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ALEGRA-MHD: Version 4.0

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HEDP Theory and ICF Target Design

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Abstract

ALEGRA is an arbitrary Lagrangian-Eulerian finite element code that emphasizes large distortion and shock propagation in inviscid fluids and solids. This document describes user options for modeling magnetohydrodynamic, thermal conduction, and radiation emission effects.

Acknowledgment

The authors wish to acknowledge the contributions of Kent Budge to early draft versions of this manual and associated algorithms in the areas of thermal conduction, emission and opacity modeling. Bob Campbell, Dan Carroll, Kyle Cochrane, Mike Desjarlais, Ray Lemke, Bryan Oliver, Steve Rosenthal, Peter Stoltz, and Erik Wemlinger have used and tested the MHD physics options in ALEGRA-MHD code and provided invaluable feedback.

We would also like to acknowledge the support of the members of the NEVADA framework development team and the rest of the ALEGRA development team. Their perpetual assistance in areas of team leadership, architecture, configuration management, regression testing, Diatom insertion, remap and advection, and more, have been invaluable.

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Nomenclature

Term	Definition
ALE	Arbitrary Lagrangian Eulerian
ALEGRA	Arbitrary Lagrangian Eulerian General Research Application
MHD	MagnetoHydroDynamics
ICF	Inertial Confinement Fusion
MMALE	Multi-Material ALE
SMALE	Single-Material ALE

ALEGRA-MHD: Version 4.0

1 Introduction to ALEGRA MHD

This manual provides a supplement to the ALEGRA Users Manual [3] and follows the pattern set therein. This manual describes the additional features that support magnetohydrodynamic (MHD) applications. This manual represents a prioritized summary of the ALEGRA MHD input options. The manual is intended as a reference guide and not as a tutorial or self-contained instruction manual.

MHD applications require a wide range of physics phenomena to be modeled. This includes hydrodynamics, solid mechanics, transient magnetics, thermal conduction, and radiation emission. Sandia's primary interest is in ICF and Z-pinch applications.

ALEGRA MHD includes only those physics capabilities which might be needed in a fairly wide range of magnetohydrodynamic applications including some Z-pinch physics applications. Only a simple radiation emission model is included for purposes of radiating excess energy. The thermal transport model is included as well as a means of smoothing the highly localized energy sources which can develop due to Joule heating. Applications which require true radiation transport coupled with MHD are not supported by the ALEGRA MHD code.

The 2D version of ALEGRA MHD supports 2D Cartesian (XY) modeling in which the magnetic field $\vec{B} = (B_x, B_y)$ may be in the plane of the mesh and the current density J_z is orthogonal to the plane, or else in which the magnetic field B_z may be orthogonal to the plane of the mesh and the current density $\vec{J} = (J_x, J_y)$ is in the plane. It also supports 2D cylindrically symmetric (RZ) modeling in which the magnetic field B_θ may be orthogonal to the plane of the mesh and the current density $\vec{J} = (J_r, J_z)$ is in the plane. The 2D code supports unstructured quadrilateral grids.

The 3D version of ALEGRA MHD supports 3D Cartesian (XYZ) modeling on fully unstructured grids. The 3D code implements a magnetic diffusion solution based on edge and face elements [2]. A discretely divergence free property is maintained both in the magnetics solve and during a constrained transport algorithm in the remap phase. The magnetic flux density is represented in terms of face elements with the element magnetic flux on faces as degrees of freedom. The 3D code supports unstructured hexahedral grids.

Self-consistent transfer of energy to and from external lumped element circuit equations may be modeled. Coupled circuit equations allow a set of differential-algebraic equations to

be coupled to the transient magnetic or MHD simulations. This is useful in situations where the simulation is driven by a known voltage source (most magnetic boundary conditions require knowledge of the current) or where the dynamics of the system being modeled feeds-back into the electrical response of the external circuit. This feature is fully described in Section 5.10.

The TRANSIENT MAGNETICS package uses the Aztec library [23] to solve the discrete partial differential equation that governs its physics. Aztec is an iterative library that greatly simplifies solving linear systems of equations. Aztec includes a number of Krylov iterative methods such as conjugate gradient (CG), generalized minimum residual (GMRES), and stabilized biconjugate gradient (BiCGSATB). An algebraic multigrid option [22] for the edge element diffusion formulation in 3D and node-centered 2D formulations are available. These features are fully described in Section 2.3.

An implicit thermal transport modeling capability is available. The current discretization is based on a support operator technique implemented by Kent Budge which has fundamental unknowns as thermal fluxes on faces. The THERMAL CONDUCTION package also uses the Aztec library. No multigrid capability is available in this case, but it is generally unnecessary.

Significant progress has been made at Sandia with respect to conductivity modeling in the solid-liquid-vapor transitions regions. Mike Desjarlais has been the principal theoretical lead in this effort. The LMD models are currently seen as the preferred capabilities. The user is advised to stay abreast of these rapidly advancing development as results are highly dependent on proper models [4, 5].

Radiation emission and opacity models are available. The emission model accounts for reabsorption by reducing the emission rate by a factor equal to one minus the probability of escape. For one group emission, the XSN opacity model can be made more accurate at lower temperatures through the use of the DYNAMIC INTEGRATION option for determining group bounds and the HAGEN RUBENS option. See Section 8.6.3 for details.

2 General Input

General input refers to keywords that appear outside the `PHYSICS ... END` block. As such they are not specific to any particular physics such as `TRANSIENT MAGNETICS` or `THERMAL CONDUCTION`. Typically these include the `TITLE` and `UNITS` keywords, `START TIME` and `TERMINATION TIME`, various `EMIT PLOT` and `EMIT OUTPUT` commands, the `PLOT VARIABLES ... END` block, as well as `MATERIAL` and material `MODEL` input. This section provides a supplement to the ALEGRA Users Manual [3].

2.1 Format and Syntax

2.1.1 Units

`UNITS, {CONSISTENT | SI | CGS | CGSEV | GAUSSIAN}`

Default units for ALEGRA are CGS units. However, the `UNITS` keyword may be used to change the default units to SI, CGSEV, or GAUSSIAN units. Systems of units can be a subject of some confusion. The source of the confusion is that the number of fundamental units and of the dimension of physical quantities is arbitrary [11, 12].

For mechanical quantities (density, velocity, acceleration, force, energy, etc.), all quantities can be expressed in terms of three fundamental units (time, length, and mass). Any simulations involving only these basic mechanical quantities can be run using any `CONSISTENT` set of units, as well as the other explicit sets of units.

Default temperatures are always Kelvin unless CGSEV units are specified. For high temperature applications where the temperature is above the thousands of Kelvin range, it is common to express the temperature in units of energy by combining Boltzmann's constant, k_B , with the temperature ($k_B T$ has dimensions of energy and 1 eV is equivalent to 11605.67 K). In the CGSEV units case, eV are the temperature units.

For `THERMAL CONDUCTION`, quantities such as the specific heat and the thermal conductivity are defined in terms of the fundamental mechanical units (time, length, and mass). Thus `THERMAL CONDUCTION` problems may be run using any `CONSISTENT` set of units, as well as the other explicit sets of units.

For `TRANSIENT MAGNETICS` a variety of electrical units may be associated with input and output quantities. This is accomplished by defining values for six units-dependent constants, κ_1 to κ_6 , at simulation start up.

For SI units, only one choice is available because the Ampere is defined to be a fundamental unit and the electrical quantities default to the standard SI units. Only SI is fully implemented at this time for 3D simulations. SI, CGS, CGSEV, and GAUSSIAN are in general supported in 2D TRANSIENT MAGNETICS simulations.

For CGS-related units, many choices are available in principle, however in ALEGRA MHD only two of these choices have been made available to the user. The default CGS units are also called Practical CGS units. Practical CGS units are a combination of SI and CGS units as found in Knoepfel's monograph [12]. Densities, lengths and velocities are expressed in CGS-like units of g/cm^3 , cm and cm/s. Charge, currents and voltages are expressed in SI-like units of coulombs, amperes and volts. Current densities, electric fields and conductivities are expressed in mixed units of amperes/cm², volts/cm and ohm-cm. Magnetic fields are in gauss. The other CGS-related set of units is the GAUSSIAN system.

The units associated with common variables are outlined in Table 1. Additional systems of units may be found in many textbooks such as Knoepfel's monograph [12] or the NRL Plasma Formulary [9].

2.2 Execution Control

2.2.1 Plot Variables

```
PLOT VARIABLES
  name [, conversion] [, AS "string"]
  name [, conversion] [, AS "string"]
END
```

This section describes additional PLOT VARIABLES available with this version of ALEGRA. Other basic plot variables for hydrodynamics, solid dynamics, and materials are listed in the ALEGRA User's Guide [3].

In Tables 2 through 4 the variable types are listed as being scalar, vector, or material. Scalar variables have only one component and may be located at the mesh cell (or element) centers or located at the mesh nodes (or vertices).

Vector variables have two or three components depending on dimensionality and may be located at the mesh cell (or element) centers or located at the mesh nodes (or vertices). In 3D Cartesian, vectors have three components. Each component appears individually in the output files and is labeled with a suffix of $_X$, $_Y$, or $_Z$. In 2D, vectors have only

Table 1. Dimensions associated with variables for various systems of units.

Variable	SI	CGS	CGSEV	GAUSSIAN
t , time	s	s	s	s
\vec{x} , position	m	cm	cm	cm
\vec{v} , velocity	m/s	cm/s	cm/s	cm/s
m , mass	kg	g	g	g
ρ , mass density	kg/m ³	g/cm ³	g/cm ³	g/cm ³
\vec{F} , force	N (Newton)	dyne	dyne	dyne
E , energy	J (Joule)	erg	erg	erg
e , specific internal energy	J/kg	erg/g	erg/g	erg/g
T , temperature	K (Kelvin)	K	eV	K
C_v , specific heat	J/(kg*K)	erg/(g*K)	erg/(g*eV)	erg/(g*K)
q , particle charge	C (Coulomb)	C	C	esu
\vec{B} , magnetic induction	T (Tesla)	G (Gauss)	G (Gauss)	G (Gauss)
\vec{J} , current density	A/m ²	A/cm ²	A/cm ²	statampere/cm ²
\vec{E} , electric field	V/m	V/cm	V/cm	statvolt/cm
σ , electrical conductivity	(Ohm-m) ⁻¹	(Ohm-cm) ⁻¹	(Ohm-cm) ⁻¹	(statohm-cm) ⁻¹
k , thermal conductivity	J/(m*s*K)	erg/(cm*s*K)	erg/(cm*s*eV)	erg/(cm*s*K)
τ_a , absorption opacity	m ⁻¹	cm ⁻¹	cm ⁻¹	cm ⁻¹
τ_s , scattering opacity	m ⁻¹	cm ⁻¹	cm ⁻¹	cm ⁻¹

two components. Each component appears individually and is labeled with a suffix of $_X$ or $_Y$ in Cartesian geometry, or with a suffix of $_R$ or $_Z$ in cylindrical geometry. Vector components orthogonal to the mesh are still necessary for 2D simulations. These variables are assigned to their own scalar variable and are listed as such in Table 2.

Material variables are associated with material properties and generally are located at the mesh cell (or element) centers. In general, all MATERIAL variables for each MODEL may be plotted by listing the variable name (with or without underscores) within the PLOT VARIABLES keyword construct. These variables are listed in the material model "Registered Plot Variables" tables for each model (see Table 18, Table 12, or Table 14, for example.)

Table 2: Plot Variables for TRANSIENT MAGNETICS.

Variable Name	Type	Description
AZ or ATHETA	scalar (2D)	A_z or A_θ component of the vector potential orthogonal to the mesh for 2D magnetics calculations
AJXB	vector	Lorentz force for 3D/2D MHD calculations
B	vector	Node-based magnetic field for 3D/2D magnetics calculations
BE	vector	Element-centered magnetic field for 3D/2D magnetics calculations
BZ or BTHETA	scalar (2D)	Node-based B_z or B_θ component of the magnetic field orthogonal to the mesh for 2D magnetics simulations
BEZ or BETHETA	scalar (2D)	Element-centered B_z or B_θ component of the magnetic field orthogonal to the mesh for 2D magnetics calculations
DIVB	scalar (3D)	Divergence of the magnetic field for 3D magnetics calculations. Should always be exactly zero to roundoff.
PHI	scalar (2D)	Node-based product of rA_θ for 2D cylindrical simulations using the FIVE R SCALED formulation
PSI	scalar (2D)	Node-based product of rB_θ for 2D cylindrical simulations using the FIVE R SCALED formulation
E	vector	Node-based electric field for 3D/2D magnetics calculations
EZ or ETHETA	scalar (2D)	Node-based E_z or E_θ component of the electric field orthogonal to the mesh for 2D magnetics calculations
J	vector	Node-based current density for 3D/2D magnetics calculations
JE	vector	Element-centered current density for 3D/2D magnetics calculations
JZ or JTHETA	scalar (2D)	Node-based J_z or J_θ component of the current density orthogonal to the mesh for 2D magnetics calculations
<i>continued on next page</i>		

<i>continued from previous page</i>		
JEZ or JETHETA	scalar (2D)	Element-centered averaged current density orthogonal to the mesh for 2D magnetics calculations
VVOL	scalar	Vertex volume for magnetics calculations
ECON	material	Electrical conductivity

Additional TRANSIENT MAGNETICS plot variables other than those listed in Table 2 are available. They are not listed in the table because they typically are not of use to the user. These variables are particular to the details of solution formulations and are primarily of use in debugging the solution method.

Table 3. Plot Variables for THERMAL CONDUCTION.

Variable Name	Type	Description
THERMAL_CON	material	Thermal conductivity
THERMAL_CON_PAR	material	Thermal conductivity component parallel to B field
THERMAL_CON_PERP	material	Thermal conductivity component perpendicular to B field

Table 4. Plot Variables for EMISSION.

Variable Name	Type	Description
EMITTED_POWER	scalar array	Radiation power (energy per time) emitted from each mesh element. Tallied by radiation energy group (gg identifier) and material (mm identifier). Tallies are also summed over energy groups and material, if there is more than one group or material.
EMITTED_POWER EMITTED_POWER_Mmm_Ggg EMITTED_POWER_Ggg EMITTED_POWER_Mmm		total power by group and material summed over materials summed over groups

2.3 Aztec Input

```
AZTEC [int]
...
END
```

Both the TRANSIENT MAGNETICS and the THERMAL CONDUCTION packages use the Aztec library [23] to solve the discrete partial differential equations that govern their physics. Aztec is an iterative library that greatly simplifies solving linear systems of equations. Aztec includes a number of Krylov iterative methods such as conjugate gradient (CG), generalized minimum residual (GMRES), and stabilized biconjugate gradient (BiCGSATB).

The AZTEC keyword set may appear as many times as desired. Different physics packages may utilize different AZTEC control sets as specified by using

```
AZTEC SET id(integer)
```

in the specific physics input section. The default AZTEC SET id-number is 0 which defaults to the conjugate gradient algorithm with symmetric diagonal scaling and other default options described below. The developers do not recommend that you blindly use the default settings as they are most likely not optimal for your particular simulations.

See the Aztec [23] and ML [22] documentation for a full descriptions of the options. Most but not all AZTEC options have been implemented in the ALEGRA interface. However only the most important and useful options are listed in this section.

Example:

```
aztec 1      $ 3D simulation ONLY, mag control
  solver     = cg
  scaling    = none
  conv norm  = rhs
  output     = none
  max iter   = 1000    $ something is wrong after a few hundred iterations
  tol        = 1.e-10  $ this may need to be reduced (problem specific)
  multilevel
    fine sweeps          = 1
    fine smoother        = Hiptmair
    coarse smoother      = LU
    multigrid levels     = 10
```

```

        interpolation algorithm = AGGREGATION
        hiptmair subsmoother    = GAUSS SEIDEL $ for serial runs
    $ hiptmair subsmoother      = MLS          $ for parallel runs > 4PE
        SMOOTH PROLONGATOR
    end
end

```

In the descriptions below the first listed option is the ALEGRA default. These are not necessarily the same as the AZTEC defaults.

2.3.1 Basic Aztec Input

```

AZTEC [int]
    [basic aztec keyword]
    ...
END

```

This section describes the basic (non-multilevel) Aztec control options.

Solver

```

SOLVER, {CG (default) | GMRES | CGS | TFQMR | BICGSTAB | LU |
        GMRESR | FIXED PT | SYMMLQ}

```

Note that CG (conjugate gradient) is applicable only to physics packages which are based on symmetric operators. These include 2D and 3D TRANSIENT MAGNETICS, and the THERMAL CONDUCTION package. The LU option uses the familiar LU-decomposition direct solution method, which is only available in serial mode and will likely quickly exhaust memory for sizeable problems. For small serial test simulations, LU is a good option. CG by itself will probably not work effectively for 3D TRANSIENT MAGNETICS solutions.

Scaling

```

SCALING, {SYM_DIAG (default) | NONE | JACOBI | BJACOBI | ROW_SUM |
        SYM_ROW_SUM}

```

The SYM_DIAG option is only available for physics packages based on symmetric operators, such as 2D TRANSIENT MAGNETICS and the THERMAL CONDUCTION package. It is highly recommended for these.

Preconditioner

PRECONDITIONER, {NONE (default) | JACOBI | NEUMANN | LS | SYM_GS |
DOM_DECOMP}

The SYM_GS option has proven quite effective for those physics packages that are based on symmetric operators. However, it has been discovered that it is possible for the actual solution accuracy to vary significantly with the preconditioner option for a given fixed tolerance value. In particular the JACOBI and SYM_GS preconditioners used with conjugate gradient may cause a significantly less accurate answer than would be obtained without the preconditioner for the same tolerance value. See the ignore scaling option.

Subdomain Solver

SUBDOMAIN SOLVER, {LU | ILUT (default) | ILU | RILU | BILU | ICC}

ICC can be used with symmetric operators.

Convergence Norm

CONVERGENCE NORM, {R0 (default) | RHS | ANORM | NOSCALE | SOL |
expected values}

Various norm options are available. Users of the code **MUST** ensure that their solutions are accurate relative to the chosen convergence norm and the chosen tolerance value. (The AZTEC weighted option is not supported in ALEGRA).

Output

OUTPUT, {NONE (default) | ALL | WARNINGS | LAST | int>0}

Note that no Aztec output is the default for ALEGRA. You must specifically request Aztec output if you want Aztec to tell you about the iterative solve. Transient magnetics will output Aztec information to the HISPLT file.

Maximum Iterations

MAXIMUM ITERATIONS, int>0 (500)

Polynomial Order

POLYNOMIAL ORDER, int>0 (3)

Overlap

OVERLAP, {DIAG | # of overlap rows (default 0)}

Not currently recommended to manipulate.

Type Overlap

TYPE OVERLAP, {STANDARD (default) | SYMMETRIC}

Not currently recommended to manipulate.

Kspace

[KSPACE int>0 (30) | KRYLOV SUBSPACE SIZE int>0 (30)]

Not currently recommended to manipulate.

Reorder

REORDER, {0 | 1 (default)}

Not currently recommended to manipulate.

Orthogonalization

ORTHOGONALIZATION, {CLASSIC (default) | MODIFIED}

Not currently recommended to manipulate.

Auxiliary Vector

AUXILIARY VECTOR, {RESID (default) | RAND}

Not currently recommended to manipulate.

Keep K Vectors

KEEP KVECTORS, int>0 (default 0)

Number of previous solution vectors in K vector orthogonalization. Not currently recommended to manipulate.

Orthogonalize K vectors

ORTHOGONALIZE KVECTORS

Not currently recommended to manipulate.

Apply K Vectors

APPLY KVECTORS

Turns on feature. Not currently recommended to manipulate.

Ignore Scaling

IGNORE SCALING

Turns off the use of scaling in the convergence norm. Not currently recommended to manipulate.

