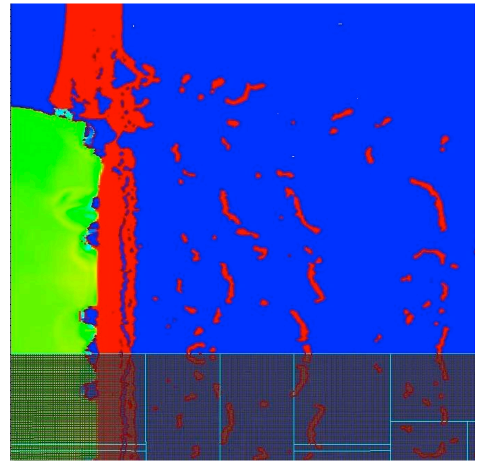
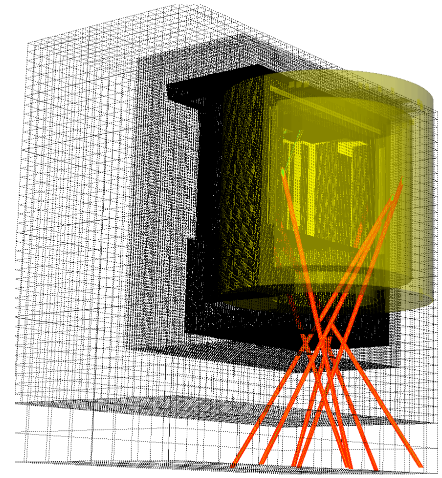
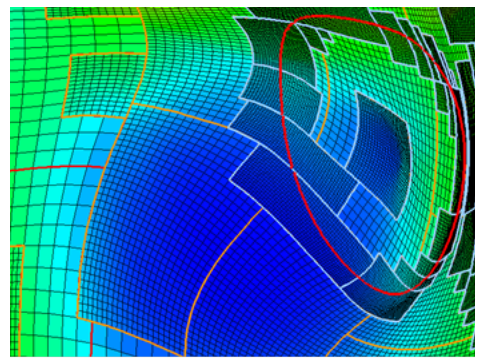
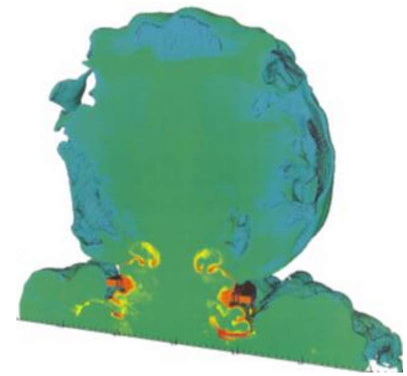
Multimaterial Multiphysics Modeling of Complex Experimental Configurations









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Center for Beam Physics Seminar

February 14, 2014

Acknowledgements

- LLNL: ALE-AMR Development and NIF Modeling
  – Robert Anderson, David Eder, Aaron Fisher, Nathan Masters
- UCLA: Surface Tension
  – Andrea Bertozzi
- UCSD: Fragmentation
  – David Benson
- LBL/LLNL: NDCX-II and Surface Tension
  – John Barnard, Alex Friedman, Wangyi Liu
- LBL/LLNL: PIC
  – Tony Drummond, David Grote, Robert Preissl, Jean-Luc Vay
- Indiana University and LSU: Asynchronous Computations
  – Hartmut Kaiser, Thomas Sterling

Outline

- Modeling for a range of experimental facilities
- Summary of multiphysics code ALE-AMR
  - ALE - Arbitrary Lagrangian Eulerian
  - AMR - Adaptive Mesh Refinement
- New surface tension model in ALE-AMR
- Sample of modeling capabilities
  - EUV Lithography
  - NDCX-II
  - National Ignition Facility
- New directions: exascale and more multiphysics
  - Coupling fluid with PIC
  - PIC challenges for exascale
  - Coupling to meso/micro scale

Multiphysics simulation code, ALE-AMR, is used to model experiments at a large range of facilities

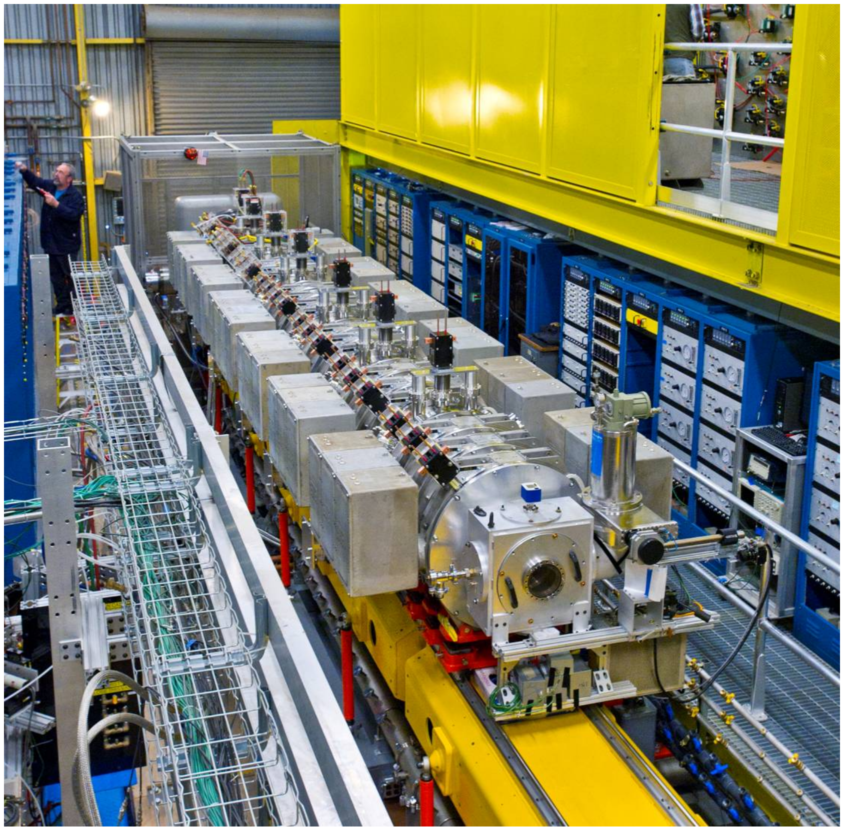
Neutralized Drift Compression Experiment (NDCX-II)

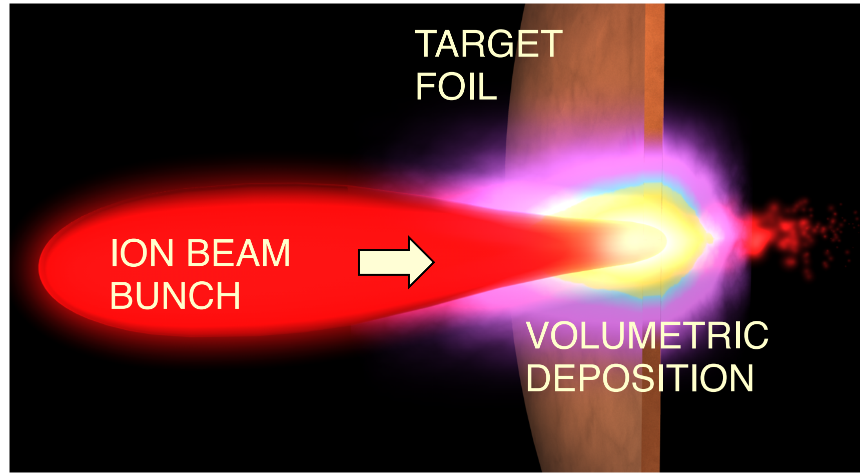
CYMER EUV Lithography System

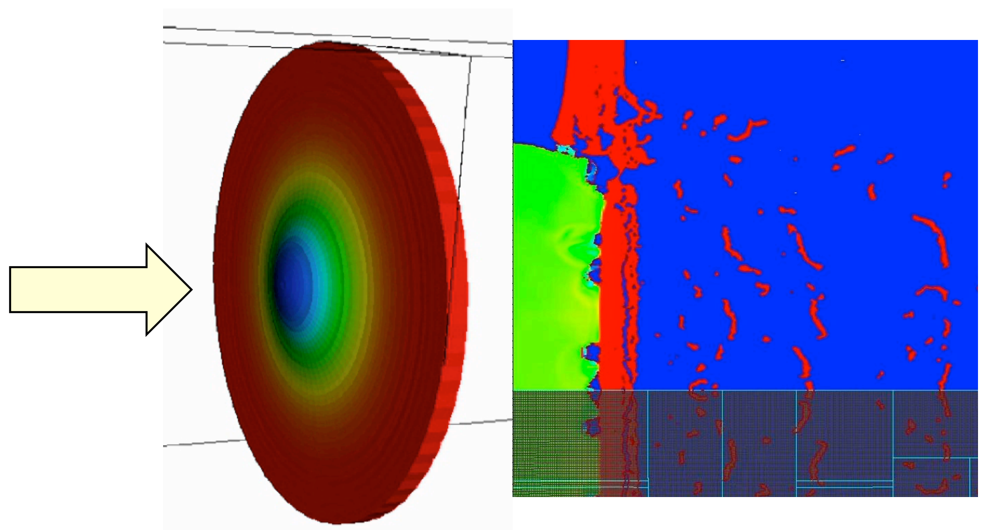
National Ignition Facility (NIF) - USA

Laser Mega Joule (LMJ) - France

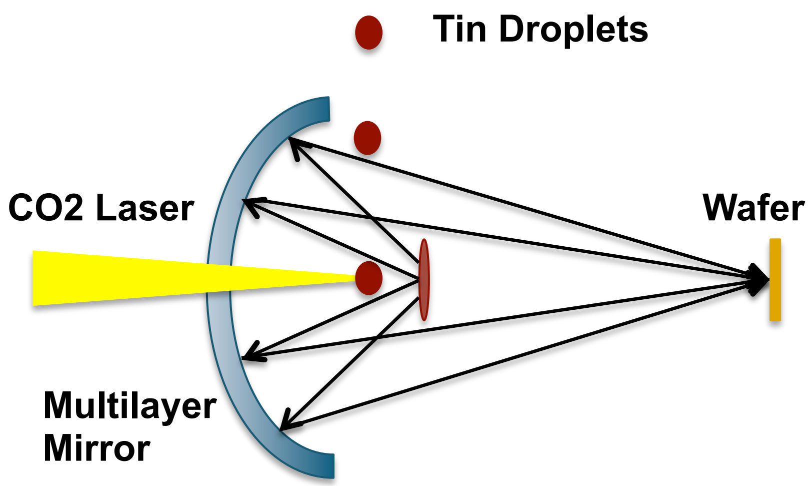
NDCX-II facility at LBNL accelerates Li ions for warm dense matter experiments



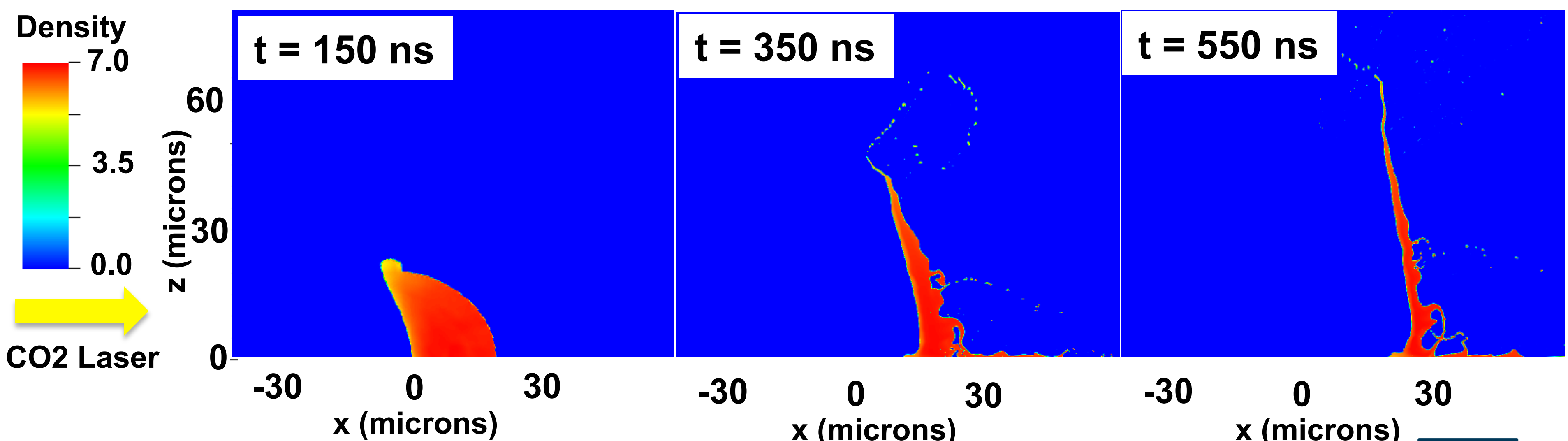




The Cymer extreme UV lithography experiment uses laser heated molten metal droplets



- Technique uses a prepulse to flatten droplet prior to main pulse
- Modeling critical to optimize process
- Surface tension affect droplet dynamics



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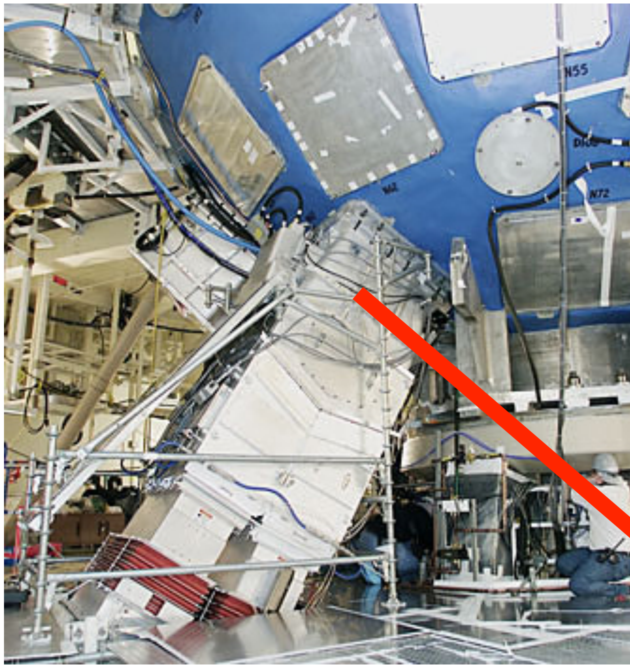
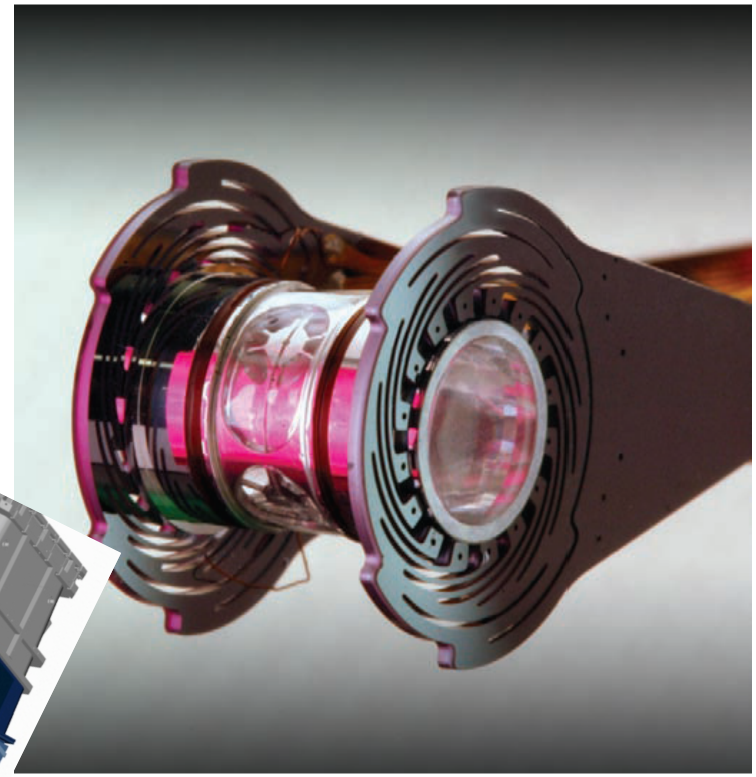
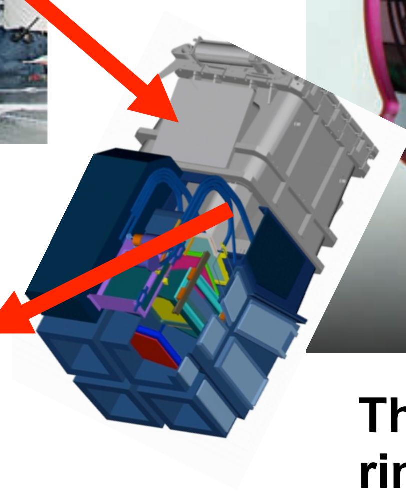
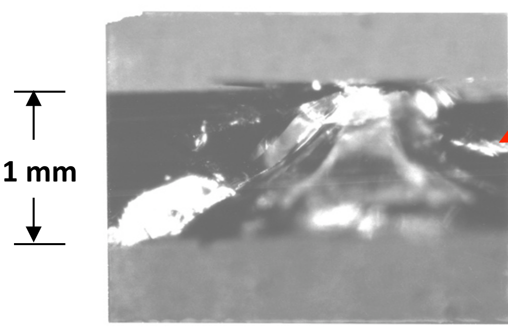
Large laser facilities, e.g., NIF and LMJ, require modeling to protect optics and diagnostics







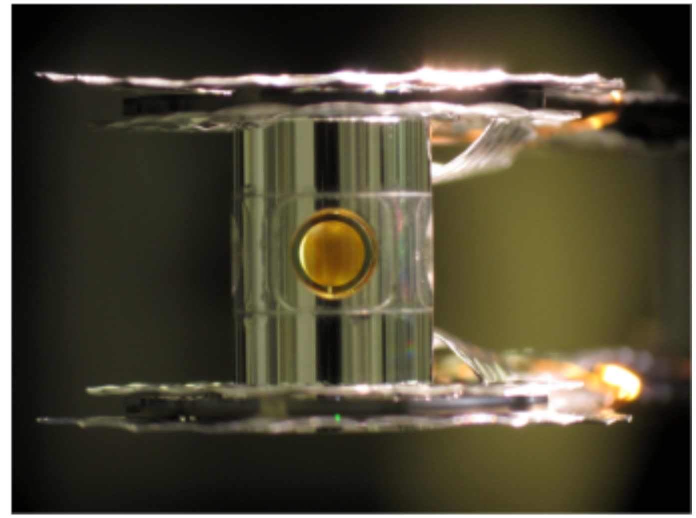


Damage to debris shields

The entire target, e. g., Si cooling rings and Al casing, must be modeled

Wide range of targets require detailed simulations for debris and shrapnel assessments/mitigations



