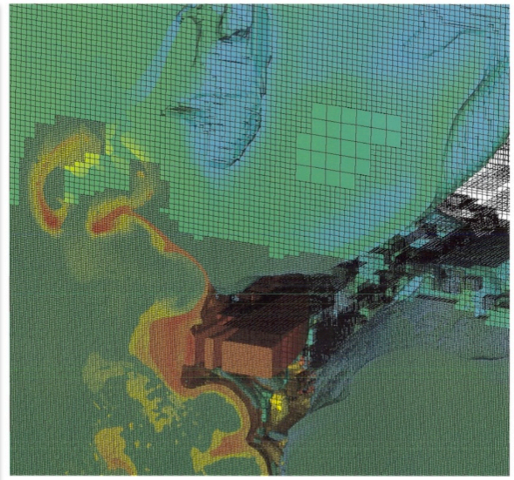
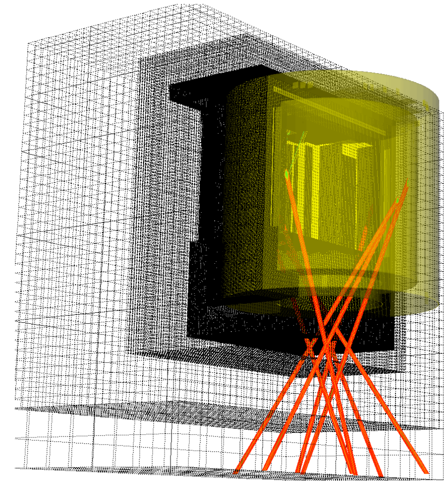
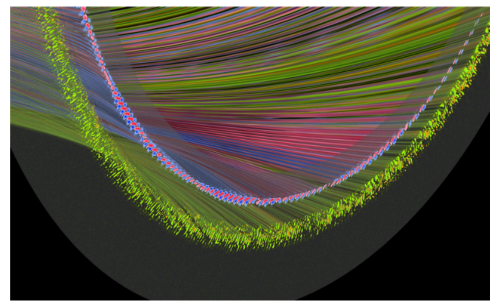
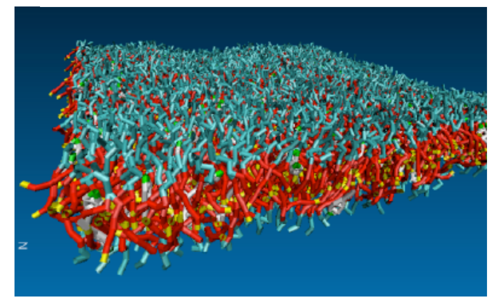
Enabling Physics insight with Multidimensional Computer Simulations

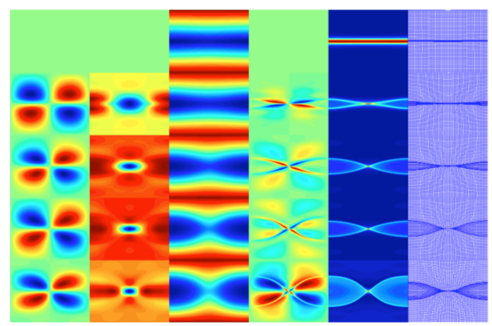


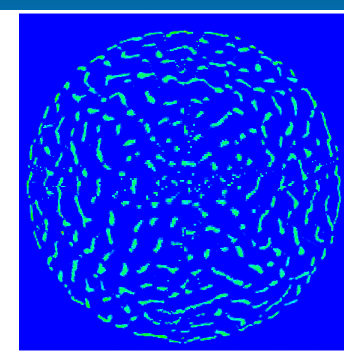






Alice E. Koniges
Berkeley Lab/NERSC





SC14 Panel
November 16, 2014

U.S. DEPARTMENT OF ENERGY | Office of Science

BERKELEY LAB
Lawrence Berkeley National Laboratory

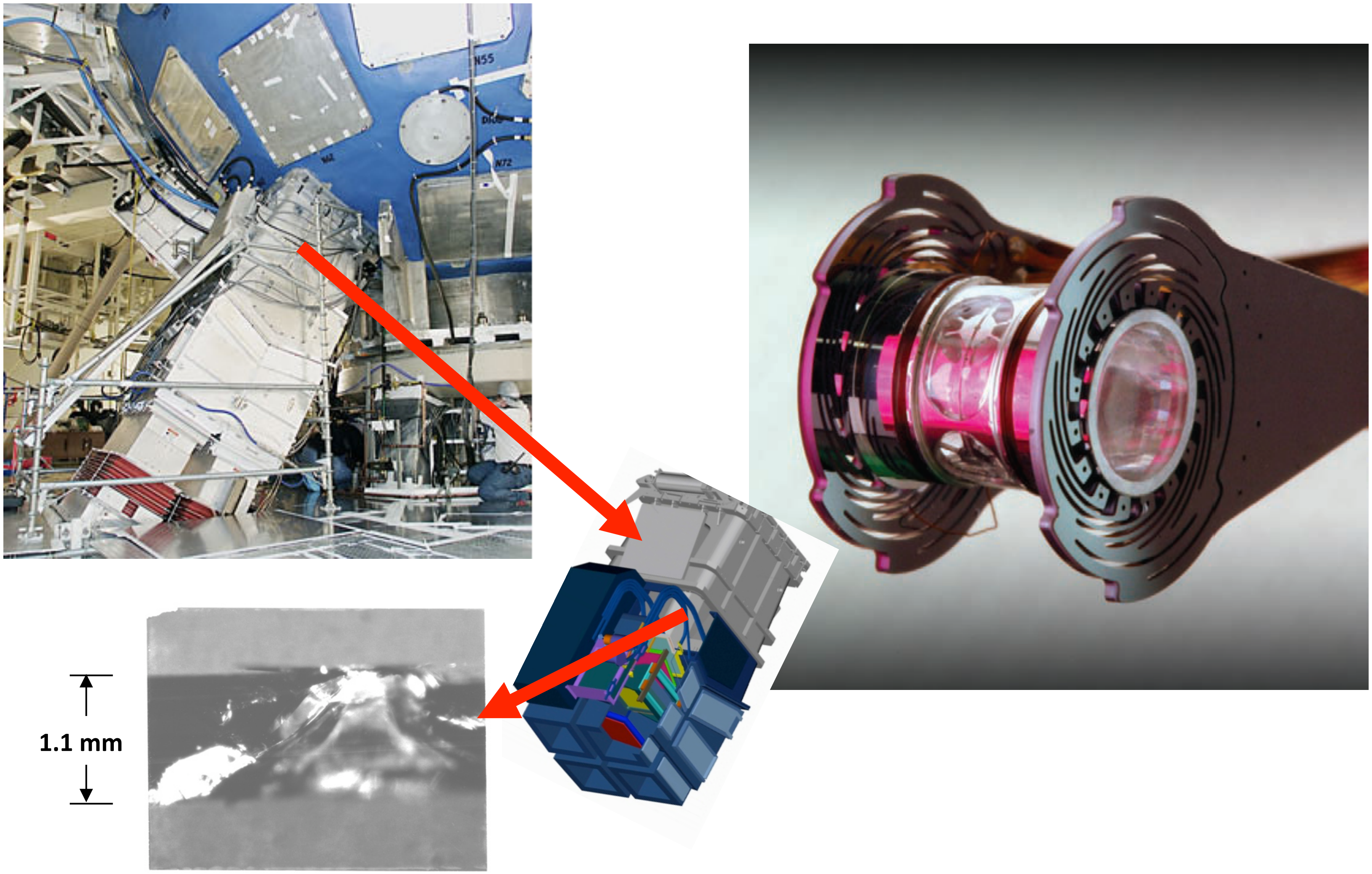
NERSC 40 YEARS at the FOREFRONT 1974-2014

