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Providing *Relevance* to an Engineering-Focused Organization: Detonator Computational Multiphysics

Sandia National Laboratories
Sharon V. Petney and Christopher J. Garasi
Sandia National Laboratories, New Mexico 87185

Problem

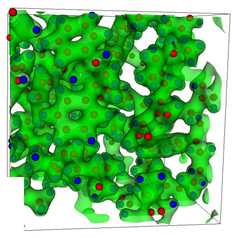
How do we deploy the wealth of R&D activities to teams trying to solve real engineering problems (e.g., evaluation of detonator designs)?

Results

Capabilities embedded in ALEGRA

BASIC RESEARCH — MISSION IMPACT

Quantum Molecular Dynamics (QMD, aka molecular dynamics with DFT forces, DFT-MD), as in the VASP code, solves a reformulation of Schrodinger's equation for the quantum state of a physical system.

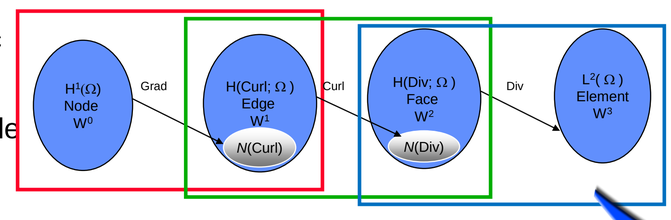


b-initio VASP ienna ackage imulation

Trilinos provides algorithms for solving large-scale, complex multi-physics engineering and scientific problems. **ML** is the preconditioner and solves large sparse linear systems of equations arising primarily from elliptic PDE discretizations.

Trilinos

The structure of the physics equations relates to geometric origins. The **deRham structure** allows compatible discretizations. This allows compatible formulations for magnetohydrodynamics, conduction.



Dakota provides an interface between analysis codes and iterative systems analysis methods. Dakota contains algorithms for advanced **optimization** methods; uncertainty quantification; parameter estimation; and sensitivity/variance analysis.

DAKOTA

An Unstructured Triangular equation of state **(UTri)** incorporates uncertainty into the equation of state as a KL expansion; the coefficients are in the table, the user can choose degree of uncertainty for a simulation.

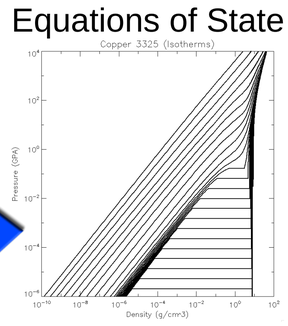
$$\mathbb{T} = \bar{\mathbb{T}} + \sum_k \xi_k \mathbb{T}_k$$

Bayes' rule:

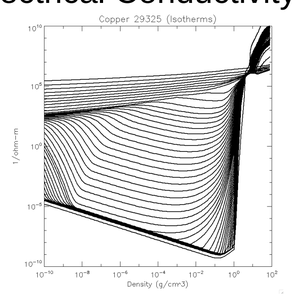
$$p(\lambda|D) = \frac{p(D|\lambda)p(\lambda)}{p(D)}$$

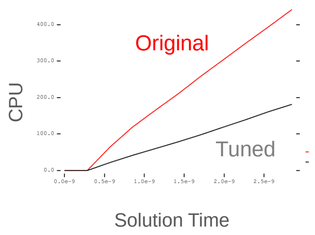
posterior — likelihood — prior — normalization

Advanced Equations of State



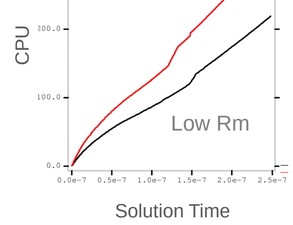
Advanced Electrical Conductivity



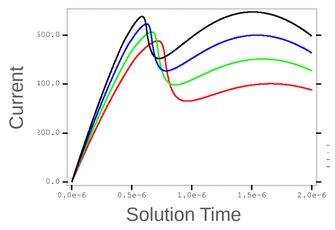


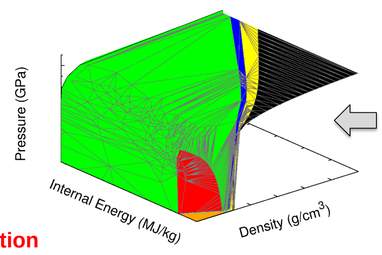
Tuned Maxwell solver; ice sheet technology for thin structures; anisotropic meshes w/large material jumps -> improvements to iterations and CPU time

MHD capability essential for modeling detonators. A special formulation for electric potential-based Joule heating allows more efficient 3D detonator design simulations (low Rm).



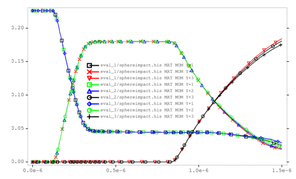
Dakota is embedded in ALEGRA, becoming the normal mode of operation. Showing current traces for various initial voltages in an exploding wire.



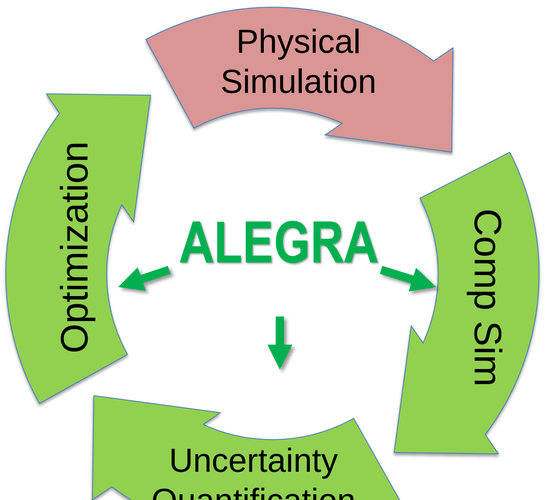


UTri builds EOS UQ into the table, double valued at phase boundaries.

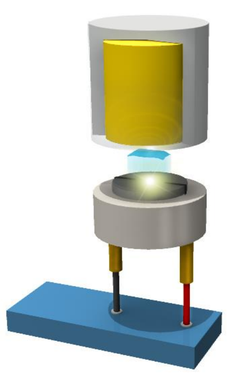
Can gain perspective from alternate sample points.

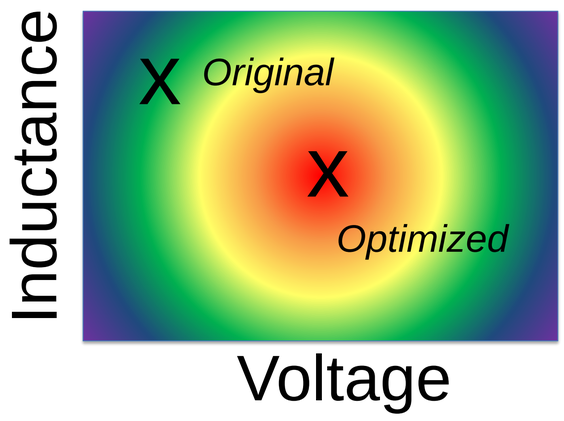


Approach



Significance





Design optimization gives insight to experimental effort to focus resources, saving time and money.

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