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"ALEGRA-MHD Applications to Solid Liner MTF/MIF Confinement Concepts,"
Authored by Enig Associates, Inc.

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4. ALEGRA-MHD CAPABILITY FOR MTF APPLICATION

4.1 Introduction

Enig Associates, Inc. ("ENIG") proposes to model the physics of MTF experiments using the ALEGRA code. ALEGRA is an Arbitrary Lagrangian-Eulerian (ALE) multi-material finite element code that emphasizes large deformations and strong shock physics [99,100,101]. As an effort to combine the modeling features of modern Eulerian shock codes with the improved numerical accuracy of modern Lagrangian finite element codes, ALEGRA is a descendant of the Pronto transient dynamics code [96,97] and contains elements of the CTH family of shock wave codes [98]. For applications involving solid phase materials, this capability permits a calculation to proceed in Lagrangian fashion until portions of the finite element mesh become too distorted, at which time the nodal points in the most deformed portion of the mesh are moved to reduce the distortion to acceptable levels. The advantage is that numerical dissipation is avoided until large deformations occur and this is limited to only those regions where severe distortions require mesh movement. For fluid dynamics applications with high shear or simulations where fluid flows through the domain, the remesh step can be a simple return to the original grid, resulting in an Eulerian simulation. The user can specify that some parts of the domain are Eulerian but others are treated as ALE or pure Lagrangian, which allows the best approach to be used on each part of the problem. In addition to mesh smoothing, the ALEGRA remesh algorithm can also move nodes to better resolve mesh regions with specific values of selected variables or their gradients.

ALEGRA solves the MHD equations using a compatible finite-element discretization that maintains the divergence-free property of the magnetic field by construction, rather than having to apply some correction that drives the divergence of the magnetic field to zero. ALEGRA includes resistive MHD terms that capture magnetic diffusion and Joule heating. It has a variety of options for specifying magnetic and electric field boundary conditions that, in combination with complete control over the part of the boundary where those conditions are enforced, provide the user with great flexibility to set up complex MHD applications. ALEGRA has a circuit solver that can be used to dynamically specify the current through the mesh boundaries. In this circuit, the mesh is itself an active element. Finally, it has multi-group flux-limited diffusion and implicit Monte Carlo radiation solvers that are available for optically thick regimes.

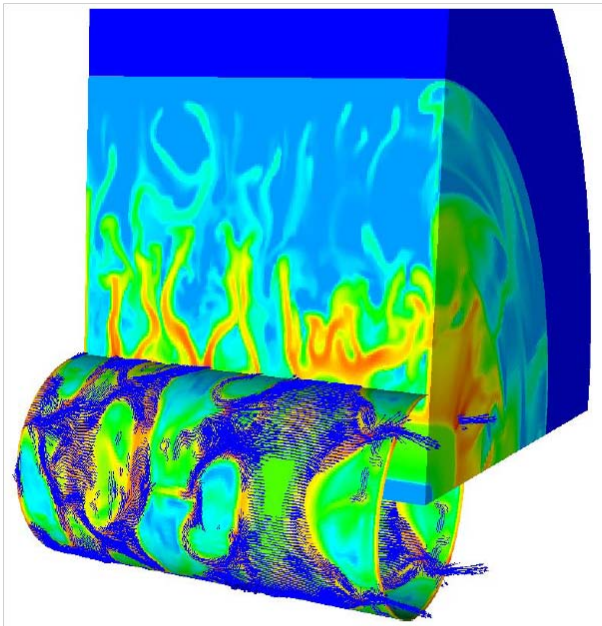

Figure 1: Density field and overlaid current-density vector contours from 3D ALEGRA simulation for a wire-array Z-pinch implosion [102].

ALEGRA is designed to run on distributed-memory parallel computers using the Single Program Multiple Data (SPMD) paradigm, in which the mesh is decomposed into sub-meshes (i.e., domain decomposition). This is done because of the need to access the enormous memories and processor speeds of massively parallel processor (MPP) computers to analyze large, three-dimensional problems. An example of a typical large 3D MHD simulation performed using ALEGRA is shown in Figure 1. Here the modeled density field resulting from a 2.5-mg tungsten wire-array implosion on Sandia's ZR pulsed power facility is plotted, with vector contours of the current density field overlaid [102].