Mathematics + Algorithms for a new Multiphysics Simulation Code applied to large experiments

Neutralized Drift Compression Experiment (NDCX-II)

CYMER EUV Lithography System

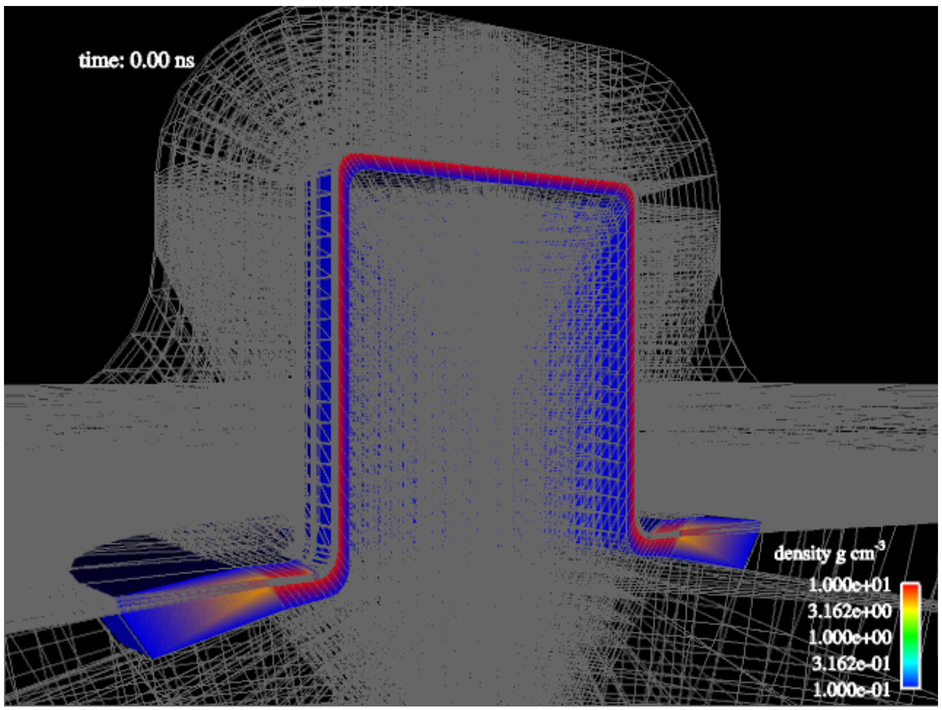
History: Predictive calculations needed for optics and diagnostics protection on NIF



