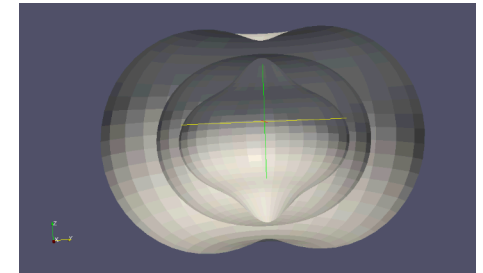
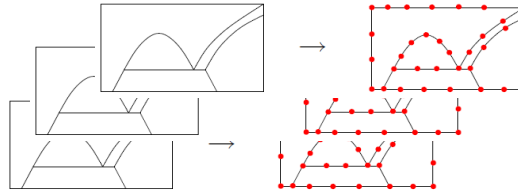
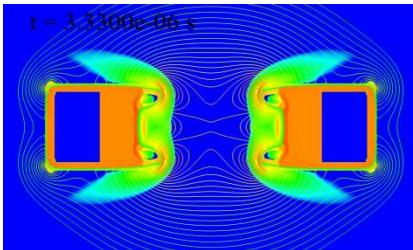
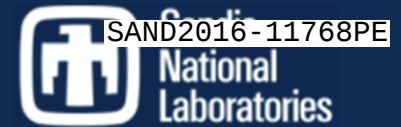


Exceptional service in the national interest



Multiphysics Shock Modeling with ALEGRA and Student Contributions

Allen C. Robinson

November 17, 2016

Fall 2016 Series Computation Mathematics at Sandia National Laboratories
UNM Department of Mathematics and Statistics

SAND2016-xxxx-PE



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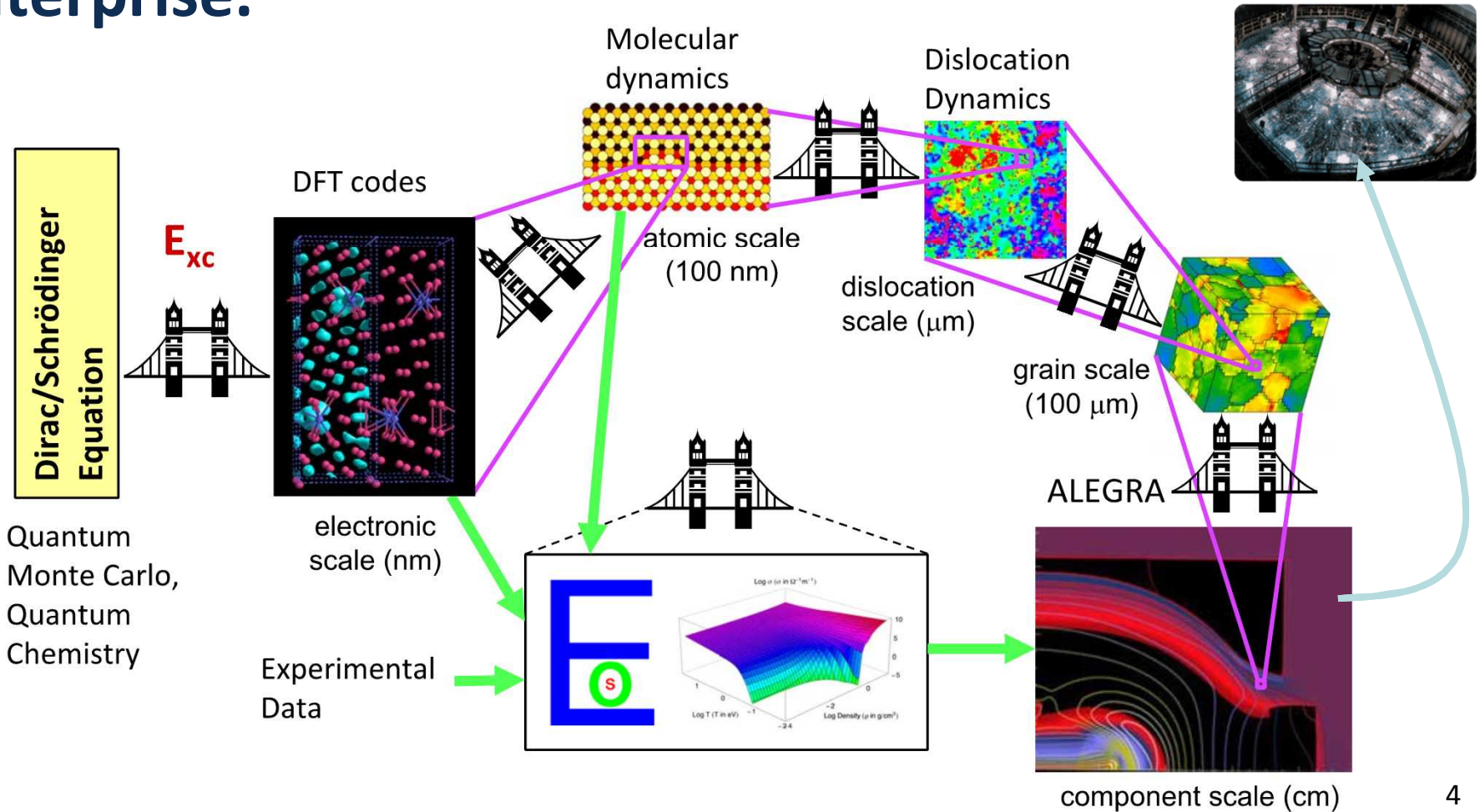
Outline

- Provide an overview of ALEGRA multi-physics capabilities and a discussion of some algorithmic approaches.
- Highlight a few undergraduate level student contributions to ALEGRA.
- Give insight into potential collaborative scope and a view into production code development challenges.

Acknowledgments

- ALEGRA development team includes many contributors over 20+ years of development.
- My contributions focus around the areas of MHD and electromechanics. My interests are now moving toward multi-fluid and generalized Ohm's Law modeling.
- Key Users: e.g. Ray Lemke, Steve Montgomery, Chris Garasi, John Niederhaus, ...
- Uncertain Tabular EOS: John Carpenter, Bert Debusschere
- Recent Students: Chace Ashcraft, Brad Hanks, Koa Fischer

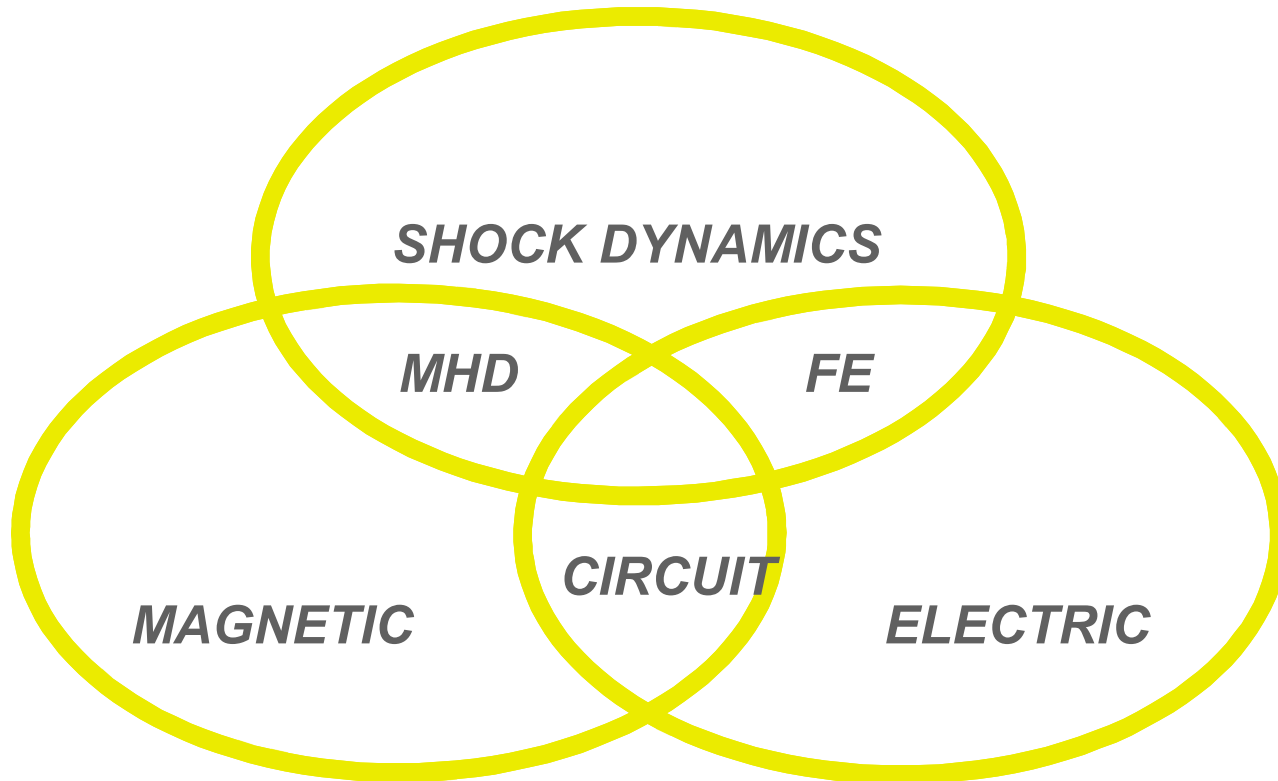
Science based engineering is the only possible way to compete in the future. It is a multi-disciplinary, multi-scale, multi-physics enterprise.





ALEGRA

SHOCK &
MULTIPHYSICS



Continuum shock algorithms (“hydrocode”)

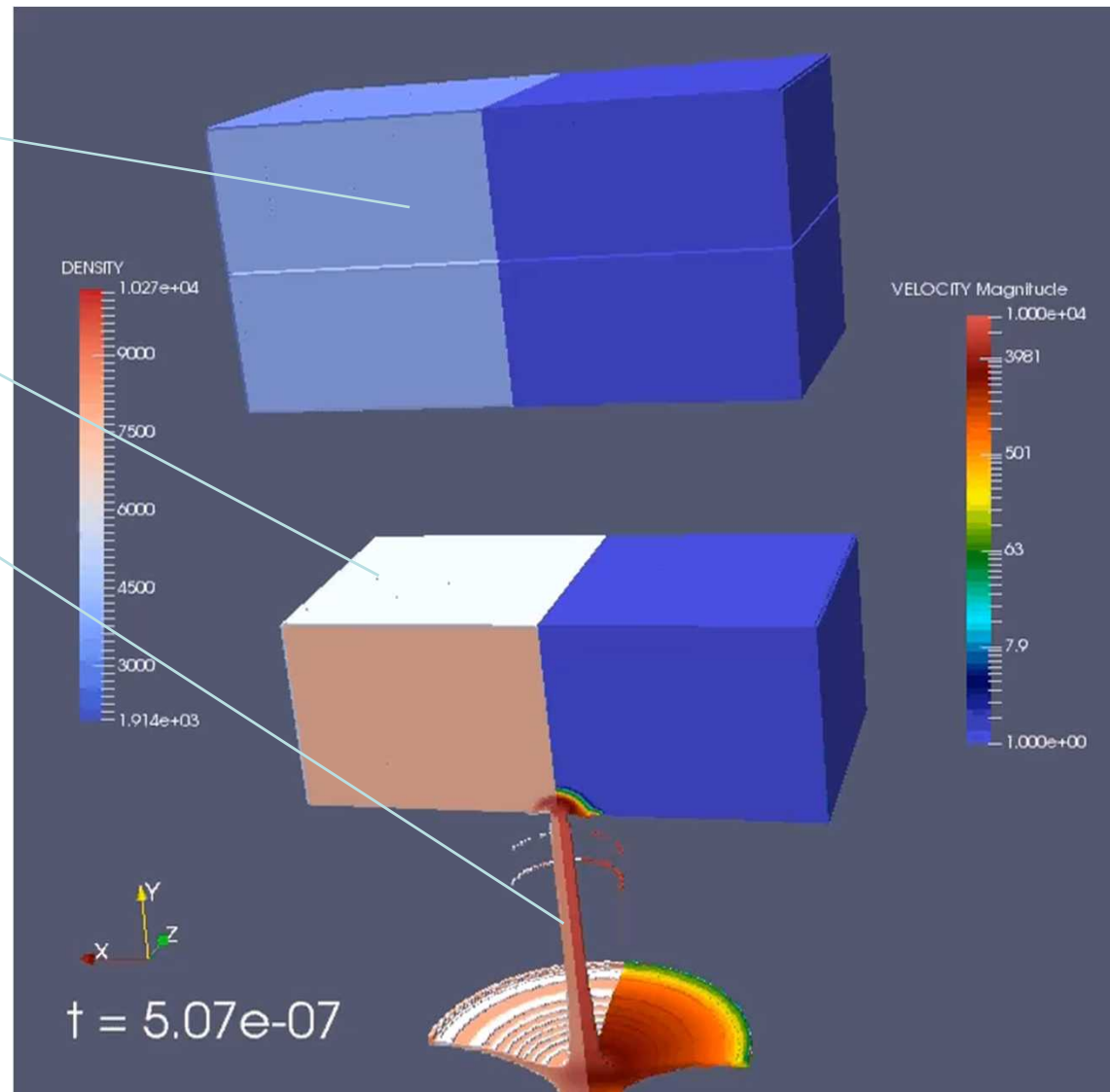
ALON panels.

