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Enabling Hydrocode Meta-Analysis: The ALEGRA-DAKOTA Experience

Allen C. Robinson, Richard R. Drake, John H. Carpenter, Raymond W. Lemke, Ann E. Wills (Mattsson)

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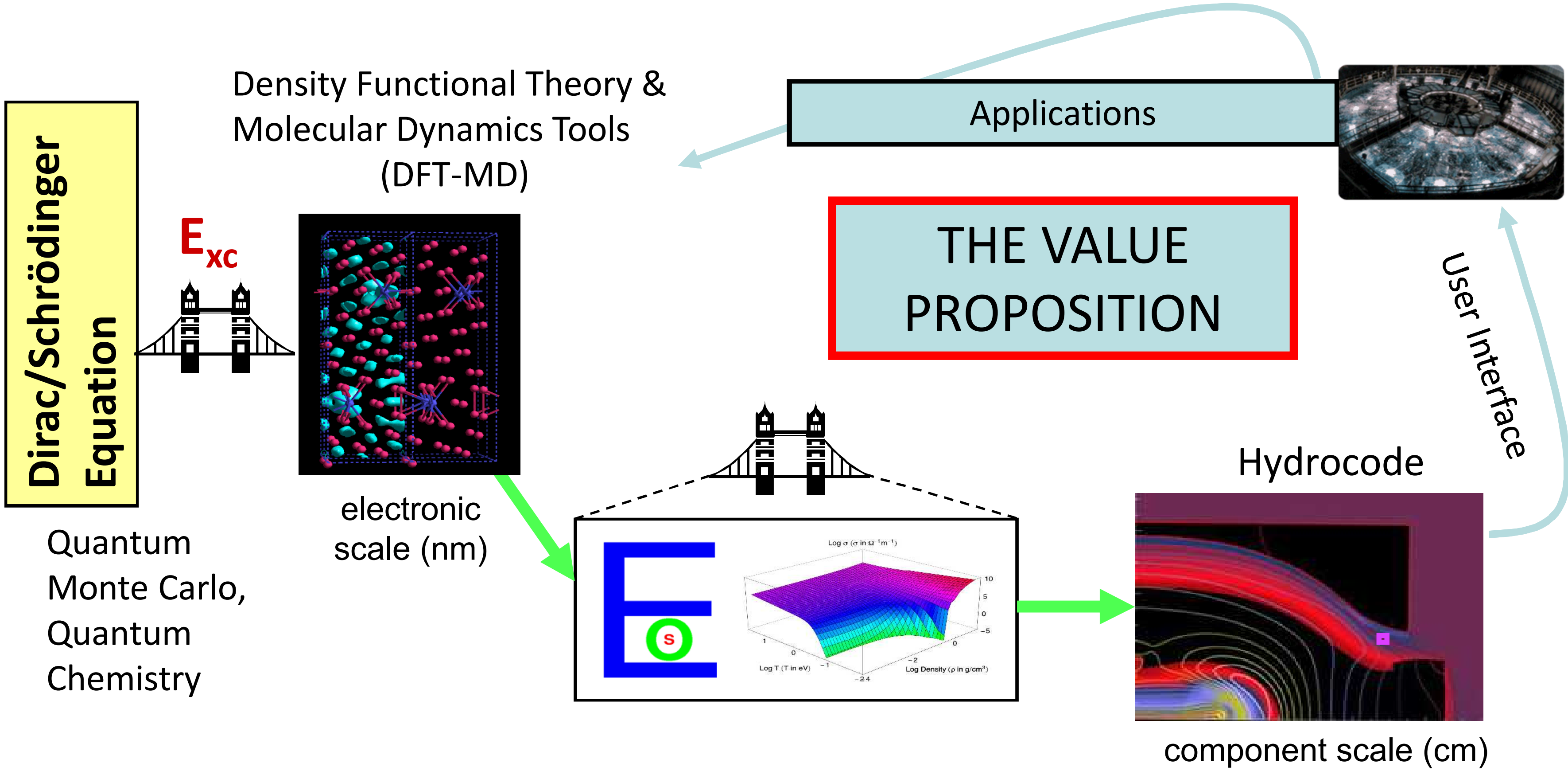
Science based engineering is a multi-scale, multi-physics, multi-parameter enterprise



How does one enable this cycle to be more effective?

Hydrocodes and Meta-Analysis

Hydrocode: Computer software which approximately solves model shock physics equations (e.g. ALEGRA)

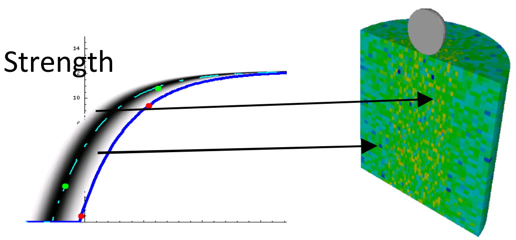
- Inputs to a hydrocode include initial geometry, closure properties and boundary conditions.
- Simulations outputs include a host of Quantities Of Interests (QOI).

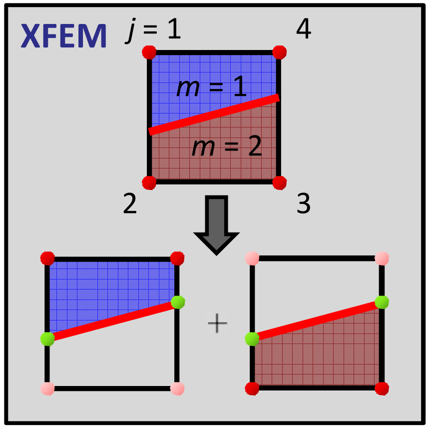
Meta-analysis: A robust, documented, and reproducible approach for sampling QOIs in a suite of forward modeling problems. (e.g. DAKOTA)

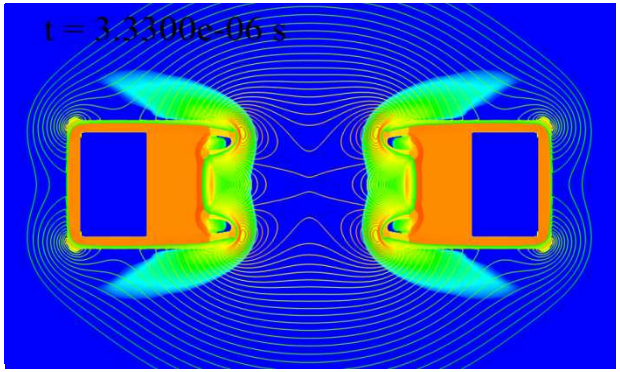
Meta-analysis is equally as difficult and scientifically involved to perform correctly and efficiently as the single hydrocode forward problem. (You need sophisticated software and users in both cases.)

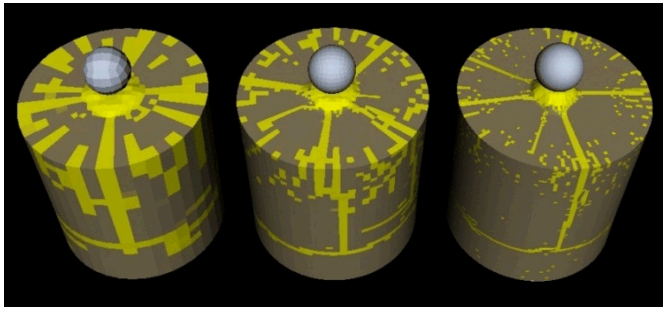
What we really need are robust modeling systems which enable meta-analysis with hydrocode forward problems.

