTIC_MODEL Namelist	125
Overview	125
Components	125
Phase	
Model	126
MTS_b	126
MTS_d	126
MTS_edot_0i	126
MTS_g_0i	127
MTS_k	127
MTS_mu_0	127
MTS_p_i	127
MTS_q_i	127
MTS_sig_a	128
MTS_sig_i	128
MTS_temp_0	128
Pwr_Law_A	128
Pwr_Law_N	128
Pwr_Law_Q	129
Pwr_Law_R	129
Bibliography	131
Index	132

# Introduction

## 1.1 Invoking Truchas

Truchas is executed in serial using a command of the form

```
truchas [-h] [-d[:n]] [-o:outdir] [-r:rstfile] infile
```

assuming truchas is the name of the executable. The brackets denote optional arguments that are described in Table 1.1. The only required argument is the path to the input file infile. This file name must end with the extension ".inp" (without the quotes). The general format of the input file is described in the next section, and the following chapters describe the various Fortran namelists that go into the input file to describe the problem to be simulated.

All of the output files are written to directory whose name is generated from the base name of the input file. For example, if the input file is myprob.inp, the output directory will be named myprob\_output. The name of the output directory can be overridden using the -o option. The directory will be created if necessary.

The precise manner of executing Truchas in parallel depends on the MPI implementation being used. This may be as simple as prefixing the serial invocation above with "mpirun -np n", where n is the number of processes. But this varies widely and providing specific instructions is beyond the scope of this document. There is no difference in the Truchas arguments between serial and parallel, however.

Table 1.1: Truchas command line options

Option	Description
-h	Print a usage summary of the command line options and exit.
-d[:n]	Sets the debug output level $n$ . The default level is 0, which produces no debug
	output, with levels 1 and 2 producing progressively more debug outputd is
	equivalent to -d:1.
$\hbox{\tt -o:} \textit{outdir}$	Causes all output files to be written to the directory $outdir$ instead of the default
	directory. The directory is created if necessary.
$ ext{-r:} rstfile$	Executes in restart mode, restarting from the data in the file rstfile. This file is
	generated from the output of a previous Truchas simulation using post-processing
	utilities.

```
This is a comment. Anything outside a namelist input is ignored.

&MESH

! Within a namelist input "!" introduces a comment.

mesh_file = "my-big-mesh.exo" ! character string value

/

Another comment.

&PHYSICS

heat_conduction = .true. ! logical values are .true./.false.

body_force = 0.0, 0.0, -9.8 ! assigning values to an array
!This would be an equivalent method ...
!body_force(1) = 0.0
!body_force(2) = 0.0
!body_force(3) = -9.8

/

Newlines in a namelist are optional.
&PHYSICAL_CONSTANTS stefan_boltzmann=0.1, absolute_zero=0.0 /
```

Figure 1.1: Fragment of a Truchas input file illustrating namelist input syntax.

#### 1.1.1 Stopping Truchas

There are occasions where one would like to gracefully terminate a running Truchas simulation before it has reached the final simulation time given in the input file. This is easily done by sending the running process the SIGURG signal:

```
kill -s SIGURG pid
```

where *pid* is the process id. When Truchas receives this signal, it continues until it reaches the end of the current time step, where it writes the final solution and then exits normally.

## 1.2 Input File Format

The Truchas input file is composed of a sequence of Fortran namelist inputs. Each namelist input has the form

```
\& namelist\text{-}group\text{-}name \\ namelist\text{-}input\text{-}body \\ /
```

The input begins with a line where the first nonblank is the character & immediately followed by the name of the namelist group. The input continues until the / character. The body of the namelist input consists of a sequence of name = value pairs, separated by

commas or newlines, that assign values to namelist variables. Namelist input is a feature of Fortran and a complete description of the syntax can be found in any Fortran reference, however the basic syntax is very intuitive and a few examples like those in Fig. 1.1 should suffice to explain its essentials.

The namelists and the variables they contain are described in the following chapters. A particular namelist will be required or optional, and it may appear only once or multiple times. Not all variables of a namelist need to be specified. Some may not be relevant in a given context, and others may have acceptable default values; only those that are used and need to be assigned a value need to be specified.

The order of the namelist inputs in the input file is not significant; they may appear in any order. Any text outside of a namelist input is ignored and can be regarded as a comment; see Fig. 1.1.

Fortran is case-insensitive when interpreting the namelist group names and variable names; they may be written in any mixture of upper and lower case. However character string values, which are interpreted by Truchas, are case-sensitive unless documented otherwise. In the event of a namelist input syntax error, Truchas will report that it was unable to read the namelist, but unfortunately it is not able to provide any specific information about the error because Fortran does not make such information available. In such cases the user will need to scan the namelist input for syntax errors: look for misspelt variable names, variables that don't belong to the namelist, blank written in place of an underscore, etc.

## 1.3 Physical Units

Truchas does not require the use any particular system of physical units, nor does it provide a means for the user to specify the dimension of a numerical value. The user is simply expected to ensure that all input values are given using a consistent system of units. To assist in this end, the dimension for all dimensional quantities is documented using the following abstract units: mass M, length L, time T, thermodynamic temperature  $\Theta$ , and electric current I. Thus mass density, for example, will be documented as having dimension  $M/L^3$ . The following derived abstract units are also used: force F (= M  $L/T^2$ ) and energy E (= M  $L^2/T^2$ ).

There are a few physical constants, like the Stefan-Boltzmann constant, that have predefined values in SI units. These constants are referenced by a few specific models, and where a model uses one of these constants this fact is noted. Use the PHYSICAL\_CONSTANTS namelist to redefine the value of these constants where necessary.

## 1.4 Working With Output Files

As described earlier, Truchas writes its output files to the directory named in the -o option, or if omitted, to a directory whose name is generated from the base name of the input file: myprob\_output if myprob.inp is the input file, for example. Two primary files are written, a .log file that is a copy of the terminal output, and a .h5 HDF5 file that contains all the simulation results. HDF5 is a widely-used format for storing and managing data, and there are a great many freely-available tools for working with these files. In this release, which is the first to feature HDF5 output, we provide only a few essential tools, described below, for

processing the .h5 file. We expect to provide additional tools in future releases.

#### 1.4.1 write\_restart

The program write\_restart is used to create Truchas restart files using data from an .h5 output file. The command syntax is

write restart [options] H5FILE

where  ${\it H5FILE}$  is the .h5 output file and the possible options are

- -h Display usage help and exit.
- -1 Print a list of the available cycles from which the restart file can be created. No restart file is written.
- -n N Data from cycle N is used to create the restart file; if not specified, the last cycle is used.
- -o FILE Write restart data to FILE. If not specified, FILE is taken to be the H5FILE name with the .h5 suffix replaced by .restart. N where N is the cycle number.
- -m FILE Create a mapped restart file using the specified ExodusII mesh FILE as the target mesh.
- -s FLOAT Scale the mapped restart mesh by the factor FLOAT.

#### 1.4.2 write\_probes

The write\_probes utility extracts probe data (see the PROBE namelist) from an .h5 output file and writes it to the terminal (where it can be redirected as needed) in a multicolumn format suitable for many line plotting programs. The command syntax is

where  ${\it H5FILE}$  is the .h5 output file and the available options are

- -h Display usage help and exit.
- -1 Print a list of the available probes.
- -n N Data for probe index N is written.

#### 1.4.3 truchas-gmv-parser.py

The python script truchas-gmv-parser.py is used to create input files for the GMV visualization tool. Formerly distributed gratis, GMV has been commercialized (http://www.generalmeshviewer.com). Earlier free versions of the tool can still be found on the internet, however, and it remains available within LANL. The command syntax is

```
python truchas-gmv-parser.py [options] H5FILE
```

where *H5FILE* is the .h5 output file. Use the option -h to get a full list of the available options.

# **ALTMESH Namelist**

#### Overview

The ALTMESH namelist specifies the alternate mesh used by the induction heating solver. This is a 3D tetrahedral mesh imported from an ExodusII format disk file.

#### **ALTMESH Namelist Features**

Required/Optional: Required when Electromagnetics is true.

Single/Multiple Instances: Single

## Components

- Altmesh\_Coordinate\_Scale\_Factor
- Altmesh File
- First\_Partition
- Grid\_Transfer\_File
- Partitioner
- Partition\_File

## Altmesh\_Coordinate\_Scale\_Factor

**Description:** An optional factor by which to scale all mesh node coordinates.

Type: real
Default: 1.0

Valid values: > 0

### Altmesh\_File

**Description:** Specifies the path to the ExodusII mesh file. If not an absolute path, it will be interpreted relative the Truchas input file directory.

Type: case-sensitive string

Default: none

### Grid Transfer File

Description: Certain fields must be mapped between the main and alternative meshes during the course of a simulation. These mappings are accomplished using some fixed grid-mapping data that depend only on the two meshes. This optional variable specifies the path of a file containing this grid mapping data. If specified, and if the file exists, it will be read and its mapping data checked to ensure that it corresponds to the two meshes being used. If it corresponds, the data will be used for the calculation. Otherwise, the grid mapping data is computed and written to the file altmesh\_mapping\_data.bin in the output directory for use in future calculations, avoiding a needless and potentially costly recomputation of the same data.

Type: case-sensitive string

Default: none

**Note:** The mapping data depends on the internal ordering of the nodes and cells of each mesh, in addition to the meshes themselves. Thus it is recommended that this file be named in such a way that reflects the identity of the two meshes *and* the number of processors used to compute the mapping data; mapping data computed with one number of processors will not be usable in a calculation with a different number of processors, even when the same pair of meshes is used.

#### Partitioner

**Description:** The partitioning method used to generate the parallel decomposition of the EM mesh.

Type: case-insensitive string

Default: "chaco"

Valid values: "chaco", "file", "block"

Notes: See the MESH namelist variable Partitioner for a description of the options.

#### Partition\_File

**Description:** Specifies the path to the EM mesh cell partition file, and is required when Partitioner is "file". If not an absolute path, it will be interpreted as a path relative to the Truchas input file directory.

**Type:** case-sensitive string

Default: none

Notes: See the Notes for the MESH namelist variable Partition\_File.

## First\_Partition

**Description:** Specifies the number given the first partition in the numbering convention

used in the partition file. Either 0-based or 1-based numbering is allowed.

Type: integer Default: 0

Valid values: 0 or 1

# **BC** Namelist

#### Overview

The BC namelist is used to define boundary conditions for the solid mechanics model at external boundaries and internal material interfaces.

The preferred method for specifying the mesh surface where a boundary condition applies is to reference a side set from the ExodusII-format mesh. Alternatively, the mesh surface can specified using a conic surface:

$$0 = p(x, y, z) = c_0 + c_x x + c_y y + c_z z + c_{xx} x^2 + c_{yy} y^2 + c_{zz} z^2 + c_{xy} xy + c_{xz} xz + c_{yz} yz$$
 (3.1)

A face belongs to the mesh surface whenever its centroid lies on this surface (see <code>Conic\_Tolerance</code>). The coefficients are specified using the <code>Conic\_\*</code> variables. Another method for solid mechanics is to specify nodes. The method is selected using <code>Surface\_Name</code>. The specified surface may also be restricted to lie within a bounding box.

#### **BC** Namelist Features

Required/Optional: Optional

Single/Multiple Instances: Multiple

## Components

- BC Name
- BC\_Table
- BC Type
- BC Value
- BC\_Variable
- Bounding\_Box
- Conic Constant
- Conic Tolerance

- Conic\_X
- Conic\_XX
- Conic\_XY
- Conic\_XZ
- Conic\_Y
- Conic\_YY
- Conic\_YZ
- Conic\_Z
- Conic ZZ
- Mesh\_Surface
- Node Disp Coords
- Surface\_Name

#### BC\_Name

**Description:** A name used to identify a particular instance of this namelist.

Type: case-sensitive string

Default: none

**Note:** This is optional and used for logging purposes only.

#### BC\_Variable

**Description:** The name of the variable to which this boundary condition applies.

Type: case-insensitive string

Default: none

Valid values: "displacement"

## BC\_Type

**Description:** The type of boundary condition.

Type: string

Default: Depends on BC Variable:

'displacement': 'x-traction', 'y-traction', 'z-traction'

Valid values: Depends on BC\_Variable:

```
'displacement': 'x-traction', 'y-traction', 'z-traction',
    'x-displacement', 'y-displacement', 'z-displacement',
    'normal-displacement', 'normal-traction', 'free-interface',
    'normal-constraint', 'contact'
```

Notes:

- The solid mechanics displacement solution defaults to a traction-free surface with no displacement constraints ('x-traction', 'y-traction', and 'z-traction' set to zero.)
- The 'free-interface', 'normal-constraint' and 'contact' types can only be specified for interfaces with gap elements.

#### BC\_Value

**Description:** Value(s) for the constant(s) used in this BC definition. See also BC Table.

Physical dimension: varies

Type: real (up to 24 values depending on BC\_Type)

**Default:** 0.0

**Notes:** The meaning of the items in the BC\_Value list depends on the particular boundary condition:

BC_Variable	BC_Type	Value Description	Physical	Number
			Dimension	of values
"displacement"	"x-displacement"	displacement	L	1
"displacement"	"y-displacement"	displacement	L	1
"displacement"	"z-displacement"	displacement	L	1
"displacement"	"x-traction"	traction (force/area)	$F/L^2$	1
"displacement"	"y-traction"	traction (force/area)	$F/L^2$	1
"displacement"	"z-traction"	traction (force/area)	$F/L^2$	1
"displacement"	"normal-displacement"	displacement	L	1
"displacement"	"free-interface"	not used	_	0
"displacement"	"normal-constraint"	not used	_	0
"displacement"	"contact"	not used	_	0

## Bounding\_Box

**Description:** The extents in each dimension of a bounding box that restricts the extent of the mesh surface where the boundary condition is applied. This does not apply in the case Surface\_Name is "node set".

Physical dimension: L

**Type:** A real array  $(x_{\min}, x_{\max}, y_{\min}, y_{\max}, z_{\min}, z_{\max})$ .

**Default:** Unlimited in each dimension.

#### Conic\_Constant

**Description:** Value of the coefficient  $c_0$  in the conic polynomial (3.1).

Type: real **Default:** 0.0

#### Conic\_Tolerance

**Description:** A mesh face is considered to lie on the conic surface when the absolute value of the conic polynomial (3.1) at the face centroid is less than the value of this parameter. Only relevant when using a conic polynomial to define the boundary condition surface.

Type: real Default:  $10^{-6}$  Valid values: > 0

**Notes:** It is important to note that this is not a tolerance on the distance of a centroid from the conic surface, but merely a tolerance on the value of the conic polynomial. Its dimension depends on that of the coefficients in the polynomial.

Most mesh generators place nodes on a bounding surface. For non-planar surfaces, this has the consequence that face centroids will not lie exactly on the surface, making the choice of this tolerance rather significant.

### Conic\_X

**Description:** Value of the coefficient  $c_x$  in the conic polynomial (3.1).

Type: real
Default: 0.0

#### Conic\_XX

**Description:** Value of the coefficient  $c_{xx}$  in the conic polynomial (3.1).

Type: real **Default:** 0.0

#### Conic\_XY

**Description:** Value of the coefficient  $c_{xy}$  in the conic polynomial (3.1).

Type: real
Default: 0.0

#### Conic\_XZ

**Description:** Value of the coefficient  $c_{xz}$  in the conic polynomial (3.1).

Type: real
Default: 0.0

#### $Conic_Y$

**Description:** Value of the coefficient  $c_y$  in the conic polynomial (3.1).

Type: real **Default:** 0.0

## Conic\_YY

**Description:** Value of the coefficient  $c_{yy}$  in the conic polynomial (3.1).

Type: real
Default: 0.0

## Conic\_YZ

**Description:** Value of the coefficient  $c_{yz}$  in the conic polynomial (3.1).

Type: real
Default: 0.0

#### Conic\_Z

**Description:** Value of the coefficient  $c_z$  in the conic polynomial (3.1).

Type: real

Default: 0.0

### Conic\_ZZ

**Description:** Value of the coefficient  $c_{zz}$  in the conic polynomial (3.1).

Type: real
Default: 0.0

## Mesh\_Surface

**Description:** Identifier of a side set defined in the ExodusII-format mesh. Only relevant when

Surface\_Name is "from mesh file".

Type: integer

Default: none

### Node\_Disp\_Coords

**Description:** List of points that identify mesh nodes where a displacement boundary condition is applied. Up to 50 points can be specified as a list of (x, y, z) coordinates. Only relevant when Surface\_Name

is "node set".

Physical dimension: L

 $\mathbf{Type:} \ \mathrm{real}$ 

# ${\tt Surface\_Name}$

**Description:** Selects the method of specifying the mesh surface where the boundary condition will be

applied.

Type: case-insensitive string

Default: none Valid values:

Value	Associated variables
"from mesh file"	Mesh_Surface. Requires that the mesh is imported from an ExodusII-format
	mesh file.
"conic"	<pre>Conic_Tolerance, Conic_Constant, Conic_X, Conic_Y, Conic_Z, Conic_XX,</pre>
	<pre>Conic_YY, Conic_ZZ, Conic_XY, Conic_XZ, Conic_YZ</pre>
"node set"	Node_Disp_Coords

# **BODY Namelist**

### Overview

The BODY namelists define initial material distributions and conditions. The BODY namelists are processed in the order they appear, and identify the specified part of the computational domain not claimed by any preceding BODY namelist. Any "background" type BODY must be listed last.

Each namelist is used to specify a geometry and initial state. The geometry is specified via the variables using an acceptable combination of surface\_name, axis, fill, height, length, mesh\_material\_number, radius, rotation\_angle, rotation\_pt, and translation\_pt, hereafter referred to as geometry-type parameters. The initial state is specified using material\_number, velocity, phi, and temperature or temperature\_function.

#### **BODY Namelist Features**

Required/Optional: Required

Single/Multiple Instances: Multiple

## Components

- axis
- fill
- height
- length
- material\_name
- mesh\_material\_number
- phi
- radius
- rotation\_angle
- rotation\_pt
- surface\_name
- temperature
- temperature\_function
- translation\_pt
- velocity

#### axis

**Description:** The axis to be used for defining a cylinder or plane.

Type: string
Default: (none)

Valid values: 'x', 'y', 'z'

#### fill

**Description:** The side of the surface to which material is to be inserted for this body.

Type: string
Default: 'inside'

Valid values: 'inside', 'outside'

### height

**Description:** Height of a cylinder body.

Physical Dimension: L

Type: real
Default: (none)

Valid values:  $(0.0, \infty)$ 

## length

**Description:** Length of each side of the box body, or the coefficients of an ellipse or ellipsoid body.

Physical Dimension: L

Type: real triplet Default: (none) Valid values:  $(0, \infty)$ 

#### material\_name

**Description:** Name of the material, or material phase in the case of a multi-phase material, that occupies the volume of this body.

Type: string
Default: (none)

#### mesh\_material\_number

**Description:** List of material numbers (element block IDs) associated with the cells as defined in the mesh file. This parameter is only meaningful when surface\_name = 'from mesh file'.

Type: integer list (16 max)

**Default:** (none)

Valid values: Existing material numbers in mesh file (if the mesh file is in Exodus/Genesis format, this is the mesh block number).

#### phi

**Description:** Initial value of the diffusion solver's multi-component scalar field in the material body.

Physical Dimension: varies

Type: real vector of Num\_Species values

**Default:** 0.0

Valid values:  $(-\infty, \infty)$ 

#### radius

**Description:** Radius of the geometric body (cylinder, sphere, ellipsoid).

Physical Dimension: L

Type: real Default: (none) Valid values:  $(0.0, \infty)$ 

#### rotation\_angle

**Description:** Angle (degrees) about the (x, y, z) axes this body is to be rotated. This variable is only supported for 'plane' and 'cylinder' body types.

Type: real triplet Default: 0.0, 0.0, 0.0 Valid values:  $(-\infty, \infty)$ 

#### rotation\_pt

**Description:** Location of the point about which this body is to be rotated. This variable is only supported for 'plane' and 'cylinder' body types.

Physical Dimension: L

Type: real triplet Default: 0.0, 0.0, 0.0 Valid values:  $(-\infty, \infty)$ 

#### surface\_name

**Description:** Type of surface characterizing the interface topology for this body. The available options are:

- "background" A background body will occupy all space which has not been claimed by previously listed BODY namelists. If provided, it must be the final BODY namelist provided. When specified, no other geometry-type parameters are relevant.
- "plane" A plane is specified using axis, rotation\_angle, rotation\_pt, and fill to define the normal direction, and translation\_pt to provide a point on the plane surface. The normal vector is an 'outward' normal, such that the region defined is in the opposite direction of the normal vector unless fill = 'outside'.
- "box" A box is specified using translation\_pt as the center, length for the length of x, y, and z sides respectively, and fill to invert the shape. This shape does not support rotation.

"sphere" A sphere is specified using translation\_pt as the center, radius, and fill to invert the shape.

"ellipsoid" An ellipsoid of the form

$$\frac{(x-x_0)^2}{l_1^2} + \frac{(y-y_0)^2}{l_2^2} + \frac{(z-z_0)^2}{l_3^2} \le 1$$

is specified using translation\_pt as the center, length for  $l_1$ ,  $l_2$ , and  $l_3$ , and fill to invert the shape. This shape does not support rotation.

"ellipse" An infinitely long elliptic cylinder of the form

$$\frac{(x-x_0)^2}{l_1^2} + \frac{(y-y_0)^2}{l_2^2} \le 1$$

is specified using translation\_pt as the center, length for  $l_1$  and  $l_2$ ,, and fill to invert the shape. This shape does not support rotation, and will be aligned with the z axis.

"cylinder" A cylinder is specified using translation\_pt as the center of the base, axis, rotation\_angle, and rotation\_pt to define the orientation, radius, height, and fill to invert the shape.

"from mesh file" This option is used to specify cells associated with element blocks in the input mesh file. mesh\_material\_number is used to list the desired element blocks. fill may be used to invert the selection.

Type: string
Default: (none)

### temperature

**Description:** Initial constant temperature of the material body.

Physical dimension:  $\Theta$ 

Type: real

Default: none

Note: Either temperature or temperature\_function must specified, but not both.

## temperature\_function

**Description:** The name of a FUNCTION namelist that defines the initial temperature function for the material body. That function is expected to be a function of (x, y, z).

Type: string
Default: none

Note: Either temperature\_function or temperature must specified, but not both.

## translation\_pt

**Description:** Location to which each surface origin of this body is translated.

Physical Dimension: L

Type: real triplet Default: 0.0, 0.0, 0.0 Valid values:  $(-\infty, \infty)$ 

# velocity

**Description:** Initial velocity of the material body.

Physical Dimension: L/T

Type: real triplet Default: 0.0, 0.0, 0.0 Valid values:  $(-\infty, \infty)$ 

# DIFFUSION\_SOLVER Namelist

#### Overview

The DIFFUSION\_SOLVER namelist sets the parameters that are specific to the heat and species transport solver. The namelist is read when either of the PHYSICS namelist options Heat\_Transport or Species\_Transport are enabled.

The solver has two time integration methods which are selected by the variable Stepping\_Method. The default is a variable step-size, implicit second-order BDF2 method that controls the local truncation error of each step to a user-defined tolerance by adaptively adjusting the step size. The step size is chosen so that an a priori estimate of the error will be within tolerance, and steps are rejected when the actual error is too large. A failed step may be retried with successively smaller step sizes.

The other integration method is a non-adaptive, implicit first-order BDF1 method specifically designed to handle the exceptional difficulties that arise when heat transfer is coupled to a fluid flow system that includes void. In this context the heat transfer domain changes from one step to the next because of the moving void region, and mesh cells may only be partially filled with material. For this method the time step is controlled by flow or other physics models.

Both methods share a common nonlinear solver and preconditioning options.

The initial step size and upper and lower bounds for the step size are set in the NUMERICS namelist. In addition, the step size selected by the adaptive solver may be further limited by other physics models or by the NUMERICS variables Dt\_Grow and Dt\_Constant. When only diffusion solver physics are enabled, it is important that these variables be set appropriately so as not to unnecessarily impede the normal functioning of the diffusion solver.

## DIFFUSION\_SOLVER Namelist Features

Required/Optional Required when heat transport and/or species transport physics is enabled. Single/Multiple Instances Single

## Components

- Abs\_Conc\_Tol
- Abs Enthalpy Tol
- Abs\_Temp\_Tol
- Cond\_Vfrac\_Threshold
- Hypre\_AMG\_Debug
- Hypre\_AMG\_Logging\_Level
- Hypre\_AMG\_Print\_Level

- Max\_NLK\_Itr
- Max\_NLK\_Vec
- Max\_Step\_Tries
- NLK\_Preconditioner
- NLK\_Tol
- NLK\_Vec\_Tol
- PC\_AMG\_Cycles
- PC\_SSOR\_Relax
- PC\_SSOR\_Sweeps
- Rel\_Conc\_Tol
- Rel\_Enthalpy\_Tol
- Rel\_Temp\_Tol
- Residual\_Atol
- Residual\_Rtol
- Stepping\_Method
- Verbose\_Stepping
- Void\_Temperature

## Abs\_Conc\_Tol

**Description:** The tolerance  $\epsilon$  for the absolute error component of the concentration error norm used by the BDF2 integrator. If  $\delta \mathbf{c}$  is a concentration field increment with reference concentration field  $\mathbf{c}$ , then this error norm is

$$|||\delta \mathbf{c}||| \equiv \max_{j} |\delta c_{j}|/(\epsilon + \eta |c_{j}|).$$

The relative error tolerance  $\eta$  is given by Rel\_Conc\_Tol. This variable is only relevant to the adaptive integrator and to diffusion systems that include concentration as a dependent variable.

Physical dimension: same as the 'concentration' variable

Type: real
Default: none
Valid values: > 0

**Notes:** The error norm is dimensionless and normalized. The BDF2 integrator will accept time steps where the estimated truncation error is less than 2, and chooses the next suggested time step so that its prediction of the next truncation error is  $\frac{1}{2}$ .

For  $c_j$  sufficiently small the norm approximates an absolute norm with tolerance  $\epsilon$ , and for  $c_j$  sufficiently large the norm approximates a relative norm with tolerance  $\eta$ . If  $\epsilon = 0$  then the norm is a pure relative norm and the concentration must be bounded away from 0.

The same tolerance is used for all concentration components.

### Abs\_Enthalpy\_Tol

**Description:** The tolerance  $\epsilon$  for the absolute error component of the enthalpy error norm used by the BDF2 integrator. If  $\delta \mathbf{H}$  is a enthalpy field increment with reference enthalpy field  $\mathbf{H}$ , then this error norm is

$$|||\delta \mathbf{H}||| \equiv \max_{j} |\delta H_{j}|/(\epsilon + \eta |H_{j}|).$$

The relative error tolerance  $\eta$  is given by Rel\_Enthalpy\_Tol. This variable is only relevant to the adaptive integrator and to diffusion systems that include enthalpy as a dependent variable.

Physical dimension:  $E/(\Theta L^3)$ 

Type: real Default: none Valid values:  $\geq 0$ 

**Notes:** The error norm is dimensionless and normalized. The BDF2 integrator will accept time steps where the estimated truncation error is less than 2, and chooses the next suggested time step so that its prediction of the next truncation error is  $\frac{1}{2}$ .

For  $H_j$  sufficiently small the norm approximates an absolute norm with tolerance  $\epsilon$ , and for  $H_j$  sufficiently large the norm approximates a relative norm with tolerance  $\eta$ . If  $\epsilon = 0$  then the norm is a pure relative norm and the enthalpy must be bounded away from 0.

## Abs\_Temp\_Tol

**Description:** The tolerance  $\epsilon$  for the absolute error component of the temperature error norm used by the BDF2 integrator. If  $\delta \mathbf{T}$  is a temperature field increment with reference temperature field  $\mathbf{T}$ , then this error norm is

$$|||\delta \mathbf{T}||| \equiv \max_{j} |\delta T_{j}|/(\epsilon + \eta |T_{j}|).$$

The relative error tolerance  $\eta$  is given by Rel\_Temp\_Tol. This variable is only relevant to the adaptive integrator and to diffusion systems that include temperature as a dependent variable.

Physical dimension:  $\Theta$ 

Type: real
Default: none
Valid values: ≥ 0

**Notes:** The error norm is dimensionless and normalized. The BDF2 integrator will accept time steps where the estimated truncation error is less than 2, and chooses the next suggested time step so that its prediction of the next truncation error is  $\frac{1}{2}$ .

For  $c_j$  sufficiently small the norm approximates an absolute norm with tolerance  $\epsilon$ , and for  $c_j$  sufficiently large the norm approximates a relative norm with tolerance  $\eta$ . If  $\epsilon = 0$  then the norm is a pure relative norm and the temperature must be bounded away from 0.

## Cond\_Vfrac\_Threshold

**Description:** Material volume fraction threshold for inclusion in heat conduction when using the non-adaptive integrator.

