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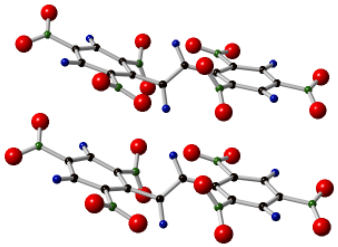

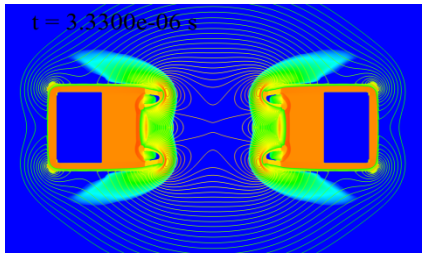

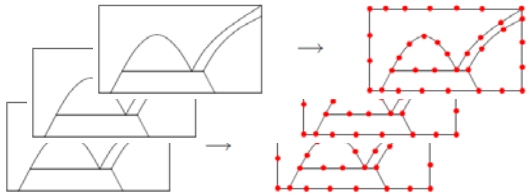

Foundations for Predictive Engineering Design in Extreme Environments in the 21st Century

Allen C. Robinson

Army Science Planning and Strategy Meeting on Materials in Extreme Environments

December 10-11, 2013, Towson, MD

SAND 2013-10341P

U.S. DEPARTMENT OF ENERGY NNSA

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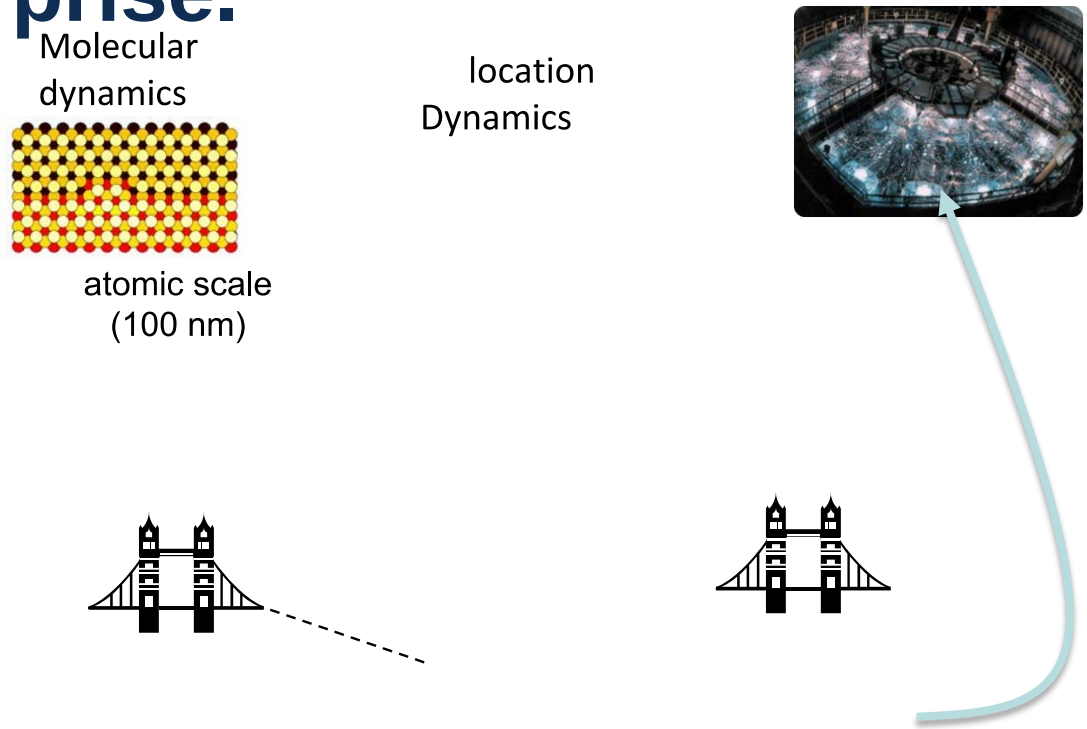
My shock multi-physics modeling viewpoint

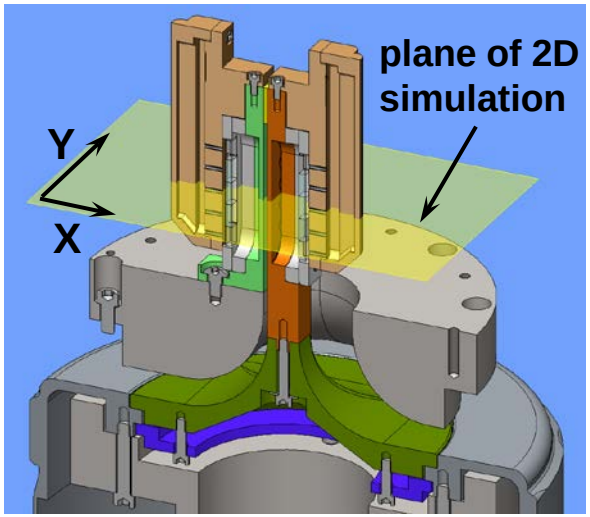
- My background (30 years at Sandia) includes hydrocode (e.g. CTH, ALEGRA) based development and modeling of material effects at extreme pressure including in the presence of high magnetic fields (ALEGRA-MHD) and also the development of ALEGRA-EMMA for modeling ferroelectrics and piezoelectrics.
- My colleagues at Sandia include experts in components engineering, quantum mechanical modeling of materials, molecular dynamics, shock and transient dynamics modeling and experimentation (including Z).
- Sandia has a long history of interaction and collaborative work with ARL.
- ARL is tasked with staying ahead of the game in an extremely complex and increasingly difficult target/threat environment.
- I will discuss what I have learned and where we need to go.

Science based engineering is the only possible way to compete in the future. It is a multi-disciplinary, multi-scale, multi-physics enterprise.

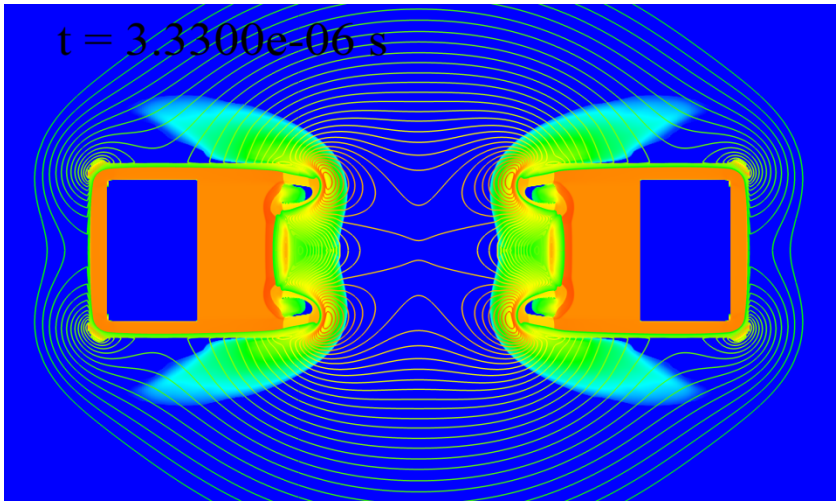


EXAMPLE: ALEGRA-MHD magnetohydrodynamic modeling provides for predictive design of flyer plate experiments

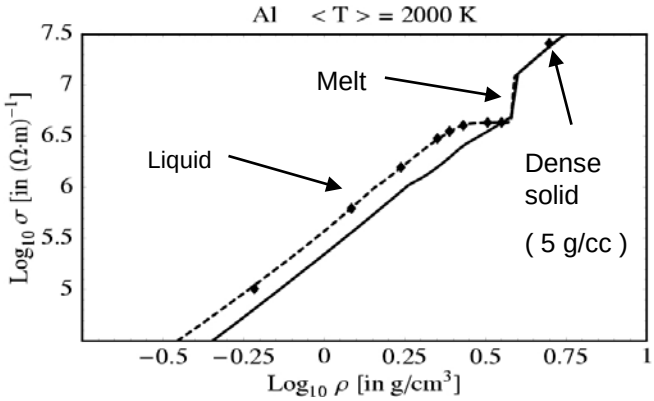
Two-sided Strip-line Flyer Plate Experiment