Like the MACH-2D/3D and ALE3D packages [103,104], ALEGRA uses an operator-split methodology for representing MHD in the context of ALE simulations. In this approach, an explicit ideal-MHD Lagrangian step is followed by a remesh/remap step where the finite-element solution, including electromagnetic fields, is mapped to the original or an arbitrarily determined mesh. ALEGRA uses a patch-recovery-based constrained transport method [105], while MACH uses the flux-conserving method described in Reference 103, and ALE3D uses the continuous remap approximation described in Reference 104.

4.2 General features and capabilities

4.2.1 Complex 3D geometries and flows

ALEGRA uses unstructured finite-element meshes in order to allow gridding around the most complex geometries [106]. This facilitates the use of both body-fitted meshes for geometrically complex structures, and meshes of arbitrary shape for complex magnetic field configurations (*e.g.*, spherical and ellipsoidal shapes, conic sections). Importantly, ALEGRA's unstructured mesh capability also facilitates Cartesian modeling of cylindrical objects that do not have azimuthal symmetry, either in a 3D Cartesian coordinate system, or a 2D Cartesian coordinate system on a section normal to the axis.

With structured meshes, one needs to maintain rows or columns throughout the domain, potentially leading to the development of insidious numerical errors and uncertainties associated with the representation of irregular surfaces on a regular mesh. For the applications of interest, this technology would be relevant to the representation of solid cylindrical liners and complex magnetic field configurations in 2D and 3D simulations. This technology would also be critical for ensuring sound modeling of the development of hydrodynamic and MHD instabilities arising during the implosion process, which can be spuriously induced by errors in the discrete representation of the geometry. A 3D cylindrical coordinate system is available in MACH-3D [103]. An unstructured-mesh capability is available in ALEGRA and ALE3D, but not the CTH or MACH packages. A typical MHD simulation on an unstructured mesh is shown in Figure 2, where a uniform magnetic field diffuses into a conducting cylinder rotating at constant speed. The rotation of the conductor produces a deviation in the field lines internal to the cylinder. A body fitted mesh is used here to discretize the circular geometry.

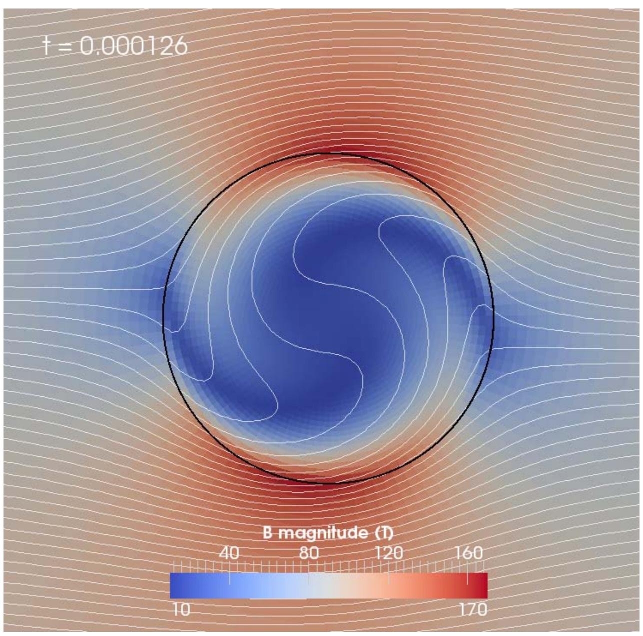

Figure 2: Magnetic field magnitude and orientation in a magnetized rotor simulation with unstructured mesh.