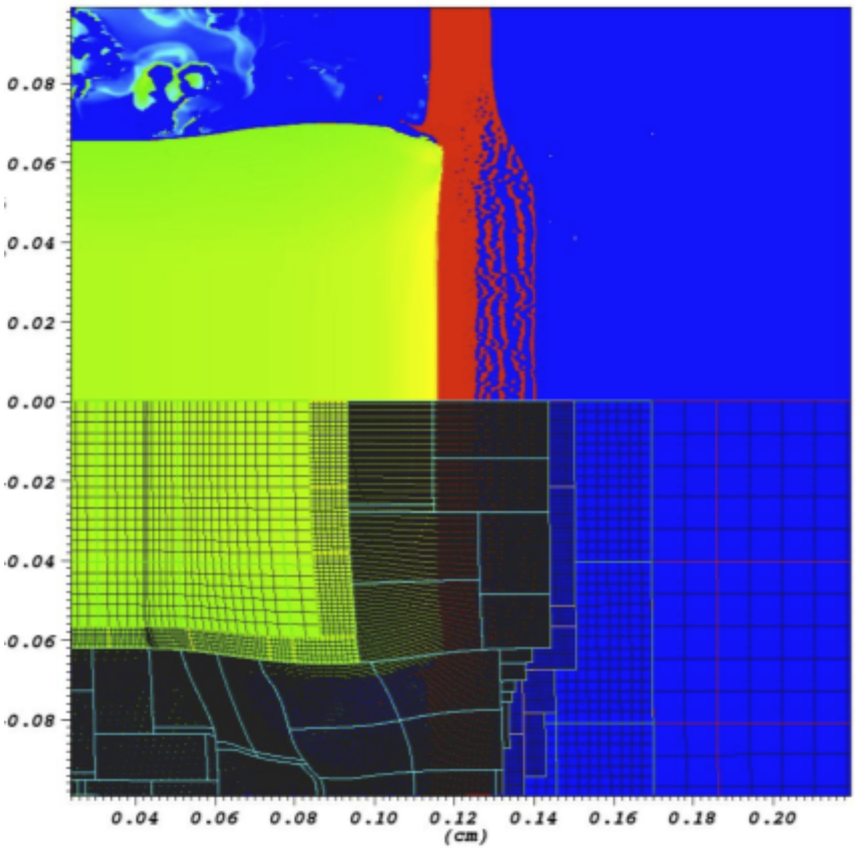






Modeling of complex experimental configurations provided by the multiphysics ALE-AMR code

Thin foil target hit from LHS



- 3D ALE hydrodynamics
- AMR (use 3X refinement)
  - With 6 levels, vol ratio 10^7 to 1
- Material interface reconstruction
- Anisotropic stress tensor
- Material failure with history
- Ion/laser deposition
- Thermal conduction
- Radiation diffusion
- Surface tension

ALE - Arbitrary Lagrangian Eulerian
AMR - Adaptive Mesh Refinement

ALE-AMR is an open science code and has no export control restrictions

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Multimateral ALE + AMR; including anisotropic stress tensor, surface tension, and sources

$$\frac{\mathrm{D}\rho}{\mathrm{D}t} = -\rho\nabla\cdot\vec{U} = -\rho U_{i,i}$$

$$\rho\frac{\mathrm{D}\vec{U}}{\mathrm{D}t} = \frac{1}{\rho}\nabla\cdot\boldsymbol{\sigma} = \frac{1}{\rho}\sigma_{ij,j}$$

$$\frac{\mathrm{D}e}{\mathrm{D}t} = \frac{1}{\rho}V\boldsymbol{s}:\dot{\boldsymbol{\varepsilon}} - P\dot{V} + \frac{1}{\rho}W_{sources} = \frac{1}{\rho}V\left(s_{ij}\dot{\varepsilon}_{ij}\right) - P\dot{V} + \frac{1}{\rho}W_{sources}$$

$$W_{sources} = W_{laser} + W_{ion} + W_{conduction} + W_{radiation}$$

$\boldsymbol{\sigma}$ is the total stress tensor (surface tension enters here), $\boldsymbol{s}$ is the deviatoric stress, and $\dot{\boldsymbol{\epsilon}}$ is the strain rate tensor with

$$s_{ij} = \sigma_{ij} + P\delta_{ij} \;\text{ and }\; \dot{\epsilon}_{\mathrm{ij}} = \frac{1}{2}\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right).$$

"Multi-Matierial ALE with AMR for Modeling Hot Plasmas and Cold Fragmenting Materials," A Koniges, N Masters, A Fisher, D Eder, Wi Liu, R Anderson, D Benson, Invited for special issue of **Plasma Science and Technology** (in review), 2014.

We model both heat conduction and radiation transport based on the diffusion approximation

Diffusion equation

$$\nabla \bullet \alpha \nabla u + \beta u = f$$

Heat Conduction

$$C_v \frac{T^{n+1} - T^n}{\Delta t} = \nabla \bullet D^n \nabla T^{n+1} - \sigma T^{n+1}$$

$$\alpha = D^n$$

$$\beta = -\sigma - \frac{C_v}{\Delta t}$$

$$f = -\frac{C_v}{\Delta t} T^n$$

Radiation Diffusion

$$\frac{E_R^{n+1} - E_R^n}{\Delta t} = \nabla \bullet \lambda \left(\frac{c}{\kappa_R} \right) \nabla E_R^{n+1} + \tilde{\kappa}_P (B^n - cE_R^{n+1})$$

$$C_v \frac{T^{n+1} - T^n}{\Delta t} = -\tilde{\kappa}_P (B^n - cE_R^{n+1})$$

$$\alpha = \lambda \left(\frac{c}{\kappa_R} \right)$$

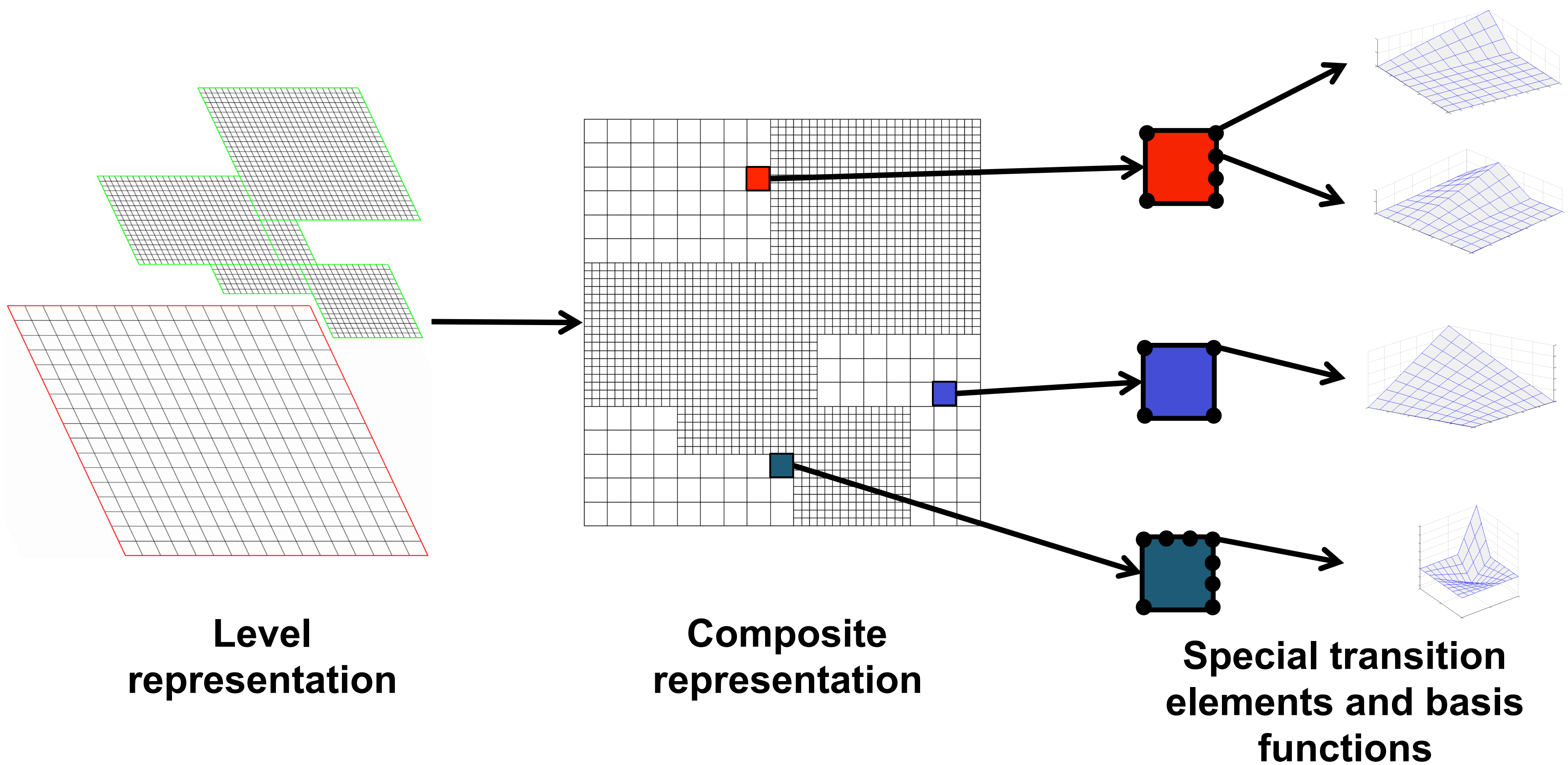
$$\beta = -\tilde{\kappa}_P c - \frac{1}{\Delta t}$$

$$f = -\frac{1}{\Delta t} - \tilde{\kappa}_P B^n$$

“An AMR Capable Finite Element Diffusion Solver for ALE Hydrocodes,” A Fisher, D Bailey, T Kaiser, D Eder, B Gunney, N Masters, A Koniges, R Anderson, Invited for special issue of **Plasma Science and Technology** (in review), 2014.

The diffusion equations are solved using Finite Element Methods accounting for AMR issues

- We map the level representation to an equivalent composite mesh
- Special nodal basis functions are constructed to handle the C-F interface



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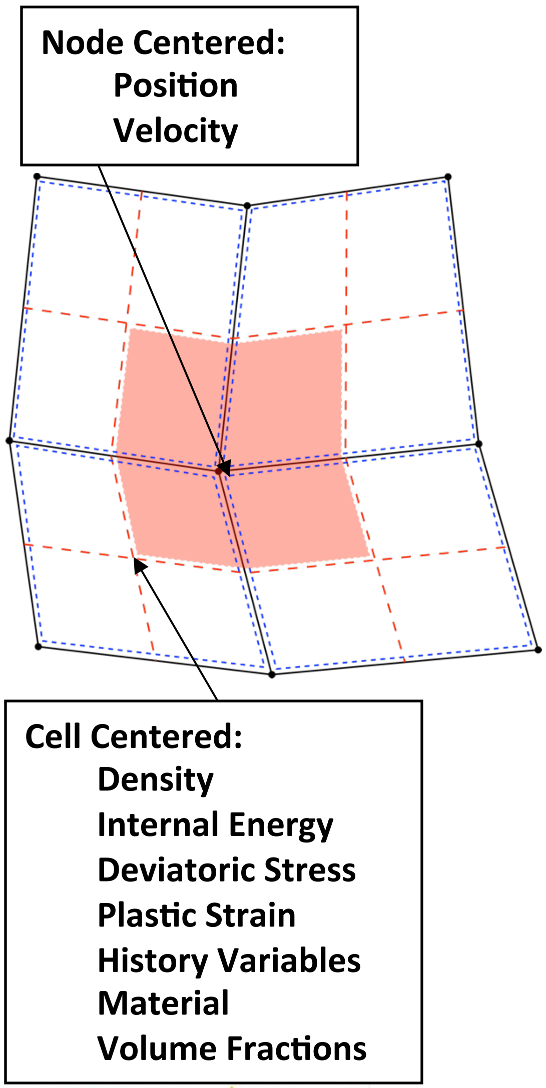
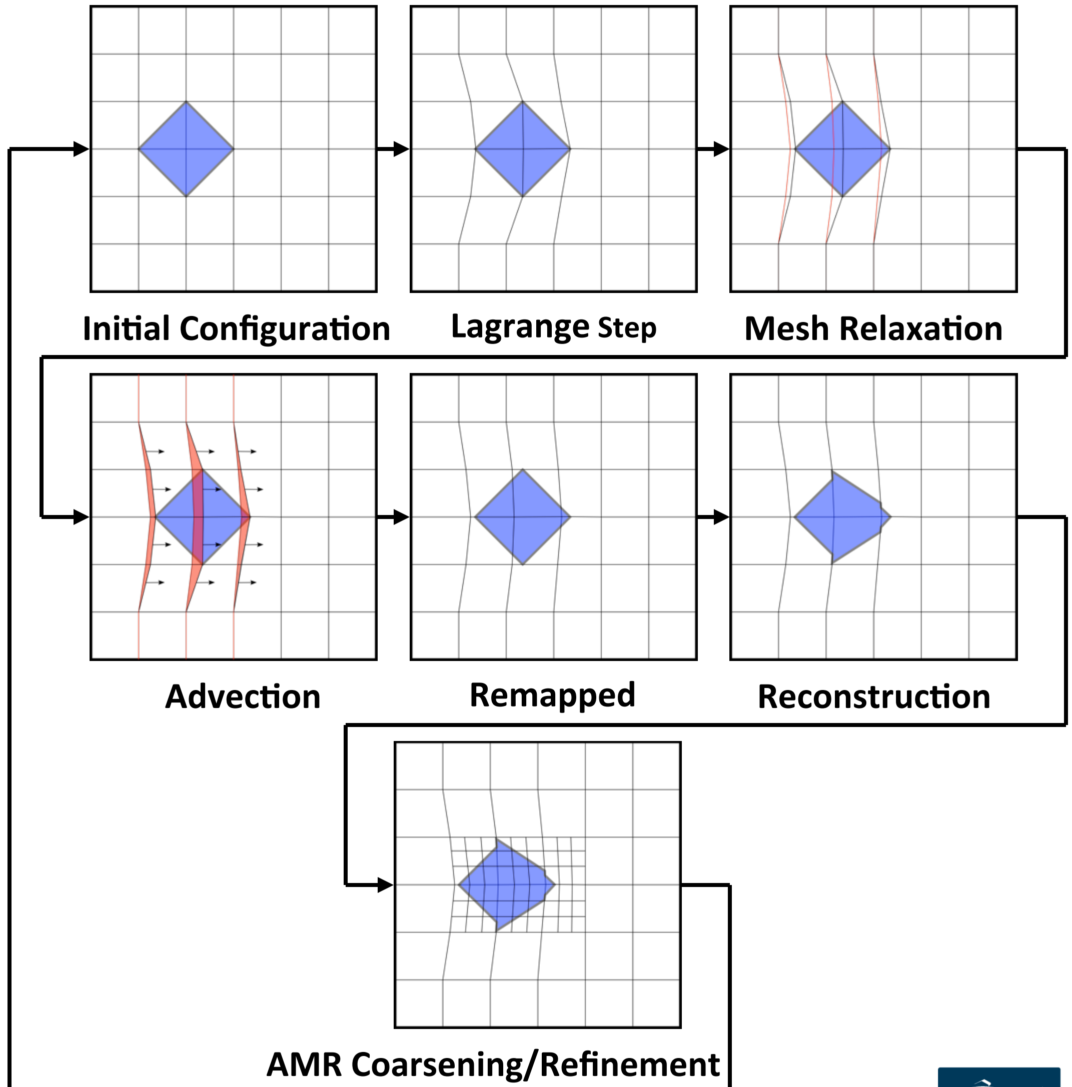
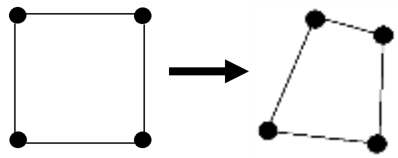
Staggered mesh Lagrange+Remap built on a structured adaptive mesh refinement framework (SAMRAI)





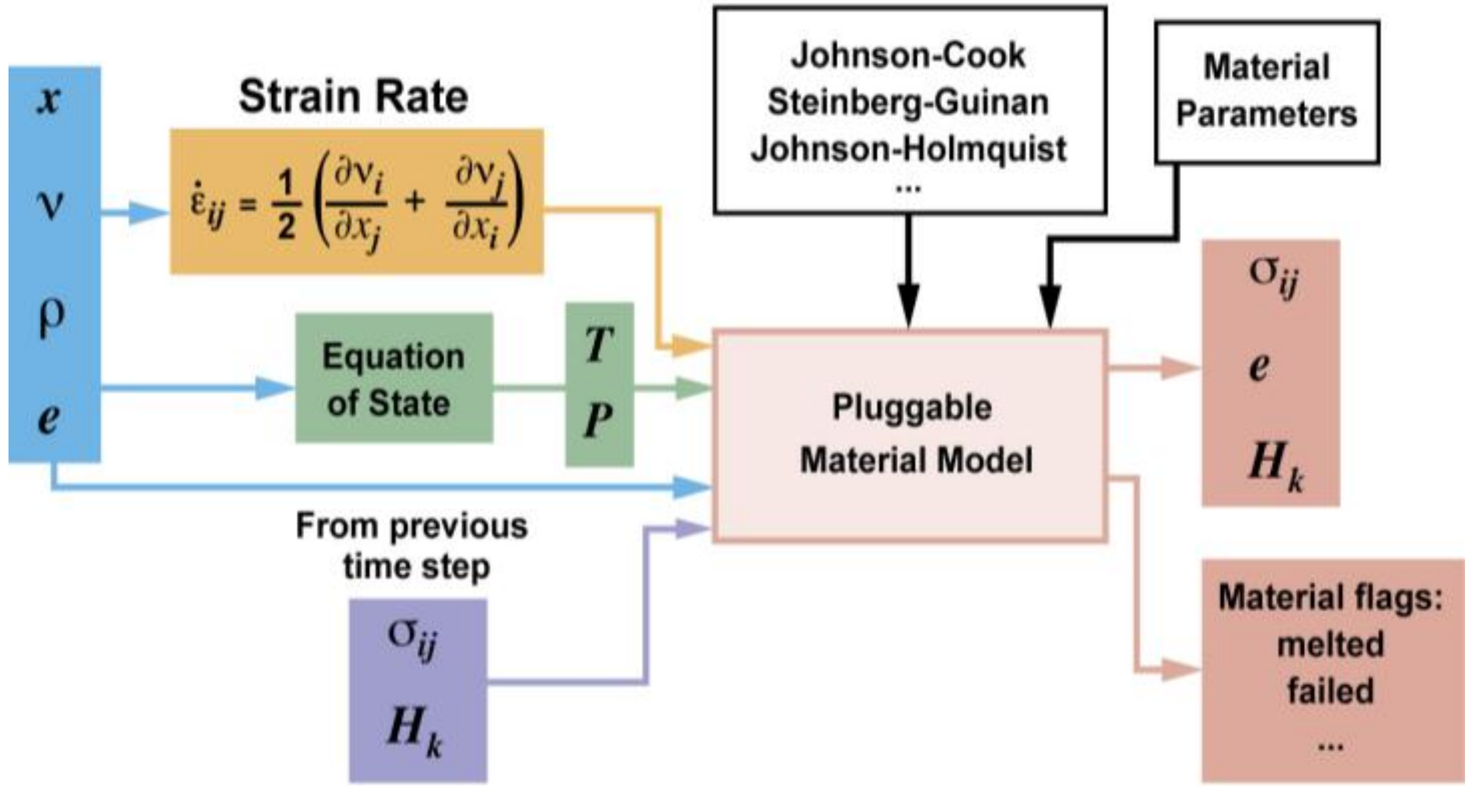
Code has a flexible framework with a new surface tension model active during the Lagrange step