2D Simulation Plane of Two-sided Strip-line

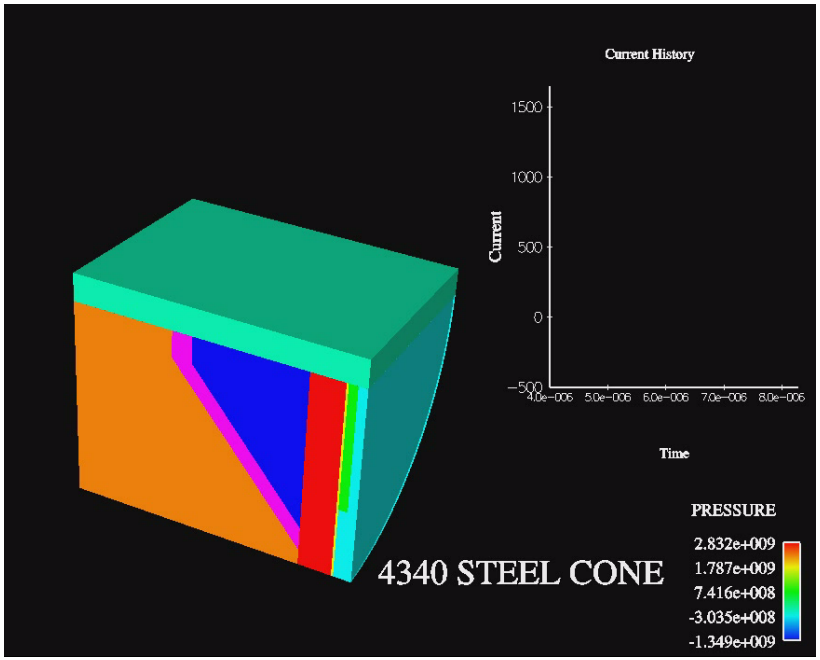


- Resistive MHD
- Accurate electrical conductivities (Desjarlais QMD/LMD).
- Sesame EOS for materials.
- Circuit model for self-consistent coupling.
- Dakota optimization loops



EXAMPLE: ALEGRA-EMMA Electromechanical analysis provides for Fuze/ Power Supply Modeling

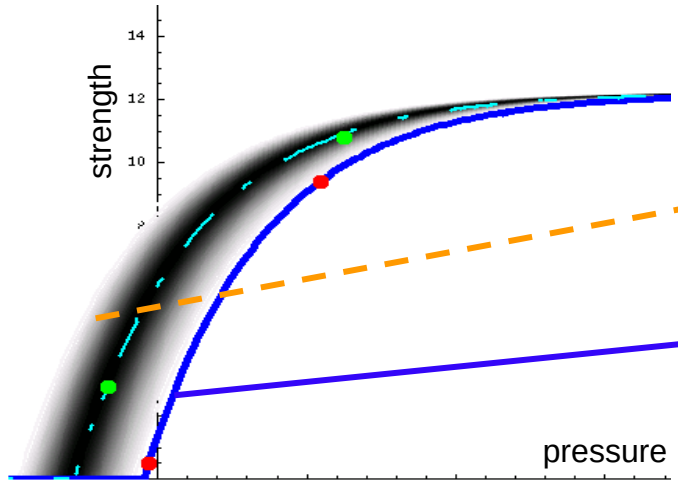
- Coupled mechanical/electric field based modeling
- Circuit coupling essential
- Advanced hydrodynamic ALE techniques are important.
- Excellent coordination between experimental data acquisition and material modeling expertise is required.

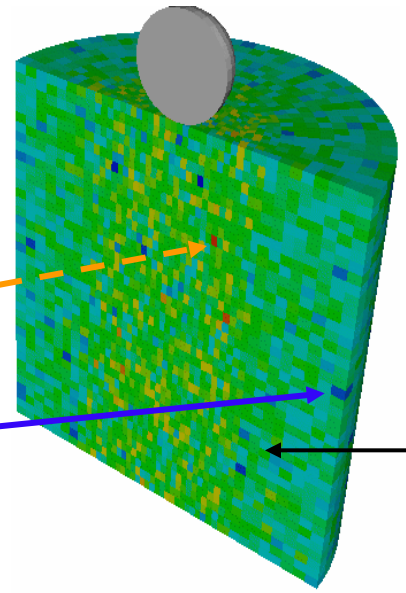


Movie shows an example simulation of a shock actuated power supply.

EXAMPLE:
Material Heterogeneity is Integral to Dynamic Failure

Spatially Variable Strength Profile for Ceramics

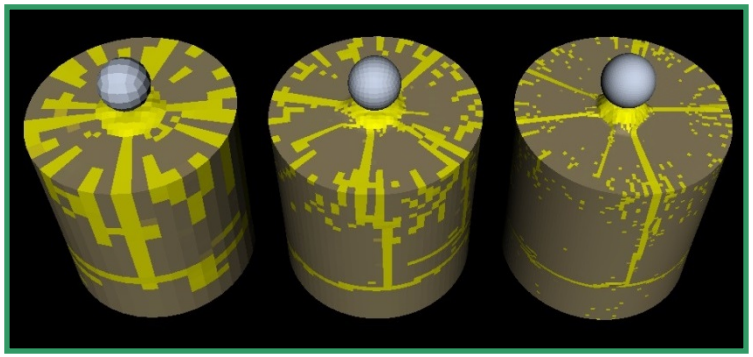




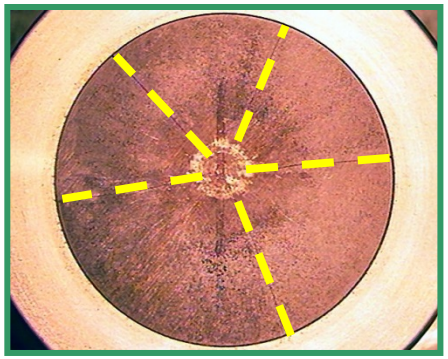
Initial state: small elements are stronger on average, but also more variable

Weibull distribution of strength*:

$$\sigma = \bar{\sigma}\left[\frac{\bar{V}\ln R}{V\ln(1/2)}\right]^{1/m}$$



Reduced Mesh Dependence: Same Model with Uncertainty, Size, and Rate Effects



Comparison to Experiment

Similar crack morphology for different mesh sizes

Formal validation and uncertainty quantification will help identify remaining issues

*Brannon, RM, Wells, JM, and Strack, OE 'Validating Theories for Brittle Damage', Metallurgical and Materials Transactions A, 38A, p. 2861-8, 2007

Continuum balance laws allow for engineering modeling (e.g. Resistive MHD Equations)

$$\dot{\rho} + \rho \nabla \cdot \mathbf{v} = 0$$

$$\rho \dot{\mathbf{v}} = \nabla \cdot \left(\mathbf{T} + \mathbf{T}^M \right) + \mathbf{f}$$

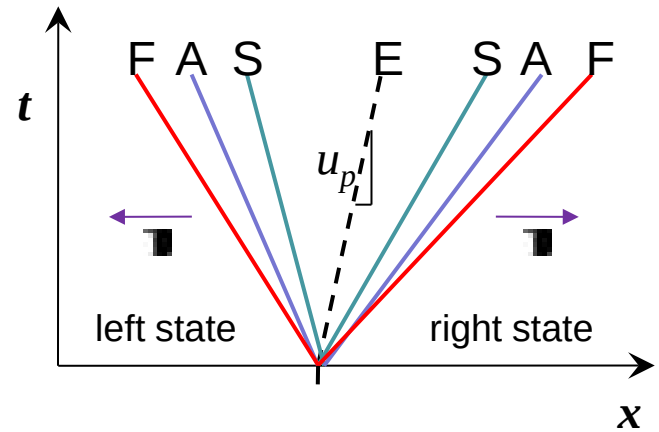
$$\rho \dot{e} = \rho s + \mathbf{T} : \mathbf{L} - \nabla \cdot \mathbf{q} + \frac{1}{\sigma} \mathbf{J} \cdot \mathbf{J}$$

$$\overset{*}{\mathbf{B}} = \frac{\partial \mathbf{B}}{\partial t} + \nabla \times (\mathbf{B} \times \mathbf{v}) + \mathbf{v}(\nabla \cdot \mathbf{B}) = -\nabla \times \frac{1}{\mu_0 \sigma} (\nabla \times \mathbf{B})$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \times \frac{\mathbf{B}}{\mu_0} = \mathbf{J}$$

$$\mathbf{T}^M = \frac{1}{\mu_0} \left(\mathbf{B}\mathbf{B}^T - \frac{1}{2} \mathbf{B}^2 \mathbf{I} \right)$$



Ideal MHD version of these equations are mathematically complicated

Closure relations for the stress, $\mathbf{T} = -p(\rho, e)I$, electrical conductivity, $\sigma(\rho, \theta)$, and heat flux, $q = -k(\rho, \theta)\nabla\theta$, are required to solve the equations.