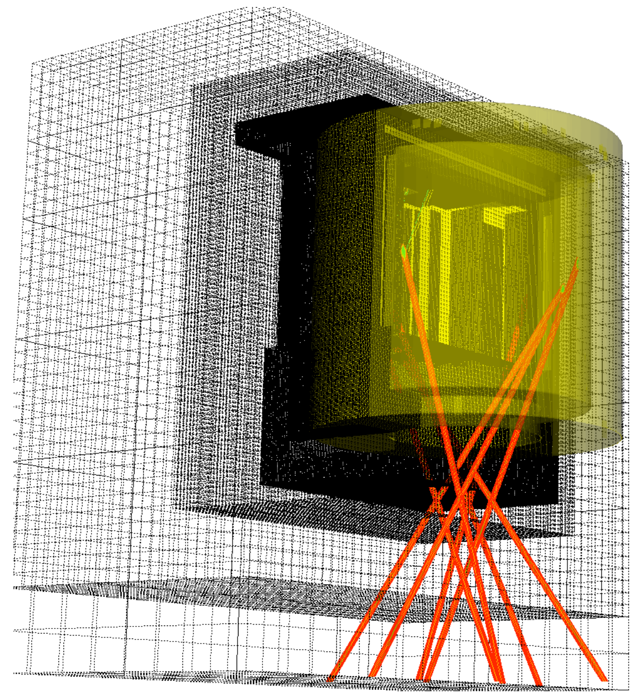
Damage to debris shields

Problem: Traditional ALE codes complicated and crashed for late-time simulations

Traditional ALE

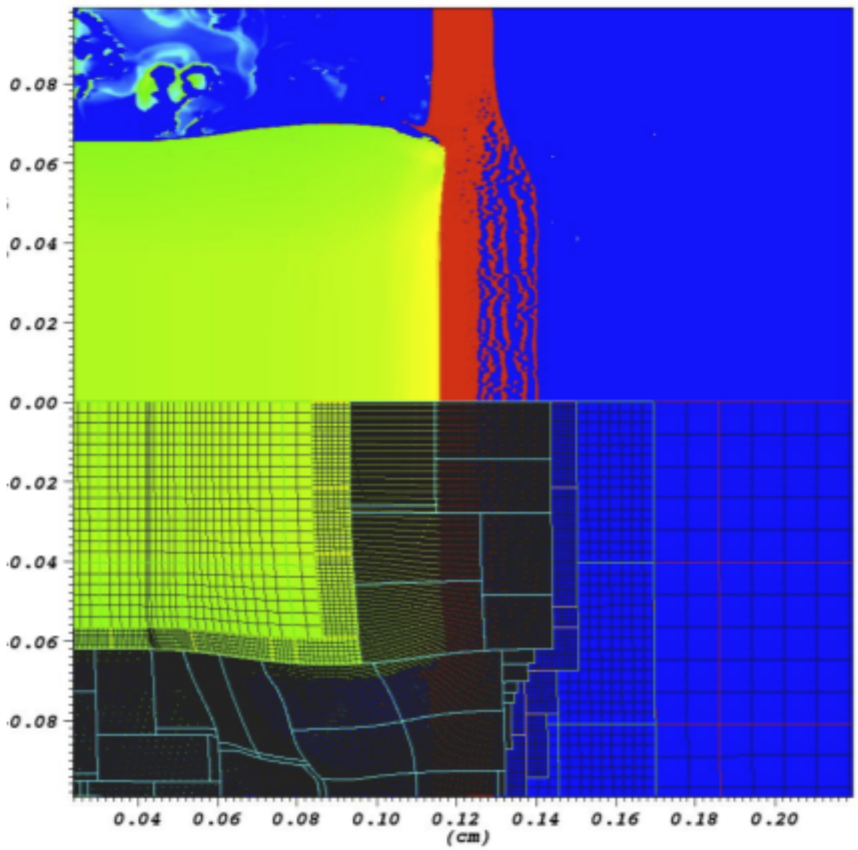


Newly Designed ALE-AMR



Led a project to design a new 3D multimaterial ALE + AMR code including substantial new physics

Simulation of soft x-rays striking foil



ALE-AMR is an open science code that runs at various computing centers including NERSC and has no export control restrictions

- **3D ALE hydrodynamics**
- **AMR (use 3X refinement)**
    - **With 6 levels, vol ratio 10^7 to 1**
- **Multi-Material (interface reconstruction)**
- **Anisotropic stress tensor**
- **Tabulated EOS and opacities**
- **Material failure with history**
- **Laser ray trace and deposition**
- **Ion deposition**
- **Thermal conduction**
- **Radiation diffusion**
- **2D Axisymmetric capability**
- **AMR with 3X in only 1 direction**
- **Surface tension**

Multimateral ALE + AMR; including anisotropic stress tensor

$$\frac{\partial \rho}{\partial t} + \nabla \bullet (\rho \vec{v}) = 0$$

Continuity equation

$$\rho \frac{\partial \vec{v}}{\partial t} = \nabla p + \nabla \bullet \Sigma' + \rho \vec{b}$$