4.2.2 Domain decomposition and parallelism

Standard domain decomposition is used to run ALEGRA on parallel machines. The finite element mesh can be generated either using an external tool (*e.g.* CUBIT), or by use of ALEGRA's inline mesh generation capability. In either case, the mesh is broken into sub-meshes to be used by each processor in a parallel calculation. This decomposition is done using preprocessing tools that either run inline with ALEGRA, or are available as part of the ALEGRA distribution.

The code also includes a capability called "diatoms," under which the user may insert complex geometrical objects onto the mesh as part of the initial conditions. In this case an algorithm based on recursive bisection is used to decompose the domain in a way that preserves optimal load balancing. All of ALEGRA's physics packages are designed for the largest parallel machines available and regularly demonstrate excellent scaling performance on DOE supercomputers, for levels of parallelism not exceeding the threshold for communication losses, which is typically encountered at the level of a few thousand elements per processor.

4.2.3 Shocks

ALEGRA has extensive shock capturing capability that has been demonstrated under a variety of circumstances. The present methodology is based on a Lagrangian method with nonlinear, monotonicity-preserving artificial viscosity [101]. ALEGRA's methods are specifically developed to compute the solution to the time-dependent form of the equations of compressible solid-mechanical-magneto-hydrodynamics. Validation studies carried out at Sandia have shown that one-dimensional MHD simulations for magnetically accelerated flyer plates reproduce experimental measurements of shock-induced motion after impact in aluminum to a high degree of accuracy, at velocities exceeding 4 km/s and under current drives exceeding 15 megaamperes [107]. Large deformations with shear are handled through the remapping methodology of an arbitrary Lagrangian-Eulerian code. The remap utilizes interface tracking of material interfaces, and a piecewise parabolic high-resolution method for other variables. The order of accuracy used in this remap operation is variable in the neighborhood of mixed elements, and Rider *et al.* (2011) have shown that using an stencil for remap that is adaptive based on the presence of mixed elements results in dramatically enhanced accuracy and robustness for multimaterial simulations involving empirical material response data and high-velocity impact [108].

4.2.4 Materials

Specification of the materials and material models used for an ALEGRA calculation is expressed in rather general terms. A material, for purposes of an ALEGRA calculation, is defined by a set of material models and initial values of critical independent variables that may differ from the default reference values. Thus, ALEGRA material specification consists of a material and a corresponding set of material models [99].

Generally, any set of material models may be specified for a material as appropriate for the physics performed in the ALEGRA calculation. This generality provides substantial flexibility for the user to describe very complex material behavior. Additionally, this model can include a fracture submodel. All materials may occupy any element in the mesh. Thus, all elements have the possibility of containing any or all materials at any point in the calculation. The element maintains an array of material volume fractions of all materials present within that element. An additional volume fraction accounts for any empty space in the element and is typically referred to as void fraction. The sum of all of the material volume fractions and the void fraction for an element must equal one. For example, an element with a material fraction of one for a particular material is completely filled with that material. Likewise an element with a void fraction of one is completely empty. An element with multiple nonzero material fractions is filled proportionally with each of those materials and is a multimaterial element. The material fractions in an element can vary throughout a calculation if the element is remapped.

The materials in a multimaterial element are assumed to occupy distinct regions of the element, *i.e.*, material interfaces exist within the element. A variety of interface reconstruction techniques are available in ALEGRA to track these material interfaces. Further, state-of-the-art multimaterial treatment ensures that the thermodynamic state of these mixed elements is handled in a way that is robust and accurate, and preserves the volumetric behavior of species with widely varying bulk modulii occupying the same mixed element [108].

4.2.5 Weakly ionized gases

ALEGRA has significant 2D and 3D capabilities for resistive magneto-hydrodynamic modeling [100,109]. This is a low electromagnetic frequency approximation that assumes that electromagnetic waves due to displacement currents and free charge may be neglected. It is thus a charge neutral model. However, low to high temperature, weakly to highly ionized flow can be effectively modeled using physically accurate closure properties for equations of state response as well as for electrical and thermal conductivities. This combined modeling capability has permitted the design of ultra-high velocity shock impact experiments at Sandia using magnetic drive such as the Z-machine. The code also supports the concept of coupling to external circuits that can be important to ensure self-consistent interaction between the mesh solution and the external world modeled by lumped-element circuits.