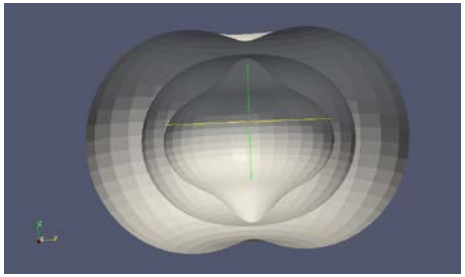
These relations are what makes the equations useful.

Example: ALEGRA-EMMA
Continuum Balance laws for Electromechanics

$$\dot{\rho} + \rho \nabla \cdot \mathbf{v} = \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

$$\rho \dot{\mathbf{v}} = \nabla \cdot \mathbf{T} + \mathbf{f}$$

$$\rho \dot{e} = \rho s + \mathbf{T} : \mathbf{L} - \nabla \cdot \mathbf{q}$$



One would like to have extreme confidence that in any 3D configuration and high pressure loading configuration that device characteristics are known and predictable

$$\nabla \cdot \mathbf{D} = 0 \qquad \nabla \times \mathbf{E} = 0 \Rightarrow \mathbf{E} = -\nabla \phi$$

$$\nabla \cdot \mathbf{D} = 0 \Rightarrow \nabla \cdot (\epsilon \nabla \phi) = \nabla \cdot \mathbf{p} \qquad \mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P} = \epsilon \mathbf{E} + \mathbf{p}$$

$$\begin{aligned} \mathbf{T} &= \mathbf{T}(\mathbf{S}, \mathbf{E}) \\ \mathbf{D} &= \mathbf{p}(\mathbf{S}) + \epsilon(\mathbf{S})\mathbf{E} \end{aligned}$$

material polarization

permittivity

remnant, permanent or spontaneous polarization

Smart applied mathematics is still needed.

$$
\begin{aligned}
\dot{\rho} + \rho \nabla \cdot \mathbf{v} &= 0 \\
\rho \dot{\mathbf{v}} &= \nabla \cdot (-p\mathbf{I} + \mathbf{T}^M) \\
\rho \theta \dot{S} &= \mathbf{J}^2/\sigma \\
\sigma \left(-\frac{\partial \mathbf{A}}{\partial t} + \mathbf{v} \times (\nabla \times \mathbf{A}) - \nabla \phi \right) &= \nabla \times \left(\frac{\nabla \times \mathbf{A}}{\mu} \right)
\end{aligned}
$$

Not very practical for some 3D applications

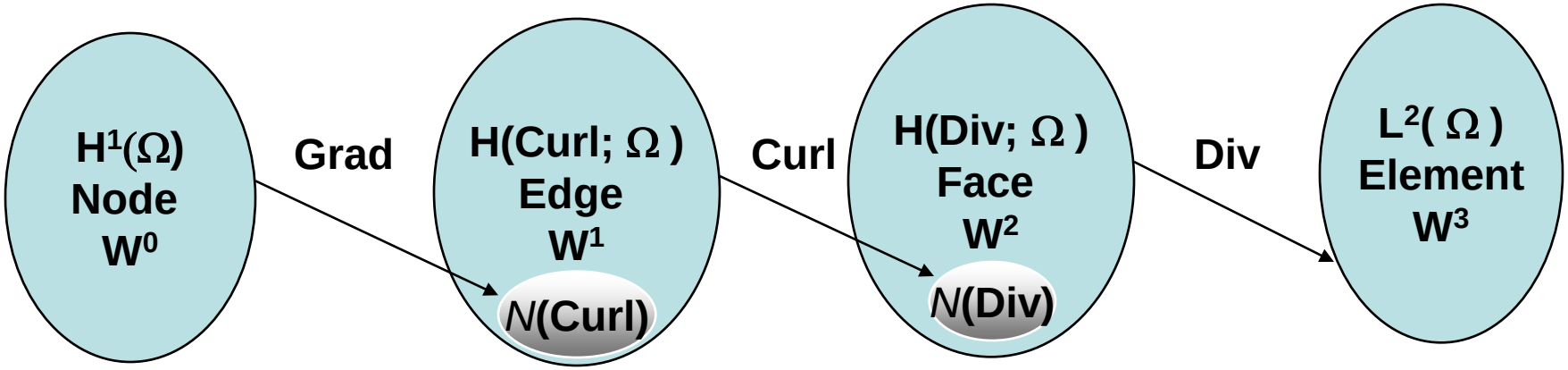
$$R_m = \frac{\mu \sigma L^2}{\tau}$$

$$R_m \ll 1$$

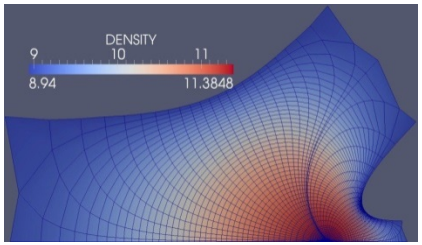
$$
\begin{aligned}
\dot{\rho} + \rho \nabla \cdot \mathbf{v} &= 0 \\
\rho \dot{\mathbf{v}} &= -\nabla p \\
\rho \theta \dot{S} &= \mathbf{J}^2/\sigma \\
\nabla \cdot \sigma \nabla \phi &= 0
\end{aligned}
$$

Practical in 3D in certain cases

Numerical methods are still advancing and the mathematics behind them is important



- Mimetic discretizations (e.g. deRham complex) are important. Implicit solvers need to understand these operators
- Hydrodynamic methods are still being improved!
- Robustness is critical.
- Detailed verification studies always pay off.



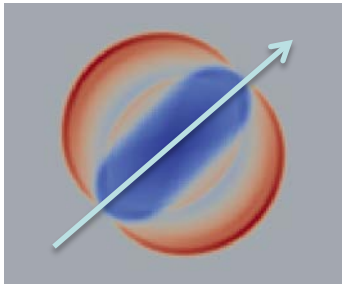
Scalable Computing Is Essential (Algorithms and Hardware)