Iteration Calls

ITERATION CALLS, int>0 (1)

AZ_iterate will be called this many times. This may be useful if the "expected values" convergence norm is used to bootstrap the weighting factors.

Not currently recommended to manipulate.

Check Update Size

CHECK UPDATE SIZE

Turn on feature. Not currently recommended to manipulate.

Tolerance

TOLERANCE, real (1.e-12)

WARNING! This default may not be appropriate for some CONVERGENCE NORM options and physics problems. The user is responsible to convince himself that the tolerance specified is sufficient for an otherwise FIXED set of AZTEC options. See the discussion under preconditioners.

Drop Tolerance

DROP TOLERANCE, real (0.0)

Not currently recommended to manipulate.

Ilut Fill

ILUT FILL, real (1.0)

Not currently recommended to manipulate.

Omega

OMEGA, real (1.0)

Not currently recommended to manipulate.

2.3.2 Multilevel Input

```
AZTEC [int]
  [basic aztec keyword]
  ...
  MULTILEVEL
    [multilevel keyword]
    ...
  END
END
```

This section describes the multilevel Aztec control options.

Multigrid Levels

MULTIGRID LEVELS, int (10)

Fine Sweeps

FINE SWEEPS, int (2)

The number of pre and post smoother sweeps to apply at each level.

Fine smoother

FINE SMOOTHER, {GAUSS SEIDEL | JACOBI | LU | AZTEC int (0) |
HIPTMAIR (Hcurl only) | MLS}

Default is automatically determined depending on matrix type. This is the type of smoother applied on each of the fine levels. The AZTEC int is the AZTEC SET int id to be used by the fine smoother.

Coarse Sweeps

COARSE SWEEPS, int (2)

Number of solver sweeps to apply at the coarse level if the coarse smoother is an iterative solver.

Coarse smoother

COARSE SMOOTHER, {GAUSS SEIDEL | JACOBI | LU (default) | AZTEC int (0) |
HIPTMAIR (Hcurl only) | MLS}

The AZTEC int is the AZTEC SET int id to be used by the coarse smoother.

Interpolation Algorithm

INTERPOLATION ALGORITHM, {UC AGGREGATION | MIS AGGREGATION |
UC MIS AGGREGATION (aka AGGREGATION, default)}

V Cycle

`{V CYCLE (default) | W CYCLE}`

Picks the style of multigrid cycling. Not currently recommended to manipulate.

FMG

`FMG`

Turns on full multigrid cycling. Not currently recommended to manipulate.

Verbose

`VERBOSE, int (0)`

Positive integer gives level of multigrid verbose output. Value ranges from 0 to 10. Used primarily to debug ML.

Damping factor

`DAMPING FACTOR, real (computed)`

Code calculates an appropriate value in general. Use only to override default. Not currently recommended to manipulate.

MLS Degree

`MLS DEGREE, int (2)`

Degree of the Tchebychev polynomial as a smoother or subsmoother. Not currently recommended to manipulate.

Full Smoother

FULL SMOOTHER (off)

Enforces extended edge-node-edge smoothing on each side of Hiptmair multigrid cycle. Not currently recommended to manipulate.

Smooth Prolongator

SMOOTH PROLONGATOR (off)

Smooth Reitzinger/Schoeberl prolongator for Hiptmair. A useful option for 3D magnetics.

Aggregate Threshold

AGGREGATE THRESHOLD, real (0.08)

Controls strength of connection in forming aggregates. Not currently recommended to manipulate.

Hiptmair Subsmoother

HIPTMAIR SUBSMOOTHER, {GAUSS SEIDEL (default) | MLS}

This is the subsmoother uses by Hiptmair smoothing.

3 Physics Input

The physics option keywords specify the physics module(s) to use for a calculation. MHD related options are listed in Table 5. Many options are actually combinations of the physics modules implemented in ALEGRA. The preferred syntax is to use the name of the desired physics module, followed by nested blocks of keywords specific to the parent physics modules, and terminated with a corresponding END keyword. For example:

```
magnetohydrodynamics conduction
  $ mhdcon is a child class formed by combining
  $ the following 3 parent classes
  hydrodynamics
    no displacement, x, nodeset 1
    [other hydrodynamics keywords]
    ...
  end

  transient magnetics
    [transient magnetics keywords]
    ...
  end

  thermal conduction
    [thermal conduction keywords]
    ...
  end

  [mhdcon specific keywords]
  ...

  [block keywords]
  ...

  [function keywords]
  ...
end

[other non-physics keywords]
...
```

Keywords pertaining to parent modules of a particular physics module are included in the problem specification by placing the keywords in an END-block introduced by the name of the parent module. Thus, a NO DISPLACEMENT keyword, which is specific to HYDRODYNAMICS (actually DYNAMICS), appears immediately within the HYDRODYNAMICS . . . END-block.

This new syntax offers certain advantages to ALEGRA code development teams. For users of ALEGRA, it offers the advantage of grouping related keywords with the particular physics module to which they are relevant.

3.1 Physics Choices

Physics modules included in ALEGRA MHD, along with their keywords and parents, are listed in Table 5.

Table 5: Physics Options and Parent Classes.

Physics Option	Parent Classes	Description
HYDRODYNAMICS	REGION UNSTRUCTURED REGION MASS PHYSICS ENERGETICS MECHANICS DYNAMICS	deformation with zero stress deviators
SOLID DYNAMICS	REGION UNSTRUCTURED REGION MASS PHYSICS ENERGETICS MECHANICS DYNAMICS	deformation with nonzero stress deviators
TRANSIENT MAGNETICS	ENERGETICS	Transient magnetics diffusion in non-moving media
THERMAL CONDUCTION	ENERGETICS	Thermal conduction in non-moving media
MAGNETOHYDRODYNAMICS	TRANSIENT MAGNETICS SOLID DYNAMICS	Transient magnetics diffusion coupled with solid dynamics
<i>continued on next page</i>		

<i>continued from previous page</i>		
MAGNETOHYDRODYNAMICS CONDUCTION	TRANSIENT MAGNETICS SOLID DYNAMICS THERMAL CONDUCTION	Transient magnetics diffusion coupled with solid dynamics and thermal conduction
HYDRODYNAMICS CONDUCTION	THERMAL CONDUCTION HYDRODYNAMICS	Thermal conduction coupled to hydrodynamics
SOLID DYNAMICS CONDUCTION	THERMAL CONDUCTION SOLID DYNAMICS	Thermal conduction coupled to solid dynamics

In addition to the various physics options, there are options available that modify or enhance the physics options. These modifiers are listed in Table 6.

Table 6. Physics Option Modifiers.

Physics Option	Parent Class Modified	Description
EMISSION	ENERGETICS	Uses a radiation emission model. Applicable to all above physics options.

3.2 Algorithm Control

Algorithm control refers to keywords that must appear within a `PHYSICS . . . END` block. They may apply specifically to a particular physics such as `TRANSIENT MAGNETICS` or `THERMAL CONDUCTION` but the syntax is the same in all cases. Typically these include the `BLOCK` and `DOMAIN` input blocks, as well as `FUNCTION` input. This section provides a supplement to the ALEGRA Users Manual [3].

3.2.1 Block

```
BLOCK int  
      [subkeyword-list]  
END
```

The `BLOCK` keyword group allows the user to specify the materials that are contained in a block and the type of mesh movement desired in the block. The default is for a block to be a voided Lagrangian block (i.e., if all subkeywords are omitted).

The specification of `LAGRANGIAN`, `MMALE`, `SMALE`, or `EULERIAN` initially sets the mesh movement for the block to these types. In particular for `MMALE` and `SMALE` meshes, additional physics based subkeywords have been defined to weight the node positions when remapping a particular block. MHD specific ALEGRA `BLOCK` subkeywords are described in Table 7. These subkeywords supplement the `BLOCK` subkeywords found in the primary ALEGRA User's Manual [3].

3.2.2 Aztec Set

```
AZTEC SET int
```

This keyword may appear as many times as desired, but if more than one type of physics is specified, then this keyword **MUST** appear within the specific physics input sections. For example, `TRANSIENT MAGNETICS` and `THERMAL CONDUCTION` solvers typically use different AZTEC control sets, therefore one must specify different `AZTEC SET int` keywords in the specific physics input sections.

The default `AZTEC SET` is 0 which defaults to the conjugate gradient algorithm with symmetric diagonal scaling and other default options. Omission of the `AZTEC SET id`

Table 7. BLOCK Remap Sub-Keywords.

Sub-Keyword	Type	Description
B MAG TRIGGER J MAG TRIGGER B MAG GRADIENT TRIGGER J MAG GRADIENT TRIGGER	real	Triggers for remesh controlled by TRANSIENT MAGNETICS quantities. Nodes will be flagged for remesh when the magnitude of the vector quantity at the node exceeds the input threshold value.
B MAG WEIGHT J MAG WEIGHT B MAG GRADIENT WEIGHT J MAG GRADIENT WEIGHT	real	Weights for remesh controlled by TRANSIENT MAGNETICS quantities. The remesh algorithm will use the maximum of the nodal value or the user specified value to bias the Tipton remesh method. The algorithm will tend to pull mesh nodes into regions where the selected physics parameter (or its gradient) are greatest.

keyword from a physics input block that requires the use of Aztec will cause that physics to use the default set. The settings for this default set may be changed by including an AZTEC SET 0 ... END block in the input file. See Section 2.3 for a descriptions of possible options.

Example:

```

magnetohydrodynamics conduction
  conduction
    ...
    scale, 1.0e10 $ do not use explicit conduction time step
    $ no explicit AZTEC SET keyword
  end
  transient magnetics
    ...
    aztec set, 1
  end
end

aztec 0      $ do NOT use ML for thermal conduction control
  solver,    cg
  scaling,   sym_diag

```

```

    conv norm, rhs
    precondition, none
    output, none
    tol, 1.e-8
    max iter, 5000
end

aztec 1      $ 2D Mag example for AZTEC/ML solver options
    solver, cg
    scaling, sym_diag $ default = sym_diag
    conv norm, rhs      $ default = r0
    tol, 1.e-8
    output, none
    multilevel          $ These settings may be overkill
        fine sweeps      = 1
        fine smoother    = GAUSS SEIDEL
        coarse smoother  = lu
        interp algorithm = AGGREGATION
    end
end

```

4 Hydrodynamics Input

HYDRODYNAMICS

```
...  
... [hydrodynamics keywords] ...  
...  
[MATERIAL FRACTION FORCE LIMIT real]  
...  
END
```

This section provides a list of supplemental keywords to the hydrodynamics section of the ALEGRA Users Manual. [3]

4.1 Solution Control

Due to numerical approximation, some physics options may compute an external force that is inordinately large compared to the material present in a mixed material/void cell, hence the user may want to limit the force in this case. Limiting only the force associated with that physics may introduce its own set of problems. The options listed here turn off all forces, both internal and external, and accelerations.

4.1.1 Material Fraction Force Limit

```
MATERIAL FRACTION FORCE LIMIT real (0.01) [POWER real (0.)]
```

Problems can arise in the calculation of forces on vertices with very little mass. The effective accelerations can become much too large causing mesh elements to become inverted and the calculation to terminate. The MATERIAL FRACTION FORCE LIMIT keyword allows the user to limit the force acting on mixed material/void elements. This difficulty arises because the force on the material in a mixed material/void element might not scale proportionately with the amount of material present in the element. In the limit that the material fraction (i.e., $mat\,frac = 1 - void\,frc$) tends to zero, the forces on the nodes surrounding the element may be disproportionately large compared to the mass of the node. In this case the acceleration of the nodes may become large causing the mesh to tangle by inverting elements. This keyword is intended to rectify this situation by limiting the forces on the nodes.

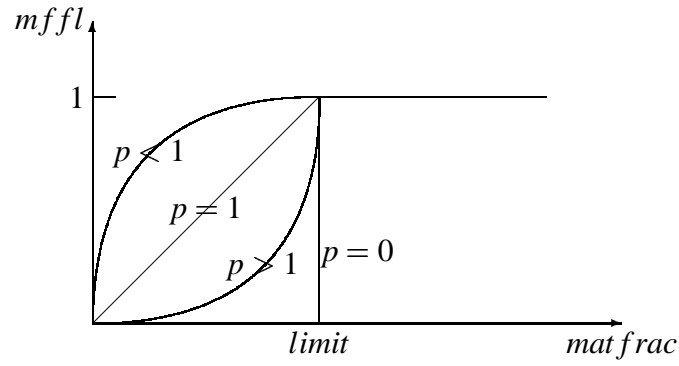


Figure 1. Material Fraction Force Limiter for Hydrodynamics.

The material fractions of attached elements are averaged. If the average material fraction is less than the specified limit, the nodal force is limited, otherwise the force is not changed. The multiplier of the nodal force used when the average material fraction (*matfrac*) is less than the specified *limit* is given by the following expression where *p* is the specified POWER.

$$mffl = \begin{cases} 0, & p = 0 \\ \left(\frac{matfrac}{limit}\right)^p, & p > 0 \end{cases} \quad (1)$$

For $p = 0$ the limiter is a step function, for $p = 1$ the limiter is linear, for $p > 1$ the limiter drops rapidly near the threshold, and for $p < 1$ the limiter drops rapidly near 0. Graphically the multiplier can be displayed as in Figure 1.

Note that TRANSIENT MAGNETICS has the same MATERIAL FRACTION FORCE LIMIT keyword. The difference in usage is that in TRANSIENT MAGNETICS this keyword limits the Lorentz force only. In HYDRODYNAMICS this keyword limits all forces, both internal (e.g., pressure) and external (e.g., gravity and Lorentz).

5 Transient Magnetics Input

TRANSIENT MAGNETICS

```
...
... [transient magnetics keywords] ...
...
END
```

The TRANSIENT MAGNETICS input controls the magnetics capability in this version of ALEGRA. This allows for modeling electromagnetic effects in the quasi-neutral, quasi-static magnetic field approximation.

$$\begin{aligned}
 \nabla \times \vec{E} &= -\kappa_3 \frac{\partial \vec{B}}{\partial t} \\
 \nabla \times \vec{H} &= \kappa_5 \vec{J} \\
 \nabla \cdot \vec{B} &= 0 \\
 \vec{B} &= \mu_0 \vec{H} \\
 \eta \vec{J} &= \vec{E} + \kappa_3 \vec{V} \times \vec{B}
 \end{aligned} \tag{2}$$

Details of the implementation can be found in various references [2].

While most input keywords are similar in 3D and 2D, there are some differences. These are noted in the following keyword descriptions. Various magnetic units are supported. See the UNITS keyword in Section 2.1.1 for more information.

3D Example:

```
transient magnetics
  formulation, whitney
  delta time = 5.e-6

  e tangent bc, sideset 10, 0., x 1. y 0. z 0.

  cyl axial slot bc, sideset 11, 1.0e6,
    x 0. y 0. z 0.,
    x 0. y 0. z 1.,
    0.00075, 0.001, 0.002, 0.00225
```

```

uniform h bc, sideset 20, 0., x 0. y 0. z 1.
uniform h bc, sideset 30, 0., x 1. y 0. z 0.

void conductivity, 1.
current density, projected
end

```

2D Example:

```

transient magnetics
  start = 0.
  stop  = 100.e-9
  delta time = 0.15e-9

  rz cyl radial slot bc, sideset 1, function 1, scale 1.,
    r 0.0, z 0.0, -2.0, -1.0, 1.0, 2.0
  centerline bc, sideset 3, 0.0,

  aztec set, 1
end

```

5.1 Formulation

FORMULATION, WHITNEY	(3D)
FORMULATION, {FIFE FIFE R SCALED}	(2D)

This keyword defines the solution formulation. In 3D, it is unnecessary.

In 2D, this input is optional and the default value is geometry dependent. In 2D Cartesian geometry, the two methods are equivalent, hence FIFE (Fully Integrated Finite Element) is chosen automatically as the default. The difference is manifested in 2D cylindrical geometry, where FIFE R SCALED is the preferred method and is chosen automatically as the default. FIFE solves for B_θ or A_θ as the fundamental variable (depending on boundary conditions) and FIFE R SCALED solves for $\Psi = rB_\theta$ or $\Phi = rA_\theta$ as the fundamental variable (depending on boundary conditions).

5.2 Time Step Control

5.2.1 Start

START real ($-\infty$) (2D only)

This keyword indicates the simulation time to start the magnetic field solution, if different from the problem START TIME. Field values are set equal to zero prior to this time. It has no effect in 3D.

5.2.2 Stop

STOP real ($+\infty$) (2D only)

This keyword indicates the simulation time to stop the magnetic field solution, if different from the problem TERMINATION TIME. Field values are set equal to zero after this time. It has no effect in 3D.

5.2.3 Delta Time

DELTA TIME real (1.e-6) [FIXED | MAGNETIC DIFFUSION | MAGDIFF] (3D)

DELTA TIME real (1.e-6) [FIXED | MAGNETIC DIFFUSION | MAGDIFF |
AUTOSTEP, TOLERANCE real, BMIN real] (2D)

The minimum of the mechanics time step and this DELTA TIME value is used as the actual magnetohydrodynamics time step. Otherwise this is the time step for the transient magnetics physics. The specified value provides an upper bound on the time step when using the non-fixed options described below. This value may also be used to give a time scale for the differential algebraic equation solver at CIRCUIT SOLVER initialization. The overall magnetics time step is reported in the DT_MAG global variable. This is the net result after considering all options described below.

The optional FIXED parameter causes transient magnetics to choose a fixed time step. This is the default.

The optional MAGNETIC DIFFUSION or MAGDIFF parameter adjusts the time step based upon the magnetic diffusion coefficient, D . Mesh element that are less than 1% material are excluded from consideration.

$$\Delta t \leq \frac{h^2}{4D} \quad (3)$$

where $D = \frac{1}{\sigma\mu_0}$, σ is the electrical conductivity, μ_0 is the permeability, and h is a characteristic cell size. The individual result of the magnetic diffusion time step is reported in the DT_MAGDIFF global variable.

The optional AUTOSTEP parameter is valid only in 2D and adjusts the time step by estimating a relative truncation error and adjusting the time step to keep the error below the specified TOLERANCE. The BMIN parameter omits mesh cells with a magnetic field value below this value from consideration.

$$\Delta t_{new} = \Delta t_{old} \sqrt{\frac{tolerance}{relerr}} \quad (4)$$

where $relerr = |\frac{\Delta B}{B}|$. Both the MAGNETIC DIFFUSION and AUTOSTEP options may be specified simultaneously.

Another factor, the Alfven speed, may control the time step when hydrodynamics is enabled. In this case, the Alfven speed is combined with a material wave speed, e.g., the sound speed, and used in a Courant condition. Keywords affecting the Alfven speed are described below. The individual result of the Alfven speed time step is reported in the DT_ALFVEN global variable.

$$\Delta t \leq \frac{h}{\sqrt{V_{hydro}^2 + V_{Alfven}^2}} \quad (5)$$

where $V_{Alfven} = \frac{B}{\sqrt{\mu_0\rho}}$ in SI units.

Example 1:

```
transient magnetics
...
delta time 0.5e-6, magnetic diffusion
...
end
```

Example 2:

```
transient magnetics
...
delta time 1., autostep, tol 0.01, bmin 1.e-4, magdiff
...
end
```

5.2.4 Alfven Density Floor

ALFVEN DENSITY FLOOR real (0.)

If this keyword is present then the Alfven speed is artificially set to zero in any element with a density below ALFVEN DENSITY FLOOR. This avoids the problem of very small time steps due to anomalously large Alfven speeds in low-density regions.

Example:

```
transient magnetics
...
alfven density floor 0.01    $ gm/cm^3
...
end
```

5.2.5 Alfven Velocity Maximum

ALFVEN VELOCITY MAXIMUM real (0.)

If this keyword is present then the Alfven speed is artificially set to zero in any element with a Alfven wave speed greater than ALFVEN VELOCITY MAXIMUM. This avoids the problem of very small time steps due to anomalously large Alfven speeds.

