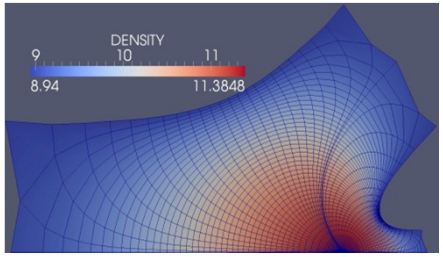
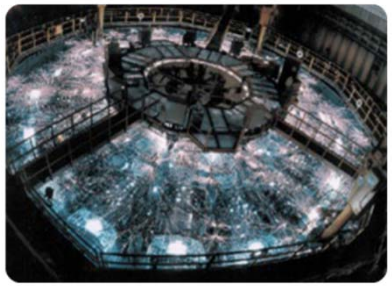
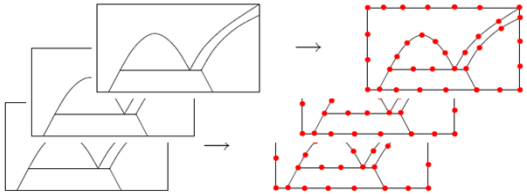
Exceptional service in the national interest

Sandia National Laboratories







Mathematical Themes in my Career at Sandia National Laboratories

Allen C. Robinson

Computational Shock & Multiphysics

Presented at Brigham Young University, Provo, UT, January 31, 2013

U.S. DEPARTMENT OF ENERGY NNSA

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND No. 2013-0597P

Outline

- What is Sandia National Laboratories?
- What do I do?
- How does mathematics relate to what I have done in my working career at Sandia? I will give interesting examples along the way.
- What should you do if you think you would like a career like mine?
- Acknowledgement: Thanks to many colleagues and student interns at Sandia.

Sandia's Governance Structure

Sandia Corporation

- AT&T: 1949–1993
- Martin Marietta: 1993–1995
- Lockheed Martin: 1995–present
- Existing contract expires: Sept. 30, 2012
- One-year contract extension: Sept. 30, 2013

Government-owned contractor-operated

Federally funded research and development center

Sandia's Sites

Albuquerque, New Mexico

Carlsbad, New Mexico

Tonopah, Nevada

Livermore, California

Amarillo, Texas

Kauai, Hawaii

National Security Challenges

1950s	1960s	1970s	1980s	1990s	2000s	2010s
Nuclear weapons	Development engineering	Multiprogram laboratory	Missile defense work	Post–Cold War transition	Post 9/11	Life Extension Programs START
Production and manufacturing engineering	Vietnam conflict	Energy crisis	Cold War	Stockpile stewardship	National security	National security challenges

Nuclear Weapons

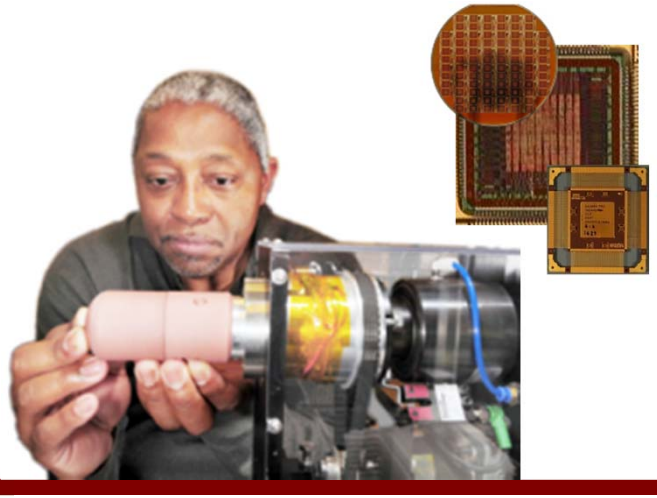
Pulsed power and radiation effects sciences

Design agency for nonnuclear components

- Neutron generators
- Arming, fuzing and firing systems
- Safety systems
- Gas transfer systems

Warhead systems engineering and integration

Production agency



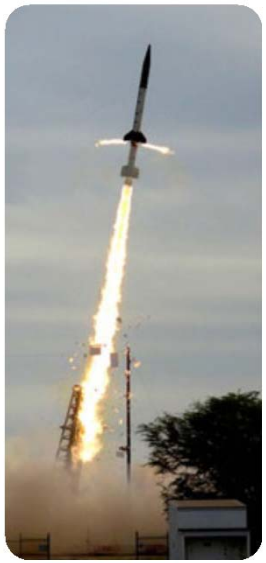
Defense Systems and Assessments

Sandia National Laboratories

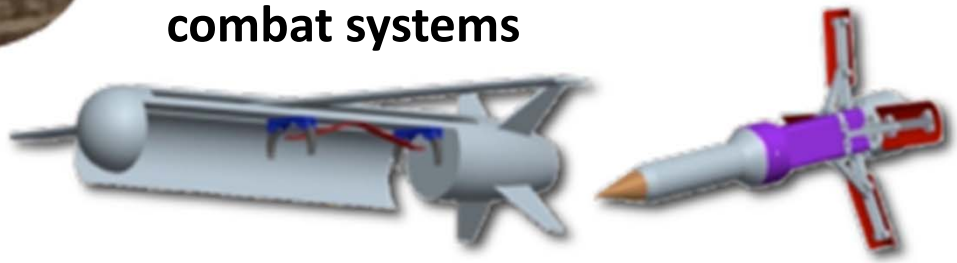
Synthetic aperture radar

Support for NASA

Support for ballistic missile defense



Ground sensors for future combat systems



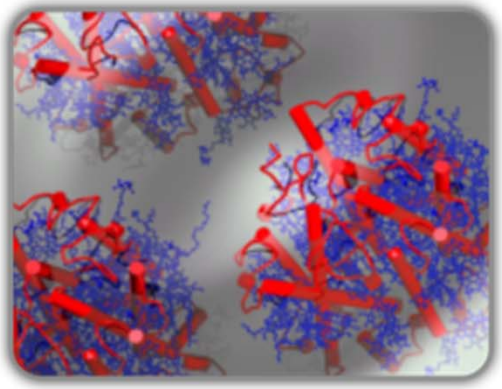
Energy, Climate, and Infrastructure Security