Lagrange Step



Calculate surface curvature using volume fractions giving additional term in stress tensor

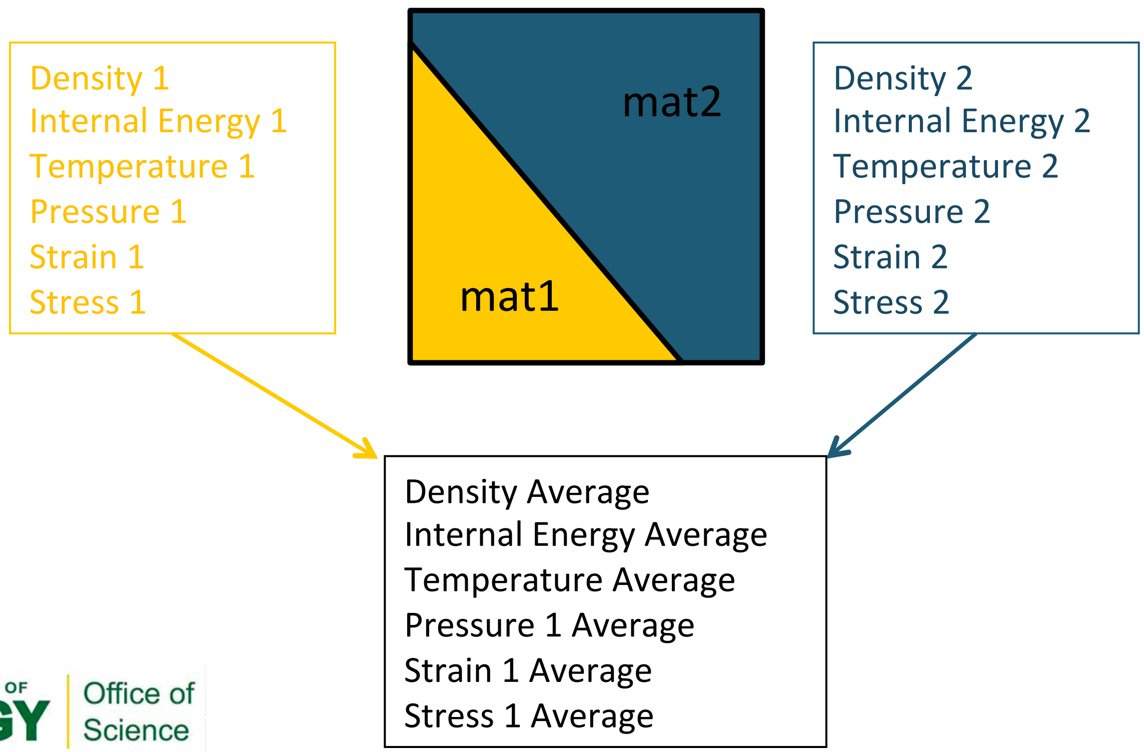
Post-Lagrange Material Update



Relax/Remap Split Physics

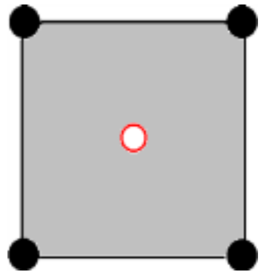
Mixed cells

- **Mixed cells have more than one material in them**
- **Volume fractions of each material in a mixed cell are tracked**
- **Interfaces are constructed using the volume fractions of nearby cells**
- **Cell based quantities are tracked for each material in the cell**
- **An average of each quantity is computed for hydro step**

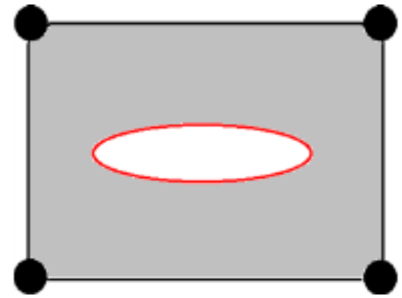


Solid fragmentation obtained using a void insertion model plus interface reconstruction

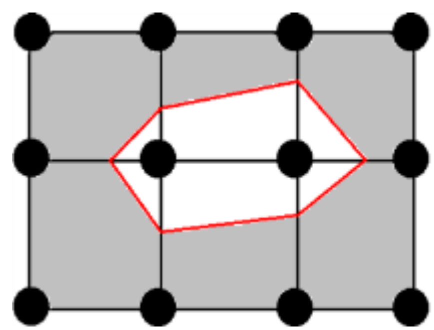
Upon failure a small volume fraction of void is introduced into the cell

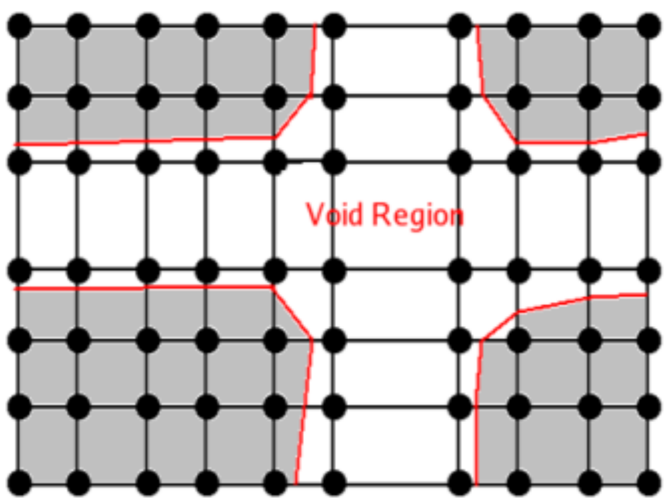


If the cell continues to grow the void enlarges to meet that growth

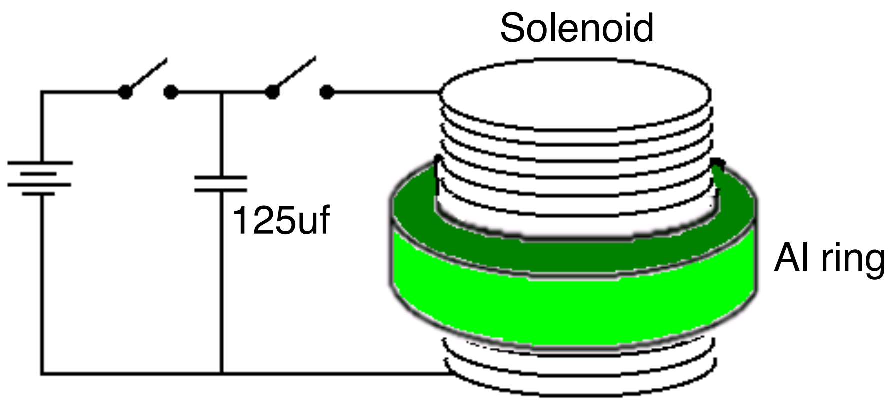


Volume fraction interface reconstruction allows voids to coalesce to form cracks

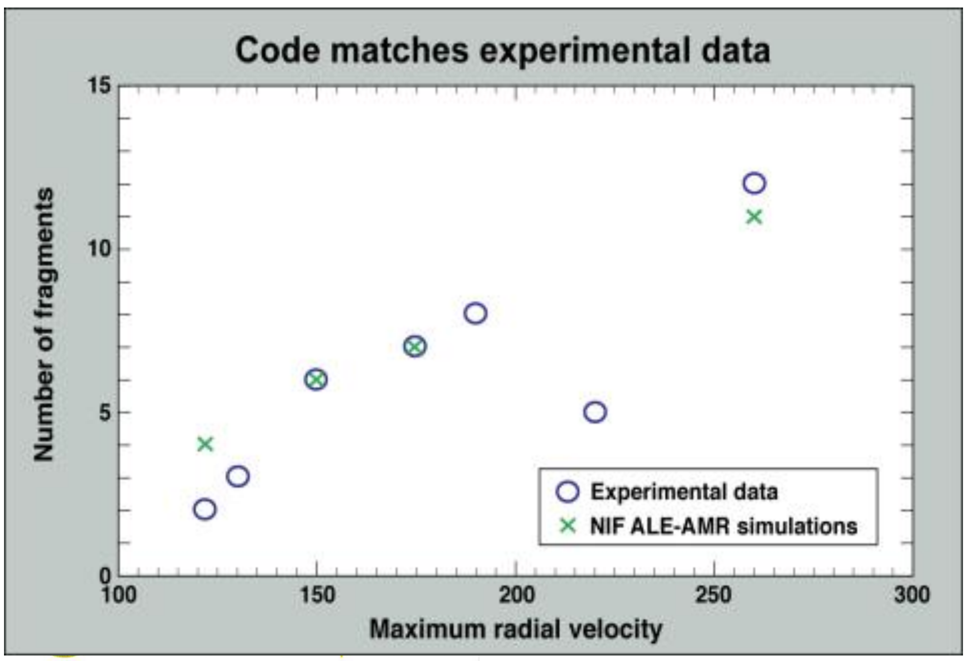




Fragmentation modeling validated against expanding ring experiment



- 15mm radius 1x1mm cross-section
- Magnetic field induces current
- Current heats and expands the ring
- Fragments are collected and counted



ALE-AMR simulations

- Use 5x5 elements by 600 elements
- Temperature from resistive heating
- Body force provides acceleration
- 6000 time steps to reach 45us

Number of calculated fragments in good agreement with data

M. Altynova, X. Hu, and G. Daehn: Increased Ductility in High Velocity Electromagnetic Ring Expansion, Metall. Material Trans. A, 27A, p1837-1844, (1996)

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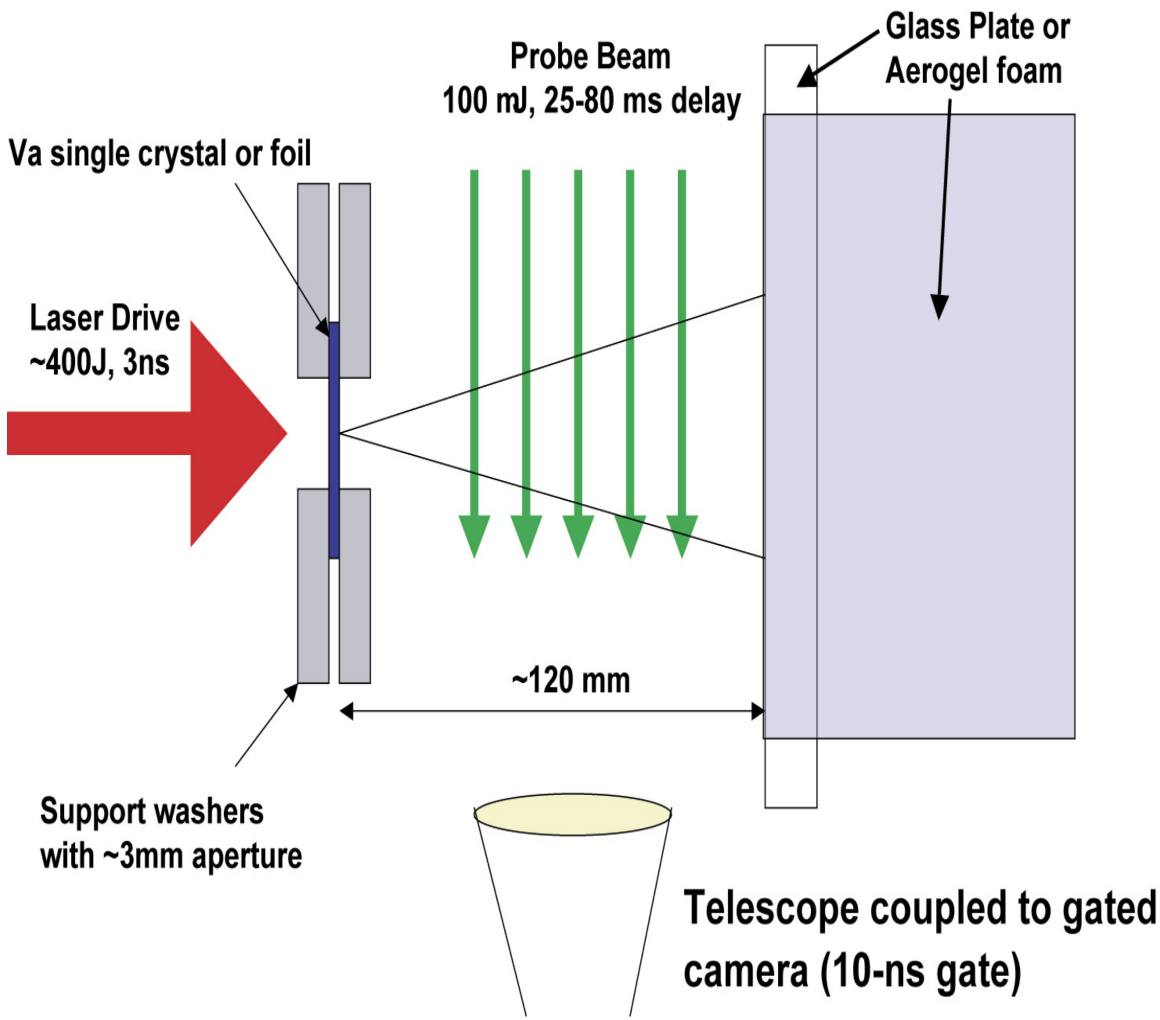
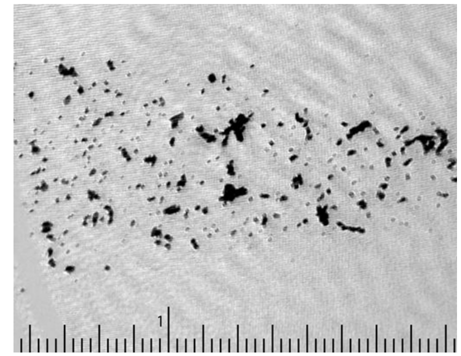
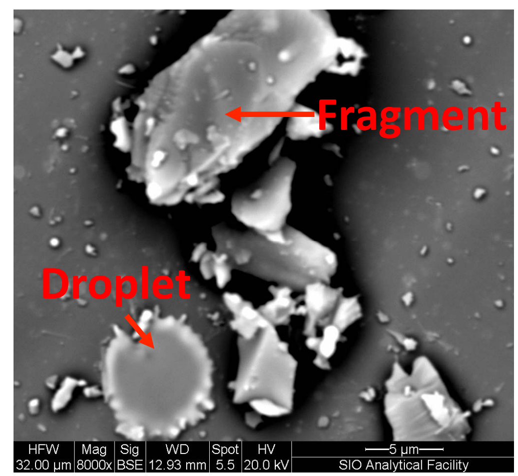
ALE-AMR fragmentation validation experiments were conducted at the Jupiter Laser Facility (Janus laser)



Fragments in flight



Collection on glass



"Experiments for the Validation of Debris and Shrapnel Calculations," A. Koniges, et al., **Journal Physics Conference Series 11**, 032072, 2008.

"Laser Compression and Fragmentation of Metals," M Meyers, H Jarmakani, B Cao, C Wei, B Kad, B Remington, E Bringa, B Maddox, D Kalantar, D Eder, A Koniges, **Proc DYMAT**, pp. 37-42, 2009.