Equations of motion

$$\rho \frac{\partial e}{\partial t} + p \nabla \bullet \vec{v} = 0$$

PdV work

$$\sum^{n+1} = f(\Sigma^n, \rho, e, \vec{v}, p, T, \vec{h})$$

Material Stress Update

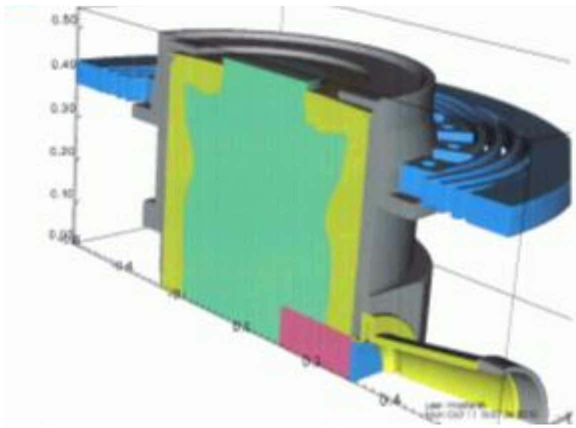
$$p = p(\rho, e)$$
$$T = T(\rho, e)$$

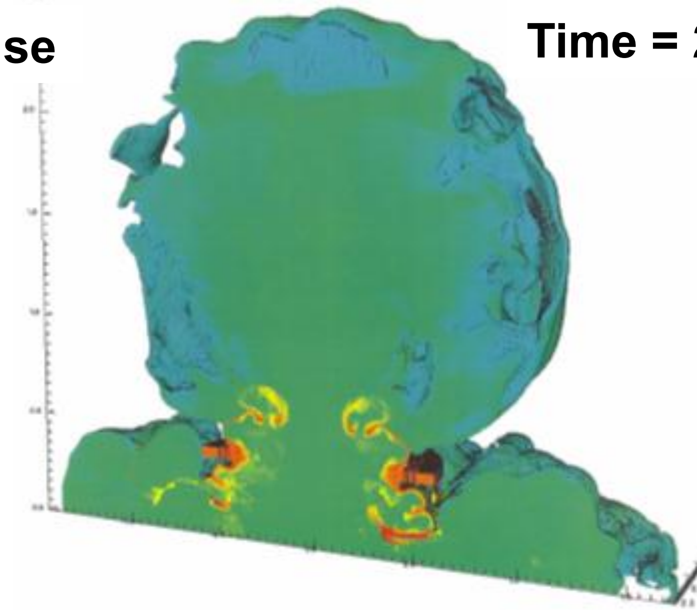
- EOS tables
- Various gas laws

Radiation Diffusion added via an operator splitting method

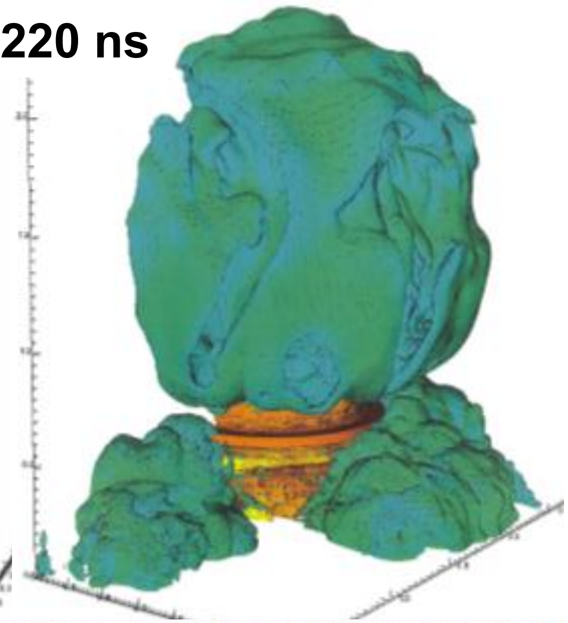
ALE-AMR was used to model the late time properties of HEDLP targets shot for National Ignition Campaign (450 M$ per year, 4B$ to construct)

