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PHYSICS APPLICATIONS IN THE ALEGRA FRAMEWORK

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Abstract

ALEGRA is a framework providing essential services for the development of discrete finite element approximations of continuum partial differential equation models of physical science. Built upon a core of solid dynamics modeling capability, with Arbitrary Lagrangian Eulerian features, ALEGRA has evolved into a vehicle to implement advanced physics modeling capabilities in a modular, object-oriented manner. These capabilities are discussed and several examples of the application of ALEGRA to physics modeling problems are presented.

Keywords: finite element; ALE; MHD; Solid Dynamics; ElectroQuasiStatics

1. Introduction

Finite element modeling of coupled physical phenomena is of great importance for understanding applications critical to the mission of Sandia National Laboratories. ALEGRA is a framework providing essential services for the development of discrete finite element approximations of continuum partial differential equation models of physical science.

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

ALEGRA was originally developed as a continuum mechanics code for modeling strong shock physics and large deformations. ALEGRA uses a Multi-Material Arbitrary Lagrangian Eulerian (MMALE) methodology for simulating these problems. This role has expanded to the current state in which a variety of finite element technologies for the spatial discretization and explicit and implicit time integration schemes are employed depending on the application. While ALEGRA partially supports several different element types, most applications employ 2D quadrilaterals or 3D hexes.

2. MMALE and Solid Dynamics

The MMALE approach allows multiple materials to be present in a single element and therefore affords additional flexibility over the traditional single material ALE method. ALEGRA supports Lagrangian, Eulerian and smoothing mesh motion within a single framework. Mesh smoothing can approach an Eulerian formulation but has the advantage of being performed less frequently. In cases of coupling a Lagrangian mesh to an Eulerian grid, smoothing of the Eulerian mesh is allowed to match the motion of the Lagrangian boundary. The mesh smoothing, or remesh, of nodes is activated by criteria related to mesh uniformity and the values of several field variables on the mesh. While several smoothing algorithms are available, the Tipton scheme [1] is most often employed. With this method, placement of the mesh nodes can be controlled with several weighting schemes based on element volume and the values of several field variables. After the remesh step, a remapping of variables to the new mesh locations is performed. Second order accurate interface reconstruction and advection methods are employed for accurate remapping.

ALEGRA has been applied to problems of deep penetration of rods into armor, using an Eulerian mesh, and the penetration of a projectile through a finite width plate, using reverse ballistics and a combination of smoothed Eulerian and Lagrangian regions. Additionally, ALEGRA has simulated shaped charges, explosively formed projectiles, underwater explosions, blast overloading of buildings and other facilities, and the propagation of a blast wave in air. In several of these categories, comparisons of experimental results with simulations have been made.

3. Advanced Physics Capabilities

The basic hydrodynamic and solid dynamics capability of ALEGRA has been leveraged in recent years to develop a framework for modeling coupled physics applications.

3.1. ElectroMechanical Physics

For coupled electromechanical applications, two approximate reduced forms of Maxwell's equations in moving media are of primary interest. The first form is the quasistatic magnetic field approximation corresponding to magnetohydrodynamic (MHD) modeling appropriate for simulating z-pinch implosions. The MHD approximation ignores displacement currents, assumes charge neutrality, and, for materials which obey an Ohm's law, a diffusion equation for the magnetic field results. The second form is the quasistatic electric field approximation (ElectroQuasiStatics or EQS) which ignores magnetic fields and can be applied, for example, in modeling poled ferroelectric power supplies.

3.1.1. Magnetics and Magnetohydrodynamics

For transient magnetics and magnetohydrodynamics in 2D, ALEGRA solves either for the normal field component B_z or B_θ in xy and rz geometry or for A_z, the normal vector potential component, if solving for field components in the xy plane. In 3D, a vector potential formulation is implemented. Isoparametric nodal finite elements are currently utilized while research focuses on edge and face element technology for representing electric field circulations on element edges and magnetic flux on faces in 3D. Example computations will be given in the presentation. A major challenge in this area is the implementation of accurate and effective advection algorithms for these new representations of the magnetic flux density in Eulerian and ALE simulations.

3.1.2 ElectroQuasiStatics Modeling

Another of ALEGRA's prime application areas is within the EQS electromechanical modeling framework. Required capability includes the ability to model shock propagation due to explosive detonation, depoling of ferroelectric ceramics, application of a parallel field solver for solving for the electric fields and coupling with an external lumped element circuit equation system. The EQS electric field approach utilizes a scalar potential for representing the electric field. Isoparametric nodal finite elements are utilized for the representation of the electric potential. This application is the most advanced in terms of coupling to the h-adaptive mesh refinement capability of ALEGRA. The presentation will show how the coupling works and how an element budgeting approach is used to avoid overflowing memory in parallel.