Steel plate.

Fully-formed shaped
charge jet imported
from 2D axisymmetric
ALEGRA simulation.

XFEM and stochastic
damage modeling
approaches in ALEGRA
will not be discussed
today.

ALEGRA is an MPI
distributed memory
parallel code.



Courtesy of J. Niederhaus (SNL) and B. Leavy (ARL)

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

$$\rho \dot{\mathbf{g}} = \nabla \cdot \mathbf{T} + \rho \mathbf{b}$$

$$\rho \dot{\epsilon} = \nabla \cdot \mathbf{T}^T \mathbf{v} + \rho \mathbf{v} \cdot \mathbf{b} + \rho h - \text{div}(\mathbf{q} + \mathcal{E} \times \mathcal{H})$$

$$\nabla \times \mathcal{H} = \mathcal{J} + \dot{\mathbf{D}}^*,$$

$$\nabla \cdot \mathbf{D} = q,$$

$$\nabla \times \mathcal{E} = -\dot{\mathbf{B}}^*,$$

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

$$\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P},$$

$$\mathbf{H} = \mathbf{B}/\mu_0 - \mathbf{M}$$

$$\dot{\mathbf{B}}^* = \frac{\partial \mathbf{B}}{\partial t} + \nabla \times (\mathbf{B} \times \mathbf{v}) + \mathbf{v}(\nabla \cdot \mathbf{B}) = \frac{\partial \mathbf{B}}{\partial t} + \nabla \times (\mathbf{B} \times \mathbf{v})$$

$$\dot{\mathbf{D}}^* = \frac{\partial \mathbf{D}}{\partial t} + \nabla \times (\mathbf{D} \times \mathbf{v}) + \mathbf{v}(\nabla \cdot \mathbf{D}) = \frac{\partial \mathbf{D}}{\partial t} + \nabla \times (\mathbf{D} \times \mathbf{v}) + q\mathbf{v}$$

$$\mathcal{E} = \mathbf{E} + \mathbf{v} \times \mathbf{B}$$

$$\mathcal{H} = \mathbf{H} - \mathbf{v} \times \mathbf{D}$$

$$\mathcal{J} = \mathbf{J} - q\mathbf{v}$$

closure relationships for $\mathbf{g}, T, \epsilon, \mathbf{q}, s, \mathcal{M}, \mathbf{P}$ and $\mathcal{J}$

Resistive MHD Equations

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

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

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

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

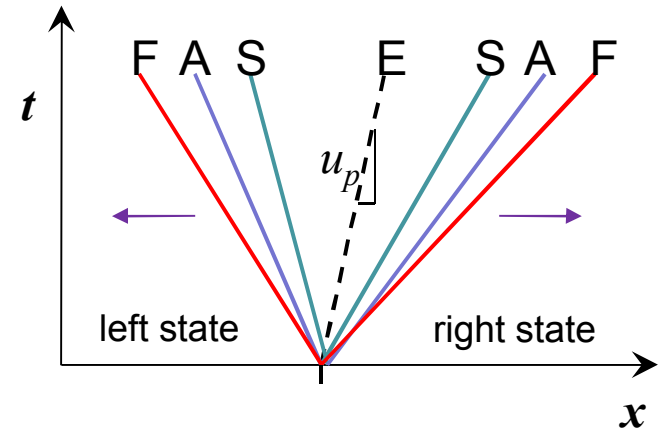
$$\nabla \times \frac{\mathbf{B}}{\mu_0} = \mathbf{J}$$

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

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

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

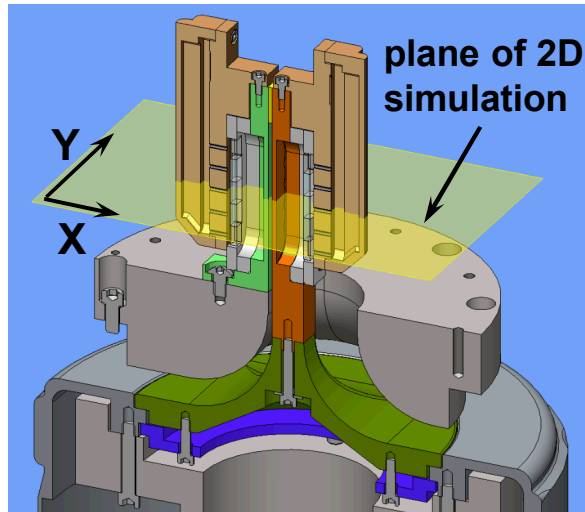
The closure relations are what makes equations useful.



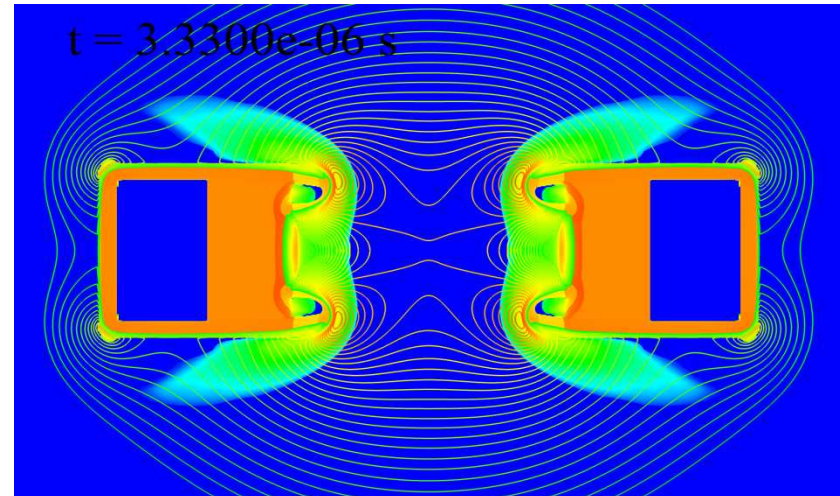
Ideal MHD wave speeds

ALEGRA magnetohydrodynamic modeling provides for predictive design of flyer plate experiments

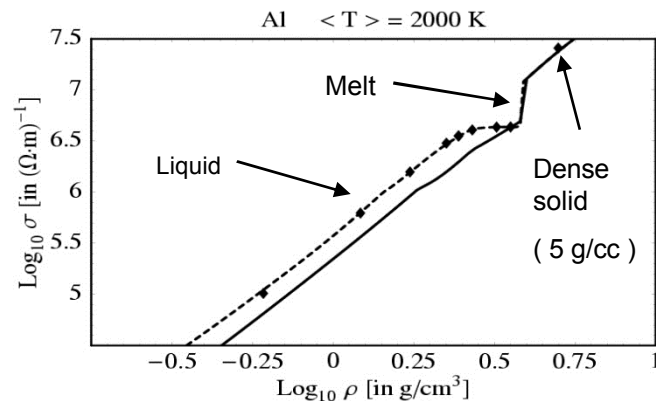
Two-sided Strip-line Flyer Plate Experiment



2D Simulation Plane of Two-sided Strip-line



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



ALEGRA implements a classical Indirect Arbitrary Lagrangian/Eulerian (ALE) Approach

- **Lagrangian**

- Mesh moves with material
- Lagrangian viewpoint is useful from a solid mechanics constitutive modeling point of view.
- Mesh-quality may deteriorate over time

- **REMESH**

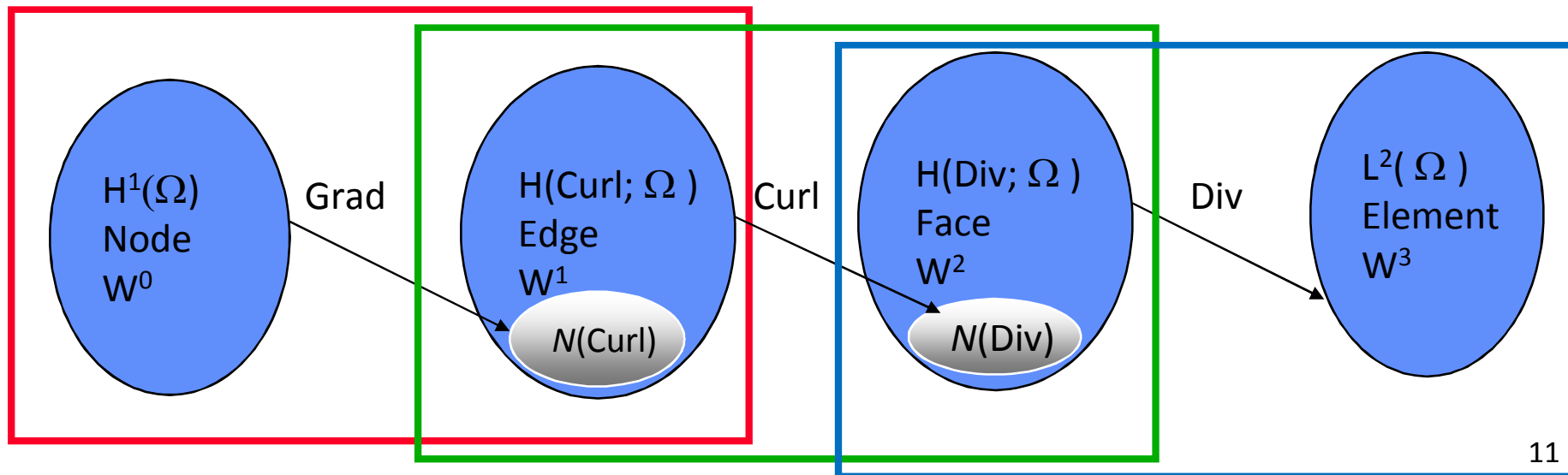
- Mesh is adjusted to improve solution-quality or robustness. Often users move the mesh back to original location (Eulerian).

- **REMAP**

- Algorithm transfers dependent variables to the new nearby mesh.

Geometric Structure and Numerical Methods

- The structure of physics equations is related to their geometric origins.
- The deRham structure shown below is used to discuss issues of “compatible discretizations.” Stable discretizations depend on maintaining proper relationships of the discrete spaces.
- FEEC (Finite Element Exterior Calculus) – See recently published “Periodic Table of Finite Elements”, Doug Arnold, et. al., femtable.org. FEEC includes discrete spaces for 0-forms, 1-forms, 2-forms and 3-forms in 3 space for example.
- Frankel, Geometry of Physics, 3rd Ed, Cambridge University Press
- Flanders, Differential Forms with Application to Physical Sciences, Dover.



Lie Derivative and Transport Theorems

Stoke's Theorem in Differential Form notation

$$\int_{\partial M^k} \alpha^{k-1} = \int_{M^k} d\alpha^{k-1}$$

Classical Transport Formulas
in Vector Notation

$$\frac{d}{dt} f = \frac{\partial f}{\partial t} + v \cdot \nabla f$$

$$\frac{d}{dt} \int_{M_t} \alpha = \int_{M_t} \frac{\partial \alpha}{\partial t} + \mathcal{L}_v \alpha = \int_{M_t} \frac{\partial \alpha}{\partial t} + \mathcal{I}_v d\alpha + d\mathcal{I}_v \alpha$$

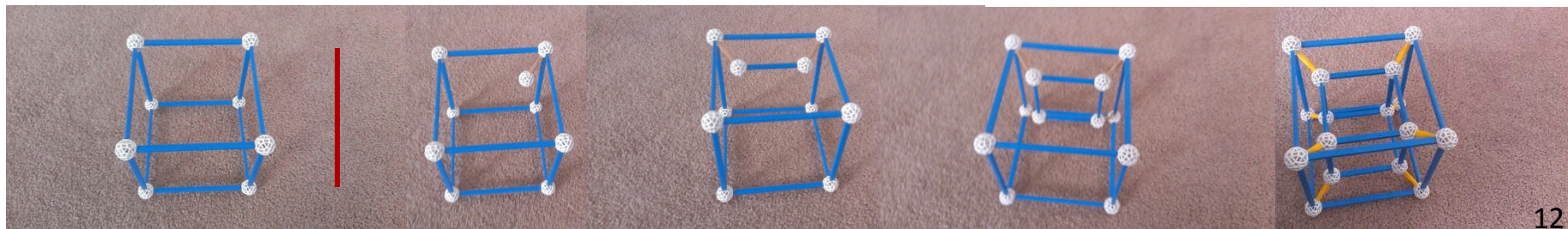


$$\frac{d}{dt} \int_{M_t^1} \mathbf{A} \cdot d\mathbf{x} = \int_{M_t^1} \left[\frac{\partial \mathbf{A}}{\partial t} - \mathbf{v} \times (\nabla \times \mathbf{A}) + \nabla(\mathbf{v} \cdot \mathbf{A}) \right] \cdot d\mathbf{x}$$