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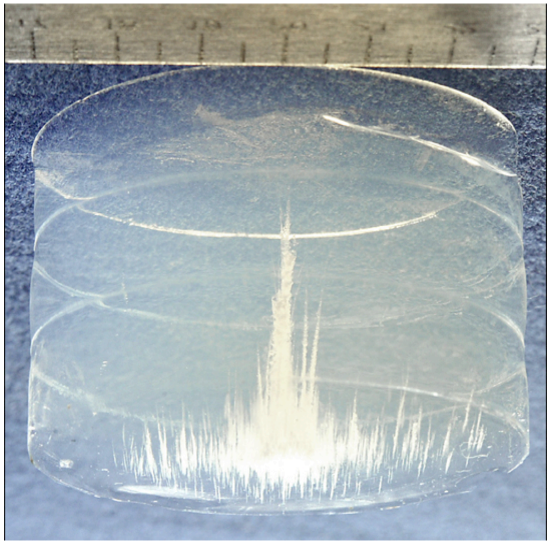
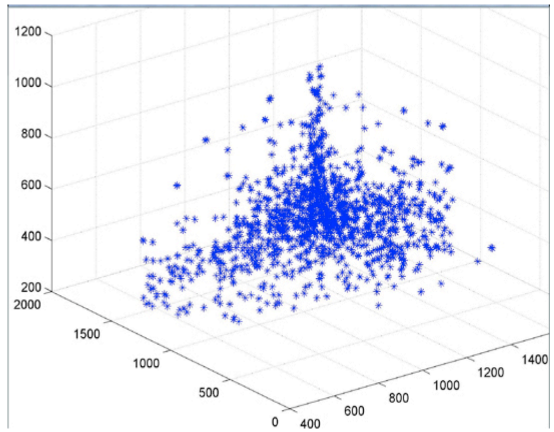
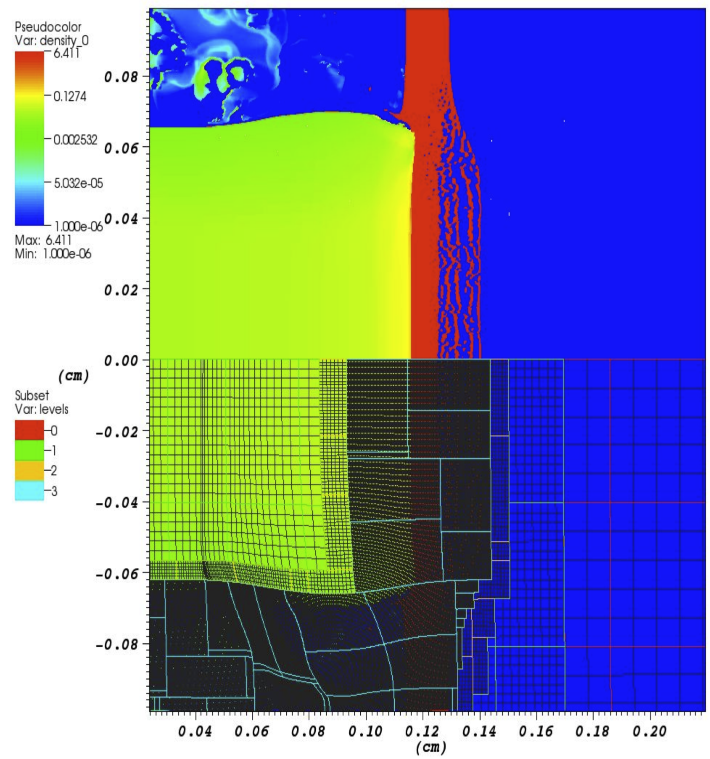
To measure the size and velocity of spalled fragments used low density aerogel in our Janus experiments



Radiographic results



Simulation with spall



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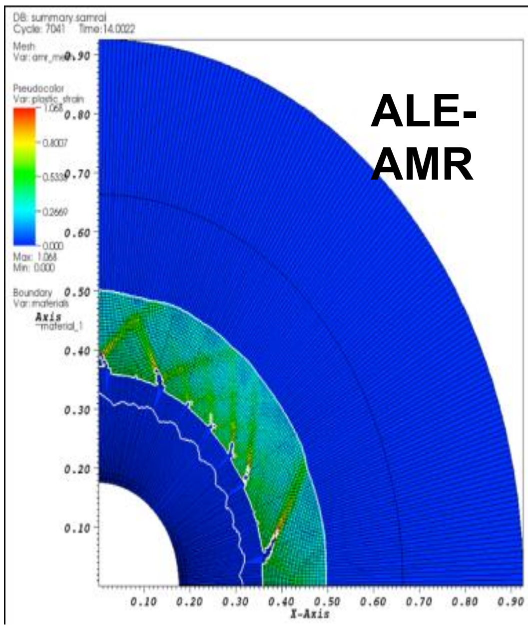
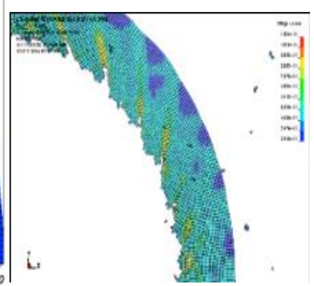
Benchmarking using other codes and test problems

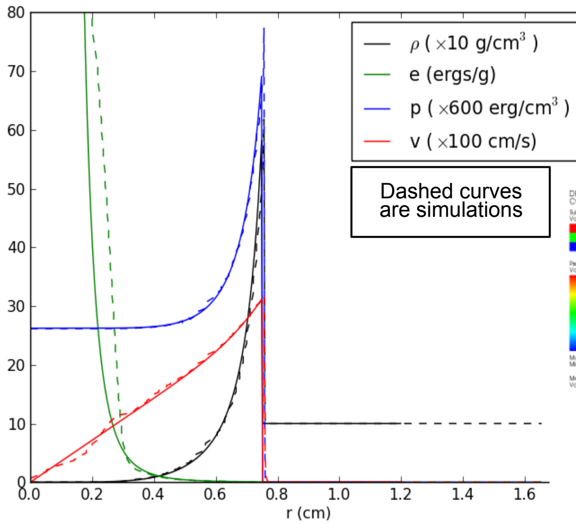
• 4-mm ring made of Al6061 surrounded by void
• Johnson-Cook strength and damage models



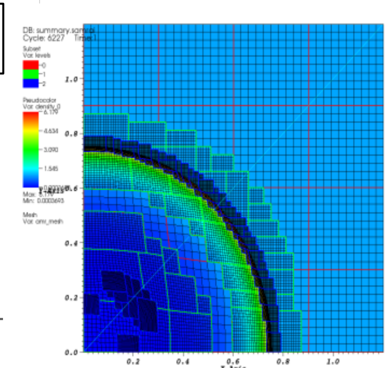
LS-DYNA



Plastic strain comparison



ALE-AMR ALE mode (3 level 360x360)



To model experiments on NDCX-II an ion deposition model was added to the code

The Bethe-Block formulation for ion deposition in ALE-AMR is

$$-\frac{dE}{dx} = \left[\frac{4\pi e^2}{m_e c^2}\right]\left[\frac{N_0 \rho_T}{A_T}\right]\left[\frac{Z_{eff}^2}{\beta^2}\right]\left[(Z_T - \bar{Z})(\mathrm{Log}\Lambda_\mathrm{B} + \mathrm{R}) + \bar{\mathrm{Z}}\mathrm{G}(\beta/\beta_\mathrm{e})(\mathrm{Log}\Lambda_\mathrm{F} + \mathrm{R}/2)\right],$$

where ρ_T, A_T, Z_T, and $\bar{Z}$ are the target density, target atomic weight, target atomic number, and target ionization state, respectively, and

$$\Lambda_B = 2m_e c^2 \beta^2 / \bar{I}$$

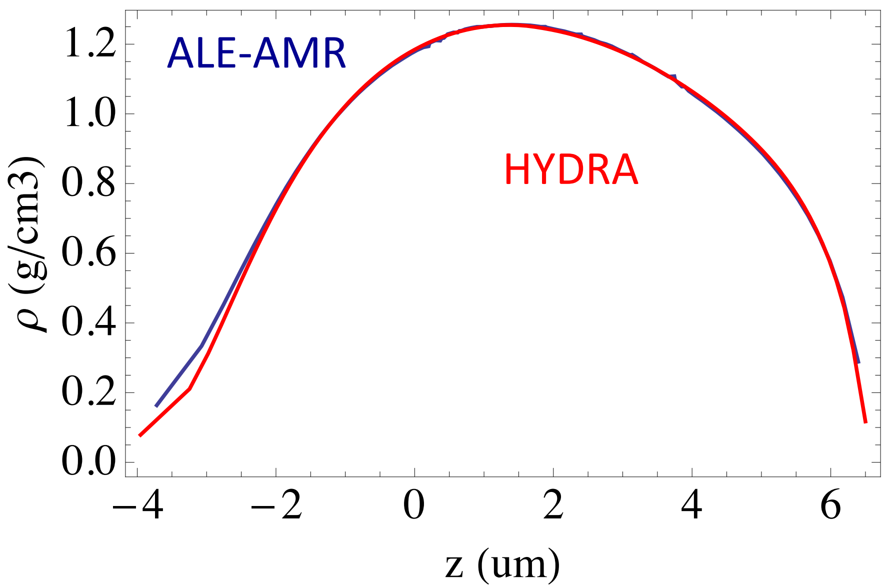
$$\Lambda_F = m_e c^2 \beta^2 / \hbar\omega_p)$$

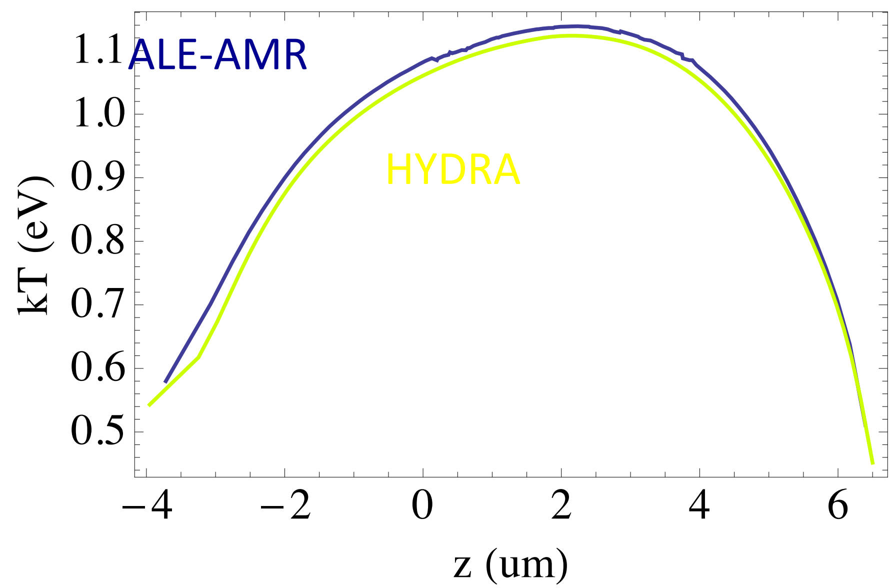
$$G(x) = \mathrm{erf(x) - xd[erf(x)]/dx}$$

$$R = 2(\log\gamma) - \beta^2$$

The ALE-AMR ion beam simulations are in excellent agreement with results from Hydra

Density and temperature profiles at the completion of the 1 ns, 2.8 MeV, Li ion heating pulse along the radial center of an Al foil. Fluence of 20 J/cm^2.



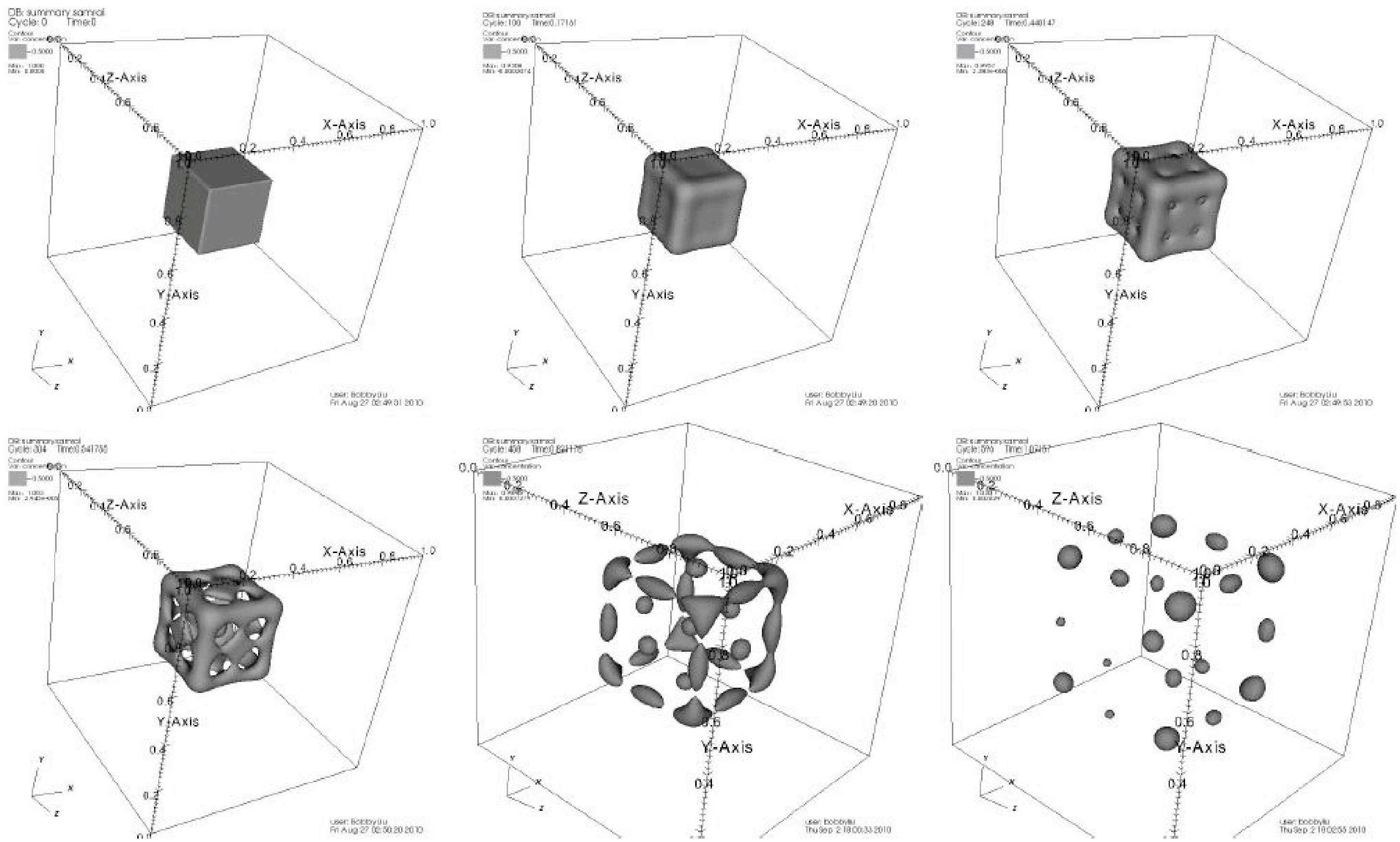


The Hydra source is not open, which limits the ability to add new packages, e.g., AMR, surface tension, fragmentation models, and new multiphysics

"Modeling Warm Dense Matter Experiments using the 3D ALE-AMR Code and the Move Toward Exascale Computing," A Koniges, D Eder, W. Liu, J Barnard, A Friedman, G Logan, A Fisher, N Masers, A Bertozzi, **EPJ Web of Conferences 59**, 09006, 2013.

Diffuse interface models for surface tension can be coupled through diffusion solver framework

Droplet break-up using Cahn-Hilliard and divergent velocity field



"Modeling droplet breakup effects in warm dense matter experiments with diffuse interface methods in ALE-AMR code," W Liu, J Bernard, A Friedman, N Masters, A Fisher, V Mlaker, A Koniges, D Eder, **Proc. SciDAC 2011**, Denver, CO, 2011.

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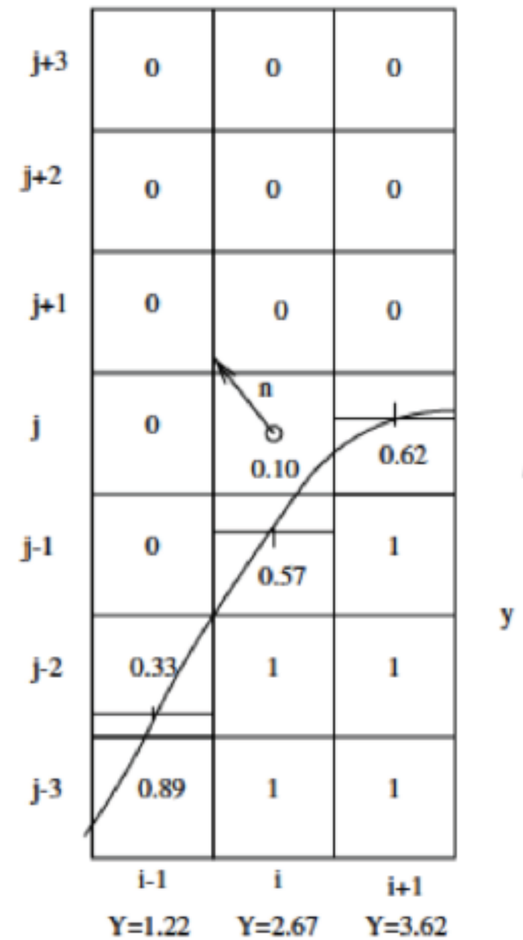
Alternative surface tension methodology using volume fractions and height function

Force $f = \gamma \kappa \vec{n}$, where γ is the surface tension coefficient, κ is the curvature, and $\vec{n}$ is normal

Calculate volume fraction of liquid in each zone and then calculate resulting height function

In 2D, we do a quadratic fit using 3 points
$y = h_1x^2 + h^2x + h_3$ and $\kappa = 2h_1 (1 + h_2^2)^{-1.5}$

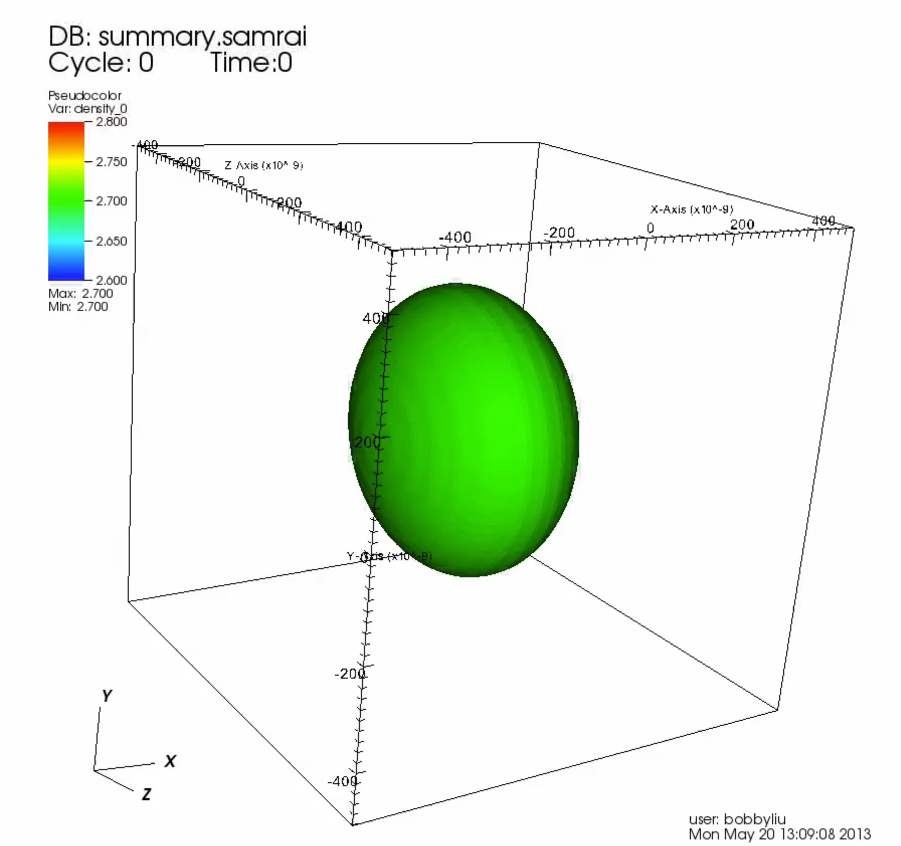
The curvature and normal are calculated in cells but the force like velocity are nodal so cell curvature is averaged to get node value



“Estimating curvature from volume fractions,” S. J. Cummins, M. M. Francois, and D. B. Kothe, Computers and Structures **83**, 425 (2005)