Type: real Default: 0.001

Valid values: (0,1)

Note: Fluid flow systems that include void will result in partially filled cells, often times with only a tiny fragment of material. Including such cells in the heat conduction problem can cause severe numerical difficulties. By excluding cells with a material volume fraction less than this threshold from participation in heat conduction we can obtain a much better conditioned system. Note that we continue to track enthalpy for such cells, including enthalpy that may be advected into or out of the cell; we just do not consider diffusive transport of enthalpy.

### Hypre\_AMG\_Debug

**Description:** Enable debugging output from Hypre's BoomerAMG solver. Only relevant when

NLK\_Preconditioner is set to 'Hypre\_AMG'.

Type: logical

Default: .false. (off)

Note: See HYPRE\_BoomerAMGSetDebugFlag in the Hypre Reference Manual.

## Hypre\_AMG\_Logging\_Level

**Description:** Enable additional diagnostic computation by Hypre's BoomerAMG solver. Only relevant when NLK\_Preconditioner is set to 'Hypre\_AMG'.

Type: integer

Default: 0 (none)

Valid values: 0, none; > 0, varying amounts. Refer to the Hypre Reference Manual description of

HYPRE\_BoomerAMGSetLogging for details.

## Hypre\_AMG\_Print\_Level

**Description:** The diagnostic output verbosity level of Hypre's BoomerAMG solver. Only relevant when NLK\_Preconditioner is set to 'Hypre\_AMG'.

Type: integer Default: 0 Valid values:

0	no output
1	write setup information
2	write solve information
3	write both setup and solve information

See HYPRE\_BoomerAMGSetPrintLevel in the Hypre Reference Manual.

## Max\_NLK\_Itr

**Description:** The maximum number of NLK nonlinear solver iterations allowed.

Type: integer Default: 5

Valid values:  $\geq 2$ 

**Notes:** This variable is used by both the adaptive and non-adaptive integrators, though the appropriate values differ significantly.

For the adaptive integrator, the failure of a nonlinear iteration to converge *is not* necessarily fatal; the BDF2 integration procedure expects that this will occur, using it as an indication that the preconditioner for the nonlinear system needs to be updated. If still unsuccessful, the step may be retried with a halved time step size, perhaps repeatedly. Therefore it is important that the maximum number of iterations not be set too high, as this merely delays the recognition that some recovery strategy needs to be taken, and can result in much wasted effort.

By contrast, a nonlinear solver convergence failure *is* fatal for the non-adaptive solver. Thus the maximum number of iterations should be set to some suitably large value; if the number of iterations ever exceeds this value the simulation is terminated.

The default value is appropriate for the adaptive integrator.

### Max NLK Vec

**Description:** The maximum number of acceleration vectors to use in the NLK nonlinear solver.

Type: integer

**Default:**  $Max_NLK_Itr - 1$ 

Valid values: > 0

Notes: The acceleration vectors are derived from the difference of successive nonlinear function iterates accumulated over the course of a nonlinear solve. Thus the maximum possible number of acceleration vectors available is one less than the maximum number of NLK iterations, and so specifying a larger number merely wastes memory. If a large number of NLK iterations is allowed (as when using the non-adaptive integrator) then it may be appropriate to use a smaller value for this parameter, otherwise the default value is fine.

### Max\_Step\_Tries

**Description:** The maximum number of attempts to successfully take a time step before giving up. The step size is reduced between each try. This is only relevant to the adaptive solver.

Type: integer
Default: 10
Valid values: > 1

**Notes:** If other physics is enabled then this variable is effectively assigned the value 1, overriding the input value. This is required for compatibility with the other physics solvers which currently have no way of recovering from a failed step.

#### NLK Preconditioner

**Description:** The choice of preconditioner for the NLK iteration. There are currently two preconditioners to choose from: SSOR and HYPRE\_AMG. The former is symmetric over relaxation, and the later is an algebraic multigrid preconditioner from the *hypre* library.

Type: string
Default: 'SSOR'

Valid values: 'SSOR' or 'Hypre\_AMG'

Notes: If SSOR is the chosen as the preconditioner, the user can set PC\_SSOR\_Relax to the over relaxation parameter and PC\_SSOR\_Sweeps to the number of SSOR sweeps. If Hypre\_AMG is the chosen as the preconditioner, the user can set PC\_AMG\_Cycles to the number of AMG cycles per preconditioning step.

### NLK\_Tol

**Description:** The convergence tolerance for the NLK nonlinear solver. The nonlinear system is considered solved by the current iterate if the BDF2 integrator norm of the last solution correction is less than this value. This variable is only relevant to the adaptive integrator.

Type: real
Default: 0.1

Valid values: (0,1)

Notes: This tolerance is relative to the dimensionless and normalized BDF2 integrator norm; see Abs\_Conc\_Tol, for example. The nonlinear system only needs to be solved to an accuracy equal to the acceptable local truncation error for the step, which is roughly 1. Solving to a greater accuracy is wasted effort. Using a tolerance in the range (0.01,0.1) is generally adequate to ensure a sufficently converged nonlinear iterate.

### NLK\_Vec\_Tol

**Description:** The NLK vector drop tolerance. When assembling the acceleration subspace vector by vector, a vector is dropped when the sine of the angle between the vector and the subspace less than this value.

Type: real
Default: 0.001
Valid values: > 0

### PC\_AMG\_Cycles

**Description:** The number of V-cycles to take per preconditioning step of the nonlinear iteration.

Physical Dimension: dimensionless

Type: integer
Default: 1

Valid values:  $\geq 1$ 

**Notes:** We use standard V(1,1) cycles. Parameters other than the number of V cycles cannot be controlled by the user.

### PC\_SSOR\_Relax

**Description:** The relaxation parameter used in the SSOR preconditioning of the nonlinear system.

Physical Dimension: dimensionless

Type: real
Default: 1.4
Valid values: (

Valid values: (0,2)

Notes: A value less than 1 gives under-relaxation and a value greater than 1 over-relaxation.

### PC\_SSOR\_Sweeps

**Description:** The number of sweeps used in the SSOR preconditioning of the nonlinear system.

Type: integer Default: 4

Valid values:  $\geq 1$ 

Notes: The effectiveness of the SSOR preconditioner (measured by the convergence rate of the nonlinear iteration) improves as the number of sweeps increases, though at increasing cost. For especially large systems where the effectiveness of SSOR deteriorates, a somewhat larger value than the default 4 sweeps may be required. Using fewer than 4 sweeps is generally not recommended.

### Rel\_Conc\_Tol

**Description:** The tolerance  $\eta$  for the relative error component of the concentration error norm used by the BDF2 integrator. If  $\delta \mathbf{c}$  is a concentration field increment with reference concentration field  $\mathbf{c}$ , then this error norm is

$$|||\delta \mathbf{c}||| \equiv \max_{j} |\delta c_{j}|/(\epsilon + \eta |c_{j}|).$$

The absolute error tolerance  $\epsilon$  is given by Abs\_Conc\_Tol. This variable is only relevant to the adaptive solver and to diffusion systems that include concentration as a dependent variable.

Physical Dimension: dimensionless

Type: real
Default: 0.0
Valid values: [0,1)

Notes: See the notes for Abs\_Conc\_Tol.

### Rel\_Enthalpy\_Tol

**Description:** The tolerance  $\eta$  for the relative error component of the enthalpy error norm used by the BDF2 integrator. If  $\delta \mathbf{c}$  is a enthalpy field increment with reference enthalpy field  $\mathbf{H}$ , then this error norm is

$$|||\delta \mathbf{H}||| \equiv \max_{j} |\delta H_{j}|/(\epsilon + \eta |H_{j}|).$$

The absolute error tolerance  $\epsilon$  is given by Abs\_Enthalpy\_Tol. This variable is only relevant to the adaptive solver and to diffusion systems that include enthalpy as a dependent variable.

Physical Dimension: dimensionless

Type: real
Default: 0.0
Valid values: [0,1)

Notes: See the notes for Abs\_Enthalpy\_Tol.

### Rel\_Temp\_Tol

**Description:** The tolerance  $\eta$  for the relative error component of the temperature error norm used by the BDF2 integrator. If  $\delta \mathbf{T}$  is a temperature field increment with reference temperature field  $\mathbf{T}$ , then this error norm is

$$|||\delta \mathbf{T}||| \equiv \max_{j} |\delta T_{j}|/(\epsilon + \eta |T_{j}|).$$

The absolute error tolerance  $\epsilon$  is given by Abs\_Temp\_Tol. This variable is only relevant to the adaptive solver and to diffusion systems that include temperature as a dependent variable.

Physical Dimension: dimensionless

Type: real
Default: 0.0

Valid values: [0,1)

Notes: See the notes for Abs\_Temp\_Tol.

### Residual\_Atol

**Description:** The absolute residual tolerance  $\epsilon_1$  used by the iterative nonlinear solver of the non-adaptive integrator. If  $r_0$  denotes the initial nonlinear residual, iteration stops when the current residual r satisfies  $||r||_2 \le \max\{\epsilon_1, \epsilon_2 ||r_0||_2\}$ .

Type: real Default: 0

Valid values:  $\geq 0$ 

Note: Ideally this tolerance should be set to 0, but in some circumstances, especially at the start of a simulation, the initial residual may be so small that it is impossible to reduce it by the factor  $\epsilon_2$  due to finite precision arithmetic. In such cases it is necessary to provide this absolute tolerance. It is impossible, however, to say what a suitable value would be, as this depends on the nature of the particular nonlinear system. Some guidance can be obtained through trial-and-error by enabling Verbose\_Stepping and observing the magnitude of the residual norms in the resulting diagnostic output file.

### Residual\_Rtol

**Description:** The relative residual tolerance  $\epsilon_2$  used by the iterative nonlinear solver of the non-adaptive integrator. If  $r_0$  denotes the initial nonlinear residual, iteration stops when the current residual r satisfies  $||r||_2 < \max\{\epsilon_1, \epsilon_2 ||r_0||_2\}$ .

Type: real
Default: none
Valid values: (0,1)

# Stepping\_Method

**Description:** The choice of time integration method.

Type: string

Default: 'Adaptive BDF2'

Valid values: 'Adaptive BDF2' or 'Non-adaptive BDF1'

**Note:** The non-adaptive integrator must be selected when fluid flow is enabled and void material is present. Otherwise use the default adaptive integrator.

# Verbose\_Stepping

**Description:** A flag that enables the output of detailed BDF2 time stepping information. The human-readable information is written to a file with the suffix .bdf2.out in the output directory.

Type: logical Default: .false.

# Void\_Temperature

**Description:** An arbitrary temperature assigned to cells that contain only the void material. The value has no effect on the simulation, and is only significant to visualization.

Type: real Default: 0

# DS\_SOURCE Namelist

The DS\_SOURCE namelist is used to define external volumetric sources for species transport model.

### Overview

### DS\_SOURCE Namelist Features

Required/Optional: Optional

Single/Multiple Instances: Multiple

# Components

• Equation

• Cell\_Set\_IDs

• Source\_Constant

• Source\_Function

### Equation

**Description:** The name of the equation this source applies to.

Type: string
Default: none

Valid values: "concentration1", "concentration2", ...

**Note:** Any name may be specified, but Truchas will only look for and use DS\_SOURCE namelists with the indicated equation names; any others are silently ignored.

### Cell\_Set\_IDs

**Description:** A list of cell set IDs that define the subdomain where the source is applied.

**Type:** a list of up to 32 integers

Default: none

Valid values: any valid mesh cell set ID

**Note:** Different instances of this namelist with a given **Equation** value must apply to disjoint subdomains; overlapping of source functions is not allowed.

Exodus II mesh element blocks are interpreted by Truchas as cell sets having the same IDs.

# Source\_Constant

**Description:** The constant value of the source function.

Type: real
Default: none

Note: Either Source\_Constant or Source\_Function must be specified, but not both.

# Source\_Function

**Description:** The name of a FUNCTION namelist that defines the source function. That function is

expected to be a function of (t, x, y, z).

Type: string
Default: none

Note: Either Source\_Function or Source\_Constant or must be specified, but not both.

# **ELECTROMAGNETICS Namelist**

### Overview

The ELECTROMAGNETICS namelist sets most of the parameters used by the electromagnetic (EM) solver to calculate the Joule heat used in induction heating simulations. Exceptions are the electrical conductivity, electric susceptibility, and magnetic susceptibility which are defined for each material phase using the MATERIAL namelist, and the induction coils hat produce an external magnetic source field, which are specified in INDUCTION\_COIL namelists. The EM calculations are performed on a tetrahedral mesh specified by the ALTMESH namelist, which is generally different than the main mesh used throughout the rest of Truchas.

A Remark on Units: The EM solver assumes SI units by default. In particular, the result of the Joule heat calculation is a *power density*—W/m<sup>3</sup> in SI units. To use a different system of units, the user must supply appropriate values for the free-space constants Vacuum\_Permittivity and Vacuum\_Permeability. In any case, the user must ensure that a consistent set of units is used throughout Truchas.

### **ELECTROMAGNETICS Namelist Features**

Required/Optional: Optional Single/Multiple Instances: Single

### Components

- CG\_Stopping\_Tolerance
- EM\_Domain\_Type
- Graphics\_Output
- Material\_Change\_Threshold
- Maximum\_CG\_Iterations
- Maximum\_Source\_Cycles
- Num\_Etasq
- Output\_Level
- Source\_Frequency
- Source\_Times
- SS\_Stopping\_Tolerance
- Steps\_Per\_Cycle
- Symmetry\_Axis
- Uniform\_Source

### CG\_Stopping\_Tolerance

**Description:** Tolerance used to determine when the conjugate gradient (CG) iteration has converged. The criterion used is that  $\|\mathbf{r}\|/\|\mathbf{r}_0\| < \mathtt{CG\_Stopping\_Tolerance}$ . The electromagnetics solver uses its own special preconditioned CG linear solver.

Type: real Default:  $10^{-5}$  Valid values: (0, 0.1)

**Notes:** The numerical characteristics of the electromagnetic system require that the linear systems be solved to significantly greater accuracy than would otherwise be required. Too loose a tolerance will manifest itself in a significant build-up of noise in the solution of the electric field over the course of the simulation. This input variable should not be greater than  $10^{-4}$ .

### EM\_Domain\_Type

**Description:** A flag specifying the type of domain geometry that is discretized by the computational mesh

Type: string
Default: none

Valid values: 'Full\_Cylinder', 'Half\_Cylinder', 'Quarter\_Cylinder'

**Notes:** At this time there is not yet a facility for specifying general boundary conditions for the electromagnetic simulation. Consequently, the computational domain  $\Omega$  is limited to the following special cases when Symmetry\_Axis='z':

```
'Full_Cylinder': \Omega = \{(x,y,z) \mid x^2 + y^2 \le r^2, \; z_1 \le z \le z_2\} 'Half_Cylinder': \Omega = \{(x,y,z) \mid x^2 + y^2 \le r^2, \; x \ge 0, \; z_1 \le z \le z_2\} 'Quarter_Cylinder': \Omega = \{(x,y,z) \mid x^2 + y^2 \le r^2, \; x,y \ge 0, \; z_1 \le z \le z_2\}
```

The values r > 0,  $z_1 < z_2$  are inferred from the mesh and are not specified directly. Dirichlet source field conditions are imposed on the boundaries  $\{x^2 + y^2 = r^2\}$  and  $\{z = z_1, z_2\}$ , and symmetry conditions on the symmetry planes  $\{x = 0\}$  and  $\{y = 0\}$  if present. See the User Manual for more details.

The analogous definitions for the other possible symmetry axes, 'x' and 'y', are obtained by the appropriate cyclic permutation of the coordinates.

For the computational mesh used in the EM simulation, see the ALTMESH namelist.

**Experimental Features**. The value 'Frustum' specifies that the domain is a frustum of a right cone

$$\Omega = \{(x, y, z) \mid x^2 + y^2 \le m^2 (z - z_0)^2, \ z_1 \le z \le z_2\}$$

or an angular wedge of a frustum. As with the other domain types the values m>0,  $z_0$  and  $z_1< z_2$  are inferred from the mesh and are not specified directly. For wedges of a frustum, the wedge sides can lie on any plane from the family of 30 degree increment planes that includes the x=0 plane. The preceding description is for the z-axis symmetry case, but the analogous functionality for the other symmetry axes is also provided.

# Graphics\_Output

**Description:** Controls the graphics output of the electromagnetic solver.

Type: logical Default: .false.

Valid values: .true.or .false.

Notes: If .true., the electromagnetic solver will generate its own graphics data files in OpenDX format (see http://www.opendx.org). The files contain the material parameter fields, the averaged Joule heat field, and the time series of the electromagnetic fields. The files are identified by the suffixes -EM.dx and -EM.bin. The value of Graphics\_Output has no impact on the normal graphics output generated by Truchas, which is determined elsewhere, and the averaged Joule heat field used in heat transport will be output there in either case.

### Material\_Change\_Threshold

**Description:** Controls, at each step, whether the Joule heat is recalculated in response to temperature-induced changes in the EM material parameter values. The Joule heat is recalculated whenever the difference between the current parameter values and those when the Joule heat was last computed exceeds this threshold value. Otherwise the previously calculated Joule heat is used. The maximum relative change is used as the difference measure.

Type: real Default: 0.3

Valid values:  $(0.0, \infty)$ 

Notes: The electric conductivity and magnetic permeability are the only values whose changes are monitored. The electric permittivity only enters the equations through the displacement current term, which is exceedingly small in this quasi-magnetostatic regime and could be dropped entirely. Thus the Joule heat is essentially independent of the permittivity and so any changes in its value are ignored.

For electric conductivity, only the conducting region (where the value is positive) is considered when computing the difference. An underlying assumption is that this region remains fixed throughout the simulation.

### Maximum\_CG\_Iterations

**Description:** Maximum number of conjugate gradient (CG) iterations allowed. The electromagnetics solver uses its own special preconditioned CG linear solver.

Type: integer Default: 500

Valid values:  $(0.0, \infty)$ 

### Maximum\_Source\_Cycles

**Description:** The electromagnetic field equations are integrated in time toward a periodic steady state. This input variable specifies the time limit, measured in cycles of the sinusoidal source field, for the Joule heat calculation.

Type: integer Default: 10

Valid values:  $(0.0, \infty)$ 

Notes: To avoid ringing, the amplitude of the external source field is ramped and is not at full strength until after approximately two cycles have passed. Consequently this input variable should not normally be < 3. Convergence to a periodic steady state is usually attained within 5 cycles; see <pre>SS\_Stopping\_Tolerance. If convergence is not attained within the limit allowed by this input variable, the last result is returned and a warning issued, but execution continues with the rest of the physics simulation.

The electromagnetic field equations are solved on an *inner* time distinct from that of the rest of the physics; see SS\_Stopping\_Tolerance.

### Num\_Etasq

**Description:** This value is used for the displacement current coefficient  $\eta^2$ , in the low-frequency, nondimensional scaling of Maxwell's equations, when its value exceeds the physical value.

Physical dimension: dimensionless

Type: real Default: 0

Valid values:  $(0.0, \infty)$ 

Notes: The quasi-magnetostatic regime is characterized by  $\eta^2 \ll 1$ . Since this value can become exceedingly small (resulting in a difficult-to-solve, ill-conditioned system), it may be helpful to use a numerical value instead, say  $\eta^2 = 10^{-6}$  or  $10^{-8}$ , without having any discernable effect on the solution. However, it is generally safe to ignore this variable and let the solver use the physical value. See the *Truchas Physics and Algorithms* for more details.

### Output\_Level

**Description:** Controls the verbosity of the electromagnetic solver

Type: integer Default: 1

Valid values: 1, 2, 3 or 4

Notes: At the default level, 1, a status message is output at the end of each source field cycle showing the progress toward steady state. Level 2 adds a summary of the CG iteration for each time step. Level 3 adds the norm of the difference between the solution and extrapolated predictor for each time step. This gives an indication of the (time) truncation error, and if noise is accumulating in the system it will be seen here; see CG\_Stopping\_Tolerance. Level 4 adds convergence info for each CG iterate. Levels 1 and 2 are typical.

# Source\_Frequency

**Description:** Frequency f (cycles per unit time) of the sinusoidally-varying magnetic source fields that drive the Joule heat calculation.

Physical dimension:  $\mathsf{T}^{-1}$ 

Type: real

Default: none

Valid values: Any single positive value, or any sequence of positive values.

**Notes:** A sequence of up to 32 values may be assigned to this variable in order to specify a time-dependent frequency; see Source\_Times and Fig. 7.1.

The source fields are due to induction coils specified through INDUCTION\_COIL namelists, and a spatially uniform source field specified by Uniform\_Source. All operate at the common frequency specified by this variable, and a common phase. The phase value is irrelevant due to the time averaging of the calculated Joule heat.

The Joule heat calculation is coupled to the rest of the physics in a manner that assumes the time scale of the electromagnetic fields,  $f^{-1}$  is  $much\ smaller$  than the time scale of the other physics (as defined by the characteristic time step). Consequently, the frequency f must not be too small.

### Source\_Times

**Description:** A sequence of times that define the time partition of the piecewise-constant functional form used in the case of time-dependent source field parameters.

Physical dimension: T

Type: real

Default: none

Valid values: Any strictly increasing sequence of values.

**Notes:** If this variable is not specified, then the source field parameters are assumed to be constant in time, with a single value assigned to Source\_Frequency, Uniform\_Source, and each Current variable in any INDUCTION\_COIL namelists. Otherwise, if n values are assigned to Source\_Times, then n+1 values must be assigned to each of those variables. See Fig. 7.1 for a description of the functional form described by these values.

At most 31 values may be specified for this variable.

### SS\_Stopping\_Tolerance

**Description:** The electromagnetic field equations are integrated in time toward a periodic steady state. Convergence to this steady state is measured by comparing the computed Joule heat field averaged over the last source field cycle,  $q_{\rm last}$ , with the result from the previous cycle,  $q_{\rm prev}$ . When  $\|q_{\rm last} - q_{\rm prev}\|_{\rm max}/\|q_{\rm last}\|_{\rm max} < {\tt SS\_Stopping\_Tolerance}$ , the Joule heat calculation is considered converged and  $q_{\rm last}$  returned.

Type: real **Default:**  $10^{-2}$ 

Valid values:  $(0.0, \infty)$ 

**Notes:** Depending on the accuracy of the other physics,  $10^{-2}$  or  $10^{-3}$  are adequate values. If the value is taken too small (approaching machine epsilon) convergence cannot be attained.

It is assumed that the time scale of the electromagnetic fields is *much shorter* than the time scale of the other physics; see Source\_Frequency. In this case it suffices to solve the electromagnetic field equations to a periodic steady state, while temporarily freezing the other physics, and averaging the rapid temporal variation in the Joule heat field over a cycle. In effect, the electromagnetic field equations are solved over an *inner* time distinct from that of the rest of the physics.

# Steps\_Per\_Cycle

**Description:** The number of time steps per cycle of the external source field used to integrate the electromagnetic field equations

Type: integer Default: 20

Valid values:  $(0.0, \infty)$ 

**Notes:** Increasing the number of time steps per cycle increases the accuracy of the Joule heat calculation, while generally increasing the execution time. A reasonable range of values is [10, 40]; anything less than 10 is *severely* discouraged.

The electromagnetic field equations are solved on an *inner* time distinct from that of the rest of the physics; see SS\_Stopping\_Tolerance.

### Symmetry\_Axis

**Description:** A flag that specifies which axis is to be used as the problem symmetry axis for the Joule heat simulation.

Type: string
Default: 'z'
Valid values: { 'x', 'y', 'z' }

Notes: The value of this variable determines the orientation of the uniform magnetic source field specified by Uniform\_Source, and the coils specified by the INDUCTION\_COIL namelists, if any. It also determines the assumed orientation of the computational domain; see EM\_Domain\_Type.

### Uniform\_Source

**Description:** Amplitude of a sinusoidally-varying, uniform magnetic source field that drives the Joule heat computation. The field is directed along the problem symmetry axis as specified by Symmetry\_Axis.

Physical dimension: I/L

Type: real Default: 0

Valid values: Any single value, or any sequence of values.

**Notes:** A sequence of up to 32 values may be assigned to this variable in order to specify a time-dependent amplitude; see **Source\_Times** and Fig. 7.1. If this variable is not specified, its value or values, as appropriate, are assumed to be zero.

The total external magnetic source field that drives the Joule heat computation will be the superposition of this field and the fields due to the coils specified in the INDUCTION\_COIL namelists, if any.

For reference, the magnitude of the magnetic field within an infinitely-long, finely-wound coil with current density I is simply I. The field magnitude at the center of a circular current loop of radius r with current I is I/2r. In both cases the field is directed along the axis of the coil/loop.

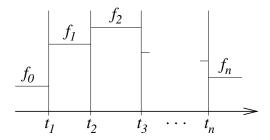


Figure 7.1: Piecewise constant function form showing the constant values  $f_0, f_1, \ldots, f_n$  in relation to the time partition  $t_1, t_2, \ldots, t_n$ .

# ENCLOSURE\_RADIATION Namelist

### Overview

### ENCLOSURE\_RADIATION Namelist Features

Required/Optional: Optional

Single/Multiple Instances: Multiple, one for each enclosure.

# Components

• Name

- Enclosure\_File
- Coord\_Scale\_Factor
- Skip\_Geometry\_Check
- Ambient\_Constant
- Ambient\_Function
- Error\_Tolerance
- Precon\_Method
- Precon\_Iter
- Precon\_Coupling\_Method
- toolpath

#### Name

**Description:** A unique name for this enclosure radiation system.

Type: string (31 characters max)

Default: none

### Enclosure\_File

**Description:** The path to the enclosure file. This is interpreted relative to the Truchas input file unless this is an absolute path. If operating in moving enclosure mode (see **toolpath**) the file name is the base name for a collection of enclosure files.

Type: string (255 characters max)

Default: none

Notes: The genre program from the RADE tool suite can be used to generate this file.

### Coord\_Scale\_Factor

Description: An optional factor with which to scale the node coordinates of the enclosure surface.

Type: real
Default: 1.0

Valid values: > 0.0

Notes: The faces of the enclosure surface must match faces from the Truchas mesh. If the coordinates of the mesh are being scaled, it is likely that the same scaling needs to be applied to the enclosure

surface.

### Ambient\_Constant

**Description:** The constant value of the ambient environment temperature.

Physical dimension:  $\Theta$ 

Type: real

Default: none

Valid values: ≥ Absolute\_Zero

Notes: Either Ambient\_Constant or Ambient\_Function must be specified, but not both. Currently this is necessary even for full enclosures, although in that case the value will not be used and any value is

acceptable.

### Ambient\_Function

**Description:** The name of a FUNCTION namelist that defines the ambient environment temperature function. That function is expected to be a function of t alone.

Type: string
Default: none
Valid values:

Notes: Either Ambient\_Function or Ambient\_Constant must be specified, but not both. Currently this is necessary even for full enclosures, although in that case the value will not be used and any

constant value is acceptable.

### Error\_Tolerance

**Description:** The error tolerance  $\epsilon$  for the iterative solution of the linear radiosity system Aq = b. Iteration stops when the approximate radiosity q satisfies  $||b - Aq||_2 < \epsilon ||b||_2$ .

Type: real

Default: 1.0e-3
Valid values: > 0

**Notes:** The Chebyshev iterative method is used when solving the radiosity system in isolation with given surface temperatures. However the usual case has the radiosity system as just one component of a larger nonlinear system that is solved by a Newton-like iteration, and this condition on the radiosity component is one necessary condition of the complete stopping criterion of the iteration.

### toolpath

**Description:** The name of a TOOLPATH namelist that defines a time-dependent motion that has been suitably partitioned. If this variable is specified it enables the moving enclosure mode of operation. This works in concert with the genre program.

### Precon\_Method (Expert Parameter)

**Description:** Preconditioning method for the radiosity system. Use the default.

Type: string
Default: "jacobi"

Valid values: "jacobi", "chebyshev"

**Notes:** The preconditioner for the fully-coupled heat transfer/enclosure radiation system NLK solver is built from smaller preconditioning pieces, one of which is a preconditioner for the radiosity system alone. The least costly and seemingly most effective is Jacobi.

### Precon\_Iter (Expert Parameter)

**Description:** The number of iterations of the Precon\_Method method to apply as the radiosity system preconditioner. *Use the default*.

Type: integer Default: 1

Valid values:  $\geq 1$ 

# Precon\_Coupling\_Method (Expert Parameter)

**Description:** Method for coupling the radiosity and heat transfer system preconditioners. Use the default.

Type: string

Default: "backward GS"

Valid values: "jacobi", "forward GS", "backward GS", "factorization"

Notes: There are several methods for combining the independent preconditionings of the radiosity system and heat transfer system to obtain a preconditioner for the fully-coupled system. If we view it as a block system with the radiosity system coming first, the first three methods correspond to block Jacobi, forward block Gauss-Seidel, and backward Gauss-Seidel updates. The factorization method is an approximate Schur complement update, that looks like block forward Gauss-Seidel followed by the second half of block backward Gauss-Seidel.