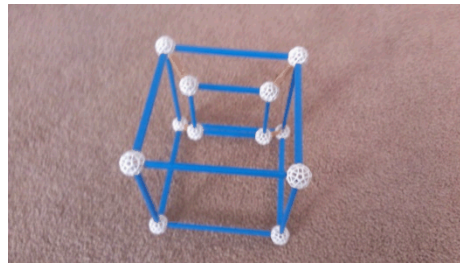
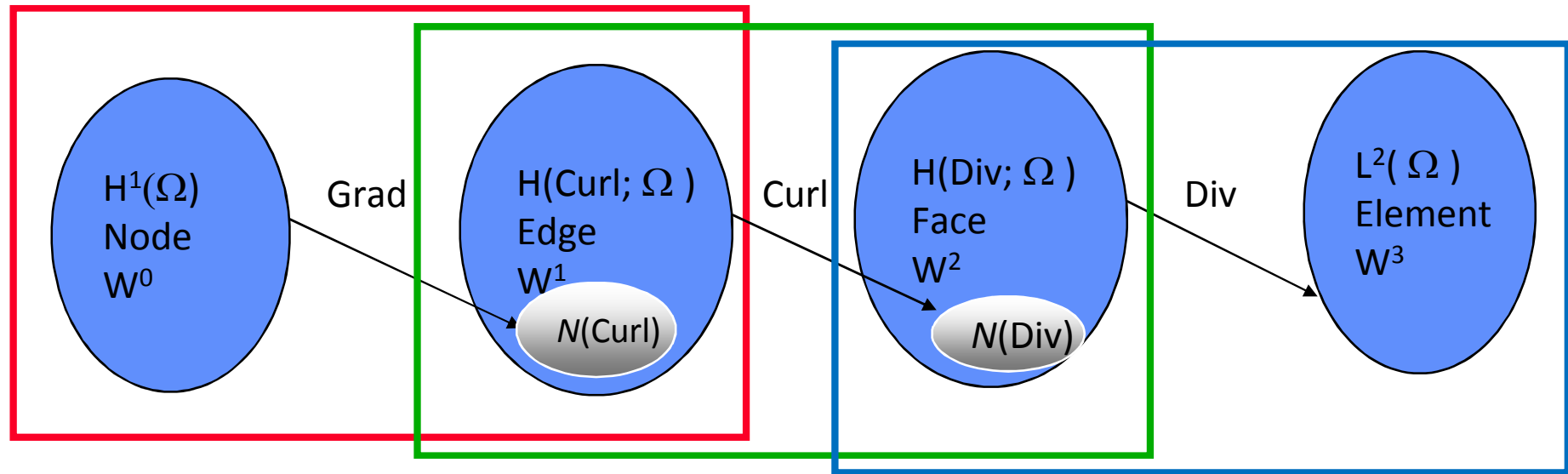
$$\frac{d}{dt} \int_{M_t^2} \mathbf{B} \cdot d\mathbf{a} = \int_{M_t^2} \left[\frac{\partial \mathbf{B}}{\partial t} + \mathbf{v}(\nabla \cdot \mathbf{B}) - \nabla \times (\mathbf{v} \times \mathbf{B}) \right] \cdot d\mathbf{a}$$

$$\frac{d}{dt} \int_{M_t^3} \rho dV = \int_{M_t^3} \left[\frac{\partial \rho}{\partial t} + \nabla \cdot (\mathbf{v} \rho) \right] dV$$

Lie Derivative and Cartan's Magic Formula



Magnetohydrodynamics



Faraday's Law (Natural operator splitting)

A straightforward **B**-field update is possible using Faraday's law.

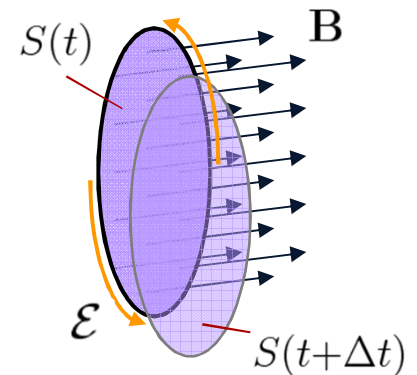
$$\nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0 \quad \mathcal{E} = \mathbf{E} + \mathbf{v} \times \mathbf{B}$$

Integrate over time-dependent surface $S(t)$, apply Stokes theorem, and discretize in time:

$$\frac{d}{dt} \int_{S(t)} \mathbf{B} \cdot d\mathbf{a} + \oint_{\partial S(t)} \mathcal{E} \cdot d\mathbf{x} = 0$$

$$\frac{1}{\Delta t} \int_{S(t+\Delta t)} (\mathbf{B}^{n+1} - \tilde{\mathbf{B}}^{n+1}) \cdot d\mathbf{a}^{n+1} + \oint_{\partial S(t+\Delta t)} \mathcal{E}^{n+1} \cdot d\mathbf{x}^{n+1}$$

$$+ \frac{1}{\Delta t} \left[\int_{S(t+\Delta t)} \tilde{\mathbf{B}}^{n+1} \cdot d\mathbf{a}^{n+1} - \int_{S(t)} \mathbf{B}^n \cdot d\mathbf{a}^n \right] = 0$$



Zero for ideal MHD by frozen-in flux theorem:

$$\frac{d}{dt} \int_{S_t} \mathbf{B} \cdot d\mathbf{a} = \int_{S_t} \mathbf{B}^* \cdot d\mathbf{a} = 0$$

Terms in red are zero for ideal MHD so nothing needs to be done if fluxes are degrees of freedom.

Solve magnetic diffusion using edge/face elements which preserve discrete divergence free property

Ω = a single conducting region in $\mathbb{R}^3$.

weakly enforced

$$\nabla \times \mathbf{H} = \mathbf{J}$$

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

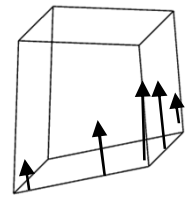
$$\mathbf{B} = \mu \mathbf{H}$$

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0 \quad \text{Exact relationship}$$

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

$$\mathbf{J} = \sigma \mathbf{E}$$

$$\text{boundary conditions} \begin{cases} \mathbf{E} \times \mathbf{n} = \mathbf{E}_b \times \mathbf{n} \text{ on } \Gamma_1 (\text{Dirichlet}), \\ \mathbf{H} \times \mathbf{n} = \mathbf{H}_b \times \mathbf{n} \text{ on } \Gamma_2 (\text{Neumann}) \end{cases}$$



Edge element

$$\int \sigma \mathbf{E}^{n+1} \cdot \hat{\mathbf{E}} dV + \Delta t \int \frac{\text{curl } \mathbf{E}^{n+1} \cdot \text{curl } \hat{\mathbf{E}}}{\mu} dV = \int \frac{\mathbf{B}^n \cdot \text{curl } \hat{\mathbf{E}}}{\mu} dV - \int \mathbf{H}_b \times \mathbf{n} \cdot \hat{\mathbf{E}} dA$$

$\mathbf{B}$ = magnetic flux density $\mathbf{E}$ = electric field $\mathbf{H}$ = magnetic field

μ = permeability σ = conductivity $\mathbf{J}$ = current density

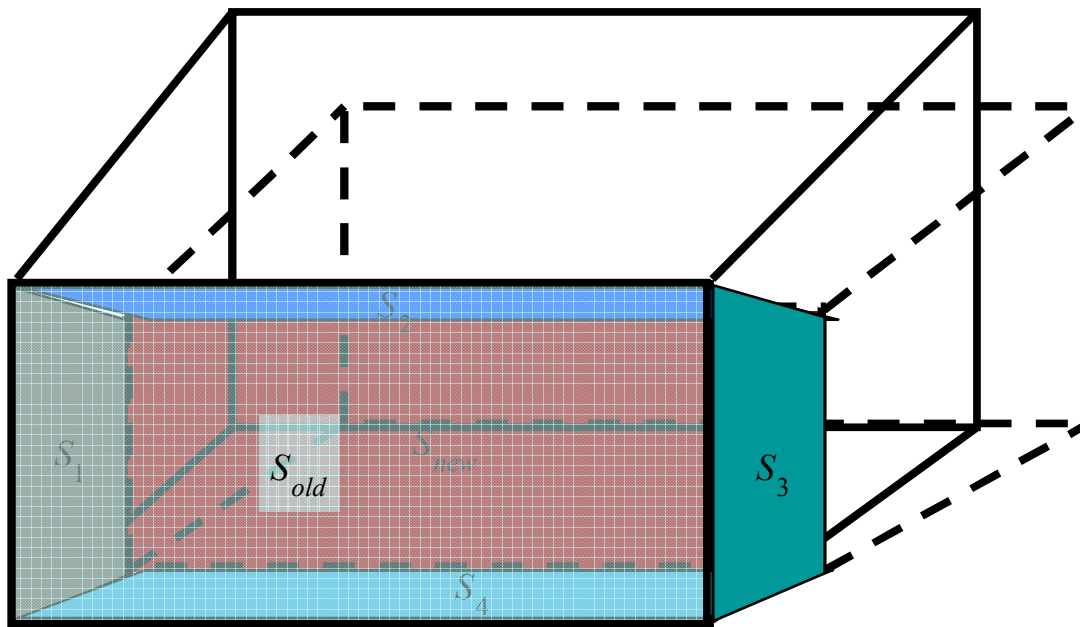
μ and σ positive and finite everywhere in W

Magnetic Flux Density Remap

- The Lagrangian step maintains the discrete divergence free property via flux density updates given only in term of discrete curls of edge circulation variables.
- The remap should not destroy this property.
- The $d\mathcal{I}_v\alpha$ part of the remap algorithm is fundamentally unsplit in order to ensure that the global divergence free property is maintained.

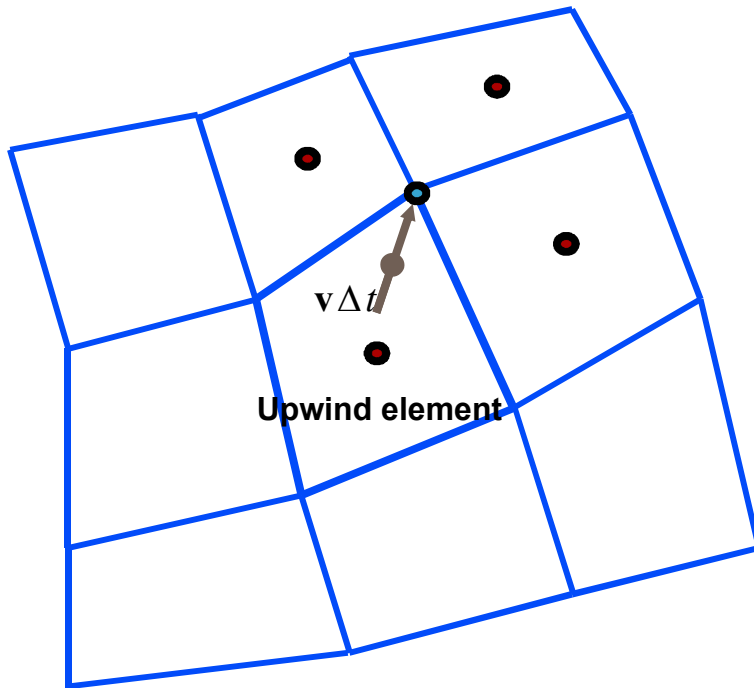
Flux remap step

$$\int_S \mathbf{B} \cdot d\mathbf{a} = 0 \quad \int_{S_{old}} \mathbf{B} \cdot d\mathbf{a} + \int_{S_{new}} \mathbf{B} \cdot d\mathbf{a} + \sum_{i=1}^4 \int_{S_i} \mathbf{B} \cdot (\mathbf{v}_g \Delta t \times d\mathbf{l}) = 0$$