Example:

```
transient magnetics
...
alfven velocity max 1.0e7    $ m/s
...
```

end

5.3 Solution Control

5.3.1 A Rezone

```
A REZONE, {CT VAN LEER (default) | CT DONOR | CT HARMONIC |  
           CT MONOTONIC | MONOA (2D only)} (2D, 3D)
```

The CT options indicate the constrained transport reconstruction option for the magnetic flux in 3D or the vector potential in 2D Cartesian. The CT options take an optional ISO and EH arguments for use by developers. CT VAN LEER is the default in 2D, but MONOA is still available as an example of a not so good algorithm. This keyword can also be used in 3D, but MONOA is not permitted.

5.3.2 Alpha

```
ALPHA real (0.) (2D only)
```

Variable weight of lumped versus consistent mass matrix. A value of 1.0 implies use of a fully consistent mass matrix and the default value of zero implies use of a lumped mass matrix. This is only active in 2D. In 3D a fully consistent vector edge element mass matrix is used.

The effect of this option can be seen in certain magnetic diffusion simulations. Use of the consistent mass matrix can result in small negative magnetic field values where none are expected. Use of the lumped avoids this behavior, thus it is the default.

5.3.3 Aztec Set

```
AZTEC SET int (0)
```

This defines the id-number of the Aztec parameter set which the magnetic solver will use.

For 2D MAG or MHD, the equations solved are formulated to always produce symmetric positive definite matrices, hence the recommended settings for Aztec parameters are:

```
AZTEC int
  SOLVER,      CG
  SCALING,     SYM_DIAG $ (or SYM_ROW_SUM)
  PRECOND,     SYM_GS   $ (used if no MULTILEVEL)
  CONV NORM,  RHS      $ (or ANORM or NOSCALED)
  OUTPUT,      NONE
  TOL,         1.E-12   $ (< 1.E-8)
  MAX ITER,   1000     $ (>500)
  MULTILEVEL
    FINE SWEEPS      = 5
    FINE SMOOTHER    = GAUSS SEIDEL
    COARSE SWEEPS    = 1      $ (because it is LU)
    COARSE SMOOTHER  = LU
    MULTIGRID LEVELS = 10
    INTERP ALGORITHM = AGGREGATION
  END
END
```

These settings for the solver, scaling and preconditioner are appropriate for symmetric positive definite matrices. A convergence norm setting of R0 is not recommended because 2D TRANSIENT MAGNETICS uses the old solution as the initial guess and this norm can easily remain greater than the tolerance, especially if the solution approaches steady state. Tighter tolerances typically produce a more accurate answer and should be the first parameter changed if the answer is not approaching the expected solution, especially for high resolution meshes. Note however that tight tolerances may cause Aztec to report convergence warnings. These appear because Aztec converges for the scaled matrices, but not necessarily for the unscaled matrices or for the convergence norm. To eliminate these messages the user can try setting the SCALING and the PRECONDITIONER to NONE to force convergence of the unscaled matrices. Finally, the iterative solver typically should not require an exceptional number of iterations. One case where high iteration counts may be necessary is if the applied boundary conditions cause a strong step function change to the solution during the initial time step.

5.3.4 Conserve Memory

CONSERVE MEMORY

If this keyword is found then the magnetic solver code releases back to the system temporary memory utilized in setting up and solving the linear equations. Otherwise, this memory is only allocated once.

5.3.5 Magnetic Field

MAGNETIC FIELD, {PROJECTED | CONSISTENT}

Variations on implementations of deriving the magnetic field from the vector potential by solving the equation $\vec{B} = \nabla \times \vec{A}$. The default is PROJECTED in 3D and CONSISTENT in 2D. The CONSISTENT option is available in 2D only.

PROJECTED solves the curl equation by treating the LHS as a lumped diagonal matrix and evaluating the RHS by a single point integration using the value of the curl at the cell center.

CONSISTENT employs a finite element approach to calculate the nodal magnetic field directly from the nodal vector potential while skipping the element-centered magnetic field as an intermediary. The LHS is treated as a lumped diagonal matrix and the RHS is evaluated by Gaussian integration of the curl using finite element basis functions.

5.3.6 Magnetic Force

MAGNETIC FORCE, {TENSOR | PJXBV | PJXPBPV | NOBFORCE}

Variations on implementations of the magnetic force. Default is PJXPBPV in 3D and TENSOR in 2D. Both the PJXPBPV and PJXBV options first compute the magnetic field and current density at the mesh vertices and then form the cross product to determine the magnetic force. The TENSOR option computes the magnetic stress tensor at the element centers and then computes a surface integral around each mesh vertex to determine the magnetic force. NOBFORCE turns off the magnetic force term in MHD simulations. Primarily for developers.

5.3.7 Material Fraction Force Limit

MATERIAL FRACTION FORCE LIMIT real (0.01) [POWER real (0.)]

Problems can arise in the calculation of Lorentz forces on vertices with very little mass. The effective accelerations can become much too large causing mesh elements to become inverted and the calculation to terminate. The MATERIAL FRACTION FORCE LIMIT keyword allows the user to limit the Lorentz force acting on mixed material/void elements. This difficulty arises because the Lorentz force on the material in a mixed material/void element might not scale proportionately with the amount of material present in the element. In the limit that the material fraction (i.e., $mat\,frac = 1 - void\,frc$) tends to zero, the forces on the nodes surrounding the element may be disproportionately large compared to the mass of the node. In this case the acceleration of the nodes may become large causing the mesh to tangle by inverting elements. This keyword is intended to rectify this situation by limiting the forces on the nodes.

After the Lorentz forces are determined for each node in the mesh, the material fractions of attached elements are averaged. If the average material fraction is less than the specified limit, the nodal force is limited, otherwise the force is not changed. The multiplier of the nodal force used when the average material fraction ($mat\,frac$) is less than the specified *limit* is given by the following expression where p is the specified POWER.

$$mffl = \begin{cases} 0, & p = 0 \\ \left(\frac{mat\,frac}{limit}\right)^p, & p > 0 \end{cases} \quad (6)$$

For $p = 0$ the limiter is a step function, for $p = 1$ the limiter is linear, for $p > 1$ the limiter drops rapidly near the threshold, and for $p < 1$ the limiter drops rapidly near 0. Graphically the multiplier can be displayed as in Figure 2.

Note that HYDRODYNAMICS has the same MATERIAL FRACTION FORCE LIMIT keyword. The difference in usage is that in TRANSIENT MAGNETICS this keyword limits the Lorentz force only. In HYDRODYNAMICS this keyword limits all forces, both internal (e.g., pressure) and external (e.g., gravity and Lorentz).

5.3.8 Current Density

CURRENT DENSITY, {PROJECTED | CONSISTENT}

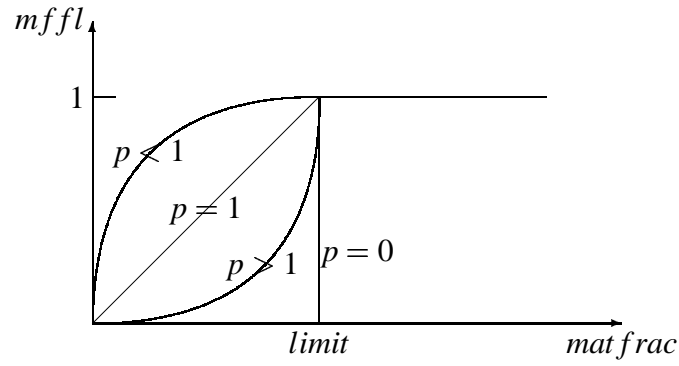


Figure 2. Material Fraction Force Limiter for Magnetics.

Various implementations of deriving the current density from either the magnetic field by solving $\vec{J} = \nabla \times \frac{1}{\mu} \vec{B}$ or from the vector potential by solving $\vec{J} = \nabla \times \frac{1}{\mu} \nabla \times \vec{A}$. The default is CONSISTENT in 2D. Only PROJECTED is available in 3D.

PROJECTED solves $\vec{J} = \nabla \times \frac{1}{\mu} \vec{B}$ by treating the LHS as a lumped diagonal matrix and evaluating the RHS by a single point integration using the value of the curl at the cell center.

CONSISTENT solves $\vec{J} = \nabla \times \frac{1}{\mu} \nabla \times \vec{A}$ by treating the LHS as a lumped diagonal matrix and evaluating the RHS by Gaussian integration using finite element basis functions. The RHS also integrates the double curl once to incorporate the boundary conditions.

5.3.9 Joule Heat

JOULE HEATING, {STANDARD | MAXSIGMA | NOHEAT}

Default is STANDARD. Joule heating is based on a fully-integrated, finite-element-based rate consistent with the discrete magnetic diffusion equations. In multi-material mesh cells, the Joule heat is partitioned among materials according to the conductivity fraction. For a simple steady state problem this gives the correct Joule heating in mixed cells.

MAXSIGMA limits Joule heating in the multi-material and mixed-void-material elements by effectively limiting the electric field by the ratio of the average conductivity to the maximum conductivity in the element. This prevents overheating of materials in mostly void cells and may allow calculations to run longer than using the STANDARD option.

$$\dot{Q}_{Joule} = \sigma_{ave} |E|^2 \approx \sigma_{ave} \left| \frac{\sigma_{ave}}{\sigma_{max}} E \right|^2 \quad (7)$$

NOHEAT turns off the Joule heating term.

5.3.10 Void Conductivity

VOID CONDUCTIVITY real (default 1.e-6)

This keyword defines the isotropic void conductivity as well as the default for materials if a conductivity model is missing. It is not a required input. The default is set to 1.E-6 $(\Omega\text{-m})^{-1}$, except for the 2D vector potential formulation, in which case the default is zero.

5.3.11 Void Reluctivity

VOID RELUCTIVITY real (default 7.957747e+5)

This keyword defines the isotropic void reluctivity, i.e. the inverse of the permeability, as the default for materials if a reluctivity models is not defined. It is not a required input. The default is set to $1/(4\pi \cdot 10^{-7} \text{ H/m})$.

5.4 Boundary Conditions

5.4.1 Cylindrical Axial Slot BC

CYLINDRICAL AXIAL SLOT BC, sideset, {function-set | CIRCUIT},
vector1, vector2, r0, r1, r2, r3 (3D)

{XY|RZ} CYLINDRICAL AXIAL SLOT BC, sideset, {function-set | CIRCUIT},
[vector1,] r0, r1, r2, r3 (2D)

Apply a current boundary condition to the given sideset which must be a planar sideset cutting a cylindrical region. The prefix XY or RZ is needed in 2D to distinguish between Cartesian and cylindrical geometries.

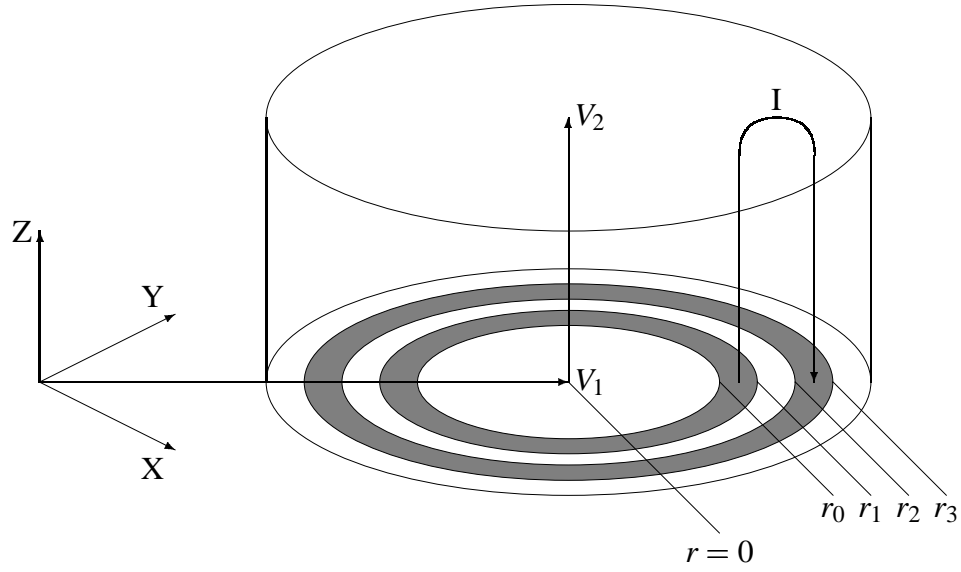


Figure 3. Geometry for the Cylindrical Axial Slot boundary condition.

The function-set keyword may be used to drive the simulation with a known current source. The direction of the current flow can be reversed by changing the sign of the function-set (i.e., setting SCALE = -1.0). The CIRCUIT keyword may be used instead of a function-set to couple the simulation to a set of circuit equations.

The vector1 defines a point on the axis of the cylinder and may displace the cylinder from the origin and also defines the $r = 0$ location. In 2D, it is used only in Cartesian geometry and is omitted in cylindrical geometry. The vector2 is used only in 3D and defines the direction of the cylindrical axis. Given a point \vec{P} on the sideset, $z = (\vec{P} - \vec{V}_1) \cdot \vec{V}_2$ and $r = |\vec{P} - \vec{V}_1 - (z \cdot \vec{V}_2)|$, assuming vector2 is normalized to unity (ALEGRA will do this).

The real parameters r0, r1, r2, and r3 specify the radial range over which this boundary condition applies. The total current is assumed to flow uniformly into the mesh between r0 and r1 and out of the mesh between r2 and r3 so that there is no net accumulation of electrical charge. In other words, the axial current density is assumed constant between r0 and r1, constant and of the opposite sign between r2 and r3, and zero elsewhere on the sideset.

Relative to the axis of the cylinder,

$$H_{\theta} = f(r) \frac{I(t)}{2\pi r} \quad (8)$$

where

$$f(r) = \begin{cases} 0, & r \leq r_0 \\ \frac{r-r_0}{r_1-r_0}, & r_0 \leq r \leq r_1 \\ 1, & r_1 \leq r \leq r_2 \\ \frac{r_3-r}{r_3-r_2}, & r_2 \leq r \leq r_3 \\ 0, & r_3 \leq r. \end{cases} \quad (9)$$

In many instances the user may wish to allow the current to diffuse naturally into the inner and outer conductors. This may be accomplished by letting the slot (or gap) between r_1 and r_2 be its own sideset. r_0 and r_1 may be equal to each other and less than the inner radius of the gap. r_2 and r_3 may be equal to each other and greater than the outer radius of the gap. Because the extent of the sideset is limited to the gap, the boundary condition will be applied only in the gap. ALEGRA will then naturally diffuse the magnetic field and current into the inner and outer conductors. The same results can also be achieved simply by setting $r_0 = r_1$ and $r_2 = r_3$.

3D Example (this example specifies a constant 1 MA current flow through the mesh):

```
cyl axial slot bc, sideset 11, 1.e6,
  x 0. y 0. z 0.,
  x 0. y 0. z 1.,
  0.00075, 0.001, 0.002, 0.00225
```

2D Cylindrical Example:

```
rz cyl axial slot bc, sideset 1, function 2, scale 0.8,
  0.0, 0.0, 1.0, 2.0
```

2D Cartesian Example:

```
xy cyl axial slot bc, sideset 300, circuit,
  x 0.0 y 0.0, 1.0, 1.0, 2.0, 2.0
```

5.4.2 Cylindrical Radial Slot BC

CYLINDRICAL RADIAL SLOT BC, sideset, {function-set | CIRCUIT},
vector1, vector2, z0, z1, z2, z3 (3D) (3D)

{XY|RZ} CYLINDRICAL RADIAL SLOT BC, sideset, {function-set | CIRCUIT},
vector1, [z0, z1, z2, z3] (2D) (2D)

Apply a current boundary condition to the given sideset which must be of cylindrical shape. The prefix XY or RZ is needed in 2D to distinguish between Cartesian and cylindrical geometries.

The function-set keyword may be used to drive the simulation with a known current source. The direction of the current flow can be reversed by changing the sign of the function-set (i.e., setting SCALE = -1.0). The CIRCUIT keyword may be used instead of a function-set to couple the simulation to a set of circuit equations.

The vector1 defines a point on the axis of the cylinder and may displace the cylinder from the origin and also defines the $z = 0$ location. In 2D cylindrical geometry, it only defines the $z = 0$ location. The vector2 is used only in 3D and defines the direction of the cylindrical axis. Given a point \vec{P} on the sideset, $z = (\vec{P} - \vec{V}_1) \cdot \vec{V}_2$ and $r = \left| \vec{P} - \vec{V}_1 - (z \cdot \vec{V}_2) \right|$, assuming vector2 is normalized to unity (ALEGRA will do this).

The real parameters z0, z1, z2, and z3 specify the axial range over which this boundary condition applies. The total current is assumed to flow uniformly into the mesh between z0 and z1 and out of the mesh between z2 and z3 so that there is no net accumulation of electrical charge. In other words, the radial current density is assumed constant between z0 and z1, constant and of the opposite sign between z2 and z3, and zero elsewhere on the sideset.

Relative to the axis of the cylinder,

$$H_\theta = f(z) \frac{I(t)}{2\pi r} \quad (10)$$

where

$$f(z) = \begin{cases} 0, & z \leq z_0 \\ \frac{z-z_0}{z_1-z_0}, & z_0 \leq z \leq z_1 \\ 1, & z_1 \leq z \leq z_2 \\ \frac{z_3-z}{z_3-z_2}, & z_2 \leq z \leq z_3 \\ 0, & z_3 \leq z. \end{cases} \quad (11)$$

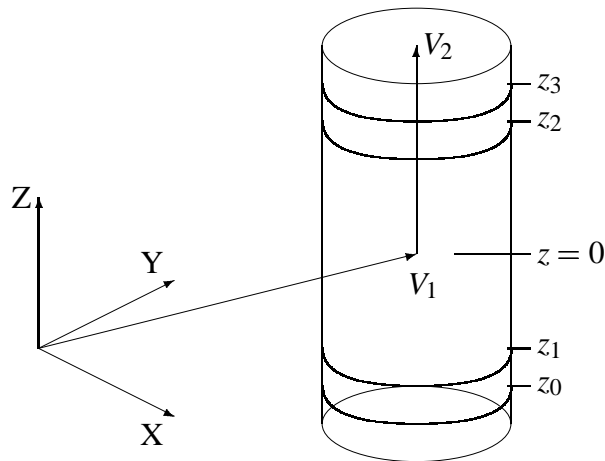


Figure 4. Geometry for the Cylindrical Radial Slot boundary condition.

In many instances the user may wish to allow the current to diffuse naturally into the lower and upper conductors. This may be accomplished by letting the slot (or gap) between z_1 and z_2 be its own sideset. z_0 and z_1 may be equal to each other and less than the lower height of the gap. z_2 and z_3 may be equal and greater than the upper height of the gap. Because the extent of the sideset is limited to the gap, the boundary condition will be applied only in the gap. ALEGRA will then naturally diffuse the magnetic field and current into the lower and upper conductors.

In situations where the upper and lower conductors are not explicitly modeled, z_0 and z_1 may be below the mesh and z_2 and z_3 may be above the mesh to model a current that effectively flows into the bottom and out of the top of the mesh.

3D Example:

```
cyl radial slot bc, sideset 30, function 1,
  x 0.0 y 0.0 z 0.0,
  x 0.0 y 0.0 z 1.0,
  -10.0, -1.0, 1.0, 10.0
```

2D Cylindrical Example:

```
rz cyl radial slot bc, sideset 1, function 2, scale 0.8,
  r 0.0 z 0.0,    -2.0, -1.0, 1.0, 2.0
```

2D Cartesian Example:

```
xy cyl radial slot bc, sideset 300, circuit,  
  r 0.0 z 0.0
```

5.4.3 E Tangent BC

E TANGENT BC, sideset, function-set, vector

Apply tangential electric field boundary conditions to set the tangential components of the electric field.

vector is the electric field direction which the code normalizes to unit magnitude and function-set gives the magnitude.