# Skip\_Geometry\_Check (Expert Parameter)

**Description:** Normally the geometry of the enclosure surface faces are compared with boundary faces of the heat conduction mesh to ensure they actually match. Setting this variable to false will disable this check, which may be necessary in some unusual use cases.

Type: logical Default: .false.

# ENCLOSURE\_SURFACE Namelist

### Overview

### **ENCLOSURE\_SURFACE** Namelist Features

Required/Optional: Required when ENCLOSURE\_RADIATION namelists are active

Single/Multiple Instances: Multiple

# Components

• Name

• Enclosure\_Name

• Face\_Block\_IDs

• Emissivity\_Constant

• Emissivity\_Function

#### Name

**Description:** A unique name for this enclosure surface.

Type: string (31 characters max)

Default: none

### Enclosure\_Name

 $\textbf{Description:} \ \ \text{The name of the } \textbf{ENCLOSURE\_RADIATION} \ \ \text{namelist that defines the enclosure radiation}$ 

system to which this surface belongs.

Type: string
Default: none

### Face\_Block\_IDs

Description: A list of face block IDs that define this enclosure surface

**Type:** a list of up to 32 integers

Default: none

Valid values: any valid face block ID from the enclosure file

Notes: The surface faces in an enclosure file are divided into blocks. When the genre program from the RADE tool suite is used to create this file, these blocks are automatically generated; each block corresponds to the Exodus II mesh side set used to defined it, and the side set ID is assigned as the face block ID. In this case, then, the IDs that can be specified here will be certain side set IDs from the Truchas Exodus II mesh file.

### Emissivity\_Constant

**Description:** The constant emissivity value for this enclosure surface.

Physical dimensions: dimensionless

Type: real
Default: none

**Valid values:** (0.0, 1.0]

Notes: Either Emissivity\_Constant or Emissivity\_Function must be specified, but not both.

### Emissivity\_Function

 $\textbf{Description:} \ \ \text{The name of a $\tt FUNCTION$ namelist that defines the emissivity function. That function is}$ 

expected to be a function of (t, x, y, z).

Type: string
Default: none

Notes: Either Emissivity\_Function or Emissivity\_Constant must be specified, but not both.

# EVAPORATION Namelist (Experimental)

### Overview

This namelist defines a special heat flux boundary condition that models heat loss due to the evaporation of material. Its intended use is in the simulation of additive manufacturing or welding processes where the laser heat source can produce localized surface temperatures approaching and exceeding the boiling temperature. The form of the heat flux is an Arrhenius-type function

$$f(T) = AT^{\beta} e^{-E_a/RT},\tag{10.1}$$

where T is temperature, R the gas constant, and A,  $\beta$ , and  $E_a$  are model parameters defined by input. When using this model, the simulation should be using Kelvin for temperature.

### **EVAPORATION Namelist Features**

Required/Optional: Optional

Single/Multiple Instances: Single

# Components

• Face\_Set\_IDs

• Prefactor

• Temp\_Exponent

• Activation\_Energy

### Face\_Set\_IDs

**Description:** A list of face set IDs that define the subset of the boundary where the evaporation boundary condition model will be imposed.

**Type:** a list of up to 32 integers

Default: none

Valid values: any valid mesh face set ID

Note: Exodus II mesh side sets are interpreted by Truchas as face sets having the same IDs.

### Prefactor

**Description:** The prefactor A.

Type: real
Default: none

# Temp\_Exponent

**Description:** The temperature exponent  $\beta$ .

Type: real
Default: none

# Activation\_Energy

**Description:** The activation energy  $E_a$ . This value must be specified in Joules per mole units, regardless

 $of \ the \ units \ used \ elsewhere \ in \ the \ simulation.$ 

Type: real

Default: none

# FLOW Namelist

### Overview

The FLOW namelist specifies the parameters for the fluid flow model and algorithm. This namelist is read whenever the PHYSICS namelist option Flow is enabled. Parameters for the linear solvers employed by the algorithm are specified using FLOW\_VISCOUS\_SOLVER and FLOW\_PRESSURE\_SOLVER namelists. Flow boundary conditions are defined using FLOW\_BC namelists.

### FLOW Namelist Features

Required/Optional: Required when flow physics is enabled.

Single/Multiple Instances: Single

# Components

### **Physics Options**

• inviscid

#### Numerical parameters

- courant\_number
- viscous\_number
- viscous\_implicitness
- track\_interfaces
- material\_priority
- vol\_track\_subcycles
- nested\_dissection (expert)
- vol\_frac\_cutoff (expert)
- fischer\_dim (expert)
- fluid\_frac\_threshold (expert)
- min\_face\_fraction (expert)
- void\_collapse (experimental)
- void\_collapse\_relaxation (experimental)

#### inviscid

**Description:** This option omits the viscous forces from the flow equations. In this case there is no viscous system to solve and the FLOW\_VISCOUS\_SOLVER namelist is not required.

Type: logical Default: .false.

### courant\_number

**Description:** This parameter sets an upper bound on the time step that is associated with stability of the explicit fluid advection algorithm. A value of 1 corresponds (roughly) to the stability limit, with smaller values resulting in proportionally smaller allowed time steps. Truchas uses the largest time step possible subject to this and other limits.

Type: real Default: 0.5

Valid values: (0.0, 1.0]

**Notes:** The Courant number for a cell is the dimensionless value  $C_i = u_i \Delta t / \Delta x_i$  where  $\Delta t$  is the time step,  $u_i$  the fluid velocity magnitude on the cell, and  $\Delta x_i$  a measure of the cell size. The time step limit is the largest  $\Delta t$  such that  $\max\{C_i\}$  equals the value of courant\_number.

The interpretation of  $u_i$  and  $\Delta x_i$  for a general cell is somewhat sticky. Currently a ratio  $u_f/h_f$  is computed for each face of a cell and the maximum taken for the value of  $u_i/\Delta x_i$ . Here  $u_f$  is the normal fluxing velocity on the face, and  $h_f$  is the inscribed cell height at the face; that is, the minimum normal distance between the face and cell nodes not belonging to the face.

### viscous\_number

**Description:** This parameter sets an upper bound on the time step that is associated with stability of an explicit treatment of viscous flow stress tensor. A value of 1 corresponds roughly to the stability limit, with smaller values resulting in proportionally smaller allowed time steps. Truchas uses the largest time step possible subject to this and other limits.

For an implicit treatment of the viscous flow stress tensor with  $viscous\_implicitness$  at least  $\frac{1}{2}$ , which is always strongly recommended, the viscous discretization is unconditionally stable and no time step limit is needed. In this case, the parameter can still be used to limit the time step for accuracy. A value of 0 will disable this limit entirely.

Type: real Default: 0

Valid values: > 0

Notes: The viscous number for a cell is the dimensionless value  $V_i = \nu_i \Delta t/\Delta x_i^2$ , where  $\Delta t$  is the time step,  $\nu_i$  the kinematic viscosity  $(\mu/\rho)$  on the cell, and  $\Delta x_i$  a measure of the cell size. The time step limit is the largest  $\Delta t$  such that  $\max\{V_i\}$  equals the value of viscous\_number. Currently the measure of cell size mirrors that used in the definition of the courant\_number, namely that  $\Delta x_i$  is taken as the minimum of the inscribed heights  $h_f$  for the faces of the cell.

### viscous\_implicitness

**Description:** The degree of time implicitness  $\theta$  used for the velocity field in the discretization of the viscous flow stress tensor in the fluid momentum conservation equation. The velocity is given by the  $\theta$ -method,  $\mathbf{u}_{\theta} = (1 - \theta)\mathbf{u}_n - \theta\mathbf{u}_{n+1}$ :  $\theta = 0$  gives an explicit discretization and  $\theta = 1$  a fully implicit discretization. In practice only the values 1,  $\frac{1}{2}$  (trapezoid method), and 0 are useful, and use of the latter explicit discretization is generally not recommended. Note that an implicit discretization,

 $\theta > 0$ , will require the solution of a linear system; see FLOW\_VISCOUS\_SOLVER. This parameter is not relevant to inviscid flow problems.

Type: real Default: 1

Valid values: [0,1]

**Notes:** The discretization is first order except for the trapezoid method  $(\theta = \frac{1}{2})$  which is second order. However note that the flow algorithm overall is only first order irrespective of the choice of  $\theta$ . The advanced velocity  $\mathbf{u}_{n+1}$  is actually the predicted velocity  $\mathbf{u}_{n+1}^{\star}$  from the predictor stage of the

flow algorithm.

### track\_interfaces

**Description:** This option enables the tracking of material interfaces. The default is to track interfaces whenever the problem involves more than one material. If the problem involves a single fluid and it is known a priori that there will never be any mixed material cells containing fluid, then this option can be set to false to short-circuit some unnecessary work, but otherwise the default should be used.

Type: logical Default: .true.

Notes:

### material\_priority

**Description:** A list of material names that defines the priority order in which material interfaces are reconstructed within a cell for volume tracking. All fluid material names must be listed, and if the problem includes any non-fluid materials, this list must include the case-sensitive keyword "SOLID", which stands for all non-fluid materials lumped together. The default is the list of fluid materials in input file order, followed by "SOLID" for the lumped non-fluids.

Type: string list

**Notes:** Different priorities will result in somewhat different results. Unfortunately there are no hard and fast rules for selecting the priorities.

### vol\_track\_subcycles

**Description:** The number of sub-time steps n taken by the volume tracker for every time step of the flow algorithm. If the flow time step size is  $\Delta t$  then the volume tracker will take n time steps of size  $\Delta t/n$  to compute the net flux volumes and advance the volume fractions for the flow step.

Type: integer Default: 2

**Notes:** With the current unsplit advection algorithm [1] it is necessary to sub-cycle the volume tracking time integration method in order to obtain good "corner coupling" of the volume flux terms.

# nested\_dissection (Expert Parameter)

**Description:** This option enables use of the nested dissection algorithm to reconstruct material interfaces in cells containing 3 or more materials. If set false the less accurate and less expensive onion skin algorithm will be used.

Type: logical Default: .true.

# vol\_frac\_cutoff (Expert Parameter)

**Description:** The smallest material volume fraction allowed. If a material volume fraction drops below this cutoff, the material is removed entirely from the cell, and its volume fraction replaced by proportional increases to the volume fractions of the remaining materials, or if the cell contains void, by increasing the void volume fraction alone.

Type: real Valid values: (0,1) Default:  $10^{-8}$ 

# fischer\_dim (Expert Parameter)

**Description:** The dimension d of the subspace used in Fischer's projection method [2] for computing an initial guess for pressure projection system based on previous solutions. Memory requirements for the method are 2(d+1) cell-based vectors. Set this variable to 0 to disable use of this method.

Type: integer Default: 6

# fluid\_frac\_threshold (Expert Parameter)

**Description:** Cells with a total fluid volume fraction less than this threshold are ignored by the flow solver, being regarded as 'solid' cells.

Type: real Valid values: (0,1) Default:  $10^{-2}$ 

# min\_face\_fraction (Expert Parameter)

**Description:** The variable sets the minimum value of the fluid density associated with a face for the pressure projection system. It is specified as a fraction of the minimum fluid density (excluding void) of any fluid in the problem.

Type: real Default:  $10^{-3}$ 

# void\_collapse (Experimental)

**Description:** The volume-of-fluid algorithm effectively treats small fragments of void entrained in fluid as incompressible, resulting in unphysical void "bubbles" that persist in the flow. A model that drives the collapse of these void fragments will be enabled when this variable is set to true. See <a href="void\_collapse\_relaxation">void\_collapse\_relaxation</a> for a model parameter.

Type: logical Default: .false.

# void\_collapse\_relaxation (Experimental)

**Description:** The relaxation parameter in the void collapse model. See void collapse.

Type: real Default: 0.1

### Valid values: [0,1]

Notes: The relaxation factor is roughly inversely proportional to the number of timesteps required for all the void in a cell to collapse as dictated by inertial forces. Thus a relaxation factor of 1 would allow for all the void in a cell to collapse over a single timestep. A factor of 0.1 would allow for the void in a cell to collapse over the course of 10 timesteps. Larger values tend to cause more mass loss (on the order of 0.5%), although the results do improve with increased subcycling.

# FLOW BC Namelist

#### Overview

The FLOW\_BC namelist is used to define boundary conditions for the fluid flow model at external boundaries. At inflow boundaries it also specifies the value of certain intensive material quantities, like temperature, that may be associated with other physics models.

Each instance of the namelist defines a particular condition to impose over a subset  $\Gamma$  of the domain boundary. The boundary subset  $\Gamma$  is specified using mesh face sets. The namelist variable <code>face\_set\_ids</code> takes a list of face set IDs, and the boundary condition is imposed on all faces belonging to those face sets. Note that ExodusII mesh sides sets are imported into Truchas as face sets with the same IDs. The following common types of boundary conditions can be defined:

- Pressure. A pressure Dirichlet condition  $p = p_b$  on  $\Gamma$  is defined by setting type to "pressure". The boundary value  $p_b$  is specified using either pressure for a constant value, or pressure\_func for a function.
- Velocity. A velocity Dirichlet condition  $\mathbf{u} = \mathbf{u}_b$  on  $\Gamma$  is defined by setting type to "velocity". The boundary value  $\mathbf{u}_b$  is specified using either velocity for a constant value, or velocity\_func for a function.
- No slip. The special velocity Dirichlet condition  $\mathbf{u} = 0$  on  $\Gamma$  is defined by setting type to "no-slip".
- Free slip. A free-slip condition where fluid is not permitted to penetrate the boundary,  $\hat{n} \cdot \mathbf{u} = 0$  on  $\Gamma$ , where  $\hat{n}$  is the unit normal to  $\Gamma$ , but is otherwise free to slide along the boundary (no tangential traction) is defined by setting type to "free-slip".
- Tangential surface tension.

These boundary condition types are mutually exclusive: namely, no two types may be defined on overlapping subsets of the boundary. Any subset of the boundary not explicitly assigned a boundary condition will be implicitly assigned a free-slip condition.

Currently it is only possible to assign boundary conditions on the external mesh boundary. However in many multiphysics applications the boundary of the fluid flow domain will not coincide with the boundary of the larger problem mesh. In some cases the boundary will coincide with an internal mesh-conforming interface that separates fluid cells and solid (non-fluid) cells, where a boundary condition could conceivably be assigned. In other cases, typically those involving phase change, the boundary is only implicit, passing through mixed fluid/solid cells, and will not conform to the mesh. In either case, the flow algorithm aims to impose an effective no-slip condition for viscous flows, or a free-slip condition for inviscid flows. A possible modeling approach in the former mesh-conforming case is to define an internal mesh interface using the MESH namelist variable interface\_side\_sets. This effectively creates new external mesh boundary where flow boundary conditions can be assigned.

### FLOW\_BC Namelist Features

Required/Optional: Optional

Single/Multiple Instances: Multiple

### Components

- name
- face\_set\_ids
- type
- pressure
- pressure\_func
- velocity
- velocity\_func
- dsigma
- inflow\_material
- inflow\_temperature

#### name

Description: A unique name used to identify a particular instance of this namelist

Type: string (31 characters max)

Default: none

#### face\_set\_ids

**Description:** A list of face set IDs that define the portion of the boundary where the boundary condition will be imposed.

Type: integer list (32 max)

Default: none

#### type

**Description:** The type of boundary condition. The available options are:

- "pressure" Pressure is prescribed on the boundary. Use pressure or pressure\_func to specify its value.
- "velocity" Velocity is prescribed on the boundary. Use velocity or velocity\_func to specify its value
- "no-slip" 0-velocity is imposed on the boundary. This is incompatible with inviscid flow.
- "free-slip" No velocity normal to the boundary, but the tangential velocity is otherwise free (no traction forces).
- "marangoni" Like "free-slip" except a tangential traction is applied that is due to temperature dependence of surface tension. Use dsigma to specify the value of  $d\sigma/dT$ . This is incompatible with inviscid flow.

Type: string Default: none

**Notes:** The different boundary condition types are mutually exclusive; no two can be specified on a common portion of the boundary.

### pressure

**Description:** The constant value of boundary pressure for a pressure-type boundary condition. To specify a function, use pressure\_func instead.

Default: none
Type: real

### pressure\_func

**Description:** The name of a FUNCTION namelist defining a function that gives the boundary pressure for a pressure-type boundary condition. The function is expected to be a function of (t, x, y, z).

Default: none
Type: string

### velocity

**Description:** The constant value of boundary velocity for a velocity-type boundary condition. To specify a function, use **velocity func** instead.

**Default:** none **Type:** real 3-vector

### velocity\_func

**Description:** The name of a VFUNCTION namelist defining a function that gives the boundary velocity for a velocity-type boundary condition. The function is expected to be a function of (t, x, y, z).

**Default:** none **Type:** string

### dsigma

**Description:** The constant value of  $d\sigma/dT$  for the marangoni-type condition. Here  $\sigma(T)$  is the temperature dependent surface tension coefficient.

Default: none
Type: real
Units: ???

### inflow\_material

**Description:** Velocity and pressure boundary conditions may result in fluid flow into the domain across the boundary. This parameter specifies the name of the fluid material to flux in. If not specified, materials are fluxed into a cell through a boundary face in the same proportion as the material volume fractions present in the cell.

Default: none

# inflow\_temperature

**Description:** Velocity and pressure boundary conditions may result in fluid flow into the domain across the boundary. This parameter specifies the temperature of the material fluxed in. If not specified, materials are fluxed into a call through a boundary face at the same temperature as the cell.

Default: none

# FLOW\_PRESSURE\_SOLVER and FLOW\_VISCOUS\_SOLVER Namelists

#### Overview

The flow algorithm requires the solution of two linear systems at each time step: the implicit viscous velocity update system and the pressure Poisson system. Truchas uses the hybrid solver from the HYPRE software library [3] to solve these systems.

The hybrid solver first uses a diagonally-scaled iterative Krylov solver. If it determines that convergence is too slow, the solver switches to a more expensive but more effective preconditioned Krylov solver that uses an algebraic multigrid (AMG) preconditioner (BoomerAMG).

The FLOW\_VISCOUS\_SOLVER namelist sets the HYPRE hybrid solver parameters for the solution of the implicit viscous velocity update system, and the FLOW\_PRESSURE\_SOLVER namelist sets the solver parameters for the solution of the pressure Poisson system. The same variables are used in both namelists.

# FLOW\_VISCOUS\_SOLVER Namelist Features

Required/Optional: Required only for viscous flow with  $viscous\_implicitness > 0$ .

Single/Multiple Instances: Single

# FLOW\_PRESSURE\_SOLVER Namelist Features

Required/Optional: Required Single/Multiple Instances: Single

### krylov\_method

**Description:** Selects the Krylov method used by the HYPRE hybrid solver. The options are "cg" (default), "gmres", and "bicgstab".

### krylov\_dim

**Description:** The Krylov subspace dimension for the restarted GMRES method.

Type: integer Valid values: > 0

Default: 5

### conv\_rate\_tol

**Description:** The convergence rate tolerance  $\theta$  where the hybrid solver switches to the more expensive AMG preconditioned Krylov solver. The average convergence rate after n iterations of the diagonally-scaled Krylov solver is  $\rho_n = \left(\|r_n\|/\|r_0\|\right)^{1/n}$ , where  $r_n = Ax_n - b$  is the residual of the linear system, and its convergence is considered too slow when

$$\left[1 - \frac{|\rho_n - \rho_{n-1}|}{\max(\rho_n, \rho_{n-1})}\right] \rho_n > \theta$$

Type: real

Valid values: (0,1)

**Default:** 0.9

### abs tol, rel tol

**Description:** The absolute and relative error tolerances  $\epsilon_1$  and  $\epsilon_2$  for the solution of the linear system. The test for convergence is  $||r|| \leq \max\{\epsilon_1, \epsilon_2 ||b||\}$ , where r = Ax - b is the residual of the linear system.

Type: real
Default: None

Note:

### max\_ds\_iter

**Description:** The maximum number of diagonally scaled Krylov iterations allowed. If convergence is not achieved within this number of iterations the hybrid solver will switch to the preconditioned Krylov solver.

Type: integer

Default:

### max\_pcg\_iter

**Description:** The maximum number of preconditioned Krylov iterations allowed.

Type: integer

**Default:** 

### print\_level

**Description:** Set this parameter to 2 to have HYPRE write diagnostic data to the terminal for each solver iteration. This is only useful in debugging situations. The default is 0, no output.

# Additional HYPRE parameters (Expert)

Some additional HYPRE solver parameters and options can be set using these namelists. Nearly all of these are associated with the BoomerAMG preconditioner, and all have reasonable defaults set by HYPRE. See the *ParCSR Hybrid Solver* section in the HYPRE reference manual [4] for details. The HYPRE user's manual [5] has some additional information. The variables that can be set are listed below. Note that the variables correspond to similarly-named HYPRE library functions and not actual HYPRE variables. Also note that there are many parameters and options that cannot currently be set by the namelists.

cg\_use\_two\_norm (logical)
amg\_strong\_threshold (real)
amg\_max\_levels (integer)
amg\_coarsen\_method (integer)
amg\_smoothing\_sweeps (integer)
amg\_smoothing\_method (integer)
amg\_interp\_method (integer)

# **FUNCTION Namelist**

#### Overview

There is often a need to specify phase properties, boundary condition data, source data, etc., as functions rather than constants. The FUNCTION namelist provides a means for defining functions that can be used in many situations.

The namelist can define several types of functions: a multi-variable polynomial, a continuous piecewise linear function defined by a table of values, a smooth step function, and with certain Truchas build configurations, a general user-provided function from a shared object library that is dynamically loaded at runtime. The functions are functions of m variables. The expected number of variables and what unknowns they represent (i.e., temperature, time, x-coordinate, etc.) depends on the context in which the function is used, and this will be detailed by the documentation of those namelists where these functions can be used.

**Polynomial Function.** This function is a polynomial in the variables  $\mathbf{v} = (v_1, \dots, v_m)$  of the form

$$f(\mathbf{v}) = \sum_{j=1}^{n} c_j \prod_{i=1}^{m} (v_i - a_i)^{e_{ij}}$$
(14.1)

with coefficients  $c_j$ , integer-valued exponents  $e_{ij}$ , and arbitrary reference point  $\mathbf{a} = (a_1, \dots, a_m)$ . The coefficients are specified by Poly\_Coefficients, the exponents by Poly\_Exponents, and the reference point by Poly\_Refvars.

**Tabular Function.** This is a continuous, single-variable function y = f(x) interpolated from a sequence of data points  $(x_i, y_i)$ , i = 1, ..., n, with  $x_i < x_{i+1}$ . A smooth interpolation method is available in addition to the standard linear interpolation; see **Tabular\_Interp**. There are also two different methods for extrapolating on  $x < x_1$  and  $x > x_n$ ; see **Tabular\_Extrap**.

**Smooth Step Function.** This function is a smoothed  $(C_1)$  step function in a single variable  $\mathbf{v} = (x)$  of the form

$$f(x) = \begin{cases} y_0 & \text{if } x \le x_0, \\ y_0 + (y_1 - y_0)s^2(3 - 2s), s \equiv (x - x_0)/(x_1 - x_0), & \text{when } x \in (x_0, x_1), \\ y_1 & \text{if } x \ge x_1, \end{cases}$$
 (14.2)

with parameters  $x_0$ ,  $x_1$ ,  $y_0$ , and  $y_1$ .

**Shared Library Function.** This is a function from a shared object library having a simple Fortran 77 or C compatible interface. Written in Fortran 77 the function interface must look like

```
double precision function myfun (v, p) bind(c)
double precision v(*), p(*)
```

where myfun can, of course, be any name. The equivalent C interface is

```
double myfun (double v[], double p[]);
```

The vector of variables  $\mathbf{v} = (v_1, \dots, v_m)$  is passed in the argument  $\mathbf{v}$  and a vector of parameter values specified by Parameters is passed in the argument  $\mathbf{p}$ . Instructions for compiling the code and creating a shared object library can be found in the *Truchas Installation Guide*. The path to the library is given by Library\_Path and the name of the function (myfun, e.g.) is given by Library\_Symbol. Note that the bind(c) attribute on the function declaration inhibits the Fortran compiler from mangling the function name (by appending an underscore, for example) as it normally would.

#### **FUNCTION Namelist Features**

Required/Optional: Optional

Single/Multiple Instances: Multiple

# Components

- Name
- Type
- Library\_Path
- Library\_Symbol
- Parameters
- Poly\_Coefficients
- Poly\_Exponents
- Poly\_Refvars
- Smooth\_Step\_XO
- Smooth\_Step\_X1
- Smooth\_Step\_Y0
- Smooth\_Step\_Y1
- Tabular Data
- Tabular\_Dim
- Tabular\_Extrap
- Tabular\_Interp

#### Name

**Description:** A unique name by which this function can be referenced by other namelists.

**Type:** A case-sensitive string of up to 31 characters.

Default: None

# Type

**Description:** The type of function defined by the namelist.

Type: case-sensitive string

Default: none

Valid values: "polynomial" for a polynomial function, "tabular" for a tabular function, "smooth step" for a smooth step function, or "library" for a function from a shared object library. The "library" value is not available with a Truchas executable built with the "dynamic loading" option disabled.

### Library\_Path

**Description:** The path to the shared object library that contains the function.

**Type:** A string of up to 128 characters.

Default: none

### Library\_Symbol

**Description:** The symbol name of the function within the shared object file.

**Type:** A string of up to 128 characters.

Default: none

Notes: Unless the Fortran function is declared with the BIND(C) attribute, which is the recommended practice, a Fortran compiler will almost always mangle the name of the function so that the symbol name is not quite the same as the name in the source code. Use the UNIX/Linux command-line utility nm to list the symbol names in the library file to determine the correct name to use here.

#### Parameters

**Description:** Optional parameter values to pass to the shared library function.

Type: real vector of up to 16 values

Default: None

# Poly\_Coefficients

**Description:** The coefficients  $c_j$  of the polynomial (14.1).

**Type:** real vector of up to 64 values

Default: None

# Poly\_Exponents

**Description:** The exponents  $e_{ij}$  of the polynomial (14.1).

Type: integer array

Default: None

Notes: Namelist array input is very flexible. The syntax

```
Poly_Exponents(i,j) = ...
```

defines the value for exponent  $e_{ij}$ . All the variable exponents for coefficient j can be defined at once by listing their values with the syntax

```
Poly_Exponents(:,j) = ...
```

In some circumstances it is possible to omit providing 0-exponents for variables that are unused. For example, if the function is expected to be a function of (t, x, y, z), but a polynomial in only t is desired, one can just define a 1-variable polynomial and entirely ignore the remaining variables. On the other hand, if a polynomial in z is desired, one must specify 0-valued exponents for all the preceding variables.

### Poly\_Refvars

**Description:** The optional reference point **a** of the polynomial (14.1).

Type: real vector **Default:** 0.0

#### Tabular\_Data

**Description:** The table of values  $(x_i, y_i)$  defining a tabular function y = f(x). See also Tabular\_Dim, Tabular\_Interp, and Tabular\_Extrap for additional variables that define the function.

Type: real array Default: none

**Notes:** This is a  $2 \times n$  array with  $n \le 100$ . Namelist array input is very flexible and the values can be specified in several ways. For example, the syntax

```
Tabular_Data(1,:) = x_1, x_2, ..., x_n
Tabular_Data(2,:) = y_1, y_2, ..., y_n
```

specifies the  $x_i$  and  $y_i$  values as separate lists. Or the values can be input naturally as a table

The line breaks are unnecessary, of course, and are there only for readability as a table.

# Tabular Dim

**Description:** The dimension in the m-vector of independent variables that serves as the independent variable for the single-variable tabular function.

Type: integer Default: 1

Notes: Functions defined by this namelist are generally functions of m variables  $(v_1, v_2, \ldots, v_m)$ . The number of variables and the unknowns to which they correspond depend on the context where the function is used. One of these variables needs to be selected to be the independent variable used for the tabular function. In typical use cases the desired tabular function will depend on time or temperature. Those unknowns are often the first variable, and the default value of Tabular\_Dim is appropriate.

# Tabular\_Extrap

**Description:** Specifies the method used for extrapolating outside the range of tabular function data points.

Type: case-insensitive string

Default: "nearest"

Valid values: "nearest", "linear"

**Notes:** Nearest extrapolation continues the y value at the first or last data point. Linear extrapolation uses the slope of the first or last data interval, or if Akima smoothing is used (see Tabular\_Interp) the computed slope at the first or last data point.

### Tabular\_Interp

**Description:** Specifies the method used for interpolating between tabular function data points.

Type: case-insensitive string

Default: "linear"

Valid values: "linear", "akima"

Notes: Akima interpolation [6] uses Hermit cubic interpolation on each data interval, with the slope at each data point computed from the linear slopes on the neighboring four intervals. The resulting function is  $C^1$  smooth. To determine the slope at the first two and last two data points, two virtual data intervals are generated at the beginning and at the end using quadratic extrapolation.