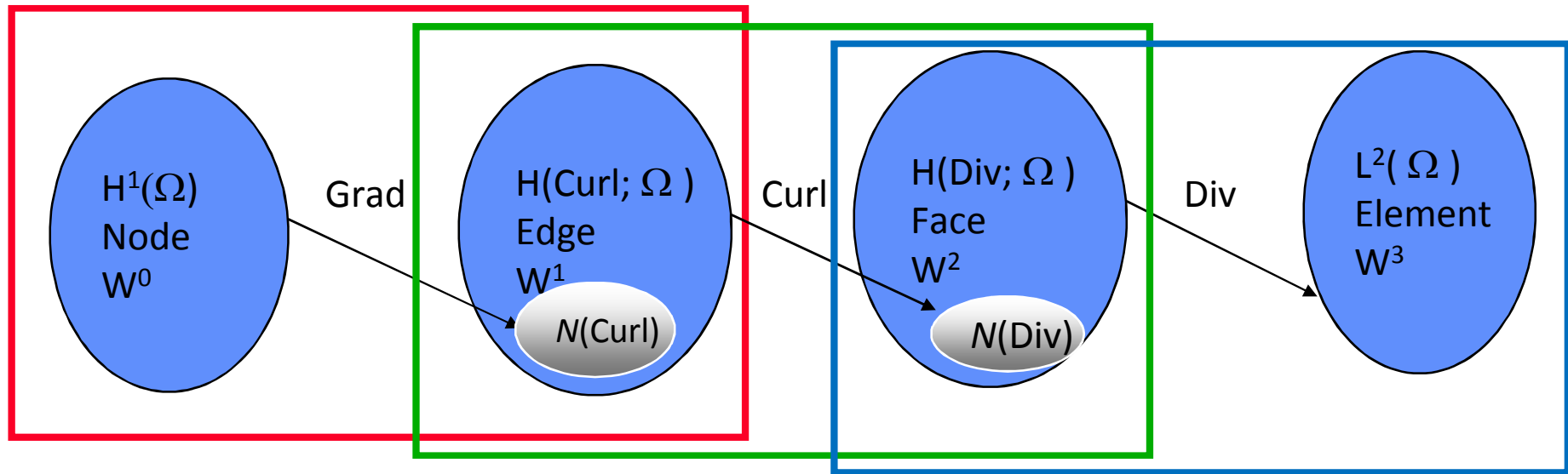
$$\int_{S_{old}} \mathbf{B} \cdot d\mathbf{a} + \int_{S_{new}} \mathbf{B} \cdot d\mathbf{a} + \sum_{i=1}^4 \int_{S_i} d\mathbf{l} \cdot (\mathbf{B} \times \mathbf{v}_g \Delta t) = 0$$

Constrained Transport Type Algorithm



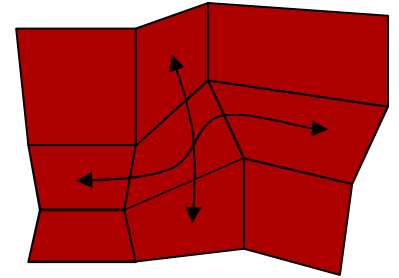
- Compute B at nodes from the face element representation at element centers. This must be **second order accurate**.
 - Compute trial cross face element flux coefficients on each face using these nodal B .
 - Limit on each face to obtain cross face flux coefficients which contribute zero total flux.
 - Compute the edge flux contributions in the upwind element by a midpoint integration rule at the center of the edge centered motion vector.
-
- "Arbitrary Lagrangian-Eulerian 3D Ideal MHD Algorithms," Int. Journal Numerical Methods in Fluids, 2011;65:1438-1450. (remap and deBar energy conservation discussed)

Mass Conservation



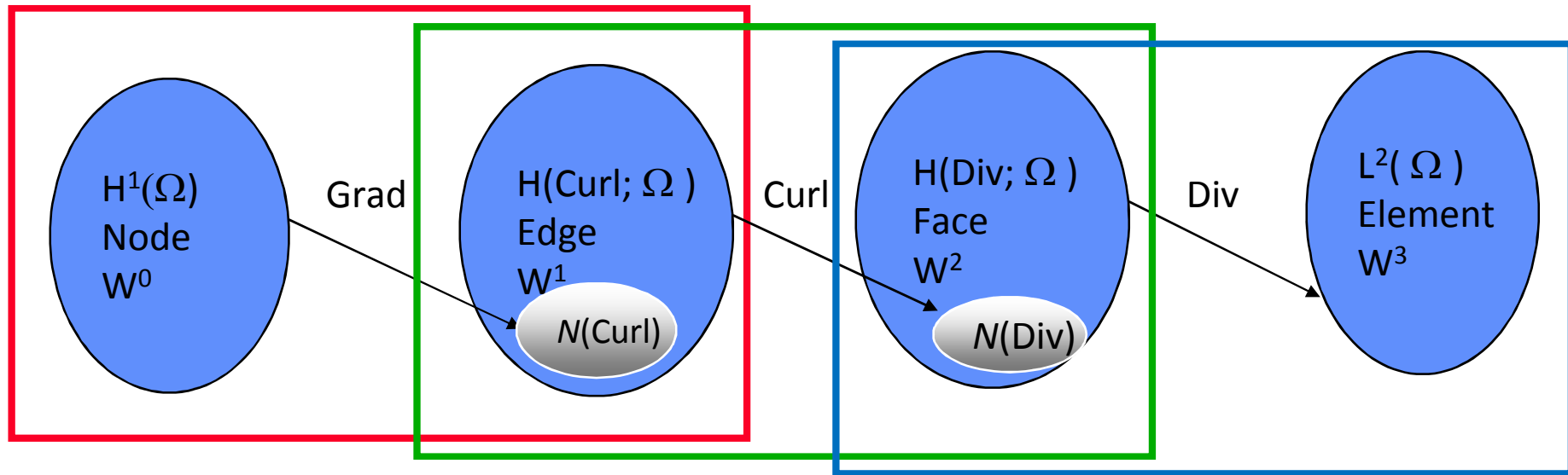
Mass Conservation

- Lagrangian Step
 - Mass is conserved in the Lagrangian frame.
 - Discrete Lagrangian continuity equation is trivial.
- Remap Step
 - Integration of reconstructed densities over swept surfaces or intersecting grids yield conservative mass changes.

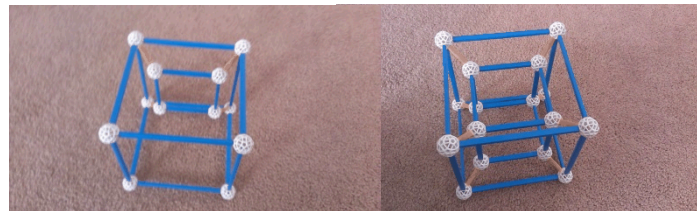


Cartan Magic Formula has Two Parts:

When might one need both parts for remap?

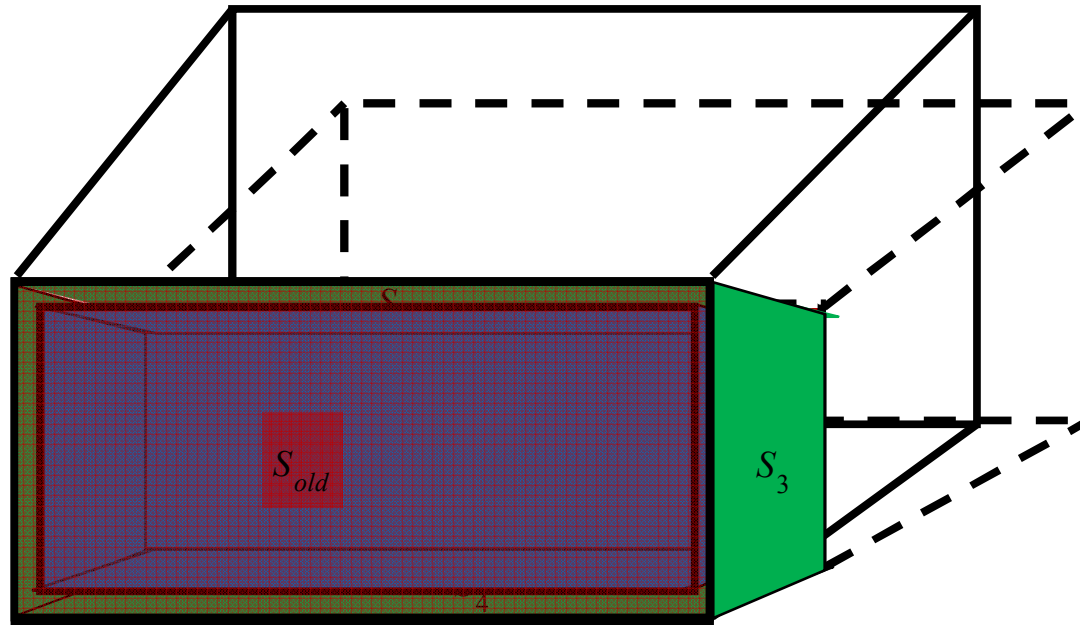


Full Maxwell equations associated with generalized Ohm's Law xMHD model is a possible example.



How would this work?

$$\frac{\partial \mathbf{D}}{\partial t} + \boxed{\nabla \times (\mathbf{D} \times \mathbf{v})} + \boxed{\mathbf{v}(\nabla \cdot \mathbf{D})}$$



New electric displacement flux is the oriented **sum of swept edge contributions which do not change the charge** plus **swept volume contributions which do**.
This is simply the divergence theorem (generalized Stoke's theorem).

Reduced models are extremely useful in the right context.

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

Not very practical for 3D detonator modeling.

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

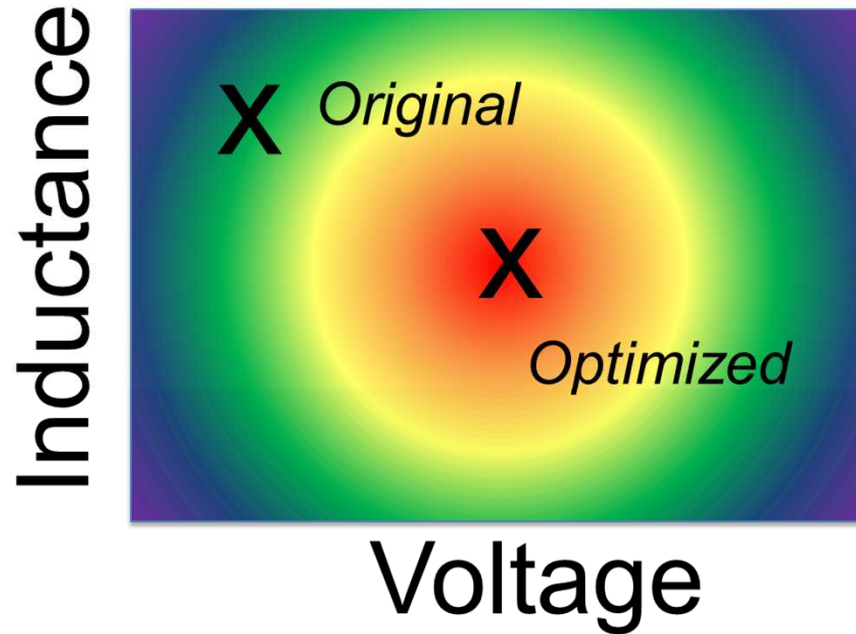
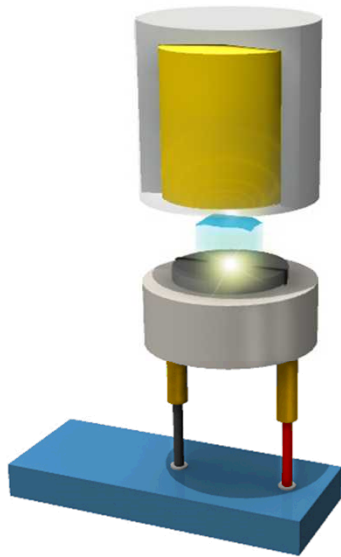


$$R_m \ll 1$$

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

Practical 3D detonator modeling

A sufficient and efficient model enables parameter scans and optimization.



