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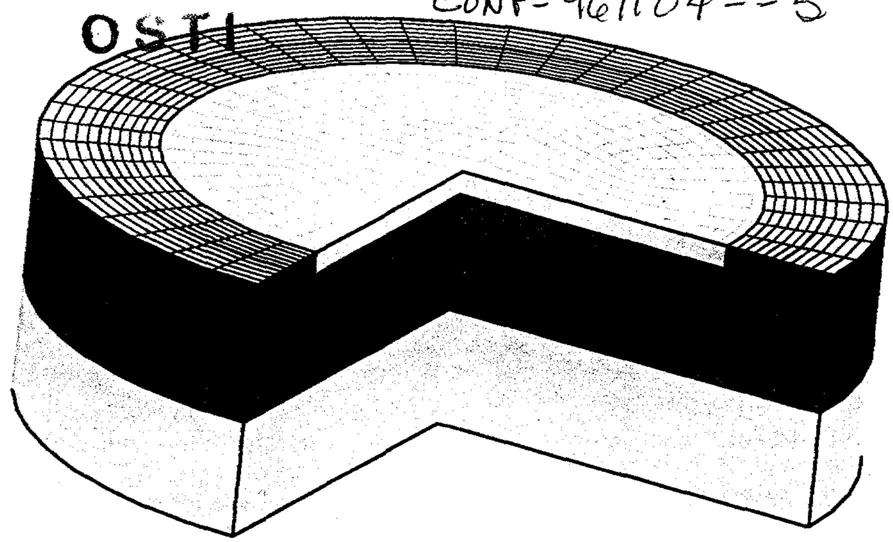
EMMA Electromechanical Modeling in ALEGRA



Electromechanical simulation technology is being developed at Sandia National Laboratories in order to model the function of devices designed using piezoelectric and ferrocerramic materials. The figure shows a cutaway view of a quartz gauge mesh.

Objective

EMMA (ElectroMechanical Modeling in Alegra) is a simulation capability being developed at Sandia National Laboratories for high-fidelity modeling of electromechanical devices. These devices can produce electrical current arising from material changes due to shock impact or explosive detonation.

Impact

EMMA can be used to help design important Department of Energy components and to investigate possible failure modes. To this end critical material model development is facilitated by using accurately resolved numerical simulations running on high performance parallel platforms.

To ensure high levels of deterrent capability in the 21st century, new stockpile stewardship principles are being embraced at Sandia National Laboratories. The Department of Energy ASCI (Accelerated Strategic Computing Initiative) program is providing the computational capacity and capability as well as funding the system and simulation software infrastructure necessary to provide accurate, precise and predictive modeling of important components and devices. An important class of components require modeling of piezoelectric and ferroceramic materials. The capability to run highly resolved simulations of these types of components on the ASCI parallel computers is being developed at Sandia in the EMMA (ElectroMechanical Modeling in Alegra) code. We wish to be able to routinely run coupled electromechanical shock-physics simulations containing on the order of 10 to 100 million elements which will allow us to better resolve shock waves and calculate system capacitances and currents accurately. With this capability material models will be precisely tuned to give accurate predictions for complex three-dimensional problems.

EMMA modeling combines several software technologies to provide the desired electromechanical simulations. The mechanics of shock propagation and material motion are solved using the ALEGRA framework developed at Sandia. The ALEGRA code is a C++ software infrastructure for parallel shock-physics calculations. The EMMA code uses class derivation and multiple inheritance to bring together solid dynamics and electric field modeling. The electric field is represented as the gradient of a potential, ϕ, which satisfies the elliptic equation:

$$\nabla \bullet (\varepsilon \bullet \nabla \phi) = \nabla \bullet P$$

where P is the polarization vector and ε is the dielectric tensor. The field equations are solved using a finite element technique and the AZTEC parallel linear equation solver capability developed at Sandia. A circuit equation capability connects the finite element electromechanics with an external circuit equation system. The DASPK differential-algebraic equation package developed at Lawrence Livermore National Laboratories is used to solve the circuit equation system. Development of properly characterized piezoelectric and ferroceramic material models will be an ongoing concern at Sandia. The EMMA capability brings together the required software technology for high fidelity parallel simulations of electromechanical devices on the ASCI parallel computers.

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