3D Example:

```
e tangent bc, sideset 100, 0.0, x 1. y 0. z 0.
```

2D Example:

```
e tangent bc, sideset 2, 200.0, r 0. z 1.
```

5.4.4 Uniform H BC

UNIFORM H BC, sideset, function-set, vector, [LENGTH real]

Apply $\vec{H} = \vec{B}/\mu_0$ boundary conditions to the given sideset assuming the vector is tangential to the sideset. If it is not then the tangential component will be imposed. The function-set specifies the magnitude of the magnetic field H when no LENGTH keyword is present. If a LENGTH is given then the function-set is assumed to be a current rather than a magnetic field and LENGTH is used to change current to magnetic field units according to:

$$B(t) = \mu_0 H(t) = \frac{\mu_0 I(t)}{L} \quad (12)$$

In 2D, a vector is specified as:

[X real, Y real,] [Z real]	(Cartesian geometry)
[R real, Z real,] [THETA real]	(cylindrical geometry)

depending upon geometry. The first two components or third component may be optional.

It is often useful to specify $SCALE = 7.957747e5$ in the function-set, especially when working in SI units and the magnetic induction B is given. This SCALE is $1/\mu_0$ and scales $H = B/\mu_0$.

3D Examples:

```
uniform h bc, sideset 10, 1.0, scale 7.957747e5, x 0. y 0. z -1.
uniform h bc, sideset 11, 1.0, scale 7.957747e5, x 0. y 0. z 1.
```

2D Example (1 Tesla magnetic field in the plane of a Cartesian mesh):

```
uniform h bc, sideset 10, 1.0, scale 7.957747e5, x 0. y -1.
```

2D Example (1 Tesla magnetic field orthogonal to the plane of a Cartesian mesh):

```
uniform h bc, sideset 20, 1.0, scale 7.957747e5, z 1.
```

5.4.5 Centerline BC

CENTERLINE BC, {sideset | NONE} (2D RZ only)

Zero the magnetic field or the vector potential along the given sideset. In 2D cylindrical geometry, the value of the magnetic field B_θ , the vector potential A_θ , and their products with the radius r are identically zero along the centerline of the mesh. Multiple occurrences of this command are allowed when the centerline is comprised of more than one sideset.

This is the only boundary condition for magnetic field simulations that can be known *a priori* and was historically provided for the user. The method devised to implement the boundary condition, however, is rather inefficient for large meshes, requiring a loop over the entire mesh every time step. The historic method is still used in cylindrically symmetric problems when no CENTERLINE BCs are specified. Use of this boundary condition suppresses the historic method.

This boundary condition is valid along the inner edge of cylindrical meshes that do not extend to the centerline, but still have the field equal to zero because there is no enclosed current. It is also valid along the outer edge of cylindrical meshes where there is zero net current (i.e., there may be oppositely directed currents that cancel one another).

The keyword `NONE` specifies that there is no such applicable boundary condition. Such may be the case if there is an interior current-carrying conductor that is not explicitly modeled. The intent of the `NONE` keyword is to suppress the historic method in cases where there is no zero-field inner boundary.

2D RZ Examples:

```
centerline bc, sideset 11
centerline bc, sideset 12
```

5.4.6 E Normal Return Current BC

```
E NORMAL RETURN CURRENT BC, real,
  CATHODE BLOCK id-list, ANODE BLOCK id-list,
  {function-set | CIRCUIT} (2D XY only)
```

```
E NORMAL RETURN CURRENT BC, real,
  CATHODE MATERIAL id-list, ANODE MATERIAL id-list,
  {function-set | CIRCUIT} (2D XY only)
```

This boundary condition allows the modeling of a cross-section of a cathode-anode configuration where the normal current in the cathode is balanced by the return current in the anode. Specification of the cathode and anode may be accomplished using either block-ids or material-ids. Block and material specifications may not be mixed in a single simulation, however.

The first `real` is the length of the return current in the Z direction orthogonal to the plane of the mesh. **IMPORTANT:** The region keyword `VOLUMETRIC SCALE FACTOR` must also be set to the product of this length and any planar geometrical symmetries. This is because the codes divides the volumetric scale factor by this normal length in order to compute the planar symmetry for scaling the current.

If the block specification is used, the cathode and anode `id-lists` need to include all blocks which may contain cathode or anode material during the course of the calculation.

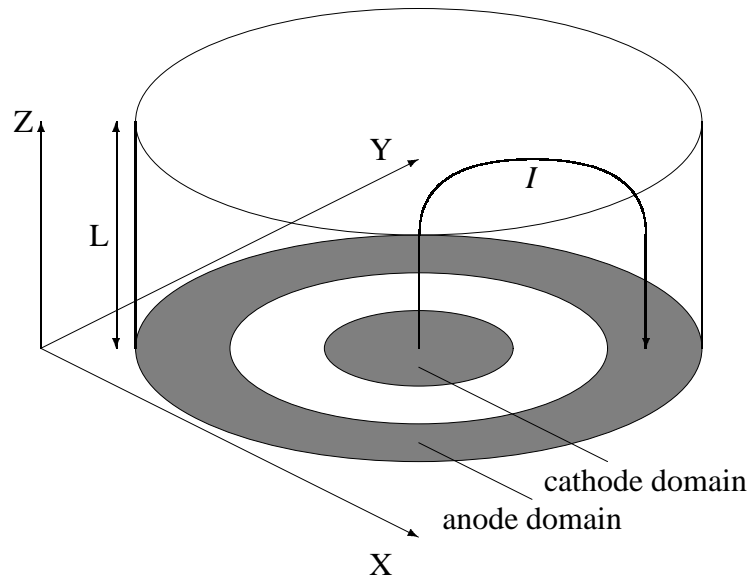


Figure 5. Geometry for the E Normal Current Return boundary condition.

It is desirable to have void (blocks not specified in the cathode or anode lists and having no material) separating the two regions. The code will give warning messages if any material enters these void regions. The code cannot otherwise determine if the anode and cathode regions physically touch, causing an electrical short and thus invalidating the modeling assumptions.

If the material specification is used, the cathode and anode id-lists must be distinct. If the cathode and anode materials are the same, two MATERIAL keyword groups must still be defined, but may reference the same set of MODEL subkeywords. The number of mesh blocks is immaterial. No separating void blocks are needed. Cathode and anode materials may coexist in the same mesh block. Other materials may be present in addition to the anode and cathode materials. These materials may represent insulators or perhaps electrically isolated conductors. The code will abort should cathode and anode materials coexist in the same mesh cell. This situation indicates an electrical short and again invalidates the modeling assumptions.

The function-set is representative of a voltage drop driver. Alternatively the mesh may be coupled to an external CIRCUIT model.

Finally, this boundary condition is incompatible with H-tangent boundary conditions such as the CYLINDRICAL AXIAL SLOT BC, CYLINDRICAL RADIAL SLOT BC, or UNIFORM

H BC.

Example 1:

```
e normal return current bc, 1.0,  
    cathode block 5, anode block 1 2 3 4, function 1
```

Example 2:

```
e normal return current bc, 0.036,  
    cathode material 11 12, anode material 13, circuit
```

The equations which describe this boundary conditions and the coupling to an external circuit equation have been documented [15].

5.5 Current Tally

```
CURRENT TALLY, int,  
    sideset1 [SYMMETRY FACTOR real] [sideset2 ...]  
END                                                    (3D/2D)  
  
CURRENT TALLY, int,  
    block-id1 [SYMMETRY FACTOR real] [block-id2 ...]  
END                                                    (2D only)
```

This option allows the user to tally the total current flowing through a collection of sidesets or blocks as a function of time. Multiple sidesets may be included in a single tally. The *int* is used to identify the tally in the EXODUS and HISPLT output files. In 2D, the user may specify a set of blocks to tally the total current flow perpendicular to the mesh. sidesets and block-ids may not be mixed in the same tally, although both may appear in separate CURRENT TALLY commands in the same input deck. Both the incoming and outgoing currents are reported for each tally. The names of the tallies in the output files are *I_IN_int* and *I_OUT_int*.

The optional SYMMETRY FACTOR keyword allows the user to individually scale the current tally of each sideset or block in situations where a symmetry is present and a reduced simulation is modeled. This keyword is necessary because sidesets (which are areas) may

not scale in the same manner as volumes (e.g., the `VOLUMETRIC SCALE FACTOR` keyword).

Coding internal to ALEGRA attempts to force the user to specify a completed set of tallies. The code checks to see that the incoming and outgoing currents are equal, or else that one is zero in the case of a partial tally. If the two values differ by more than some tolerance (currently 1.E-5), a warning message is issued.

Assuming the specified tallies represent the total current, ALEGRA also reports the total current in the variable `CURRENT`, the total mesh inductance in the variable `INDUCTANCE`, and the total mesh resistance in the variable `RESISTANCE`.

Examples:

```
current tally, 1, sideset 3, sideset 4, end
current tally, 2, block 12, end
```

5.6 Initial Magnetic Flux Density

Generally speaking initial magnetic flux density initial conditions must be used with care and consideration. In most real problems the interior magnetic field should be generated as a consequence of boundary conditions. However, sometimes it is convenient to input initial conditions and then view the evolution of the field from that point on. The diffuse initial field option can also be used to smooth the initial conditions if desired before the actual start of the simulation. The general format for initial magnetic flux density initial conditions is

```
INITIAL B FIELD, [block-id,] {option}
```

This specifies the application of an initial condition by `block-id`. The `block-id` determines the mesh block to which the initial condition applies. If omitted, the initial condition will apply to all mesh blocks. `block-ids` are required to be positive.

The `option` keyword allows the user to choose from the following initial conditions. If no initial conditions are specified, then the initial magnetic field is set equal to zero.

If multiple initial conditions are specified, then the fields are added according to the superposition principle.

5.6.1 Uniform Initial Field

INITIAL B FIELD, [block-id,] UNIFORM, vector1,
[symtensor], [CONSTANT vector2] (3D)

INITIAL B FIELD, [block-id,] UNIFORM, vector1,
[CONSTANT real] (2D)

Uniform magnetic flux density value. block-id specifies the input block to which the field applies. If block-id is missing the field applies to all blocks.

The value, \vec{B} , vector1, specifies the magnitude and direction of the initial magnetic field. Units for the magnitude are Tesla in SI units, or Gauss in practical CGS units, or Gauss in GAUSSIAN units.

In 3D the symtensor, $\vec{\vec{S}}$, contributes an extra term to the vector potential to give certain continuity properties to the vector potential at block boundaries. It does not affect the magnetic field density except at block boundaries. The vector2, \vec{C} , is a constant vector offset to the vector potential available to match the vector potential across block boundaries.

$$\vec{A} = \vec{C} + .5(\vec{\vec{S}}\vec{x} + \vec{B} \times \vec{x}) \quad (13)$$

In 2D, a vector is specified as

[X real, Y real,] [Z real] (Cartesian geometry)
[R real, Z real,] [THETA real] (cylindrical geometry)

depending upon geometry. The first two components or third component may be optional. The CONSTANT is an offset to the vector potential component to match the vector potential across block boundaries.

5.6.2 Uniform Planar Current

INITIAL B FIELD, UNIFORM PLANAR CURRENT, vector1, vector2, vector3
(Cartesian only)

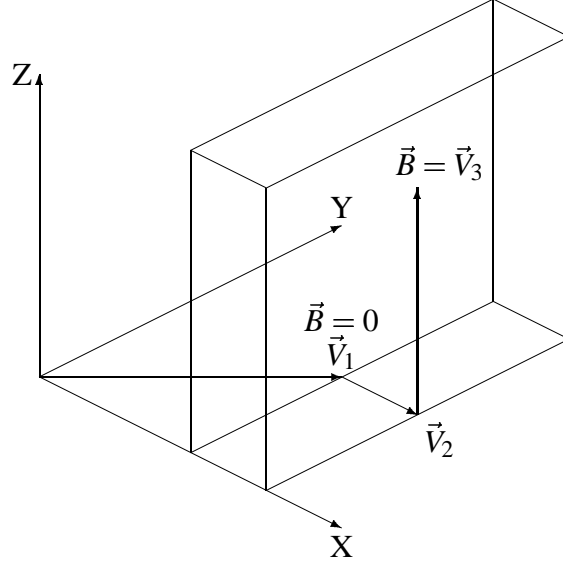


Figure 6. Geometry for the Uniform Planar Current initial condition.

This keyword defines a planar magnetic flux density generated by a planar sheath of uniform current density. The magnetic field is zero on one side of the sheath (called the negative side), is uniform on the other side of the sheath (called the positive side), and varies linearly within the sheath. This initial condition applies to all mesh blocks and is not meaningful in 2D cylindrical geometry.

vector1 specifies a point on the negative face of the sheath. vector2 orients the sheath normal. Its magnitude equals the thickness of the sheath. Its direction points toward the positive side of the sheath where the magnetic field is non-zero. vector3 defines the direction and magnitude of the magnetic field.

In 2D, vector1 and vector2 have only (X,Y) components, while vector3 may have all three components and is specified as:

```
[X real, Y real,] [Z real]
```

The analytic formulas for this initial condition are as follows. Given a point \vec{P} in the mesh, the coordinate relative to the negative face of the sheath is $x = (\vec{P} - \vec{V}_1) \cdot \vec{V}_2 / |\vec{V}_2|$. The magnetic field and vector potential are:

$$\vec{B}(x) = B_0 \frac{\vec{V}_3}{|\vec{V}_3|} \begin{cases} 0, & x \leq 0 \\ x/|\vec{V}_2|, & 0 \leq x \leq |\vec{V}_2| \\ 1, & |\vec{V}_2| \leq x \end{cases} \quad (14)$$

$$\vec{A}(x) = B_0 \frac{\vec{V}_2 \times \vec{V}_3}{|\vec{V}_2 \times \vec{V}_3|} \begin{cases} 0, & x \leq 0 \\ -x^2/(2|\vec{V}_2|), & 0 \leq x \leq |\vec{V}_2| \\ -\frac{1}{2}|\vec{V}_2| - (x - |\vec{V}_2|), & |\vec{V}_2| \leq x \end{cases} \quad (15)$$

where $B_0 = |\vec{V}_3|$ has been called out for clarity.

For example in 2D Cartesian geometry, a 0.5 mm sheath perpendicular to the x axis and centered at 2.0 cm and with a 200 T magnetic field on its positive side is specified using SI units as:

```
initial b field, uniform planar current,
  x 0.01975 y 0., $ sheath face
  x 0.0005 y 0., $ sheath normal/thickness
  z 200.          $ magnetic field
```

5.6.3 Uniform Axial Current

```
INITIAL B FIELD, [block-id,] AXIAL CURRENT,
  [R0 real] [R1 real] [B0 real] [B1 real] [CONSTANT vector,]
  vector1, vector2, z0, z1, z2, z3 \quad (3D)
```

```
INITIAL B FIELD, [block-id,] AXIAL CURRENT,
  [R0 real] [R1 real] [B0 real] [B1 real] [CONSTANT real,]
  vector1, [z0, z1, z2, z3] \quad (2D)
```

This keyword defines an azimuthal magnetic flux density generated by a uniform axial current. All optional parameters default to zero if they are not specified.

block-id specifies the input block to which the field applies. If block-id is missing the field applies to all blocks.

R0 and R1 specify the inner and outer radii of the annular region where the axial current flows. The current density is assumed to be uniform for $R_0 \leq r \leq R_1$ and zero elsewhere.

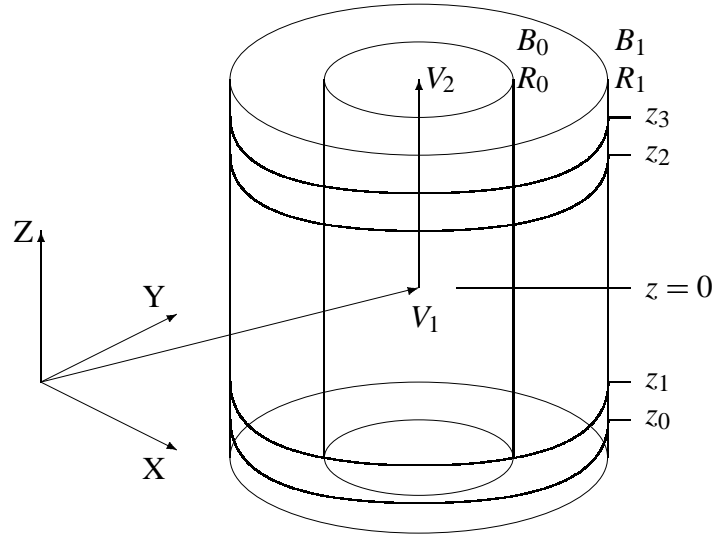


Figure 7. Geometry for the Axial Current initial condition.

B_0 and B_1 specify the magnitude of the azimuthal magnetic field at the radii R_0 and R_1 , respectively.

The optional `CONSTANT` keyword is added to the vector potential to allow continuity of the vector potential across block boundaries.

`vector1` defines a point on the axis of the cylinder which displaces the annular region from the origin and defines the $z = 0$ point along the axis. `vector2` defines the direction of the axis of the region in 3D (ALEGRA will normalize `vector2`). These parameters are similar to the `CYLINDRICAL RADIAL SLOT BC` boundary condition (see Figure 7).

The real numbers z_0 , z_1 , z_2 , and z_3 define the axial extent of the initial field. The magnetic field is modified by a factor $f(z)$ that increases linearly from zero to one between z_0 and z_1 , is unity between z_1 and z_2 , and decreases linearly back to zero between z_2 and z_3 . It is zero outside this range. This models a positive uniform current density entering the mesh through a cylindrical slot between z_0 and z_1 and exiting the mesh through a cylindrical slot between z_2 and z_3 . z_0 and z_1 can be below the mesh and z_2 and z_3 above the mesh to model a current that flows into the bottom and out of the top of the mesh.

$$f(z) = \begin{cases} 0, & z \leq z_0 \\ \frac{z-z_0}{z_1-z_0}, & z_0 \leq z \leq z_1 \\ 1, & z_1 \leq z \leq z_2 \\ \frac{z_3-z}{z_3-z_2}, & z_2 \leq z \leq z_3 \\ 0, & z_3 \leq z. \end{cases} \quad (16)$$

In 2D, vector1 is a point on the axis of the cylindrical region. In Cartesian geometry it can be used to displace the center of the region from the origin. In cylindrical geometry, it defines the $z = 0$ point along the axis. No second vector is needed because the direction of the cylindrical axis can only be parallel to the z axis. The real numbers z_0 , z_1 , z_2 , and z_3 are only needed in 2D for cylindrical geometry and have the same meaning as in 3D.

The analytic formulate for this initial condition are as follows. Given a point \vec{P} on the sideset, the location along the axis is $z = (\vec{P} - \vec{V}_1) \cdot \vec{V}_2$ and the radial distance from the cylindrical axis is $r = |\vec{P} - \vec{V}_1 - (z \cdot \vec{V}_2)|$. The azimuthal magnetic field and vector potential are:

$$B_\theta(r) = \begin{cases} 0, & r < R_0 \\ \frac{1}{r} \left(R_0 B_0 \frac{R_1^2 - r^2}{R_1^2 - R_0^2} + R_1 B_1 \frac{r^2 - R_0^2}{R_1^2 - R_0^2} \right), & R_0 \leq r \leq R_1 \\ B_1 \frac{R_1}{r}, & R_1 \leq r \end{cases} \quad (17)$$

$$\vec{A}(r) = \vec{A}_0 + \vec{n} \begin{cases} 0, & r < R_0 \\ \frac{R_0 B_0 - R_1 B_1}{2} \left(\frac{r^2 - R_0^2}{R_1^2 - R_0^2} \right) + \frac{(R_0 B_1 - R_1 B_0) R_0 R_1}{R_1^2 - R_0^2} \ln \left(\frac{r}{R_0} \right), & R_0 \leq r \leq R_1 \\ \frac{R_0 B_0 - R_1 B_1}{2} + \frac{(R_0 B_1 - R_1 B_0) R_0 R_1}{R_1^2 - R_0^2} \ln \left(\frac{R_1}{R_0} \right) - R_1 B_1 \ln \left(\frac{r}{R_1} \right), & R_1 \leq r \end{cases} \quad (18)$$

where \vec{A}_0 is the optional CONSTANT and \vec{n} is the unit vector in the direction of vector2. \vec{A}_0 is added to the vector potential to allow continuity of the vector potential across block boundaries. Quite often, $R_0 = 0$ and/or $B_0 = 0$ and the above expressions simplify tremendously. In 2D, \vec{A}_0 and \vec{n} have only a z component.