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

ALEGRA (FE) Quasi-static electric field approximation to Maxwell Equations

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

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

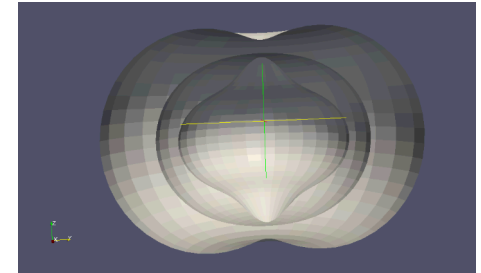
$$\rho \dot{e} = \rho s + \mathbf{T} : \mathbf{L} - \nabla \cdot \mathbf{q}$$

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

$$\nabla \cdot \mathbf{D} = 0 \Rightarrow \nabla \cdot (\epsilon \nabla \phi) = \nabla \cdot \mathbf{p}$$

$$\mathbf{T} = \mathbf{T}(\mathbf{S}, \mathbf{E})$$

$$\mathbf{D} = \mathbf{p}(\mathbf{S}) + \epsilon(\mathbf{S}) \mathbf{E}$$



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

$$\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P} = \epsilon \mathbf{E} + \mathbf{p}$$

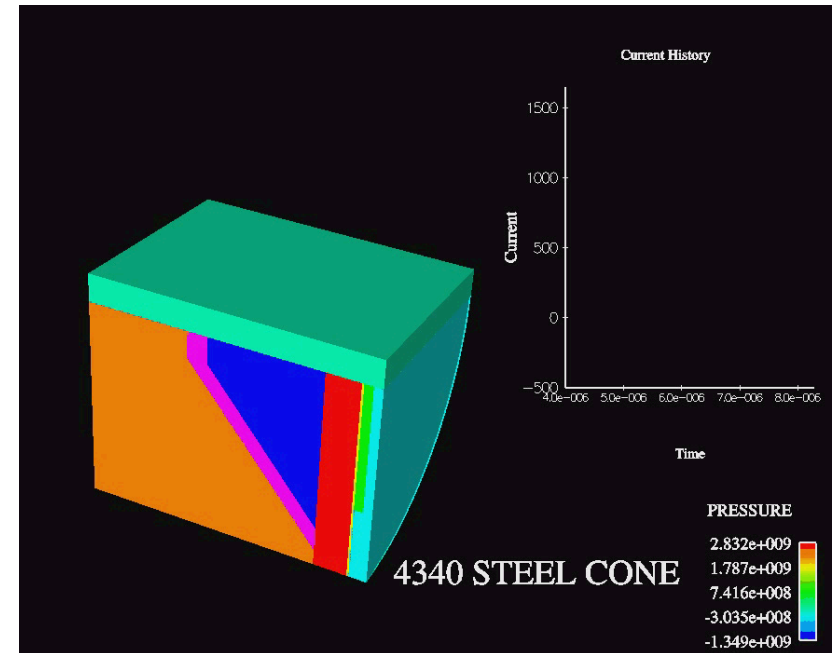
material
polarization

permittivity

remnant, permanent or spontaneous
polarization

ALEGRA (FE) electromechanical analysis provides for Fuze/ Power Supply Modeling

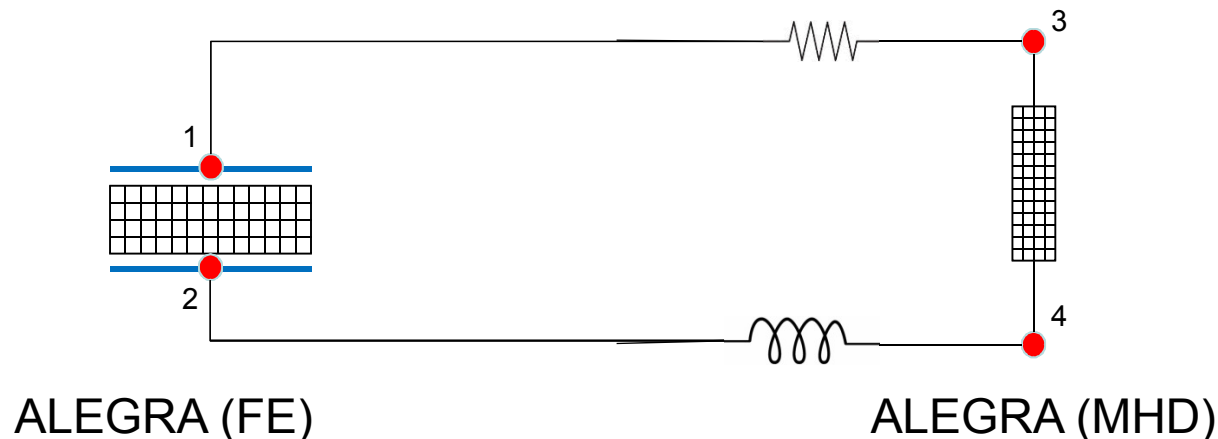
- Coupled mechanical/electric field based modeling
- Circuit coupling essential
- Advanced hydrodynamic ALE techniques are important.
- Excellent coordination between experimental data acquisition and material modeling expertise is required.



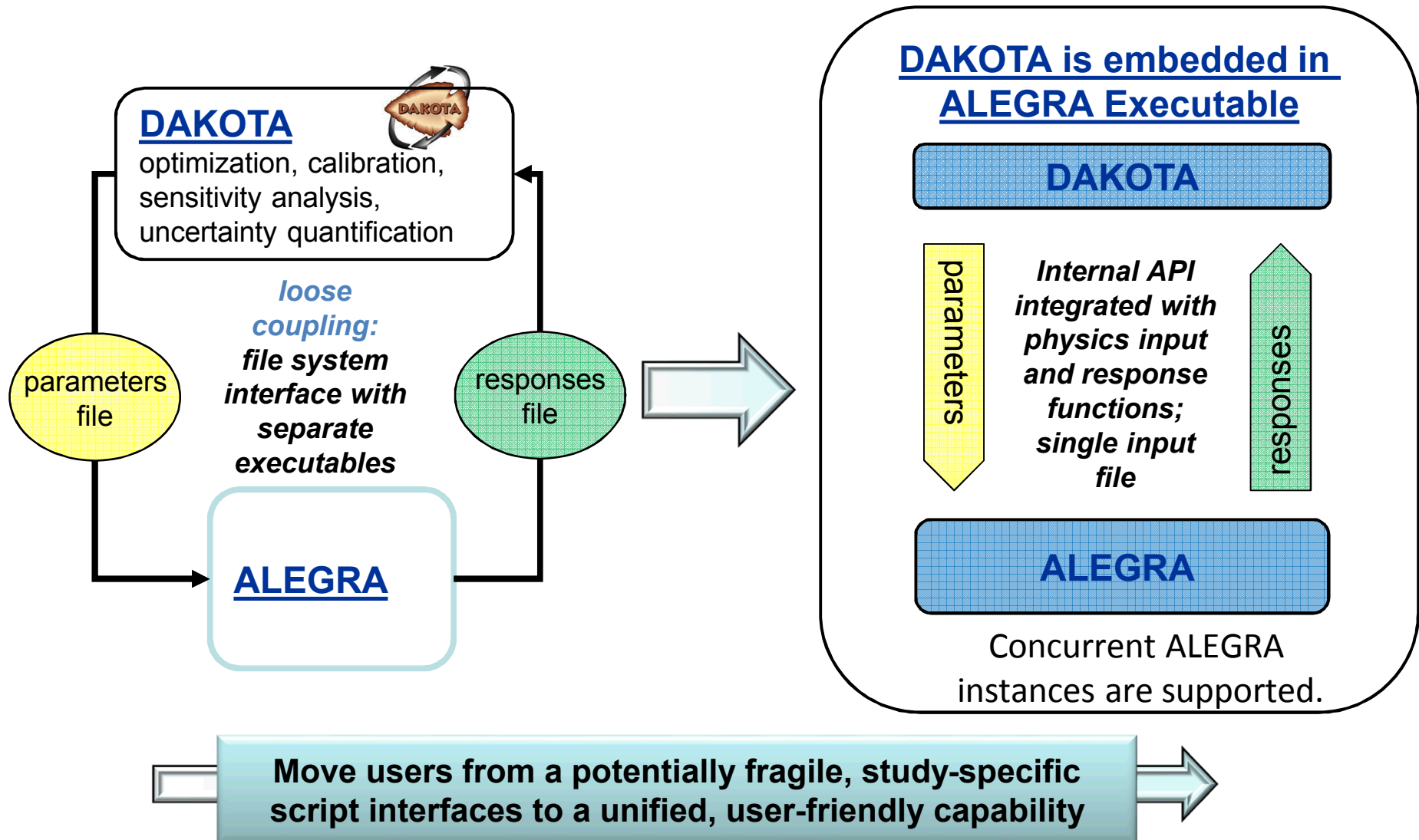
Movie shows an example simulation of a shock actuated power supply.

Electrically Coupled Modeling

- Full system component models can be usefully connected via external circuits. One directional coupling is not always defensible.
- MPI communicator technology allows for simultaneous circuit coupled ALEGRA models. Multiple executables appear on the MPIrun command line.
- Run different geometry (2D/3D) and/or electromagnetic physics problems synchronously and with external circuit.



Sampling based meta-analysis approach for enabling users

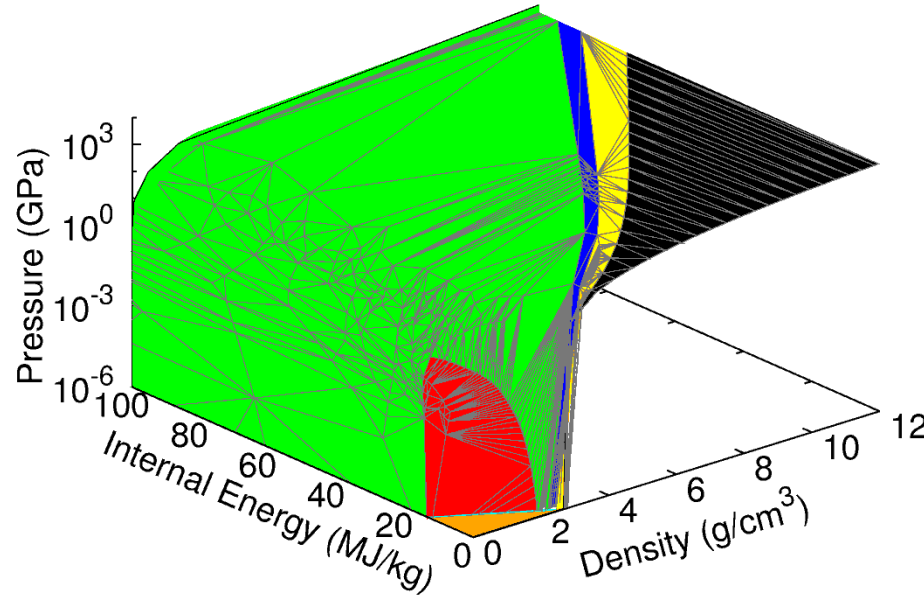


Example: UQ Representation of EOS

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

Tabular EOS with Uncertainty Available



Phases:

off table

solid

fluid

melt

vaporization

sublimation

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

- N sample tables with consistent topological meshing step is the starting point
- Export a truncated set of mode tables that capture most of the details (i.e. eigenspectrum energy)
- 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. We must provide means for the user to sample properly with independent random variables provided by DAKOTA.

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

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

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

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



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

Undergraduate Students

- Undergraduate student can be extremely helpful and they also benefit tremendously from Sandia internship program.
- Contributions generally focus on verification related activities. I will mention only 3 examples:
 - Chace Ashcraft – Transient magnetics verification
 - Brad Hanks – Testing of ALEGRA in a difficult 2D isentropic flow test problem.
 - Koa Fischer – Forced shock Burger's QOI's.

Axisymmetric magnetic diffusion (SAND2016-0804)

$$\frac{\partial B_\theta}{\partial t} = \frac{\partial}{\partial r} \left(\frac{\eta}{\mu r} \frac{\partial (r B_\theta)}{\partial r} \right) + \frac{\partial}{\partial z} \left(\frac{\eta}{\mu} \frac{\partial B_\theta}{\partial z} \right)$$

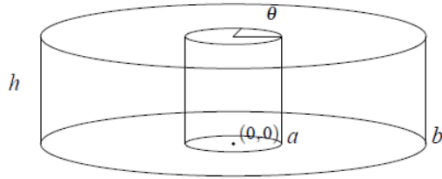
$$\psi = r B_\theta$$

$$\frac{\partial \psi}{\partial t} = r \frac{\partial}{\partial r} \left(\frac{\eta}{\mu r} \frac{\partial \psi}{\partial r} \right) + \frac{\partial}{\partial z} \left(\frac{\eta}{\mu} \frac{\partial \psi}{\partial z} \right)$$

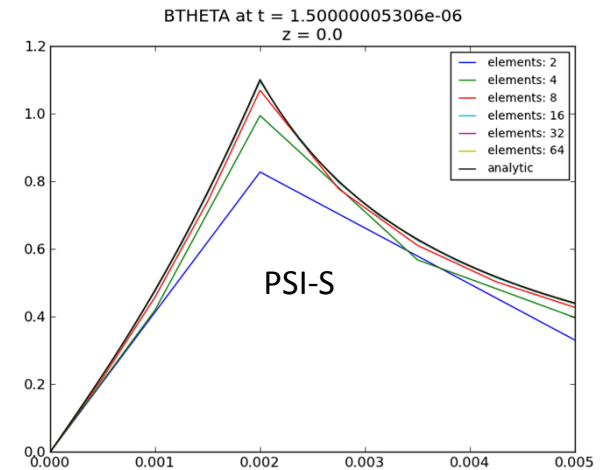
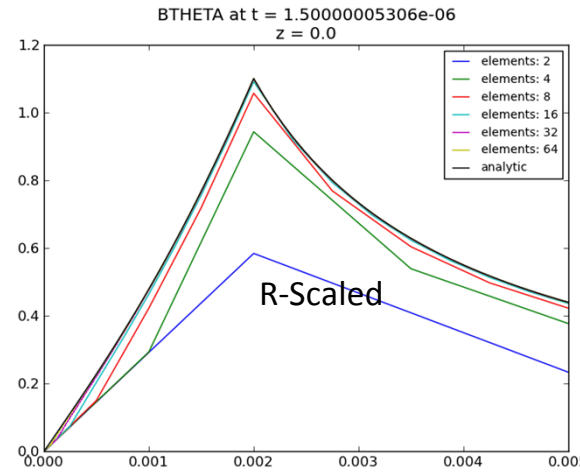
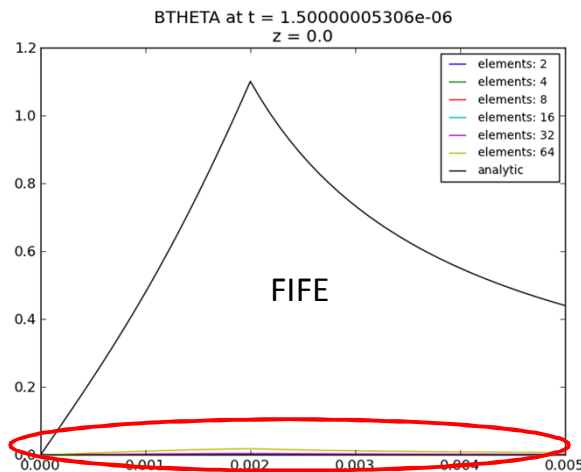
$$s = r^2$$

$$\frac{1}{2s} \frac{\partial \psi}{\partial t} = \frac{\partial}{\partial s} \left(\frac{2\eta}{\mu} \frac{\partial \psi}{\partial s} \right) + \frac{\partial}{\partial z} \left(\frac{\eta}{2s\mu} \frac{\partial \psi}{\partial z} \right)$$

Mellissen and Simkin, 1990



- We developed a two region fully time dependent transient magnetic solution to mimic an exploding wire configuration with a separation of variables approach for verification purposes.