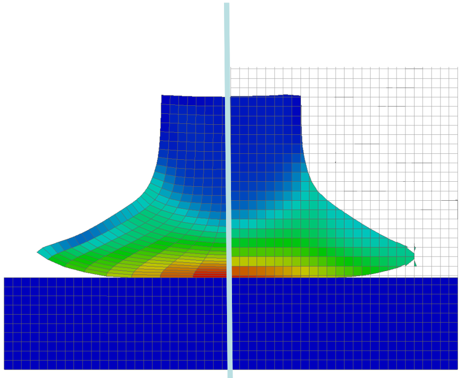
ALEGRA:
Sandia ALE hydrocode technology providing new approaches in solid dynamics and multiphysics



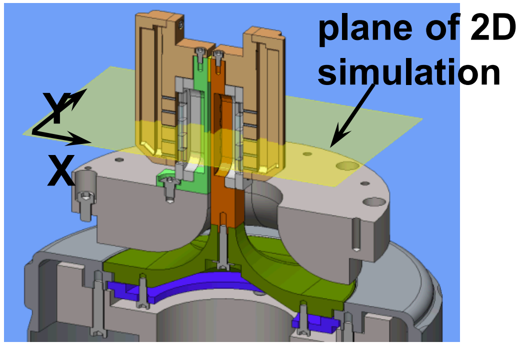








Lagrangian | XFEM Eulerian



Stochastic damage modeling

XFEM interface modeling

Stripline design on Z

DAKOTA: Design Analysis Kit for Optimization and Terascale Applications

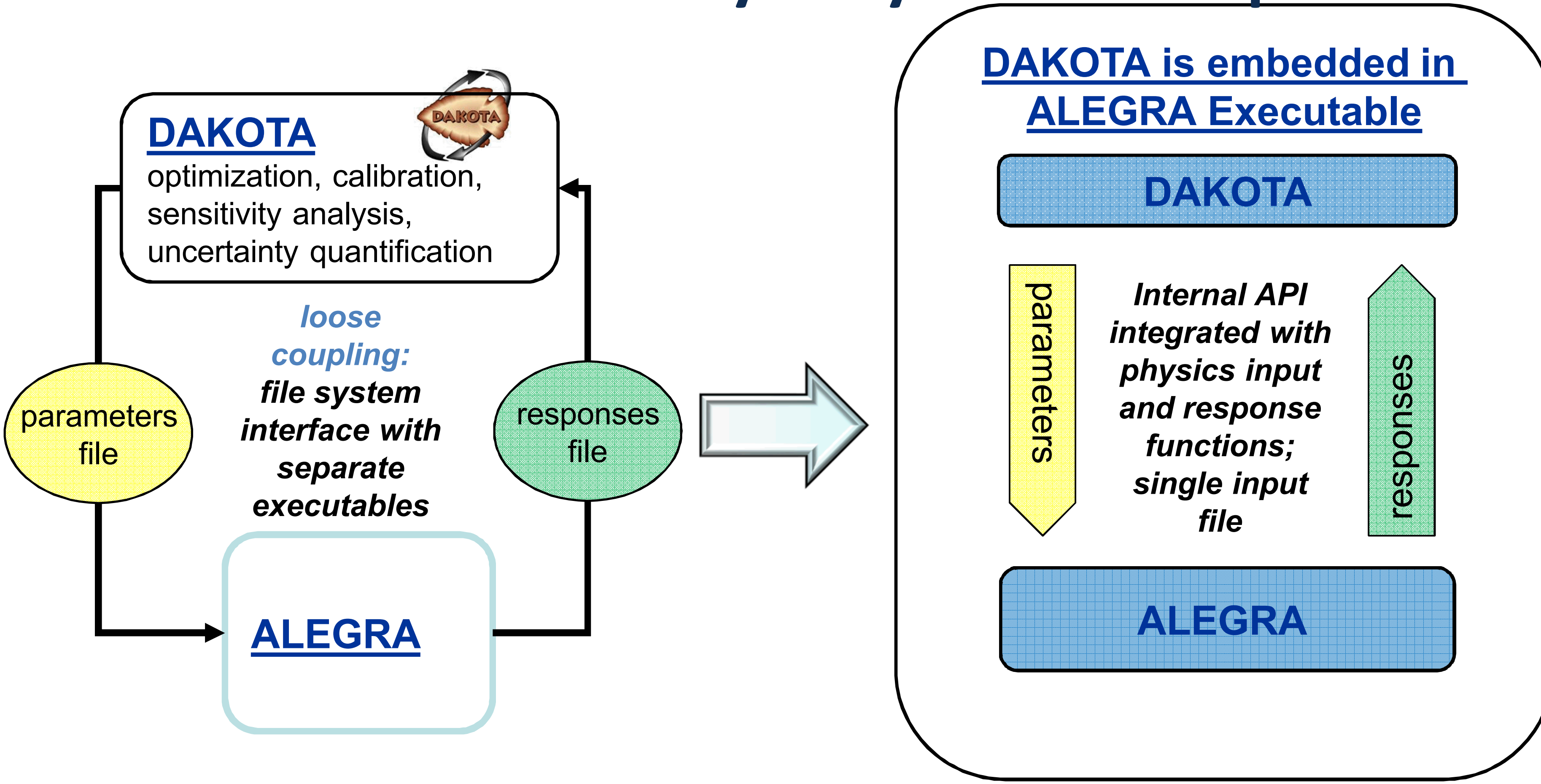
DAKOTA contains algorithms for:

- optimization with gradient and nongradient-based methods;
- uncertainty quantification with sampling, reliability, stochastic expansion, and epistemic methods;
- parameter estimation with nonlinear least squares methods;
- sensitivity/variance analysis with design of experiments and parameter study methods.

These capabilities may be used on their own or as components within advanced strategies such as hybrid optimization, surrogate-based optimization, mixed integer nonlinear programming, or optimization under uncertainty.

How are they used together?

How can this meta-analysis system be improved?



Move users from a potentially fragile, study-specific script interfaces to a unified, user-friendly capability

Why the embedded DAKOTA in ALEGRA approach?

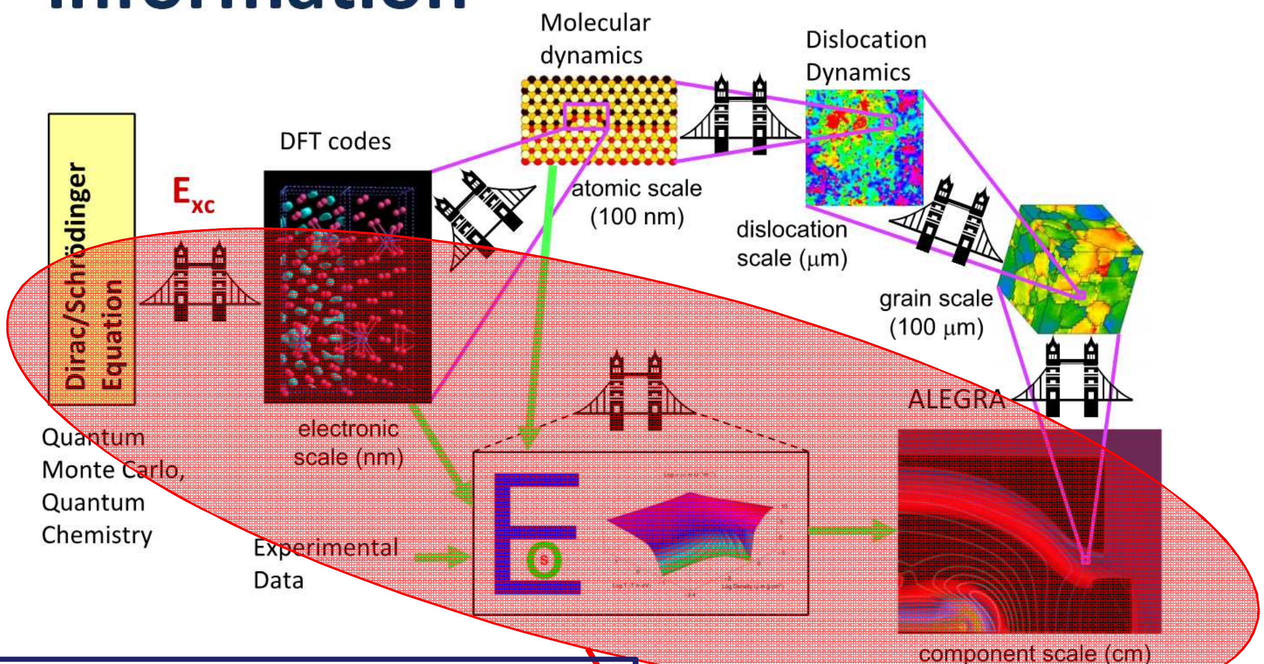
Design Goal:

- Make it so easy for ALEGRA users to put together a useful meta-analysis that such work will be natural and expected.