4.2.6 Radiation

ALEGRA presently contains two different treatments of photon radiation transport [110]. One is deterministic and the other is statistical in nature. Both address the optically thick regime. One approach is multigroup flux-limited radiation diffusion. Depending on the mean free path, and detailed nature of the radiation field, this approach may be the most useful. ALEGRA also has an implicit Monte Carlo method, which can be used more widely albeit at a higher computational cost. If a deterministic solution is required in physical circumstances that render the diffusion approximation invalid, a discrete ordinates method could be used, but this would require an extensive effort to develop such a method. ALEGRA's radiation capability, though functional, is not currently subjected to the same degree of effort in development and testing as are other components of the code. Therefore, results computed using the radiation transport capability in ALEGRA should be treated with caution.

4.2.7 Time accurate simulation of transient phenomena including start-up

The majority of ALEGRA's applications are transient in nature ranging from z-pinch to shaped-charge simulations. The individual physics within ALEGRA are separated using operator splitting to produce a first-order temporal scheme. This splitting allows some of the physics to be advanced individually without constraints from other physics, and new physics can be easily incorporated. Additionally this splitting allows the appropriate time-integration method to be used on the individual physics (*e.g.*, explicit for hydrodynamics, and implicit for magnetic diffusion, radiation and thermal conduction). The hydrodynamic and ideal MHD physics within ALEGRA are second-order time accurate, which provides a reduction in the error for the given time step size. Also for given problems, a quasi-static magnetic-diffusion solve removes time step size constraining materials from the transient solves, thus allowing larger time steps and faster solution times. Multilevel preconditioning for these direct linear solves is implemented in ALEGRA, preserving the parallel scaling of ALEGRA multiphysics simulations performed on highly parallelized computing platforms.

For MHD, an implicit linear-solve operation is performed on every time step after the Lagrangian ideal-MHD step. The transient boundary value problem associated with a weak formulation of the eddy current diffusion equation is solved on edge and face elements whose arrangement within a DeRham complex ensures preservation of the divergence-free character of the magnetic flux density [109]. Supercycling is also implemented for situations where the the magnetic diffusion time vastly exceeds the limiting time step required by the CFL condition.

Results from a typical simulation showing the development of complex 3D effects in an MHD system are shown in Figure 3. Here, an initially solid single tungsten wire is simulated using periodic boundary conditions to represent a 30-wire array in a z-pinch implosion [111]. A sinusoidal perturbation is imposed on the wire. As magaampere levels of current flow through the wire, the perturbation gives rise to concentrations of the magnetic pressure later in time, and plumes of ablated material flowing toward the axis under the influence of Lorentz forces.