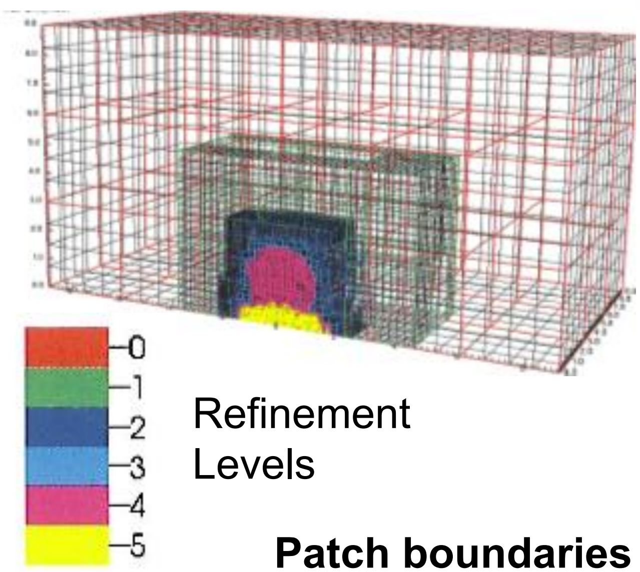
Materials at end of laser pulse



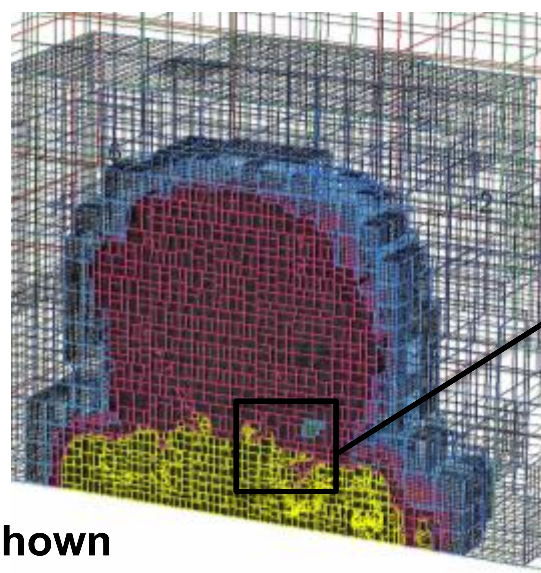


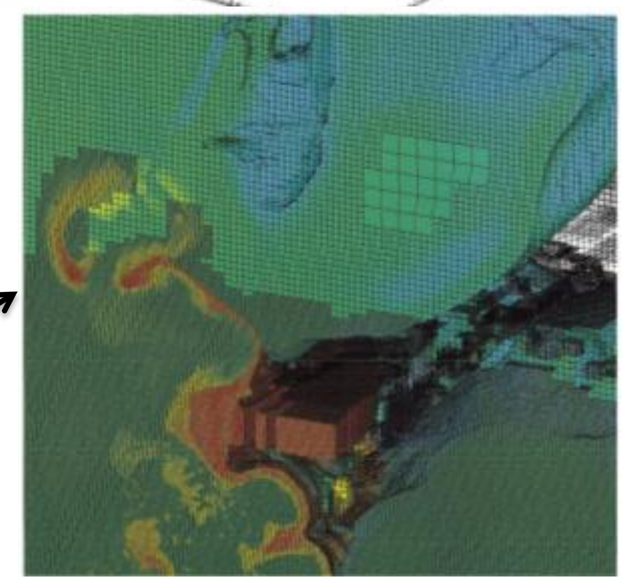
Time = 220 ns





Refinement
Levels

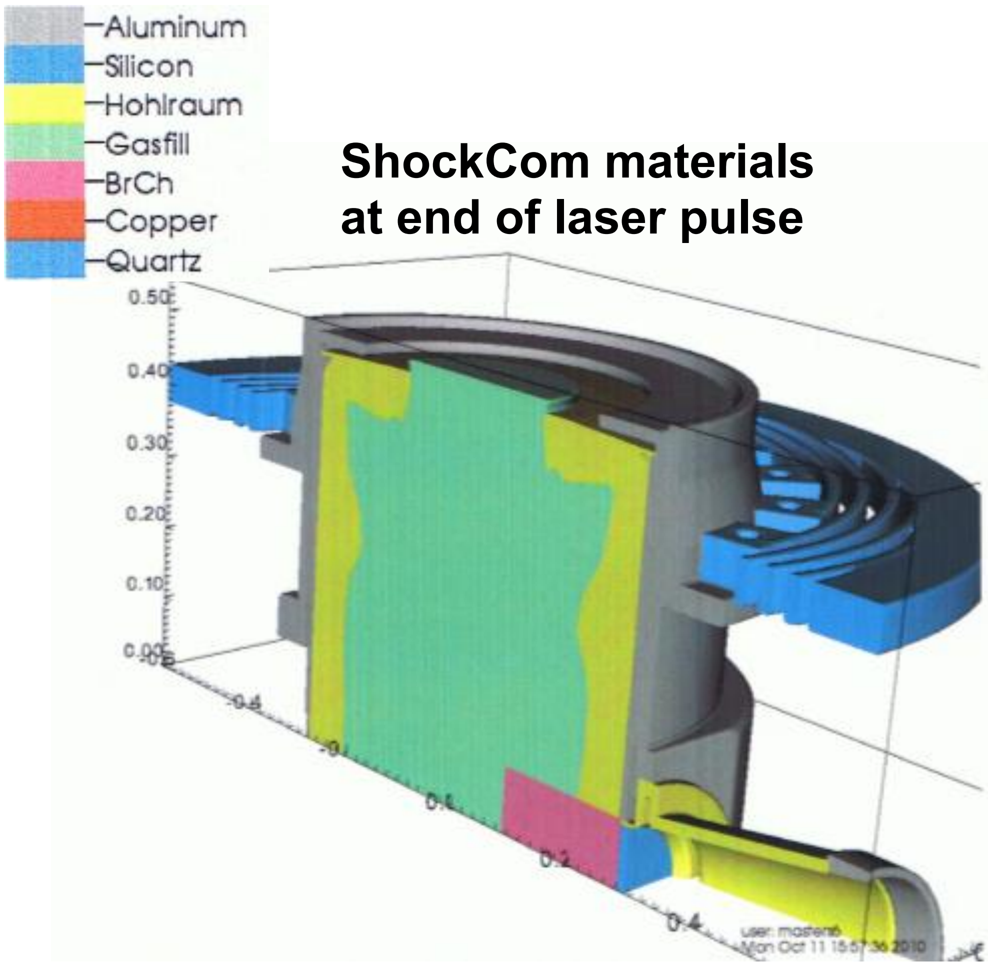




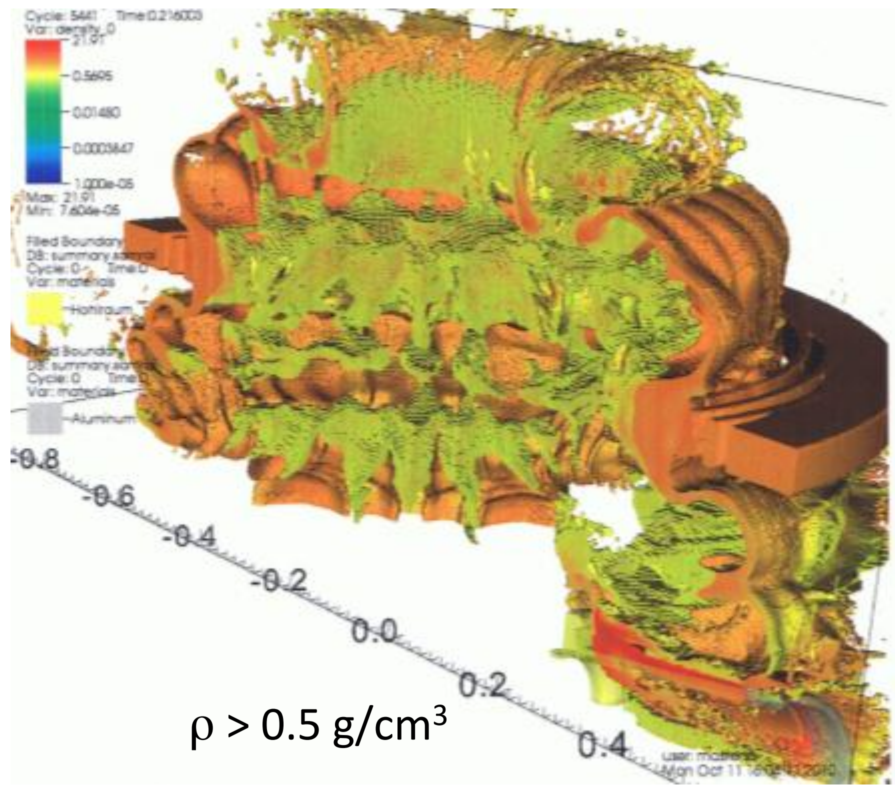
Patch boundaries shown

Multimaterial interface reconstruction + AMR allows fast and accurate modeling of complex targets