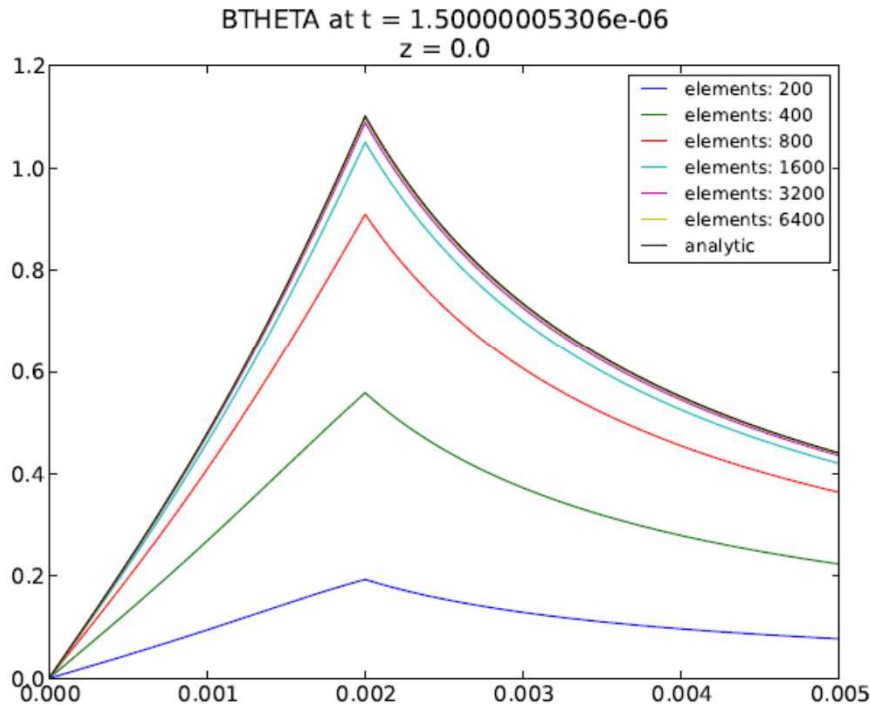


Elements/block	Convergence Order
1	2.09611e-01
2	2.09611e-01
4	7.31077e-02
8	2.16658e-02
16	1.01580e-02
32	2.09721e-02

Elements/block	Convergence Order
1	1.59109e00
2	1.59109e00
4	1.60632e00
8	1.66119e00
16	1.53120e00
32	1.45542e00

Elements/block	Convergence Order
1	1.52672e00
2	1.52672e00
4	1.75725e00
8	2.24243e00
16	2.33500e00
32	2.03655e00

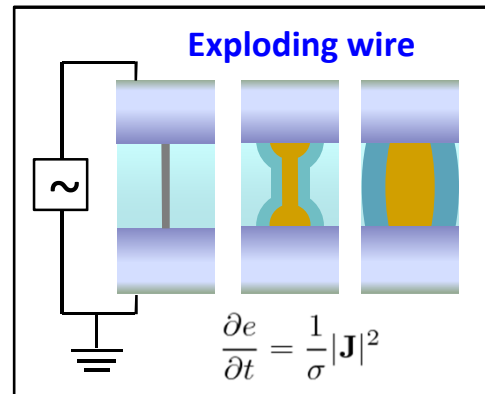
A second order convergent method (FIFE) may still be practically useless on some problems.



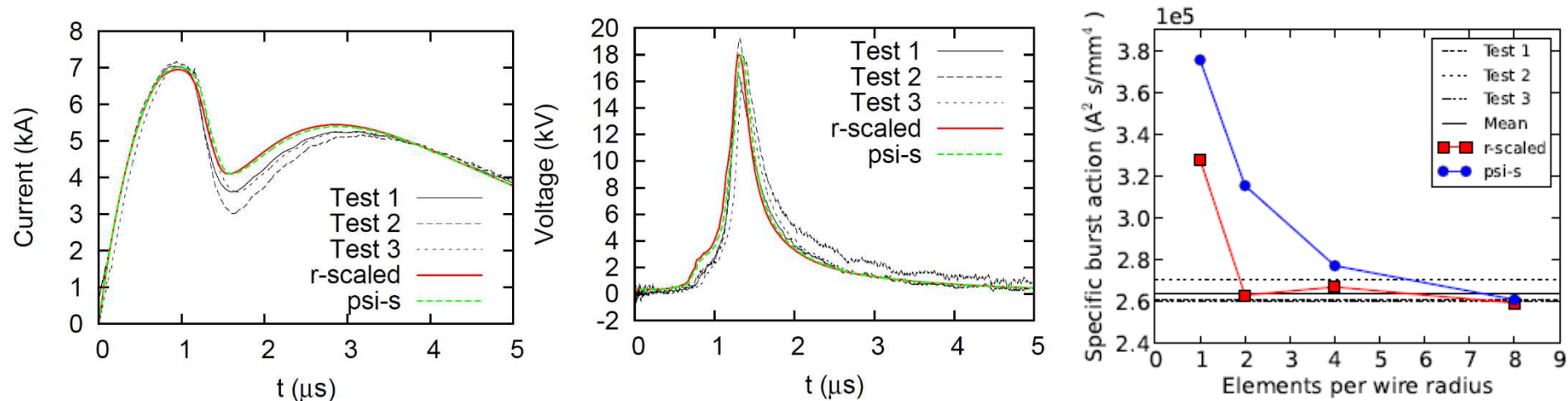
Number of elements per block	Order of convergence
100	7.60723e-01
200	7.60723e-01
400	1.50851e+00
800	1.91023e+00
1600	2.01595e+00
3200	2.00151e+00

Straightforward discretization of first equation using linear finite elements is completely inadequate.

Validation testing for exploding aluminum wire

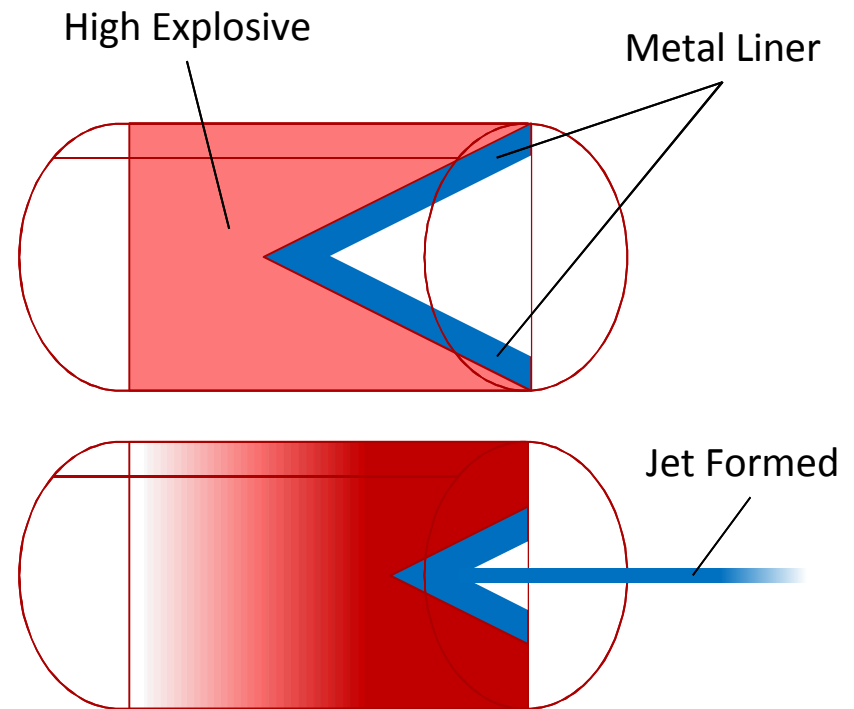


Validation work published in January (SAND2016-0804) compares ALEGRA results using two axisymmetric MHD formulations (“r-scaled” and “psi-s”) to experimental tests conducted by ARL:



Investigation of ALEGRA Shock Hydrocode Algorithms Using an Exact Free Surface Jet Solution (SAND2014-0479)

- A shaped charge is a cylinder packed with high explosive around a metal liner.
- Detonation of explosive material causes the collapse of a liner which forms a metal jet.
- Shaped charges have been used for armor penetration.
- Subsonic collapse speed of the liner is necessary for coherent jets
- We will be modeling a flow that mimics a shaped charge in planar geometry.



The idea is to stress a shock code in a two dimensional shockless regime.

Planar Analytic Solution

- Irrotational, subsonic, steady, and isentropic
- Flow is solved in the hodograph plane with the velocity and flow angle, q and θ respectively.
- Conservation of mass implies the existence of a stream function from which a separable second order linear equation is formed.
- Complex variable techniques for the incompressible case lead to the form of the solution in the compressible case.
- Solution is integrated to obtain the physical plane.

$$dz = dx + i dy = \frac{e^{i\theta}}{q} \left(d\phi + \frac{i}{\rho} d\psi \right)$$

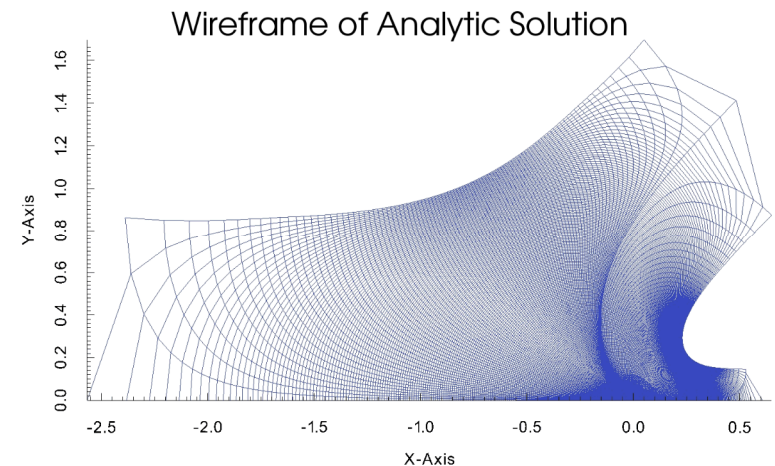
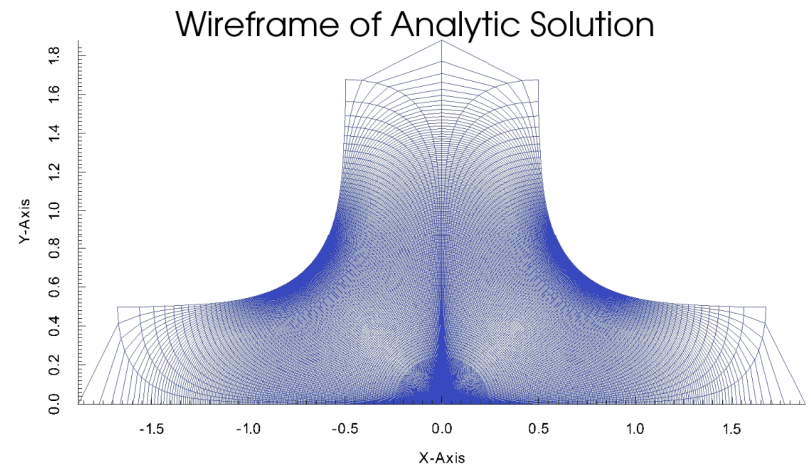
$$\frac{\partial \phi}{\partial \theta} = \frac{q}{\rho} \frac{\partial \psi}{\partial q} \qquad \frac{\partial \phi}{\partial q} = -\frac{(1 - M^2)}{q\rho} \frac{\partial \psi}{\partial \theta}$$

$$q^2 \frac{\partial^2 \psi}{\partial q^2} + q(1 + M^2) \frac{\partial \psi}{\partial q} + (1 - M^2) \frac{\partial^2 \psi}{\partial \theta^2} = 0$$

$$\psi = ((\rho_1 q_1)/\pi) \left\{ \sum_{n=2}^{\infty} \frac{1}{n} \frac{\psi_n(\tau)}{\psi_n(\tau_1)} \sin n(\theta - \beta + \pi) \right. \\ + \sum_{n=2}^{\infty} \frac{1}{n} \frac{\psi_n(\tau)}{\psi_n(\tau_1)} \sin n(\theta + \beta - \pi) \\ - (1 - \cos \beta) \sum_{n=2}^{\infty} \frac{1}{n} \frac{\psi_n(\tau)}{\psi_n(\tau_1)} \sin n\theta \\ \left. + (1 + \cos \beta) \sum_{n=2}^{\infty} \frac{1}{n} \frac{\psi_n(\tau)}{\psi_n(\tau_1)} \sin n(\theta - \pi) \right\}$$