Sandia National Laboratories

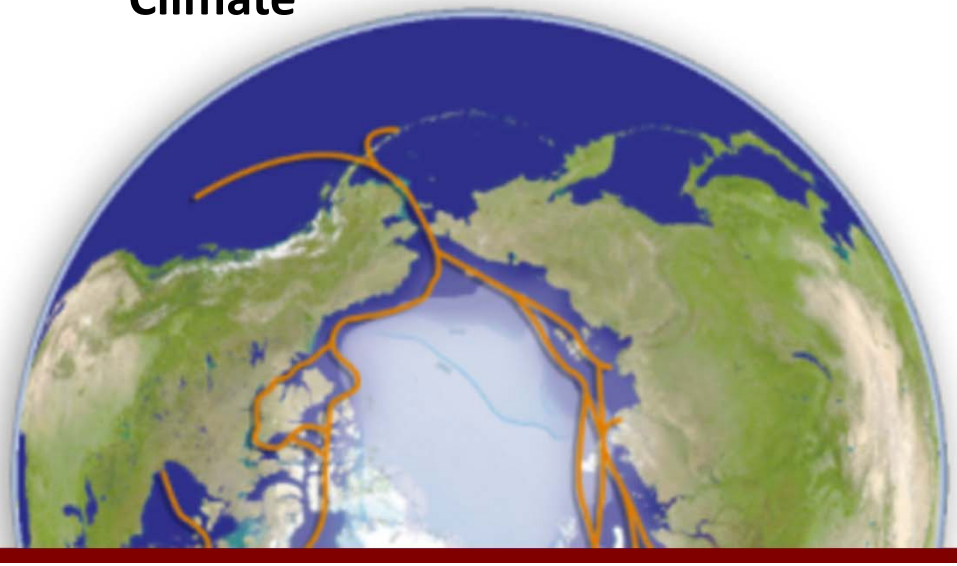
Energy

Infrastructure

Crosscuts and enablers



Climate



jbei
Joint BioEnergy Institute

International, Homeland, and Nuclear Security

Critical asset protection

Homeland defense and force protection

Homeland security programs

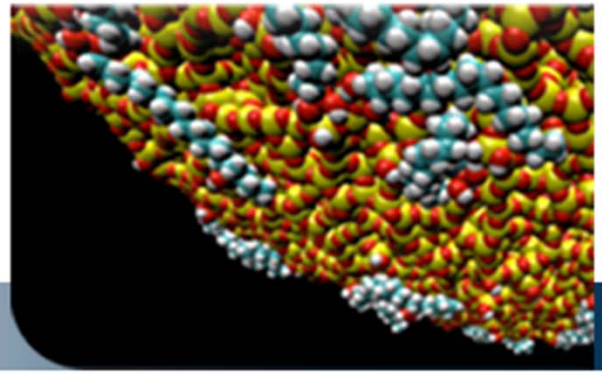
Global security

Science and Engineering Foundations

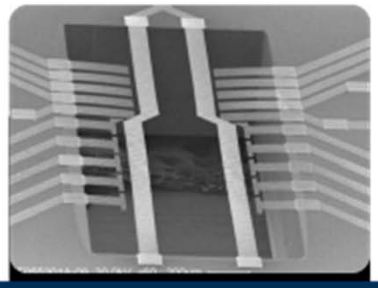
Sandia National Laboratories

Computing and information science

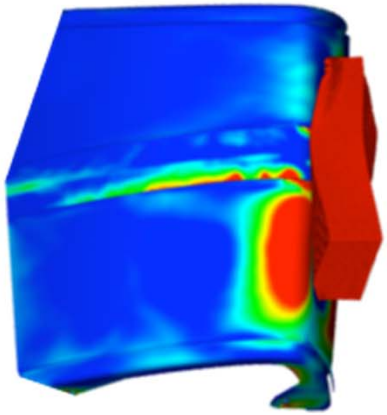
Materials science



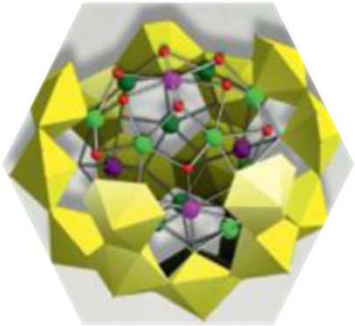
Nanodevices and microsystems



Engineering sciences

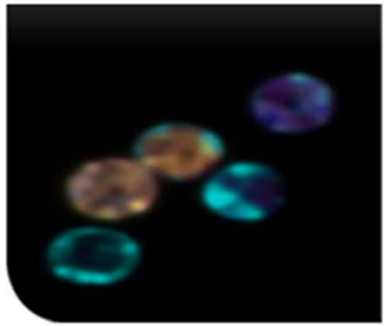


Geoscience



Radiation effects and high-energy density science

Bioscience



SNL Workforce

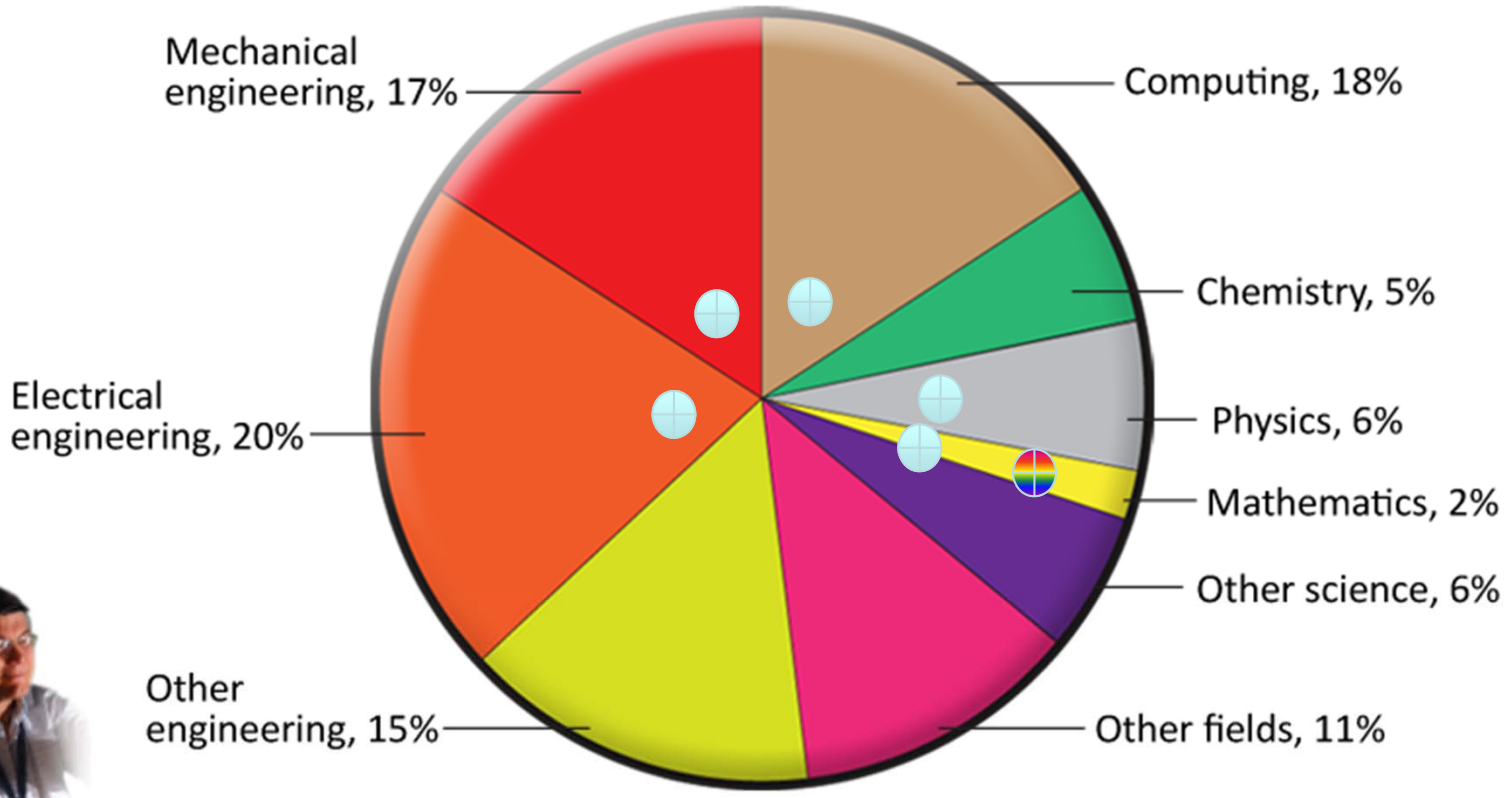
- Onsite workforce: 11,711
- Regular employees: 9,238
- Gross payroll: ~$981M