ShockCom materials at end of laser pulse



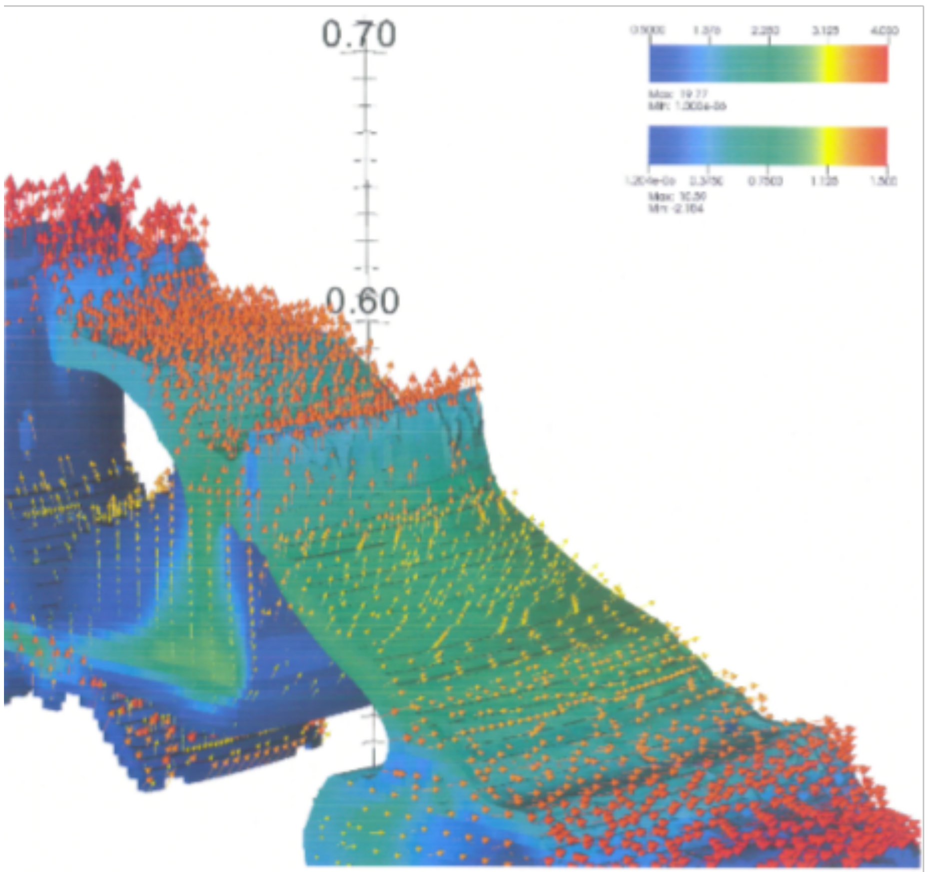
Density 216 ns after end of laser pulse



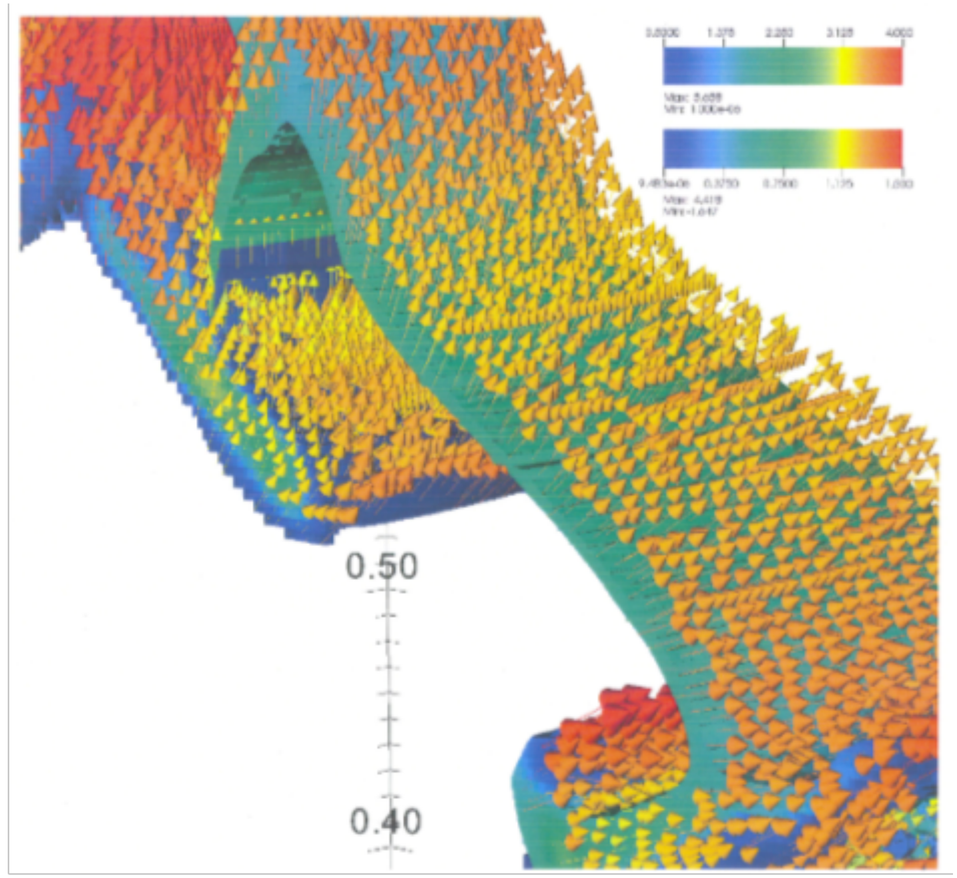
$\rho > 0.5$ g/cm^3

Molten Al in a Keyhole wedge simulation expands and drops in density in a divergent velocity field