The algorithm seeks to avoid undulations in the interpolated function where the data suggests a flat region though its choice of slopes at data points. Figure 14.1A shows the typical smooth Akima interpolation. If the first interval was expected to be flat, the exhibited undulation would likely be unacceptable. By inserting an additional data point to create successive intervals with the same slope, as in Figure 14.1BC, the algorithm identifies it as a flat region and preserves it in the interpolation. Where two flat regions with differing slopes meet, it is impossible to simultaneously retain smoothness and preserve flatness. In this case a modification to the Akima algorithm used by Matlab's tablelookup function is adopted, which gives preference to the region with smaller slope as shown in Figure 14.1D.

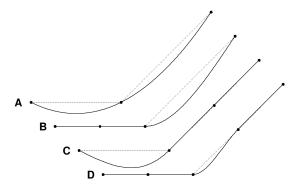


Figure 14.1: Examples of smooth Akima interpolation.

### Smooth\_Step\_X0

**Description:** The parameter  $x_0$  of the function (14.2).

Type: real
Default: none

**Valid values:** Require only  $x_0 < x_1$ .

#### Smooth\_Step\_X1

**Description:** The parameter  $x_1$  of the function (14.2).

Type: real
Default: none

**Valid values:** Require only  $x_0 < x_1$ .

# ${\tt Smooth\_Step\_YO}$

**Description:** The parameter  $y_0$  of the function (14.2).

Type: real
Default: none

# ${\tt Smooth\_Step\_Y1}$

**Description:** The parameter  $y_1$  of the function (14.2).

Type: real
Default: none

# INDUCTION\_COIL Namelist

### Overview

The variables in an INDUCTION\_COIL namelist specify the physical characteristics of an induction coil that is to produce an external magnetic field to drive the electromagnetic Joule heat calculation. Figure 15.1 shows the idealized model of a coil that is used to analytically evaluate the driving field. The coil axis is assumed to be oriented with the problem symmetry axis as defined in the ELECTROMAGNETICS namelist. Multiple coils may be specified; the net driving field is the superposition of the fields due to the individual coils, and a spatially uniform field that can be specified in the ELECTROMAGNETICS namelist. The coils carry a sinusoidally-varying current with a common frequency and phase. The frequency is specified in the ELECTROMAGNETICS namelist, while the phase value is irrelevant due to the time averaging of the calculated Joule heat. Each coil, however, has an independent current amplitude which is specified here. In addition, the current and frequency may be piecewise constant functions of time.

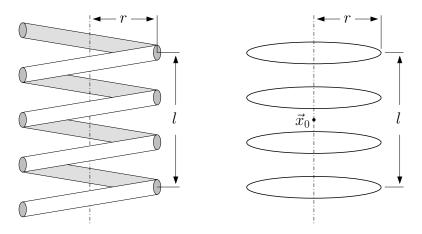


Figure 15.1: Physical 4-turn helical coil with extended wire cross section (left), and its idealized model as a stacked array of circular current loops (right).

# INDUCTION\_COIL Namelist Features

Required/Optional: Optional

Single/Multiple Instances: Multiple

# Components

- Center
- Current
- Length
- NTurns
- Radius

#### Center

**Description:** A 3-vector  $\mathbf{x}_0$  giving the position of the center of the coil; cf. Figure 15.1.

Physical dimension: L

Type: real Default: (0,0,0)

Valid values: any 3-vector

#### Current

**Description:** Amplitude of the sinusoidally-varying current in the coil.

Physical dimension: |

Type: real
Default: none

Valid values: Any single value, or any sequence of values.

**Notes:** A sequence of up to 32 values may be assigned to this variable in order to specify a time-dependent current amplitude; see Source\_Times in the ELECTROMAGNETICS namelist and Fig. 7.1.

### Length

**Description:** Length l of the coil; cf. Figure 15.1.

Physical dimension: L

Type: real Default: none Valid values:  $(0, \infty)$ 

Notes: Length is not required, nor meaningful, if NTurns is 1.

#### NTurns

**Description:** Number of turns of the coil; cf. Figure 15.1.

Type: integer Default: none

Valid values: Any positive integer.

# Radius

**Description:** Radius r of the coil; cf. Figure 15.1.

Physical dimension: L

Type: real
Default: none

Valid values:  $(0, \infty)$ 

# MATERIAL and PHASE Namelists

#### Overview

A database of materials, their properties and attributes are defined using the MATERIAL, PHASE, and PHASE\_CHANGE namelists. Not all materials are necessarily included in the simulation, but only those specified by the PHYSICS namelist variable materials. This allows one to reuse material input blocks without needing to prune out unused materials which would otherwise negatively impact performance. In Truchas usage, one or more phases comprise a material. A single-phase material is defined by a MATERIAL namelist specifies all properties and attributes of the material. A multi-phase material is defined by a MATERIAL namelist and an optional PHASE namelist for each of the material phases. Properties and attributes that apply to all phases can be defined in the MATERIAL namelist. Properties and attributes specific to a given phase are defined in the PHASE namelist for the phase, and these supercede any that might be defined in the MATERIAL namelist for the phase. Additional information that defines the transformation between phases is specified using the PHASE CHANGE namelist.

#### The MATERIAL Namelist

The MATERIAL namelist defines a material, either single-phase or multi-phase, that is available to be used in a simulation. In addition to the property and attribute variables described below, the namelist has the following variables.

#### name

A unique name for the material used to reference it.

#### phases

A multi-phase material is defined by assigning a value to **phases**. This is a list of two or more unique phase names that comprise the material. The phases must be listed in order from low to high temperature phases. The phase names will be referenced by PHASE\_CHANGE namelists and by optional PHASE namelists. Consecutive pairs of phases must be accompanied by a corresponding PHASE\_CHANGE namelist.

#### The PHASE Namelist

The PHASE namelist defines properties and attributes specific to one phase of a multi-phase material. It is optional. Any properties or attributes defined here supersede those defined in the parent MATERIAL namelist. In addition to the property and attribute variables described below, the PHASE namelist has the following variable.

#### name

The name of the phase. This is one of the names assigned to the **phases** variable of the MATERIAL namelist for the parent material.

# Property and Attribute Variables

The following variables specify the values of material properties and attributes. Unless otherwise noted, they may appear in both the MATERIAL and PHASE namelists. Many properties can be either constant-valued or a function. Variables ending with the suffix **\_func** specify the name of a FUNCTION namelist that defines a function that computes the value of the property.

### Thermodynamic Properties

The following property variables are used by the heat transport model:

- density
- specific\_heat, specific\_heat\_func, ref\_temp, and ref\_enthalpy
- specific\_enthalpy\_func
- conductivity, conductivity\_func

The material mass density (mass per volume) is specified by **density**. It is limited to constant values and all phases in a multi-phase material are currently constrained to have the same density (but see **density\_delta\_func** for flow and **tm\_linear\_cte** for solid mechanics.) Consequently this variable may only appear in the MATERIAL namelist.

There are two options for defining the temperature-dependent specific enthalpy function h(T) of a material or phase. The first specifies the specific heat  $C_p(T)$  (energy per unit mass per degree temperature) using **specific\_heat** for a constant or **specific\_heat\_func** for a function of temperature. In the latter case it must either be a tabular function or a polynomial without a  $T^{-1}$  term. An analytic antiderivative of the specific heat will be generated by Truchas and used for h(T). For a single-phase material or the lowest-temperature phase of a multi-phase material, there is an arbitrary constant of integration. By default it is chosen such that h(0) = 0. It can be chosen instead such that  $h(T_{ref}) = h_{ref}$  by specifying values for the optional variables **ref\_temp** and **ref\_enthalpy**, which default to 0. These latter two variables may only appear in the MATERIAL namelist.

The second option is to specify the specific enthalpy function h(T) (energy per unit mass) directly using **specific\_enthalpy\_func**. The function must be strictly increasing, and when used for a phase of a multi-phase material, it must incorporate the latent heat associated with the transformation from the adjacent lower-temperature phase (when there is one).

The thermal conductivity (power per unit length per degree temperature) of a material or phase is specified by **conductivity** for a constant or **conductivity\_func** for a function. The function is assumed to be a function of temperature T, or  $(T, \phi_1, \ldots, \phi_n)$  when coupled with solutal species transport.

#### Fluid Flow Properties

The following attribute and property variables are used by the fluid flow model:

- is\_fluid
- density
- density\_delta\_func
- viscosity, viscosity\_func

The boolean attribute is\_fluid is used to indicate whether or not the material or phase is a fluid. Its default value is F (or .false.) Materials and phases marked as fluid are included in the fluid flow model. The constant reference density  $\rho_0$  of a fluid material or phase is specified by density. This is the same density value used for heat transport. A temperature-dependent fluid density  $\rho(T)$  can be defined by giving its deviation from the reference density,  $\delta\rho(T) = \rho(T) - \rho_0$  using the variable density\_delta\_func. This

is used only to compute the buoyancy body force of the Boussinesq approximation in the flow model. If not specified, no deviation from the reference density is assumed.

The dynamic viscosity (mass per length per time) of a material or phase is specified by **viscosity** for a constant or **viscosity\_func** for a function of temperature. This is required for viscous flow problems (FLOW namelist variable inviscid = F).

#### **Electromagnetic Properties**

The following property variables are used by the induction heating model:

- electrical conductivity, electrical conductivity func
- electric susceptibility, electric susceptibility func
- magnetic\_susceptibility, magnetic\_susceptibility\_func

The electrical conductivity of a material or phase is specified using either electrical\_conductivity for a constant, or electrical\_conductivity\_func for a function of temperature. The default value is 0. The electromagnetics solver assumes SI units by default and the units of electrical conductivity are Siemens per meter. To use different units, the values for the PHYSICAL\_CONSTANTS namelist variables vacuum\_permeability and vacuum\_permittivity must be redefined appropriately.

The electric susceptibility  $\chi_e$  of a material or phase is specified using either **electric\_susceptibility** for a constant, or **electric\_susceptibility\_func** for a function of temperature. The relative permittivity is  $1 + \chi_e$ . This property has a default value of zero, which is appropriate in most cases.

The magnetic susceptibility  $\chi_m$  of a material or phase is specified using either magnetic\_susceptibility for a constant, or magnetic\_susceptibility\_func for a function of temperature. The relative permeability is  $1 + \chi_m$ . This property has a default value of zero, which is appropriate in most cases.

### Thermomechanical Properties

The following properties are used by the solid mechanics model, and are only relevant to non-fluid materials and phases. Additional viscoplasticity parameters may be defined using the VISCOPLASTIC\_MODEL namelist.

- tm\_ref\_density
- tm\_ref\_temp
- tm\_linear\_cte, tm\_linear\_cte\_func
- tm\_lame1, tm\_lame1\_func
- tm\_lame2, tm\_lame2\_func

The temperature at which a material or phase is stress-free is specified by tm\_ref\_temp and its density (mass per volume) at that temperature specified by tm\_ref\_density. Its linear coefficient of thermal expansion (inverse time) is specified by tm\_linear\_cte for a constant or tm\_linear\_cte\_func for a function of temperature.

The first and second Lamé constants  $\lambda$  and G (force per area) for a material or phase is specified by  $tm_lame1$  and  $tm_lame2$  for constants or  $tm_lame1_func$  and  $tm_lame2_func$  for functions of temperature.

#### **Species Transport Properties**

The following property variables are relevant to the solutal species transport model. The model allows for an arbitrary number of species with concentrations  $\{\phi_i\}_{i=1}^n$ , and the variables are arrays of length n with each element being the property for the corresponding species.

- diffusivity, diffusivity\_func
- soret, soret\_func

The diffusivity (area per time) of a species component in a material or phase is specified by the corresponding element of **diffusivity** for a constant or **diffusivity\_func** for a function. A function is expected to be a function of all the species concentrations  $(\phi_1, \ldots, \phi_n)$ , or when coupled with heat transfer, a function of temperature and concentrations  $(T, \phi_1, \ldots, \phi_n)$ .

When coupled with heat transfer, the Soret coefficient (inverse temperature) of the thermodiffusion term for a species component in a material or phase is specified by the corresponding element of **soret** for a constant or **soret\_func** for a function. A function is expected to be a function of temperature and concentrations  $(T, \phi_1, \ldots, \phi_n)$ . This is optional. If not specified, thermodiffusion of the species component is not included in the model, but if defined for one phase of a multi-phase material, it must be defined for all its phases.

# MESH Namelist

#### Overview

The MESH namelist specifies the common mesh used by all physics models other than the induction heating model, which uses a separate tetrahedral mesh specified by the ALTMESH namelist. For simple demonstration problems, a rectilinear hexahedral mesh of a brick domain can be defined, but for most applications the mesh will need to be generated beforehand by some third party tool or tools and saved as a file that Truchas will read. At this time Exodus II [7] is the only supported mesh format (also sometimes known as Genesis). This well-known format is used by some mesh generation tools (Cubit [8], for example) and utilities exist for translating from other formats to Exodus II. The unstructured 3D mesh may be a general mixed-element mesh consisting of non-degenerate hexehedral, tetrahedral, pyramid, and wedge/prism elements. The Exodus II format supports a partitioning of the elements into element blocks and also supports the definition of side sets, which are collections of oriented element faces that describe mesh surfaces, either internal or boundary. Extensive use is made of this additional mesh metadata in assigning materials, initial conditions, boundary conditions, etc., to the mesh.

#### MESH Namelist Features

Required/Optional: Required Single/Multiple Instances: Single

# Components

#### External mesh file

- mesh\_file
- interface\_side\_sets
- gap\_element\_blocks
- exodus block modulus

#### Internally generated mesh

- x\_axis
- y\_axis
- z axis
- noise\_factor

#### Common parameters

- coordinate\_scale\_factor
- partitioner
- partition\_file
- first\_partition

#### External Mesh File

In typical usage, the mesh will be read from a specified Exodus II mesh file. Other input variables that follow specify optional modifications that can be made to the mesh after it is read.

#### mesh file

**Description:** Specifies the path to the Exodus II mesh file. If not an absolute path, it will be interpreted as a path relative to the Truchas input file directory.

**Type:** case-sensitive string

Default: none

# interface\_side\_sets

**Description:** A list of side set IDs from the ExodusII mesh identifying internal mesh surfaces that will be treated specially by the heat/species transport solver.

Type: integer list

**Default:** An empty list of side set IDs.

Valid values: Any side set ID whose faces are internal to the mesh.

Notes: The heat/species transport solver requires that boundary conditions are imposed along the specified surface. Typically these will be interface conditions defined by THERMAL\_BC namelists, but in unusual use cases they could also be external boundary conditions defined by the same namelists. In the latter case it is necessary to understand that the solver views the mesh as having been sliced open along the specified internal surfaces creating matching pairs of additional external boundary and, where interface conditions are not imposed, boundary conditions must be imposed on both sides of the interface.

# gap\_element\_blocks (deprecated)

**Description:** A list of element block IDs from an Exodus II mesh that are to be treated as gap elements.

Type: integer list

**Default:** An empty list of element block IDs.

Valid values: Any element block ID.

Notes: Any element block ID in the mesh file can be specified, but elements that are not connected such that they can function as gap elements or are not consistent with side set definitions will almost certainly result in incorrect behavior. The code does not check for these inconsistencies.

The heat/species transport solver drops these elements from its view of the mesh and treats them instead as an internal interface; see the notes to <code>interface\_side\_sets</code>. The block IDs specified here can be used as values for <code>face\_set\_ids</code> from the <code>THERMAL\_BC</code> namelist.

#### exodus\_block\_modulus

**Description:** When importing an Exodus II mesh, the element block IDs are replaced by their value modulo this parameter. Set the parameter to 0 to disable this procedure.

Type: integer Default: 10000 Valid values:  $\geq 0$ 

Notes: This parameter helps solve a problem posed by mixed-element meshes created by Cubit and Trelis. In those tools a user may define an element block comprising multiple element types. But when exported in the Exodus II format, which doesn't support blocks with mixed element types, the element block will be written as multiple Exodus II blocks, one for each type of element. One of the blocks will retain the user-specified ID of the original block. The IDs of the others will be that ID plus an offset specific to the element type. For example, if the original block ID was 1, hexahedra in the block will be written to a block with ID 1, tetrahedra to a block with ID 10001, pyramids to a block with ID 100001, and wedges to a block with ID 200001. These are the default offset values, and they can be set in Cubit/Trelis; see their documentation for details on how the IDs are generated. It is important to note that this reorganization of element blocks occurs silently and so the user may be unaware that it has happened. In order to reduce the potential for input errors, Truchas will by default convert the block IDs to congruent values modulo N in the interval [1, N-1] where N is the value of this parameter. The default value 10000 is appropriate for the default configuration of Cubit/Trellis, and restores the original user-specified block IDs. Note that this effectively limits the range of element block IDs to [1, N-1].

The element block IDs are modified immediately after reading the file. Any input parameters that refer to block IDs must refer to the modified IDs.

# **Internally Generated Mesh**

A rectilinear hexahedral mesh for a brick domain  $[x_{\min}, x_{\max}] \times [y_{\min}, y_{\max}] \times [z_{\min}, z_{\max}]$  can be generated internally as part of a Truchas simulation using the following input variables. The mesh is the tensor product of 1D grids in each of the coordinate directions. Each coordinate grid is defined by a coarse grid whose intervals are subdivided into subintervals, optionally with biased sizes. The generated Exodus II mesh consists of a single element block with ID 1, and a side set is defined for each of the six sides of the domain with IDs 1 through 6 for the  $x = x_{\min}, x = x_{\max}, y = y_{\min}, y = y_{\max}, z = z_{\min}$ , and  $z = z_{\max}$  sides, respectively. Note that while the mesh is formally structured, it is represented internally as a general unstructured mesh.

### x\_axis, y\_axis, z\_axis

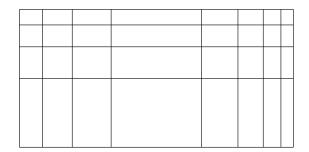
Data that describes the grid in each of the coordinate directions. The tensor product of these grids define the nodes of the 3D mesh. The data for each coordinate grid consists of these three component arrays:

**%coarse\_grid:** A strictly increasing list of two or more real values that define the points of the coarse grid for the coordinate direction. The first and last values define the extent of the domain in this direction.

**%intervals:** A list of postive integers defining the number of subintervals into which each corresponding coarse grid interval should be subdivided. The number of values must be one less than the number of coarse grid points.

**%ratio:** An optional list of positive real values that define the ratio of the lengths of successive subintervals for each coarse grid interval. The default is to subdivide into equal length subintervals. If specified, the number of values must be one less than the number of coarse grid points.

See Figure 17 for an example.



```
x_axis%coarse_grid = 0.0, 0.67, 1.33, 2.0
x_axis%intervals = 3, 1, 4
x_axis%ratio = 1.3, 1.0, 0.7
y_axis%coarse_grid = 0.0, 0.5, 1.0
y_axis%intervals = 1, 3
y_axis%ratio = 0.7
z_axis%coarse_grid = 0.0, 1.0
z_axis%intervals = 1
```

Figure 17.1: Top xy surface of the rectilinear mesh generated by the example input shown.

# noise\_factor (expert)

**Description:** If specified with a positive value, the coordinates of each mesh node will be perturbed by uniformly distributed random amount whose magnitude will not exceed this value times the local cell size at the node. Nodes on the boundary are not perturbed in directions normal to the boundary. This is only useful for testing.

Valid values:  $\in [0, 0.3]$ 

**Default:** 0

#### Common Variables

The following variables apply to both types of meshes.

# coordinate\_scale\_factor

**Description:** An optional factor by which to scale all mesh node coordinates.

Type: real
Default: 1.0
Valid values: > 0

### partitioner

Description: The partitioning method used to generate the parallel decomposition of the mesh.

 $\mathbf{Type:} \ \ \mathrm{case\text{-}insensitive \ string}$ 

Default: "chaco"

Valid values: "chaco", "file", "block"

Notes:

"chaco" uses a graph partitioning method from the Chaco library [9] to compute the mesh decomposition at run time. This is the standard method long used by Truchas.

"file" reads the partitioning of the mesh cells from a disk file; see partition\_file.

"block" partitions the mesh cells into nearly equal-sized blocks of consecutively numbered cells according their numbering in the mesh file. The quality of this naive decomposition entirely depends on the given ordering of mesh cells, and thus this option is not generally recommended.

### partition\_file

**Description:** Specifies the path to the mesh cell partition file, and is required when **partitioner** is "file". If not an absolute path, it will be interpreted as a path relative to the Truchas input file directory.

Type: case-sensitive string

Default: none

Notes: The format of this text file consists of a sequence of integer values, one value or multiple values per line. The first value is the partition number of the first cell, the second value the partition number of the second cell, and so forth. The number of values must equal the number of mesh cells. The file may use either a 0-based or 1-based numbering convention for the partitions. Popular mesh partitioning tools typically use 0-based partition numbering, and so the default is to assume 0-based numbering; use first\_partition to specify 1-based numbering.

# first\_partition

**Description:** Specifies the number given the first partition in the numbering convention used in the partition file. Either 0-based or 1-based numbering is allowed.

Type: integer Default: 0

Valid values: 0 or 1

# NUMERICS Namelist

#### Overview

The NUMERICS namelist specifies general numerical parameters not specific to any particular physics, especially those controlling the overall time stepping of the Truchas model.

#### **NUMERICS Namelist Features**

Required/Optional: Required Single/Multiple Instances: Single

# Components

- Alittle
- Cutvof
- Cycle\_Max
- Cycle\_Number
- Discrete\_Ops\_Type
- Dt\_Constant
- Dt\_Grow
- Dt\_Init
- Dt\_Max
- Dt\_Min
- t

#### Alittle

**Description:** A small, positive real number (relative to unity) used to avoid division by zero or to compare against other numbers to deduce relative significance.

Physical dimension: dimensionless

Type: real

**Default:** EPSILON(x), where x is of type real. If the precision of x is double, EPSILON(x) returns  $1.0^{-16}$  for most combinations of software (Fortran 90 compiler) and hardware platforms tested.

**Valid values:** (0.0, 0.001]

#### Cutvof

**Description:** The value of a material cell volume fraction below which that material is ignored. If any material has a cell volume fraction less than **Cutvof**, then that material is deleted from that cell, with all other materials present receiving a proportional increase in volume fraction. The only exception is the "background" material, which if present receives the entire allocation (equal to the volume fraction deleted).

Physical dimension: dimensionless

Type: real Default:  $10^{-8}$ 

Valid values: (0.0, 1.0)

Notes: Relative to most other volume-fraction-based algorithms, Cutvof is defaulted and used at a much lower value. If a prototypical value of Cutvof equal to  $10^{-4}$  were used, as is the case in most commercial software, local and global mass conservation would suffer, and lack of algorithmic robustness would be masked. The default  $10^{-8}$  value for Cutvof yields good results, hence setting it higher is generally not necessary.

### Cycle\_Max

**Description:** The maximum cycle number allowed in the given simulation, where one "cycle" corresponds to one integration time step over all physical model equations. The simulation will terminate gracefully when the cycle number reaches Cycle\_Max.

Type: integer Default: 1000000 Valid values:  $(0, \infty)$ 

Notes: A simulation will also terminate gracefully if the last entry in the Output\_T input variable (real) array (in the OUTPUTS namelist) is exceeded by the current simulation time t.

### Cycle\_Number

**Description:** The cycle number to be used just prior to the first actual cycle (time step) taken in the given simulation. The first simulation cycle number is then taken to be cycle\_number + 1.

Type: integer Default: 0

Valid values:  $[1, \infty)$ 

**Notes:** The default value of 0 results in the first computational cycle taken to be 1. This input variable is most useful when starting simulations from a restart file that already contains a restart cycle number > 0.

# Discrete\_Ops\_Type

**Description:** Flag for choosing the numerical reconstruction method used in estimating face-centered (located at cell face centroids) spatial gradients and values of discrete cell-centered data. Specifically, face pressure gradients, face velocity values, and face velocity gradients are all controlled by this flag.

Type: string

Default: "default"

Valid values: "default", "ortho", "nonortho"

Notes: Face-centered pressure gradients are needed for cell-centered estimates of the pressure Laplacian (used in the pressure Poisson solve) and for enforcement of solenoidal face-centered velocities. Face-centered velocity gradients are needed for cell-centered estimates of the stress tensor, and face-centered velocity values are needed for estimation of fluxing velocities. If this variable does not appear in the NUMERICS namelist, or if it appears and is set to 'default', the type of discrete operators to use is chosen by testing the orthogonality of the mesh cells. When all mesh cells are found to be orthogonal (to roundoff error) and thus hexahedral, then Discrete\_Ops\_Type defaults to an 'ortho' method. Otherwise, Discrete\_Ops\_Type defaults to a 'nonortho' method, namely the Least Squares Linear Reconstruction (LSLR) method. For a detailed discussion of discrete operators in Truchas, consult the Truchas Physics and Algorithms. If 'ortho' or 'nonortho' is set, the chosen operator type is used, whatever the mesh.

The user can set an overall discrete operator type as above and choose an alternative discrete operator type for the projection step in fluid flow (FF). To override the overall default or explicit overall setting, set the variable FF\_Discrete\_Ops\_Type to the desired value. Setting this variable leaves the overall setting Discrete\_Ops\_Type unmodified for all remaining parts of the code.

#### Dt\_Constant

**Description:** A constant integration time step value to be used for all time steps in the simulation

Physical dimension: T

Type: real Default: none Valid values:  $(0, \infty)$ 

Notes: This Dt\_Constant input variable should be used with extreme caution, as its specification overrules all other time step choices that are controlled by linear stability and accuracy considerations. In particular, NUMERICS namelist input variables Dt\_Grow, Dt\_Init, Dt\_Max, and Dt\_Min are all ignored if Dt\_Constant is specified. Use of Dt\_Constant is therefore advised only for controlled numerical algorithm experiments, and not for simulations intended for applications analysis and validation.

#### Dt\_Grow

**Description:** A factor to multiply the current integration time step  $(\delta t)$  for the purpose of estimating the time step used during the next cycle  $(\delta t_g = Dt\_Grow * \delta t)$ . This candidate time step  $(\delta t_g)$  is chosen only if all other currently active time step restrictions have not already limited its value below  $\delta t_g$ .

Physical dimension: dimensionless

Type: real Default: 1.05 Valid values:  $[1, \infty)$ 

Notes: Dt\_Grow is *ignored* if Dt\_Constant is specified.

#### $\mathtt{Dt}_{\mathtt{Init}}$

**Description:** Integration time step value used for the first computational cycle

Physical dimension: T

Type: real Default:  $10^{-6}$ 

Valid values:  $(0, \infty)$ 

Notes: The default value of <code>Dt\_Init</code> is completely arbitrary, as it is <code>always</code> problem dependent. Unless a constant time step is desired (via specification of <code>Dt\_Constant</code>), then, a value for <code>Dt\_Init</code> should be specified (instead of relying on the default) that is consistent with the time scales of interest for the simulation at hand. A general rule of thumb is to set <code>Dt\_Init</code> smaller than the time step ultimately desired, thereby allowing the time step to grow gradually and steadily (say, over 10-20 cycles) to the desired time step value.

For restart calculations, the initial time step size is extracted from the restart file and used instead of Dt Init, unless Ignore Dt in the RESTART namelist has been set to true.

Dt\_Init is ignored if Dt\_Constant is specified.

### Dt\_Max

Description: Maximum allowable value for the time step

Physical dimension: T

Type: real
Default: 10

Valid values:  $(0, \infty)$ 

Notes: The time step is *not* allowed to exceed this value, even if other accuracy- or stability-based criteria would permit it. The default value of <code>Dt\_Max</code> is completely arbitrary, as it is <code>always</code> problem dependent. Unless a constant time step is desired (via specification of <code>Dt\_Constant</code>), then, a value for <code>Dt\_Max</code> should be specified (instead of relying on the default) that is consistent with the time scales of interest for the simulation at hand.

Dt\_Max is ignored if Dt\_Constant is specified.

#### Dt\_Min

**Description:** Minimum allowable value for the time step

Physical dimension: T

Type: real Default:  $10^{-6}$  Valid values:  $(0, \infty)$ 

Notes: If the time step falls below this value, the user is informed as such and the simulation terminates gracefully. Termination occurs at this condition because is it very probable that either numerical algorithm or physical model problems have occurred and the simulation is unable to recover. The default value of Dt\_Min is completely arbitrary, as it is always problem dependent. Unless a constant time step is desired (via specification of Dt\_Constant), then, a value for Dt\_Min should be specified (instead of relying on the default) that is consistent with the time scales of interest for the simulation at hand. A good rule of thumb to use for Dt\_Min is to use a value several orders of magnitude below the time scale of interest.

Dt\_Min is ignored if Dt\_Constant is specified.

#### t

**Description:** The simulation time to be used at the beginning of the first computational cycle.

Physical dimension: T

Type: real Default: 0

# **OUTPUTS** Namelist

### Overview

The OUTPUTS namelist defines the problem end time and various output options.