Data for FY12 through end of September

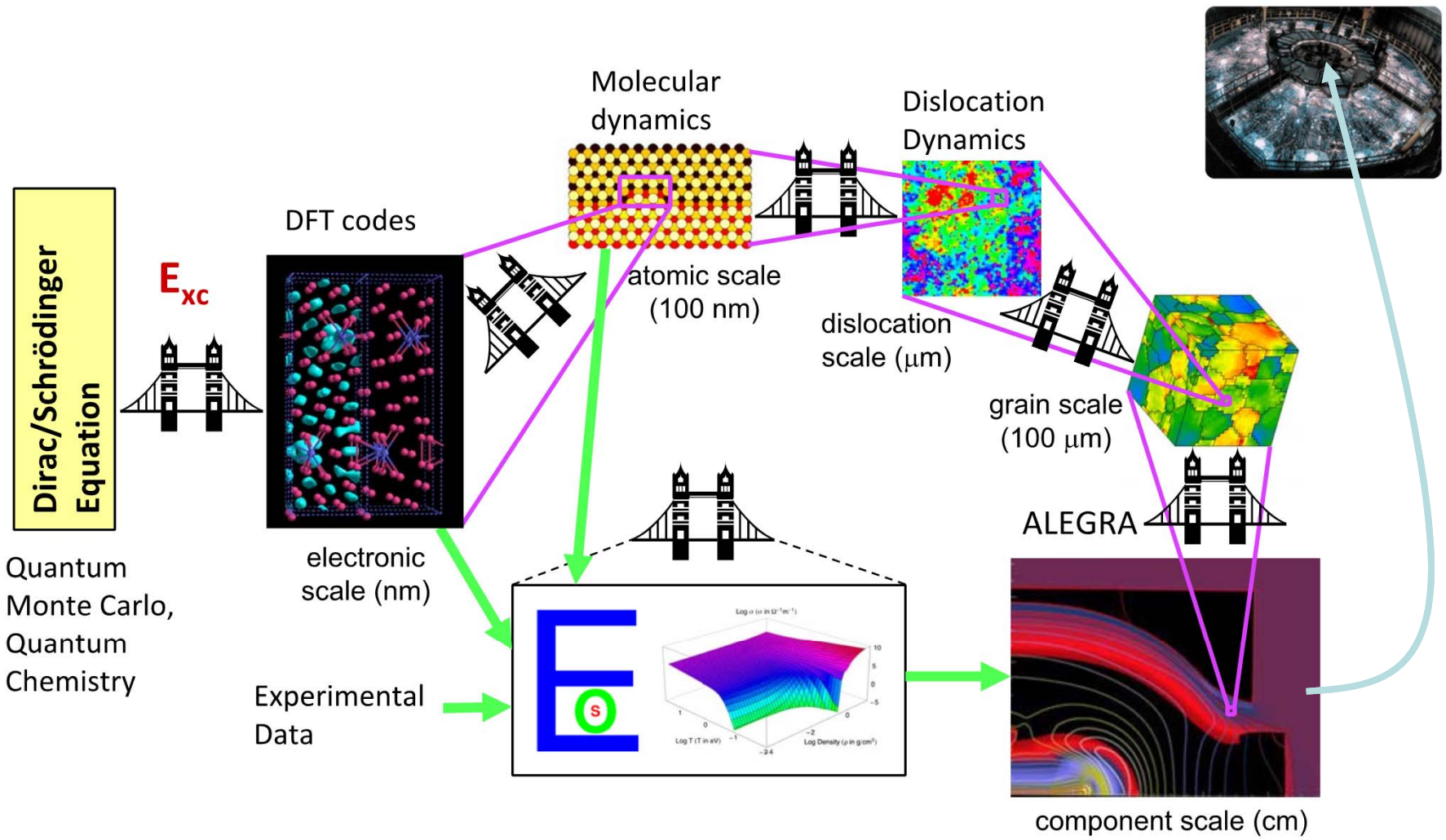
I hired in as a "mathematician" with a Ph.D. in Applied Math

This is what I really do

Research & Development staff(4,682) by discipline

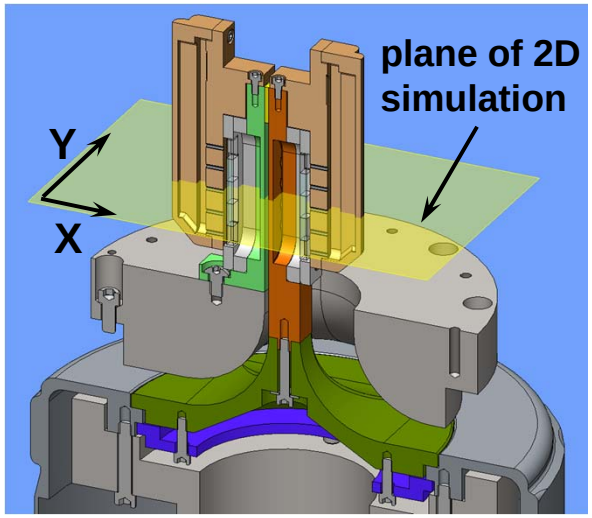


Science based engineering is the future and it is a multiscale enterprise.

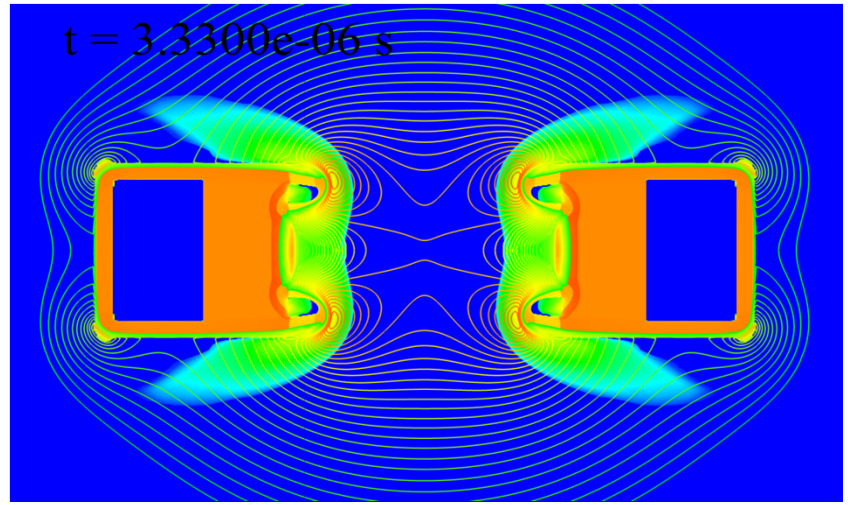


ALEGRA magnetohydrodynamic (MHD) modeling provides for predictive design of flyer plate experiments (Ray Lemke)

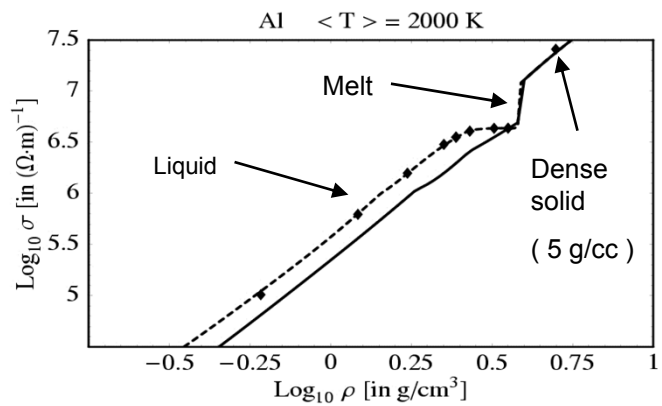
Two-sided Strip-line Flyer Plate Experiment



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



Continuum Balance laws for Resistive MHD (Non-linear Partial Differential Equation Set)

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

Conservation of mass

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

Conservation of momentum including JxB forces

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

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

Conservation of energy

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

Conservation of magnetic Flux (involution)

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

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

Reduced Ampere's Law

Additional 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.