For example, if block 3 is an annular region located between two perfect cylindrical conductors at radii 0.002 meters and 0.02 meters and 1000 Amperes of current flows on the inner conductor and -1000 Amperes flows on the outer conductor, the magnetic field in block 3 is described in 3D by:

\$ calculate A as a superposition of fields

```
$ block 1 (inner conductor) defaults to zero
$ block 2 (outer conductor)
```

```
initial b field, block 2, axial current, r1 0.02, b1 0.0,
constant, x 0., y 0., z -5.605e-4,
x 0., y 0., z 0., x 0., y 0., z 1., -2., -1., 1., 2.
```

```
$ block 3 (annular region)
```

```
initial b field, block 3, axial current, r1 0.002, b1 0.1,
x 0., y 0., z 0., x 0., y 0., z 1., -2., -1., 1., 2.
```

or in 2D cylindrical by:

```
$ Btheta (not Atheta) is the fundamental variable
$ blocks 1 and 2 (inner and outer conductors) default to zero
$ block 3 (annular region)
```

```
initial b field, block 3, axial current, b 0.1, r 0.002,
r 0., z 0., -2., -1., 1., 2.
```

5.6.4 Mean Initial Field

INITIAL B FIELD, MEAN, vector

This keyword is intended to be used for vector potential solutions on periodic meshes. One cannot represent a constant magnetic field with a periodic vector potential. In 2D, this means that the magnetic field must be in the plane of the mesh, orthogonal components are not allowed. The vector is a magnetic field vector that is constant in both space and time. There is no block-id subkeyword with this command. To be constant in space, this command must apply to all blocks. This keyword is typically used in conjunction with other initial fields and/or boundary conditions to represent the total magnetic field.

In 3D, the vector is specified as:

```
X real, Y real, Z real (Cartesian geometry)
```

In 2D, the vector is specified as either:

X real, Y real	(Cartesian geometry)
R real, Z real	(cylindrical geometry)

Orthogonal components to the mesh are not allowed. Only a non-zero Z component makes physical sense in cylindrical geometry.

Example:

```

initial b field, block 1, uniform, x 0.0 y 0.001120998243 $ left
initial b field, block 2, uniform, x 0.0 y -0.001120998243 $ right

initial b field, mean, x 0.0008407486825 y 0.0

uniform h bc, sideset 21, 0.001120998243, scale 7.957747e5,
                        x 0.0 y 1.0                        $ left
uniform h bc, sideset 22, -0.001120998243, scale 7.957747e5,
                        x 0.0 y 1.0                        $ right

```

5.6.5 Diffuse Initial Field

DIFFUSE INITIAL FIELD, [real]

This options invokes a transient magnetics solve before startup whereby the relevant magnetic field distribution may be computed for a given span of time. This option is particularly useful when using initial conditions from another simulation requiring a self-consistent initialization of the magnetic field. The real number represents the time interval for the magnetic field diffusion. The size of the time interval relative to the magnetic diffusion time, $\tau_d = l^2/4D$, where $D = 1/\sigma\mu_0$, determines the amount of diffusion that takes place.

5.7 1D Test Options

The following three options are designed specifically for one dimensional vector potential advection tests on a periodic mesh.

5.7.1 1D Square Vector Potential

```
INITIAL B FIELD, SQUARE A,  
    vector (y-component is magnitude)  
    central-position  
    half-width
```

The keyword initializes the z-component of the vector potential.

Example:

```
initial b field, square a,  
    x 0. y 0.5e-3,  
    0.5  
    0.25
```

5.7.2 1D Triangle Vector Potential

```
INITIAL B FIELD, TRIANGLE A,  
    vector (y-component is magnitude)  
    central-position  
    half-width
```

This option initializes the z-component of the vector potential.

Example:

```
initial b field, triangle a,  
    x 0. y 0.5e-3,  
    0.5  
    0.25
```

5.7.3 1D Gaussian Vector Potential

```
INITIAL B FIELD, GAUSSIAN A,  
    vector (y-component is magnitude)
```

```
central-position  
half-width
```

This keyword initializes the z-component of the vector potential.

Example:

```
initial b field, gaussian a,  
  x 0. y 0.5e-3,  
  0.5  
  0.25
```

5.8 2D/3D Test Options

5.8.1 2D Gaussian Vector Potential

```
INITIAL B FIELD, GAUSS2D A,  
  vector (y-component is magnitude)  
  x-central-position  
  y-central-position  
  half-width-at-half-max
```

This keyword initializes the z-component of the vector potential.

Example:

```
initial b field, gauss2d a,  
  x 0. y 0.5e-3,  
  0.0  
  0.0  
  0.25
```

5.8.2 Random Field

```
INITIAL B FIELD, RANDOM, vector
```

Gives a random field with magnitudes scaled by components of vector. Useful for testing solvers.

Example:

```
initial b field, random, x 0. y 0.5e-3,
```

5.8.3 Sinusoid Vector Potential

```
INITIAL B FIELD, GAUSS2D A,  
    vector (y-component is magnitude)  
    x-central-position  
    y-central-position  
    half-width-at-half-max
```

This keyword initializes the z-component of the vector potential.

Example:

```
initial b field, gauss2d a,  
    x 0. y 0.5e-3,  
    0.0  
    0.0  
    0.25
```

5.8.4 Tearing Option

```
INITIAL B FIELD, TEARING,  
    vector (y-component is magnitude)  
    central-position
```

This keyword initializes the z-component of the vector potential.

Example:

```
initial b field, tearing a,  
    x 0. y 0.5e-3,  
    0.25
```

5.8.5 Vortex Option

INITIAL B FIELD, VORTEX, vector, length-scale (Cartesian only)

This keyword initializes the vector potential according to Reference [24]. In 3D, often only one component of the vector is non-zero. This non-zero component becomes the amplitude of the magnetic field that lies in the plane orthogonal to the vector. The length-scale is the full spatial wavelength. The vector potential is:

$$\begin{aligned} A_x &= \frac{LV_x}{2\pi} \sin\left(\frac{2\pi y}{L}\right) \sin\left(\frac{2\pi z}{L}\right) \\ A_y &= \frac{LV_y}{2\pi} \sin\left(\frac{2\pi x}{L}\right) \sin\left(\frac{2\pi z}{L}\right) \\ A_z &= \frac{LV_z}{2\pi} \sin\left(\frac{2\pi x}{L}\right) \sin\left(\frac{2\pi y}{L}\right) \end{aligned} \quad (19)$$

3D example:

```
initial b field, vortex,
  x 1. y 1. z 1.,
  1.0
```

In 2D, the x-component of the vector is becomes the amplitude of the magnetic field. The length-scale is one-half the spatial wavelength. The vector potential and magnetic field are:

$$\begin{aligned} A_z &= -\frac{LV_x}{\pi} \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{\pi y}{L}\right) \\ B_x &= -V_x \sin\left(\frac{\pi x}{L}\right) \cos\left(\frac{\pi y}{L}\right) \\ B_y &= V_x \cos\left(\frac{\pi x}{L}\right) \sin\left(\frac{\pi y}{L}\right) \end{aligned} \quad (20)$$

2D example shown in Figure 8:

```
initial b field, vortex,
  x 0.5e-3 y 0.,
  0.5
```

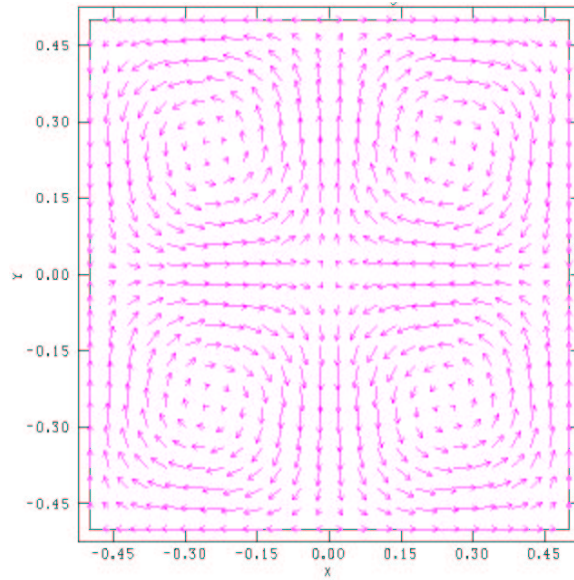


Figure 8. 2D Initial Vortex Magnetic Field.

5.9 Other Initial Fields

Other initial fields may be easily implemented as required by applications.

5.10 Coupled Circuit Equations

Coupled circuit equations allow a set of differential-algebraic equations to be coupled to the transient magnetic or MHD simulations. These equations are solved using DASPK. [16, 6, 19] This is useful in situations where the simulation is driven by a known voltage source (most magnetic boundary conditions require knowledge of the current) or where the dynamics of the system being modeled feeds back into the electrical response of the external circuit. The circuit solver may be used in both 2D and 3D, and in either SI or CGS (Practical CGS) units.

Coupled circuit equations are fairly simple to set up and the method is outlined using the following steps.

1. Sketch a diagram of the equivalent circuit (see Figure 9).

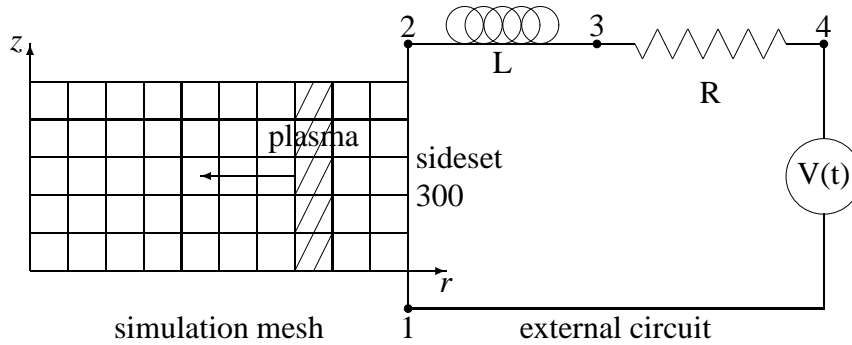


Figure 9. Simple circuit model for the Z accelerator.

2. Label the junctions between the circuit components with numbers. Each junction becomes a `CIRCUIT NODE` in the input deck. The numerical labels become the node numbers in the input deck. Circuit nodes can connect more than two circuit elements, that is, parallel circuits are allowed.
3. Each circuit component becomes a `CIRCUIT ELEMENT` in the input deck. Most circuit element connect two nodes and these are designated as the input and output nodes. A few circuit elements connect three nodes. Positive currents flow from the input node to the output node. If the order of the nodes happen to be mislabeled, no matter, ALEGRA will report a negative current flowing in the element.
4. ALEGRA will automatically construct a set of equations consistent with Kirchhoff's laws for the equivalent circuit, namely that the sum of the voltages around a loop is zero, $\sum V = 0$, and that the sum of the currents into a node is zero, $\sum I = 0$.

For example, the Z accelerator in the Pulsed Power Center at Sandia National Laboratories can be modeled using an equivalent circuit. The simplest such model has only a time-dependent voltage source, an external resistance and an external inductance. The Z pinch plasma (load) collapses and stagnates onto its axis, the inductance of the load rises dramatically causing a current drop in the external circuit. Voltage monitors along the accelerator reliably measure the voltage at a significant distance from the load. The actual current through the load is not known to the same accuracy. Both of these aspects can be modeled using a coupled circuit equation.

Example:

\$ external circuit loop

```

circuit solver, relerr 1.e-4, abserr 1.e-4

circuit node, 1, fixedv 0. $ ground
circuit node, 2
circuit node, 3
circuit node, 4, function 1 $ source voltage

$ circuit element, 1 4 $ represented by source voltage
circuit element, 4 3, resistor 0.120 $ ohms
circuit element, 3 2, inductor 12.05e-9 $ henrys
circuit element, 2 1, mesh

rz cyl radial slot bc, sideset 300, circuit,
  r 0. z 0., -10., -1., 1., 10.

```

5.10.1 Circuit Solver

```
CIRCUIT SOLVER, [RELERR real (0.01)] [ABSERR real (0.01)]
```

Circuit solver error criteria passed to DASPK. The error values typically used range from 1.E-4 to 1.E-6. The DASPK solution procedure is somewhat sensitive and it is recommended that the user adjust these error parameters to gain a feel for solution response and carefully monitor the actual solutions obtained.

5.10.2 Circuit Node

```

CIRCUIT NODE node_#
  [sideset]
  [ STARTV real |
    FIXEDV real |
    function-set |
    DAMPED SINUSOID amplitude damping_rate frequency phase |
    DOUBLE EXPONENTIAL A_amplitude a_exponent B_amplitude b_exponent]

```

This input defines a circuit node and associated voltage. A node may be attached to one or more CIRCUIT ELEMENTS. According to Kirchhoff's law the sum of the currents flowing

from each circuit element into the node must sum to zero. If a node connects to only one circuit element then that node must have its voltage specified.

The sideset, if specified, is constant potential surface in the ALEGRA mesh. The voltage at this surface is defined by one of the following voltage options. The potential is linked to the ALEGRA simulation through an E TANGENT BC boundary condition.

The remaining set of optional keywords allow a choice of the voltage behavior of the node. Note that the user is not required to specify a voltage option. In that case, the voltage is allow to vary and the values are computed by the circuit model.

STARTV sets the initial voltage of the node. Subsequent voltage values are computed by the circuit model. This option is useful for specifying an initial voltage across a capacitor element.

FIXEDV fixes the voltage of the node at a constant value. At least one node must have a constant zero voltage. This node provides the ground for the circuit model.

function-set or FUNCTIONV specifies a tabular voltage input for the node. The table_# refers to a standard ALEGRA FUNCTION and the optional SCALE parameter is a voltage multiplier.

DAMPED SINUSOID requires four real values and specifies a time dependent voltage of the form

$$V(t) = A \cdot e^{-a \cdot t} \cdot \sin(\omega \cdot t + \theta) \quad , \quad (21)$$

where A is the voltage amplitude, a is the damping_rate, ω is the frequency (radians/second) and θ is the phase (radians).

DOUBLE EXPONENTIAL requires four real values and specifies a time dependent voltage of the form

$$V(t) = A \cdot e^{-a \cdot t} - B \cdot e^{-b \cdot t} \quad . \quad (22)$$

5.10.3 Circuit Element

```
CIRCUIT ELEMENT input_node output_node
{ MESH |
```

```

CAPACITOR real_capacitance |
INDUCTOR  real_inductance  |
RESISTOR  real_resistance  |
SOURCE,   function-set     |
SWITCH,   function-set     |
VARISTOR  real_vref real_iref real_alpha |
ZFLOW,    {function-set} real_gmin real_gmax }

```

This line defines each circuit element and its characteristics. Many circuit element input values are order dependent and have no keywords.

The `input_node` and the `output_node` are integer numbers correspond to nodes defined by the `CIRCUIT NODE` keyword. A positive current flows through the circuit element from the `input_node` to the `output_node`.

One of the remaining keywords is required to specify the type of circuit element. Valid options are specified in the following list.

`MESH` specifies that this circuit element represents the mesh. This circuit element couples to a `TRANSIENT MAGNETICS` boundary condition that specifies the `CIRCUIT` keyword such as the `CYLINDRICAL RADIAL SLOT BC`.

`CAPACITOR` specifies a standard electrical capacitor with a capacitance value of `real_capacitance`.

`INDUCTOR` specifies a standard electrical inductor with a inductance value of `real_inductance`.

`RESISTOR` specifies a standard electrical resistor with a resistance value of `real_resistance`.

`SOURCE` specifies a prescribed current source defined by the `function-set`.

`SWITCH` specifies a resistor with a time dependent resistance value given by a `function-set`.

`ZFLOW` specifies a Zflow resistor with a Zflow value given by the `function-set`. Minimum and maximum conductance values are also required. The first node in the element node list specifies the Zflow loss node. The model requires that the Zflow loss node have a circuit element connectivity of 3. The conductance for the Zflow element is given by

$$\frac{I_{upstream} - I_{downstream}}{Z_{flow} \sqrt{I_{upstream}^2 - I_{downstream}^2}} \quad (23)$$

Example:

```

circuit solver, relerr=1.e-4, abserr 1.e-4

$ mesh loop
$ capacitor-mesh $ mesh has inductance and resistance

circuit node 1 fixedv 0.
circuit node 2 startv 1.  $ initial capacitor voltage

circuit element, 1 2, capacitor 5.e-6    $ Farads
circuit element, 2 1, mesh

xy cyl radial slot bc, sideset 300, circuit,
  r 0. z 0.

$ test loop - independent of mesh
$ capacitor-inductor-resistor

circuit node 3 fixedv 0.
circuit node 4 startv 1.  $ initial capacitor voltage
circuit node 5

circuit element, 3 4, capacitor 5.e-6    $ Farads
circuit element, 4 5, inductor 18.64e-9  $ Henrys
circuit element, 5 3, resistor 5.09e-2   $ Ohms

```

This example is from a problem that computes the behavior of a section of coaxial cable (the mesh) driven by the voltage stored in a capacitor. This is represented by nodes 1 and 2 and the associated circuit elements. For comparison a simple test RLC circuit is also modeled by node 3, 4, and 5, and the associated elements. Note that this test circuit is completely independent of the mesh demonstrating the flexibility of the circuit model.

6 Thermal Conduction Input

```
THERMAL CONDUCTION
...
... [thermal conduction keywords] ...
...
END
```

The THERMAL CONDUCTION keyword group specifies controls for the implicit thermal solver routines.

$$\rho C_v \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) \quad (24)$$

where T is the temperature, ρ is the density, C_v is the specific heat, and k is the thermal conductivity.

6.1 Time Step Control

The thermal conductivity time step is given by

$$\Delta t_{con} = f \min(\Delta t_k, \Delta t_c) \quad (25)$$

where

$$\Delta t_k = \frac{\rho C_v h^2}{k} \quad (26)$$

where h is a characteristic cell size and

$$\Delta t_c = \Delta t (.05) |T + T_{min}| / |T - T_{old}| \quad (27)$$

6.1.1 Time Step Scale, f

```
TIME STEP SCALE real (default 10.)
```

The keyword TIME STEP SCALE can be set to control the scale, f , applied to the time step. The time step is calculated using an explicit criteria, but can be increased by any

desired factor f since the actual calculation is implicit, by use of the TIME STEP SCALE keyword. The default value is 10.

The thermal conduction time step is reported in the DT_CON global variable. Note that this time step is reported in the output file without the TIME STEP SCALE factor.

6.1.2 Minimum Temperature, T_{min}

MINIMUM TEMPERATURE real (default 1000 K) T_{min} is the cutoff temperature for temperature change control.

6.1.3 Minimum Density, ρ_{min}

MINIMUM DENSITY real (default 0.) ρ_{min} is the cutoff thermal conductivity density. This keyword is needed when the thermal solves are taking too many iterations due to a stiffness rather than mass dominated matrix corresponding to extremely high thermal diffusion speeds. This can happen for very small densities occurring in the problem. No multigrid is available for the face centered discretization employed so to make progress this keyword can be employed to essentially turn off diffusion in very low density regimes. This is internally in the code by setting the thermal conductivity k to very small values.