3.2 Transient ElectroMagnetics

In order to solve increasingly large and complex coupled-physics applications, full-wave, transient electromagnetics has been integrated into the ALEGRA framework. Here, all terms in Maxwell's equations are retained, making no approximations, and the full vector electric and magnetic fields in the solution volume are obtained, subject to the boundary conditions. One ultimate goal is to predict the induced current delivered to an internal system component due to microwave or ionizing radiation incident on the system exterior. Ionizing radiation drives system-generated electromagnetic pulse (SGEMP), which might represent the most significant source of electrical energy to sensitive internal electronics because outer layers of electromagnetic shielding are bypassed. For other applications, ALEGRA can predict antenna response as well as the behavior of microwave integrated circuits.

Both unconditionally stable Helmholtz [2] and conditionally stable curl-curl [3] formulations have been implemented, using both edge-based and face-based basis functions on tetrahedral elements. Thin-wire and thin-slot sub-cell algorithms have been implemented to avoid meshing fine details. For additional efficiency, a classical structured finite-difference time-domain (FDTD) algorithm is incorporated into the ALEGRA framework. The goal is to hybridize multiple regions of unstructured elements with one or more rectilinear FDTD regions. Geometry that involves billions of structured elements and millions of unstructured elements will be solvable using current massively parallel computing platforms. Eventually, particle-in-cell algorithms will be added for surface emission and other applications.

The benefits to the developer of using the ALEGRA framework for these new applications include the use of an established, rigorous configuration management system, access to mesh and variable database management, automated regression testing, and framework support for parallelization. Perhaps more important is the ability to couple self-consistently with other physical drivers, such as ionizing radiation for the SGEMP application and radiation diffusion and thermal conduction for Z pinch applications. Even though

ALEGRA was initially designed as a continuum mechanics code, integration of electromagnetics into the new Version 4 framework has been very straightforward.

4. Material Modeling

All of the physics applications supported in ALEGRA require material modeling to complete the particular equations. To allow for maximum flexibility and accommodation of the various physics algorithms, a material is defined in ALEGRA as a collection of material models that describe appropriate response for the physics being modeled. For example, in modeling poled ferroelectric ceramics, a sophisticated material model accounts for mechanical stress-strain response and also the response due to polarization and electrical permittivity. In other physics, several physical phenomena may be simulated, requiring several material models to completely evaluate all the variables of interest.

In such cases, a series of material models are specified for a particular material. For example, MHD with conduction and strength would require a series of models describing the equation of state, deviatoric response, yielding, plastic flow, and electrical and thermal conductivities. In this manner, complex material modeling requirements may be accommodated for all of the various physics methods and the coupled physics methods. Currently, the ALEGRA material model library contains models for equation of state (i.e., ideal gas, Mie-Gruneisen U_s-u_p, Mie-Gruneisen power law, tabular SESAME, JWL), mechanical stress-strain response (e.g., linear elastic, elastic plastic, Johnson-Cook, Steinberg-Guinan-Lund, Baummann, Zerilli-Armstrong), electrical conductivity (e.g., Modified Lee More, Spitzer, Knoepfel), thermal conductivity (Modified Lee More, Spitzer, polynomial), opacity (e.g., Kramer, Princeton XSN), electromechanical response (e.g., piezoelectric, etc.), and two temperature equations of state (tabular SESAME).

Additionally, a combined material model may comprise a set of individual material models and manage the interaction between these models. For example, one mechanical response model in ALEGRA has as submodels, an equation of state model, a yield stress model, and a plastic flow model. The model uses the submodels to compute the current mechanical state of the material. However, the specific equation of state and yield submodels are user selected from among a set of submodels available to this particular combined model.

5. Conclusions

ALEGRA is a modern object-oriented code framework in which many coupled or standalone physics modeling capabilities can reside. Current capability includes ALE solid dynamics, transient magnetics, magnetohydrodynamics, electro-quasi-static electromechanics, transient electromagnetics and thermal conduction. A broad set of material models for a wide variety of physics applications is available in the code. Such capabilities are available in isolation or as needed in concert, using the object-oriented method of multiple inheritance. Several application examples concerned with the advanced physics capabilities of ALEGRA are presented.

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