<u>These relations are what makes the equations useful.</u>

A non-linear hyperbolic equation

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0$$

White board discussion: The method of characteristics and why shocks appear for non-linear hyperbolic equations.

A parabolic equation

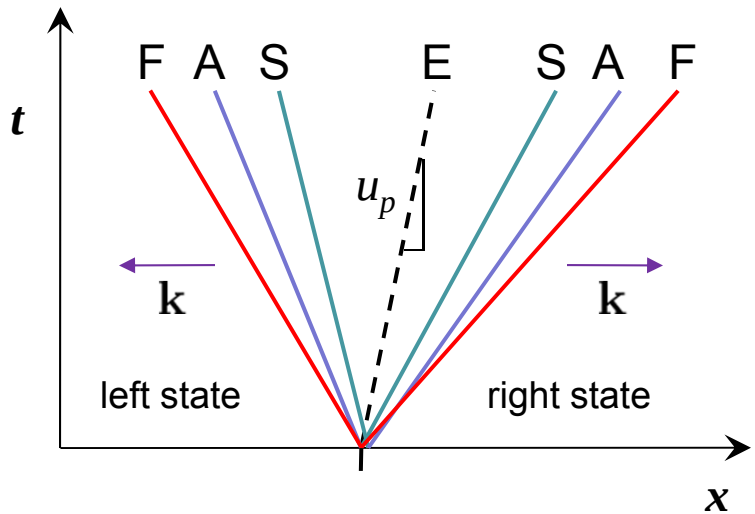
$$\frac{\partial u}{\partial t} = \nu\frac{\partial^2 u}{\partial x^2}$$

Burger's equation

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu\frac{\partial^2 u}{\partial x^2}$$

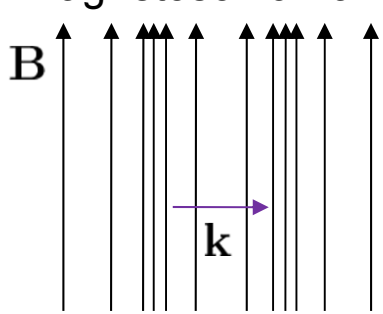
Ideal MHD wave propagation

The equations of ideal MHD are hyperbolic and have seven real eigenvalues, corresponding to seven characteristics or modes:

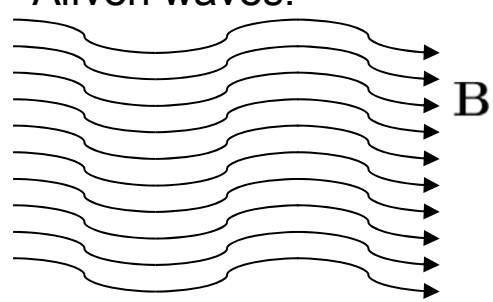


- 2 "fast" magnetosonic modes
- 2 Alfvén modes
- 2 "slow" magnetosonic modes
- 1 contact or "entropy" mode
- [In pure gas dynamics: only 3 real eigenvalues → only 3 modes.]

Magnetosonic waves:



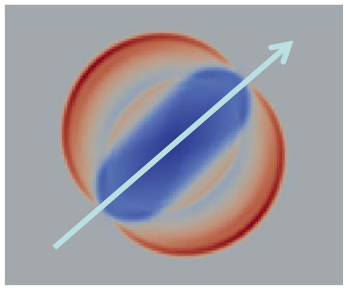
Alfvén waves:



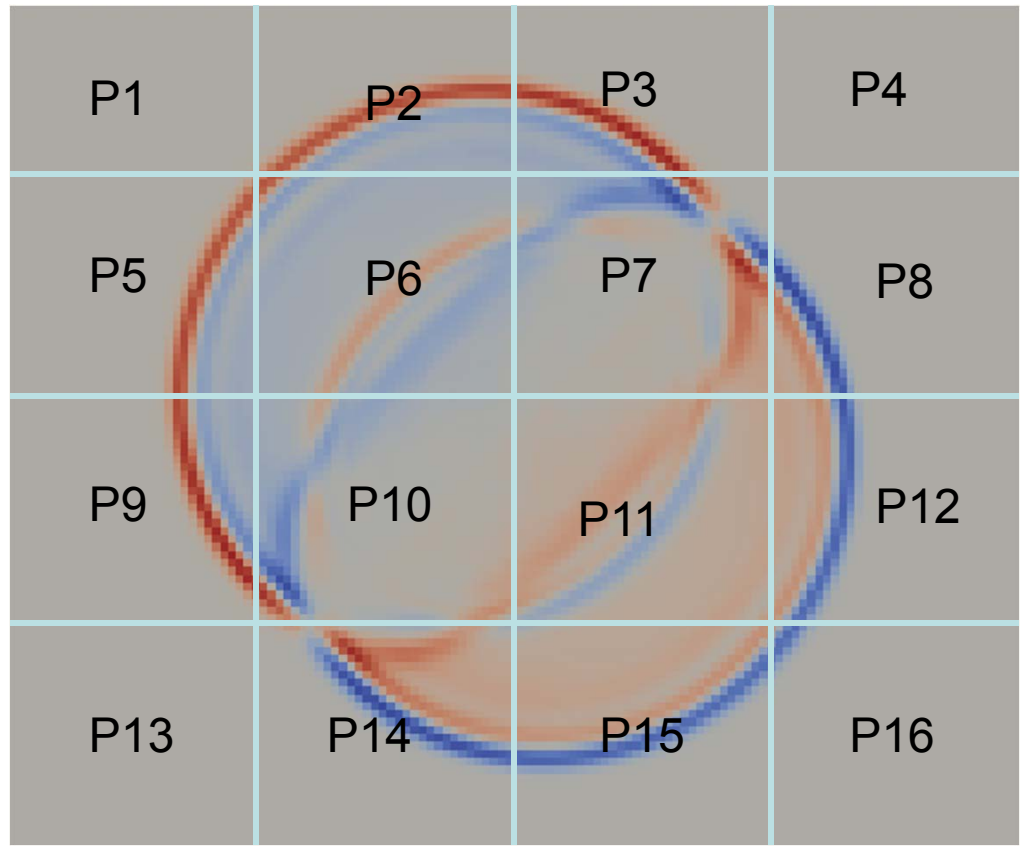
How to Solve MHD on a Computer?