#### **OUTPUTS Namelist Features**

Required/Optional: Required Single/Multiple Instances: Single

# Components

- Int\_Output\_Dt\_Multiplier
- Output\_Dt
- Output\_Dt\_Multiplier
- Output\_T
- Probe\_Output\_Cycle\_Multiplier
- Short\_Output\_Dt\_Multiplier
- Move\_Block\_IDs
- Move\_Toolpath\_Name

# Int\_Output\_Dt\_Multiplier

Description: Factor multiplying Output\_Dt for time interval to write interface output data.

Type: integer array Default: none Valid values:  $\geq 0$ 

## Output\_Dt

**Description:** Output time interval for each output time span.

Physical dimension: T

Type: real array
Default: none
Valid values: > 0

### Output\_T

**Description:** A sequence of time values for defining time spans that have distinct output time intervals.

The last time is the problem end time.

Physical dimension: T

Type: real array Default: none

Valid values: strictly increasing sequence of two or more values

## Probe\_Output\_Cycle\_Multiplier

**Description:** Factor multiplying truchas cycle to determine frequency of writing probe output.

Type: integer Default: 1

Valid values: > 0

# Short\_Output\_Dt\_Multiplier

Description: Factor multiplying Output\_Dt for time interval to write short edits

Type: integer array

**Default:** 0

Valid values:  $\geq 0$ 

# Output\_Dt\_Multiplier

Description: Factor multiplying Output\_Dt for time interval to write output.

Type: integer array

Default: 0

Valid values:  $\geq 0$ 

#### Move\_Block\_IDs

**Description:** A list of element block IDs that are associated with a translation written to the output file. Use Move\_Toolpath\_Name to specify the translation.

**Type:** a list of up to 32 integers

Default: none

Notes: Use of this feature does not alter the mesh data that is written to the HDF5 output file. It merely adds some additional data that associates a time-dependent translation with element blocks. Use of the data, if any, is left to users of the file. At this time the Paraview Truchas output reader (post version 5.2) uses this information to translate the mesh blocks for visualization.

## Move\_Toolpath\_Name

**Description:** The name of a TOOLPATH namelist that defines the translation to apply to the element blocks given by Move\_Block\_IDs.

Type: string
Default: none

# PHASE\_CHANGE Namelist

#### Overview

The PHASE\_CHANGE namelist defines the phase change model used for the transformation between two phases of a multi-phase material. An instance of this namelist is required for each consecutive pair of phases specified by the phases variable of a MATERIAL namelist.

Truchas models the transformation from low temperature phase ("solid") to high temperature phase ("liquid") using a "solid fraction" function  $f_{\rm sol}(T)$  that gives the fraction of low temperature phase as a function of temperature. There are two temperatures  $T_{\rm sol} < T_{\rm liq}$  such that  $f_{\rm sol} = 1$  for  $T \le T_{\rm sol}$ ,  $f_{\rm sol} = 0$  for  $T \ge T_{\rm liq}$ , and  $0 < f_{\rm sol} < 1$  for  $T_{\rm sol} < T < T_{\rm liq}$ . There are two alternative methods for specifying this function.

The first simple, but non-physical, method uses a smooth Hermite cubic polynomial to interpolate  $f_{\text{sol}}$  between  $T_{\text{sol}}$  and  $T_{\text{liq}}$ . This is pictured below. The second method uses a table of  $(T, f_{\text{sol}})$  values to define  $f_{\text{sol}}(T)$ . This allows physics-based phase change models like lever and Scheil to be defined, and data from CALPHAD-type tools to be used directly.

Note that while described in terms of solid and liquid, these phase change models also apply to solid-solid transformations with the obvious reinterpretation of notation.

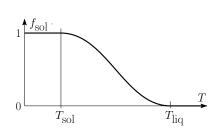
#### Namelist Variables

low\_temp\_phase, high\_temp\_phase

These are the names of the two material phases.

solidus\_temp, liquidus\_temp

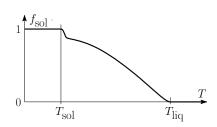
The solidus and liquidus temperatures,  $T_{\rm sol}$  and  $T_{\rm liq}$ . If these variables are defined, the simple solid fraction model is used, which interpolates the solid fraction over the interval  $[T_{\rm sol}, T_{\rm liq}]$  using a smooth Hermite cubic polynomial. These variables are incompatible with solid\_frac\_table.



#### solid\_frac\_table

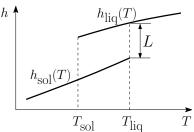
A table of temperature-solid fraction values. The format is the same as described for the FUNCTION namelist Tabular\_Data variable. However the table may be given in either increasing or decreasing temperature order, and the solid fraction values must be strictly monotone. The table endpoints must specify the 1 and 0 solid fractions, and the corresponding temperatures are taken to be  $T_{\rm sol}$  and  $T_{\rm liq}$ , respectively. The solid fraction function is interpolated from this table using Akima smoothing; see the FUNCTION namelist Tabular\_Interp. Additional data points outside the interval  $[T_{\rm sol}, T_{\rm liq}]$  are automatically added to ensure that the solid fraction is constant outside the transformation interval. This variable is incompatible with solidus\_temp and liquidus\_temp.

solid\_frac\_table = 930.0 1.00 931.0 0.95 ... 940.0 0.00



#### latent\_heat

The energy per unit mass L absorbed during the transformation of the material from the low temperature phase to the high temperature phase at the liquidus temperature  $T_{\text{liq}}$ . This property is required when the specific enthalpy of the high temperature phase is defined from its specific heat. Otherwise it is ignored.



# PHYSICAL\_CONSTANTS Namelist

#### Overview

The values of physical constants used in Truchas' physics models are set through this namelist. The default for all these constants is their value in SI units. If a different system of units is used, these may need to be assigned the appropriate values.

## PHYSICAL\_CONSTANTS Namelist Features

Required/Optional: Optional Single/Multiple Instances: Single

# Components

- Absolute\_Zero
- Stefan Boltzmann
- Vacuum\_Permeability
- Vacuum\_Permittivity

# Absolute\_Zero

**Description:** The value of absolute-zero in the temperature scale used. The default value is 0 for Kelvin. Centigrade would use the value -273.15, for example. This constant is used by thermal radiation boundary conditions and enclosure (view factor) radiation.

Physical dimension:  $\Theta$ 

Type: real Default: 0 K

Valid values: any value

#### Stefan\_Boltzmann

**Description:** Stefan-Boltzmann constant for thermal radiation. The default is its value in SI units. This constant is used by thermal radiation boundary condititions and enclosure (view factor) radiation.

Physical dimension:  $E/(T L^2 \Theta^4)$ 

Type: real

**Default:**  $5.67 \times 10^{-8} \text{ W/(m}^2 \text{ K}^4)$ **Valid values:** any positive value

# Vacuum\_Permeability

Description: The magnetic permeability of free space. The default is its value in SI units. This

parameter is used by the electromagnetics solver.

Physical dimension:  $M L T^{-2} I^{-2}$ 

Type: real

**Default:**  $4\pi \times 10^{-7} \text{ H/m}$ 

Valid values: any positive value

# Vacuum\_Permittivity

Description: The electric permittivity of free space. The default is its value in SI units. This parameter

is used by the electromagnetics solver.

Physical dimension:  $M^{-1} L^{-3} T^4 I^2$ 

Type: real

**Default:**  $8.854188 \times 10^{-12} \text{ F/m}$  **Valid values:** any positive value

# PHYSICS Namelist

#### Overview

The PHYSICS namelist specifies which physics models are active in the simulation. The models are implemented by the four primary physics kernels — fluid flow, heat/species transport, induction heating, and solid mechanics — which are weakly coupled using time splitting. A brief overview of the physics kernels follows; see *Truchas Physics and Algorithms* for more details.

Fluid Flow. The fluid flow physics model simulates multi-material, incompressible flow with interface tracking. A gravitational body force is defined using the Body\_Force\_Density variable. See the MATERIAL namelist for a description of the material properties required by the fluid flow model.

Heat and Species Transport. The heat and species transport physics kernel models both heat conduction with thermal (view factor) radiation, and solutal species diffusion and thermodiffusion. These (primarily) diffusive transport processes are fully coupled; advection of enthalpy and solutal species are handled by the fluid flow physics kernel and incorporated as loosely-coupled source terms. Heat transport is enabled using the Heat\_Transport flag, and solves the heat equation

$$\frac{\partial H}{\partial t} = \nabla \cdot K \nabla T + Q + Q_{\text{joule}} + Q_{\text{adv}}, \tag{22.1}$$

with dependent variables temperature T and enthalpy density H. The enthalpy density is algebraically related to temperature as H = f(T) where  $f'(T) = \rho \, c_p$  is the volumetric heat capacity. See the MATERIAL namelist for a description of the material properties required by the heat equation. The optional volumetric heat source Q is defined through the DS\_SOURCE namelist using "temperature" as the equation name. The Joule heating source  $Q_{\text{joule}}$  is computed by the induction heating kernel, and the advected heat  $Q_{\text{adv}}$  by the flow kernel. The boundary conditions on T are defined through the THERMAL\_BC namelists. The initial value of T are defined through the Temperature variable of the BODY namelists. View factor radiation systems which couple to the heat equation are defined using ENCLOSURE\_RADIATION namelists. Solutal species transport is enabled using the Species\_Transport flag, which solves the n coupled equations

$$\frac{\partial \phi_i}{\partial t} = \nabla \cdot D_i(\nabla \phi_i [+S_i \nabla T]) + Q_i + Q_{i,adv}, \quad i = 1, \dots, n,$$
(22.2)

for species concentrations  $\phi_i$ . The number of components n is defined by Number\_of\_Species. The thermodiffusion term in  $[\cdot]$  is only included when coupled with heat transport. See the MATERIAL namelist for defining the diffusivities  $D_i$  and Soret coefficients  $S_i$ . The optional volumetric source  $Q_i$  is defined through the DS\_SOURCE namelist using "concentration i" as the equation name. The advected species source  $Q_{i,\text{adv}}$  is computed by the flow kernel. Boundary conditions on  $\phi_i$  are defined through the SPECIES\_BC namelists. The initial value of the  $\phi_i$  are defined through the Phi variable of the BODY namelists.

**Induction Heating.** The induction heating physics kernel solves for the Joule heat that is used as a source in heat transport. It is enabled using the **Electromagnetics** flag. See the MATERIAL namelist for a description of the material properties required by the electromagnetics solver. The **ELECTROMAGNETICS** namelist is used to describe the induction heating problem.

Solid Mechanics. The solid mechanics physics kernel models small strain elastic and plastic deformation of solid material phases, including deformations induced by temperature changes and solid state phase changes. It is enabled using the Solid\_Mechanics flag. See the MATERIAL namelist for a description of the material properties required by the solid mechanics kernel. Parameters which define the plasticity model are defined using the VISCOPLASTIC\_MODEL namelist. Displacement and traction boundary conditions are defined using the BC namelist. The effect of the gravitational body force defined by Body\_Force\_Density can be included by enabling the Solid\_Mechanics\_Body\_Force flag.

#### PHYSICS Namelist Features

Required/Optional: Required Single/Multiple Instances: Single

# Components

- Body\_Force\_Density
- Electromagnetics
- Flow
- Heat\_Transport
- Materials
- Number\_of\_Species
- Solid\_Mechanics
- Species\_Transport

#### Materials

Description: A list of materials to include in the simulation. These are material names defined in MATERIAL namelists. The list must include all materials assigned to a region in a BODY namelist, or specified as an <code>inflow\_material</code> in a fluid flow boundary condition, but it need not include all materials defined in the input file. Use the reserved name "VOID" to refer to the built-in void pseudo-material.

Type: string list

#### Flow

**Description:** Enables the simulation of fluid flow.

Type: logical

Default: false

### Body\_Force\_Density

**Description:** A constant force per unit mass, **g**, that acts throughout material volumes. The net force on a volume is the integral of its density times **g** over the volume. Typically **g** is the gravitational

acceleration.

Physical dimension:  $L/T^2$ 

Type: real 3-vector **Default:** (0, 0, 0)

Note: The fluid flow model always includes this body force.

The solid mechanics model has the option of including this body force or not; see

Solid\_Mechanics\_Body\_Force.

### Heat\_Transport

**Description:** Enables the calculation of heat conduction, advection, and radiation using the heat/species

transport physics kernel.

Type: logical **Default:** false

### Species\_Transport

**Description:** Enables the calculation of species diffusion and advection using the heat/species transport physics kernel. The number of species components must be specified using Number\_of\_Species.

Type: logical Default: false

### Number\_of\_Species

Description: The number of species components. Required when Species\_Transport is enabled.

Type: integer Default: 0

Valid values: > 0

## Solid\_Mechanics

**Description:** Enables the calculation of solid material stresses and strains.

Type: logical **Default:** false

#### Electromagnetics

**Description:** Enables the calculation of Joule heating.

Type: logical

Default: false

# PROBE Namelist

#### Overview

The PROBE namelist is used to define the location in the computational domain where the value of specific solution quantities will be recorded at every time step. The data is written to a standard multi-column text file specified by the namelist. The solution time is written to the first column and the specified solution quantities to the remaining columns. Useful metadata about the probe is written to the first few lines of the file. These lines begin with a # character and would be treated as comment lines by many post-processors. As many probes as desired may be defined, but each must write to a different file.

#### **Probe Namelist Features**

Required/Optional: Optional

Single/Multiple Instances: Multiple

# Components

- coord
- coord\_scale\_factor
- data
- data\_file
- description
- digits

#### coord

**Description:** The spatial coordinates of the location of the probe. These coordinates may be further scaled by an optional scaling factor; see coord\_scale\_factor.

Type: real 3-vector

Default: none

**Notes:** For cell-centered quantities, data will be taken from the cell whose centroid is nearest this location, and for node-centered quantities data will be taken from the nearest node.

### coord\_scale\_factor

**Description:** A multiplicative scaling factor applied to the coordinates of the probe.

Type: real
Default: 1.0

#### data

**Description:** The data quantity whose value will be recorded. The available options are:

"temperature" Cell-centered temperature
"pressure" Cell-centered fluid pressure
"velocity" Cell-centered fluid velocity

Type: string
Default: none

# data\_file

**Description:** The name of the probe output file. The file will be created in the output directory, and any existing file will be overwritten. Each probe must write to a different output file.

Type: string
Default: none

## description

**Description:** An optional text string that will be written to the header of the output file.

Type: string
Default: none

## digits

**Description:** The number of significant digits in the output data.

Type: integer
Default: 6

### RESTART Namelist

#### Overview

Truchas is able to use data from a previous calculation to initialize a new calculation. Such a *restart* calculation is invoked by using the '-r' commandline argument to the executable with the path name of the restart data file. By default, all appropriate data from the restart file is used. This optional namelist provides variables to limit the restart data that will be used.

#### **RESTART Namelist Features**

Required/Optional: Optional Single/Multiple Instances: Single

#### Components

- Ignore\_T
- Ignore Dt
- Ignore\_Joule\_Heat
- Ignore\_Solid\_Mechanics

#### Ignore\_T

**Description:** When restarting, the initial time and starting cycle count are normally extracted from the restart file. If this flag is true, then those values are ignored and the first value of the <code>Output\_T</code> array is used as the initial time and the cycle count starts at 0, as happens with a non-restart run.

Type: logical **Default:** false

#### Ignore\_Dt

Description: When restarting, the initial time step size is normally extracted from the restart file. If this flag is true, then that value is ignored and the value specified by Dt\_Init from the NUMERICS namelist is used instead. Note that if Dt\_Constant in the NUMERICS namelist is specified then its value is used regardless.

Type: logical

Default: false

#### Ignore\_Joule\_Heat

**Description:** If this flag is true, the Joule heat data in the restart file (if any) will be ignored when initializing the code. This variable is only relevant for restart calculations with **Electromagnetics** enabled in the **PHYSICS** namelist.

Type: logical **Default:** false

#### Ignore\_Solid\_Mechanics

**Description:** If this flag is true, the solid mechanics data in the restart file (if any) will be ingored when initializing the code. This variable is only relevant for restart calculations with Solid\_Mechanics enabled in the PHYSICS namelist.

Type: logical **Default:** false

# SIMULATION\_CONTROL Namelist (Experimental)

#### Overview

There may be points in time during a simulation when something changes abruptly; a boundary condition or source turns on/off, or a physics model is enabled/disabled, for example. In such circumstances it is best to hit these times precisely with a time step and then continue from that point with a reduced step size appropriate to resolving the time transients that result from the impulsive forcing of the model—in essence, to split the simulation seamlessly into a sequence of phases where each phase is a new simulation whose initial state is the final state of the preceding phase. This experimental namelist provides a means for achieving this. The start time of each additional phase subsequent to the initial phase is specified using the Phase\_Start\_Times array, and the initial step size using either the Phase\_Init\_Dt or Phase\_Init\_Dt\_Factor variables. Truchas will hit those times precisely with a time step, smoothly adjusting the step size in advance to avoid abrupt step size changes, and then effectively "restart" the time stepping. Currently this only effects the second-order diffusion solver which maintains a (smooth) history of states at recent time steps. When restarting that history is deleted and time stepping begins fresh using only the current state.

#### SIMULATION\_CONTROL Namelist Features

Required/Optional: Optional

Single/Multiple Instances: Single

#### Components

- Phase\_Init\_Dt
- Phase\_Init\_Dt\_Factor
- Phase\_Start\_Times

#### Phase\_Init\_Dt

Description: The initial time step size to use for each of the simulation phases. This is the analog of Dt\_Init, which is used for the initial (and default) phase of the simulation. Either Phase\_Init\_Dt or Phase\_Init\_Dt\_Factor must be specified, but not both.

Type: real

Default: none

#### Phase\_Init\_Dt\_Factor

**Description:** The initial time step size used for each of the simulation phases is this factor times the last step size of the preceding phase. Either Phase\_Init\_Dt\_Factor or Phase\_Init\_Dt must be

specified, but not both.

Type: real
Default: none

#### Phase\_Start\_Times

**Description:** The list of starting times of each of the phases.

Type: real array
Default: none

**Note:** The initial simulation phase, which is otherwise the only phase, need not be included in this list, though it may be. The provided list of times is sorted, and the first time greater than the initial time is taken as the start of the first phase following the default initial phase; earlier times are ignored.

# SOLID\_MECHANICS Namelist

#### Overview

The SOLID\_MECHANICS namelist sets parameters that are specific to the solid mechanics model and algorithm. This namelist is read whenever the PHYSICS namelist option Solid\_Mechanics is enabled. Parameters for the nonlinear solver used by the algorithm and its preconditioner are specified in NONLINEAR\_SOLVER and LINEAR\_SOLVER namelists. Optional material viscoplasticity models are defined in VISCOPLASTIC\_MODEL namelists.

#### SOLID\_MECHANICS Namelist Features

Required/Optional Required when solid mechanics physics is enabled. Single/Multiple Instances Single

#### Components

- Contact\_Distance
- Contact\_Norm\_Trac
- Contact\_Penalty
- Displacement\_Nonlinear\_Solution
- Solid\_Mechanics\_Body\_Force
- Stress\_Reduced\_Integration
- Strain\_Limit

#### Contact\_Distance

**Description:** A length scale parameter  $\beta$  for the contact function

$$\lambda = \lambda_s * \lambda_\tau$$

where

$$\lambda_s = \begin{cases} 1 & \text{if } s < 0 \\ 0 & \text{if } s > \beta \\ 2(\frac{s}{\beta} - 1)^3 + 3(\frac{s}{\beta} - 1)^2 & \text{if } 0 < s < \beta \end{cases}$$

and

$$\lambda_{\tau} = \begin{cases} 1 & \text{if } \tau_n < 0 \\ 0 & \text{if } \tau_n > \tau^* \\ 2(\frac{\tau_n}{\tau^*} - 1)^3 + 3(\frac{\tau_n}{\tau^*} - 1)^2 & \text{if } 0 < \tau_n < \tau^* \end{cases}$$

$$s = \hat{n} \cdot (u_k - u_i)$$

Physical dimension: L

Type: real Default: 1.0e-7 Valid values:  $(0, \infty]$ 

Notes: The default value is usually a good value for mesh cell sizes in the 1 - 10 mm size range.

#### Contact\_Norm\_Trac

**Description:** A parameter  $\tau^*$  for the contact function

$$\lambda = \lambda_s * \lambda_{\tau}$$

where

$$\lambda_s = \begin{cases} 1 & \text{if } s < 0 \\ 0 & \text{if } s > \beta \\ 2(\frac{s}{\beta} - 1)^3 + 3(\frac{s}{\beta} - 1)^2 & \text{if } 0 < s < \beta \end{cases}$$

and

$$\lambda_{\tau} = \begin{cases} 1 & \text{if } \tau_n < 0 \\ 0 & \text{if } \tau_n > \tau^* \\ 2(\frac{\tau_n}{\tau^*} - 1)^3 + 3(\frac{\tau_n}{\tau^*} - 1)^2 & \text{if } 0 < \tau_n < \tau^* \end{cases}$$

 $\tau_n$  is the normal traction at the interface where a positive value corresponds to a tensile force normal to the surface.

Physical dimension: F/L<sup>2</sup>

Type: real Default: 1.0e4 Valid values:  $[0, \infty]$ 

**Notes:** The default value is probably appropriate for materials with elastic constants in the range  $10^9$  -  $10^{11}$ . This parameter should probably be scaled proportionately for elastic constants that differ from this range.

#### Contact\_Penalty

**Description:** A penalty factor for the penetration constraint in the contact algorithm. Changing this is probably not a good idea in the current version.

Physical dimension: dimensionless

Type: real Default: 1.0e3 Valid values:  $[0, \infty]$ 

Notes:

#### Displacement\_Nonlinear\_Solution

**Description:** A character string pointer to the nonlinear solution algorithm parameters to be used in a Newton-Krylov solution of the nonlinear thermo-elastic viscoplastic equations. This string "points" to a particular NONLINEAR\_SOLVER namelist if it matches the Name input variable string in the NONLINEAR\_SOLVER namelist.

Type: string

Default: "default"

Valid values: arbitrary string

Notes: If this string does not match a Name input variable string specified in a NONLINEAR\_SOLVER namelist, then the default set of nonlinear solution algorithm parameters is used for the thermo-elastic viscoplastic equations.

#### Solid\_Mechanics\_Body\_Force

**Description:** Body forces will be included in the solid mechanics calculation.

Physical dimension:

Type: logical Default: .false.

#### Strain\_Limit

**Description:** This parameter controls the use of the ODE integrator in the plastic strain calculation. It should be set to the minimum significant value of the plastic strain increment for a time step. If convergence seems poor when a viscoplastic material model is used, it may help to reduce the value.

Physical dimension: L/L

 $\mathbf{Type:} \ \mathrm{real}$ 

**Default:** 1.0e-10 **Valid values:**  $\geq 0$ 

**Notes:** This parameter can not be currently used to control the time step. It may be used for such

purposes in future releases.

# SPECIES\_BC Namelist

#### Overview

The SPECIES\_BC namelist is used to define boundary conditions for the species diffusion model at external boundaries. Each instance of the namelist defines a particular condition to impose on a species component over a subset of the domain boundary. The boundary subset  $\Gamma$  is specified using mesh face sets. The namelist variable <code>face\_set\_ids</code> takes a list of face set IDs, and the boundary condition is imposed on all faces belonging to those face sets. Note that ExodusII mesh side sets are imported into Truchas as face sets with the same IDs. The species component is specified using the <code>comp</code> namelist variable. The following types of boundary conditions can be defined. The outward unit normal to the boundary  $\Gamma$  is denoted  $\hat{n}$ .

• Concentration. A concentration Dirichlet condition for species component j

$$\phi_j = c \text{ on } \Gamma \tag{27.1}$$

is defined by setting type to "concentration". The boundary value c is specified using either conc for a constant value, or conc\_func for a function.

 $\bullet$  Flux. A total concentration flux condition for species component j

$$-D_i \nabla \phi_i \cdot \hat{n} = q \text{ on } \Gamma, \tag{27.2}$$

when the system does not include temperature as a dependent variable, or

$$-D_{i}(\nabla \phi_{i} + S_{i}\nabla T) \cdot \hat{n} = q \text{ on } \Gamma$$
(27.3)

when it does, is defined by setting type to "flux". The concentration flux q is specified using either flux for a constant value, or flux\_func for a function.

The specified species concentration boundary conditions are not allowed to overlap, and they must completely cover the computational boundary.

#### SPECIES\_BC Namelist Features

Required/Optional: Required

Single/Multiple Instances: Multiple

#### Components

name

- face\_set\_ids
- comp
- type
- conc
- conc\_func
- flux
- flux\_func

#### name

**Description:** A unique name used to identify a particular instance of this namelist.

Type: string (31 characters max)

Default: none

#### comp

**Description:** The species component this boundary condition applies to.

Type: integer
Default: 1

#### face\_set\_ids

**Description:** A list of face set IDs that define the portion of the boundary where the boundary condition will be imposed.

Type: integer list (32 max)

Default: none

#### type

**Description:** The type of boundary condition. The available options are:

"concentration" Concentration is prescribed on the boundary. Use conc or conc\_func to specify its value.

"flux" Total outward concentration flux is prescribed on the boundary. Use flux or flux\_func to specify its value.

Type: string

Default: none

#### conc

**Description:** The constant value of boundary concentration for a concentration-type boundary condition. To specify a function, use **conc\_func** instead.

Default: none
Type: real

#### conc\_func

**Description:** The name of a FUNCTION namelist defining a function that gives the boundary concentration for a concentration-type boundary condition. The function is expected to be a function of (t, x, y, z).

Default: none
Type: string

#### flux

**Description:** The constant value of the total outward boundary concentration flux for a flux-type boundary condition. To specify a function, use flux\_func instead.

Default: none
Type: real

#### flux\_func

**Description:** The name of a FUNCTION namelist defining a function that gives the total outward boundary concentration flux for a flux-type boundary condition. The function is expected to be a function of (t, x, y, z).

Default: none
Type: string

# THERMAL\_BC Namelist

#### Overview

The THERMAL\_BC namelist is used to define boundary conditions for the heat transfer model at external boundaries and internal interfaces. Each instance of the namelist defines a particular condition to impose over a subset of the domain boundary. The boundary subset  $\Gamma$  is specified using mesh face sets. The namelist variable <code>face\_set\_ids</code> takes a list of face set IDs, and the boundary condition is imposed on all faces belonging to those face sets. Note that ExodusII mesh side sets are imported into Truchas as face sets with the same IDs.

#### External boundaries

The following types of external boundary conditions can be defined. The outward unit normal to the boundary  $\Gamma$  is denoted  $\hat{n}$ .

• Temperature. A temperature Dirichlet condition

$$T = T_b \text{ on } \Gamma$$
 (28.1)

is defined by setting type to "temperature". The boundary value  $T_b$  is specified using either temp for a constant value, or temp\_func for a function.

• Total Flux. A heat flux condition

$$-\kappa \nabla T \cdot \hat{n} = q_b \text{ on } \Gamma \tag{28.2}$$

is defined by setting type to "flux". The heat flux  $q_b$  is specified using either flux for a constant value, or flux func for a function.

• Heat Transfer. An external heat transfer flux condition

$$-\kappa \nabla T \cdot \hat{n} = \alpha (T - T_{\infty}) \text{ on } \Gamma$$
 (28.3)

is defined by setting type to "htc". The heat transfer coefficient  $\alpha$  is specified using either htc for a constant value, or htc\_func for a function, and the ambient temperature  $T_{\infty}$  is specified using either ambient\_temp for a constant value, or ambient\_temp\_func for a function.

• Ambient Radiation. A simple ambient thermal radiation condition

$$-\kappa \nabla T \cdot \hat{n} = \epsilon \sigma \left( (T - T_0)^4 - (T_\infty - T_0)^4 \right) \text{ on } \Gamma$$
(28.4)

is defined by setting type to "radiation". The emissivity  $\epsilon$  is specified using either emissivity for a constant value or emissivity\_func for a function, and the temperature of the ambient environment  $T_{\infty}$  is specified using either ambient\_temp for a constant value, or ambient\_temp\_func for a function. Here  $\sigma$  is the Stefan-Boltzmann constant and  $T_0$  is the absolute-zero temperature, both of which can be redefined if the problem units differ from the default SI units using the Stefan Boltzmann and Absolute Zero components of the PHYSICAL CONSTANTS namelist.

The specified boundary conditions are not generally allowed to overlap. It is not permitted, for example, to imposed both a temperature and a flux condition on the same part of boundary. The one exception is that heat transfer and ambient radiation conditions can be superimposed; the net flux in this case will be the sum of the heat transfer and radiation fluxes.

It is also generally required that the specified boundary conditions completely cover the computational boundary. When enclosure radiation systems are present, however, no boundary condition should be imposed on the part of the boundary that belongs to the enclosures unless it is a heat transfer condition. In that case the net flux is the sum of the heat transfer and radiative (from enclosure radiation) fluxes.

#### Internal interfaces

Internal interfaces are merely coincident pairs of conforming external mesh boundaries. These are modifications to the mesh created by Truchas and are defined using the Interface\_Side\_Sets parameter from the MESH namelist. Only the face set IDs referenced there can be used in the definition of the following interface conditions. The following types of internal interface conditions can be defined.