6.2 Solution Control

6.2.1 Aztec Set

AZTEC SET int

This keyword sets the identification number of the Aztec parameter set which the implicit thermal solver will use. The actual parameters used are specified by the AZTEC keyword group. The default value is 0.

6.2.2 Conserve Memory

CONSERVE MEMORY

Requests that all solver memory for conduction be returned to the system and reallocated the next cycle. By default the memory is retained across cycles. **WARNING:** It is possible that excessive allocations and deallocations can have a detrimental effect on code performance.

6.3 Boundary Conditions

6.3.1 No Heat Flux

NO HEAT FLUX, sideset

This keyword allows the user to specify zero heat flux through a surface defined by the sideset argument.

6.3.2 Prescribed Heat Flux

PRESCRIBED HEAT FLUX, sideset, function-set

This keyword allows the user to prescribe the heat flux on a surface defined by the sideset keyword as a function of time.

6.3.3 Temperature BC

TEMPERATURE BC, sideset, function-set

This keyword allows the user to specify the temperature on a surface defined by the sideset keyword as a function of time.

7 Emission Input

```

EMISSION
  {BLACKBODY | PLANCK | BREMSSTRAHLUNG}
  GROUP BOUNDS
    ...
  END
  [EMISSION ENERGY FLOOR, 0.0]
  [MAXIMUM EMISSION DENSITY, 0.0]
  [MINIMUM TEMPERATURE, 0.0]
  [NEWTON | BISECT]
  [MAXIMUM NEWTON ITERATIONS, 1]
  [TOLERANCE, 1.0e-6]
END

```

The emission model is a way to keep material heating under control by radiating photon energy using an approximate radiation emission model. The net radiation emission is typically a balance between energy emitted and energy absorbed,

$$\frac{de_m}{dt} = - \sum_g [R(T_m, g) - A(g)] \cdot f_\rho \cdot f_T \quad (28)$$

for each group g and each material m . Here $\frac{de_m}{dt}$ is the time rate of change of the material specific energy, T_m is the material temperature, g is the group number, $R(T_m, g)$ is a radiation emission rate function, and $A(g)$ is a radiation absorption rate function. f_ρ and f_T are density and temperature dependent multipliers described below. Simple one-dimensional considerations allow us to approximate the probability of escape after a distance x as $e^{-\tau_{ag}d}$ where $\tau_{ag}d$ is known as the optical depth, τ_{ag} is the absorption opacity, and the distance d is the mean distance to void. We approximate the absorption rate as the emission rate times the probability of reabsorption (i.e., not escaping).

$$A(g) = \left(1 - e^{-\tau_{ag}d}\right) R(T_m, g) \quad (29)$$

Thus, the net emission rate becomes the total emission rate reduced by the probability of escape.

$$\frac{de_m}{dt} = - \sum_g e^{-\tau_{ag}d} R(T_m, g) \cdot f_\rho \cdot f_T \quad (30)$$

Because ALEGRA is an energy-based code, the actual discrete algorithm approximates the material temperature variation in terms of the specific energy.

$$T_m^{n+1} = T_m^n + \frac{(e_m^{n+1} - e_m^n)}{C_v^n} \quad (31)$$

where C_v is the material heat capacity. The first Newton iterate is used to calculate the change in e_m . The derivative of $R(T_m, g)$ with respect to temperature is then required. The Newton correction is intended to provide a mechanism for avoiding excessive cooling.

7.1 Emission Model Options

There are currently two emission options within ALEGRA:

- BLACKBODY or PLANCK - Blackbody emission model using the Planck function
- BREMSSTRAHLUNG - thermal Bremsstrahlung emission model

One or the other emission model must be specified.

7.1.1 Planck Emission

{BLACKBODY | PLANCK}

These two keywords both refer to the same emission model. The BLACKBODY or PLANCK emission model defines the radiation emission rate function in units of *energy/mass/time* as

$$R(T_m, g) = \sigma_{ag} B(T_m, g) = \frac{\tau_{ag}}{\rho} B(T_m, g) \quad (32)$$

where σ_{ag} is the group absorption cross section in units of *area/mass*, $\tau_{ag} = \rho\sigma_{ag}$ is the group absorption opacity in units of *1/length* (τ_{ag} is the variable that ALEGRA stores), ρ is

the mass density, and $B(T_m, g)$ is the Planck function integral in units of *energy/area/time* given by

$$B(T_m, g) = 4\pi \int_{\epsilon_g}^{\epsilon_{g+1}} B(\epsilon, T_m) d\epsilon = 4\pi \int_{\epsilon_g}^{\epsilon_{g+1}} \frac{2}{h^3 c^2} \frac{\epsilon^3}{\exp\left(\frac{\epsilon}{kT_m}\right) - 1} d\epsilon \quad (33)$$

This emission model requires that all MATERIALs have an opacity model specified. Scattering opacity values are ignored. See "Opacity Models" in Section 8.6.

7.1.2 Bremsstrahlung Emission

BREMSSTRAHLUNG

The Bremsstrahlung emission model is pertinent to astrophysical X-ray cluster cooling flows and is defined by the White and Sarazin prescription for a half-solar abundance cooling function [10]. The radiation emission rate function is given by

$$R(T_m, g) = \frac{10^{-35} \rho}{(\mu m_p)^2} \begin{cases} 2.35 \cdot e^{-\left(\frac{T_m}{3.5 \cdot 10^5}\right)^{4.5}} + \frac{5 \cdot e^{-\left(\frac{T_m}{2.8 \cdot 10^6}\right)^{4.4}}}{T_m^{0.17}} \\ \quad + \frac{0.05 \cdot e^{-\left(\frac{T_m}{1.55 \cdot 10^7}\right)^4}}{T_m^{0.08}} + 2.4 \cdot 10^{-5} \sqrt{T_m} & , \quad T_m > 10^5 \\ 3.18 \left(\frac{T_m}{10^5}\right)^{1.6} - \frac{150}{T_m}, & \text{otherwise} \end{cases} \quad (34)$$

It is recommended that the BISECT option be enabled for this emission model since the cooling function is not monotonic with temperature.

BREMSSTRAHLUNG does not require any opacity models and should only be called with a single energy group. The limits of this group are irrelevant. Use of the probability of escape does require an opacity model however, unless the OPTICAL MULTIPLIER is set to zero.

7.2 Group Boundaries

GROUP BOUNDS

```
LOG real TO real BY int, [SCALE real (1.0)]  
LINEAR real TO real BY int, [SCALE real (1.0)]  
...
```

END

This required keyword defines the photon energy group bounds in keV. The photon energy spectrum is divided into regions. The package further subdivides regions into the actual photon groups using either LINEAR or logarithmic (LOG) intervals within the region. The optional SCALE keyword is used as an opacity multiplier. Its default value is 1.0

For example, a specification of

```
group bounds  
  log 1. to 32. by 5  
end
```

will cause the spectral region from 1.0 to 32.0 keV to be divided into five photon groups whose bounds are 1.0 to 2.0, 2.0 to 4.0, 4.0 to 8.0, 8.0 to 16.0, and 16.0 to 32.0 keV.

The GROUP BOUNDS input is required for both models.

7.3 Algorithm Control

7.3.1 Emission Multiplier

EMISSION MULTIPLIER real (1.0)

If this optional keyword is present then the net emission rate is scaled by this factor. The main purpose of this factor is to allow the user to perform sensitivity studies relative to the natural emission rate.

7.3.2 Optical Multiplier

OPTICAL MULTIPLIER real (1.0)

If this optional keyword is present then the optical depth τ_{ag-x} in the probability of escape is scaled by this factor. This factor may be used for sensitivity studies or to adjust the estimate of the mean-distance-to-void x should there be a systematic error.

7.3.3 Mean Distance to Void

MDTV, {RMS (default) | MIN MAX}

This optional keyword selects the method used to estimate of the mean-distance-to-void d . The default method is RMS.

The RMS method computes the root-mean-square size of the material and the mesh about the mean material and mesh locations for each orthogonal coordinate, respectively. The RMS mesh sizes are used as weights for the RMS material sizes in the standard distance formula to account for one-dimensional simulations.

$$\begin{aligned}
 d &= 2\sqrt{w_x^2 x_{rms}^2 + w_y^2 y_{rms}^2 + w_z^2 z_{rms}^2} \\
 w_x &= X_{rms} / \sqrt{X_{rms}^2 + Y_{rms}^2 + Z_{rms}^2} \\
 w_y &= Y_{rms} / \sqrt{X_{rms}^2 + Y_{rms}^2 + Z_{rms}^2} \\
 w_z &= Z_{rms} / \sqrt{X_{rms}^2 + Y_{rms}^2 + Z_{rms}^2}
 \end{aligned} \tag{35}$$

where x_{rms} , y_{rms} , and z_{rms} are the root-mean-square size of the material, and X_{rms} , Y_{rms} , and Z_{rms} are the root-mean-square size of the mesh.

The MIN MAX method uses the difference between the maximum and minimum material coordinates and the difference between the maximum and minimum mesh coordinates as the size of the material and mesh respectively. The min-max mesh sizes are used as weights for the min-max material sizes in the standard distance formula to account for one-dimensional simulations.

$$\begin{aligned}
d &= \sqrt{w_x^2(x_{max} - x_{min})^2 + w_y^2(y_{max} - y_{min})^2 + w_z^2(z_{max} - z_{min})^2} \\
w_x &= (X_{max} - X_{min}) / \sqrt{(X_{max} - X_{min})^2 + (Y_{max} - Y_{min})^2 + (Z_{max} - Z_{min})^2} \\
w_y &= (Y_{max} - Y_{min}) / \sqrt{(X_{max} - X_{min})^2 + (Y_{max} - Y_{min})^2 + (Z_{max} - Z_{min})^2} \\
w_z &= (Z_{max} - Z_{min}) / \sqrt{(X_{max} - X_{min})^2 + (Y_{max} - Y_{min})^2 + (Z_{max} - Z_{min})^2}
\end{aligned} \tag{36}$$

where x_{min} , y_{min} , z_{min} , x_{max} , y_{max} , and z_{max} are the minimum and maximum values where material is present, and X_{min} , Y_{min} , Z_{min} , X_{max} , Y_{max} , and Z_{max} are the minimum and maximum values of the mesh.

For uniform meshes the RMS method yields a smaller mean-distance-to-void than the MIN MAX method. The MIN MAX method is better for highly non-uniform meshes.

7.3.4 Emission Energy Floor

EMISSION ENERGY FLOOR real (0.0)

If this optional keyword is present then the available energy in an element will not drop below the percentage given by the EMISSION ENERGY FLOOR. This floor may help to avoid the problem of an element obtaining a negative temperature by emitting more energy than is available. The available energy is defined by a linear extrapolation to the material specific internal energy down to zero temperature.

$$e_{avail} = e_m(T_m) - e_m(0) = C_v(T_m - 0) = C_v T_m \tag{37}$$

For example, to keep the energy available in an element from dropping below 1% of its starting value, one would use the EMISSION ENERGY FLOOR as follows:

```

emission
...
  emission energy floor 0.01
end

```

Emission down to this energy floor is allowed.

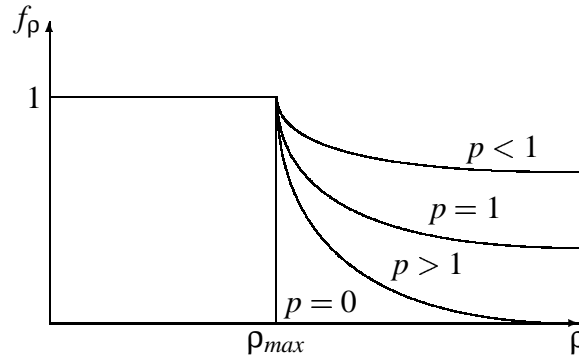


Figure 10. Maximum Emission Density Multiplier.

7.3.5 Maximum Emission Density

MAXIMUM EMISSION DENSITY real (0.0) [POWER real (0.0)]

If this optional keyword is present and the density value is non-zero, then only material densities less than the input value will emit at the prescribed rate. A zero value implies emission at all densities. The assumption is that above this density the material is optically thick and some portion of the emitted energy is immediately reabsorbed. The multiplier of the net emission rate when the density is greater than the specified limit is given by the following expression where p is the specified POWER.

$$f_{\rho} = \begin{cases} 1, & \rho \leq \rho_{max} \\ 0, & \rho > \rho_{max}, p = 0 \\ \left(\frac{\rho_{max}}{\rho}\right)^p, & \rho > \rho_{max}, p > 0 \end{cases} \quad (38)$$

Graphically the multiplier can be displayed as in Figure 10. This option should only be used when the probability of escape factor is insufficient to limit the net emission rate at high densities.

Example:

```
emission
...
  max emission density 0.1
end
```

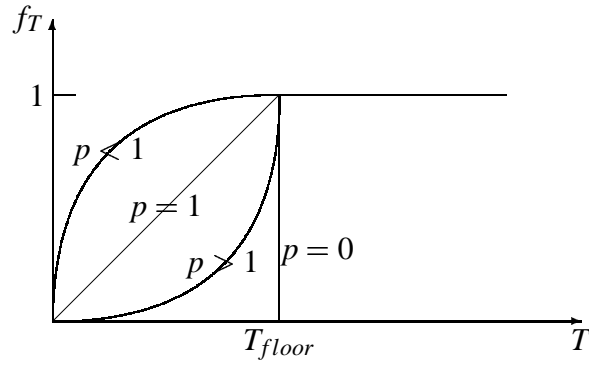


Figure 11. Minimum Emission Temperature Multiplier.

7.3.6 Minimum Emission Temperature

MINIMUM TEMPERATURE real (0.0) [POWER real (0.0)]

The optional MINIMUM TEMPERATURE specification is such that if emission model would cool an element below this temperature, the emission model turns itself off. Emission down to this minimum temperature is allowed. If the temperature value is non-zero, then only material temperatures greater than the input value will emit at the prescribed rate. A zero value implies emission at all temperatures. The assumption is that the material is too cold to emit. The multiplier of the net emission rate when the temperature is less than the specified limit is given by the following expression where p is the specified POWER.

$$f_T = \begin{cases} 1, & T \geq T_{floor} \\ 0, & T < T_{floor}, p = 0 \\ \left(\frac{T}{T_{floor}}\right)^p, & T < T_{floor}, p > 0 \end{cases} \quad (39)$$

Graphically the multiplier can be displayed as in Figure 11. This option should only be used when the probability of escape factor is insufficient to limit the net emission rate at low temperatures.

Example:

```
emission
...
```

```
min temperature 933. $ Kelvin
end
```

7.3.7 Solution Method

```
{NEWTON (default) | BISECT}
```

If the `NEWTON` keyword is present, it explicitly forces use of the default Newton iteration method.

If the `BISECT` keyword is present then the Newton algorithm will incorporate a bisection step into it. Use this for the `BREMSSTRAHLUNG` emission option as the cooling function is non-monotonic. This option does not need to be specified for the `BLACKBODY` or `PLANCK` option.

7.3.8 Maximum Newton Iterations

```
MAXIMUM NEWTON ITERATIONS int (1)
```

Optionally specifies the maximum number of Newton iterations. A warning will occur if the maximum number of Newton iterations is exceeded and the solution tolerance remains less than the tolerance specified by the `TOLERANCE` keyword. Quite often it is sufficient to give this parameter a value of just 2.

7.3.9 Newton Iteration Tolerance

```
TOLERANCE real (1.0e-6)
```

Optional accuracy level setting for Newton iteration solution of emission energy equation. The default value is 1.0e-6.

8 Material Models Input

8.1 Materials

The MATERIAL keyword is explained fully the basic ALEGRA manual [3]. In this version of ALEGRA, some of the material models get some of their information from the MATERIAL keyword block, namely the atomic composition as defined by the NUMBER OF ELEMENTS keyword. This allows each material to be treated consistently and with a minimum of input required from the user. Currently, QEOS requires the material composition to be entered here. The XSN material composition may be entered here or under the XSN model. The material input format is:

```
MATERIAL int [string]
  MODEL int
  [MODEL int]
  variable_name real
  [variable_name real]
  [NUMBER OF ELEMENTS int
    ELEMENT int, MASS real, FRACTION real
    ...
  END]
END
```

Example of material input:

```
block 1
  material 201 $ see BLOCK input for this item
end

material 201 "Air"
  model 11      $ QEOS
  model 12      $ XSN
  number of elements 3
    element 7, mass 14.007, fraction 0.7809
    element 8, mass 16.000, fraction 0.2095
    element 18, mass 39.948, fraction 0.0096
  end
end
```

8.2 Material Models

```
MODEL int model_name
    parameter [int|real]
    parameter = [int|real]
    ...
END
```

The following sections describe the various material models that support MHD applications. In each of the material model descriptions that follow, two tables are presented for each MODEL. The first table lists and defines the user specifiable input parameters. These parameters are to be listed withing the MODEL ... END keyword block in the input deck. The second table lists the registered code variables input to and output from the various models. These variables are available for plotting and are to be listed within the PLOT VARIABLES ... END keyword block in the input deck.

A list of the currently available models is provided in Table 8. The models are categorized into general model types.

Table 8. Material Model Types and Model Names.

General Material Model Type	Model Name
Combined Electrical/Thermal Conductivity	LMD SPITZER
Electrical Conductivity	EC ANOMALOUS EC KNOEPFEL
Thermal Conductivity	CONSTANT THERMAL CONDUCTIVITY PLASMA POLYNOMIAL
Opacity	BIGGS LIGHTHILL KRAMERS FITTED XSN
Ionization State	SAHA IONIZATION

The material models listed in Table 9 are considered to be obsolete and may be deleted from ALEGRA in the near future.

Table 9. Obsolete Material Model Types and Model Names.

General Material Model Type	Model Name
Electrical Conductivity	KEC SESAME
Thermal Conductivity	KTC SESAME
Ionization State	KZB SESAME

8.3 Combined Electrical and Thermal Conductivity Models

Electrical conductivity models are used by TRANSIENT MAGNETICS to close the coupled set of hydrodynamics and Maxwell's equations by using Ohm's law which relates the current density \vec{J} to the electric field \vec{E} and the cross product of the velocity \vec{V} and magnetic field \vec{B} ,

$$\vec{J} = \sigma \left(\vec{E} + \vec{V} \times \vec{B} \right). \quad (40)$$

where σ is the electrical conductivity. This is the simplest form of Ohm's law.

THERMAL CONDUCTION physics solves the thermal heat conduction equation. The heat flux \vec{q} is related to the temperature gradient by

$$\vec{q} = -k \nabla T, \quad (41)$$

where the constant of proportionality k is the thermal conductivity. The heat flux \vec{q} has dimensions of energy/area/time, the temperature has dimensions of Kelvin (K), so the thermal conductivity k has dimensions energy/length/time/K.

Some models provide both electrical and thermal conductivities. Others provide only one or the other. The user must provide a set of models which will uniquely provide the required parameters for the physics which is requested. NOTE: If overlapping models are requested in the sense that two models provide the same output, then the code will use the last model listed to provide that given output.