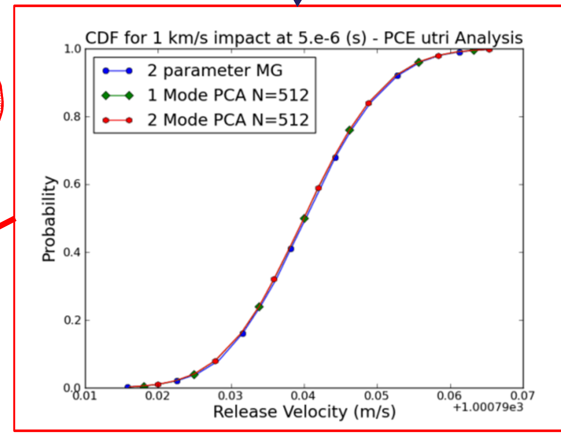
Strategic Solution:

+ DAKOTA is linked in as part of ALEGRA
- ALEGRA had to be made effectively reentrant (lots of work)
+ Multiple ALEGRA samples can occur in parallel (users should consider parallel load balance of sample runs)
+ Parameter substitutions happen naturally in the input stream using a standardized user environment.
+ We have built in an extensive set of standardized set of QOI (response functions) including the ability to build in user defined QOI's via a run-time "C type language" interpreted interface.
+ Helps solves the reproducible meta-analysis requirement.
+ Evidence from users is that it encourages and enables meta-analysis.

Example I: Propagation of uncertain EOS information



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.

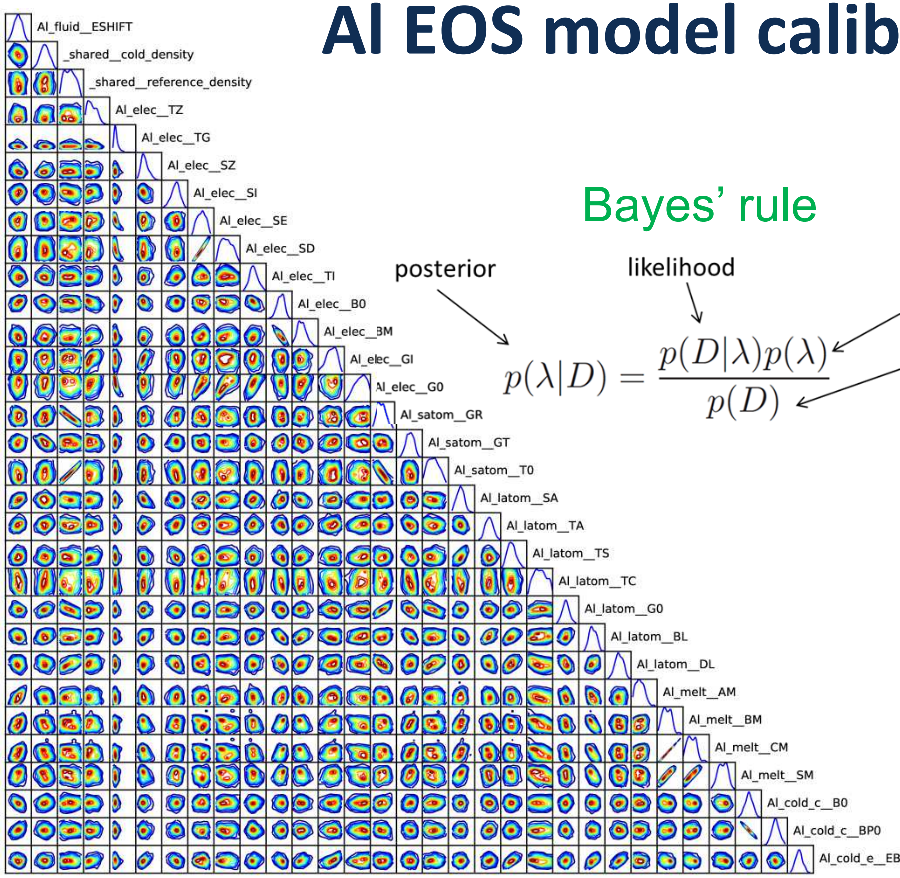
Example: Propagate uncertainty due to statistically equivalent possible EOS fits to the same data, to the analyst.

Our proposed solution

Robinson, Berry, Carpenter, Debusschere, Drake, Mattsson, Rider, “Fundamental issues in the representation and propagation of uncertain equation of state information in shock hydrodynamics”, Computers and Fluids, 83, (2013) p. 187–193.

Software Package	Output
EOS model library and data	Proposal Model (XML input deck)
Bayesian Inference using Markov Chain Monte Carlo	Extensive Sampling of the posterior distribution function (PDF)
EOS Table Building	Topologically equivalent tables for each sample
PCA Analysis	Mean EOS table + most significant perturbations
Hydrocode + Dakota	Cumulative Distribution Function (CDF) for quantities of interest