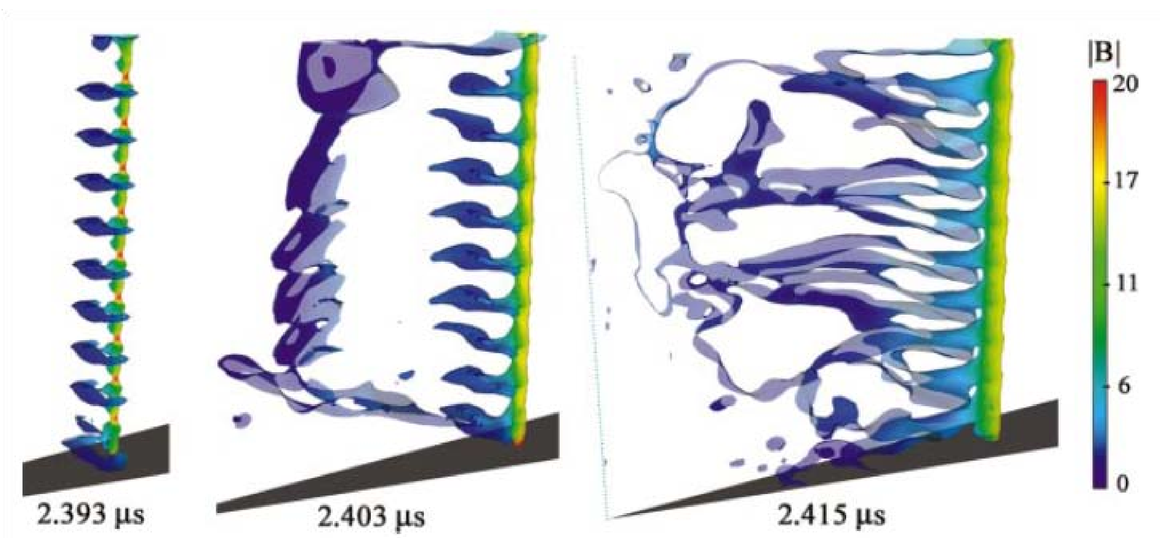

Figure 3: 3D-periodic ALEGRA simulation for a single tungsten wire in a 30-wire array implosion, showing magnetic flux density magnitude on material isosurfaces indicating the development of complex 3D structure [111].

4.2.8 Development/Validation

ALEGRA has been validated under a number of challenging circumstances including high energy density physics, electromagnetically driven problems, and high-speed impact. In each of these cases the fidelity of the solution and quality of the modeling has been interrogated by a comparison with experimental data. ALEGRA has shown to produce high-quality simulations in the most challenging circumstances such as wire-array implosions when compared with the radiation output, timing, and general character of the phenomena. ALEGRA has also been the subject of validation studies for exploding wires, where Ohmic heating from a more modest current pulse (approximately 6-kA peak current, 1-μs rise time) is used to vaporize a metallic wire. ALEGRA MHD simulations for this problem used a 2D axisymmetric finite-element mesh, with energy transmitted to the simulation domain using the lumped-element circuit model. The recorded voltage and current pulses for multiple realizations of an exploding wire experiment, whose features are very sensitive to the details and timing of the phase changes undergone by the wire, were compared to the simulation data with very favorable results [112]. ALEGRA has also been the subject of extensive verification testing [105]. The development practices used by the ALEGRA development team, are based on the recursive automated exercising of these verification and validation tests as development proceeds, in an effort to ensure sustainable advancement of code capabilities and accuracy.

4.3 MTF-specific capabilities

4.3.1 MHD modeling for matter in the warm-dense and hot plasma regimes

A critical capability for simulating MTF systems is sound modeling of the electrical conductivity of material in the warm dense matter regime. This is the regime where the material has the properties of neither a solid at room temperature, nor a hot ionized plasma. Rather, its state is near the metal-insulator transition, where the electrical conductivity is both poorly characterized and highly sensitive to the material state. This is the situation in the initially solid liner in MTF systems. As the conducting liner heats up Ohmically, its conductivity plummets, leading to even greater rates of Ohmic heating. The runaway situation leads to a scenario in which energy can be deposited very quickly, and the character of the solution can change dramatically as a result of only a small change in the material state or the material parameters.

This was recognized in early work on the Lee-More-Desjarlais (LMD) conductivity model, which is implemented and very heavily used in ALEGRA for MHD simulations. It was discovered that with appropriate treatment of ionization potentials, and with density-functional-theory-based corrections to the model for individual materials, agreement between ALEGRA simulations and the 15-MA, 40-km/s flyer plate experiment was remarkable. This is documented in Reference 107. These improvements allowed modelers for the first time to reproduce measured shock velocities using an MHD simulation that was initialized using a metallic liner at ambient temperature. Electrical conductivities had been too low in the metal-insulator transition region, resulting in overheated and melted material [113], which failed to produce the expected shock pressures and velocities. This is shown here in Figure 4.