• Interface Heat Transfer. An interface heat transfer condition models heat transfer across an imperfect contact between two bodies or across a thin subscale material layer lying along an interface  $\Gamma$ . It imposes continuity of the heat flux  $-\kappa\nabla T \cdot \hat{n}$  across the interface  $\Gamma$  and gives this flux as

$$-\kappa \nabla T \cdot \hat{n} = -\alpha[T] \text{ on } \Gamma, \tag{28.5}$$

where [T] is the jump in T across  $\Gamma$  in the direction  $\hat{n}$ . It is defined by setting type to "interface-htc". The heat transfer coefficient  $\alpha$  is specified using either htc for a constant value, or htc func for a function.

• Gap Radiation. A gap radiation condition models radiative heat transfer across a thin open gap lying along an interface  $\Gamma$ . It imposes continuity of the heat flux  $-\kappa \nabla T \cdot \hat{n}$  across  $\Gamma$  and gives the flux as

$$-\kappa \nabla T \cdot \hat{n} = \epsilon_{\Gamma} \sigma \left( (T_{-} - T_{0})^{4} - (T_{+} - T_{0})^{4} \right) \text{ on } \Gamma, \tag{28.6}$$

where  $T_-$  and  $T_+$  denote the values of T on the inside and outside gap surfaces with respect to the normal  $\hat{n}$  to  $\Gamma$ . It is defined by setting type to "gap-radiation". The gap emissivity  $\epsilon_{\Gamma}$  is specified using either emissivity for a constant value, or emissivity\_func for a function. The effective gap emissivity  $\epsilon_{\Gamma}$  depends on the emissivities  $\epsilon_-$  and  $\epsilon_+$  of the surfaces on either side of the gap and is given by

$$\epsilon_{\Gamma} = \frac{\epsilon_{-}\epsilon_{+}}{\epsilon_{-} + \epsilon_{+} - \epsilon_{-}\epsilon_{+}}.$$
(28.7)

The value of the Stefan-Boltzmann constant  $\sigma$  and the absolute-zero temperature  $T_0$  can be redefined if the problem units differ from the default SI units using the Stefan\_Boltzmann and Absolute\_Zero components of the PHYSICAL\_CONSTANTS namelist.

#### THERMAL\_BC Namelist Features

Required/Optional: Required

Single/Multiple Instances: Multiple

#### Components

- name
- face\_set\_ids
- type
- temp

- temp\_func
- flux
- flux\_func
- htc
- htc\_func
- ambient\_temp
- ambient\_temp\_func
- emissivity
- emissivity\_func

#### name

**Description:** A unique name used to identify a particular instance of this namelist.

Type: string (31 characters max)

Default: none

#### face\_set\_ids

**Description:** A list of face set IDs that define the portion of the boundary where the boundary condition will be imposed.

Type: integer list (32 max)

Default: none

#### type

**Description:** The type of boundary condition. The available options are:

- "temperature" Temperature is prescribed on the boundary. Use temp or temp\_func to specify its value.
- "flux" Outward heat flux is prescribed on the boundary. Use flux or flux\_func to set its value.
- "htc" External heat transfer condition. Use htc or htc\_func to set the heat transfer coefficient, and ambient\_temp or ambient\_temp\_func to set the ambient temperature.
- "radiation" A simple ambient thermal radiation condition. Use emissivity or emissivity\_func to set the emissivity, and ambient\_temp or ambient\_temp\_func to set the temperature of the ambient environment.
- "interface-htc" An internal interface heat transfer condition. Use htc or htc\_func to set the heat transfer coefficient.
- "gap-radiation" A gap thermal radiation condition. Use emissivity or emissivity\_func to set the emissivity.

Type: string
Default: none

#### temp

**Description:** The constant value of boundary temperature for a temperature-type boundary condition. To specify a function, use temp\_func instead.

**Default:** none **Type:** real

#### temp\_func

**Description:** The name of a FUNCTION namelist defining a function that gives the boundary temperature for a temperature-type boundary condition. The function is expected to be a function of (t, x, y, z).

**Default:** none **Type:** string

#### flux

**Description:** The constant value of the outward boundary heat flux for a flux-type boundary condition. To specify a function, use **flux func** instead.

Default: none
Type: real

#### flux\_func

**Description:** The name of a FUNCTION namelist defining a function that gives the outward boundary heat flux for a flux-type boundary condition. The function is expected to be a function of (t, x, y, z).

**Default:** none **Type:** string

#### htc

**Description:** The constant value of the heat transfer coefficient for either an external or interface heat transfer-type boundary condition. To specify a function, use <a href="https://http

Default: none
Type: real

#### htc\_func

**Description:** The name of a FUNCTION namelist defining a function that gives the heat transfer coefficient for either an external or interface heat transfer-type boundary condition. The function is expected to be a function of (t, x, y, z) for an external heat transfer-type boundary condition, and a function of (T, t, x, y, z) for an interface heat transfer-type boundary condition. In the latter case T is taken to be the maximum of the two temperatures on either side of the interface.

Default: none Type: string

#### ambient\_temp

**Description:** The constant value of the ambient temperature for external heat transfer or radiation-type boundary condition. To specify a function, use ambient\_temp\_func instead.

Default: none
Type: real

### ambient\_temp\_func

**Description:** The name of a FUNCTION namelist defining a function that gives the ambient temperature for external heat transfer or radiation-type boundary condition. The function is expected to be a function of (t, x, y, z).

Default: none
Type: string

#### emissivity

**Description:** The constant value of emissivity for a radiation-type boundary condition. To specify a function, use emissivity\_func instead.

Default: none
Type: real

#### emissivity\_func

**Description:** The name of a FUNCTION namelist defining a function that gives the emissivity for a radiation-type boundary condition. The function is expected to be a function of (t, x, y, z).

Default: none
Type: string

# THERMAL\_SOURCE Namelist

#### Overview

The THERMAL\_SOURCE namelist is used to define external volumetric heat sources (power per unit volume). This source is in addition to any other sources coming from other physics, such as a Joule heat source. Each instance of this namelist defines a source, and the final source is the sum of all such sources (subject to some limitations).

Two forms of sources q can be defined:

- (1)  $q(t, \mathbf{x}) = f(t, \mathbf{x}) \chi_S(\mathbf{x})$ , where f is a user-defined function and S is a subdomain corresponding to one or more user-specified mesh cell sets. Here  $\chi_S$  is the characteristic function on S:  $\chi_S = 1$  for  $\mathbf{x} \in S$  and  $\chi_S = 0$  for  $\mathbf{x} \notin S$ . Sources of this form can be summed as long as the interiors of their subdomains do not intersect.
- (2)  $q(t, \mathbf{x}) = A(t) \sum_{j} q_{j} \chi_{j}(\mathbf{x})$ , where A is a user-defined time-dependent prefactor,  $q_{j}$  is a constant source on mesh cell j, and  $\chi_{j}$  is the characteristic function on cell j. The collection of values  $\{q_{j}\}$  is read from a data file.

#### THERMAL\_SOURCE Namelist Features

Required/Optional: Optional

Single/Multiple Instances: Multiple

#### Components

- name
- cell\_set\_ids
- data\_file
- prefactor
- prefactor\_func
- source
- source\_func

#### name

**Description:** A unique name used to identify a particular instance of this namelist.

**Type:** string (31 characters max)

Default: none

#### cell\_set\_ids

**Description:** A list of cell set IDs that define the subdomain where the source is applied.

**Type:** a list of up to 32 integers

Default: none

Valid values: any valid mesh cell set ID

Note: Different instances of this namelist must apply to disjoint subdomains; overlapping of source

functions of this form is not supported.

Exodus II mesh element blocks are interpreted by Truchas as cell sets having the same IDs.

#### source

**Description:** The constant value of the heat source. To specify a function, use source\_func instead.

Physical dimension:  $E/T L^3$ 

Type: real
Default: none

#### source\_func

**Description:** The name of a FUNCTION namelist that defines the source function. That function is

expected to be a function of (t, x, y, z).

Type: string
Default: none

#### data\_file

**Description:** The path to the data file. It is expected to be a raw binary file consisting of a sequence of 8-byte floating point values, the number of which equals the number of mesh cells. The order of the values is assumed to correspond to the external ordering of the mesh cells. The file can be created with most any programming language. In Fortran use an unformatted stream access file.

#### prefactor

**Description:** The constant value of the prefactor A. For a function use prefactor\_func.

#### prefactor\_func

**Description:** The name of a FUNCTION namelist that defines the function that computes the value of the time dependent prefactor A(t).

# TOOLPATH Namelist (Experimental)

#### Overview

The TOOLPATH namelist defines a path through space, especially that taken by a machine tool, such as a laser or build platform, in the course of a manufacturing process. Its use is not limited to such cases, however. The path is specified using a simple command language that is adapted to common CNC machine languages. The current implementation is limited to a path through Cartesian 3-space (3-axis). The command language is described at the end of the chapter.

#### **TOOLPATH Namelist Features**

Required/Optional: Optional

Single/Multiple Instances: Multiple

#### Components

- Name
- Command\_String
- Command\_File
- Start\_Time
- Start\_Coord
- Time\_Scale\_Factor
- Coord\_Scale\_Factor
- Write\_Plotfile
- Plotfile\_Dt
- Partition\_Ds

#### Name

**Description:** A unique name used to identify a particular instance of this namelist. Clients will reference the toolpath using this name.

**Type:** case sensitive string (31 characters max)

Default: none

#### Command\_String

**Description:** A string from which to read the commands that define the toolpath. This is only suitable for relatively simple paths; use Command\_File instead for more complex paths.

Type: string (1000 characters max)

Default: none

Notes: Use single quotes to delimit the string to avoid conflicts with double quotes used within the

commands.

#### Command\_File

**Description:** The path to a file from which to read the commands that define the toolpath. If not an absolute path, it will be interpreted as a path relative to the Truchas input file directory.

Type: string

Default: none

Notes: C++ style comments may used in the file; all text from the '//' to the end of the line is ignored.

#### Start\_Time

**Description:** The starting time of the toolpath.

Type: real
Default: 0

#### Start\_Coord

**Description:** The starting coordinates of the toolpath.

Type: real 3-vector **Default:** (0,0,0)

#### Time\_Scale\_Factor

**Description:** An optional multiplicative factor by which to scale all time values. This applies to all namelist variables as well as toolpath commands.

Type: real
Default: 1

Valid values: > 0

**Notes:** This is applied appropriately to speeds and accelerations in the toolpath commands.

#### Coord\_Scale\_Factor

**Description:** An optional multiplicative factor by which to scale all coordinate values. This applies to all namelist variables as well as toolpath commands.

Type: real
Default: 1

Valid values: > 0

**Notes:** This is applied appropriately to speeds and accelerations in the toolpath commands.

#### Write\_Plotfile

**Description:** Enable this flag to have a discrete version of the toolpath written to a disk file. The file will be located in the Truchas output directory and be named toolpath-name.dat, where name is the name assigned to the namelist. If enabled, Plotfile\_Dt must be specified.

Type: logical

Default: .false.

Notes: The file is a multi-column text file where each line gives the toolpath data at a specific time. The columns are, in order, the segment index, the time, the three position coordinates, and the flag settings (0 for clear and 1 for set). Not all flags are written, only those that were set at some point. The initial comment line starting with a '#' labels the columns. Data is written at the end point times of each path segment, and at zero or more equally spaced times within each segment interval. The latter frequency is determined by Plotfile\_Dt.

#### Plotfile\_Dt

**Description:** Output time frequency used when writing the toolpath to a disk file. See Write Plotfile.

Type: real
Default: none
Valid values: > 0

#### Partition\_Ds

**Description:** Assign a value to this parameter to generate an additional discrete version of the toolpath that is required by some clients. The value specifies the desired spacing in path length. Refer to the client's documentation on whether this is needed and for further information.

Type: real
Default: none
Valid values: > 0

Notes: Some clients require a discrete version of the toolpath that consists of a time-ordered sequence of (time, coordinate) pairs. The sequence includes the end points of the segments. In addition each segment is partitioned into one or more parts of equal path length approximately equal to, but no greater than Partition\_Ds.

#### The Toolpath Command Language

A toolpath is represented as a sequence of n+2 continuous path segments defined on time intervals  $(-\infty, t_0]$ ,  $[t_0, t_1]$ ,  $[t_1, t_2]$ , ...,  $[t_n, \infty)$ . The individual segments are simple paths (e.g., no motion or linear motion) that are defined by path commands. A set of flags (0 through 31) is associated with each path segment. Clients of a toolpath can use the setting of a flag (set or clear) for a variety of purposes; for example, to indicate that a device is on or off for the duration of the segment.

The toolpath command language is expressed using JSON text. The specification of a toolpath takes the form

```
[command, command, ...]
```

where *command* is one of the following:

```
["dwell",dt]
```

Remain at the current position for the time interval dt.

```
["moverel", [dx, dy, dz], s, a, d]
```

Linear displacement from the current position. Motion accelerates from rest to a constant speed, and then decelerates to rest at the position (dx, dy, dz) relative to the current position. The linear speed, acceleration, and deceleration are s, a, and d, respectively. If d is omitted, its value is taken to be a. If both a and d are omitted then instantaneous acceleration/deceleration to speed s is assumed.

```
["setflag",n_1,n_2,...]
```

Sets or clears the listed flags. 32 flags (0 through 31) are available. The setting of a flag holds for all subsequent motions (above) until changed.

Except for the integer flag numbers, the real numeric values may be entered as integer or floating point numbers; that is, "1" is an acceptable alternative to "1.0".

The initial and final unbounded path segments are automatically generated and are not specified. The initial segment is a dwell at the position given by  $Start\_Coord$  that ends at time  $t_0$  given by  $Start\_Time$ . Likewise the final segment is a dwell starting at a time and at a position determined by the preceding sequence of path segments. All flags start clear in the initial segment.

# TURBULENCE Namelist

#### Overview

The presence of the TURBULENCE namelist enables a simple algebraic turbulence model for viscous flow problems. The turbulent kinetic viscosity  $\nu_t$  ( =  $\mu_t/\rho$ ) is taken to be

$$\nu_t = c_\mu k^{\frac{1}{2}} l \tag{31.1}$$

where  $c_{\mu}$  is a proportionality constant, l is a length scale corresponding to the eddy size, and

$$k = f \cdot \frac{1}{2}u^2 \tag{31.2}$$

is the local turbulent kinetic energy per unit mass, modeled as a fraction f of the mean kinetic energy. The namelist variables give values for the model parameters. See  $Truchas\ Physics\ and\ Algorithms$  for more details.

#### TURBULENCE Namelist Features

Required/Optional: Optional

Single/Multiple Instances: Single

#### Components

• CMU

• KE\_fraction

• Length

#### Turbulence\_CMU

**Description:** Value of the parameter  $c_{\mu}$  in (31.1).

Type: real
Default: 0.05
Valid values: > 0

**Notes:** The default value is appropriate in most situations.

#### Turbulence\_KE\_Fraction

**Description:** Value of the parameter f in (31.2).

Type: real
Default: 0.1

Valid values: (0,1)

**Notes:** The default value is appropriate in most situations.

#### Turbulence\_Length

**Description:** Value of the length scale parameter l in (31.1).

Physical dimension: L

Type: real
Default: none
Valid values: > 0

Notes: The value should correspond to the size of the turbulent eddies. In turbulent pipe flow, for

example, this would be one third the pipe radius.

# **VFUNCTION Namelist**

#### Overview

Similar to the FUNCTION namelist, the VFUNCTION namelist is used to define a vector-valued function that can be used in some situations where vector-valued data is needed, such as the specification of the boundary velocity in a flow boundary condition.

These are general vector-valued functions of one or more variables,  $\mathbf{y} = (y_1, \dots, y_m) = \mathbf{f}(x_1, \dots, x_n)$ . The dimension of the value, the number of variables, and the unknowns they represent (i.e., time, position, temperature, etc.) all depend on the context in which the function is used, and that is described in the documentation of those namelists where these functions can be used. Currently only a single function type can be defined:

**Tabular Function.** This is a continuous, single-variable function  $\mathbf{y} = \mathbf{f}(s)$  linearly interpolated from a sequence of data points  $(s_i, \mathbf{y}_i)$ ,  $i = 1, \ldots, p$ , with  $s_i < s_{i+1}$ . The variable  $x_d$  that is identified with s is specified by tabular\_dim.

#### FUNCTION Namelist Features

Required/Optional: Optional

Single/Multiple Instances: Multiple

#### Components

- Name
- Type
- Tabular\_Data
- Tabular\_Dim

#### Name

**Description:** A unique name by which this vector function can be referenced by other namelists.

**Type:** A case-sensitive string of up to 31 characters.

Default: None

#### Type

**Description:** The type of function defined by the namelist.

 $\mathbf{Type:}\ \mathrm{case}\text{-sensitive string}$ 

Default: none

Valid values: "tabular" for a tabular function

#### Tabular\_Data

**Description:** The table of values  $(s_i, \mathbf{y}_i)$  defining a tabular function  $\mathbf{y} = \mathbf{f}(s)$ . Use **Tabular\_Dim** to set the variable identified with s.

Type: real array
Default: none

**Notes:** This is a  $(m+1) \times p$  array that is most easily specified in the following manner

```
\begin{split} \text{Tabular\_Data(:,1)} &= s_1, \ y_{11}, \ \dots, \ y_{m1} \\ \text{Tabular\_Data(:,2)} &= s_2, \ y_{12}, \ \dots, \ y_{m2} \\ &\vdots \\ \text{Tabular\_Data(:,p)} &= s_p, \ y_{1p}, \ \dots, \ y_{mp} \end{split}
```

#### Tabular\_Dim

**Description:** The dimension in the m-vector of independent variables that serves as the independent variable for the single-variable tabular function.

Type: integer Default: 1

# VISCOPLASTIC\_MODEL Namelist

#### Overview

The VISCOPLASTIC\_MODEL namelist defines the viscoplastic model to be used for a particular solid material phase in material stress-strain calculations. Two viscoplastic models are available: a mechanical threshold stress (MTS) model and a power law model. When no model is given for a solid material phase, it is modeled as a purely elastic material. The models specify a relation for the effective plastic strain rate  $\dot{\epsilon}$  as a function of temperature T and von Mises stress  $\sigma$ . For more details on the models see the Truchas Physics and Algorithms manual. Briefly:

Power Law Model. In the simple power law model, the strain rate relation is

$$\dot{\epsilon} = A \exp(-Q/RT) \,\sigma^n,\tag{33.1}$$

where A, n, Q, and R are parameters given by this namelist. **MTS Model**. The MTS model uses the strain rate relation

$$\dot{\epsilon} = \dot{\epsilon}_{0i} \exp\left[-\frac{\mu b^3 g_{0i}}{kT} \left(1 - \left(\frac{\mu_0}{\mu \sigma_i} (\sigma - \sigma_a)\right)^{p_i}\right)^{q_i}\right], \qquad \mu = \mu_0 - \frac{D}{\exp(T_0/T) - 1}$$
(33.2)

where  $\dot{\epsilon}_{0i}$ ,  $g_{0i}$ , b, k, D,  $\mu_0$ ,  $T_0$ ,  $\sigma_i$ ,  $\sigma_a$ ,  $p_i$ , and  $q_i$  are parameters given by this namelist. When  $\sigma < \sigma_a$  we instead use  $\dot{\epsilon} = K \sigma^5$ , where K is chosen to give continuity with the previous relation at  $\sigma = \sigma_a$ . And when  $\sigma - \sigma_a > \mu \sigma_i/\mu_0$  we take  $\dot{\epsilon} = \dot{\epsilon}_{0i}$ .

#### SURFACE\_TENSION Namelist Features

Required/Optional: Optional; only relevant when Solid\_Mechanics is true. Single/Multiple Instances: Multiple; at most one per solid material phase.

#### Components

- Phase
- Model
- MTS\_b
- MTS\_d
- MTS\_edot\_0i
- MTS\_g\_Oi
- MTS\_k
- MTS\_mu\_0

- MTS\_p\_i
- MTS\_q\_i
- MTS\_sig\_a
- MTS\_sig\_i
- MTS\_temp\_0
- Pwr\_Law\_A
- Pwr\_Law\_N
- Pwr\_Law\_Q
- Pwr\_Law\_R

#### Phase

Description: The name of the material PHASE to which this viscoplastic model applies.

Type: case-sensitive string

Default: none

#### Model

**Description:** The type of viscoplastic strain rate model.

Type: case-insensitive string

Default: none

Valid values: "MTS", "power law", "elastic"

Notes: The effect of the "elastic" option is equivalent to not specifying a viscoplastic model at all; it is

provided as a convenience.

#### MTS\_b

**Description:** Burger's vector length b in (33.2).

Physical dimension: L

Type: real
Default: none
Valid values: > 0

#### MTS\_d

**Description:** Constant D used in (33.2).

Physical dimension: F/L<sup>2</sup>

Type: real

Default: none

#### MTS\_edot\_0i

**Description:** Reference strain rate  $\dot{\epsilon}_{0i}$  used in (33.2).

Physical dimension:  $\mathsf{T}^{-1}$ 

Type: real
Default: none
Valid values: > 0

#### MTS\_g\_0i

**Description:** Material constant  $g_{0i}$  used in (33.2).

Type: real
Default: none
Valid values: > 0

#### MTS\_k

**Description:** Boltzmann's constant k used in (33.2).

Physical dimension:  $E/\Theta$ 

Type: real
Default: none
Valid values: > 0

**Note:** Temperature should be expressed in Kelvin, or other temperature scale where 0 corresponds to absolute zero. If SI units are being used, k should be  $1.38 \times 10^{-23}$ . Use a value appropriate to the

units used in (33.2).

#### MTS\_mu\_0

**Description:** Reference value  $\mu_0$  for the temperature dependent shear modulus used in (33.2).

Physical dimension: F/L<sup>2</sup>

Type: real
Default: none
Valid values: > 0

#### MTS\_p\_i

**Description:** Exponent term  $p_i$  used in (33.2).

Type: real
Default: none
Valid values: > 0

#### MTS\_q\_i

**Description:** Exponent term  $q_i$  used in (33.2).

Type: real
Default: none
Valid values: > 0

#### MTS\_sig\_a

**Description:** The athermal stress term  $\sigma_a$  in (33.2).

Physical dimension: F/L<sup>2</sup>

Type: real Default: none Valid values:  $\geq 0$ 

#### MTS\_sig\_i

**Description:** A stress term  $\sigma_i$  related to obstacles to dislocation motion in (33.2).

Physical dimension:  $F/L^2$ 

Type: real
Default: none
Valid values: > 0

#### MTS\_temp\_0

**Description:** Constant  $T_0$  used in the temperature dependent shear modulus equation in (33.2).

Physical dimension:  $\Theta$ 

Type: real
Default: none
Valid values: > 0

#### Pwr\_Law\_A

**Description:** Constant term A in (33.1).

Physical dimension: F/L<sup>2</sup>

#### Pwr\_Law\_N

**Description:** Stress exponent term n in (33.1).

Type: real
Default: none
Valid values: > 0

#### Pwr\_Law\_Q

**Description:** Activation energy Q in (33.1).

 ${\bf Physical\ dimension:}\ {\sf E/mol}$ 

Type: real Default: none Valid values:  $\geq 0$ 

#### Pwr\_Law\_R

**Description:** Gas constant R in (33.1).

Physical dimension:  $E/(\Theta \text{ mol})$ 

Type: real  $\mathbf{Default:}$  none  $\mathbf{Valid\ values:} > 0$ 

Note: Temperature should be expressed in Kelvin, or other temperature scale where 0 corresponds to

absolute zero. Use the value for R appropriate to the units used in (33.1).

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# Index

Abs_Conc_Tol, 21, 22, 26, 27	BC_Name, 9, 10
Abs_Enthalpy_Tol, 21, 22, 27	BC_Table, 9, 11
Abs_Temp_To1, 21, 23, 28	BC_Type, 9-11
abs_tol, 58	BC_Value, 9, 11
Absolute_Zero, 40, 89, 109, 110	BC_Variable, 9-11
Activation_Energy, 45, 46	BODY, 15, 91, 92
Alittle, 81	axis, 15-18
ALTMESH, 5, 33, 34, 75	fill, 15-18
Altmesh_Coordinate_Scale_Factor, 5	height, $15, 16, 18$
${\tt Altmesh\_File},  5$	length, 15-18
First_Partition, 5, 7	$\mathtt{material\_name},\ 15,\ 16$
${ t Grid\_Transfer\_File,5,6}$	$\mathtt{material\_number}, 15$
Partition_File, $5$ , $6$	$mesh_material_number, 15, 16, 18$
Partitioner, $5, 6$	$\mathtt{Phi},91$
Altmesh_Coordinate_Scale_Factor, 5	$\mathtt{phi},15,17$
Altmesh_File, 5	radius, 15, 17, 18
Ambient_Constant, 39, 40	$rotation\_angle, 15, 17, 18$
Ambient_Function, 39, 40	$rotation_pt, 15, 17, 18$
ambient_temp, 109, 111, 112	$surface_name, 15, 17$
ambient_temp_func, 109, 111-113	Temperature, $91$
axis, 15-18	temperature, $15$ , $18$
	$temperature\_function, 15, 18$
BC, 9, 92	$\mathtt{translation\_pt}, 15, 17, 18$
$BC_Name, 9, 10$	velocity, $15$ , $19$
BC_Table, 9, 11	Body_Force_Density, 91, 92
BC_Type, 9-11	Bounding_Box, 9, 11
$BC_Value, 9, 11$	
BC_Variable, 9-11	Cell_Set_IDs, 31
Bounding_Box, $9$ , $11$	$\mathtt{cell\_set\_ids}, 115, 116$
${\tt Conic\_Constant},9,11,14$	Center, 68
${\tt Conic\_Tolerance,9,11,14}$	CG_Stopping_Tolerance, 33, 34, 36
$\mathtt{Conic}_{\mathtt{X}},\ 10,\ 12,\ 14$	CMU, 121
$\texttt{Conic}_XX, 10, 12, 14$	Command_File, 117, 118
$\texttt{Conic}_XY, 10, 12, 14$	Command_String, 117
$\texttt{Conic}_XZ, 10, 12, 14$	comp, 105, 106
$\mathtt{Conic}_{\mathtt{Y}}, 10, 12, 14$	conc, 105, 106
$\mathtt{Conic}_{\mathtt{YY}}, 10, 12, 14$	$\mathtt{conc\_func}, 105107$
$\texttt{Conic}_{YZ}, 10, 13, 14$	${\tt Cond\_Vfrac\_Threshold}, {\tt 21}, {\tt 23}$
$\texttt{Conic}_{2}, 10, 13, 14$	Conic_Constant, 9, 11, 14
${\tt Conic\_ZZ}, 10, 13, 14$	Conic_Tolerance, 9, 11, 14
$\texttt{Mesh\_Surface},\ 10,\ 13,\ 14$	Conic_X, 10, 12, 14
${\tt Node\_Disp\_Coords}, 10, 13, 14$	Conic_XX, 10, 12, 14
$Surface_Name, 9-11, 13$	Conic_XY, 10, 12, 14