Al EOS model calibration and inference

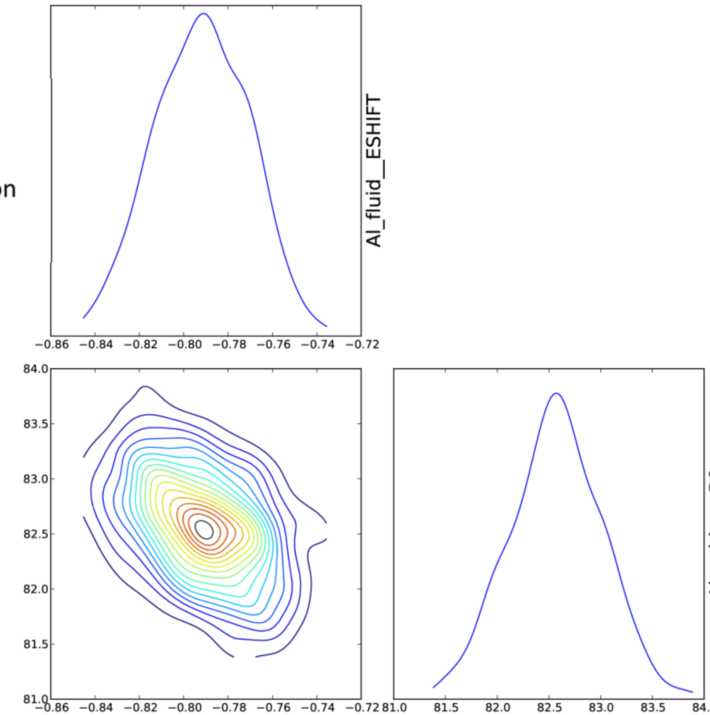


Al model EOS inference

Bayes' rule

posterior — likelihood — prior — normalization

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



A marginal distribution

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

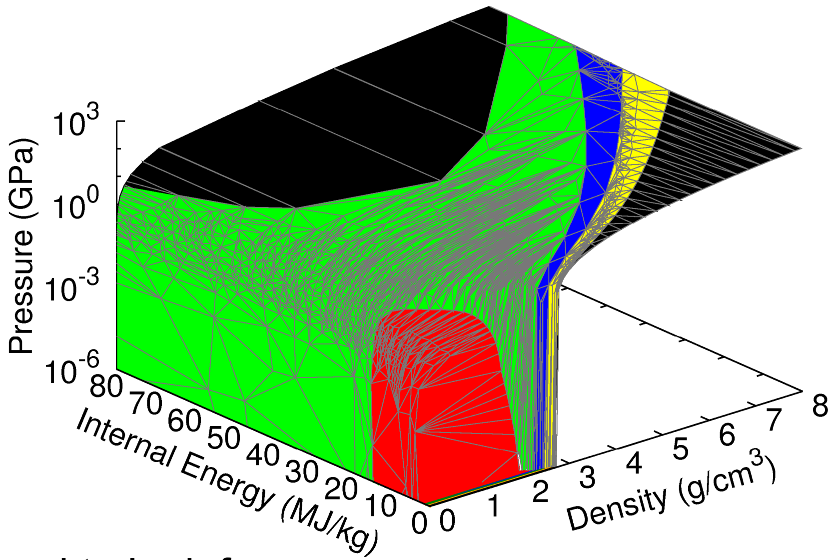
- Use adaptive Markov Chain Monte Carlo (MCMC) scheme to reduce number of steps
- Use optimization to find Maximum A Posteriori (MAP) parameters from which to start chain
- Each posterior evaluation is roughly equivalent to generating an entire EOS table

Tabular EOS generation and UQ representation

Simultaneously tabulate N parameterizations of an EOS 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

Example PCA mean pressure table at 0.1 tolerance



phases:

off table
solid
fluid
melt
vaporization

Principal Component Analysis (PCA) is 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 is necessary due to dynamic range of multi-phase tables.
- Log density and log energy used in PCA analysis (also ensures positivity)
- Random variables ξ are uncorrelated, with zero mean and unit standard deviation, but not necessarily independent

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

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

$$\begin{aligned} z &= \bar{z} + U\Sigma\xi = \bar{z} + \tilde{U}\Sigma\xi \\ &= \bar{z} + (Z - \bar{z}\mathbf{1}^T)H^{1/2}\tilde{V}\xi \end{aligned}$$

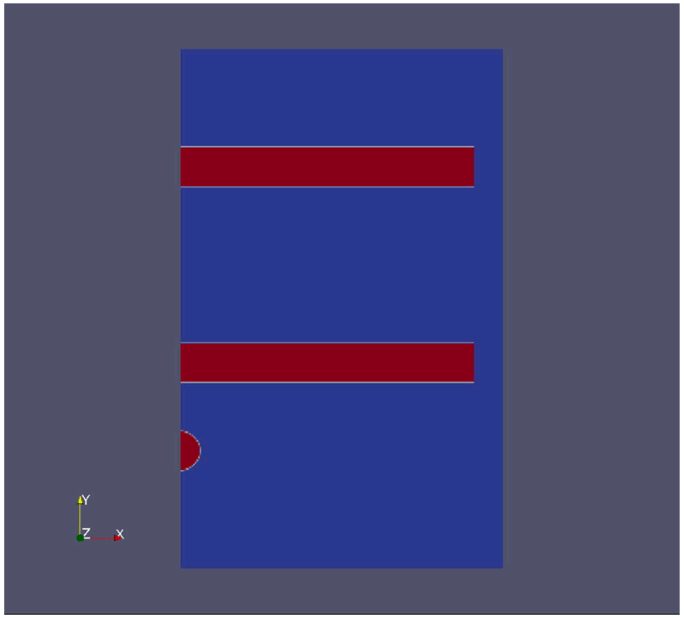
$$\mathbb{T} = \bar{\mathbb{T}} + \sum_k \xi_k \mathbb{T}_k$$

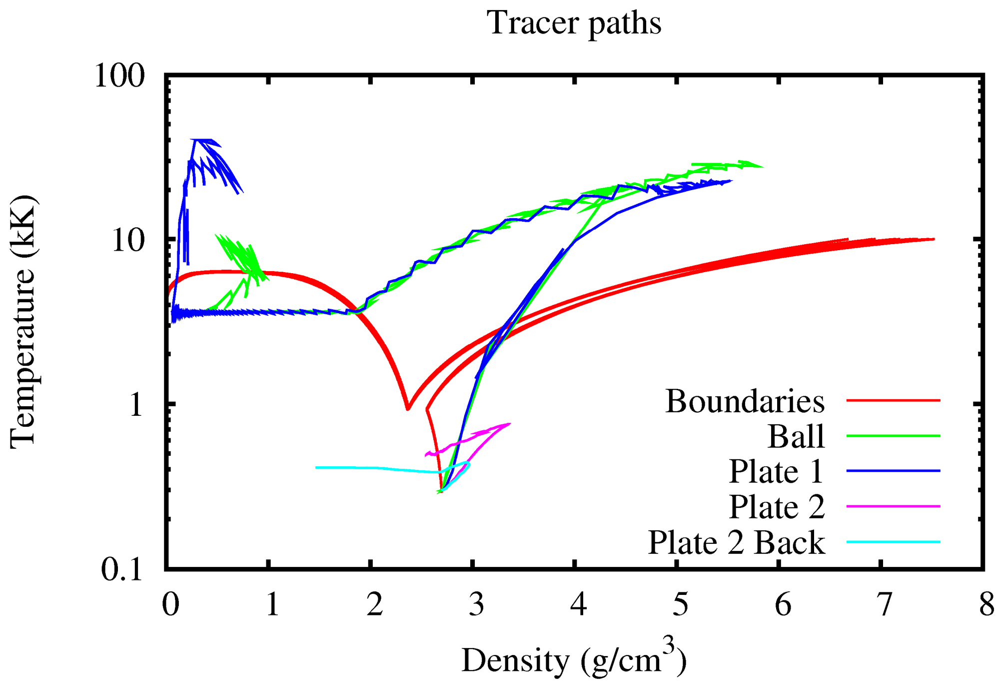
Multiphase Tabular Generation and Representation: Initial AL UQ enabled table

$$T = \bar{T} + \xi_1 T_1 + \xi_2 T_2 + \xi_3 T_3 + \cdots$$

- Wide range UQ AL EOS with 6 phase regions in the density-energy table.
- With the current multi-phase model there are 37 free parameters.
- 6 parameters were fixed due to insufficient constraining data.
- The MCMC inference samples 31 parameters
- We took 400 samples from the chain. Due to unresolved topology issues in the table generation process, only 6 of those were successfully tabulated simultaneously. There were 3 significant modes at 1e-6 cutoff in the PCA analysis. Work still in progress.
- Accuracy of the tables is set at a relative tolerance of 0.1.
- PCA solver currently scales as N^2 so this limits practical number of samples.