CJETB Code

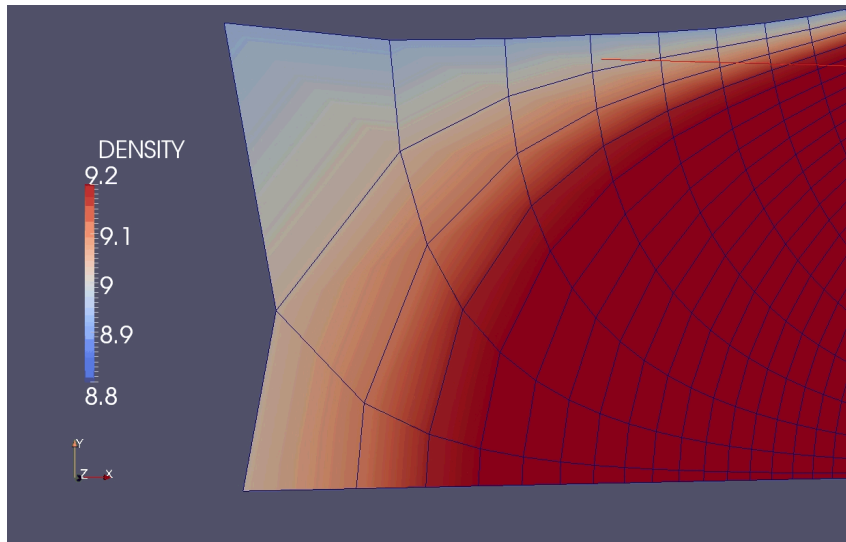
- Plane Subsonic Isentropic Fluid Flow, no strength
- Exodus solution from CJETB code – Robinson SAND2002-1015
- Exodus file contains two timesteps
 - Timestep 1 - $\beta = 90^\circ$
 - Timestep 2 - $\beta = 45^\circ$
- Mach number 0.9 with a pressure shifted ideal gas EOS matching copper properties.



Diatom – Exodus Solution Import

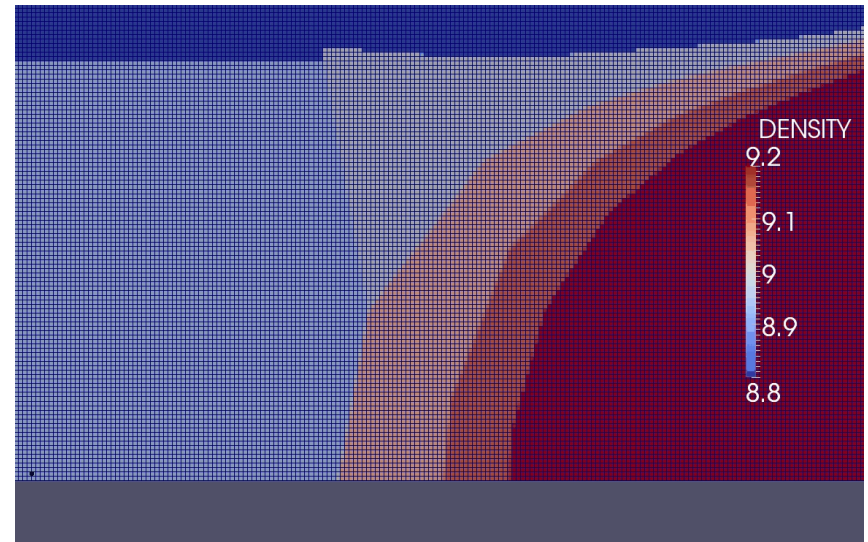
Exact Solution

- Created in CJETB code
- Mesh based on (q, θ) space
- Contains information throughout cells



Imported Solution

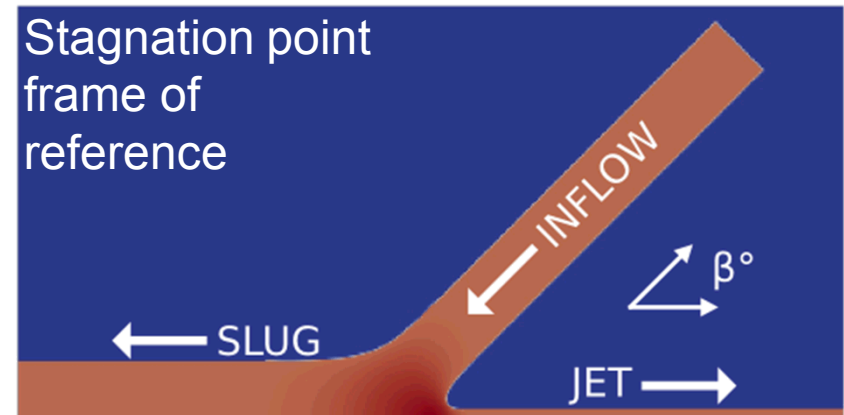
- Mesh more resolved than exact solution
- No interpolation
- Value taken from cell center



Errors may occur when ALEGRA mesh resolution is more refined than the exact solution. Issue resolved by increasing the resolution of the exact solution.

Verification Testing in ALEGRA

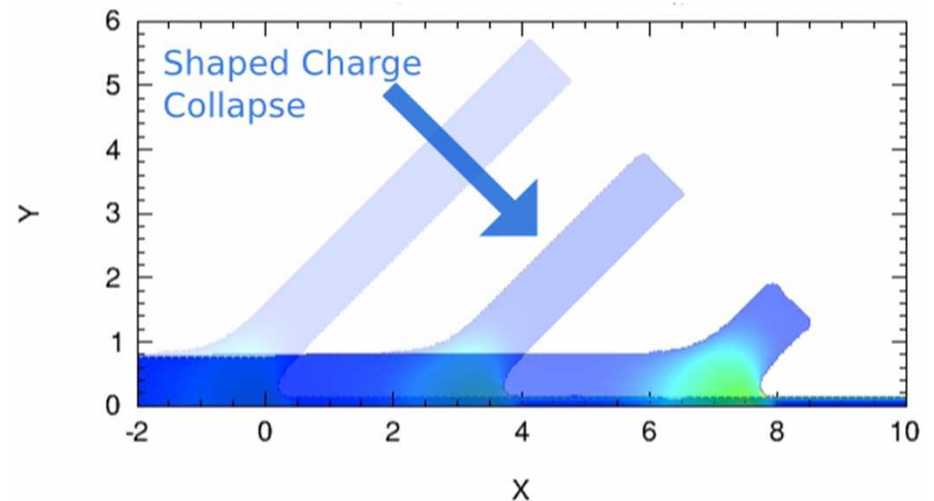
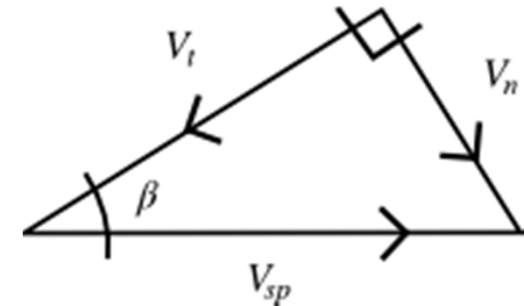
- Two incident angles and frames of reference
 - $\beta = 90^\circ$ & 45°
 - Stagnation point and Laboratory frame of reference
- Mesh resolution is displayed by the number of elements across the jet.
- Initial state should remain unchanged due to steady state isentropic flow.



Verification Testing in ALEGRA

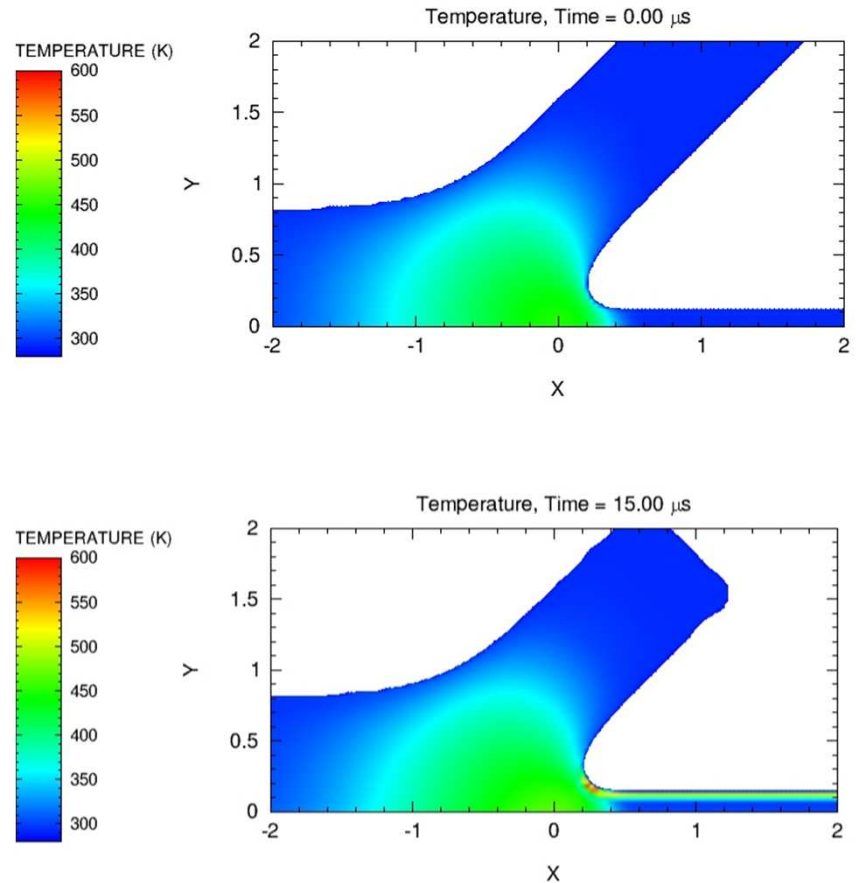
- Laboratory frame of reference
 - It is a traditional way of viewing a shaped charge with the liner collapsing to form the jet.
 - Slightly more complex than the stagnation point frame of reference.

$$V_{sp} = \frac{V_t}{\cos \beta} = \frac{V_n}{\sin \beta}$$



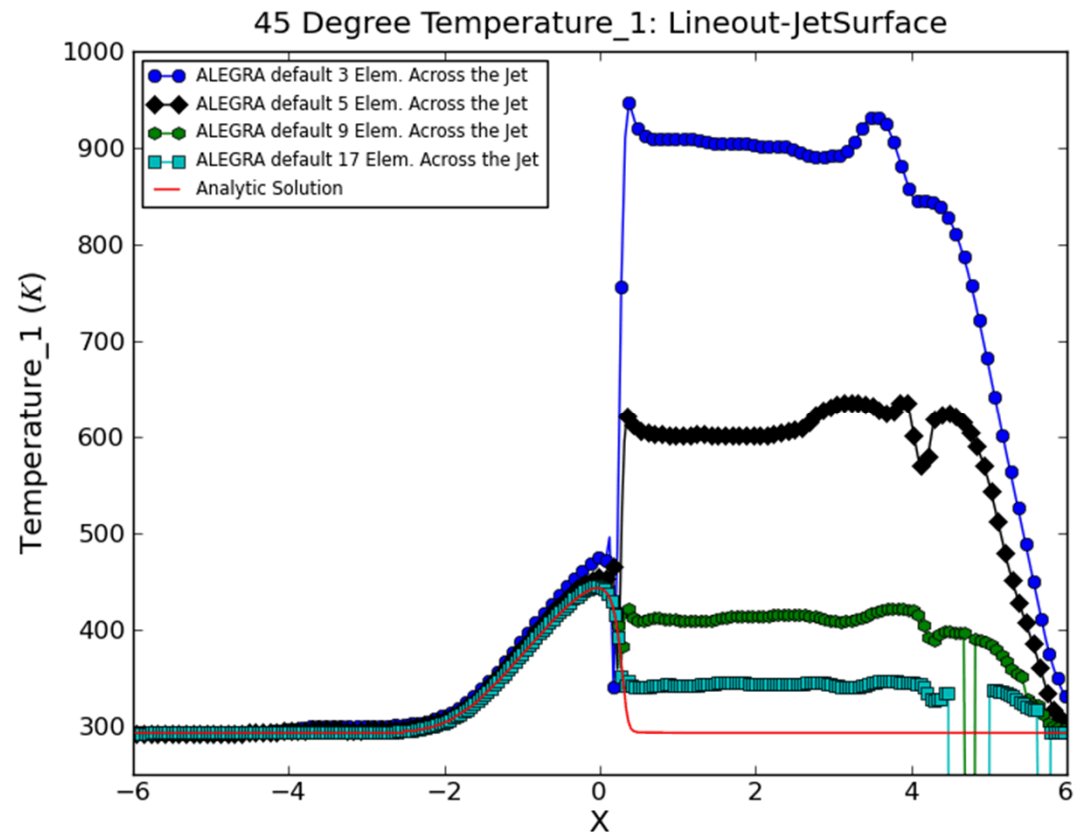
Some results with ALEGRA

- Small initial oscillations occurred based on imperfections with the exact solution and initial conditions for the equation of state
- Quasi-steady state achieved and errors from initial oscillations are pushed out as more material moves through the stagnation point region
- Anomalous heating found specifically in the tight corner and along the jet surface