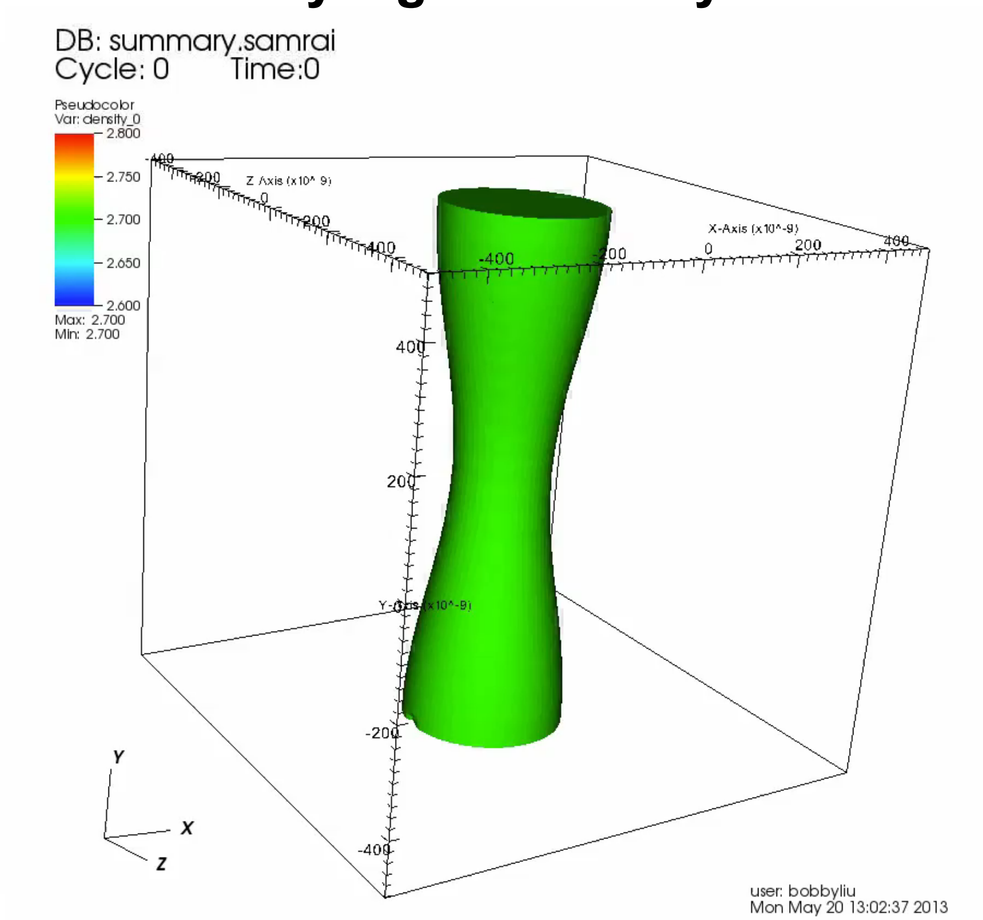
We have validated the surface tension model using different test cases with analytic solutions

Ellipsoid oscillation



Level of damping depends on the surrounding material

Rayleigh instability



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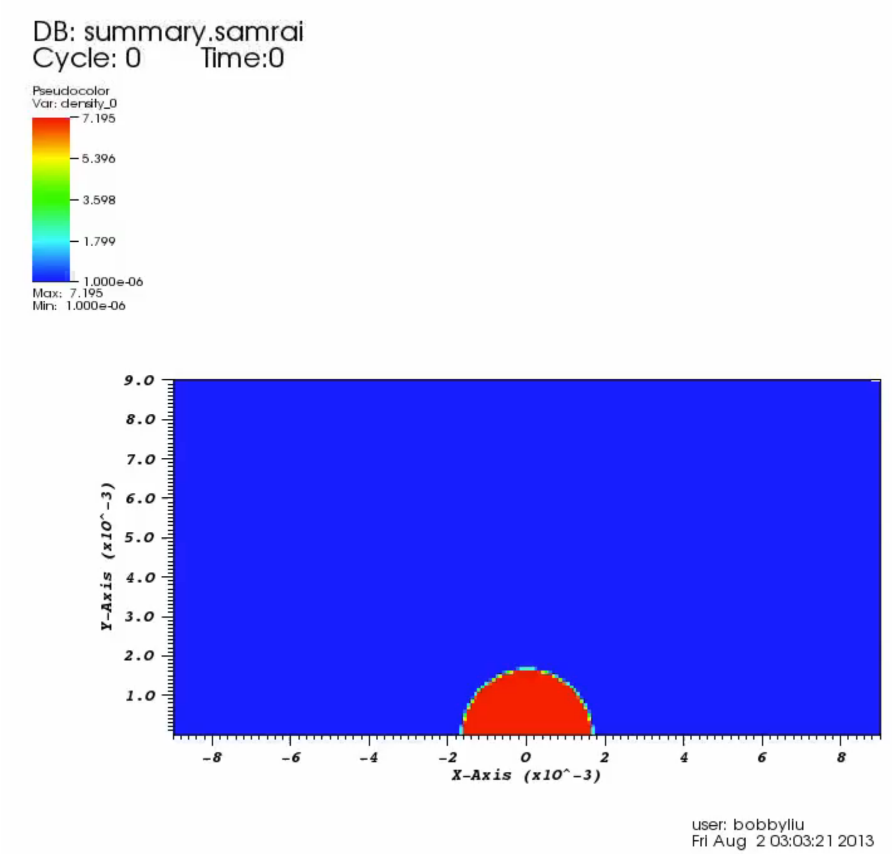
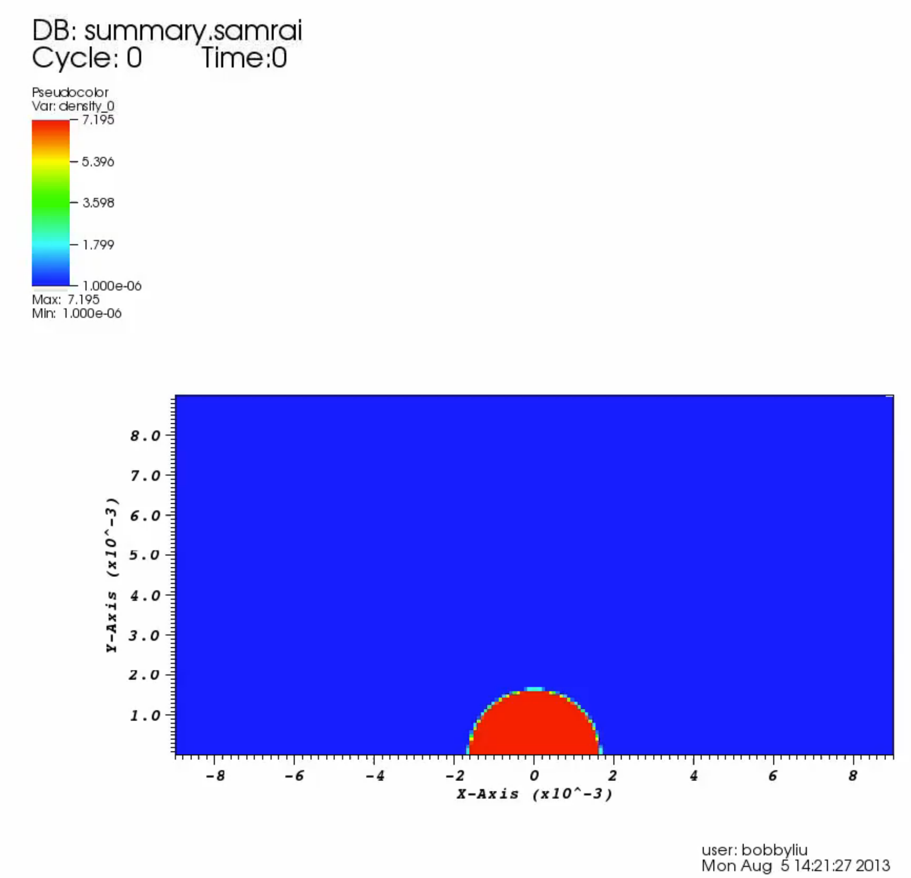
We are exploring different ways to define the liquid vapor interface in the simulations

Without surface tension

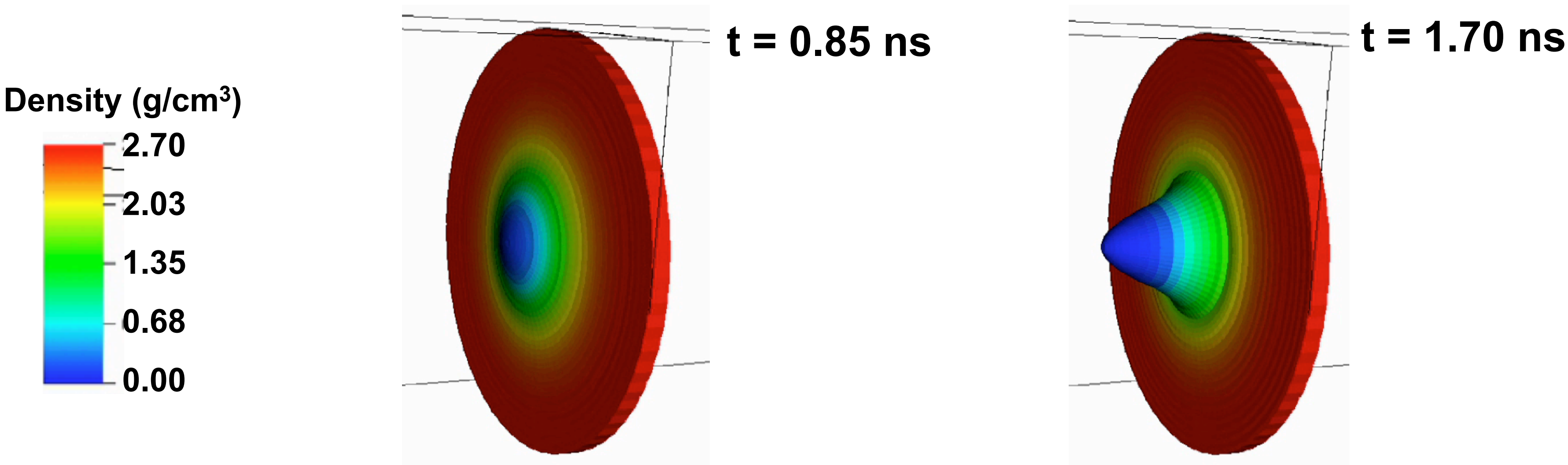


With surface tension



These simulations use a density criteria to define interface

ALE-AMR can be used to design future NDCX II experiments with sub ns high-energy pulses

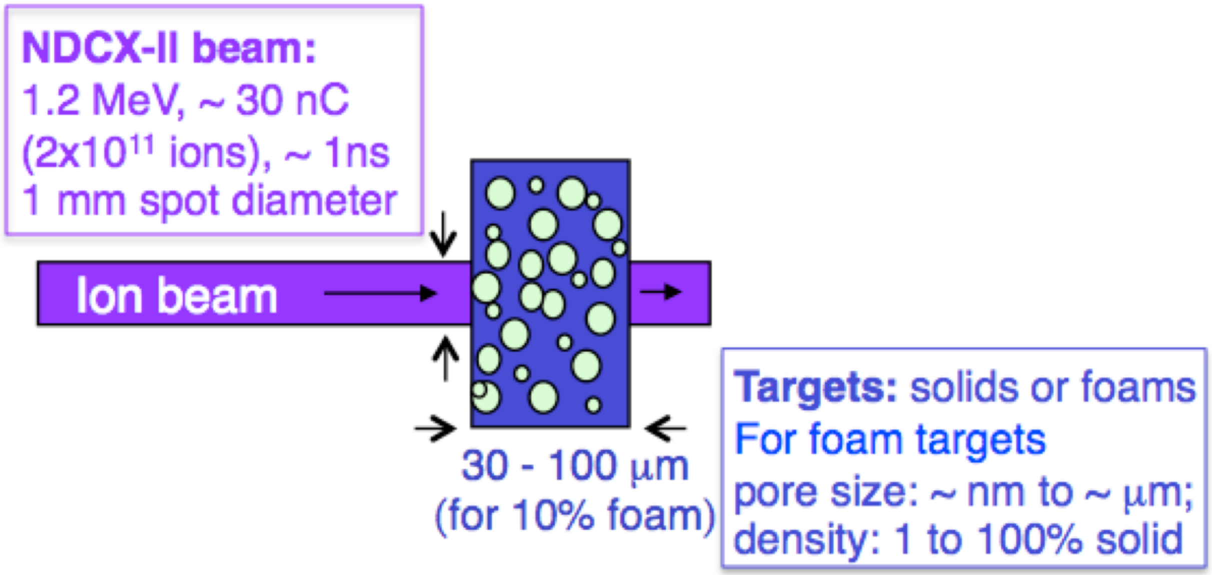


- **2D simulation of thin (1 micron) foil at end of heating pulse (left) and at 2X the pulse duration (right)**
- **The longitudinal scale is exaggerated relative to the transverse**
- **The radius of the simulated target is 1 mm**
- **Simulations confirm heating within hydrodynamic expansion times**

"Advanced Target Effects Modeling for Ion Accelerators and other High-Energy-Density Experiments," A Koniges, W Liu, S Lidia, T Schenkel, J Barnard, A Friedman, D Eder, A Fisher, and N Masters, **The Eighth International Conference on Inertial Fusion Sciences and Application** (in review), 2014.

Proposed experiments on NDCX II can study a wide range of warm dense matter regimes

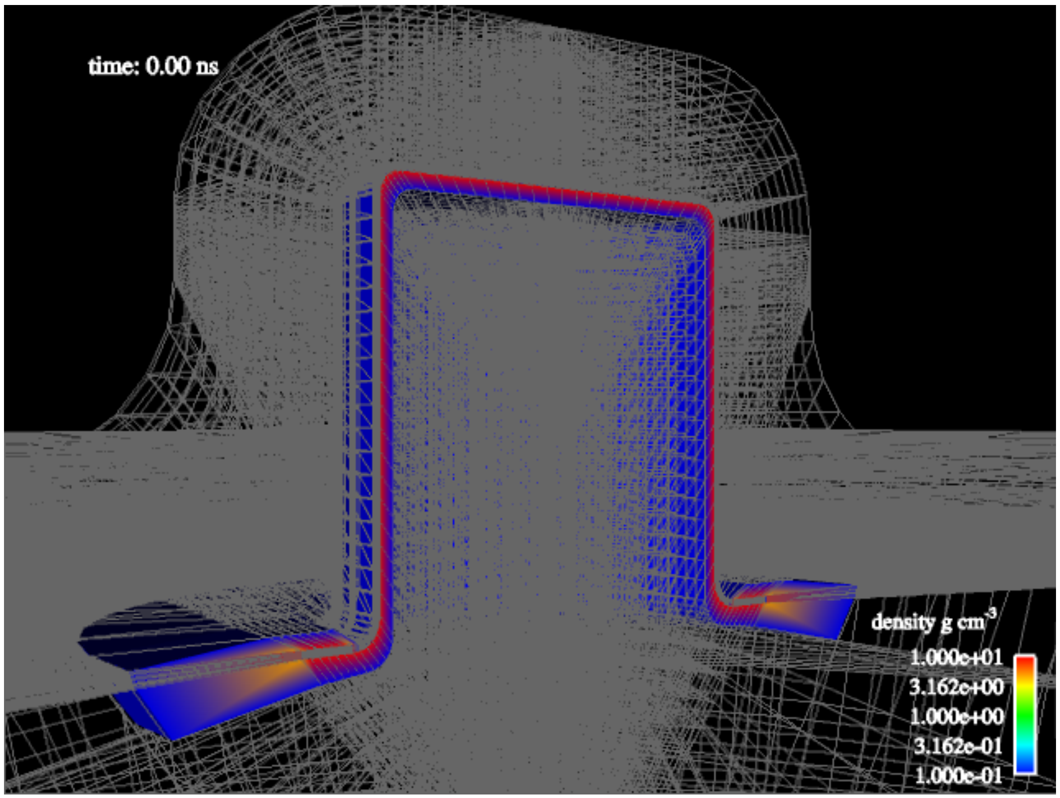
- **Diagnostics could measure properties of hot expanding matter including droplet size, droplet rate formation, homogeneity of temperature, hydrodynamics instabilities growth rate, etc.**
- **New modeling techniques will allow the design and analysis of these experiments, which can include both solid and foam targets**



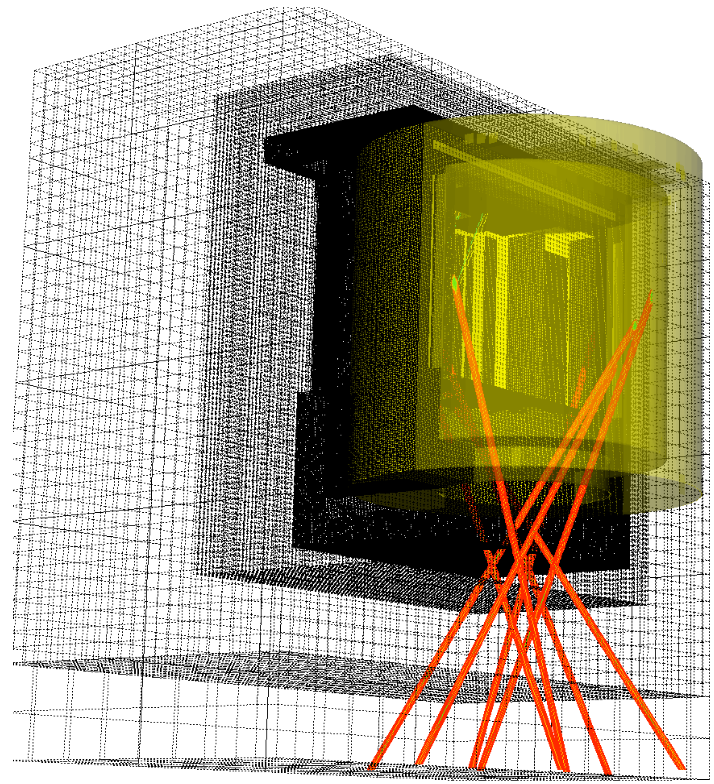
"NDCX-II target experiments and simulations," J Barnard, R More, M Terry, A Friedman, E Henestroza, A Koniges, J Kwan, A Ng, P Ni, W Liu, B Logan, E Startsev, A Yuen, **Nuclear Instruments and Methods in Physics Research 733**, 45, 2014.