2D plane ideal MHD problem with initially pressured region

Magnitude of planar B field



Normal current density Jz



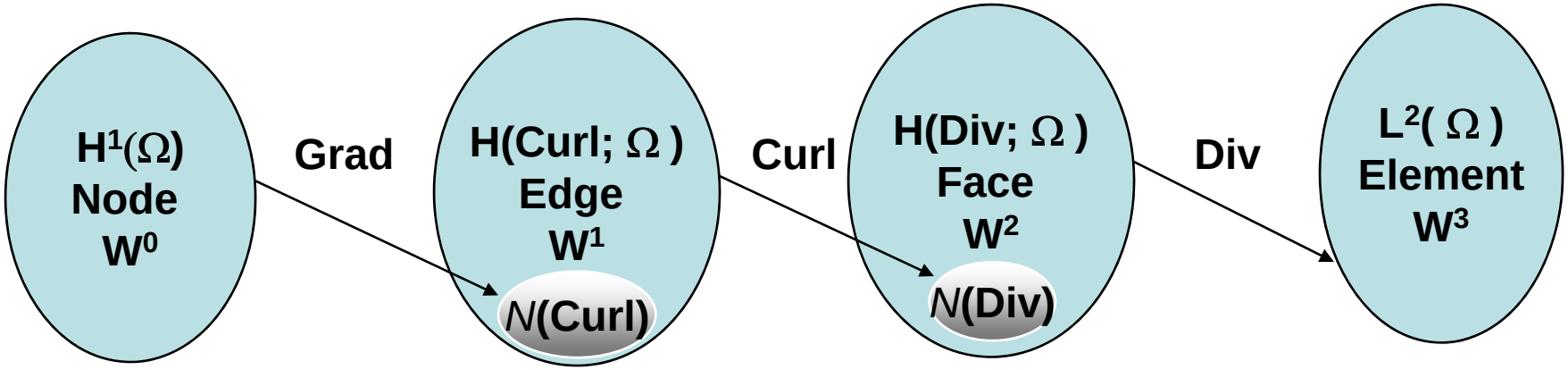
Demonstration of Local Communication Algorithm

Parallel Computing – O(N) <u>scalable</u> algorithms

Hybrid Parallel Computing Revolution is in Progress

Comments on “Speaking” Computer Languages and Software Engineering

Mimetic discretizations (deRham complex) are natural for MHD

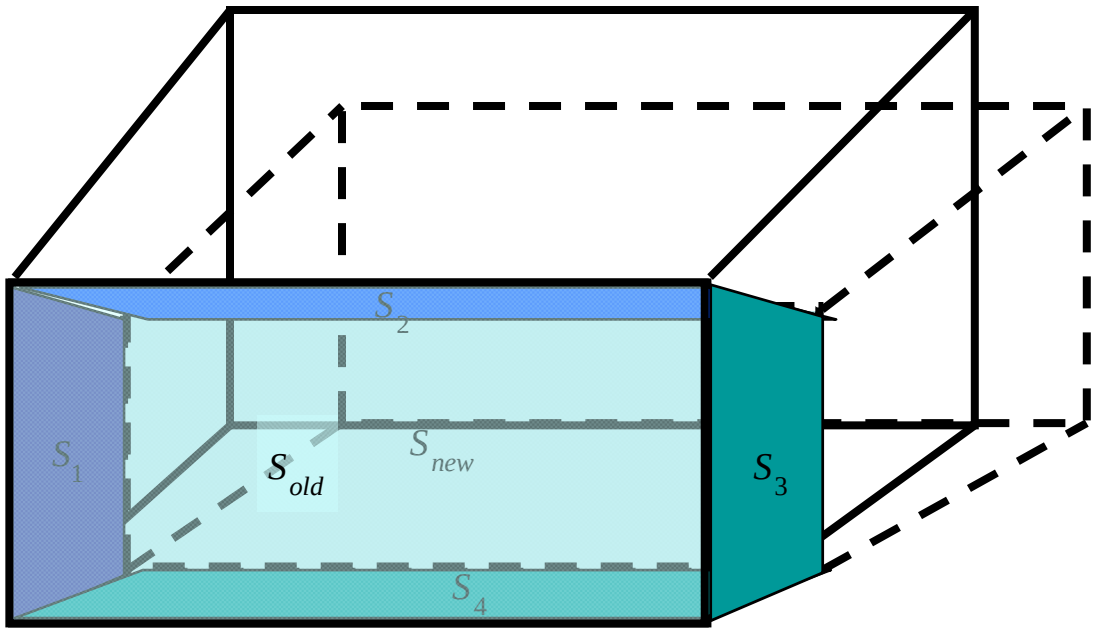


- **Magnetic flux and vector potential circulation are invariants in ideal MHD and thus natural degrees of freedom.**
- **Circulation is the degree of freedom for the edge element.**
- **Flux is the degree of freedom for the face element.**
- **Discrete node, edge, face element representations matching these properties are possible using mimetic finite elements to solve the magnetic diffusion equation in an operator split context.**
- **MATH: Function Spaces, Details of the null space of the diffusion operator turn out to be very important from a discrete modeling point of view.**

Constrained Transport Flux Remap
Math: Calculus; Divergence Theorem

$$\int_S \mathbf{B} \bullet d\mathbf{a} = 0$$

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



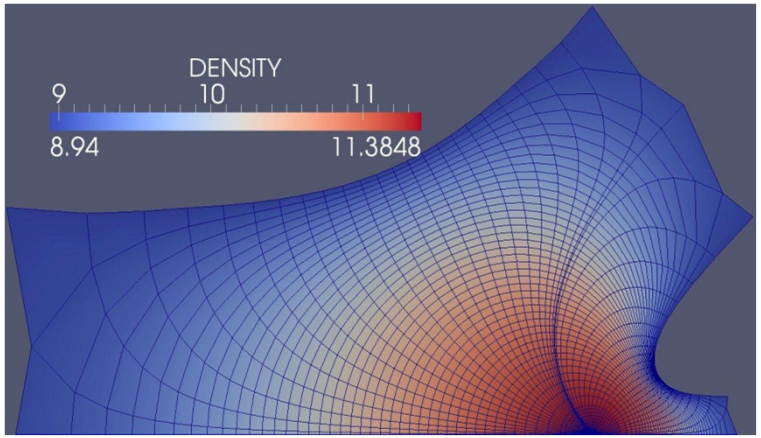
$$\int_{S_{old}} \mathbf{B} \bullet d\mathbf{a} + \int_{S_{new}} \mathbf{B} \bullet d\mathbf{a} + \sum_{i=1}^{4} \int_{S_i} \mathbf{dl} \bullet (\mathbf{B} \times \mathbf{v}_g \Delta t) = 0$$

Verification: Solving the equations right (correctly)

- Student: Brad Hanks
- Plane Subsonic Isentropic Fluid Flow with low compression EOS model
- Import my complex analytical representation of the solution into a more general code for <u>verification</u> testing.
- MATH: Complex variables, special functions (hypergeometric), series summation acceleration techniques, this verification work pushes other researchers in numerical methods
- Incompressible Solution:

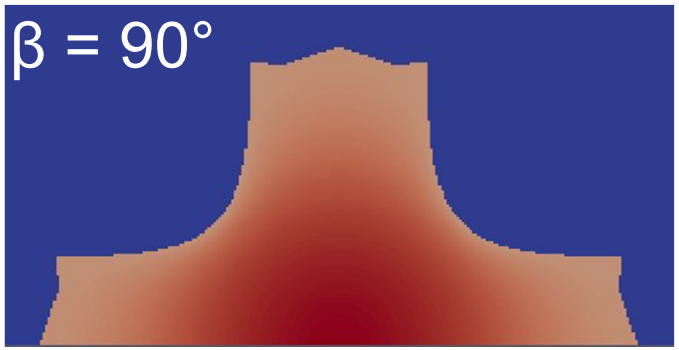
$$W(\Omega) = (q_1/\pi)\left\{\log(1+\Omega e^{i\beta}) + \log(1+\Omega e^{-i\beta}) - (1-\cos\beta)\log(1-\Omega) - (1+\cos\beta)\log(1+\Omega)\right\}$$

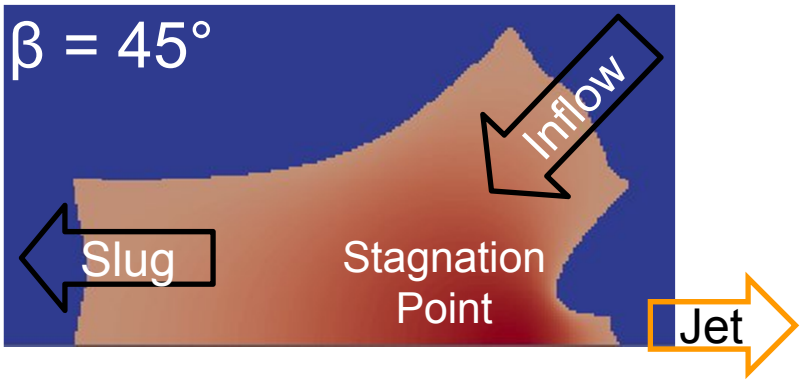
$$\psi = ((\rho_1 q_1)/\pi)\left\{\sum_{n=2}^{\infty}\frac{1}{n}\frac{\psi_n(\tau)}{\psi_n(\tau_1)}\sin n(\theta-\beta+\pi) + \sum_{n=2}^{\infty}\frac{1}{n}\frac{\psi_n(\tau)}{\psi_n(\tau_1)}\sin n(\theta+\beta-\pi) - (1-\cos\beta)\sum_{n=2}^{\infty}\frac{1}{n}\frac{\psi_n(\tau)}{\psi_n(\tau_1)}\sin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



Can the general code match the exact solution?

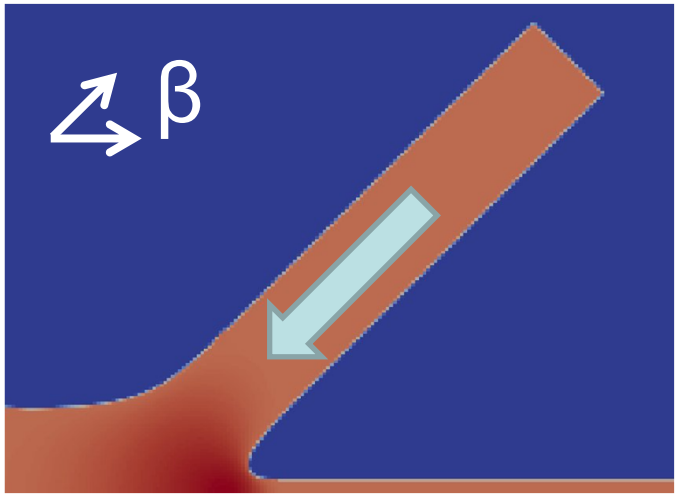
- Verification code solutions

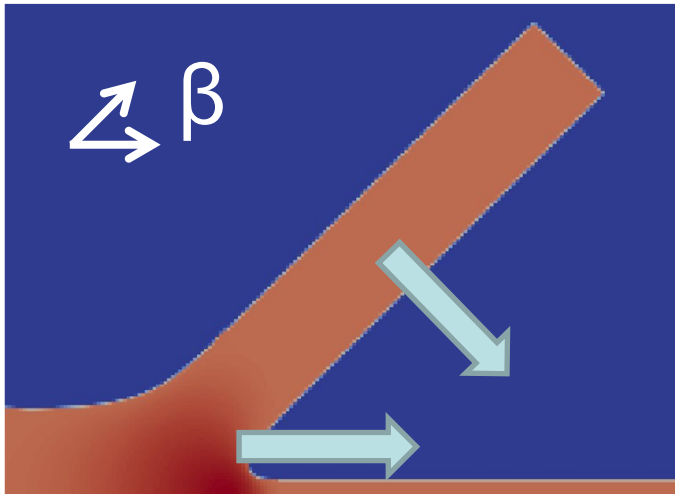




- **Simulations – 2 incident angles, 2 frames of reference**

Stagnation Point Frame of Reference





Laboratory Frame of Reference

Validation: Solving the Right Equations

- Modeling equations are not set in stone:
  - Sometimes simplified equations can be justified through asymptotic analysis.
  - A common set of equations may also not be good enough for the desired purpose and may need to be improved.
  - Answering this question is termed VALIDATION.
  - Math: Dimensional Analysis, Asymptotic analysis