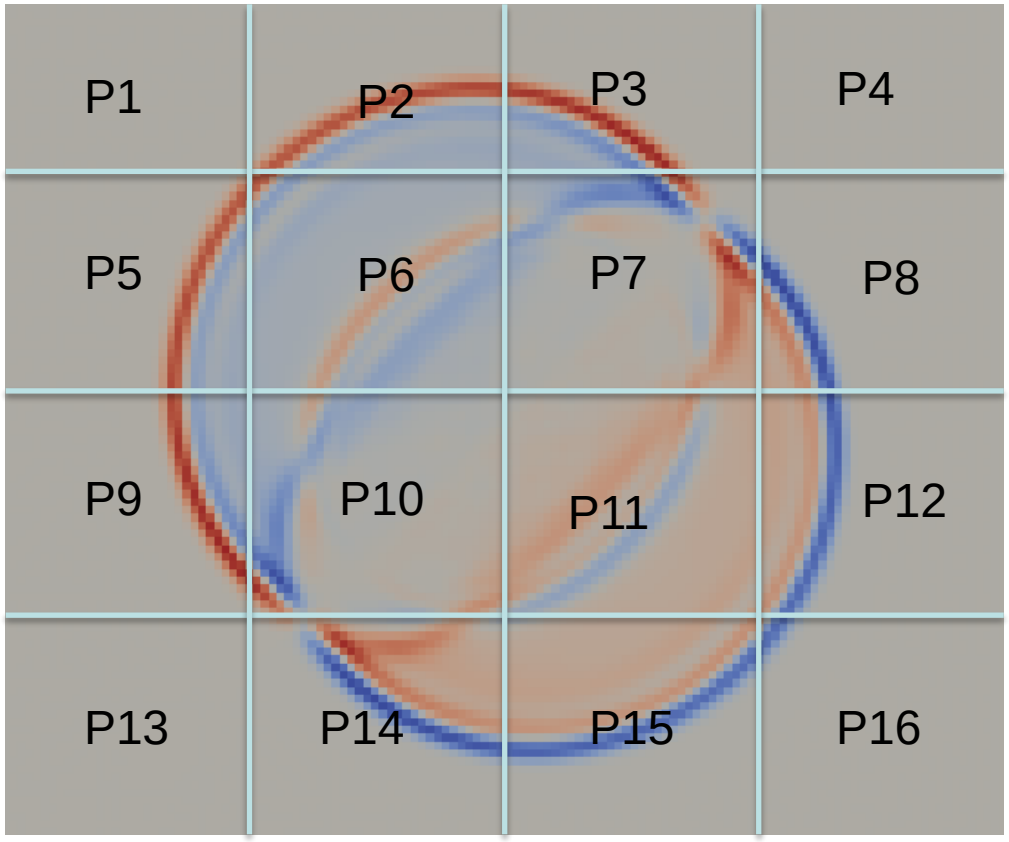
O(N) <u>scalable</u> algorithms are required

Parallel computing has and will undergo profound shifts.

Quality software engineering with embedded flexibility is not an optional requirement to deal with the future.

Large teams working together effectively is required.





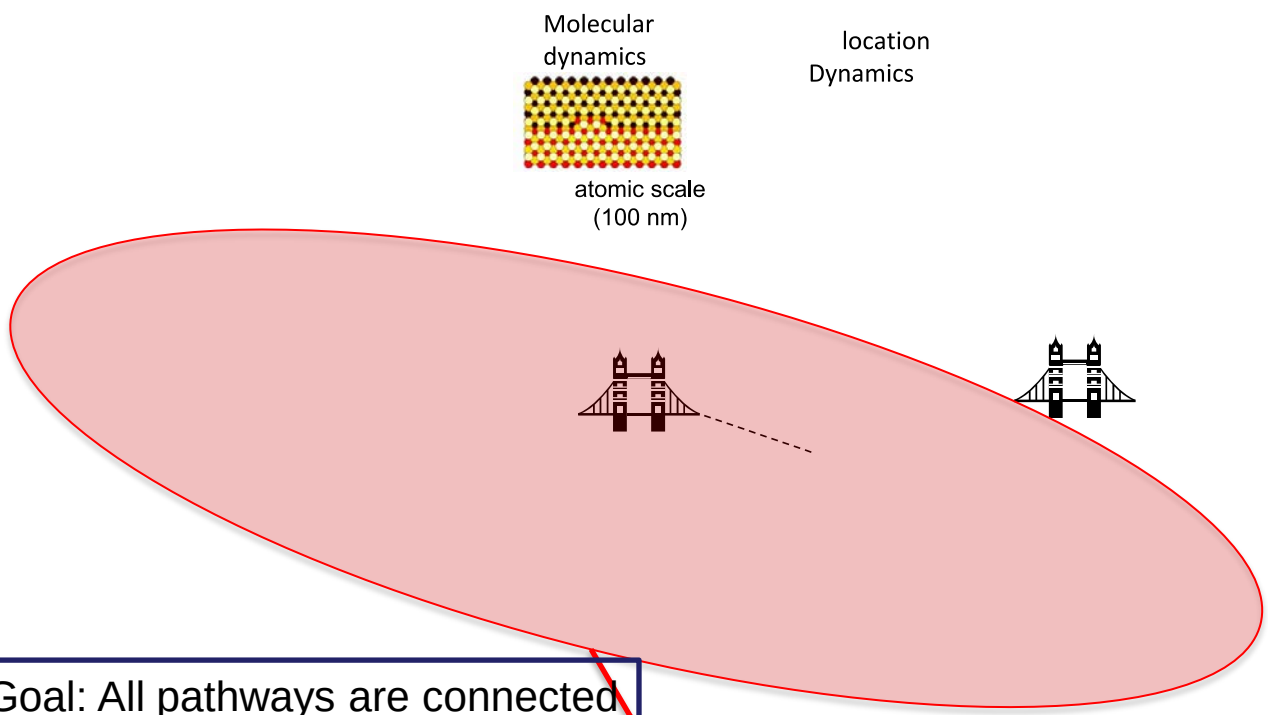
Meta-Computing is the Future: Uncertainty Quantification, Optimization and Inverse Problems

- Given a set of modeling equations with initial conditions, boundary conditions and closures, we can solve them on a computer and get an answer. (Forward problem)
- Actually… the modeling equations, initial and boundary conditions and are uncertain on both an epistemic (reducible) and aleatory (irreducible) level. (Uncertainty Quantification (UQ))
- Engineers want to optimize configurations and easily compute optimized design or inverse problems while taking into account uncertainty.
- What does this future look like?

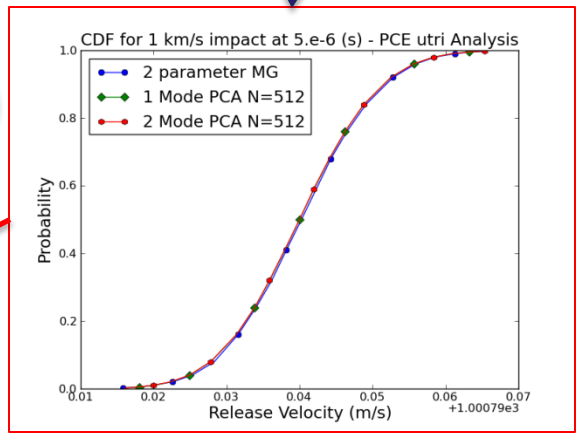
The Big Picture Strategy

- 0-20 Year Solution: (SAMPLING BASED ANALYSIS)
  - Sample Based Uncertainty Quantification (UQ) and Optimization using forward tools as a black box. (DAKOTA)
  - Can use current technology and evolve it.
  - Poor scaling with parametric dimension.
- 5-30+ year solution; (ADJOINT BASED ANALYSIS)
  - Numerical tools which naturally compute derivatives with respect to parametric choices.
  - Much less certain how much current technology can be evolved forward.
  - Excellent scaling with parametric dimension.
- All solutions must be obtained with an increasingly integrated multi-scale physics modeling stack.

Building UQ Enabled Bridges between Fundamental Laws of Nature and Engineering



Goal: The analyst running the continuum code should easily get results that can be transformed into the equivalent of “50% chance of rain” to give to the decision maker.



Goal: All pathways are connected in a unified engineering process and iteratively improved. Upscaling bridges must be built with embedded UQ information.