Historical development of ALE-AMR: Traditional ALE (like Hydra) inappropriate for late-time

Traditional ALE

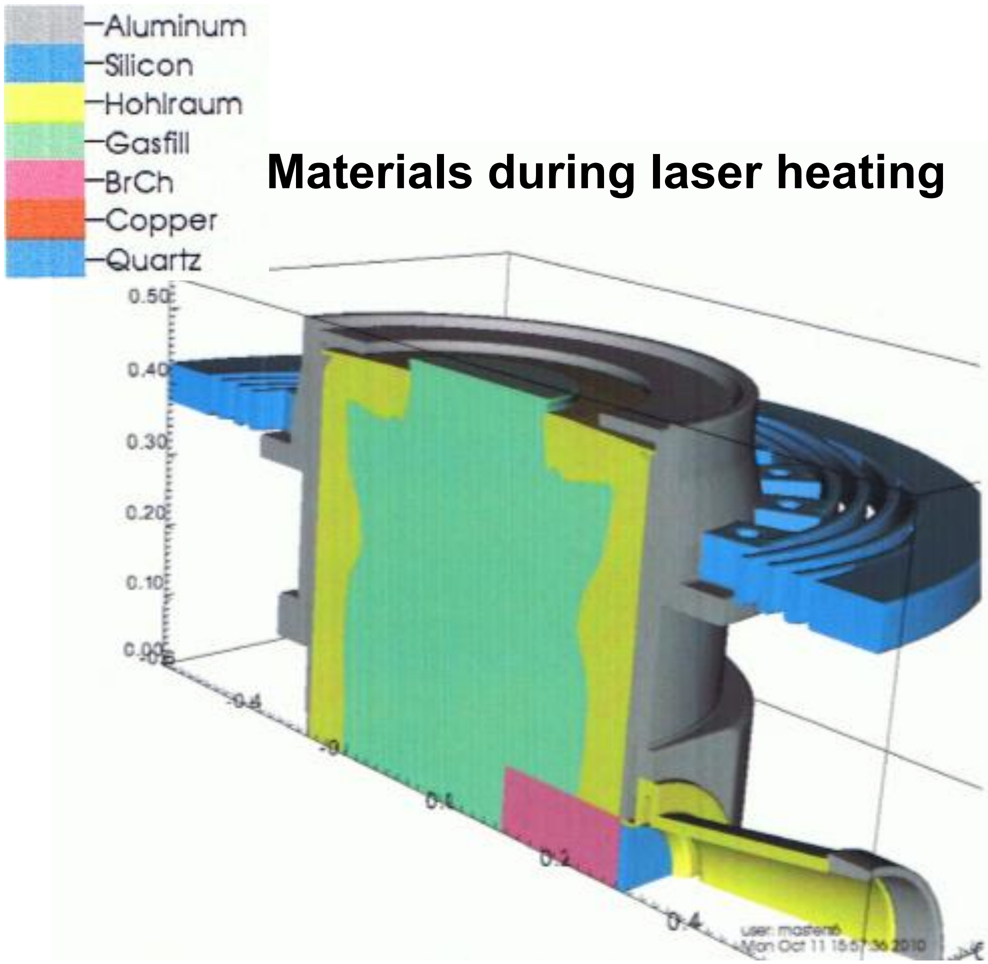


Newly Designed ALE-AMR

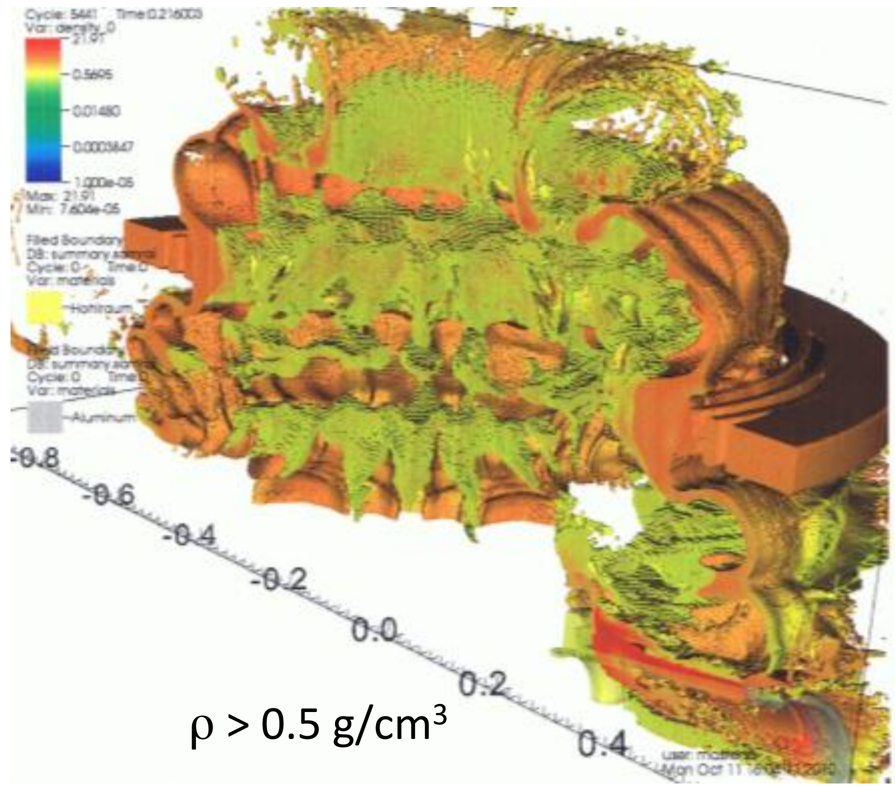


ALE-AMR was developed initially for late-time whole-target (not just hohlraum) NIF simulations

Materials during laser heating



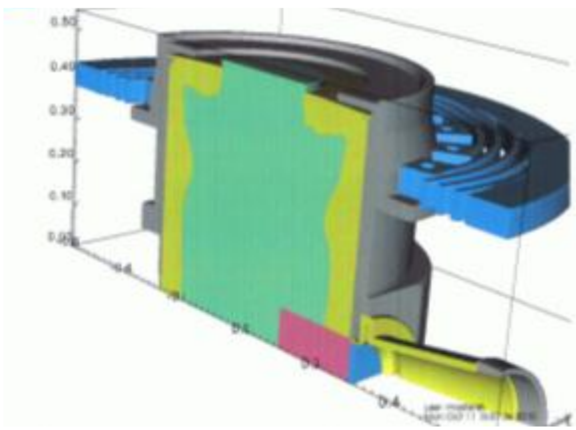
Threshold density at 220 ns

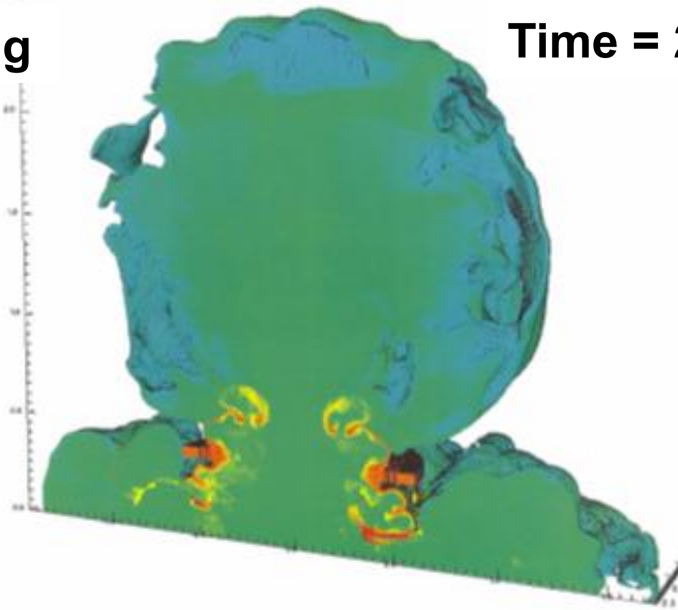


"Modelling debris and shrapnel generation in inertial confinement fusion experiments," D Eder, A Fisher, A Koniges and N Masters, **Nuclear Fusion 53**, 113037, 2013.

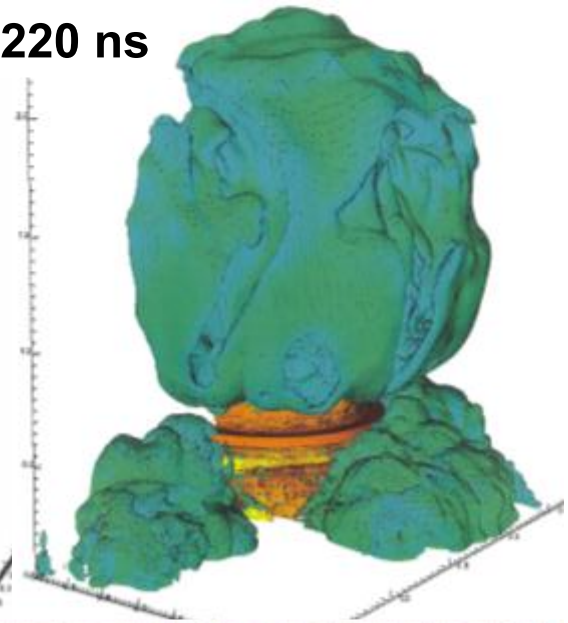
The use of AMR with six levels of refinement is critical to model plasma plume expansion

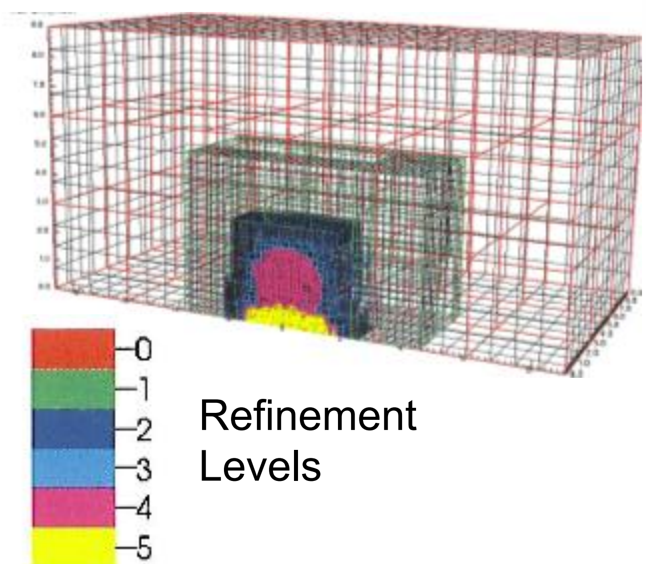
Materials during laser heating



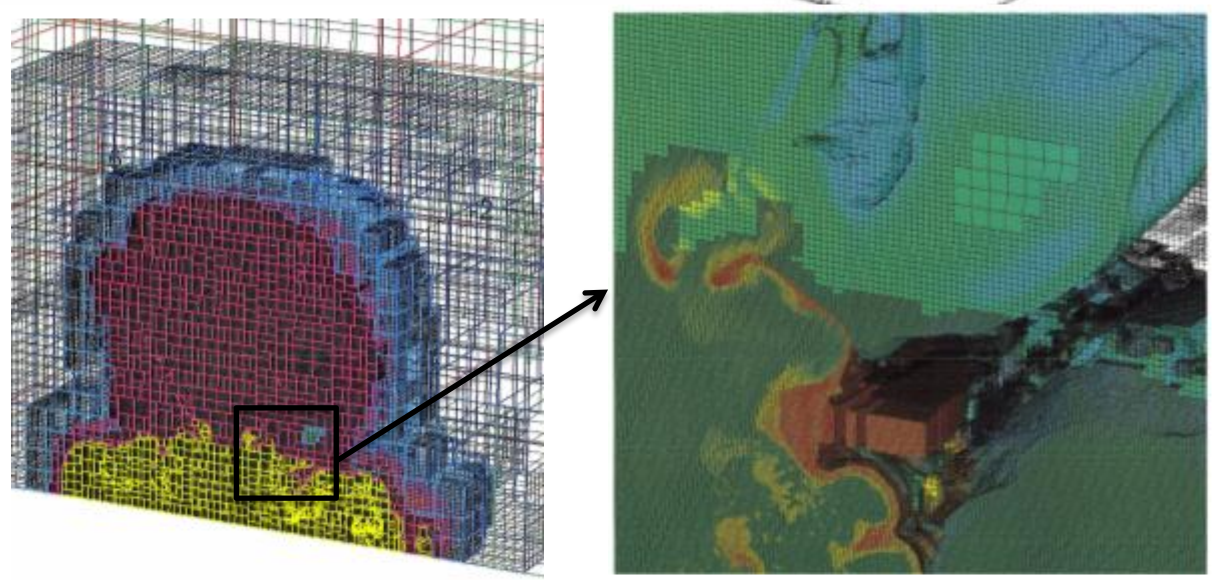


Time = 220 ns





Refinement Levels



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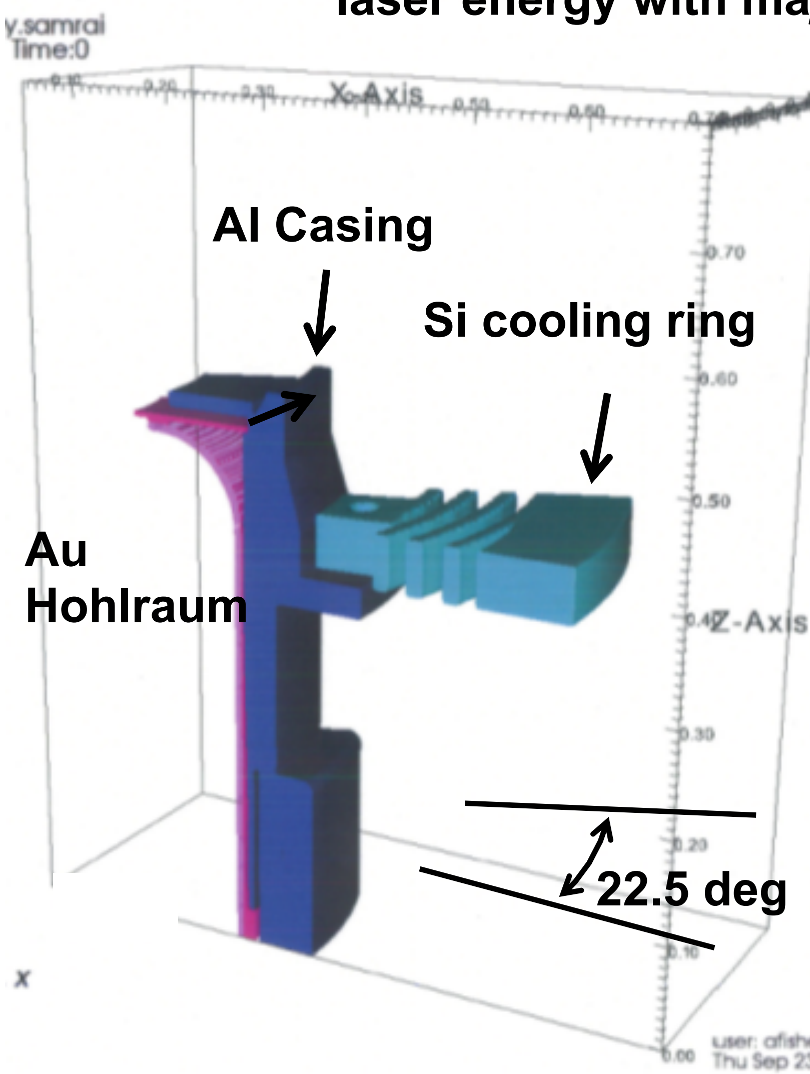
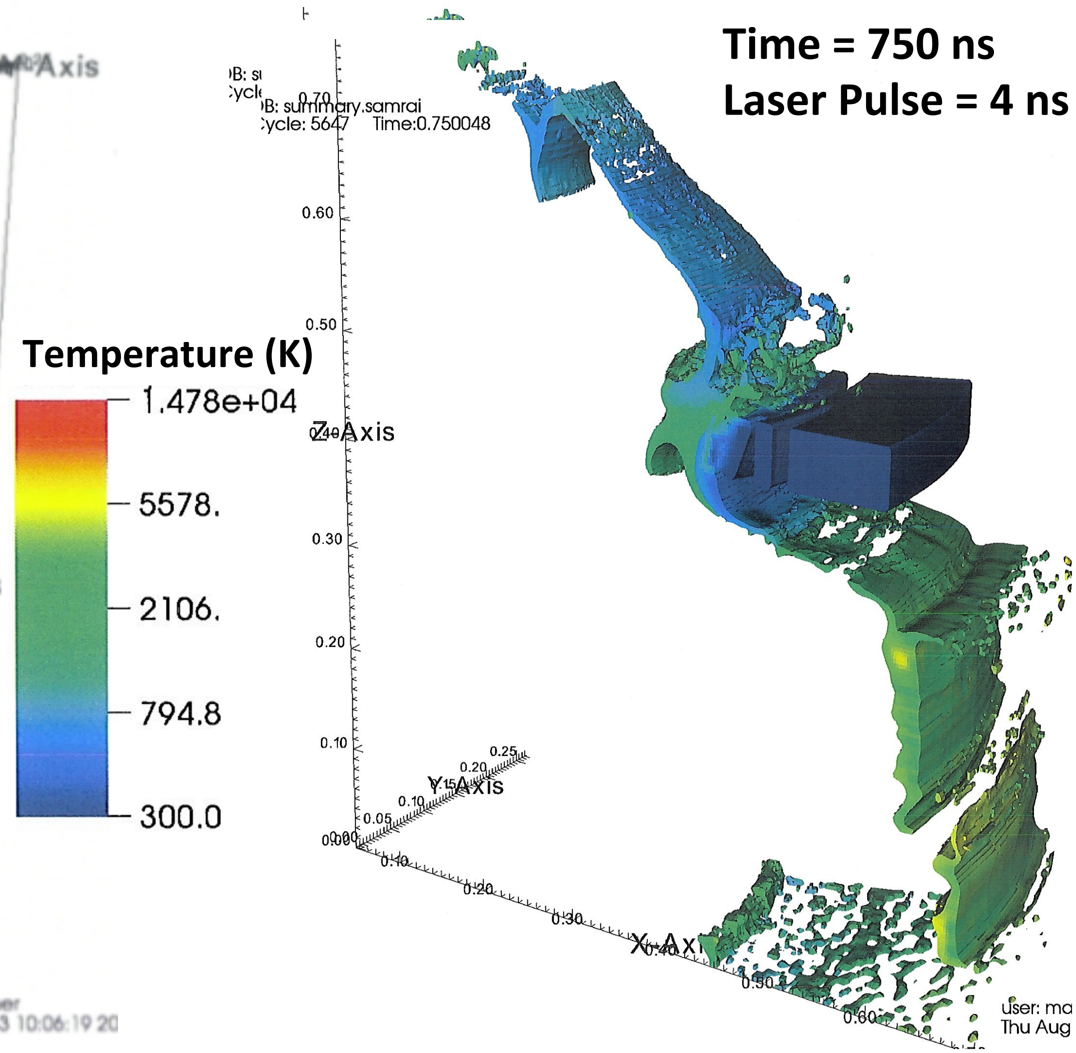
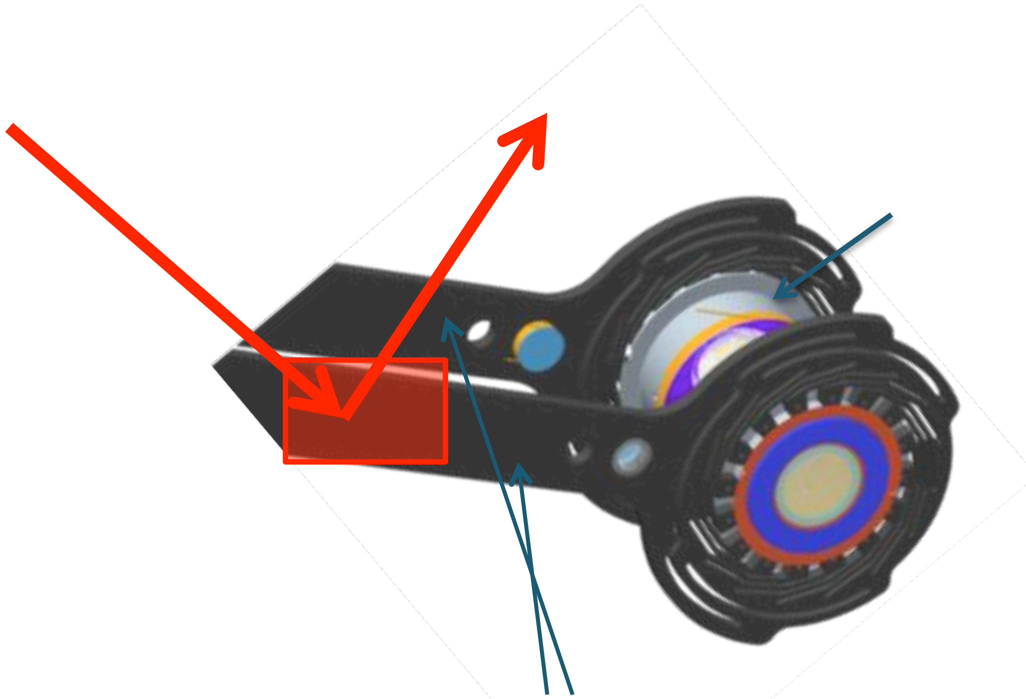
Sample NIF target where fragmentation modeling is needed for protection of optics/diagnostics