Conic_XZ, 10, 12, 14	Equation, $31$
Conic_Y, 10, 12, 14	Source_Constant, 31, 32
Conic_YY, 10, 12, 14	Source_Function, $31$ , $32$
Conic_YZ, 10, 13, 14	$\mathtt{dsigma}, 54, 55$
Conic_Z, 10, 13, 14	Dt_Constant, 21, 81, 83, 84, 97
Conic_ZZ, 10, 13, 14	Dt_Grow, 21, 81, 83
Contact_Distance, 101	Dt_Init, 81, 83, 84, 97, 99
Contact_Norm_Trac, 101, 102	Dt_Max, 81, 83, 84
Contact_Penalty, 101, 102	Dt_Min, 81, 83, 84
conv_rate_tol, 58	_ , , , , , , , , , , , , , , , , , , ,
coord, 95	ELECTROMAGNETICS, 33, 67, 68, 92
Coord_Scale_Factor, 39, 40, 117, 118	CG_Stopping_Tolerance, 33, 34, 36
coord_scale_factor, 95, 96	EM_Domain_Type, 33, 34, 38
coordinate_scale_factor, 76, 78	Graphics_Output, 33, 34
courant_number, 47, 48	Material_Change_Threshold, 33, 35
Current, 37, 68	Maximum_CG_Iterations, 33, 35
Cutvof, 81, 82	Maximum_Source_Cycles, 33, 35
Cycle_Max, 81, 82	Num_Etasq, 33, 36
Cycle_Number, 81, 82	Output_Level, 33, 36
Cycle_Number, 81, 82	Source_Frequency, 33, 36, 37
data, 95, 96	Source_Times, 33, 36-38, 68
data_file, 95, 96, 115, 116	SS_Stopping_Tolerance, 33, 35-37
data_iiie, 35, 36, 115, 116 description, 95, 96	Steps_Per_Cycle, 33, 37
DIFFUSION_SOLVER, 21	Symmetry_Axis, 33, 34, 38
Abs_Conc_Tol, 21, 22, 26, 27	Uniform_Source, 33, 36-38
Abs_Enthalpy_Tol, 21, 22, 27	Electromagnetics, 5, 92, 93, 98
Abs_Temp_Tol, 21, 23, 28	EM_Domain_Type, 33, 34, 38
Cond_Vfrac_Threshold, 21, 23	emissivity, 109-111, 113
Hypre_AMG_Debug, 21, 24	Emissivity_Constant, 43, 44
Hypre_AMG_Logging_Level, 21, 24	emissivity_func, 109-111, 113
Hypre_AMG_Print_Level, 21, 24	Emissivity_Function, 43, 44
Max_NLK_Itr, 22, 24	Enclosure_File, 39
Max_NLK_Vec, 22, 25	Enclosure_Name, 43
Max_Step_Tries, 22, 25	ENCLOSURE_RADIATION, 39, 43, 91
NLK_Preconditioner, 22, 24, 25	Ambient_Constant, 39, 40
NLK_To1, 22, 26	Ambient_Function, 39, 40
NLK_Vec_Tol, 22, 26	Coord_Scale_Factor, 39, 40
Num_Species, 17	Enclosure_File, 39
${\tt PC\_AMG\_Cycles}, 22, 26$	Error_Tolerance, $39,40$
${\tt PC\_SSOR\_Relax,22,26}$	Name, $39$
$PC\_SSOR\_Sweeps, 22, 26$	${\tt Precon\_Coupling\_Method}, 39, 41$
$\texttt{Rel\_Conc\_Tol}, 22, 27$	$\texttt{Precon\_Iter},\ 39,\ 41$
$\mathtt{Rel\_Enthalpy\_Tol},\ 22,\ 23,\ 27$	${\tt Precon\_Method}, 39, 41$
$\mathtt{Rel\_Temp\_Tol},\ 22,\ 23,\ 27$	Skip_Geometry_Check, $39, 41$
Residual_Atol, $22$ , $28$	$\mathtt{toolpath},\ 39,\ 41$
${\tt Residual\_Rtol}, 22, 28$	ENCLOSURE_SURFACE, 43
${\tt Stepping\_Method}, 21, 22, 28$	Emissivity_Constant, $43$ , $44$
Verbose_Stepping, $22, 28$	Emissivity_Function, 43, 44
${\tt Void\_Temperature}, 22, 29$	${\tt Enclosure\_Name},43$
$\mathtt{digits},95,96$	${\tt Face\_Block\_IDs},43$
Discrete_Ops_Type, $81-83$	$\mathtt{Name},43$
Displacement_Nonlinear_Solution, 101, 103	Equation, $31$
DS_SOURCE, 31, 91	Error_Tolerance, 39, 40
Cell_Set_IDs, 31	EVAPORATION, $45$

Activation_Energy, $45$ , $46$	FUNCTION, 18, 32, 40, 44, 55, 61, 72, 88, 107, 112,
Face_Set_IDs, 45	113, 116, 123
Prefactor, 45	Library_Path, 62
Temp_Exponent, 45, 46	Library_Symbol, 62, 63
exodus_block_modulus, 75, 76	Name, $62$
, ,	Parameters, $62$ , $63$
Face_Block_IDs, 43	Poly_Coefficients, 61-63
Face_Set_IDs, 45	Poly_Exponents, 61-63
face_set_ids, 53, 54, 76, 105, 106, 109-111	Poly_Refvars, 61-63
FF_Discrete_Ops_Type, 83	Smooth_Step_X0, 62, 65
fill, 15–18	Smooth_Step_X1, 62, 65
First_Partition, 5, 7	Smooth_Step_Y0, 62, 65
first_partition, 76, 79	Smooth_Step_Y1, 62, 66
fischer_dim, 47, 50	Tabular_Data, 62, 64, 88
FLOW, 47, 73	Tabular_Dim, 62, 64
courant_number, 47, 48	Tabular_Extrap, 61, 62, 64
fischer_dim, 47, 50	Tabular_Interp, 61, 62, 64, 88
fluid_frac_threshold, 47, 50	Type, 62
	1ype, 02
inviscid, 47-49	gap_element_blocks, 75, 76
material_priority, 47, 49	Graphics_Output, 33, 34
min_face_fraction, 47, 50	Grid_Transfer_File, 5, 6
nested_dissection, 47, 49	d11d_11d1b1b1_1110, 0, 0
track_interfaces, 47, 49	$\texttt{Heat\_Transport},\ 21,\ 91-93$
viscous_implicitness, 47, 48, 57	height, 15, 16, 18
viscous_number, 47, 48	high_temp_phase, 87
void_collapse, 47, 50	htc, 109-112
void_collapse_relaxation, 47, 50	htc_func, 109-112
vol_frac_cutoff, 47, 50	Hypre_AMG_Debug, 21, 24
vol_track_subcycles, 47, 49	Hypre_AMG_Logging_Level, 21, 24
Flow, 47, 92	Hypre_AMG_Print_Level, 21, 24
FLOW_BC, 47, 53	mypro_mid_rrino_dever, zr, zr
$\mathtt{dsigma}, 54, 55$	Ignore_Dt, 84, 97
$\mathtt{face\_set\_ids}, 53, 54$	Ignore_Joule_Heat, 97, 98
${\tt inflow\_material}, 54, 55, 92$	Ignore_Solid_Mechanics, 97, 98
${ t inflow\_temperature},\ 54,\ 56$	Ignore_T, 97
$\mathtt{name}, 54$	INDUCTION_COIL, 33, 36-38, 67
$\mathtt{pressure}, 5355$	Center, 68
${\tt pressure\_func}, 5355$	Current, 37, 68
${\tt type,}\ 53,\ 54$	Length, 68
velocity, $53-55$	NTurns, 68
$\verb velocity_func , 53-55 $	Radius, 68
FLOW_PRESSURE_SOLVER, 47, 57	inflow_material, $54$ , $55$ , $92$
flow_solvers	inflow_temperature, 54, 56
$abs\_tol, 58$	Int_Output_Dt_Multiplier, 85
$\verb"conv_rate_tol", 58"$	Interface_Side_Sets, 110
krylov_dim, 57	interface_side_sets, 53, 75, 76
${\tt krylov\_method}, 57$	inviscid, 47-49
$ exttt{max\_ds\_iter}, 58$	Invitora, iv io
print_level, 58	KE_fraction, 121
rel_tol, 58	krylov_dim, 57
FLOW_VISCOUS_SOLVER, 47-49, 57	krylov_method, 57
fluid_frac_threshold, 47, 50	J
flux, 105–107, 109, 111, 112	latent_heat, 88
flux func 105–107 109 111 112	I.E.GACY FI.OW

FF_Discrete_Ops_Type, $83$	$\mathtt{MTS}_{\mathtt{p}}\mathtt{i},\ 126,\ 127$
Length, 68, 121	$MTS_q_i, 126, 127$
length, 15-18	MTS_sig_a, 126, 128
Library_Path, 62	MTS_sig_i, 126, 128
Library_Symbol, 62, 63	MTS_temp_0, 126, 128
LINEAR_SOLVER, 101	_ ,_ ,
liquidus_temp, 87	Name, $39, 43, 62, 103, 117, 123$
low_temp_phase, 87	$\mathtt{name}, 71$
1 -1 · · · · · · · · · · · · · · · · · ·	name, 54, 105, 106, 110, 111, 115
MATERIAL, 33, 71, 87, 91, 92	$\mathtt{nested\_dissection},\ 47,\ 49$
$\mathtt{name}, 71$	$\mathtt{NLK\_Preconditioner},\ 22,\ 24,\ 25$
phases, 71	$NLK_{Tol}, 22, 26$
phases, 87	$\texttt{NLK\_Vec\_Tol},\ 22,\ 26$
Material_Change_Threshold, 33, 35	${ t Node\_Disp\_Coords}, 10, 13, 14$
material_name, 15, 16	$noise\_factor, 75, 78$
material_number, 15	NONLINEAR_SOLVER, 101, 103
material_priority, 47, 49	Name, $103$
Materials, 92	NTurns, 68
	Num_Etasq, 33, 36
materials, 71	Num_Species, 17
max_ds_iter, 58	Number_of_Species, 91-93
Max_NLK_Itr, 22, 24	NUMERICS, 21, 81, 83, 97
Max_NLK_Vec, 22, 25	Alittle, 81
Max_Step_Tries, 22, 25	Cutvof, 81, 82
Maximum_CG_Iterations, 33, 35	Cycle_Max, 81, 82
Maximum_Source_Cycles, 33, 35	Cycle_Number, 81, 82
MESH, 53, 75, 110	Discrete_Ops_Type, 81-83
coordinate_scale_factor, 76, 78	Dt_Constant, 21, 81, 83, 84, 97
exodus_block_modulus, 75, 76	Dt_Grow, 21, 81, 83
first_partition, 76, 79	Dt_Init, 81, 83, 84, 97, 99
gap_element_blocks, 75, 76	Dt_Max, 81, 83, 84
${\tt Interface\_Side\_Sets}, 110$	Dt_Min, 81, 83, 84
${\tt interface\_side\_sets}, 53, 75, 76$	t, 81, 82, 84
$\mathtt{mesh\_file},\ 75,\ 76$	0, 01, 02, 04
$\verb"noise_factor", 75, 78"$	Output_Dt, 85
Partition_File, 7	Output_Dt_Multiplier, 85, 86
$partition_file, 76, 78$	Output_Level, 33, 36
Partitioner, $6$	Output_T, 82, 85, 86, 97
partitioner, $76$ , $78$ , $79$	OUTPUTS, 82, 85
$x_{axis}, 75, 77$	Int_Output_Dt_Multiplier, 85
$y_{axis}, 75, 77$	Move_Block_IDs, 85, 86
z_axis, 75, 77	Move_Toolpath_Name, 85, 86
$mesh\_file, 75, 76$	Output_Dt, 85
mesh_material_number, 15, 16, 18	Output_Dt_Multiplier, 85, 86
Mesh_Surface, 10, 13, 14	Output_T, 82, 85, 86, 97
min_face_fraction, 47, 50	Probe_Output_Cycle_Multiplier, 85, 86
Model, 125, 126	Short_Output_Dt_Multiplier, 85, 86
Move_Block_IDs, 85, 86	Short_dutput_bt_nartipiler, 89, 80
Move_Toolpath_Name, 85, 86	Parameters, $62$ , $63$
MTS_b, 125, 126	Partition_Ds, 117, 119
MTS_d, 125, 126	Partition_File, 5-7
MTS_edot_0i, 125, 126	partition_file, 76, 78
MTS_g_0i, 125, 127	Partitioner, 5, 6
MTS_k, 125, 127	partitioner, 76, 78, 79
MTS_mu_0, 125, 127	PC_AMG_Cycles, 22, 26
	- 0a_0j 0±00, ±2, ±0

PC_SSOR_Relax, 22, 26	$\mathtt{digits},95,96$
PC_SSOR_Sweeps, 22, 26	Probe_Output_Cycle_Multiplier, 85, 86
PHASE, 71, 126	Pwr_Law_A, 126, 128
$\mathtt{name}, 71$	Pwr_Law_N, 126, 128
Phase, 125, 126	Pwr_Law_Q, 126, 129
PHASE_CHANGE, 71, 87	Pwr_Law_R, 126, 129
high_temp_phase, 87	, ,
latent_heat, 88	Radius, 68
liquidus_temp, 87	radius, 15, 17, 18
low_temp_phase, 87	Rel_Conc_Tol, 22, 27
solid_frac_table, 88	Rel_Enthalpy_Tol, 22, 23, 27
solidus_temp, 87	Rel_Temp_Tol, 22, 23, 27
Phase_Init_Dt, 99	rel_tol, 58
Phase_Init_Dt_Factor, 99, 100	Residual_Atol, 22, 28
Phase_Start_Times, 99, 100	Residual_Rtol, 22, 28
phases, 71	RESTART, 84, 97
phases, 87	Ignore_Dt, 84, 97
Phi, 91	
	Ignore_Joule_Heat, 97, 98
phi, 15, 17	Ignore_Solid_Mechanics, 97, 98
PHYSICAL_CONSTANTS, 3, 73, 89, 109, 110	Ignore_T, 97
Absolute_Zero, 40, 89, 109, 110	rotation_angle, 15, 17, 18
Stefan_Boltzmann, 89, 109, 110	rotation_pt, 15, 17, 18
Vacuum_Permeability, 33, 89, 90	01 . 0 D. W.J.: J: 05 06
Vacuum_Permittivity, 33, 89, 90	Short_Output_Dt_Multiplier, 85, 86
PHYSICS, 21, 47, 91, 98, 101	SIMULATION_CONTROL, 99
Body_Force_Density, 91, 92	Phase_Init_Dt, 99
Electromagnetics, $5$ , $92$ , $93$ , $98$	Phase_Init_Dt_Factor, 99, 100
Flow, $47$ , $92$	Phase_Start_Times, 99, 100
${ t Heat\_Transport,21,91-93}$	Skip_Geometry_Check, 39, 41
Materials, $92$	Smooth_Step_XO, 62, 65
$\mathtt{materials}, 71$	${\tt Smooth\_Step\_X1},  62,  65$
Number_of_Species, $91-93$	${\tt Smooth\_Step\_Y0, 62, 65}$
${\tt Solid\_Mechanics},92,93,98,101,125$	${\tt Smooth\_Step\_Y1, 62, 66}$
Species_Transport, $21$ , $91$ – $93$	${\tt solid\_frac\_table}, 88$
Turbulence_CMU, 121	SOLID_MECHANICS, 101
Plotfile_Dt, 117, 119	${\tt Contact\_Distance}, 101$
Poly_Coefficients, 61-63	${\tt Contact\_Norm\_Trac,\ 101,\ 102}$
Poly_Exponents, 61-63	${\tt Contact\_Penalty}, 101, 102$
Poly_Refvars, 61-63	Displacement_Nonlinear_Solution, 101, 103
Precon_Coupling_Method, 39, 41	Solid_Mechanics_Body_Force, 92, 93, 101, 103
Precon_Iter, 39, 41	${\tt Strain\_Limit}, 101, 103$
Precon_Method, 39, 41	${\tt Stress\_Reduced\_Integration}, 101$
Prefactor, 45	Solid_Mechanics, 92, 93, 98, 101, 125
prefactor, 115, 116	Solid_Mechanics_Body_Force, 92, 93, 101, 103
prefactor_func, 115, 116	solidus_temp, 87
pressure, 53-55	source, 115, 116
pressure_func, 53-55	Source_Constant, 31, 32
print_level, 58	Source_Frequency, 33, 36, 37
PROBE, 4, 95	source_func, 115, 116
coord, 95	Source_Function, 31, 32
coord_scale_factor, 95, 96	Source_Times, 33, 36-38, 68
data, 95, 96	SPECIES
data_file, 95, 96	flux, 105
description, 95, 96	SPECIES_BC, 91, 105
accertperon, 50, 50	DI 101110_10, 01, 100