Mesh Resolution study

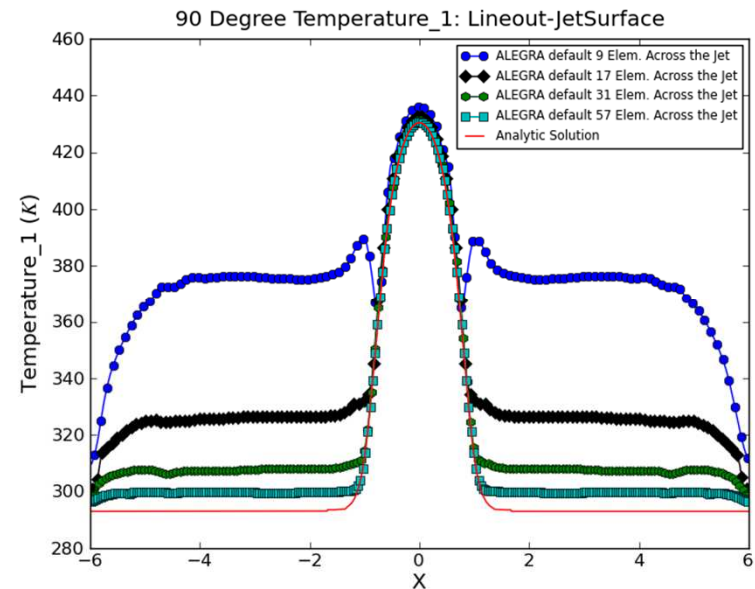
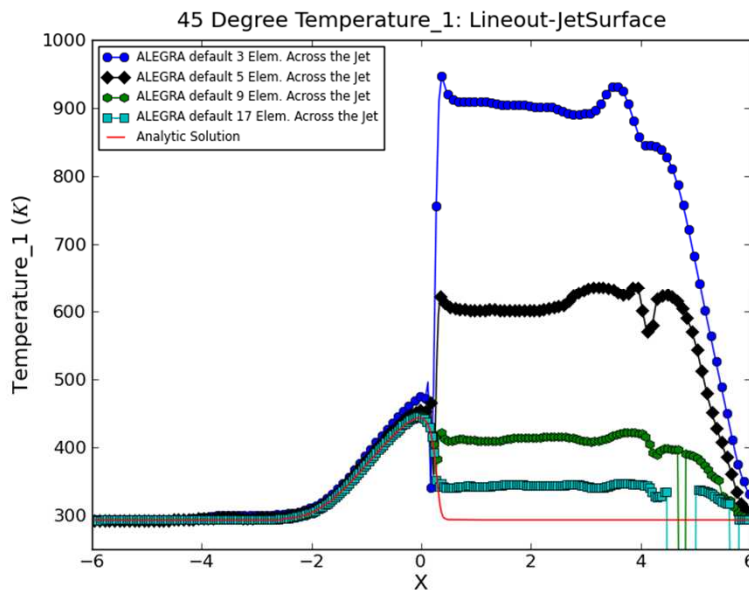
- Quasi-steady solution and initial oscillations are shown.
- Simulation improves with increasing mesh resolution.



Effect of inflow angle

A comparison of various inflow angles appears to show that error increases with a tighter corner.

Note variation in temperature scales



Testing methodology is permanently stored in test suite as a challenge to develop better numerical methods.

Verification of a Forced Burger's Equation

- Forced Burger's Equation
- Solve through the method of characteristics using a particular initial condition.
- This work is looking toward careful verification of adjoint based methodologies in next generation codes.

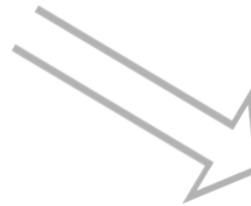


$$\frac{\partial u}{\partial t} + \frac{\partial(\frac{1}{2}u^2)}{\partial x} = s$$



$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = s$$

$$\frac{du}{dt} = s \text{ on } \frac{dx}{dt} = u$$

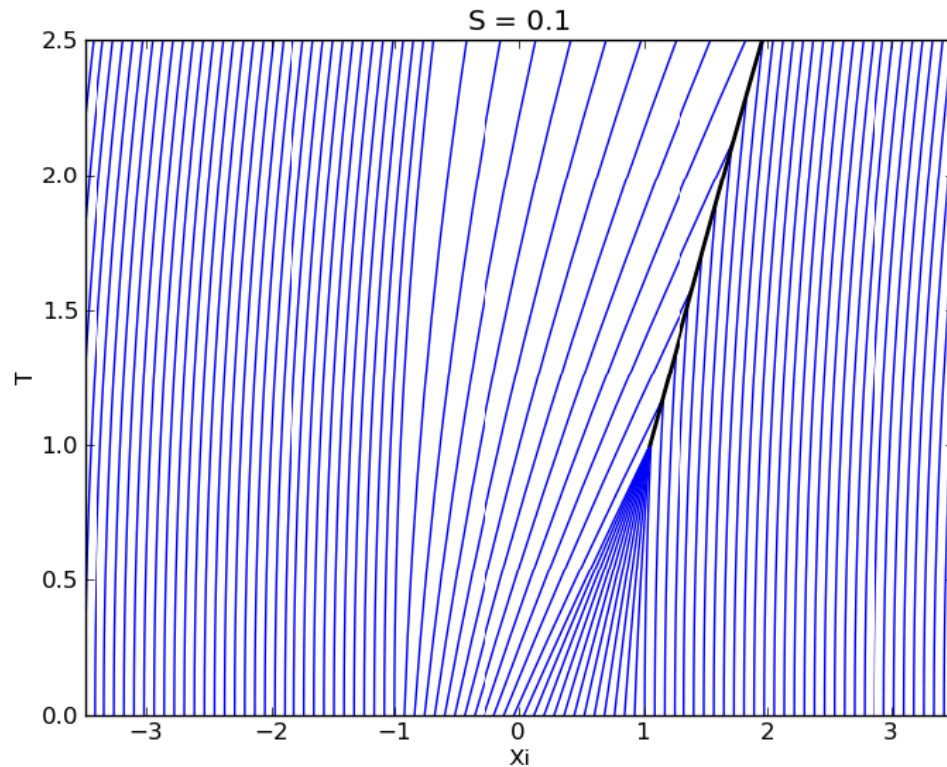


$$u = st + f(\xi),$$

$$x = \frac{1}{2}st^2 + f(\xi)t + \xi$$

$$f(\xi) = \begin{cases} 0 & \text{if } \xi < -1, \\ (1 + \xi) & \text{if } -1 \leq \xi < 0, \\ (1 - \xi) & \text{if } 0 \leq \xi < 1, \\ 0 & \text{if } 1 \leq \xi \end{cases}$$

Forced Burger's Equation Shock Curve



Shock jump condition

$$-\dot{x}_s[u] + \left[\frac{1}{2}u^2\right] = 0$$

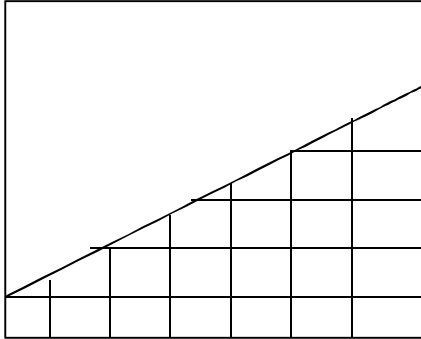
We have the solutions on either side of where we want to fit the shock.

Substitution gives an ODE which can be solved for the shock curve.

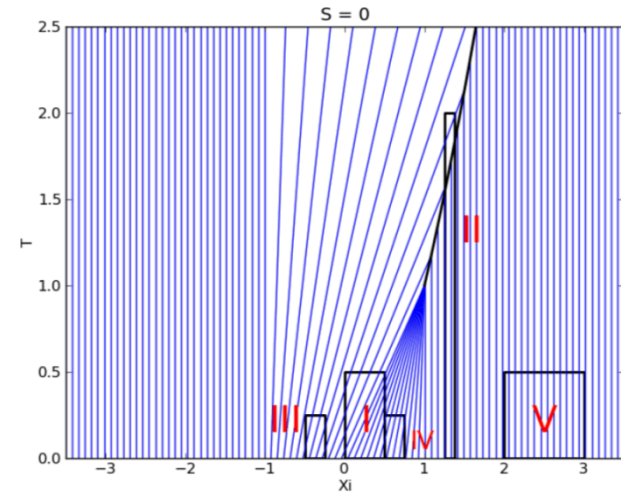
$$x_s = \frac{st^2}{2} + (1 + \xi_-)t + \xi_-, \quad u_- = st + (1 + \xi_-) \quad x_s = \frac{st^2}{2} + \xi_+, \quad u_+ = st$$

$$x_s = \frac{1}{2}st^2 - 1 + \sqrt{2}(1 + t)^{\frac{1}{2}}$$

Example computation via numerical integration of integral quantities of interest.



$$t(x, s) = \frac{2x}{1 + \sqrt{1 + 2sx}}$$



$$Q_I(s; u) = \int_0^{\frac{1}{2}} \left(\int_0^{t(x,s)} st + \left(1 - \frac{x - \frac{1}{2}st^2 - t}{(1-t)}\right) dt + \int_{t(x,s)}^{\frac{1}{2}} st + \left(1 + \frac{x - \frac{1}{2}st^2 - t}{(1+t)}\right) dt \right) dx$$

Linear and non-linear quantities of interest and derivatives with respect to parameters. This is useful for testing adjoint methodologies across bounding characteristics and shocks.

Exact $Q_i(s; u)$						
		1	2	3	4	5
s	0	0.210624	0.033201	0.034866	0.026970	0.000000
	0.1	0.216675	0.080950	0.035593	0.027832	0.012500
	0.2	0.222693	0.118001	0.036319	0.028693	0.025000
	0.3	0.228681	0.150004	0.037045	0.029555	0.037500

TABLE 3.1

Exact $Q'_i(s; u^2)$						
		1	2	3	4	5
s	0	0.104167	0.385417	0.007812	0.007813	0.000000
	0.1	0.107292	0.418750	0.008034	0.008138	0.008333
	0.2	0.110417	0.452083	0.008255	0.008464	0.016667
	0.3	0.113542	0.485417	0.008477	0.008789	0.025000

TABLE 3.16

What are useful skill sets for students?

- Classical applied math/physics (E&M)/engineering
- Programming skills, e.g. Python, C++, ...
- Concepts in linear and non-linear wave propagation and PDEs.
- Numerical analysis and methods for ODE and PDE.
- Abilities to work well with others and communicate effectively.
- Test Driven Development, Source Code Management and code quality concepts

Principles for a Successful Multiphysics Production Code

- Pay attention to user's needs and keep your paying customers happy.
- Pay attention to getting the physics right (Closure properties)
- Algorithmic robustness and quality is important.
- A general code leads to many software libraries and multiple initial, boundary condition, circuit coupling, algorithmic choices approaches. Software quality will catch up to you.
- Code team culture/disciplined software process is key. Use a team software platform effectively (e.g. Teamforge, GitHub, GitLab)
- Commitment to high quality testing and a clean comprehensive test suite is essential.
- You can't do it alone. Value everyone's strengths.
- A team ethic of continuous improvement will serve you well.

Summary

- ALEGRA is an arbitrary Lagrangian-Eulerian multiphysics code able to deal with difficult and sophisticated applications.
- Modern compatible discretization concepts fit naturally and effectively fit into an ALE multiphysics approach.
- Representing uncertainties in closure properties are being considered and meta analysis can be effectively enabled.
- Extensive V&V and continual code improvement is the natural permanent state for both developers and users.
- Undergraduate students can play an important and valued part of this process.