Example calculation: 2mm diameter Al ball impacting spaced Al plates at 20 km/s in air background. Termination at 1.5 microsec

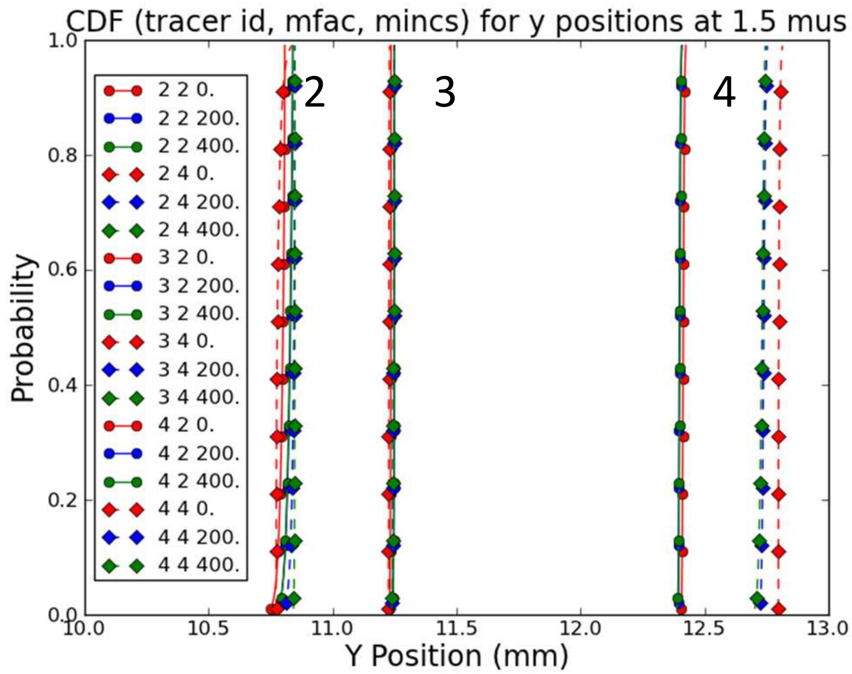




Phase boundary lines of PCA source EOS files are shown along with phase space trajectory of tracers (mean table, csmin=0)

Example uncertainty analysis using UQ enabled AL EOS

3 PCE (polynomial chaos expansion) quadrature points and 1 tabular mode



Lessons Learned:

1) UQ EOS information can be comparable to other model uncertainty (e.g. mesh resolution (mfac), numerical or modeling constants (mincs))
2) UQ enabled table capability tends to drive useful verification and numerical work
3) Formal approach leads to more precise and detailed thinking.

Example II:
Optimization based Equation of State calibration

Key Idea:

Use hydrocode to calibrate off Hugoniot EOS information based on accurate boundary velocity measurements in a well characterized experiment.

The ZR accelerator delivers up to 25 MA current & several MJ magnetic energy to short circuit load

22 MJ stored energy; ~10 TW peak power

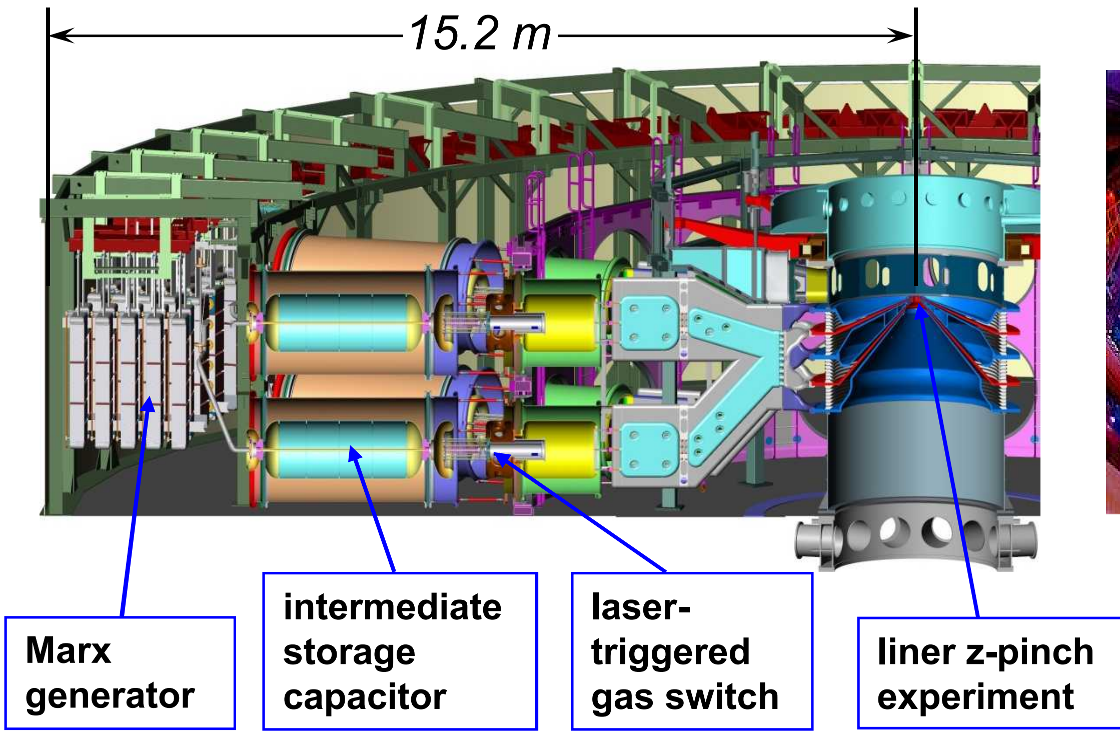
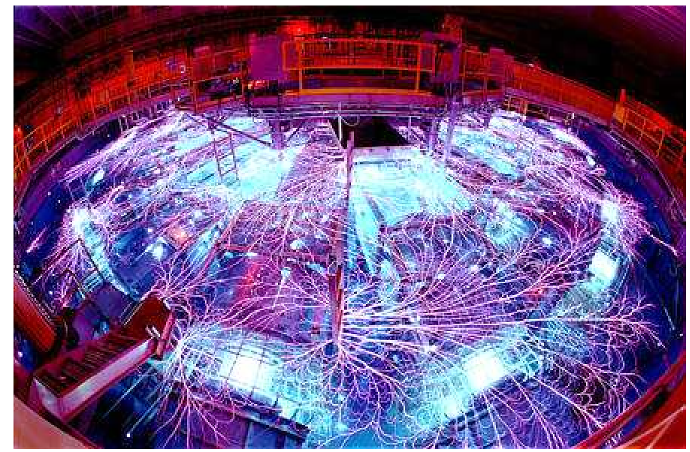


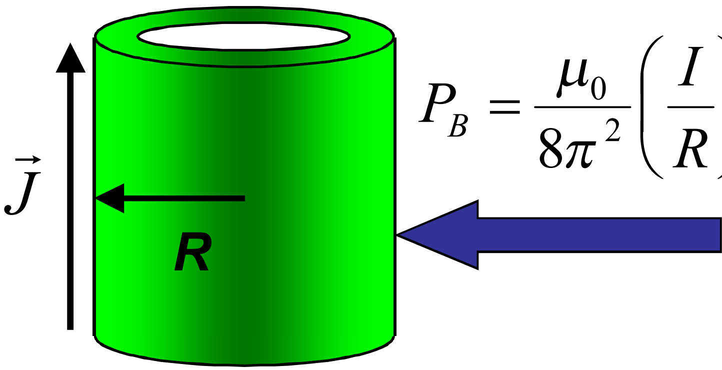
Photo of Z experiment



Current rise times of 100-1000 ns possible via independent timing of 36 laser triggered switches.