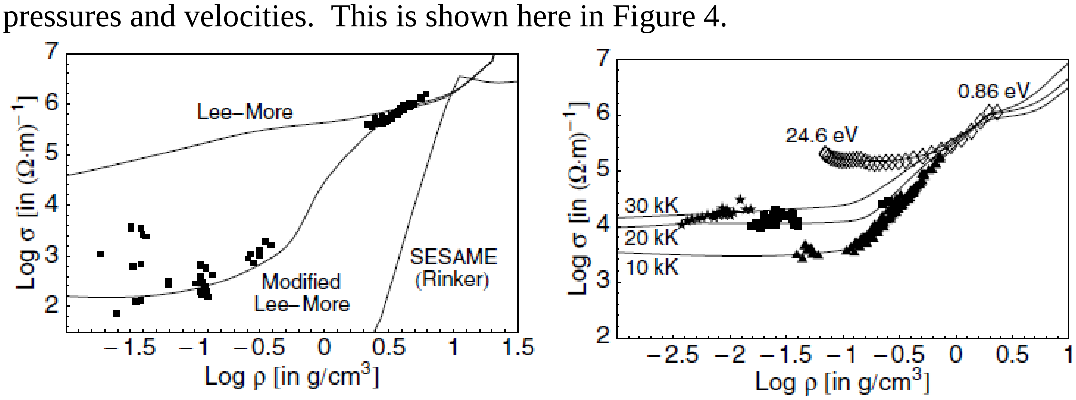

Figure 4: LMD model for aluminum electrical conductivity ("modified Lee-More"), compared to experimental data and to alternative models, showing that LMD dramatically increases model realism at high temperature and low density. Plots are taken Desjarlais (2001) [113]. Left: copper at 6000 K; right: aluminum.

This capability is also crucial for MTF modeling, as the liner is initialized in the solid state, and must maintain self-consistent electrical conductivity as it varies in phase due to heating via enormous currents. This makes ALEGRA, coupled to the LMD conductivity model, ideal for modeling of these systems.

As for hot, ionized plasmas, such as the plasma in a field-reversed configuration device, or internal to the liner in an MTF device, ALEGRA incorporates numerous models for ionization, opacity, and thermal conductivity. These have been used successfully in modeling Z-pinch wire array implosions, gas-puff experiments, exploding wires, and other scenarios involving hot ionized plasmas.

4.3.2 Material response across transitions between solid, liquid, gas, and plasma phases

In addition to handling the electrical conductivity accurately, numerical modeling for MTF devices must appropriately handle the constitutive response for materials whose phase must traverse from the solid state to vaporized metal and ionized plasma. This must be represented in a way that is both robust and accurate. Further, the modeling must be able to handle the presence of materials at different phases in the same element. This situation is the scenario for which ALEGRA was designed. The code incorporates constitutive models that have been built over decades of materials research, including the Sesame equation of state models, the Johnson-Cook, Steinberg-Guinan, and other strength models, and advanced fracture models. These empirical and semi-empirical models span the necessary ranges of temperatures and densities needed for modeling MTF devices, and account for phase changes correctly. Further, ALEGRA includes specialized controls that allow the modeler to ensure that the simulation will respond correctly in situations where a material melts but subsequently resolidifies, or where errors in the tabular model data lead to unrealistic states. The combination of a broad selection of material response models available in the code, with the appropriate tools and controls for constraining the models correctly, will enable modeling for MTF devices where liners will melt and vaporize to proceed with good accuracy and robustness.