Simulation of NIF experiment using 1% of full laser energy with majority of target not vaporized





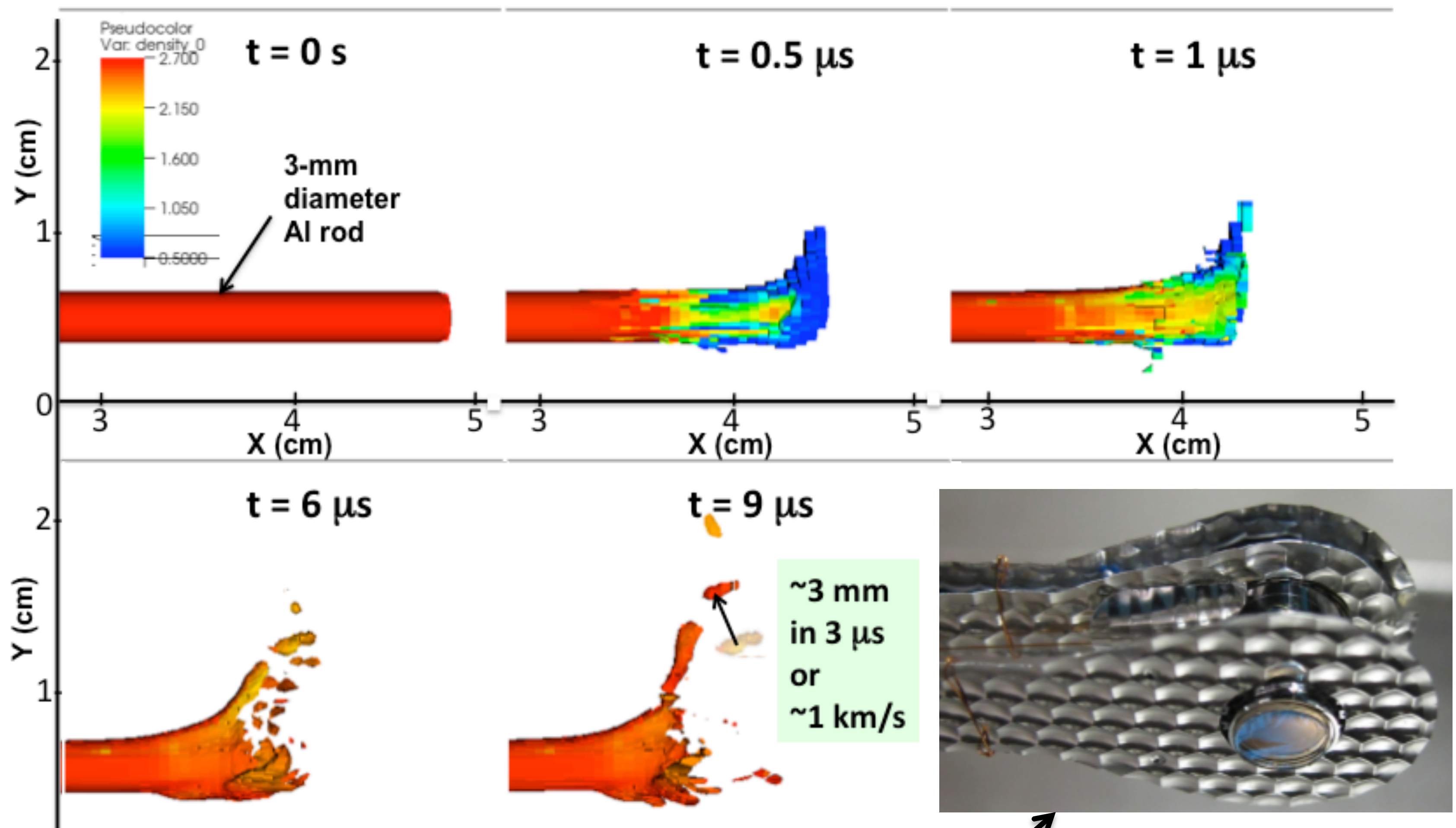
Code instrumental in redesign of several experimental configurations to meet safety/performance standards



Si cooling arms

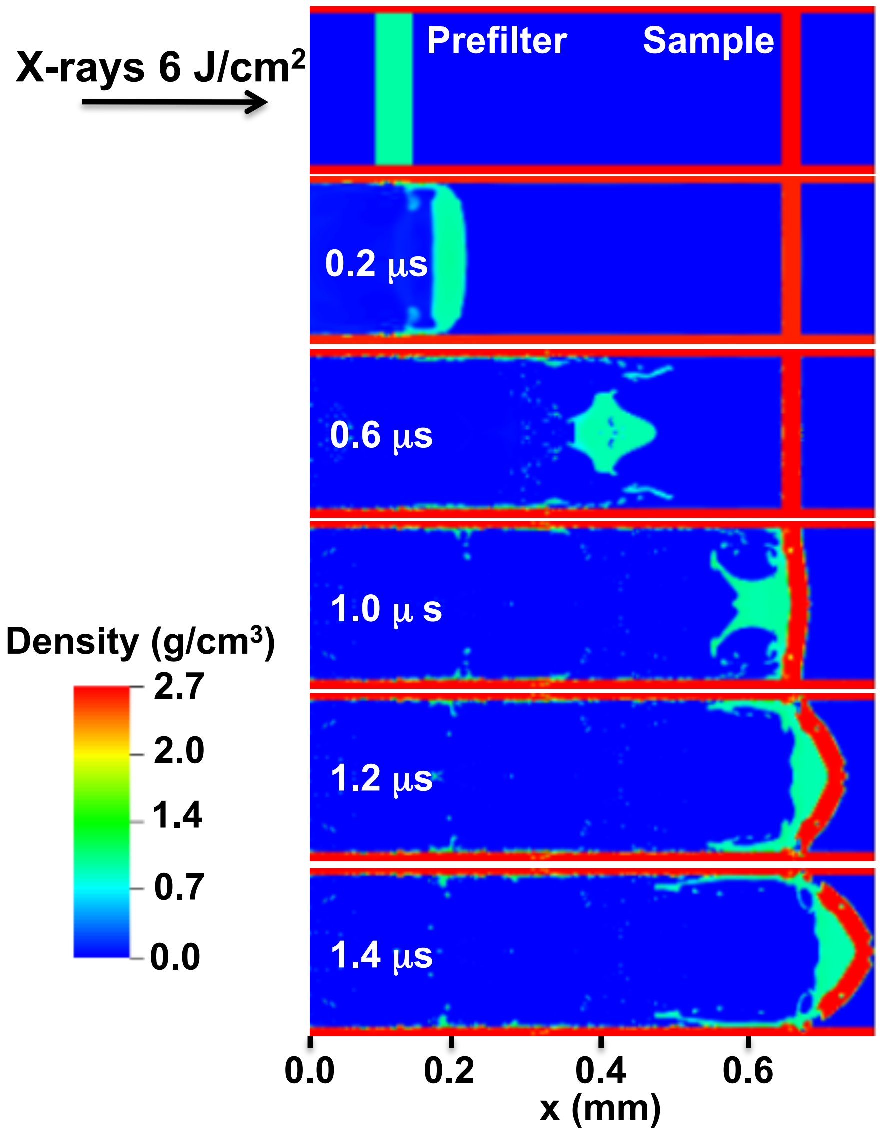
- Early experiments observed reflect of 1w light towards other beamlines
- Proposed modification was to replace flat Si supports with two Al rods
- Curved surface of rods would disperse the reflected laser light

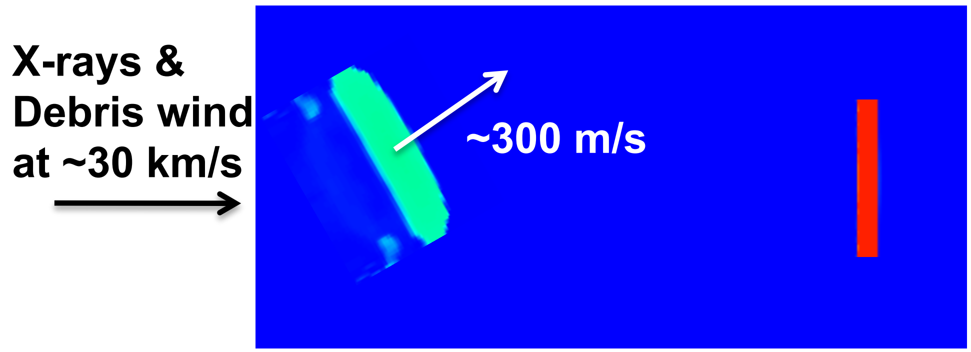
ALE-AMR simulations of Al rods driven by plasma debris wind predicted optical damage



A redesigned using waffled Al foils covering Si surfaces was developed

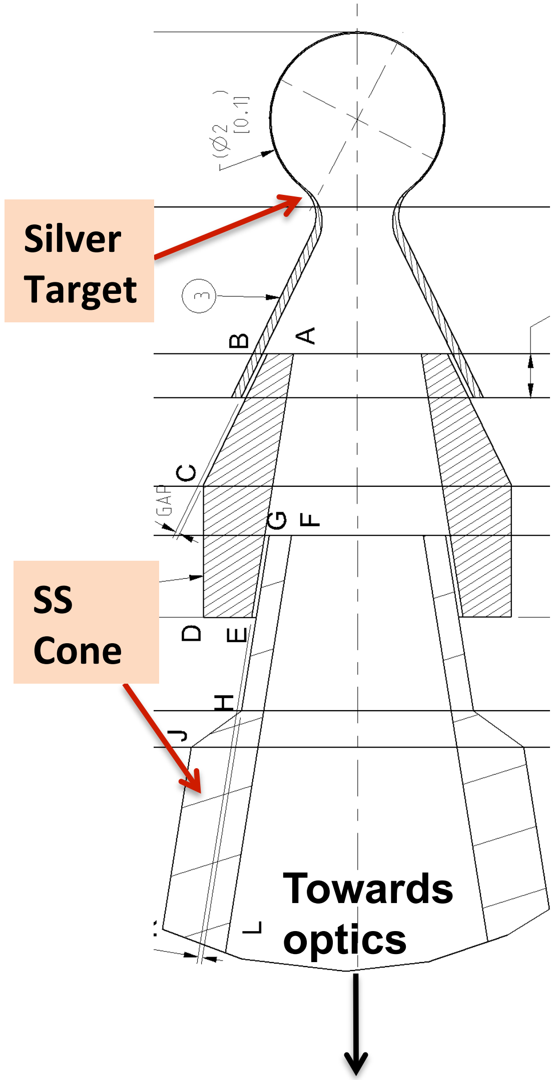
Simulations showed that x-ray loading in initial design damaged thin samples and tilted redesign protects samples from x-rays and fast debris wind from target

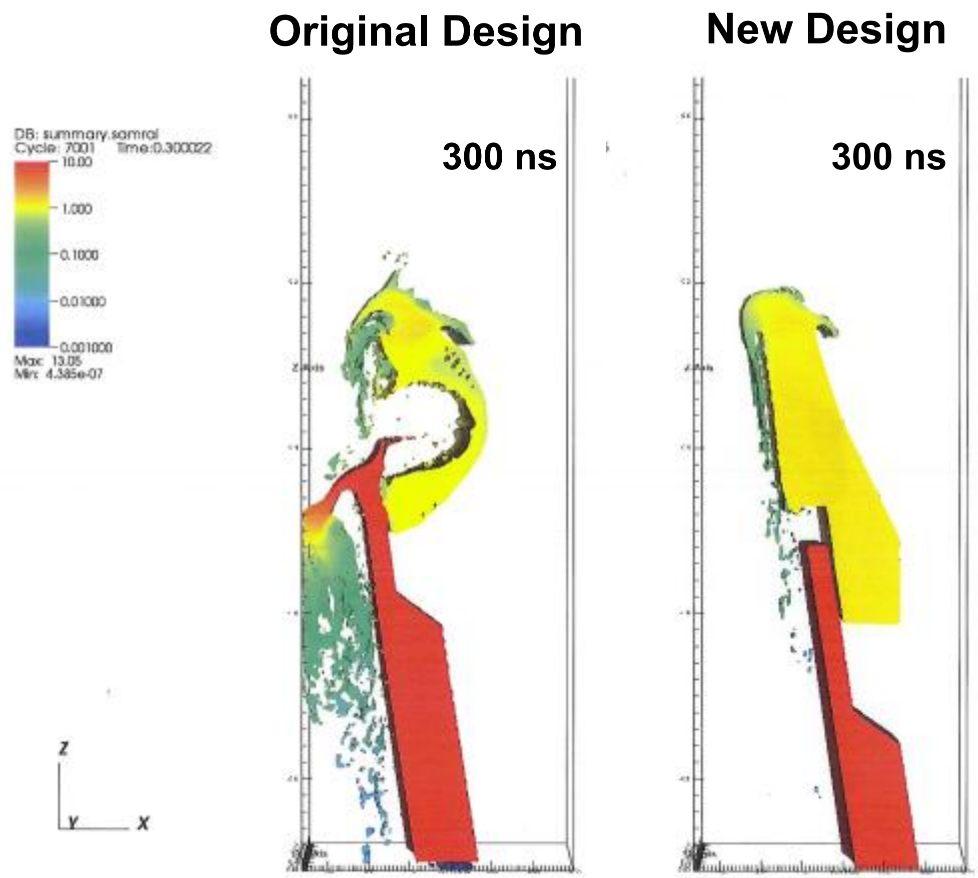




Redesigned Sample Holder

A redesign based on ALE-AMR simulations reduces material directed towards optics



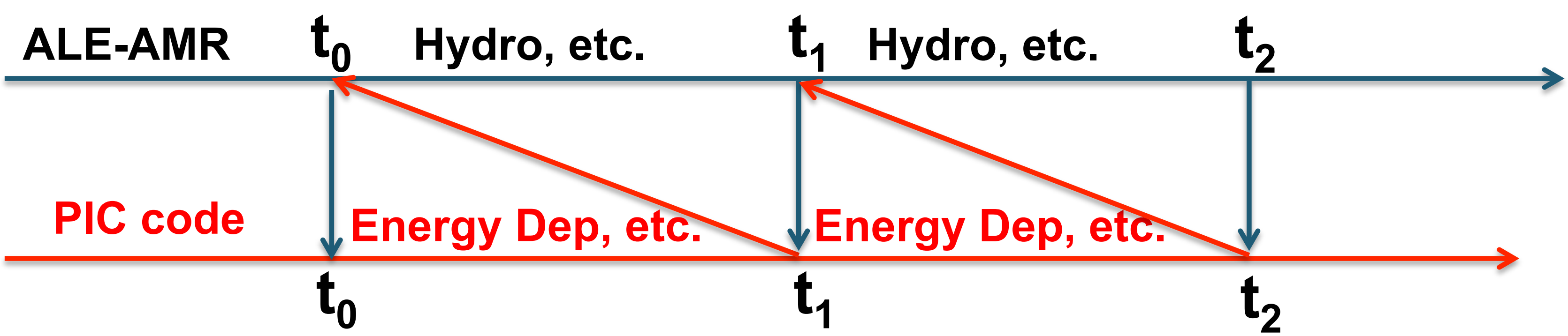


Outline

- Modeling for a range of experimental facilities
- Summary of multiphysics code ALE-AMR
  - ALE - Arbitrary Lagrangian Eulerian
  - AMR - Adaptive Mesh Refinement
- New surface tension model in ALE-AMR
- Sample of modeling capabilities
  - EUV Lithography
  - NDCX-II
  - National Ignition Facility
- **New directions: exascale and more multiphysics**
  - **Coupling fluid with PIC**
  - **PIC challenges for exascale**
  - **Coupling to meso/micro scale**

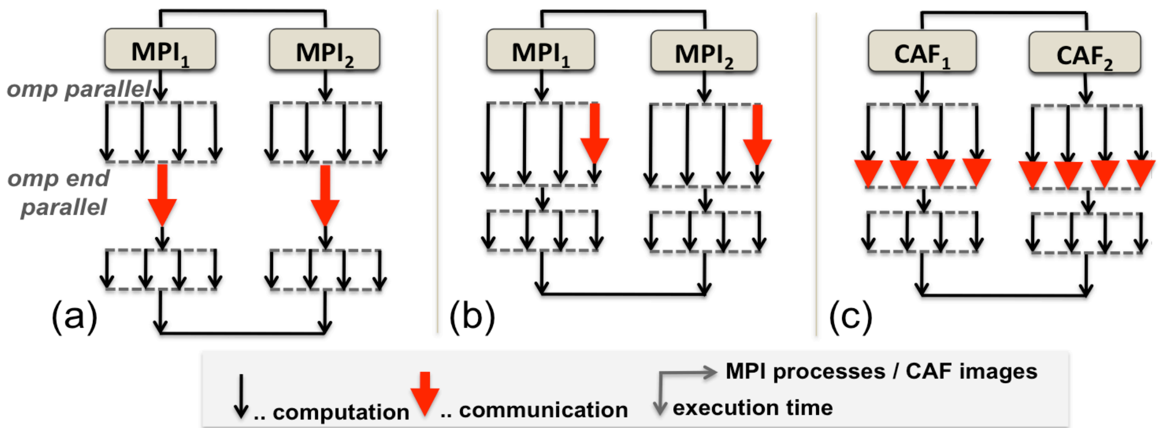
Coupling ALE-AMR to a PIC code allows additional physics to be added to simulations

- For short-pulse wakefield experiments, e.g., BELLA, the plasma formation using capillary discharges or lasers could be modeled with ALE-AMR with results coupled to a PIC code
  - Foot on the short pulse can also cause hydro effects
- We have explored the idea of coupling ALE-AMR to a PIC code in a quasi continuous mode to model CO_2 pulse chains
  - Have 5-10 3 ps pulses with 10 ps spacing interacting with a gas jet
  - PIC to calculate hot electrons, energy deposition, etc. for 1st pulse
  - Couple PIC results to ALE-AMR to calculate hydro for next pulse

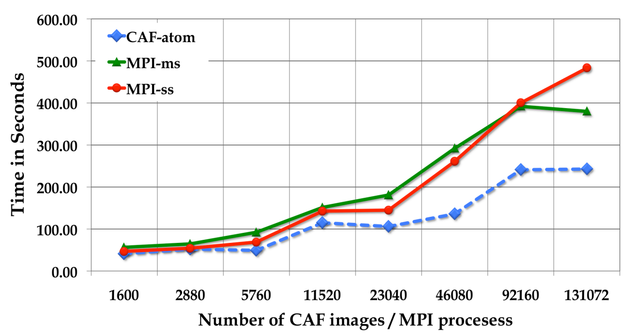


Note: PIC code Zuma coupled to Hydra for fast ignition studies
D. Strozzi, et al., Phys. Plasmas 19, 072711, 2012.