8.3.1 LMD Conductivities

```
MODEL model_id_number LMD
    [parameter = value]
    ...
END
```

The Lee-More-Desjarlais (LMD) model [4, 5] is an extension of the Lee-More model [14] that provides much better agreement with measured electrical conductivities in the vicinity of the metal-insulator transition and yet smoothly blends with the Lee-More model away from this regime. The conductivities generated by the two models can differ by several

orders of magnitude with the largest differences occurring for densities one to two orders of magnitude below solid density and temperatures below 2 eV. The model also outputs the thermal conductivities, as well as the ionization state, so that no separate thermal conductivity need be computed. This conductivity model also includes the effect of magnetic fields on the conductivity. The conductivities returned are those parallel and perpendicular to the magnetic field. The proper coordinate transformation between this magnetically oriented system and the computational coordinates needs to be ensured. The most significant changes in this model, relative to the Lee-More model, are an improved ionization model and a new expression for the minimum allowed collision time. The new ionization model blends the Thomas-Fermi ionization with a first-ionization Saha model. The Saha contribution is non-ideal in that a pressure ionization term is used to reduce the ionization energy near solid densities. The ionization state calculated with this model is a significant improvement over the Thomas-Fermi ionization in the vicinity of the metal-insulator transition, particularly for temperatures below 3 eV or so. The new expression for the minimum allowed collision time introduces a power law dependence on density through the P_2 parameter. This dependence is in agreement with the measured conductivities at low temperatures and densities below solid and effectively bridges the metal, liquid, and plasma conductivity regimes. It is anticipated that for most applications the user will make use of predefined parameter sets for each material of interest, linked to the Z for the material. These parameters may be overridden if the user wishes to experiment with modeling unsupported materials. The model is sufficiently robust that if the user supplies Z , A , RHO , $SOLID$, $TMELT$, and $XIEV$, and accepts the defaults for the other parameters, reasonably good metallic conductivities will be generated.

In place of the P_2 , P_3 , and P_4 parameters of the generic Lee-More model, we now have

$$p_2 = \min \left[p_{2a} + \frac{p_{2b}}{p_T}, \frac{\bar{V}_e}{\sqrt{2E_F/m_e}} \left(\frac{n_a}{2 \cdot 10^{22}} \right)^{2/p_T} \right], \quad (42)$$

$$p_3 = \frac{p_{3a}}{2} \left(1 + \left(\frac{T_m}{T} \right)^{p_{3b} \cdot r_{fact}} \right), \text{ and} \quad (43)$$

$$p_4 = \frac{p_{4a}}{2} \left(1 + \left(\frac{T_m}{T} \right)^{p_{4b} \cdot r_{fact}} \right) \quad (44)$$

where

$$p_T = 1 + \exp \left(\frac{T - 25000}{10000} \right), \text{ and} \quad (45)$$

$$r_{fact} = \sqrt{2 / \left(\left(\frac{\rho}{\rho_s} \right)^2 + \left(\frac{\rho_s}{\rho} \right)^2 \right)}. \quad (46)$$

T_m is the melt temperature and ρ_s is the material solid density. These constructions for P3 and P4 are used primarily for fine tuning the solid density conductivity as a function of temperature, including the drop in conductivity at melt which is determined by the relation:

$$\tau_{liq} = \frac{\tau_{BG}}{p_4} \frac{T}{T + p_5} \quad (47)$$

for $T \geq T_m$. The net effect of these changes to P3 and P4 are relatively minor. Note the new parameter P5 which is useful for matching the conductivity above melt for some materials, notably aluminum.

The correct parameters for some materials have been incorporated into the model. For these materials, one needs only to specify the atomic number, Z, or in the case of deuterium, also specify the atomic mass, A as 2. The code will set the remaining parameters correctly. Currently featured materials include those found in Table 10.

Table 10. Predefined Materials for LMD.

Z	A	Symbol	Material
1	2.	D	Deuterium
13	-	Al	Aluminum
22	-	Ti	Titanium
29	-	Cu	Copper
47	-	Ag	Silver
74	-	W	Tungsten

Example:

```
model 1 lmd
  Z = 13.
end
```

Note: there is no option for reverting to the original Lee More model for comparison purposes.

- Modules: material_libs/ec
 - ec_lmd.h
 - ec_lmd.C
 - lmd_setup.h
 - lmd.F
 - coulomb_logarithm.C
- Physics:
 - transient magnetics
 - all magnetohydrodynamics physics options

Table 11: Input Parameters for LMD.

Parameter Name	Type	Description
Z	real	Atomic number (this is the only required parameter)
A	real	Atomic mass
RHO SOLID	real	Material solid density
TMELT	real	Specifies the solid density melt temperature. This scales the usual Cowan melt temperature calculation so that the melt temperature will be correct at solid density, but is still a function of density. Calculated if TMELT .le. 0.
XIEV	real	The energy of the first ionization in eV
LOG LAMBDA MIN	real	The minimum allowed value of the Coulomb logarithm
G0, G1	real	The spin level degeneracy factors $(2J + 1)$ for the ground state and first ionization, respectively
P1	real	Multiplier on the average distance between ions $R_0 = (4\pi\rho/3Am_i)^{-1/3}$, used when comparing to the Debye-Huckel screening length and choosing the larger value to be the maximum impact parameter for the Coulomb logarithm
<i>continued on next page</i>		

<i>continued from previous page</i>		
P2A, P2B	real	Used to construct the multiplier P2 on the minimum electron relaxation time which is equal to the average distance between ion divided by the mean electron thermal velocity, $(3kT/m_e)^{1/2}$
P3A, P3B	real	Used to construct the multiplier P3 on the electron relaxation time in the Bloch-Gruneisen regime (below the melt temperature).
P4A	real	Used to construct the multiplier P4 on the electron relaxation time in the Bloch-Gruneisen regime (above the melt temperature)
P5	real	Used to fine tune the solid density conductivity above melt
EC FLOOR	real	Minimum electrical conductivity value (default = 0.)
EC MULTIPLIER	real	Electrical conductivity multiplier (default = 1.)
TC FLOOR	real	Minimum thermal conductivity value (default = 0.)
TC MULTIPLIER	real	Thermal conductivity multiplier (default = 1.)
ANOMALOUS	real	If greater than 0., will enable an anomalous collisionality in low density, high temperature regions. A value of 1.0 is nominal. See the SPITZER model for details. (default = 0.)
TEMPERATURE CUTOFF	real	The minimum temperature used to evaluate the conductivities (default = 0.)
USE PARALLEL CONDUCTIVITY	real	The LMD model returns the values of the conductivities perpendicular to the magnetic field by default. If not equal to 0., the LMD model will return the values of the conductivities parallel to the magnetic field. (default = 0.)

Table 12. Registered Plot Variables for LMD.

Variable Name	Type	Mode	Description
DENSITY	real	INPUT	Material density
TEMPERATURE	real	INPUT	Material temperature
ECON	real	OUTPUT	Electrical conductivity used
ECON_PAR	real	OUTPUT	Electrical conductivity parallel to the magnetic field
ECON_PERP	real	OUTPUT	Electrical conductivity transverse to the magnetic field
THERMAL_CON	real	OUTPUT	Thermal conductivity used
THERMAL_CON_PAR	real	OUTPUT	Thermal conductivity parallel to the magnetic field
THERMAL_CON_PERP	real	OUTPUT	Thermal conductivity transverse to the magnetic field
ZBAR	real	OUTPUT	Average ionization state

8.3.2 Spitzer Conductivities

```
MODEL model_id_number SPITZER
  [parameter = value]
  ...
END
```

The SPITZER conductivity model [13] is valid for high temperature plasmas above 1 eV temperature. The model computes electrical conductivity components parallel and perpendicular to the magnetic field.

$$\sigma_{\parallel}(\rho, T) = (\gamma_E) \frac{2(2kT)^{3/2}}{\pi^{3/2} m_e^{1/2} Z e^2 c^2 \ln \Lambda} \cdot \frac{1}{f_{anom}} \quad (48)$$

$$\sigma_{\perp}(\rho, T) = \left(\frac{3\pi}{32} \right) \frac{2(2kT)^{3/2}}{\pi^{3/2} m_e^{1/2} Z e^2 c^2 \ln \Lambda} \cdot \frac{1}{f_{anom}} \quad (49)$$

By default, the model returns the values of the perpendicular electric conductivity.

The model also computes thermal conductivity components parallel and perpendicular to the magnetic field.

$$\kappa_{\parallel}(\rho, T) = (\delta_T) 20 \left(\frac{2}{\pi} \right)^{3/2} \frac{(kT)^{5/2} k}{m_e^{1/2} e^4 Z \ln \Lambda} \cdot \frac{1}{f_{anom}} \quad (50)$$

$$\begin{aligned} \kappa_{\perp}(\rho, T) &= \frac{8}{3} \frac{(\pi m_i k)^{1/2} n_i^2 Z^2 e^2 c^2 \ln \Lambda}{T^{1/2} B^2} \cdot f_{anom} \\ &= \frac{8}{3} (\pi m_{amu} k)^{1/2} N_A^2 e^2 c^2 \left(\frac{\rho^2 Z^2 \ln \Lambda}{A^{3/2} T^{1/2} B^2} \right) \cdot f_{anom} \end{aligned} \quad (51)$$

By default, the model returns the minimum of these two thermal conductivities.

In low-density, high-temperature plasmas in a strong magnetic field, the electrical conductivity may be reduced by an anomalous factor, $f_{anom} \geq 1$. [21] This factor also enhances the value of the perpendicular thermal conductivity, and reduces the value of the parallel thermal conductivity as shown in the above formulas. These anomalous conductivities are

enabled by setting the input parameter `ANOMALOUS` $> 0.$, where a value of 1.0 is nominal. A value greater than 1 increases this effect and a value less than 1 reduces this effect. In CGS units with the electron temperature expressed in eV, then the anomalous factor is:

$$\begin{aligned}
 f_{anom} &= 1 + P_{anomalous} \frac{v^*}{v_{ei}} \\
 v^* &= \Omega_e \sqrt{(\bar{Z} m_e) / (A m_{amu})} (V_d / V_{th})^2 \\
 v_{ei} &= 2.9 \cdot 10^{-6} (\bar{Z}^2 N_i \log \Lambda) / (T_e^{3/2}) \\
 V_d &= |\vec{J}| / (\bar{Z} e N_i) \\
 V_{th} &= \sqrt{(2 k_B T_i) / (A m_{amu})}
 \end{aligned} \tag{52}$$

where $P_{anomalous}$ is the `ANOMALOUS` input parameter, v^* is an anomalous collision frequency, v_{ei} is the electron-ion collision frequency, $\Omega_e = (e|\vec{B}|) / (m_e c)$ is the electron cyclotron frequency, V_d is a drift velocity, V_{th} is the ion thermal velocity, \bar{Z} is the average ionization state, A is the atomic mass, and N_i is the ion number density.

The parameters `COLD ECON` and `COLD TCON` are a simplified attempt to extend the `SPITZER` model below the Spitzer regime. A better approach is to use the `LMD` model. If these paramters are non-zero and if the ionization state \bar{Z} is less than 1, this model model will use \bar{Z} to linearly interpolate between the cold value and the Spitzer value with $\bar{Z} = 1$.

$$\sigma = \begin{cases} (1 - \bar{Z}) \sigma_{cold} + \bar{Z} \sigma_{Spitzer}, & \bar{Z} < 1 \\ \sigma_{Spitzer}, & \bar{Z} \geq 1 \end{cases} \tag{53}$$

$$\kappa = \begin{cases} (1 - \bar{Z}) \kappa_{cold} + \bar{Z} \kappa_{Spitzer}, & \bar{Z} < 1 \\ \kappa_{Spitzer}, & \bar{Z} \geq 1 \end{cases} \tag{54}$$

- Modules: `material_libs/ec`
 - `ec_spitzer.h`
 - `ec_spitzer.C`
 - `coulomb_logarithm.C`
- Physics:

- transient magnetics
- all magnetohydrodynamics physics options

Table 13: Input Parameters for SPITZER.

Parameter Name	Type	Description
A	real	Atomic mass
Z	real	Atomic number
FIXED ZBAR	real	Overrides any ionization model with a constant value for the ionization state (optional)
FIXED COULOG	real	Overrides the coulomb logarithm calculation with a constant value (optional)
EC MULTIPLIER	real	May be used to scale the electrical conductivity (optional)
TC MULTIPLIER	real	May be used to scale the thermal conductivity (optional)
COLD ECON	real	Electrical conductivity value when ZBAR<1.0 (optional)
COLD TCON	real	Thermal conductivity value when ZBAR<1.0 (optional)
ANOMALOUS	real	If greater than 0., will enable an anomalous collisionality in low density, high temperature regions. A value of 1.0 is nominal. (default = 0.)
TEMPERATURE CUTOFF	real	Model is called with the maximum of the material temperature or the cutoff temperature. (optional)
USE PARALLEL CONDUCTIVITY	real	Setting this parameter to be non-zero causes the parallel value of the conductivity will be used. (optional)
USE PERPENDICULAR CONDUCTIVITY	real	Setting this parameter to be non-zero causes the perpendicular value of the conductivity will be used. (optional)

Table 14. Registered Plot Variables for SPITZER.

Variable Name	Type	Mode	Description
DENSITY	real	INPUT	Material density
TEMPERATURE	real	INPUT	Material temperature
ECON ECON_PAR ECON_PERP	real	OUTPUT	Electrical conductivity
THERMAL_CON THERMAL_CON_PAR THERMAL_CON_PERP	real	OUTPUT	Thermal conductivity
COULOG	real	OUTPUT	Coulomb logarithm

8.4 Electrical Conductivity Models

8.4.1 EC Anomalous Conductivity

```
MODEL model_id_number EC ANOMALOUS
  [parameter = value]
  ...
END
```

This is a density and temperature independent model that returns one of two user specified values for the conductivity depending upon the value of the cell-centered current density, J_E . This model is given by

$$\sigma(\rho, T) = \begin{cases} \sigma_0, & |\vec{J}_E| \leq J_{anom} \\ \sigma_1, & |\vec{J}_E| > J_{anom} \end{cases} \quad (55)$$

The model is parametrized by the constants σ_0 , σ_1 , and the magnitude of the current density J_{anom} . The orientation of the current density is inconsequential.

- Modules: material_libs/ec
 - ec_anomalous.h
 - ec_anomalous.C
- Physics:
 - transient magnetics
 - all magnetohydrodynamics physics options

Table 15. Input Parameters for EC ANOMALOUS.

Parameter Name	Type	Description
SIGMA0	real	Reference conductivity, σ_0
SIGMA1	real	Reference conductivity, σ_1
JANOM	real	Threshold current density , J_{anom}

Table 16. Registered Plot Variables for EC ANOMALOUS.

Variable Name	Type	Mode	Description
DENSITY	real	INPUT	Material density
TEMPERATURE	real	INPUT	Material temperature
ECON	real	OUTPUT	Electrical conductivity

8.4.2 EC Knoepfel Conductivity

```
MODEL model_id_number EC KNOEPFEL
  [parameter = value]
  ...
END
```

A low temperature model called the Knoepfel model [12] is reasonable for metals from about 100 K up to the melting point. This model is given by

$$\sigma(\rho, T) = \max \left(\frac{\sigma_0}{1 + \beta C_v (T - T_0)} \left(\frac{\rho}{\rho_0} \right)^\alpha, \sigma_{min} \right) \quad (56)$$

The model is parametrized by the constants σ_0 , ρ_0 , α , and βC_v . A constant conductivity may be obtained by setting $\alpha = 0$ and $\beta C_v = 0$. A reasonable guess for α given no other information is twice the Gruneisen coefficient for the material. At a minimum this model can achieve a drop in conductivity with temperature. It cannot deal with the melt transition however. The conductivity floor is not part of the model given by Knoepfel, but is added for additional flexibility.

- Modules: material_libs/ec
 - ec_knoepfel.h
 - ec_knoepfel.C
- Physics:
 - transient magnetics
 - all magnetohydrodynamics physics options

Table 17. Input Parameters for EC KNOEPFEL.

Parameter Name	Type	Description
SIGMA0	real	Reference conductivity, σ_0
RHO0	real	Model reference density, ρ_0
T0	real	Model reference temperature, T_0
ALPHA	real	Density exponent, α
BETACV	real	Temperature coefficient, βC_v
SIGMAMIN	real	Minimum conductivity, σ_{min}
TEMPERATURE CUTOFF	real	Model is called with the maximum of the material temperature or the cutoff temperature

Table 18. Registered Plot Variables for EC KNOEPFEL.

Variable Name	Type	Mode	Description
DENSITY	real	INPUT	Material density
TEMPERATURE	real	INPUT	Material temperature
ECON	real	OUTPUT	Electrical conductivity

8.4.3 KEC Sesame Conductivity

```

MODEL model_id_number KEC SESAME
  [parameter = value]
  ...
END

```

Electrical conductivity as found in tabular form in Kerley Sesame format. [8] Internally this is the 602 Sesame table. This is not really a model. It is a software interface. The origins of any table used here must be carefully researched and understood.

- Modules: material_libs/kerley_eos/sesame
 - sec_mig.h
 - sec_mig.C
 - secmig.F
- Physics:

- transient magnetics
- all magnetohydrodynamics physics options

Table 19. Input Parameters for KEC SESAME.

Parameter Name	Type	Description
FEC	string	Table file name
NEC	integer	Table Number
TEMPERATURE CUTOFF	real	Model is called with the maximum of the material temperature or the cutoff temperature.

Table 20. Registered Plot Variables for KEC SESAME.

Variable Name	Type	Mode	Description
DENSITY	real	INPUT	Material density
TEMPERATURE	real	INPUT	Material temperature
ECON	real	OUTPUT	Electrical conductivity

Example:

```
model, 2, kec sesame
    fec = 'ses600'
    nec = 3109
end
```

8.5 Thermal Conductivity Models

8.5.1 Constant Thermal Conductivity

```
MODEL model_id_number CONSTANT THERMAL CONDUCTIVITY
  [parameter = value]
  ...
END
```

The CONSTANT THERMAL CONDUCTIVITY model allows the user to specify a simple constant conductivity.

$$\kappa(\rho, T) = \kappa_0 \quad (57)$$

- Modules: material_libs/thermal_con_models
 - constant_con.h
 - constant_con.C
- Physics: thermal conduction and its derivatives

Table 21. Input Parameters for CONSTANT THERMAL CONDUCTIVITY.

Parameter Name	Type	Description
THERMAL_CONSTANT	real	Constant thermal conductivity, κ_0

Table 22. Registered Plot Variables of CONSTANT THERMAL CONDUCTIVITY.

Variable Name	Type	Mode	Description
TEMPERATURE	real	INPUT	Material temperature
DENSITY	real	INPUT	Material density
THERMAL_CON	real	OUTPUT	Thermal conductivity

8.5.2 Plasma Thermal Conductivity

```
MODEL model_id_number PLASMA
  [parameter = value]
  ...
END
```

The PLASMA thermal conductivity model is a simple power law of the form:

$$\kappa(\rho, T) = A\rho^B T^C. \quad (58)$$

Similar to the SPITZER conductivity model if $B = 0$ and $C = 5/2$, it can be used to study deviations from pure Spitzer-like behavior. It can also be used to specify a constant conductivity.

- Modules: material_libs/thermal_con_models
 - plasma.h
 - plasma.C
- Physics: thermal conduction and its derivatives

Table 23. Input Parameters for PLASMA.

Parameter Name	Type	Description
A	real	Thermal conductivity coefficient (note that conductivities obtained from tables may need to be scaled if B or C are nonzero)
B	real	Density exponent
C	real	Temperature exponent

8.5.3 Polynomial Thermal Conductivity

```
MODEL model_id_number POLYNOMIAL
  [parameter = value]
  ...
END
```

Table 24. Registered Plot Variables of PLASMA.

Variable Name	Type	Mode	Description
DENSITY	real	INPUT	Material density
TEMPERATURE	real	INPUT	Material temperature
THERMAL_CON	real	OUTPUT	Thermal conductivity

The POLYNOMIAL thermal conductivity model is a simple power law model that depends only on temperature:

$$\kappa(\rho, T) = A_0 + A_1 \cdot T^{N_1} + A_2 \cdot T^{N_2} + A_3 \cdot T^{N_3}. \quad (59)$$

- Modules: material_libs/thermal_con_models
 - polynomial_con.h
 - polynomial_con.C
- Physics: thermal conduction and its derivatives

Table 25. Input Parameters for POLYNOMIAL.