comp, 105, 106 conc, func, 105-107 conc, func, 105-107 face_set_ids, 105, 106 flux_func, 105-107 name, 105, 106 type, 105, 106 Species_Transport, 21, 91-93 SS_Stopping_Tolerance, 33, 35-37 Start_Coord, 117, 118, 120 Steafa_Boltzmann, 89, 109, 110 Stepping_Method, 21, 22, 28 Stress_Reduced_Integration, 101 Surface_name, 15, 17 Symmetry_Axis, 33, 34, 38 Tsrain_Limit, 101, 103 Strace_name, 15, 17 Symmetry_Axis, 33, 34, 38 Tt, 81, 82, 84 Tabular_Dim, 62, 64, 123, 124 Tabular_Interp, 61, 62, 64 Tabular_Interp, 61, 62, 64 Tabular_Interp, 61, 62, 64, 88 temp_109-111 Temp_Exponent, 45, 46 temp=func, 109, 111, 112 Temperature, 15, 18 temperature, 15, 18 temperature, 109, 111, 112 Temperature, 19 temperature, 19 temperature, 19, 110 ambient_temp, 109, 111, 112 flux_func, 109-112 name, 110, 111 temp_func, 109, 111, 112 thc_inon-112 thc_inon-113 face_set_ids, 76, 109-111 temp_func, 109, 111, 112 thc_inon-112 thc_inon-112 thc_inon-113 face_set_ids, 16, 116 data_file_ils, 116, 116 aname, 115 prefactor_func, 115, 116 source, 115, 116 sourc		. 115 110
conc_func, 105-107 face_set_ids, 105, 106 flux, 106, 107 flux_func, 105-107 name, 105, 106 type, 105, 106 Species_Transport, 21, 91-93 SS_Stopping_Tolerance, 33, 35-37 Start_Coord, 117, 118, 120 Sterfan_Boltzmann, 89, 109, 110 Stepping_Method, 21, 22, 28 Stepp_Per_Cycle, 33, 37 Strain_Limit, 101, 103 Stress_Reduced_Integration, 101 Surface_name, 9-11, 13 surface_name, 15, 17 Symmetry_Axis, 33, 34, 38  t_ 81, 82, 84 Tabular_Data, 62, 64, 88, 123, 124 Tabular_Data, 62, 64, 123, 124 Tabular_Dim, 62, 64, 123, 124 Tabular_Dim, 62, 64, 123, 124 Tabular_Interp, 61, 62, 64 Tabular_Interp,	comp, 105, 106	source_func, 115, 116
face_set_ids, 105, 106 flux, 106, 107 flux, 106, 107 flux, 106, 107 flux, 106, 106 type, 105, 106 type, 105, 106 Species_Transport, 21, 91-93 SS_Stopping_Tolerance, 33, 35-37 Start_Coord, 117, 118, 120 Start_Time, 117, 118, 120 Stertam_Boltzmann, 89, 109, 110 Stepping_Method, 21, 22, 28 Stepping_thethod, 21, 22, 28 Steps_Per_Cycle, 33, 37 Strain_Limit, 101, 103 Stersam_Beduced_Integration, 101 Surface_Name, 9-11, 13 surface_name, 15, 17 Symmetry_Axis, 33, 34, 38  Tabular_Data, 62, 64, 88, 123, 124 Tabular_Data, 62, 64, 88, 123, 124 Tabular_Data, 62, 64, 123, 124 Tabular_Interp, 61, 62, 64 Tabular_Interp, 61, 62, 64, 88 temp_func, 109, 111, 112 Temp_Exponent, 45, 46 temp_func, 109, 111, 112 Temperature, 91 temperature, 91 temperature, 15, 18 temperature function, 15, 18 THERMAL_BC, 76, 91, 109 ambient_temp_func, 109, 111, 112 emissivity_func, 109-111, 113 emissivity_func, 109-111, 113 emissivity_func, 109-111 flux, 109, 111, 112 flux_func, 109, 111, 112 thc_func, 109-112 htc_func, 109-112 htc_func, 109-112 htc_func, 109-111 temp_func, 109, 111, 112 three, 109-112 three, 109-111 temp_func, 109, 111, 112 three, 109-112 htc_func, 109-111 temp_func, 109, 111, 112 three, 109-112 three, 109-11		
flux, 106, 107 flux_func, 105-107 name, 105, 106 Species_Transport, 21, 91-93 SS_Stopping_Tolerance, 33, 35-37 Start_Coord, 117, 118, 120 Start_Time, 117, 118, 120 Steps_Per_Cycle, 33, 37 Strain_Limit, 101, 103 Stress_Reduced_Integration, 101 Surface_Name, 9-11, 13 surface_name, 15, 17 Symmetry_Axis, 33, 34, 38  t. 81, 82, 84 Tabular_Data, 62, 64, 88, 123, 124 Tabular_Data, 62, 64, 123, 124 Tabular_Dim, 62, 64, 123, 124 Tabular_Linterp, 61, 62, 64 Tabular_Interp, 61, 62, 64, 88 temp_func, 109, 111, 112 Temperature, 91 temperature, 91 temperature, 15, 18 temperature, 19, 109 ambient_temp_func, 109, 111, 112 ambient_temp_func, 109, 111, 112 flux_func, 109-112 htc_func, 109-111 temp_func, 109, 111, 112 type, 109-111 THERMAL_SOURCE, 115 coll_set_ids, 115, 116 name, 115 prefactor_func, 115, 116 prefact		
flux_func, 105-107     name, 105, 106     type, 105, 106     Species_Transport, 21, 91-93     SS_Stopping_Tolerance, 33, 35-37     Start_Coord, 117, 118, 120     Start_Time, 117, 118, 120     Start_Time, 117, 118, 120     Start_Doord, 117, 118, 120     Start_Doord, 117, 118, 120     Start_Doord, 117, 118, 120     Start_Time, 117, 118, 120     Start_Time, 117, 118, 120     Start_Doord, 117, 118, 120     Start_Time, 117, 118, 120     Start_Time, 117, 118, 120     Start_Doord, 117, 118, 120     Start_Time, 117, 118, 120     Start_Coord, 117, 118, 120     Start_Coord, 117, 118, 120     Start_Coord, 117, 118, 120     Start_Coord, 117, 118, 120     Start_Time, 117, 118, 120     Start_Time, 117, 118, 120     Start_Coord, 117, 118, 120     Start_Time, 117, 118, 120     Start_Coord, 117, 118, 120     Start_Coord, 117, 118, 120     Start_Coord, 117, 118, 120     Start_Coord, 117, 118, 120     Start_Time, 117, 118, 120     Start_Coord, 117, 118, 120     Time Scale_Factor, 117, 118     Write_Plottine, 117, 119     tolopath, 39, 41     track_interfaces, 47, 49		
name, 105, 106 type, 105, 106 Species_Transport, 21, 91-93 SS Stopping_Tolerance, 33, 35-37 Start_Coord, 117, 118, 120 Start_Time, 117, 118, 120 Start_Time, 117, 118, 120 Stepping_Method, 21, 22, 28 Stepping_Method, 21, 22, 28 Steps_Per_Cycle, 33, 37 Strain_Limit, 101, 103 Stress_Reduced_Integration, 101 Surface_Name, 9-11, 13 surface_name, 15, 17 Symmetry_Axis, 33, 34, 38  Length, 121 Tabular_Data, 62, 64, 88, 123, 124 Tabular_Dim, 62, 64, 123, 124 Tabular_Dim, 62, 64, 123, 124 Tabular_Interp, 61, 62, 64 Tabular_Interp, 61, 62, 64, 88 temp_func, 109, 111, 112 Temp_Exponent, 45, 46 temp_func, 109, 111, 112 Temperature, 15, 18 temperature, 15, 19, 53-55 velocity, 15, 19, 53-55 velocity, 15, 19, 53-55 velocity, 15, 19,		_
Species_Transport, 21, 91-93 Species_Transport, 21, 91-94 Species_Transport, 11, 119 S		
Species_Transport, 21, 91-93 Species_Transport, 21, 91-93 Start_Coord, 117, 118, 120 Start_Coord, 117, 118, 120 Start_Time, 117, 118, 120 Start_Time, 117, 118, 120 Stefan_Boltzmann, 89, 109, 110 Stepping_Method, 21, 22, 28 Steps_Per_Cycle, 33, 37 Strain_Limit, 101, 103 Stress_Reduced_Integration, 101 Surface_Name, 9-11, 13 Surface_name, 15, 17 Symmetry_Axis, 33, 34, 38 Tabular_Data, 62, 64, 88, 123, 124 Tabular_Data, 62, 64, 88, 123, 124 Tabular_Dim, 62, 64, 123, 124 Tabular_Dim, 62, 64, 123, 124 Tabular_Limetr, 61, 62, 64 Tabular_Interp, 61, 62, 64, 88 temp, 109-111 Temp_Exponent, 45, 46 temp_func, 109, 111, 112 Temperature, 91 temperature, 15, 18 temperature, 109, 111, 112 ambient_temp_func, 109, 111, 113 emissivity, 109-111, 113 emissivity, 109-111, 113 emissivity_func, 109-111, 113 face_set_ids, 76, 109-111 flux, 109, 111, 112 htc, 109-112 htc_func, 109, 111, 112 type, 109-111 temp_func, 109, 111, 112 type, 109-111 type, 109-112 type, 109-112 type, 109-112 type, 109-112 type, 109-112 type, 109-112 type, 1		
SS_Stopping_Tolerance, 33, 35-37 Start_Coord, 117, 118, 120 Start_Time, 117, 118, 120 Stefan_Boltzmann, 89, 109, 110 Stepping_Method, 21, 22, 28 Steps_Per_Cycle, 33, 37 Strain_Limit, 101, 103 Stress_Reduced_Integration, 101 Surface_Name, 9-11, 13 surface_name, 15, 17 Symmetry_Axis, 33, 34, 38  Tabular_Data, 62, 64, 88, 123, 124 Tabular_Dim, 62, 64, 123, 124 Tabular_Dim, 62, 64, 123, 124 Tabular_Interp, 61, 62, 64 Tabular_Interp, 61, 62, 64, 88 temp_109-111 Temp_Exponent, 45, 46 temp_func, 109, 111, 112 Temperature, 91 temperature, 15, 18 TEMENAL_SC, 76, 91, 109 ambient_temp_func, 109, 111, 112 ambient_temp_func, 109, 111, 112 flux_func, 109, 111, 112 flux_func, 109, 111, 112 flux_func, 109, 111, 112 htc, 109-112 htc, 109-112 htc, 109-111 temp_func, 109, 111, 112 flux_func, 109, 111, 112 temp_func, 109, 111, 112 htc, 109-112 htc, 109-112 htc, 109-112 htc, 109-111 temp_func, 109, 111, 112 temp_func, 109, 111, 112 temp_func, 109, 111, 112 htc, 109-112 htc, 109-111 temp_func, 109, 111, 112 htc, 109-112 htc, 109-111 temp_func, 109, 111, 112 htc, 109-112 htc, 109-111 temp_func, 109, 111, 112 htc, 109-112 htcfunc, 109-111 temp_func, 109, 111, 112 htc, 109-112 htcfunc, 109-111 temp_func, 109, 111, 112 htc, 109-112 htcfunc, 109-111 htemp_func, 109, 111, 112 htc, 109-112 htcfunc, 109-111 htm, 109-112 htm, 109-111 htm, 109-111 htm, 109-112 htm, 109-111 htm, 109-111 htm, 109-112 htm, 109-111 htm, 109-112 htm, 109-111 htm, 109-112 htm, 109-11	¥ =	
Start_Cord, 117, 118, 120		
Start_Time, 117, 118, 120         Time_Scale_Factor, 117, 118           Stepfing_Method, 21, 22, 28         toolpath, 39, 41           Stepping_Method, 21, 22, 28         toolpath, 39, 41           Stresp_Per_Cycle, 33, 37         track_interfaces, 47, 49           Strass_Reduced_Integration, 101         TURBULENCE, 121           Surface_Name, 9-11, 13         CMU, 121           Symmetry_Axis, 33, 34, 38         Length, 121           t, 81, 82, 84         Turbulence_KE_Fraction, 121           Tabular_Data, 62, 64, 88, 123, 124         Turbulence_KE_Fraction, 121           Tabular_Dim, 62, 64, 123, 124         Turbulence_KE_Fraction, 121           Tabular_Extrap, 61, 62, 64         Turbulence_KE_Fraction, 121           Turbulence_KE_Fraction, 121		
Stefan_Boltzmann, 89, 100, 110         Write_Plotfile, 117, 119           Stepspeng_Method, 21, 22, 28         toolpath, 39, 41           Stepsper_Cycle, 33, 37         track_interfaces, 47, 49           Strain_Limit, 101, 103         translation_pt, 15, 17, 18           Stress_Reduced_Integration, 101         TURBULENCE, 121           Surface_Name, 9-11, 13         CMU, 121           Surface_name, 15, 17         KE_fraction, 121           Symmetry_Axis, 33, 34, 38         Length, 121           Turbulence_Length, 122         Turbulence_Length, 122           Tabular_Data, 62, 64, 88, 123, 124         Turbulence_Length, 122           Tabular_Dim, 62, 64, 123, 124         Turbulence_Length, 122           Turbulence_KE_Fraction, 121         Turbulence_Length, 122           Turbulence_Length, 122		
Stepping_Method, 21, 22, 28   toolpath, 39, 41   Stepping_Method, 21, 22, 28   track_interfaces, 47, 49   Strain_Linit, 101, 103   translation_pt, 15, 17, 18   Stress_Reduced_Integration, 101   TURBULENCE, 121   Surface_Name, 9-11, 13   CMU, 121   Surface_name, 15, 17   KE_fraction, 121   Symmetry_Axis, 33, 34, 38   Length, 121   Turbulence_KE_Fraction, 121   Turbulence_CMU, 121   Turbulence_KE_Fraction, 121   Turbulence_CMU, 112   Turbulence_Cmu, 112   Turbulence_CMU, 121   Turbulence_Cmu, 112   Turbulence_Cmu, 112   Turbulence_Cmu, 112   Turbulence_Cmu, 112   Turbulence_Cmu, 121   Turbulence_Cmu, 121   Turbulence_Cmu, 121   Turbulence_Cmu, 121   Turbulence_Cmu, 121   Turbulence_Cmu, 121   Turbulence_Cmenth, 122   Turbulence_Cmu, 121   Turbulence_Cmenth, 122   Turbulence_Cmenth,		
Steps_Per_Cycle, 33, 37         track_interfaces, 47, 49           Strain_Limit, 101, 103         translation_pt, 15, 17, 18           Surface_Name, 9-11, 13         TURBULENCE, 121           Symmetry_Axis, 33, 34, 38         CMU, 121           KE_fraction, 121         KE_fraction, 121           t, 81, 82, 84         Turbulence_KE_Fraction, 121           Tabular_Dim, 62, 64, 123, 124         Turbulence_CMU, 121           Tabular_Dim, 62, 64, 123, 124         Turbulence_Length, 122           Tabular_Interp, 61, 62, 64         Turbulence_Length, 122           Tabular_Interp, 61, 62, 64, 88         type, 62, 123, 124           temp, 109-111         Turbulence_Length, 122           Type, 62, 123, 124         type, 53, 54, 105, 106, 109-111           Temperature, 91         Vacuum_Permeability, 33, 89, 90           temperature, 15, 18         Vacuum_Permeability, 33, 89, 90           temperature_function, 15, 18         Vacuum_Permeability, 33, 89, 90           velocity, 15, 19, 53-55         velocity, 15, 19, 53-55           velocity, 15, 19, 53-55         Velocity, 109-111           flux_func, 109, 111, 112         Tabular_Data, 123, 124           ambient_temp_func, 109, 111, 112         Tabular_Data, 123, 124           tabular_dim, 123         Tabular_Dim, 123, 124           tabular_dim, 123		
Strain_Limit, 101, 103         translation_pt, 15, 17, 18           Stress_Reduced_Integration, 101         TURBULENCE, 121           Surface_Name, 9-11, 13         CMU, 121           surface_name, 15, 17         KE_fraction, 121           Symmetry_Axis, 33, 34, 38         Length, 121           t, 81, 82, 84         Turbulence_KE_Fraction, 121           Tabular_Data, 62, 64, 88, 123, 124         Turbulence_CMU, 121           Tabular_dim, 123         Turbulence_Length, 122           Tabular_Extrap, 61, 62, 64         Turbulence_Length, 122           Tabular_Interp, 61, 62, 64, 88         type, 62, 123, 124           temp, 109-111         temp, 109, 111, 112           Temp_Exponent, 45, 46         Uniform_Source, 33, 36-38           temperature, 91         Vacuum_Permeability, 33, 89, 90           temperature, 15, 18         velocity, 15, 19, 53-55           THERMAL_BC, 76, 91, 109         velocity, 15, 19, 53-55           THERMAL_BC, 76, 91, 109         velocity, 15, 19, 53-55           welocity, 109-111, 113         meissivity, 109-111, 113           face_set_ids, 76, 109-111         Tabular_Data, 123, 124           flux_func, 109, 111, 112         Model, 125, 126           htc, 109-112         Model, 125, 126           name, 110, 111         MTS_b, 125, 126 <td< td=""><td></td><td><u>-</u></td></td<>		<u>-</u>
Stress_Reduced_Integration, 101         TURBULENCE, 121           Surface_Name, 9-11, 13         CMU, 121           Surface_name, 15, 17         KE_fraction, 121           Symmetry_Axis, 33, 34, 38         Length, 121           t, 81, 82, 84         Turbulence_KE_Fraction, 121           Tabular_Data, 62, 64, 88, 123, 124         Turbulence_CMU, 121           Tabular_Dim, 62, 64, 123, 124         Turbulence_KE_Fraction, 121           Tabular_Extrap, 61, 62, 64         Type, 62, 123, 124           Tabular_Interp, 61, 62, 64         Type, 62, 123, 124           Temp_func, 109, 111, 112         Uniform_Source, 33, 36-38           temp_func, 109, 111, 112         Uniform_Source, 33, 36-38           temp_func, 109, 111, 112         Vacuum_Permeability, 33, 89, 90           temperature, 51, 18         Velocity, 15, 19, 53-55           temperature, 109, 111, 112         Verbose_Stepping, 22, 28           ambient_temp_func, 109, 111, 112         Verbose_Stepping, 22, 28           velocity_func, 53-55         Verbose_Stepping, 22, 28           VFUNCTION, 55, 123         Tabular_Data, 123, 124           flux_func, 109-111, 113         Tabular_Data, 123, 124           flux_func, 109, 111, 112         Model, 125, 126           thc_func, 109, 111, 112         Model, 125, 126           temp_func, 109, 111, 112	-	
Surface_Name, 9-11, 13 surface_name, 15, 17 Symmetry_Axis, 33, 34, 38  Length, 121  t, 81, 82, 84 Tabular_Data, 62, 64, 88, 123, 124 Tabular_Dim, 62, 64, 123, 124 Tabular_Latin, 123 Tabular_Extrap, 61, 62, 64 Tabular_Interp, 61, 62, 64, 88 temp_func, 109, 111, 112 Temperature, 91 temperature, 91 temperature, 15, 18 ThermAL_BC, 76, 91, 109 ambient_temp, 109, 111, 112 ambient_temp_func, 109, 111, 113 emissivity_func, 109-111, 113 emissivity_func, 109-111, 113 face_set_ids, 76, 109-111 flux_func, 109, 111, 112 htc, 109-112 htc_func, 109, 111, 112 thep_func, 109, 111, 112 thep_func, 109, 111, 112 thep_func, 109, 111, 112 htc, 109-112 htc_func, 109, 111, 112 htc, 109-111 THERMAL_SOURCE, 115 cell_set_ids, 115, 116 data_file, 115, 116 name, 115 prefactor_func, 115, 116 prefactor_func, 115, 116  MTS_sig_i, 126, 128		_ · · · · · · · · · · · · · · · · · · ·
surface_name, 15, 17       KE_fraction, 121         Symmetry_Axis, 33, 34, 38       Length, 121         t, 81, 82, 84       Turbulence_Length, 122         Tabular_Data, 62, 64, 88, 123, 124       Turbulence_CMU, 121         Tabular_Dim, 62, 64, 123, 124       Turbulence_KE_Fraction, 121         tabular_Extrap, 61, 62, 64       Turbulence_Length, 122         Tabular_Extrap, 61, 62, 64       Type, 62, 123, 124         Tabular_Interp, 61, 62, 64, 88       type, 53, 54, 105, 106, 109-111         temp, 109-111       Uniform_Source, 33, 36-38         temp_func, 109, 111, 112       Vacuum_Permeability, 33, 89, 90         temperature, 91       Vacuum_Permeability, 33, 89, 90         temperature function, 15, 18       Vacuum_Permittivity, 33, 89, 90         temperature function, 15, 18       Vacuum_Permittivity, 33, 89, 90         temperature function, 15, 18       Vacuum_Permittivity, 33, 89, 90         temperature function, 109, 111, 112       Verbose_Stepping, 22, 28         ambient_temp_func, 109, 111, 113       Verbose_Stepping, 22, 28         wFUNCTION, 55, 123       Name, 123         nemissivity, 109-111, 113       Tabular_Data, 123, 124         flux, 109, 111, 112       Tabular_Data, 123, 124         thc_func, 109-112       Model, 125, 126         name, 110, 111       MTS_cl, 125, 126 </td <td></td> <td>,</td>		,
Symmetry_Axis, 33, 34, 38  Legth, 121 Turbulence_KE_Fraction, 121 Turbulence_Length, 122 Tabular_Data, 62, 64, 88, 123, 124 Tabular_Dim, 62, 64, 123, 124 Tabular_Latrap, 61, 62, 64 Tabular_Extrap, 61, 62, 64 Tabular_Interp, 61, 62, 64, 88 Temp, 109-111 Temp_Exponent, 45, 46 temp-func, 109, 111, 112 Temperature, 91 temperature, 15, 18 temperature, 15, 18 temperature, 15, 18 temperature, 15, 18 temperature, 109, 111, 112 THERMAL_BC, 76, 91, 109 ambient_temp, 109, 111, 113 emissivity, 109-111, 113 emissivity, 109-111, 113 emissivity, 109-111, 113 face_set_ids, 76, 109-111 flux, 109, 111, 112 flux_func, 109, 111, 112 htc, 109-112 htc_func, 109-112 htc_func, 109-111 temp, 109-111 temp, 109-111 temp, 109-111 temp, 109-111 temp, 109-111 THERMAL_SOURCE, 115 cell_set_ids, 115, 116 anae, 115 prefactor_func, 115, 116 prefactor_func, 115, 116 mrs_sig_i, 126, 128  MTS_sig_a, 126, 128	_ :	
t, 81, 82, 84 Turbulence_KE_Fraction, 121 Tabular_Data, 62, 64, 88, 123, 124 Tabular_Dim, 62, 64, 123, 124 Tabular_Dim, 62, 64, 123, 124 Tabular_dim, 123 Turbulence_KE_Fraction, 121 Turbulence_Length, 122 Turbulence_KE_Fraction, 121 Turbulence_KE_Fraction, 121 Turbulence_KE_Fraction, 121 Turbulence_KE_Fraction, 121 Turbulence_Length, 122 Turbulence_KE_Fraction, 121 Turbulence_KE_Fraction, 121 Turbulence_KE_Fraction, 121 Turbulence_KE_Fraction, 121 Turbulence_Length, 122 Turbulence_CMU, 121 Turbulence_CMU, 121 Turbulence_KE_Fraction, 121 Turbulence_KE_Fraction, 121 Turbulence_KE_Fraction, 121 Turbulence_KE_Fraction, 121 Turbulence_KE_Fraction, 121 Turbulence_CMU, 121 Turbulence_CMU, 121 Turbulence_CMU, 121 Turbulence_CMU, 122 Turbulence_CMU, 122 Turbulence_CMU, 123 Turbulence_CMU, 125 Turbulence_Cete, 125 Turbulence_Cete, 125 Turbulence_Cete, 125 Turbulence_Cete, 125 Turbulence_CMu, 125 Turbulence_Cunden, 125 Turbulence_Cete, 126 Turbulence_Cete, 12	_ : :	
t, 81, 82, 84 Turbulence_Length, 122 Tabular_Data, 62, 64, 88, 123, 124 Tabular_Dim, 62, 64, 123, 124 Tabular_dim, 123 Tabular_textrap, 61, 62, 64 Turbulence_Length, 122 Tabular_dim, 123 Tabular_textrap, 61, 62, 64 Type, 62, 123, 124 Tabular_Interp, 61, 62, 64 Type, 62, 123, 124 Tabular_Interp, 61, 62, 64, 88 temp, 109-111 Temp_Exponent, 45, 46 temp_func, 109, 111, 112 Temperature, 91 temperature, 15, 18 temperature, 15, 18 temperature, 15, 18 temperature, 109, 111, 112 ambient_temp, 109, 111, 112 ambient_temp_func, 109, 111-113 emissivity, 109-111, 113 emissivity_func, 109-111 flux, 109, 111, 112 flux, 109, 111, 112 flux, 109, 111, 112 flux, 109-112 htc, 109-112 htc, 109-112 htc, 109-111 htc, 109-111 ThermAl_SOURCE, 115 cell_set_ids, 115, 116 data_file, 115, 116 name, 115 prefactor_func, 115, 116 prefactor_func, 115, 116 mTS_sig_a, 126, 128 mTS_sig_a, 126, 128 mTS_sig_a, 126, 128	Symmetry_Axis, 33, 34, 38	_
Tabular_Data, 62, 64, 88, 123, 124 Tabular_Dim, 62, 64, 123, 124 Tabular_Dim, 62, 64, 123, 124 Tabular_Latrap, 61, 62, 64 Tabular_Interp, 61, 62, 64, 88 Type, 62, 123, 124 Type, 62, 123, 124 Type, 62, 123, 124 Type, 62, 123, 124 Type, 53, 54, 105, 106, 109-111 Temp_Exponent, 45, 46 Temp_func, 109, 111, 112 Temperature, 91 Temperature, 15, 18 Temperature function, 15, 18 THERMAL_BC, 76, 91, 109 Temberature_func, 109, 111, 112 Tempissivity_func, 109-111, 113 Tabular_Data, 123, 124 Turbulence_KE_Fraction, 121 Turbulence_Length, 122 Type, 62, 123, 124 Type, 62, 123, 124 Type, 62, 123, 124 Type, 53, 54, 105, 106, 109-111 Temperature, 15, 18 Temperature, 15, 18 Vacuum_Permeability, 33, 89, 90 Vacuum_Permittivity, 33, 89, 90 Vacuum_Permeability, 32, 92 Vacuum_Per	+ 01 00 04	
Tabular_Dim, 62, 64, 123, 124  tabular_dim, 123  Turbulence_KE_Fraction, 121  Turbulence_Length, 122  Type, 62, 123, 124  Type, 63, 54, 105, 106, 109-111  Type, 61, 62, 64, 88  Type, 53, 54, 105, 106, 109-111  Type, 62, 123, 124  Type, 13, 126  Type, 13, 126  Type, 13, 126  Type, 13, 126  Type, 12, 126  Type, 123, 124  T		
Tabular_dim, 123 Tabular_Extrap, 61, 62, 64 Tabular_Interp, 61, 62, 64, 88 Type, 62, 123, 124 Type, 62, 123, 106, 109-111 Temp_Exponent, 45, 46 temp_func, 109, 111, 112 Temperature, 91 temperature, 15, 18 THERMAL_BC, 76, 91, 109 ambient_temp_func, 109, 111, 112 emissivity, 109-111, 113 emissivity, 109-111, 113 emissivity_func, 109-111, 113 face_set_ids, 76, 109-111 flux_func, 109, 111, 112 htc, 109-112 htc_func, 109-112 name, 110, 111 temp_func, 109, 111, 112 type, 109-111 THERMAL_SOURCE, 115 cell_set_ids, 115, 116 data_file, 115, 116 prefactor_func, 115, 116 prefactor_func, 115, 116 mrs_sig_i, 126, 128  Turbulence_Length, 122 Type, 62, 123, 124 type, 53, 54, 105, 106, 109-111 type, 53, 54, 105, 106, 109-111 type, 53, 54, 105, 106, 109-111 tvaluer_Bource, 33, 36-38  Uniform_Source, 33, 36-38  Vacuum_Permittivity, 33, 89, 90 velocity, 15, 19, 53-55 velocity_func, 53-50 velocity_func, 53-50 velocity_func, 53-50 velocity_func, 53-50 velocity_func, 53-50 velocity_func, 53-50 velocity_f		
Tabular_Extrap, 61, 62, 64 Tabular_Interp, 61, 62, 64, 88 Type, 62, 123, 124 Tabular_Interp, 61, 62, 64, 88 type, 53, 54, 105, 106, 109-111  Temp_Exponent, 45, 46 temp_func, 109, 111, 112 Temperature, 91 Vacuum_Permeability, 33, 89, 90 temperature_function, 15, 18 THERMAL_BC, 76, 91, 109 ambient_temp, 109, 111, 112 amissivity, 109-111, 113 emissivity, 109-111, 113 emissivity, func, 109-111, 113 face_set_ids, 76, 109-111 flux_func, 109, 111, 112 flux_func, 109, 111, 112 htc, 109-112 htc_func, 109-112 htc_func, 109-111 temp_func, 109, 111, 112 type, 123, 124 temp_func, 109, 111, 112 type, 109-111 temp_func, 109, 111, 112 type, 109-111 THERMAL_SOURCE, 115 cell_set_ids, 115, 116 data_file, 115, 116 mame, 115 prefactor, 115, 116 mTS_eig_i, 126, 128  Type, 22, 28 Vacuum_Permeability, 33, 89, 90 Vacuum_Permittivity, 91, 126 Vacuum_Permittivity, 33, 89, 90 Vacuum_Permittivity, 10e, 102 Vacuum_Permit		
Tabular_Interp, 61, 62, 64, 88		
temp, 109-111 Temp_Exponent, 45, 46 temp_func, 109, 111, 112 Temperature, 91 temperature, 15, 18 temperature_function, 15, 18 THERMAL_BC, 76, 91, 109 ambient_temp_func, 109, 111, 112 emissivity, 109-111, 113 emissivity_func, 109-111, 113 emissivity_func, 109-111 flux_func, 109, 111, 112 flux_func, 109, 111, 112 htc_func, 109-112 htc_func, 109-112 htc_func, 109-111 temp_func, 109, 111, 112 themp_func, 109, 111 temp_func, 109, 111, 112 themp_func, 109, 111 temp_func, 109, 111 temp_fu	<del>-</del> ' ' ' ' ' ' ' ' ' ' ' ' ' ' ' ' ' ' '	
Temp_Exponent, 45, 46 temp_func, 109, 111, 112 Temperature, 91 temperature, 15, 18 temp_remonerature, 15, 18 temperature, 15, 18 temperature_function, 15, 18 THERMAL_BC, 76, 91, 109 ambient_temp, 109, 111, 112 emissivity, 109-111, 113 emissivity_func, 109-111, 113 emissivity_func, 109-111, 113 face_set_ids, 76, 109-111 flux, 109, 111, 112 flux_func, 109, 111, 112 flux_func, 109-112 htc_func, 109-112 htc_func, 109-111 temp_func, 109, 111, 112 tabular_dim, 123 flux_func, 109-112 htc_func, 109-111 temp_func, 109, 111, 112 tabular_dim, 123 Type, 123, 124 VISCOPLASTIC_MODEL, 73, 92, 101, 125 Model, 125, 126 MTS_b, 125, 126 MTS_b, 125, 126 THERMAL_SOURCE, 115 cell_set_ids, 115, 116 mTS_p, 125, 127 data_file, 115, 116 mTS_p, 126, 127 mTS_q, 126, 127 mTS_sig_a, 126, 128 mTS_sig_i, 126, 128	<del>-</del> ' ' ' ' ' ' ' ' ' ' ' ' ' ' ' ' ' ' '	type, 53, 54, 105, 106, 109-111
temp_func, 109, 111, 112 Temperature, 91	= '	W-: 0 22 26 20
Temperature, 91 temperature, 15, 18 temperature, 15, 18 temperature_function, 15, 18 THERMAL_BC, 76, 91, 109 ambient_temp, 109, 111, 112 ambient_temp_func, 109, 111-113 emissivity, 109-111, 113 emissivity_func, 109-111, 113 face_set_ids, 76, 109-111 flux, 109, 111, 112 flux_func, 109, 111, 112 flux_func, 109, 111, 112 htc_func, 109-112 name, 110, 111 temp_func, 109, 111, 112 flemp, 109-111 THERMAL_SOURCE, 115 cell_set_ids, 115, 116 mane, 115 prefactor_func, 115, 116 mrs_sig_i, 126, 128		Uniform_Source, 33, 30-38
temperature, 15, 18  temperature_function, 15, 18  THERMAL_BC, 76, 91, 109  ambient_temp, 109, 111, 112  emissivity, 109-111, 113  emissivity_func, 109-111, 113  face_set_ids, 76, 109-111  flux_func, 109, 111, 112  flux_func, 109-112  name, 110, 111  temp, 109-111  THERMAL_SUURCE, 115  cell_set_ids, 115, 116  prefactor_func, 115, 116  mrs_sig_i, 126, 128  Telocity, 15, 19, 53-55  velocity_func, 53-55  velocity_func, 53-55  Verbose_Stepping, 22, 28  VFUNCTION, 55, 123  Name, 123  PVFUNCTION, 55, 123  Name, 123  Tabular_Data, 123, 124  Tabular_Dim, 123  Tabular_Dim, 123, 124  Tabular_Dim, 123  Tabular_Dim, 123  Tabular_Dim, 123  Tabular_Dim, 123  Tabular_Dim, 126, 124  Tabular_Dim, 126  Tabular_Dim	<del>-</del>	Vacuum Darmachility 22 00 00
temperature_function, 15, 18 THERMAL_BC, 76, 91, 109     ambient_temp, 109, 111, 112     ambient_temp_func, 109, 111-113     emissivity, 109-111, 113     emissivity_func, 109-111, 113     emissivity_func, 109-111     face_set_ids, 76, 109-111     flux, 109, 111, 112     flux_func, 109, 111, 112     flux_func, 109-112     htc_func, 109-112     htc_func, 109-111     temp, 109-111     temp, 109-111     temp, 109-111     temp, 109-111     flux_delta, 125, 126     mame, 110, 111     temp_func, 109, 111, 112     mys_d, 125, 126     type, 109-111     mys_d, 125, 126     mys_g_oi, 125, 127     mys_k, 125, 127     cell_set_ids, 115, 116     mys_p_i, 126, 127     mane, 115     prefactor, 115, 116     mys_sig_a, 126, 128     mys_sig_i, 126, 128		
THERMAL_BC, 76, 91, 109     ambient_temp, 109, 111, 112     ambient_temp_func, 109, 111-113     emissivity, 109-111, 113     emissivity_func, 109-111, 113     emissivity_func, 109-111, 113     emissivity_func, 109-111     face_set_ids, 76, 109-111     flux, 109, 111, 112     flux_func, 109, 111, 112     flux_func, 109, 111, 112     flux_func, 109-112     htc_func, 109-112     htc_func, 109-112     htc_func, 109-111     temp, 109-111     temp, 109-111     temp, 109-111     temp, 109-111     temp_func, 109, 111, 112     model, 125, 126     mame, 110, 111     model, 125, 126     mod	<del>-</del>	
ambient_temp, 109, 111, 112  ambient_temp_func, 109, 111-113  emissivity, 109-111, 113  emissivity_func, 109-111, 113  emissivity_func, 109-111, 113  face_set_ids, 76, 109-111  flux, 109, 111, 112  flux_func, 109, 111, 112  flux_func, 109, 111, 112  htc_func, 109-112  htc_func, 109-112  htc_func, 109-111  temp, 109-111  temp, 109-111  flum_func, 109, 111, 112  flum_func, 109, 112, 126  flum_func, 109, 112, 126  flum_func, 109, 112, 126  flum_func, 109, 112, 126  flum_func, 109, 125, 127  flum_func, 125, 126  flum_func, 128  flum_func, 123, 124  flum_func, 123	<del>-</del>	• • • • • • • • • • • • • • • • • • • •
ambient_temp_func, 109, 111-113 emissivity, 109-111, 113 emissivity_func, 109-111, 113 face_set_ids, 76, 109-111 flux, 109, 111, 112 flux_func, 109, 111, 112 flux_func, 109, 111, 112 htc, 109-112 htc, 109-112 htc, 109-112 mame, 110, 111 temp_func, 109, 111, 112 temp_func, 109, 111, 112 temp_func, 109, 111, 112 flux_func, 109-111 flux_func, 109-111 flux_func, 109, 111, 112 flux_func, 109-111 flux_func, 109, 111, 112 flux_func, 109-111 flux_func, 109-112 flux_func, 109-111 flux_func, 109-112 flux_func, 109-112 flux_func, 109-112 flux_func, 109-112 flux_func, 109-111 flux_func, 109-112 flux_func, 109-111 flux_func, 109-112 flux_func, 109-111 flux_func, 109-1		* - · · ·
emissivity, 109-111, 113 emissivity_func, 109-111, 113 face_set_ids, 76, 109-111 flux, 109, 111, 112 flux_func, 109, 111, 112 htc, 109-112 htc_func, 109-112 htc_func, 109-111 temp, 109-111 temp, 109-111 temp, 109-111 temp, 109-111 THERMAL_SOURCE, 115 cell_set_ids, 115, 116 emissivity_func, 109, 115, 116 emissivity_func, 109-111 temp, 109-111 Thermal_source, 115, 116 mrs_edot_oi, 125, 127 mrs_edot_oi, 125, 126 mrs_e		
$\begin{array}{llllllllllllllllllllllllllllllllllll$	_ • - · · · · · · · · · · · · · · · · · ·	
$\begin{array}{llllllllllllllllllllllllllllllllllll$		
$\begin{array}{llllllllllllllllllllllllllllllllllll$	<b>* -</b>	
$\begin{array}{llllllllllllllllllllllllllllllllllll$		<del>-</del> , ,
htc, 109-112 VISCOPLASTIC_MODEL, 73, 92, 101, 125 htc_func, 109-112 Model, 125, 126 mame, 110, 111 MTS_b, 125, 126 temp, 109-111 MTS_d, 125, 126 temp_func, 109, 111, 112 MTS_edot_0i, 125, 126 type, 109-111 MTS_g_0i, 125, 127 THERMAL_SOURCE, 115 MTS_k, 125, 127 cell_set_ids, 115, 116 MTS_mu_0, 125, 127 data_file, 115, 116 MTS_p_i, 126, 127 name, 115 MTS_q_i, 126, 127 prefactor, 115, 116 MTS_sig_a, 126, 128 prefactor_func, 115, 116 MTS_sig_i, 126, 128		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		
$\begin{array}{llllllllllllllllllllllllllllllllllll$		_
$\begin{array}{llll} \text{temp, } 109-111 & \text{MTS\_d, } 125,  126 \\ \text{temp\_func, } 109,  111,  112 & \text{MTS\_edot\_0i, } 125,  126 \\ \text{type, } 109-111 & \text{MTS\_g\_0i, } 125,  127 \\ \text{THERMAL\_SOURCE, } 115 & \text{MTS\_k, } 125,  127 \\ \text{cell\_set\_ids, } 115,  116 & \text{MTS\_mu\_0, } 125,  127 \\ \text{data\_file, } 115,  116 & \text{MTS\_p\_i, } 126,  127 \\ \text{name, } 115 & \text{MTS\_q\_i, } 126,  127 \\ \text{prefactor, } 115,  116 & \text{MTS\_sig\_a, } 126,  128 \\ \text{prefactor\_func, } 115,  116 & \text{MTS\_sig\_i, } 126,  128 \\ \end{array}$		
$\begin{array}{llll} \texttt{temp\_func}, \ 109, \ 111, \ 112 & \texttt{MTS\_edot\_Oi}, \ 125, \ 126 \\ \texttt{type}, \ 109-111 & \texttt{MTS\_g\_Oi}, \ 125, \ 127 \\ \texttt{THERMAL\_SOURCE}, \ 115 & \texttt{MTS\_k}, \ 125, \ 127 \\ \texttt{cell\_set\_ids}, \ 115, \ 116 & \texttt{MTS\_mu\_O}, \ 125, \ 127 \\ \texttt{data\_file}, \ 115, \ 116 & \texttt{MTS\_p\_i}, \ 126, \ 127 \\ \texttt{name}, \ 115 & \texttt{MTS\_q\_i}, \ 126, \ 127 \\ \texttt{prefactor}, \ 115, \ 116 & \texttt{MTS\_sig\_a}, \ 126, \ 128 \\ \texttt{prefactor\_func}, \ 115, \ 116 & \texttt{MTS\_sig\_i}, \ 126, \ 128 \\ \end{array}$		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	= ·	
THERMAL_SOURCE, 115  cell_set_ids, 115, 116  data_file, 115, 116  mts_k, 125, 127  mts_mu_0, 125, 127  mts_p_i, 126, 127  mts_q_i, 126, 127  mts_q_i, 126, 127  mts_sig_a, 126, 128  prefactor_func, 115, 116  mts_sig_i, 126, 128		
cell_set_ids, 115, 116       MTS_mu_0, 125, 127         data_file, 115, 116       MTS_p_i, 126, 127         name, 115       MTS_q_i, 126, 127         prefactor, 115, 116       MTS_sig_a, 126, 128         prefactor_func, 115, 116       MTS_sig_i, 126, 128	V 2 /	
data_file, 115, 116       MTS_p_i, 126, 127         name, 115       MTS_q_i, 126, 127         prefactor, 115, 116       MTS_sig_a, 126, 128         prefactor_func, 115, 116       MTS_sig_i, 126, 128		
name, 115       MTS_q_i, 126, 127         prefactor, 115, 116       MTS_sig_a, 126, 128         prefactor_func, 115, 116       MTS_sig_i, 126, 128		·
prefactor, 115, 116 MTS_sig_a, 126, 128 prefactor_func, 115, 116 MTS_sig_i, 126, 128		- <b>-</b> - · · · ·
prefactor_func, 115, 116 MTS_sig_i, 126, 128		
	<del>-</del>	
50urce, 110, 110 mis_temp_0, 120, 120		
	500100, 110, 110	1110_00mp_0, 120, 120

```
\mathtt{Phase},\, 125,\, 126
    Pwr_Law_A, 126, 128
    {\tt Pwr\_Law\_N},\, 126,\, 128
    {\tt Pwr\_Law\_Q},\, 126,\, 129
     Pwr_Law_R, 126, 129
{\tt viscous\_implicitness},\,47,\,48,\,57
viscous_number, 47, 48
void_collapse, 47, 50
void\_collapse\_relaxation, 47, 50
Void_Temperature, 22, 29
vol_frac_cutoff, 47, 50
vol\_track\_subcycles, 47, 49
{\tt Write\_Plotfile},\, 117,\, 119
x_axis, 75, 77
y_axis, 75, 77
z_axis, 75, 77
```