- Example: Low Magnetic Reynolds Number Approximation

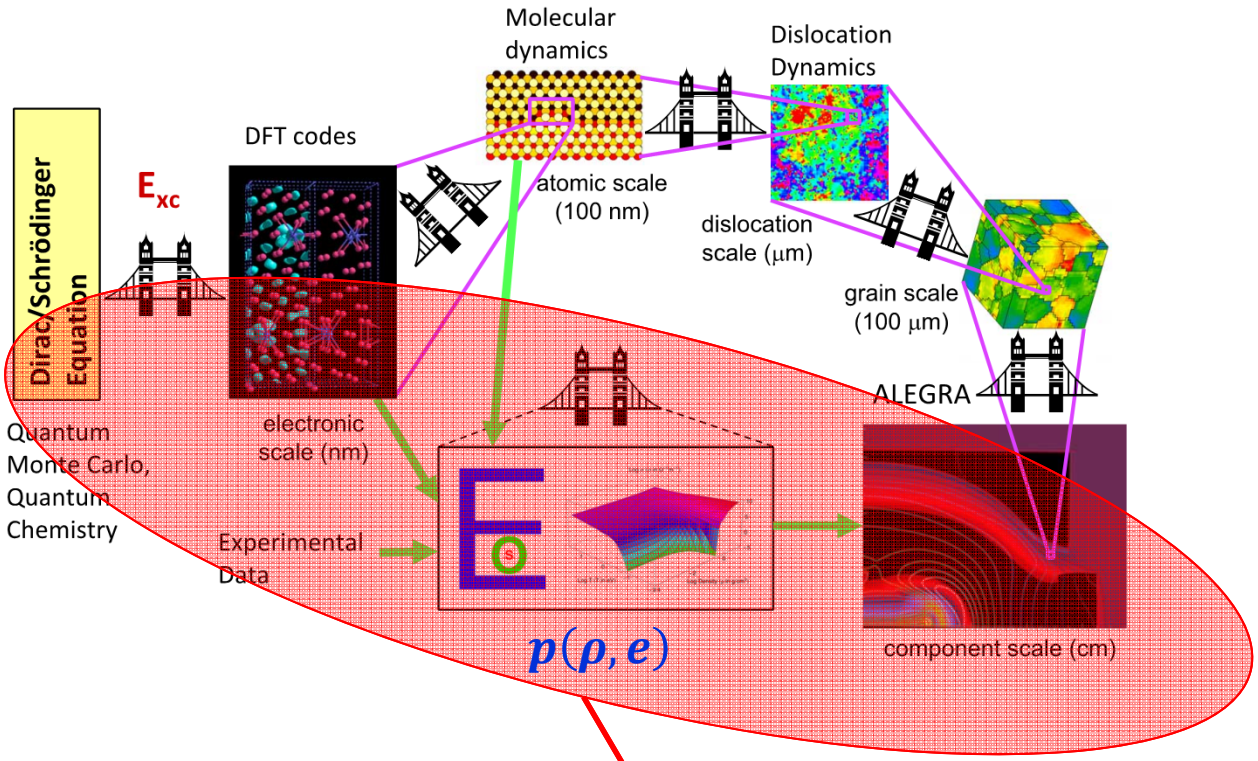
$$R_m = \frac{\mu\sigma L^2}{\tau}$$

$$\begin{aligned}
\dot{\rho} + \rho\nabla\cdot\mathbf{v} &= 0 \\
\rho\dot{\mathbf{v}} &= \nabla\cdot(-p\mathbf{I} + \mathbf{T}^M) \\
\rho\theta\dot{S} &= \mathbf{J}^2/\sigma \\
\sigma\left(-\frac{\partial\mathbf{A}}{\partial t} + \mathbf{v}\times(\nabla\times\mathbf{A}) - \nabla\phi\right) &= \nabla\times\left(\frac{\nabla\times\mathbf{A}}{\mu}\right)
\end{aligned}
\quad \xrightarrow{R_m \ll 1} \quad
\begin{aligned}
\dot{\rho} + \rho\nabla\cdot\mathbf{v} &= 0 \\
\rho\dot{\mathbf{v}} &= -\nabla p \\
\rho\theta\dot{S} &= \mathbf{J}^2/\sigma \\
\nabla\cdot\sigma\nabla\phi &= 0
\end{aligned}$$

What can be done about uncertainties in engineering?

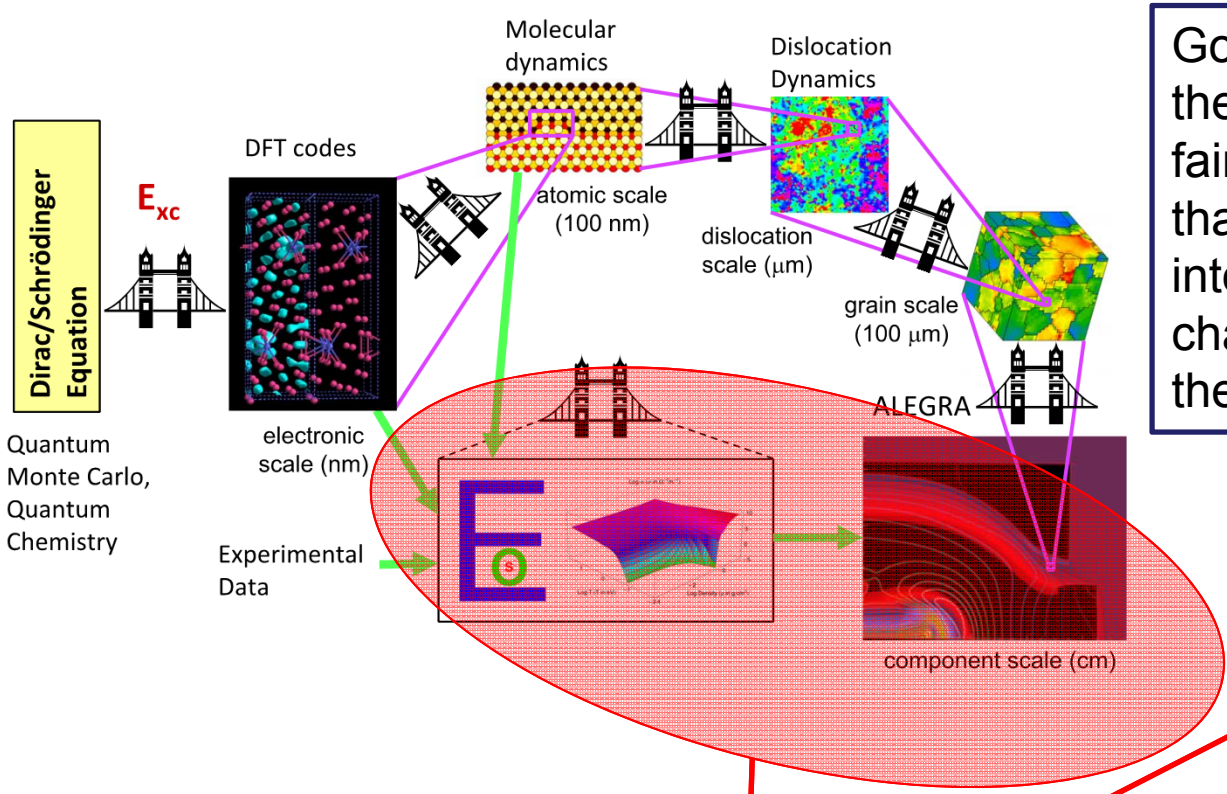
- For example, the U.S no longer does nuclear weapon testing. You want nuclear weapons to be <u>very</u> <u>safe</u> and <u>credible</u>.
- Given a set of modeling equations with inputs including initial conditions, boundary conditions and closures, we can in principle solve them on a computer.
- Actually… modeling equations and inputs are uncertain at some level. Enter the field of "Uncertainty Quantification" (UQ)
- Math: Probability Theory, Bayesian Analysis, Markov Chain Monte Carlo, Random Fields and Variables
- Find solution $Y(x, t, \omega)$ where ω is a vector of random variables or alternatively, find cumulative distribution function of Quantities of Interest (QOIs).
- Technology: Black Box Uncertainty Quantification
  - See dakota.sandia.gov

Building Bridges between Fundamental Laws of Nature and Engineering

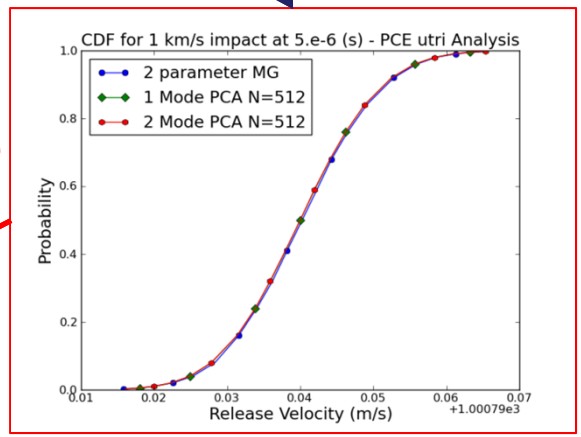


Propagating uncertainty in experimental and DFT data to the analyst using the continuum code.

Building Bridges between Fundamental Law of Nature and Engineering



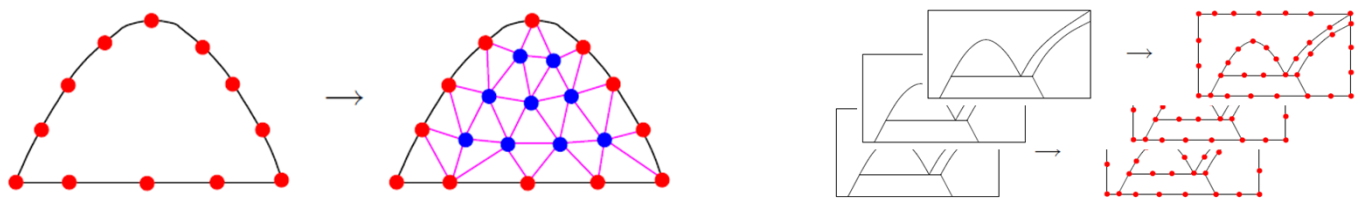
Goal: The analyst running the continuum code should fairly easily get results out that can be transformed into the equivalent of "50% chance of rain" to give to the decision maker.