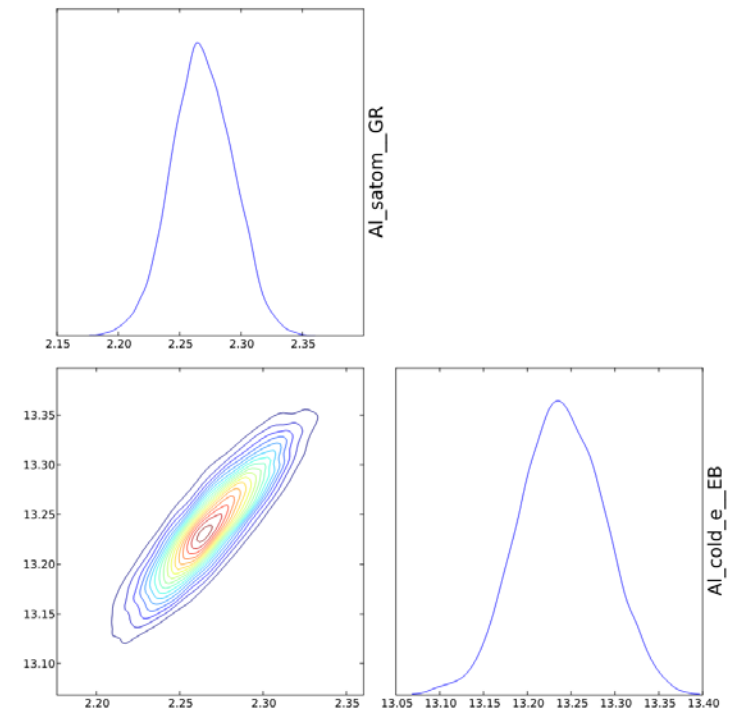
Example: Propagate uncertainty due to statistically equivalent possible EOS fits to the same data, to the analyst.

Al EOS model calibration and inference

Bayes' rule

posterior likelihood prior normalization

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



18 parameter Al model EOS inference

A marginal distribution

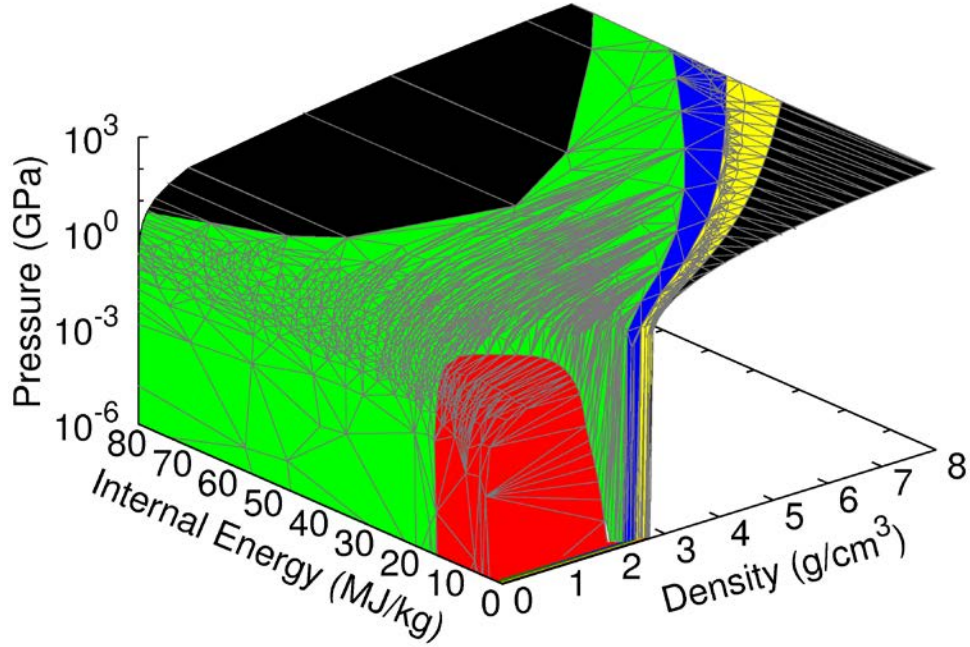
Bayesian inference to determine posterior distribution function of parameters is costly:

- Use adaptive Markov Chain Monte Carlo (MCMC) scheme to reduce number of steps
- Use optimization to find Maximum A Posteriori (MAP) parameters from which to start chain
- Each posterior evaluation is roughly equivalent to generating an entire EOS table
  - Between 2-10 seconds for the aluminum model on a single cluster processor
  - MCMC is a serial process, but prior and likelihood evaluation can be parallelized to some degree
  - Al model includes stability and smoothness conditions across the range of interest in the prior, as well as 16 sets of data in the likelihood

Tabular EOS generation and UQ representation

Simultaneously tabulate N parameterizations of an EOS model (N=808 for the Al model):

- New UTri format uses linear interpolation on triangles to capture salient features
- Each tabulation is topologically equivalent (smooth mapping of nodes)
- Optimized node placement is costly but can reduce table size
- PCA mean pressure table at 0.1 tolerance shown with overlaid triangulation (phases: off table, solid, fluid, melt, vaporization)



Principal Component Analysis (PCA) used to look for a tabular representation with reduced dimensionality:

- N tables from previous meshing step are starting point
- Export a truncated set of mode tables that capture most of the details (i.e. eigenspectrum energy)
- Multi-precision floating point necessary due to dynamic range of multi-phase tables
- Aluminum model had a single significant mode
- Random variables ξ are uncorrelated, with zero mean and unit standard deviation, but not necessarily independent

$$\bar{z} = ZH\mathbf{1}/\mathbf{1}^T H\mathbf{1}$$

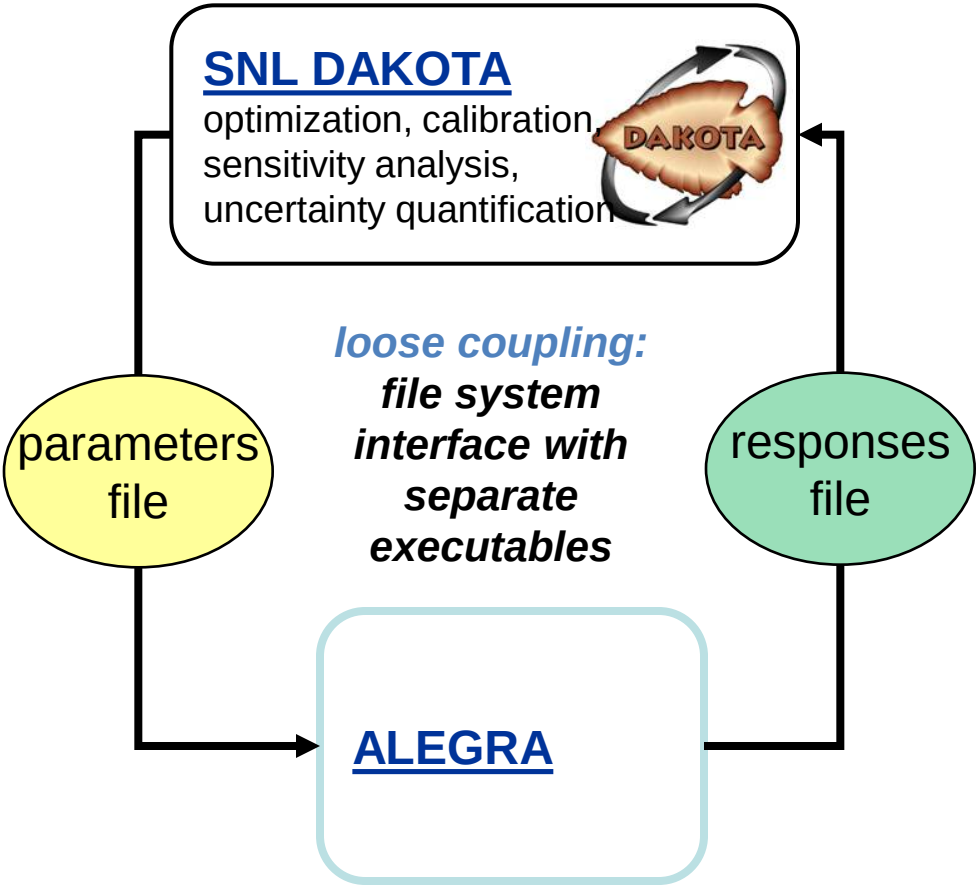
$$(Z - \bar{z}\mathbf{1}^T)H^{1/2} = \tilde{U}\Sigma\tilde{V}^T$$