t = 116 ns

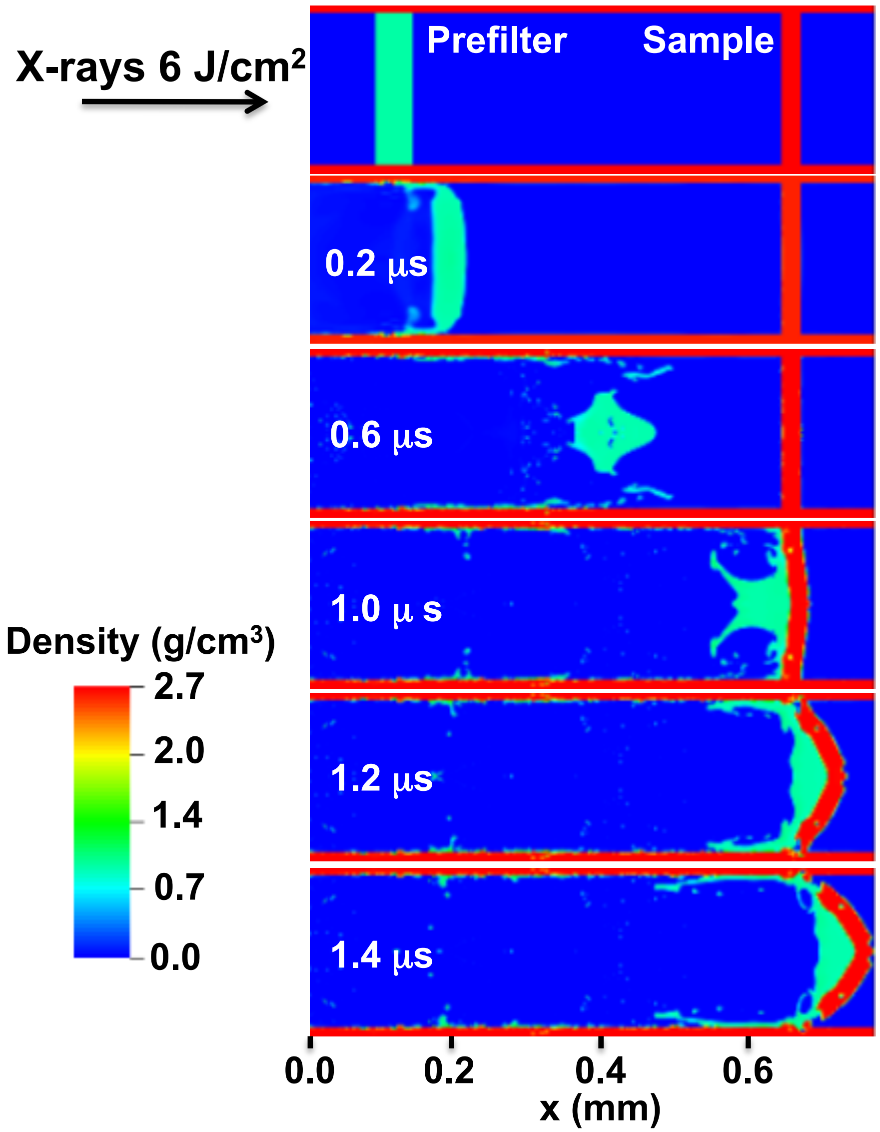


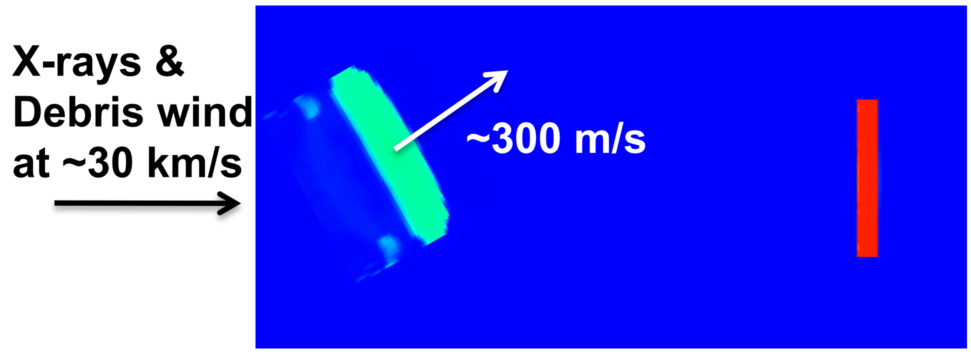
t = 235 ns



Need to estimate droplet sizes in divergent velocity fields motivated effort on surface tension

Simulations showed that x-ray loading in initial design damaged thin samples and tilted redesign protects samples from x-rays and fast debris wind from target

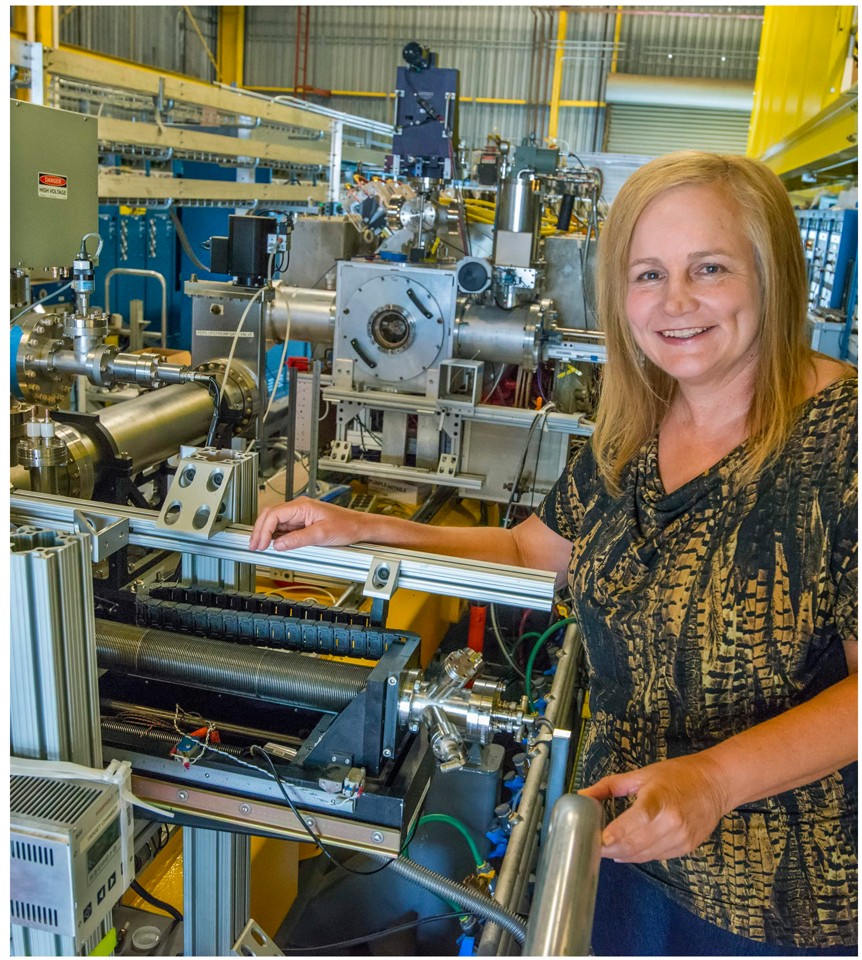




Redesigned Sample Holder

Some stuff about me

- 1st Woman to get a PhD in Applied Mathematics at Princeton
- Approximately 100 Papers and 1000 Citations
- PI on a few million dollars of research grants
- Raised 3 Kids, have a physicist spouse (34 years)
- Worked part time a bit – but don't tell anyone ☺
- Had 9 post-docs in last 6 years
- Try to make time to – ride my horse, do an occasional sprint triathlon, play piccolo



Leader/PI, Petascale Initiative in Computational Science and Engineering

Project:	Post Doc	Start Date	Eductation (PhD)
EFRC: Q-Chem parallelization and GPU Optimization	J Kim	Oct-09	Univ. IL Urbana-Champaign
Fusion: GTS for ITER-Scale; Programming Models	R Preissl	Feb-10	J. Kepler Univ. (Austria)
Multiphase Flow in Porous Media for Carbon Sequestration	K Fagnan	Mar-10	Univ. of Washington
Modeling for Next Generation Advanced Light Source	B Austin	Jun-10	UC Berkeley
Advanced Light Source and Geophysical Imaging with GPU's	F Maia	Jul-10	Uppsala Univ. (Sweden)
Benchmarking and Optimization of Energy-Related Applications	P Narayanan	Sep-10	Univ. of Maryland
ARRA-funded LBL NDCX-II modeling with ALE-AMR	W Liu	Jan-11	UC Los Angeles
Linear Solvers and Hybrid Programming	X Yuan	Mar-11	Columbia University
Poission Solver for Nano-Control EFRC	C Kavouklis	Jun-11	Univ. of Texas Austin