Quasi-isentropic compression to peak stresses ≈20 Mbar possible in cylindrical liner implosions on Z

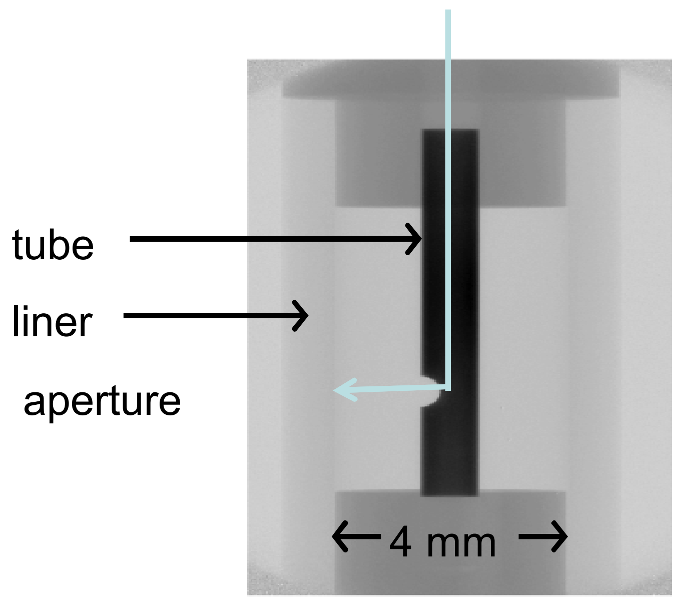
Liner Z-Pinch Implosion



$$P_B = \frac{\mu_0}{8\pi^2}\left(\frac{I}{R}\right)^2$$

I=20 MA; R=0.1 cm;
P_B≈64 Mbar.

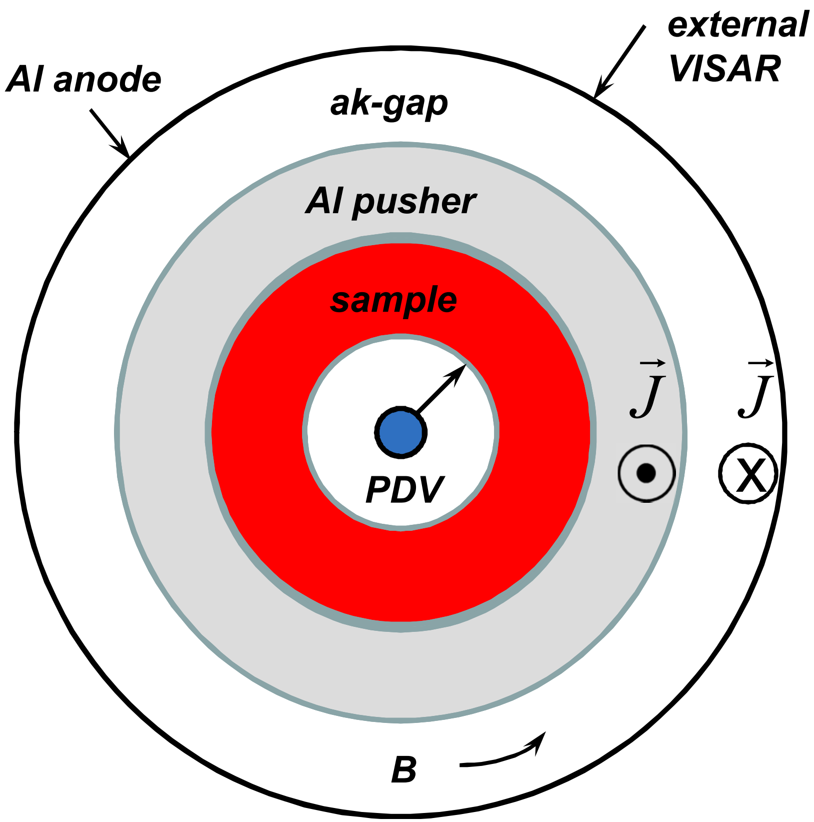
- 3-4 times greater stress than in planar geometry.
- Material stress increases monotonically.
- Shockless compression achieved by shaping current.
- Diagnosing compressed state is challenging.
- ***Successfully fielded accurate photonic Doppler velocimetry (PDV)***.



Radial Photonic Doppler Velocimetry (PDV) successfully measures liner surface implosion velocity in experiments on Z.

Use the data to infer information about the sample equation of state.

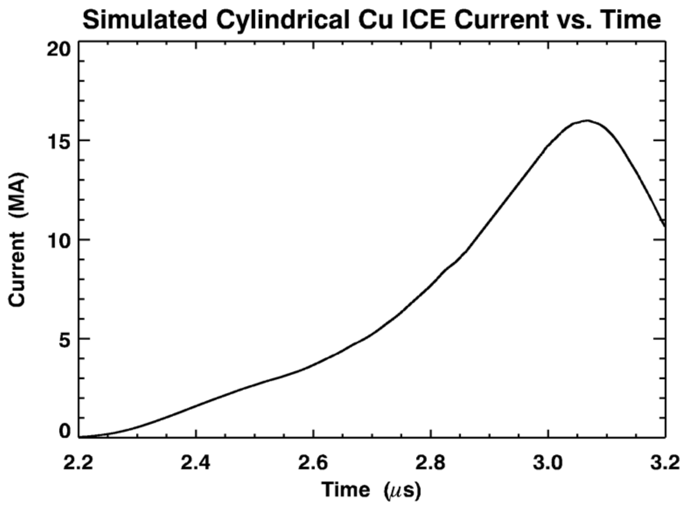
Cylindrical quasi-isentropic compression experiment.

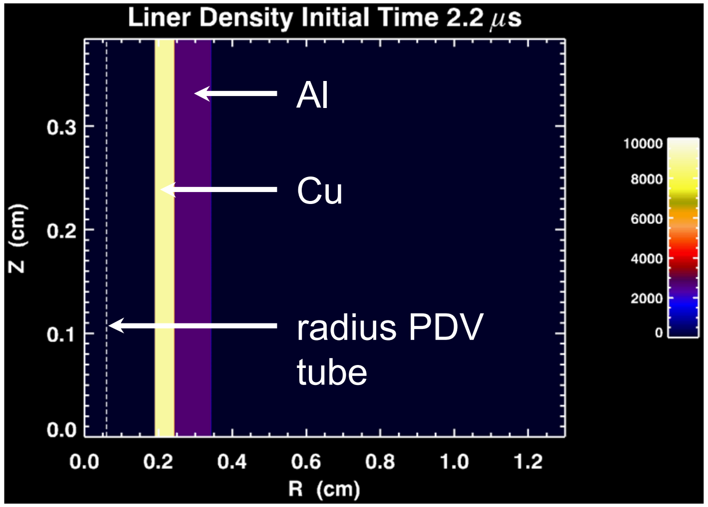


- Goal is to measure off-Hugoniot density and pressure.
- Pressure and density in sample inferred from velocimetry data + MHD code + mathematical optimization.
  - Current is inferred from external VISAR.
  - Velocity of sample inner surface is obtained from PDV.
  - Velocity of inner surface is a function of the assumed EOS of the pusher and the unknown EOS of the sample.
  - Choose the coefficients in the sample EOS model to match the inner surface velocity history via optimization.