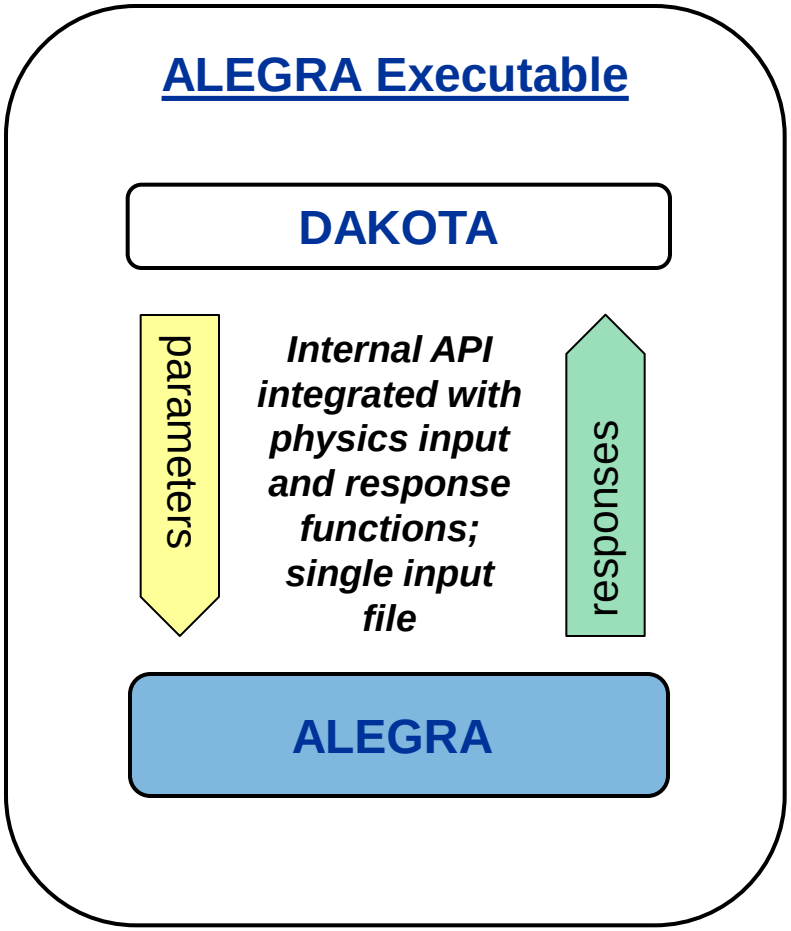
$$z = \bar{z} + U\Sigma\xi = \bar{z} + \tilde{U}\Sigma\xi$$

$$= \bar{z} + (Z - \bar{z}\mathbf{1}^T)H^{1/2}\tilde{V}\xi$$

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

Reduction of practical barriers to sampling based meta-analysis is critical for predictive engineering.

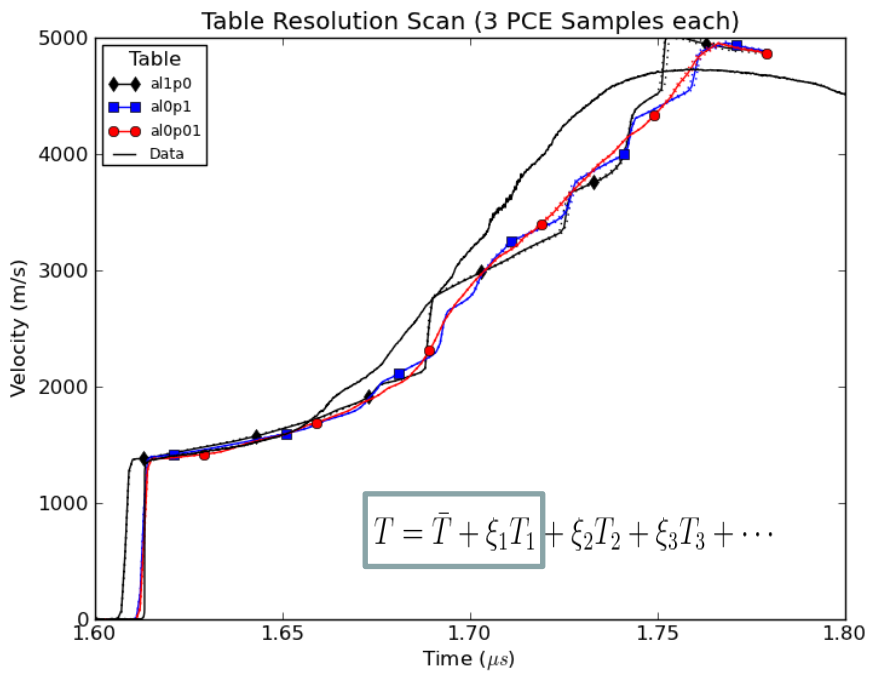




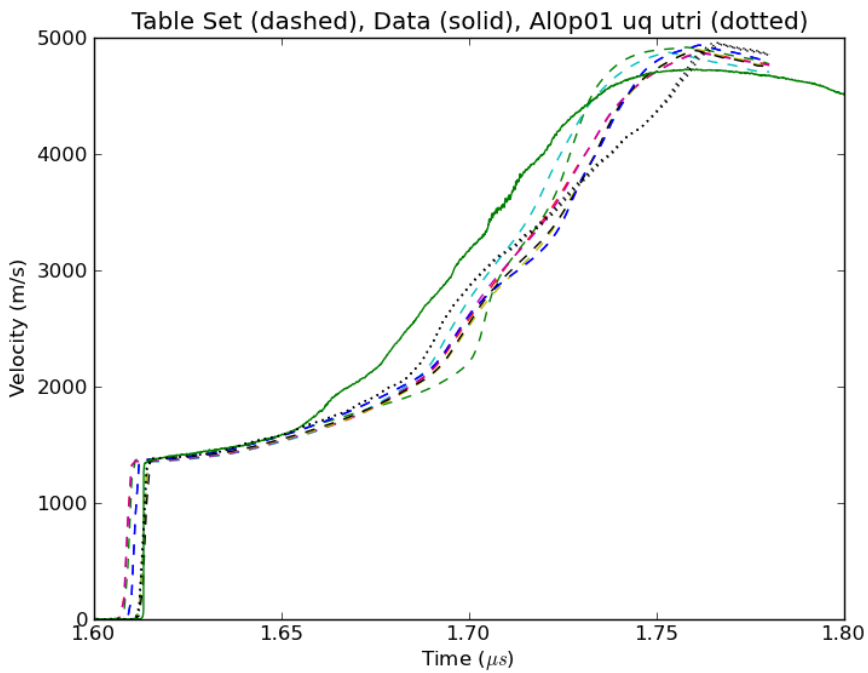
Current → **Moving from potentially fragile, study-specific script interfaces to a unified, user-friendly capability** → *Future*

Example: Al Shock Ramp Experiment

UQ enabled (UTri) AL EOS tables



SESAME EOS tables



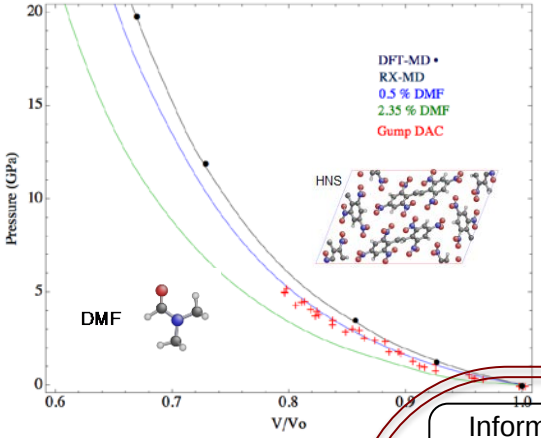
Can one surmise why the SESAME and UTri models differ?

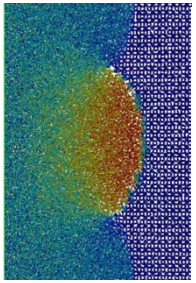
- Structure in the curves is of the same order as seen in low resolution UQ tables.
- Failure to reproduce the shock timing also was seen in low resolution UQ tables.
- UTri tables use linear C0 interpolation leading to sharp corners in the structure of the 1.0 tolerance curve, whereas the SESAME tables use a smoother quasi-C1 interpolation
- One cannot determine if differences between SESAME tables are due to their models or their tabulation. (Often exacerbated by the inability to reproduce the original model.)
- Understanding model inadequacy in a quantitative way is an important next step.