Parameter Name	Type	Description
A0	real	Constant coefficient
A1	real	Coefficient of first temperature term
A2	real	Coefficient of second temperature term
A3	real	Coefficient of third temperature term
N1	real	Power of first temperature term
N2	real	Power of second temperature term
N3	real	Power of third temperature term

8.5.4 KTC Sesame Thermal Conductivity

```

MODEL model_id_number KTC SESAME
  [parameter = value]
  ...
END

```

Table 26. Registered Plot Variables of POLYNOMIAL.

Variable Name	Type	Mode	Description
DENSITY	real	INPUT	Material density
TEMPERATURE	real	INPUT	Material temperature
THERMAL_CON	real	OUTPUT	Thermal conductivity

Thermal conductivity as found in tabular form in Kerley Sesame format. [8] Internally this is the 603 Sesame table. This is not really a model. It is a software interface. The origins of any table used here must be carefully researched and understood.

- Modules: material_libs/kerley_eos/sesame
 - stc_mig.h
 - stc_mig.C
 - stcmig.F
- Physics: thermal conduction and its derivatives

Table 27. Input Parameters for KTC SESAME.

Parameter Name	Type	Description
FTC	String	Table file name
NTC	int	Table Number
TEMPERATURE CUTOFF	real	Minimum temperature

Table 28. Registered Plot Variables of KTC SESAME.

Variable Name	Type	Mode	Description
DENSITY	real	INPUT	Material density
TEMPERATURE	real	INPUT	Material temperature
THERMAL_CON	real	OUTPUT	Electrical conductivity

Example:

```
model, 4, ktc sesame  
    ftc = 'ses600'  
    ntc = 3109  
end
```

8.6 Opacity Models

Opacity models calculate radiation absorption and emission coefficients for radiation and radiation hydrodynamics simulations. Currently recognized opacity model names are:

- BIGGS LIDTHILL
- KRAMERS FITTED
- XSN

8.6.1 Biggs Lighthill Opacity

```
MODEL model_id_number BIGGS LIDTHILL
  NUMBER OF ELEMENTS int
    ELEMENT int, MASS real, FRACTION real
  END
  [parameter = value]
  ...
END
```

The Biggs Lighthill opacity [1] provides convenient analytical approximations to photoelectric absorption and incoherent scattering cross sections (cm^2/g) of photons by atoms. The cross sections σ are scaled by the density ρ to return opacity, $\tau = \rho\sigma$, of dimensions of inverse length ($1/L$).

This opacity model applies to atoms of atomic numbers between 1 and 100 and is designed for photon energies $10 \text{ eV} < E < 1 \text{ MeV}$ and material temperatures that result in an average ionization < 1 . The cross sections are material temperature independent and are calculated only once during setup. At each time step, the cross sections are scaled by the new density to obtain the density dependent opacities.

The photoelectric cross sections σ_a for each element are approximated by four-term polynomials in reciprocal powers of the photon energy E (in keV) on numerous fitting intervals.

$$\sigma_a = \frac{A_1}{E} + \frac{A_2}{E^2} + \frac{A_3}{E^3} + \frac{A_4}{E^4} \quad (60)$$

The incoherent scattering cross sections σ_s are based on the Klein-Nishina relation, but use simpler approximate equations for efficient computer evaluation.

For composite materials the total opacities are computed by mixing the atomic cross sections according to the mass fractions f_m of the elements. Mass fractions are determined by the code from the input atomic fractions f_a as specified MATERIAL keyword NUMBER OF ELEMENTS.

$$\sigma_{mixed} = \sum_e f_{m,e} \sigma_e \quad (61)$$

- Modules: material_libs/opac_models
 - Biggs_Lighthill.h
 - Biggs_Lighthill.C
 - biggs.h
 - biggs.C
 - biggs_*.h
- Data Files: /pr/alegra/mig_data
 - biggs_pp_coef.dat
 - biggs_pe_coef.dat
- Physics:
 - emission
 - radiation and all derived physics classes

Example 1:

```
model 1 biggs lighthill
  legendre          = 1  $ default
  secondary radiation = 2  $ default
  integration intervals = 40 $ default
  number of elements = 3
    element 1,  mass 1.0079, fraction 0.01
    element 13, mass 26.981, fraction 0.98
```

Table 29. Input Parameters for BIGGS LIGHTHILL.

Parameter Name	Type	Description
INTEGRATION INTERVALS	int	Number of integration intervals in each group (Default = 40)
LEGENDRE	int	Number of Legendre moments used. 1 = Isentropic
NUMBER OF ELEMENTS	int	Overrides material model definition.
SECONDARY RADIATION	int	0 = None 1 = fluorescence only 2 = fluorescence and annihilation (default) 3 = annihilation only
WEIGHTING	real	User defined group weighting. Not yet available.

Table 30. Registered Plot Variables for BIGGS LIGHTHILL.

Variable Name	Type	Mode	Description
DENSITY	Scalar	INPUT	Material density
OPACA	Opacity	OUTPUT	τ_a - Absorption opacity - units of $\frac{1}{length}$
OPACS	Opacity	OUTPUT	τ_s - Scattering opacity - units of $\frac{1}{length}$

```

        element 100, mass 257.00, fraction 0.01 $ max Z allowed
    end
end

```

Example 2:

```

model 1 biggs lighthill
end

```

8.6.2 Kramers Fitted Opacity

```

MODEL model_id_number KRAMERS FITTED
    [parameter = value]
    ...
END

```

The Kramers fitted opacity [25] uses the simple analytic expressions

$$\tau_a = \rho \sigma_a = C_a \rho^{a+1} T^b \nu^c \quad (62)$$

$$\tau_s = \rho \sigma_s = C_s \rho^{d+1} T^e \nu^f \quad (63)$$

to calculate the true absorption σ_a and scattering σ_s mass coefficients (units are area per mass).

- Modules: material_libs/opac_models
 - kramers_fitted.h
 - kramers_fitted.C
- Physics:
 - emission
 - radiation and all derived physics classes

Table 31. Input Parameters for KRAMERS FITTED.

Parameter Name	Type	Description
KAP COEF	real	C_a - Coefficient of true absorption
KAP RHO EXP	real	a - Density exponent for absorption
KAP T EXP	real	b - Temperature exponent for absorption
KAP NU EXP	real	c - Photon energy exponent for absorption
SIG COEF	real	C_s - Coefficient of scattering
SIG RHO EXP	real	d - Density exponent for scattering
SIG T EXP	real	e - Temperature exponent for scattering
SIG NU EXP	real	f - Photon energy exponent for scattering

For example, free-free absorption and Thompson scattering in a completely ionized plasma could be specified as:

```
model 1 kramers fitted
  kap coef      = 2.22e32
```

Table 32. Registered Plot Variables for KRAMERS_FITTED.

Variable Name	Type	Mode	Description
DENSITY	Scalar	INPUT	Density
TEMPERATURE	Scalar	INPUT	Temperature
NU(j)	Scalar	INPUT	Left frequency bound in j-th group
OLD_DENSITY	Scalar	OUTPUT	Previous density (not used)
OLD_TEMP	Scalar	OUTPUT	Previous temperature (not used)
OPACA	Opacity	OUTPUT	τ_a - Absorption opacity - units of $\frac{1}{length}$
OPACS	Opacity	OUTPUT	τ_s - Scattering opacity - units of $\frac{1}{length}$

```

kap rho exp = 1.0
kap t exp  = -0.5
kap nu exp = -3.0
sig coef   = 3.99
sig rho exp = 0.0
sig t exp  = 0.0
sig nu exp = 0.0
end

```

This model is particularly useful for calculations where the opacity in the regime of interest can be approximated reasonably well by the above analytical form and computational speed is desired.

8.6.3 XSN Opacity

```

MODEL model_id_number XSN
  NUMBER OF ELEMENTS int
    ELEMENT int, MASS real, FRACTION real
  END
  [parameter = value]
  ...
END

```

XSN [17, 18, 20] provides frequency-dependent emission and absorption coefficients for a material that may or may not be in LTE (local thermodynamic equilibrium). The model assumes an average ion approximation and can handle the case of multiple elements

in a composite material. The XSN package is highly compute intensive compared to other opacity models.

In LTE, the required inputs are the mass density ρ , the atomic molar fraction f_a , and the electron temperature T_e .

In non-LTE, additional inputs are needed (see below).

Material composition information listed under the XSN model will override the composition information listed under the MATERIAL model.

- Modules: material_libs/opac_models
 - xsn.h
 - xsn.C
 - xsn_interface.h
 - xsn_interface.C
- Physics:
 - emission
 - radiation and all derived physics classes

Table 33: Input Parameters for XSN.

Parameter Name	Type	Description
ATOMIC VOLUME MULTIPLIER	real	Fudge factor for atomic volumes (default = 1.0)
BOUND BOUND MULTIPLIER	real	Fudge factor for bound-bound opacity (default = 1.0)
CONTINUUM LOWERING MULTIPLIER	real	Fudge factor for continuum lowering (default = 1.0)
CONTINUUM LOWERING TYPE	int	Continuum lowering model to use: 1 = use no continuum lowering (default) 2 = ion-sphere model
DOPPLER WIDTH OPTION	int	Use Doppler line width model (default = 0)
ENERGY LEVEL TYPE	int	Energy level model to use: 1 = Bohr with Pauli corrections (default) 2 = Dirac energy levels
<i>continued on next page</i>		

<i>continued from previous page</i>		
FREE BOUND MULTIPLIER	real	Fudge factor for free-bound emission (default = 1.0)
HAGEN RUBENS	none	This is NOT an ice cream sandwich. Modifies the low photon energy opacities using the value of the electrical conductivity and is recommended primarily for metals. [7] NOTE! THE USER MUST SPECIFY THE ELECTRICAL CONDUCTIVITY MODEL BEFORE THE XSN MODEL IN THE INPUT DECK!
LINE OPTION	int	(default = 0)
LINE WIDTH MULTIPLIER	real	Fudge factor for line widths (default = 1.0)
MINIMUM NUCLEAR Z	real	(default = 10.0)
MAXIMUM DENSITY	real	Cutoff density for bound-bound opacity fudge factor (default = 100.0)
NUMBER OF ELEMENTS	int	(default = 0, maximum = 5)
NUMBER OF LEVELS	int	(default = 7, maximum = 10)
NUMBER OF SUBGROUPS PER GROUP	int	(default = 100, maximum = 560)
OPACITY AVG LIMIT	int	(default = 1)
PLANCK OPACITY OPTION	int	(default = 1)
STRAIGHT OPACITY AVERAGE	int	(default = 1)
TEMPERATURE CUTOFF	real	(default = 0.0, code units)
TWO BAND OPTION	int	(default = 0)

Table 34. Registered Plot Variables for XSN.

Variable Name	Type	Mode	Description
DENSITY	Scalar	INPUT	Material density
TEMPERATURE	Scalar	INPUT	Material temperature
OLD_DENSITY	Scalar	OUTPUT	Old density
OLD_TEMP	Scalar	OUTPUT	Old temperature
OPACA	Opacity	OUTPUT	τ_a - Absorption opacity - units of $\frac{1}{length}$
OPACS	Opacity	OUTPUT	τ_s - Scattering opacity - units of $\frac{1}{length}$

For example,

```

material 1 DDGAS
    ...
    model = 2
    ...
end

model 2 xsn $ DD-GAS
    number of elements 1
        element 1, mass 2.0, fraction 1.0
    end
end

material 3 CH
    ...
    model = 6
    ...
end

model 6 xsn $ CH + 5% O + 0.25% Br
    number of elements 4
        element 1, mass 1.0079, fraction 0.47375
        element 6, mass 12.0110, fraction 0.47375
        element 8, mass 15.9994, fraction 0.05
        element 35, mass 79.9040, fraction 0.0025
    end
end

```

8.7 Ionization Models

8.7.1 Saha Ionization

```
MODEL model_id_number SAHA IONIZATION
  [parameter = value]
  ...
END
```

The SAHA IONIZATION model [25] solves for the relative abundance of nuclei in adjacent charge states and for the average ionization state, \bar{Z} , of a hot material. This model obtains its necessary information from the NUMBER OF ELEMENTS ... END block of the MATERIAL specification.

The ionization state is found by solving a nonlinear set of equations relating the fractional number of ions in each ionization state.

$$\frac{\alpha_{m+1}\alpha_e}{\alpha_m} = C_{Saha} \left(\frac{A}{\rho} \right) \left(\frac{u_{m+1}}{u_m} \right) (T^{3/2}) \exp \left(\frac{-I_{m+1}}{T} \right) \quad (64)$$

$$1 = \sum_{m=0}^Z \alpha_m \quad \text{and} \quad \alpha_e = \sum_{m=0}^Z m\alpha_m \quad (65)$$

where $\alpha_m = N_m/N$ represents the fraction of ions in the m^{th} charge state and $N = \rho N_A/A$ is the number density of nuclei. N_m represents the number density of nuclei in the m^{th} charge state. $\alpha_e = N_e/N$ represents the ratio of free electrons to nuclei and also the average ionization state, \bar{Z} . A is the atomic mass, ρ is the density in g/cm^3 , u_m is essentially the electronic partition function (assumed to be equal to the statistical weight of the statistical weight of the ground state, i.e., 2 for the two electron spin states), T is the temperature in keV, and I_m is the ionization potential of the m^{th} charge state also in keV.

$$C_{Saha} = \frac{2}{N_A} \left(\frac{2\pi m_e k_B}{h^2} \right)^{3/2} = 317.013 \quad (66)$$

where N_A is the Avogadro's number, m_e is the electron mass, h is Planck's constant, and k_B is essentially Boltzmann's constant converting the temperature from keV to ergs.

- Modules: material_libs/ec
 - matmod_saha.h
 - matmod_saha.C
 - saha_equation.F
- Physics: any physics requiring ionized materials

Table 35. Input Parameters for SAHA IONIZATION.

Parameter Name	Type	Description
TEMPERATURE CUTOFF	real	Minimum temperature used to evaluate the ionization state

Table 36. Registered Plot Variables of SAHA IONIZATION.

Variable Name	Type	Mode	Description
DENSITY	real	INPUT	Material density
TEMPERATURE	real	INPUT	Material temperature
ZBAR	real	OUTPUT	Ionization state

Example:

```
model, 5, saha ionization
  $ no parameters necessary
end
```

8.7.2 KZB Sesame Ionization

```
MODEL model_id_number KZB SESAME
  [parameter = value]
  ...
END
```

Ionization state as found in tabular form in Kerley Sesame format. [8] Internally this is the 601 Sesame table. This is not really a model. It is a software interface. The origins of any table used here must be carefully researched and understood.

- Modules: material_libs/kerley_eos/sesame
 - szb_mig.h
 - szb_mig.C
 - szbmig.F
- Physics: any physics requiring ionized materials

Table 37. Input Parameters for KZB SESAME.

Parameter Name	Type	Description
FZB	String	Table file name
NZB	int	Table Number

Table 38. Registered Plot Variables of KZB SESAME.

Variable Name	Type	Mode	Description
DENSITY	real	INPUT	Material density
TEMPERATURE	real	INPUT	Material temperature
ZBAR	real	OUTPUT	Ionization state

Example:

```
model, 5, kzb sesame
  fzb = 'ses600'
  nzb = 3109
end
```

9 Diagnostics

9.1 Global Tallies

In many problems of interest it is often desirable to know the energy budget. How much energy is related to a given physical process? What are the values of the kinetic, internal, magnetic, and radiation energies? How much energy is supplied by a given source or is lost to a given sink? How fast does energy change from one form to another? A global energy balance can be constructed as follows.

$$E_{error}(t) = E_{tot}(t) - [E_{tot}(0) + E_{sources}(t) - E_{losses}(t)] = 0 \quad (67)$$

where

$$E_{tot}(t) = E_{int}(t) + E_{kin}(t) + E_{mag}(t) \quad (68)$$

Ideally the error in this energy balance should be zero, or at least small compared to most energy tallies. Deviations from zero are typically due to missing energy tallies, numerical inaccuracies, or perhaps too large of a time step.

Table 39. Global Tallies for REGION (All Physics Options).

Global Variable Name	Explanation
ETOT	Total of the kinetic internal, magnetic, and radiation energies
PTOT*	and the rate of total energy change.

Table 40: Global Tallies for TRANSIENT MAGNETICS.

Global Variable Name	Explanation
DT_MAG	Overall limiting time step for TRANSIENT MAGNETICS
DT_MAGDIFF	Suggested limiting time step for resolving magnetic diffusion. It is essentially one e-folding time for problems where the magnetic field varies exponentially in time. In SI units, $\tau_{magdiff} = (\mu\sigma h^2)/4$, where μ is the permeability, σ is the conductivity, and h is a characteristic cell size.
DT_ALFVEN	Limiting time step based upon Alfven wave speed.
CURRENT	Current flowing in the mesh as tallied by the CURRENT TALLY boundary conditions. Present only if CURRENT TALLY commands are specified.
<i>continued on next page</i>	

<i>continued from previous page</i>	
INDUCTANCE	Inductance of the mesh computed from the total magnetic field energy, EMAG, and the total CURRENT tally. Present only if CURRENT TALLY boundary conditions are specified. In SI units, $\frac{1}{2}LI^2 = E_{mag} = \frac{1}{2\mu_0} \int B^2 dV$.
RESISTANCE	Resistance of the mesh computed from the total joule heating rate, PJOULE, and the total CURRENT tally. Present only if CURRENT TALLY boundary conditions are specified. In SI units, $RI^2 = P_{Joule} = \int \eta J^2 dV$.
EMAG PMAG	Magnetic field energy and rate of change.
EJOULE PJOULE	Cumulative tally of the energy transferred to the material via Joule heating and rate of heating.
EJOULV PJOULV	Cumulative tally of the energy transferred to the void via Joule heating and rate of heating as a consequence of small, but finite, void conductivities. This energy and power should be small compared to other energies and powers for a valid solution.
EUDJXB PUDJXB	Cumulative tally of the energy transferred to the material via work done by $\vec{J} \times \vec{B}$ forces and rate of change.
EMAGHYDRO PMAGHYDRO	Cumulative tally of the change in magnetic field energy due to Lagrangian motion of the mesh and rate of change. (2D only)
EMAGWORK PMAGWORK	Cumulative tally of the energy transferred to the material via work done by forces and rate of change. Typically these tallies equal the sum of the EUDJXB and EMAGHYDRO tallies (2D only)
EPOYNT PPOYNT	Cumulative tally of the energy transferred to the system via Poynting flux through the boundary of the mesh and rate of change. Since this tally typically represents a source of energy, it should be added to the energy balance equation. This tally is positive if energy is added to the mesh and negative if energy is lost from the mesh.
<i>continued on next page</i>	

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ETDERR PTDERR	Time discretization energy and rate of change. This energy error originates naturally when constructing the fully-implicit numerical algorithm used to solve the MHD equations. It should be small compared to other energies and powers for a valid solution. (2D only)
EMAGRZERR	Error in the magnetic field energy as a result of advection, i.e., remap. It should be small compared to other energies for a valid solution. There is no corresponding power.

Table 41. Global Tallies for THERMAL CONDUCTION.

Global Variable Name	Explanation
DT_CON	Overall limiting time step for THERMAL CONDUCTION. The reported time step does not include scaling by the TIME STEP SCALE keyword so the user may readily see the time step that thermal conduction would normally employ.

Table 42. Global Tallies for EMISSION.

Global Variable Name	Explanation
ERADEMIT PRADEMIT*	Cumulative tally of the radiation energy emitted by the material and the rate of emission due to the EMISSION model. Since this tally represents a gain to the radiation energy, it should be added to the initial radiation energy in energy balance equations.
DIST_TO_VOID	A report of the mean-distance-to-void used to compute the reabsorption factor in the emission model.
OPTICAL_DEPTH_MIN OPTICAL_DEPTH_MAX	A report of the minimum and maximum optical depth used to compute the reabsorption factor in the emission model. The optical depth is defined to be the absorption opacity times the mean-distance-to-void.

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