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

Uncertainty Quantification for EOS - $p(\rho, e; \omega)$

- In this project we need a compact equation-of-state (EOS) representation of an uncertain EOS surface.
- Laplace-Beltrami equation can be used to compute a smooth mapping of one domain to a perturbed domain.



$$\frac{1}{\sqrt{g}}\frac{\partial}{\partial \xi^\alpha}\left(\sqrt{g}g^{\alpha\beta}\frac{\partial x^i}{\partial \xi^\alpha}\right) = 0$$

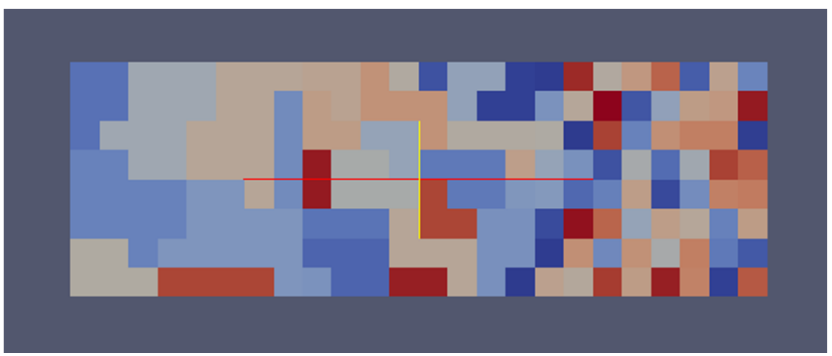
- Try to reduce the random dimension of the tabular space.
- Math: Differential Geometry, Calculus of Variations, Finite Elements, Singular Value Decomposition or Principal Component Analysis

Random Random Field Theory and Initial Conditions: Students Project: Dale Koenig and Emily Fischer

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

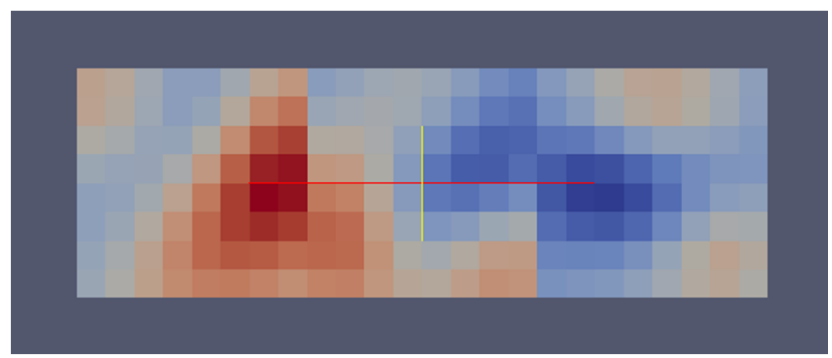
$$R(\mathbf{x},\mathbf{y}) = E\left(\left(f(\mathbf{x}) - \bar{f}(\mathbf{x})\right)\left(f(\mathbf{y}) - \bar{f}(\mathbf{y})\right)\right) = \sum_{i=1}^{N} \sigma_i^2 \phi_i(\mathbf{x})\phi_i(\mathbf{y})$$

Space- filling curves and Random Rotations



Karhunen-Loeve Expansion

Useful math: Symmetric eigenvalue problems and Invariant Subspaces (debug story)



Applied Mathematics in the 21 Century

- Computer simulation and modeling will be key to success in overcoming the challenges of the upcoming century. Mathematics is the "lingua franca."
  - Challenge: Can you find any significant/difficult problem which is not substantially benefitted by mathematically based modeling.
- Honesty about what modeling can and cannot do is essential. This is the driver behind the UQ theme in predictive science and engineering today. What is the confidence in your modeling results?
- End to end multi-scale modeling will become more common and required for most competitive enterprises. A confluence of modeling and math, computer science and experimental science is the theme of the future.

My BYU undergraduate training

- Math major with computational emphasis.
  - Built microcomputer
  - Physics Minor
  - Mathematical Statistics
  - Chemistry
  - No material science or topology or functional spaces. ☹
  - Richard A. Hansen was my numerical analysis professor and thought enough of me to offer me a job. ☺
- Internship opportunities
  - Eyring Research Institute. Minuteman Missile Simulations including Honors project. (Math: Numerical ODEs, Rigid Body Mechanics)
  - Solution manual for calculus text. (Gurcharan S. Gill)
- I believe my applied internship work was one key for entrance to a great graduate school.

My Caltech graduate training

- I went to Caltech in the Applied Math Department.
- I was introduced to theoretical fluid mechanics.
- Other: Complex analysis and asymptotic analysis; probability theory, matrix theory, basic practical concepts of classical applied math including linearized stability analysis for problems in fluid mechanics; numerical methods
- Research work: Existence and Stability of Vortices and Vortex Arrays under Philip Saffman.
- I probably should have taken a theoretical continuum mechanics class ☹
- Graduated with PhD and entered the world of shock physics modeling at Sandia ☺

What should you do now as an undergraduate if you think you would like a career similar to mine?

- Try to get a conceptual grasp of as much relevant mathematics, physics, computer science, material science, statistics and chemistry as you can. Realize that you will not learn everything but breadth is important.
- Become well-versed in scientific computer languages and environments. (Linux, editors, C++, Fortran, Python, Latex, Matlab, …)
  - Learn to learn as required
- Learn work-group skills (interpersonal and group software management (VCS)). An advanced educational program should make you practice these skills. (Hint to professors ☺)
- Find a job (summer and/or part time) where you are really stretched to deliver in a real world application area.
  - One job will usually translate to more work.
  - Telecommuting.
- Plan now to go to graduate school.

How do you get an internship as an undergraduate?

- Work as hard as you can in your classwork so that you are prepared and so your professors can recommend you and lobby for you. Ask them to help you make contacts.
- Make sure you have basic useful skills ASAP.
- Don't be afraid to ask "stupid" questions in order to clear up your views about any subject. Learning never ends.
- Talk to professors and other older adults that you cross paths with about their work and what they do. You need to ask.
- Ask your contacts for help in sharing your resume with the right people and ask for permission to contact directly.
- FOLLOW UP! This is the first practical test of a key interpersonal work skill. Be appreciative and personal.

How do you get an internship at Sandia?

- Sandia has a large and extensive summer internship program with excellent pay.
  - www.sandia.gov/careers/students_postdocs/index.html
- You submit your resume online and as summer jobs are posted you can apply to any of them as they come up.
- You will significantly improve your chances if you have done your networking homework early so that you know ahead of time of relevant postings and when they will appear.
- A number of summer students come to work every year at the Computer Science Research Institute where I work.
  - csri.sandia.gov/index.htm
  - A seminar series for students covering a variety of topics is created each summer and the CSRI students are expected to attend.
  - Students learn a lot and make significant contributions.
- Questions and comments?