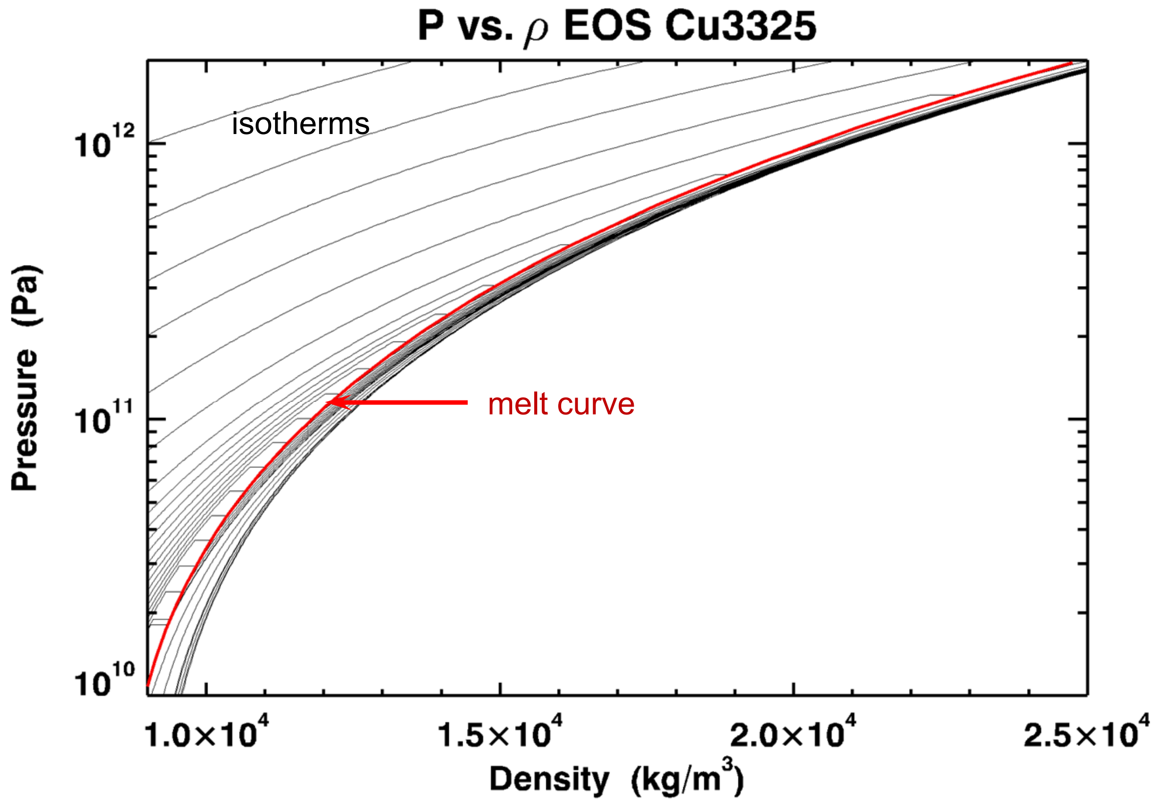
A simulated cylindrical experiment illustrates the technique for shockless compression of copper

- Current shaped to compress Cu quasi-isentropically.
- Cu: R_i=1.9 mm, R_o=2.43 mm, Δ=530 μm; Al: R_o=3.43 mm.
- 2D ALEGRA, resistive MHD+conduction+material models.
- 50 μm perturbation, random in z, on outer surface aluminum.



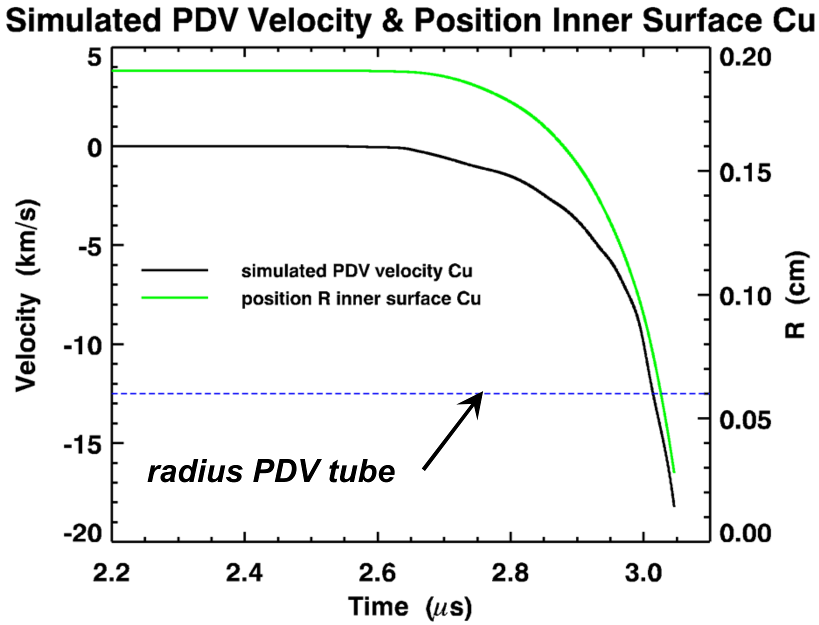


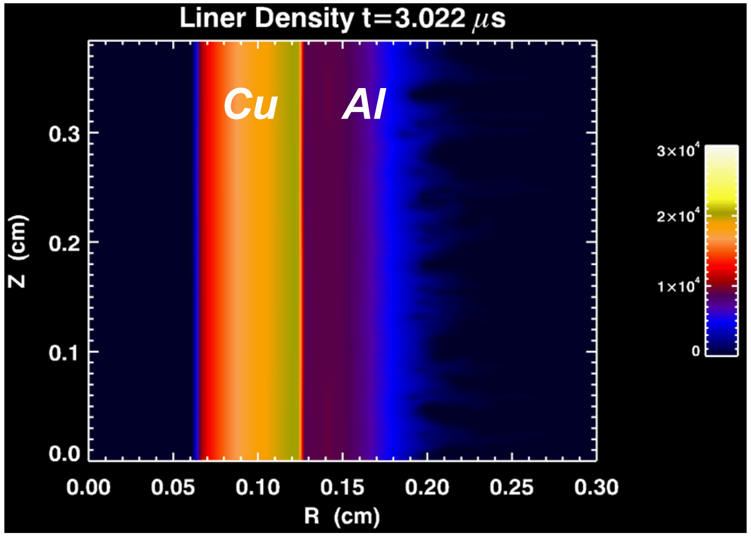
Copper equation of state 3325 developed at SNL using density functional theory is used to develop the surrogate data.

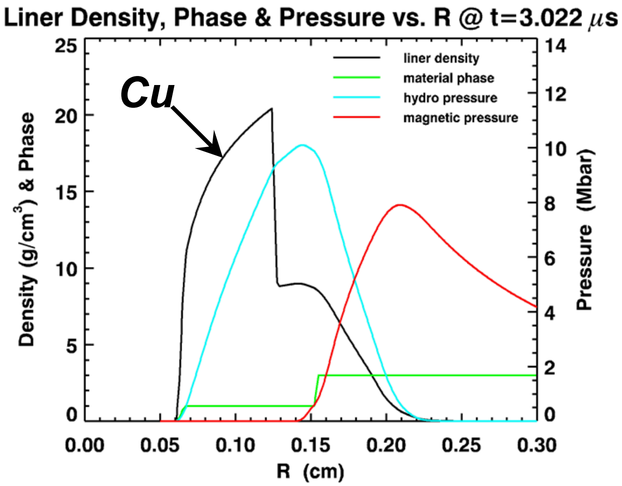


* John Carpenter and Kyle Cochrane (SNL).