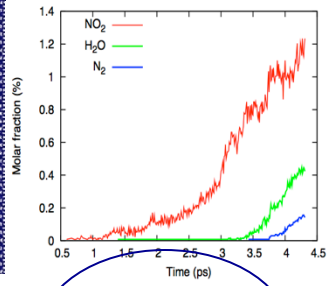
What are the requirements for upscaled material modeling with embedded uncertainty? (Carpenter/Mattsson/Magyar)

- In extreme environments, experimental data is increasingly difficult to obtain for fitting model parameters. We need to develop our ability to calculate and thus bridge model data in a much more automated and connected way.
- We MUST invest in building and reinforcing the multiscale bridges as engineering tools.
  - Improved DFT functional formulations including account history effects (TDDFT).
  - Fully coupled modeling of thermodynamic and transport properties (e.g. EOS+conductivity)
  - (Re-)Coupling of constitutive models with the EOS. This can have several directions, including properly handling metastable states such as tension, understanding the kinetics of phase transitions (melt and polymorphic), and improved modeling of porosity.
    - Rethink/improve the form and thermodynamic foundation of our models? (e.g. Peshkov research)
  - Properly producing EOSs for multi-component systems (i.e. alloys)
  - A predictive reactive burn model (See next slide)
- UQ as an integral part of all the above activities. At a minimum, this means extending beyond the parametric tabular EOS form described to include model uncertainty as well as constitutive model parameters.
- Design Goal:: "Material models always come with error bars"

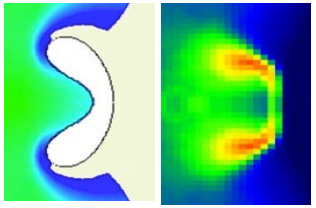
The multi-scale quest is close to being bridged at some level for energetic materials (Thompson).

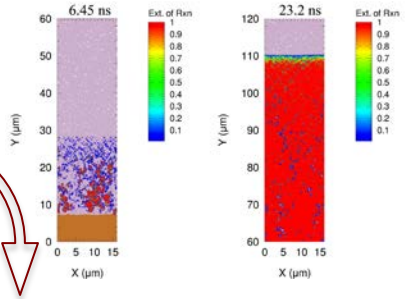






Hydrocode RMD





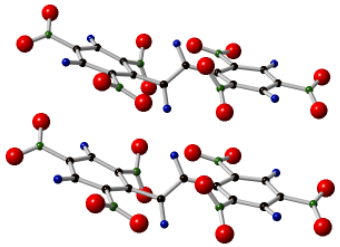
Inform/Calibrate via e.g. E.O.S. calculations

Reactive Molecular Dynamics

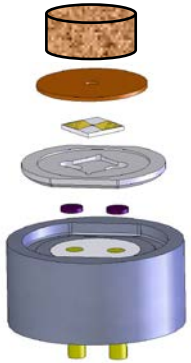
Inform/Calibrate via direct comparison

Quantum Mechanical Methods

Continuum Hydro-dynamics

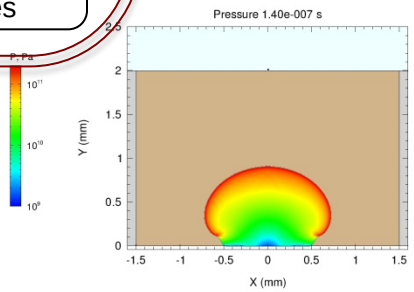


HNS



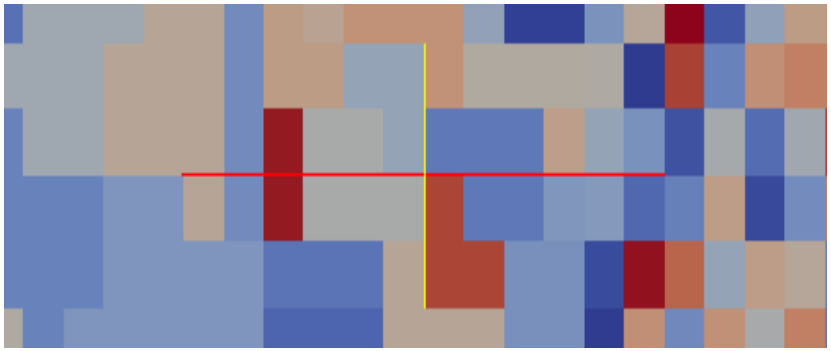
Real Devices

Accurate description/prediction of real devices



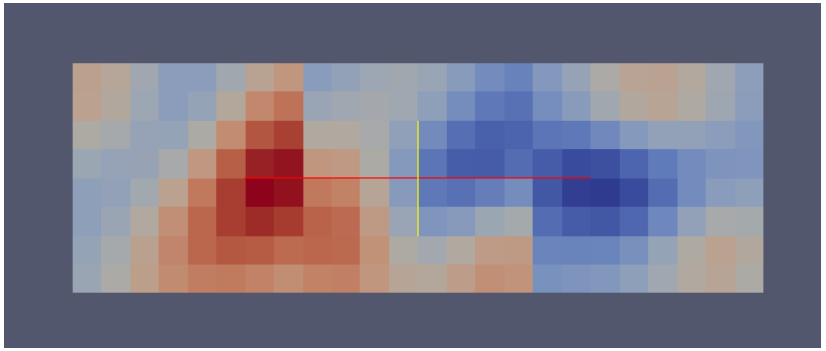
At the continuum end, such a vision will also require robust computational support for aleatory material uncertainty

Example1: Weibull Material Distributions (Weakest link theories)



Example 2: Random Field Representations (KL expansions)

$$f(\mathbf{x}) = \bar{f}(\mathbf{x}) + \sum_{i=1}^{N} \xi_i \phi_i(\mathbf{x})$$



- The material distributions for such continuum analyses MUST be derived from realistic data to be of any real use. Tight collaboration with experimentalists is fundamentally required.
- Outputs from forward models are stochastic variables.
- Random field theory is useful.

Next generation multi-physics modeling

- The various electromechanical approximations are highly useful and efficient. What is being lost?
  - Modeling of transitions between Maxwell regimes and additional diagnostic information.
- Can we build a numerical method for the full Maxwell's equations coupled to shock-hydro that naturally transitions between the electro-quasi-static and magneto-quasi-static regimes, that is reasonably efficient and would give useful electromagnetic wave propagation couplings?
- This would open up many opportunities for additional diagnostic and validation modalities.
- Similarly for other multi-physics: radiation transport, chemistry
- We also need modeling/computational software that can deal with such complexity and also move us into the future.

Example: Full Maxwell Equations and Continuum Mechanics Modeling is a Challenge

- Kovetz

$$
\begin{aligned}
\nabla \times \mathcal{H} &= \mathcal{J} + \overset{*}{\mathbf{D}}, \\
\nabla \cdot \mathbf{D} &= q, \\
\nabla \times \mathcal{E} &= -\overset{*}{\mathbf{B}}, \\
\nabla \cdot \mathbf{B} &= 0, \\
\mathbf{D} &= \epsilon_0 \mathbf{E} + \mathbf{P}, \\
\mathcal{H} &= \mu_0^{-1} \mathbf{B} - \mathbf{v} \times \epsilon_0 \mathbf{E} - \mathcal{M}
\end{aligned}
$$

- Constitutive theory provides $\mathcal{M}$, $\mathbf{P}$ and $\mathcal{J}$ with $\mathcal{E} = \mathbf{E} + \mathbf{v} \times \mathbf{B}$
- Flux derivatives fit naturally into an ALE framework

$$
\begin{aligned}
\overset{*}{\mathbf{B}} &= \frac{\partial \mathbf{B}}{\partial t} + \nabla \times (\mathbf{B} \times \mathbf{v}) + \mathbf{v}(\nabla \cdot \mathbf{B}) = \frac{\partial \mathbf{B}}{\partial t} + \nabla \times (\mathbf{B} \times \mathbf{v}) \\
\overset{*}{\mathbf{D}} &= \frac{\partial \mathbf{D}}{\partial t} + \nabla \times (\mathbf{D} \times \mathbf{v}) + \mathbf{v}(\nabla \cdot \mathbf{D}) = \frac{\partial \mathbf{D}}{\partial t} + \nabla \times (\mathbf{D} \times \mathbf{v}) + q\mathbf{v}
\end{aligned}
$$

- Fully coupled to mass, momentum and energy equations.