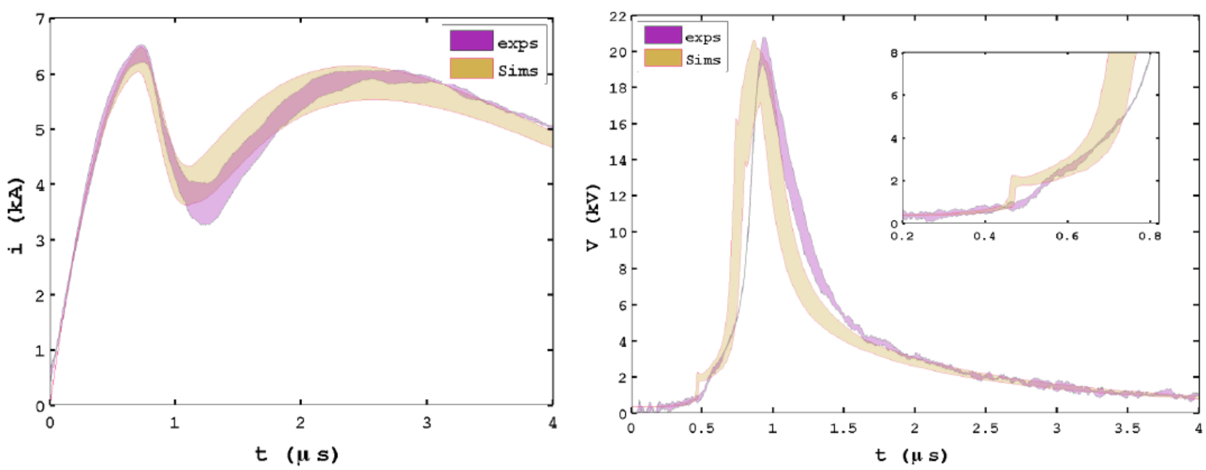

Figure 5: Comparison of experimental results and ALEGRA simulations for exploding aluminum wires, from Doney *et al.* (2010) [112]. Uncertainty ranges are included. Left: current history; right: voltage history.

The remarkable validation results obtained recently for exploding aluminum wires demonstrate that the combination of electrical conductivity models with material constitutive response models for aluminum, when used in MHD modeling using ALEGRA, yield results that reproduce laboratory observations [112]. Sample results from this study are shown in Figure 5. Aluminum material models in these simulations successfully modeled the full transition from solid-state metal at room temperature to melted, and then vaporized material. The thermodynamic state of the material and its conductivity were captured with sufficient accuracy to reproduce the observed timing of the wire explosion (indicated by the voltage collapse shown in Figure 5), as well as its electrical behavior, so that the correct voltage and current traces were obtained.

4.3.3 Nonlinear magnetic diffusion at plasma-wall interface

A third component that is anticipated to be important for modeling MTF devices correctly is that the simulation must accurately capture magnetic diffusion with nonlinear effects included. At the interface between a collapsing liner and the interior plasma in an MTF device, the simultaneous heating of the liner and diffusion of magnetic field into the liner must be resolved in space and time, with the dependence of the electrical conductivity on the thermodynamic state of the liner fully coupled. As described above, this capability is central to the MHD formulation used in ALEGRA. The MHD solution in ALEGRA is advanced on each timestep using an ideal-MHD step followed by a linear-solve operation for the diffusion of magnetic fields. The instantaneous conductivity of the materials in which the fields are diffusing is updated in time along with the other aspects of the material state such as its stress, temperature, and yield strength. This allows for nonlinear magnetic diffusion problems, even at extreme material states (*e.g.,* high temperature and/or low density), to be solved with good physical realism, so long as reliable material response data are available for the materials of interest.

4.3.4 Complex magnetic fields: initialization and boundary conditions

For simulations of MTF devices, it is also important for a modeling tool to be able to operate in axisymmetric (*r-z*) geometry, and to apply initial and boundary conditions that accurately constrain the complex magnetic fields used in these devices. ALEGRA has been used extensively in axisymmetric geometries, including for exploding wires and Z-pinch wire array implosions. This capability is not available in all MHD modeling tools that might be considered for this work. Further, as mentioned above, ALEGRA includes unstructured mesh capabilities, which allows for 2D and 3D cylindrical and circular discretizations that can still be used in the context of calculations in a Cartesian coordinate system.

ALEGRA has numerous options available for initializing magnetic fields, and all of these options enforce the divergence-free constraint by defining the field as the curl of a vector potential. An arbitrary field can also be initialized, but it must be described by the user in terms of a vector potential. This will likely be important and potentially problematic for initializing a field-reversed configuration. Boundary conditions are implemented such that the user may constrain the tangential component of the electric or magnetic field on any boundary. Here again, a user-defined field can be used, and will likely be needed for MTF modeling.

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