Copper is quasi-isentropically compressed to 9.5 Mbar, and unaffected by magnetic Rayleigh Taylor





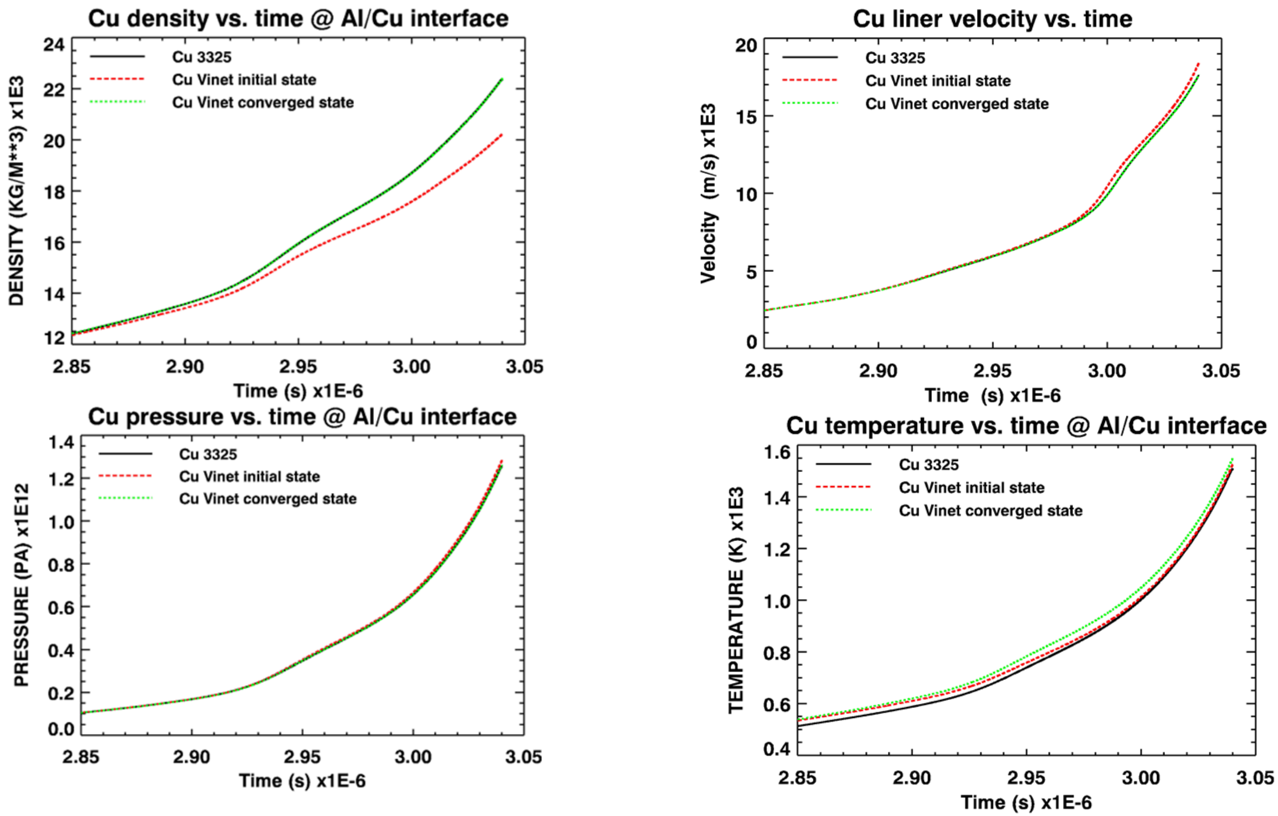


Magnetic field confined to aluminum; copper completely in solid state.

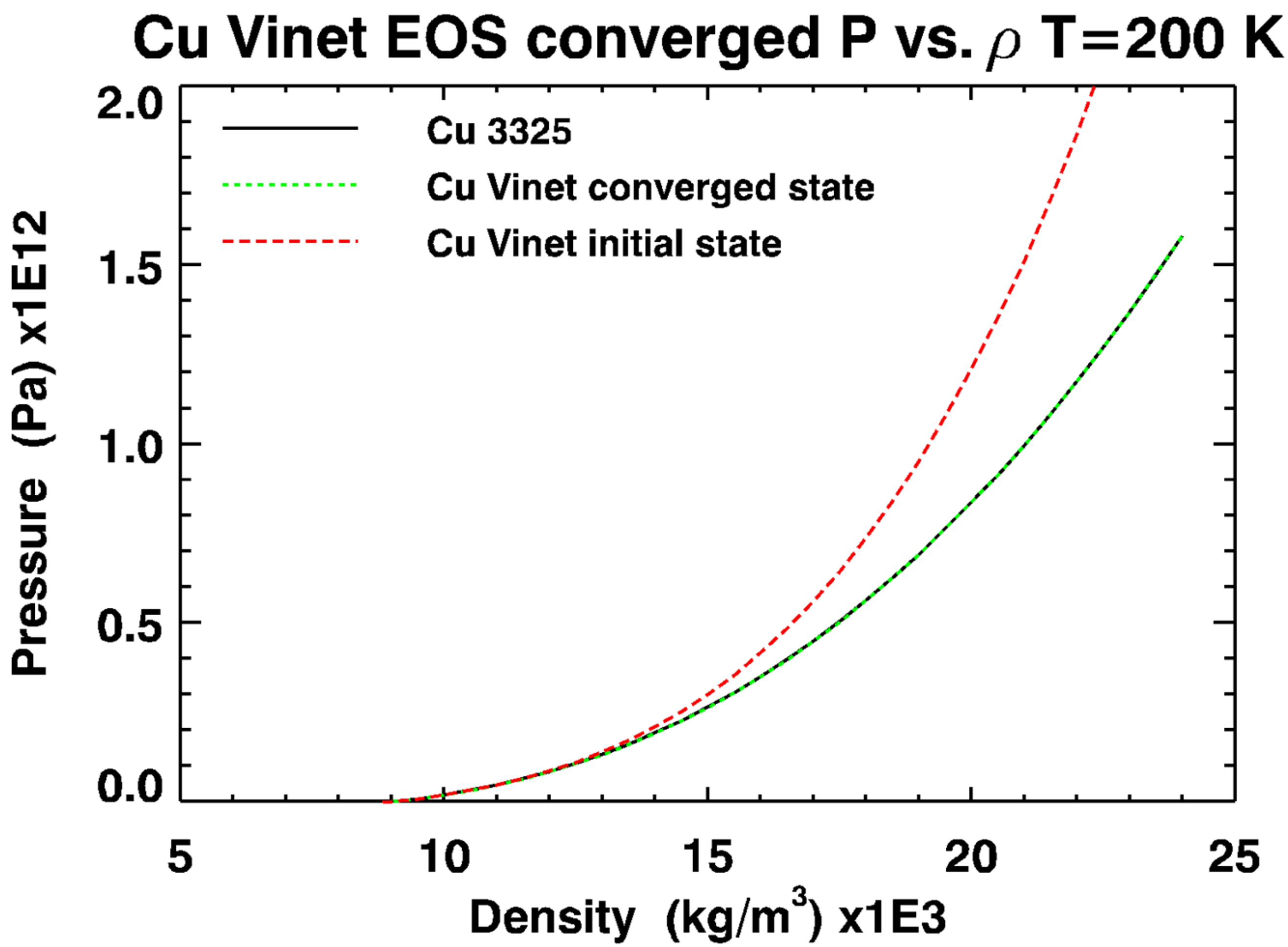
Optimize EOS parameters to match velocity

An extended Vinet type EOS with 3 free parameters has been used to match surrogate data very well.

$$P_{ref}^{extvin}(X) = \frac{3B_0}{X^2} Z \exp\left[\eta_0 Z\right] \left(1 + \sum_{n=2}^{N} d_n Z^n\right) \qquad X = \left(\frac{\rho_0}{\rho}\right)^{1/3} \qquad Z = (1 - X)$$



Extended Vinet EOS with 3 parameters works extremely well.



Lessons learned: Process is very sensitive and details must be right. Optimization error norm below the uncertainty in the measurement velocity is required (1 percent).

Looking to the future

Calibration under uncertainty would be the obvious next step and would allow uncertainties in the calibrated parameters to be captured.

This information could then enable UQ EOS development.

Consistent uncertainty information should be made available for other properties such as conductivity in the same tabular format.

Summary

The integrated ALEGRA-DAKOTA system has shown great promise for raising the bar and encouraging more meaningful meta-analysis.

Deep dives into the meta-analysis world tends to bring out substantive quality issues very effectively.

Integrated meta-analysis capabilities enable more efficient and thorough science and engineering.

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- For the ALEGRA radiation magnetohydrodynamics code see above references and following link (download PDF file):
  - http://arc.aiaa.org/doi/abs/10.2514/6.2008-1235