Current shock hydro multi-physics numerical methods

- Excellent in many ways…but
- Ad-hoc combinations of operator-splitting, semi-implicit, explicit time-integration methods and decoupled nonlinear-solvers.
  - Inaccurate and unstable results when physical mechanisms are strongly-coupled, highly-nonlinear and have overlapping time-scales,
  - Requires very small time-step sizes and make longer-time-scale integration costly and inaccurate,
  - Inflexible
  - Numerical errors and appropriate adaptive time step controls are only empirically understood,
  - Only sampling-based black-box techniques that require many expensive multi-physics solve evaluations are feasible for meta-analysis.
- This extensive code base is very useful but I do not believe it scales well into the future. What is needed?

IMEX numerical methods and Adjoint Support

- IMEX Schemes

$$\text{Forward problem: } \mathcal{L}(u;\mathbf{p}) = f(\mathbf{p})$$

$$\mathbf{u}'(\mathbf{p},t) = \mathbf{F}(\mathbf{u}(\mathbf{p},t)) + \mathbf{G}(\mathbf{u}(\mathbf{p},t));$$

$$\mathbf{R}(\mathbf{u},\mathbf{p}) = \mathbf{u}_n - \left[\sum_{j=1}^{k} a_j \mathbf{u}_{n-j} + \sum_{j=1}^{k} \hat{b}_j \Delta t \mathbf{F}(\mathbf{u}_{n-j}) + \sum_{j=0}^{k} b_j \Delta t \mathbf{G}(\mathbf{u}_{n-j})\right] = \mathbf{0}.$$

  - Stability (TVD, TVB, SSP),
  - Accuracy (e.g. 1st-5th),
  - Efficiency: partition fast (G), slow (F) operators, use explicit for slow (F) and implicit fast (G), includes fully-explicit and implicit methods. Well defined stability criteria and flexible.
  - It is possible to develop <u>adjoint</u> methodologies which play well with IMEX methods.

- Adjoint Methods

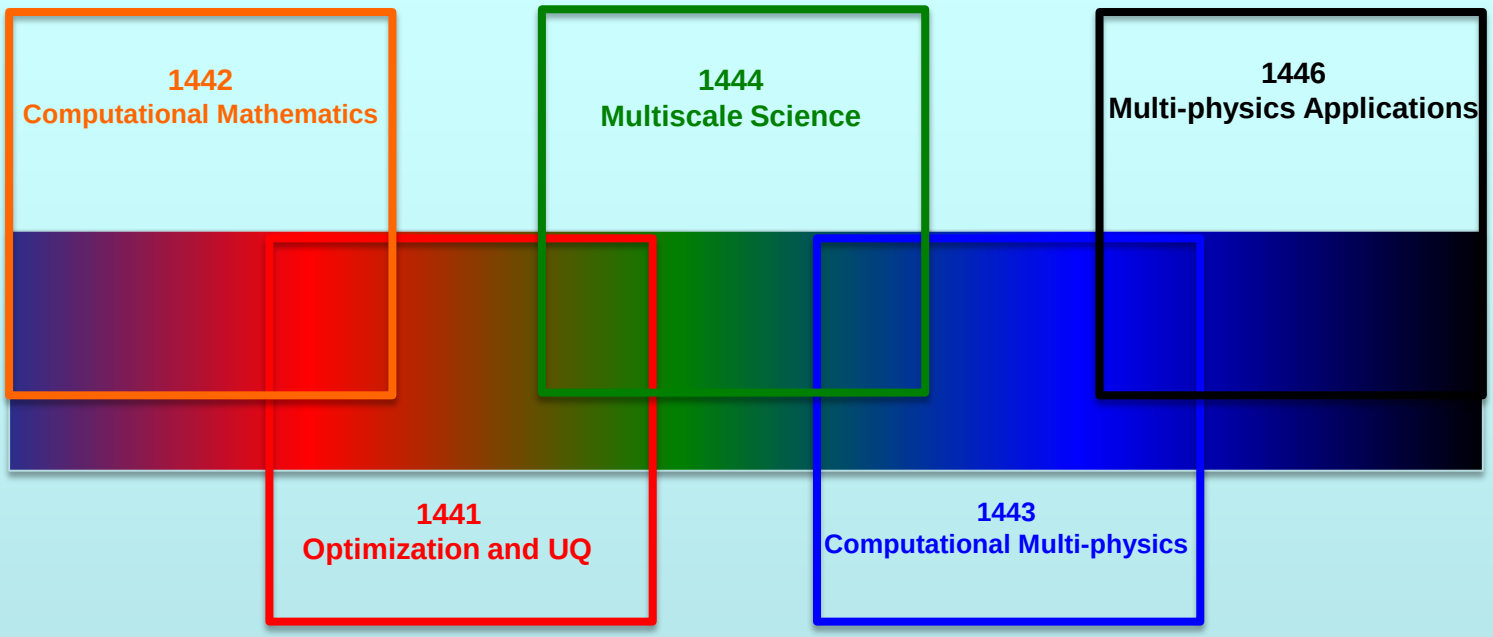
$$\text{Adjoint problem: } (\mathcal{L}'(u;\mathbf{p}))^* \psi = \partial_u g(u,\mathbf{p}).$$

$$\text{Adjoint Sensitivities: } \partial_p g(U;p) = (\psi, \partial_p \mathcal{R}(u;p)); \qquad \text{Error Estimate: } g(u;p) - g(U;p) \approx (\psi, \mathcal{R}(u;p))$$

  - Allows for smarter use of resources for UQ analysis
  - Massive efficiency benefits when number of parameters grows large (spatial material design)
  - Critical for efficient optimization:
  - Difficult implementation questions.
    - How much of our software base is reusable?

$$\min_{\mathbf{\Phi}} J(\mathbf{U},\mathbf{\Phi}) \equiv \frac{1}{2}\sum_{r=1}^{N_r} \int_{\mathsf{Q}} \xi_r(\mathbf{x}) \left\| \mathsf{R}\left(\mathbf{U} - \hat{\mathbf{U}}\right)\right\|^2 d\mathsf{Q} + \frac{\beta}{2}\int_{\Omega} \|\mathbf{\Phi}\|^2 \, d\Omega$$

The Sandia Computational Science and Math Group Strategy for Predictive Science and Engineering



Strategic Science and Engineering Experimental Partnerships
e.g. ARL, Sandia component engineering groups

Summary (10-30+ year viewpoint)

- How is this area evolving, and why is it relevant for science in the long term?
  - Basic continuum tools for shock electromechanics in various reduced approximation forms have been successful. They still need improvement.
  - Science based collaborative approaches with modeling based design and experimentation are essential.
- How and why should this topic area be a focus of defense science for the long term?
  - Defense science is all about design on a rapid iterative time scale.
  - Automated predictive modeling systems which are informed by both first principles computations and experimental data are the foundation for keeping ahead in understanding important shock/high energy environments.
- What technical elements will be required to achieve excellence in this area?
  - Multi-scale/multi-physics/UQ/optimization/inverse modeling tools which scale computationally and algorithmically and connect robustly into an increasing set of experimental modalities will be critical.
- What are recommendations for new programs, infrastructure and teams to address a prioritized list of potential grand challenges?
  - A much more integrated experimental/modeling multi-scale enterprise for shock multi-physics is required. Fund cross-cutting teams with clear objectives.
  - Next generation shock-multiphysics computational tools which scale for both forward problems and for efficiently solving optimization/inverse problems under uncertainty must now be developed.
  - Grand challenge related application suggestions:
    - Detonator physics coupled to energetic material modeling and design.
    - Fuze/power supply modeling in complicated 3D shock environments.
    - Full Maxwell/shock-hydro modeling and experiments for enhanced physics understanding and improved diagnostic modalities.

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