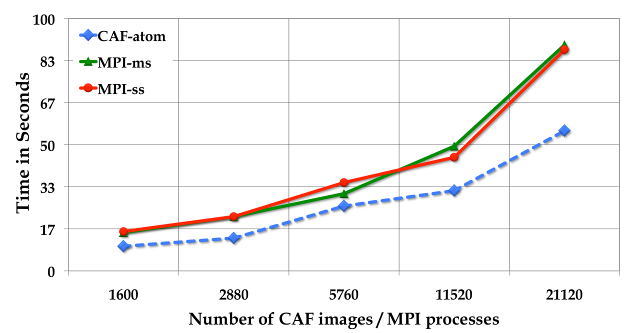
New PIC algorithm using MPI, OpenMP, and CAF gives performance improvement on 130K cores



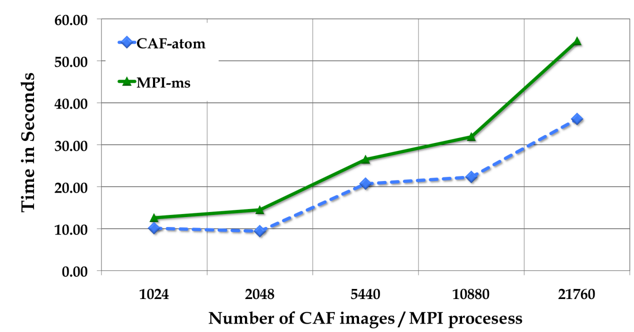
a) Classical hybrid MPI/OpenMP
b) Extension – MPI thread teams for work distribution and collective MPI function calls
c) Hybrid PGAS (CAF) / OpenMP allows ALL OpenMP threads per team to make communication calls to the thread-safe PGAS communication layer



Single-Threaded (Benchmark Suite)



Multi-Threaded (Benchmark Suite)



Multi-Threaded (GTS)

“Multithreaded Global Address Space Communication Techniques for Gyrokinetic Fusion Applications on Ultra-Scale Platforms,” R Preissl, N Wichmann, B Long, J Shalf, S Ethier, and A Koniges, **SC11** Seattle, WA, USA, 2011.

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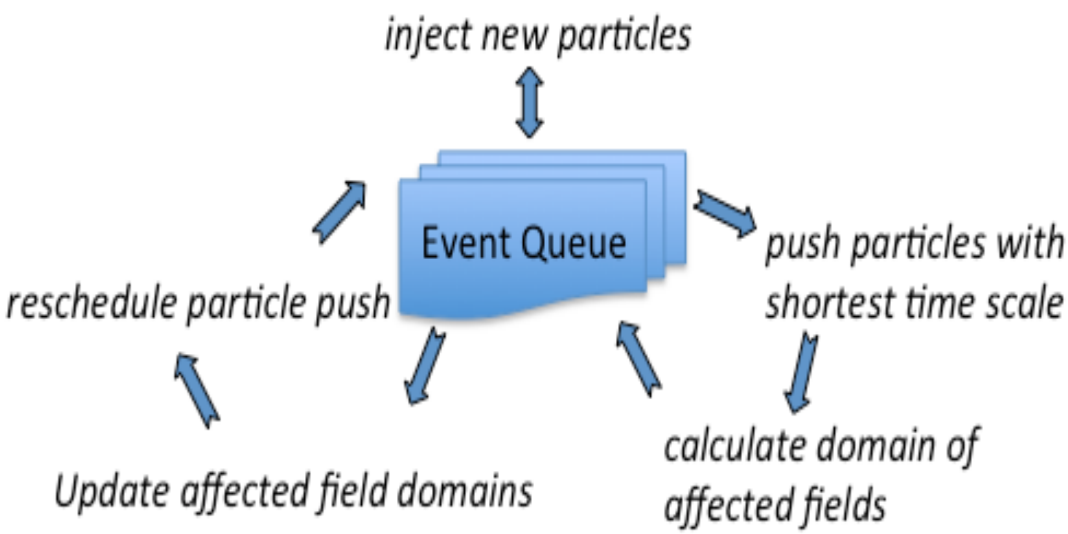
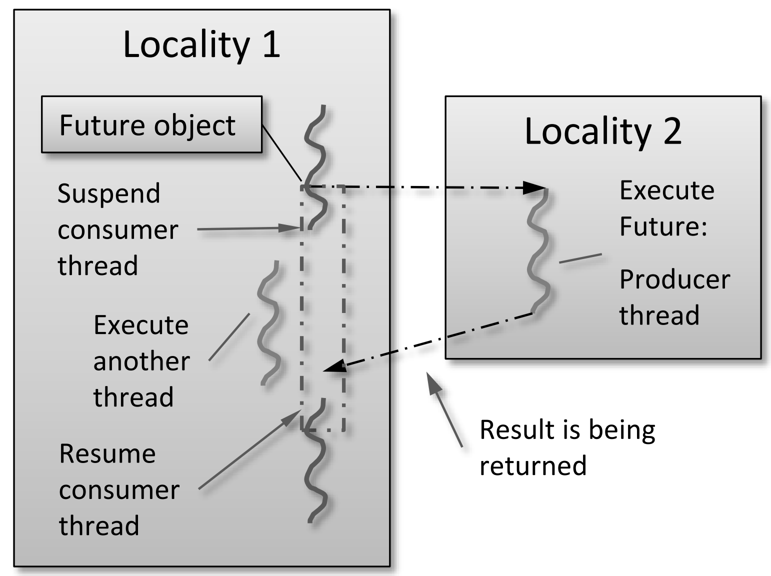
Incorporated into GTS (Princeton Gyrokinetic PIC)

BERKELEY LAB

Parallel asynchronous event-driven simulations are a promising path to exascale for certain regimes

- **Key for PIC: connect continuum to naturally event-driven particles**
  - **Continuum to discrete events can be enabled through multicore-partitioned pseudo-spectral methods using local FFTs**
- **ParalleX execution model (funded through the XPRESS project) is a excellent framework for this work using the Futures construct**

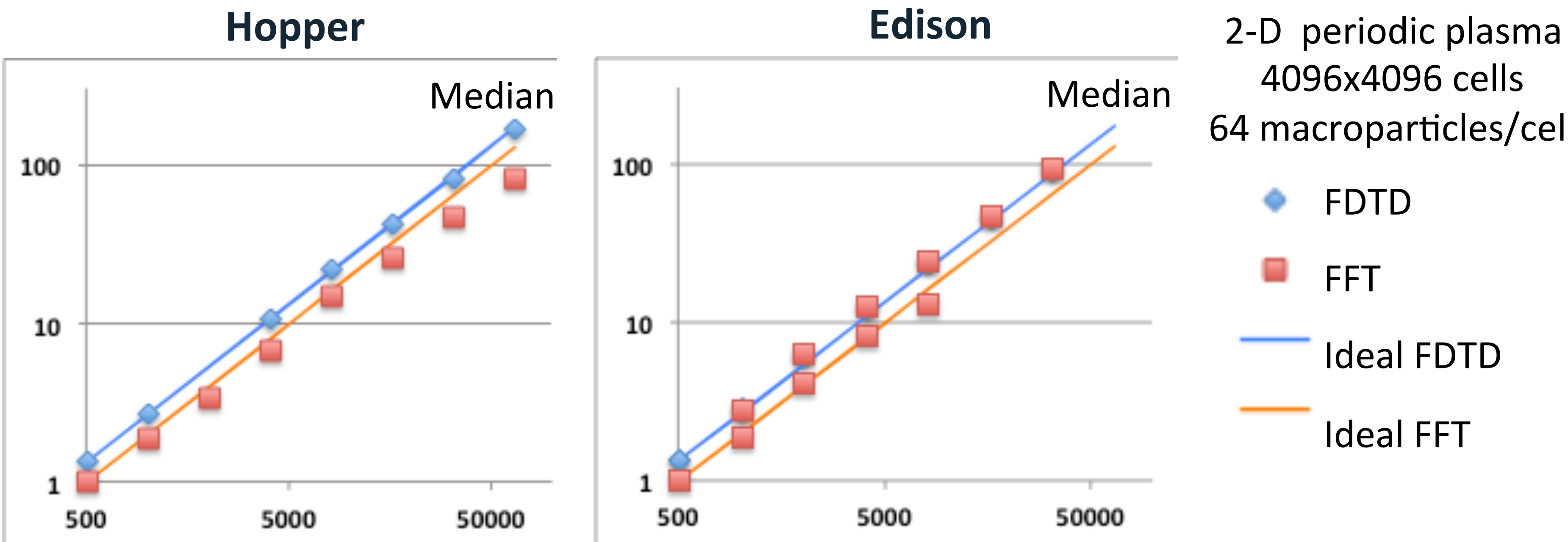




"Consideration of Asynchronous Algorithms for Particle-Grid Simulations," A Koniges, JL Vay, A Friedman, H Kaiser and T Sterling, **DOE Workshop on Applied Mathematics Research for Exascale Computing**, 2013.

As shown by Jean Luc at NUG 2014: Warp with new pseudo-spectral solver gives excellent strong scaling

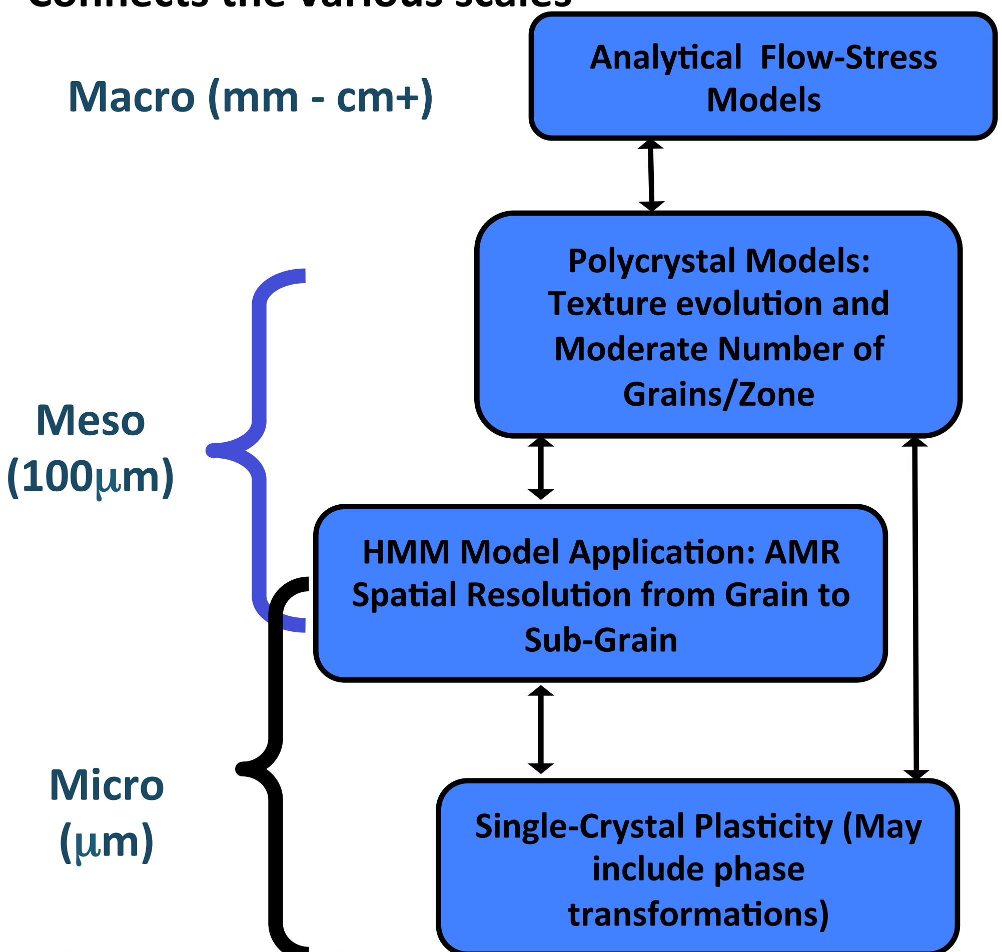
Joint AFRD/CRD/NERSC LDRD on new spectral solver decomposition

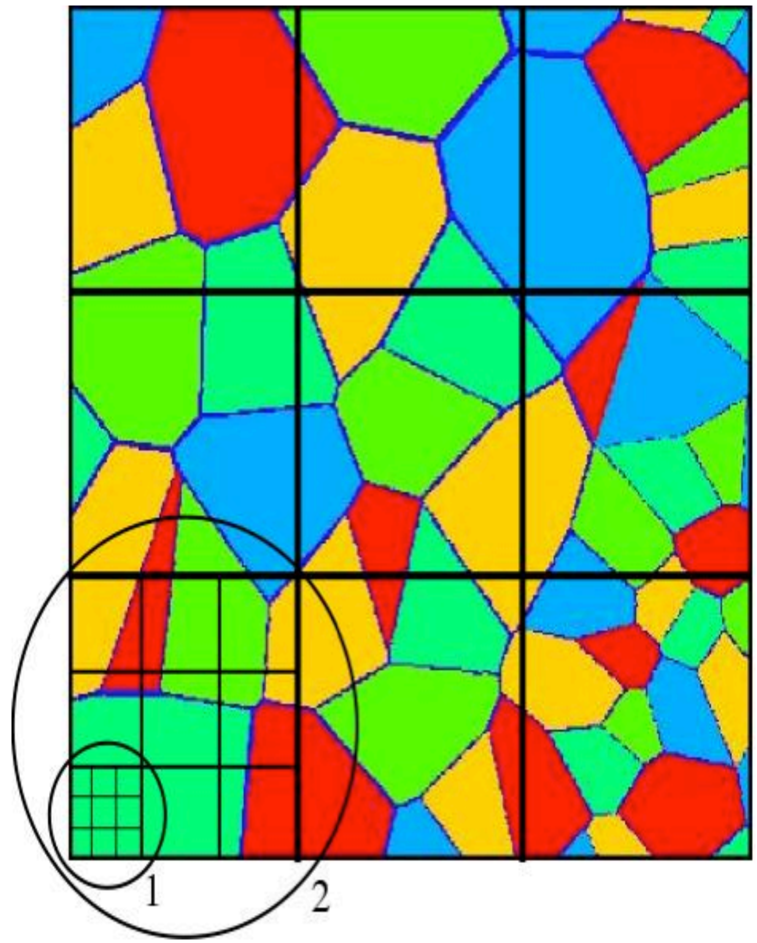


- Near linear scaling up-to 65,636 cores on Hopper, 32,768 on Edison.
- Prototype FFT Maxwell solver implemented with numpy & pyMPI.
- Optimized implementation underway; 3-D to follow (T. Drummond, CRD).

AMR allows coupling to meso/micro scale

Hierarchical Material Model (HMM)
Connects the various scales





"Multiphysics Simulations: Challenges and Opportunities," Keyes, Koniges. et al., **Int. J. of High Performance Computing Applications 27**, 4-83, 2013.

Coupling to finer scales allows modeling of additional physics regimes

- In magnetic fusion devices understanding the plasma evolution and surface erosion dynamics following a plasma transient is critical
  - NDCX-II can be used to fusion wall materials
- High power impulse magnetron sputtering experiments
  - May include B field effects (either self-generated or external) in same fashion as other ALE codes

"Scientific and computational challenges in coupled plasma edge/plasma-material interactions for fusion tokamaks," J Brooks, A. Hassanein, A. Koniges, P. Krstic, T Rognlien, T Sizyuk, V Sizyuk, D Stotler, **Contributions to Plasma Physics**, in press 2014.

Summary

- **Advanced multi-material rad/hydro/materials code ALE-AMR simulates complex experimental configurations such as**
  - **NIF optics and diagnostics**
  - **LMJ (France) new experiments**
  - **NDCX-II warm dense matter**
  - **Cymer laser-heated droplets**
- **Exascale and more multiphysics gives new opportunities**
  - **Coupling ALE-AMR with PIC, e.g., for BELLA**
  - **Programming models: overlap communication and computation**
  - **Development of asynchronous event-driven simulations**
    - **Continuum to discrete events can be enabled through multicore-partitioned pseudo-spectral methods**
  - **Coupling to meso/micro scale for new applications such as**
    - **Fusion wall material modeling**
    - **Modeling of magnetron sputtering**