Teaching, mentoring, recruiting and public outreach

SC11 Seattle, WA
Connecting communities through HPC

SC12

Program Committees

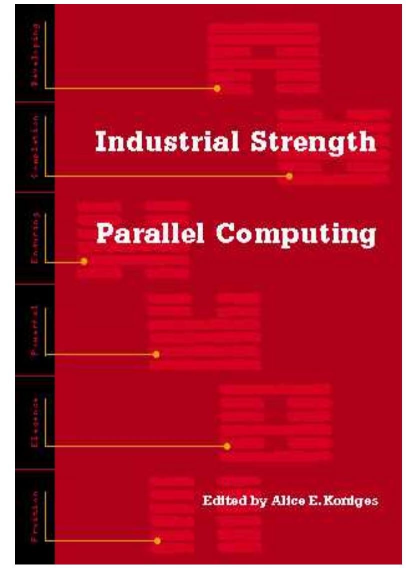
SC14 New Orleans, LA | hpc matters.

IEEE Cluster 2015
Sep. 8-11, Chicago, IL, USA

GRACE HOPPER CELEBRATION of WOMEN in COMPUTING

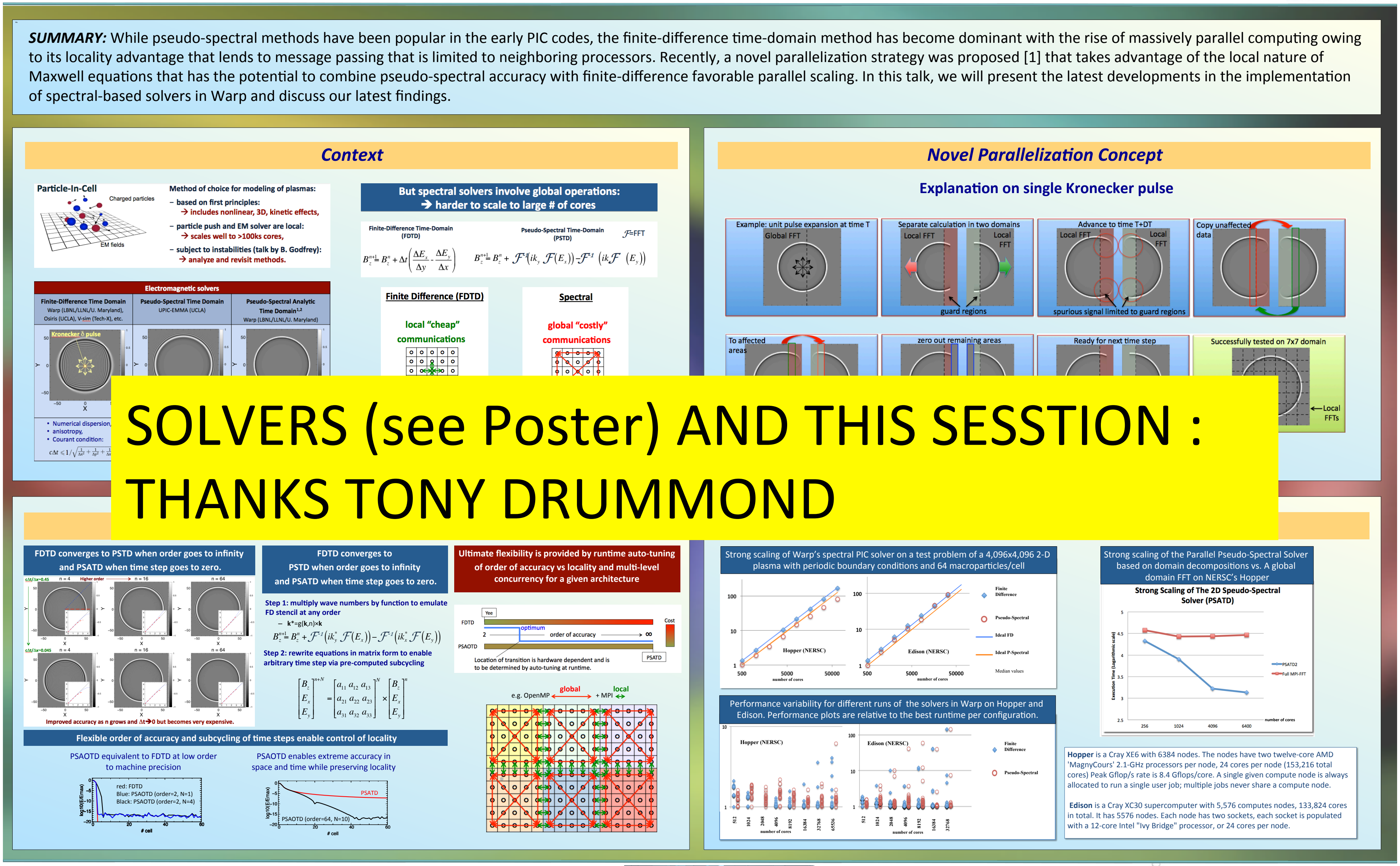
Working in the community

- Scientific Programming
  - Guest Editor
- Computational Science and Engineering
  - Invited Lead-off chapter
- International Journal of High Performance Computing
  - Associate Editor



Scalable Arbitrary-Order Pseudo-Spectral Electromagnetic Solver

J.-L. Vay[1], T. Drummond[1], A. Koniges[1], B. B. Godfrey[1,2], I. Haber[2]
[1]Lawrence Berkeley National Laboratory, [2]University of Maryland



SOLVERS (see Poster) AND THIS SESSTION : THANKS TONY DRUMMOND

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