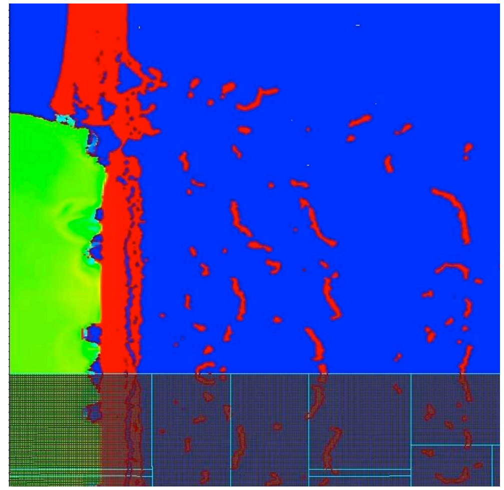
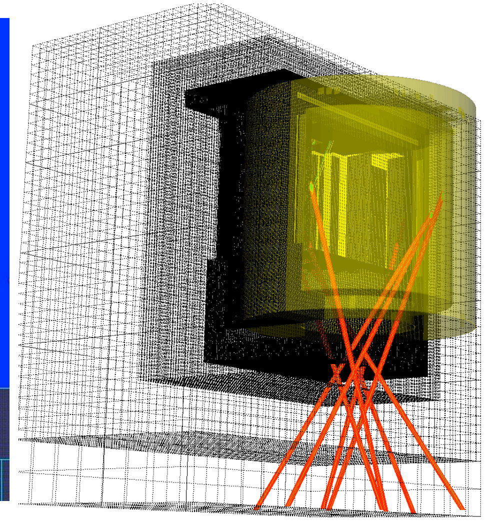
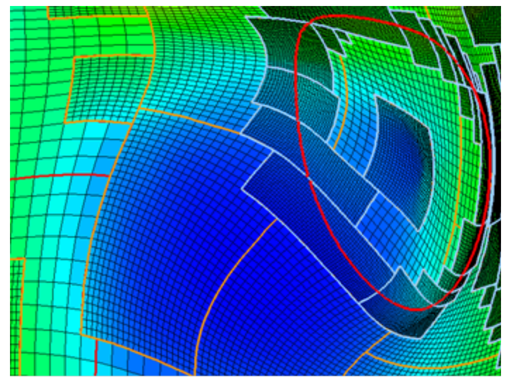
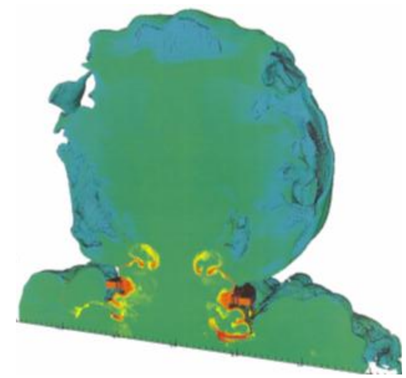
Multi-Material Plasma Modeling on HPC Platforms









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23rd International Conference on Numerical Simulation of Plasmas

Beijing, China
September 16, 2013

National Energy Research Scientific Computing Center

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What this talk is NOT about*

- **Advanced hybrid techniques to overlap communication and computation in GTS (Princeton Gyrokinetic PIC) using OpenMP tasking and the use of PGAS co-array Fortran for significantly improved performance on 160,000 cores**
- **Development of asynchronous algorithms in PIC codes in contrast to standard lock-step programming approaches**
- **Multicore-partitioned pseudo-spectral methods that take advantage of finite speed of light to allow the use of local FFTs**

***But see me if you wish more information**

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 results for different facilities**
- **Performance on new HPC platforms, e.g., Edison at NERSC**

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

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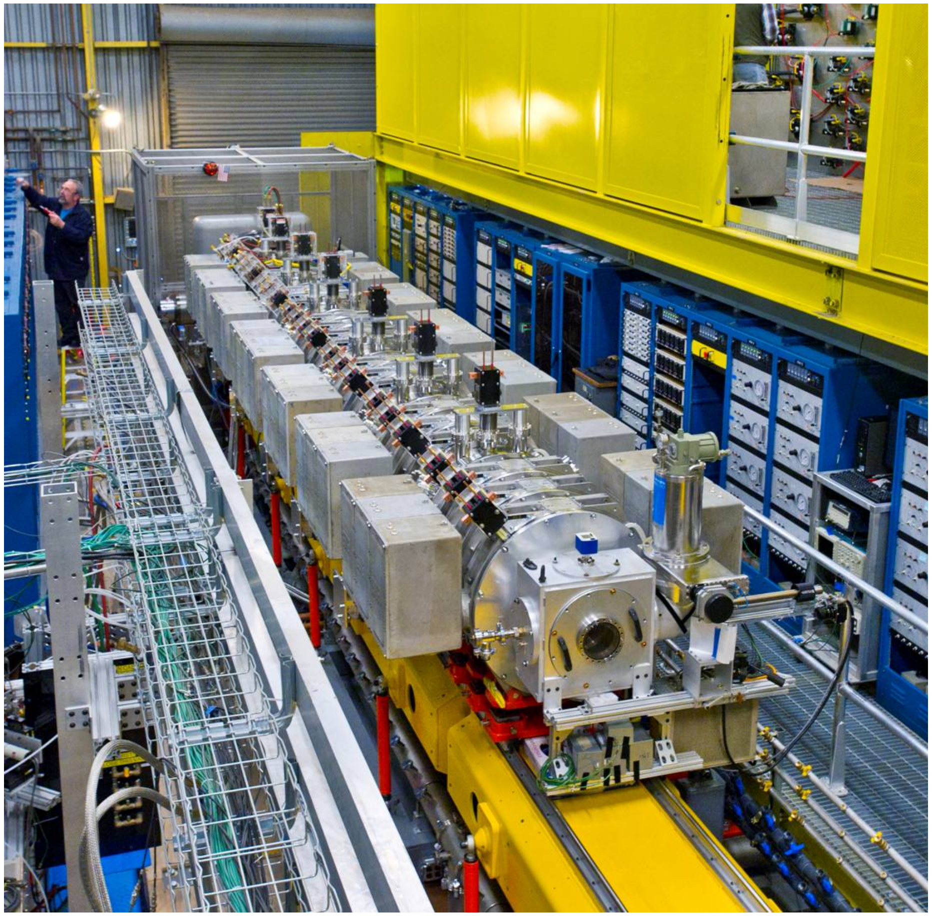
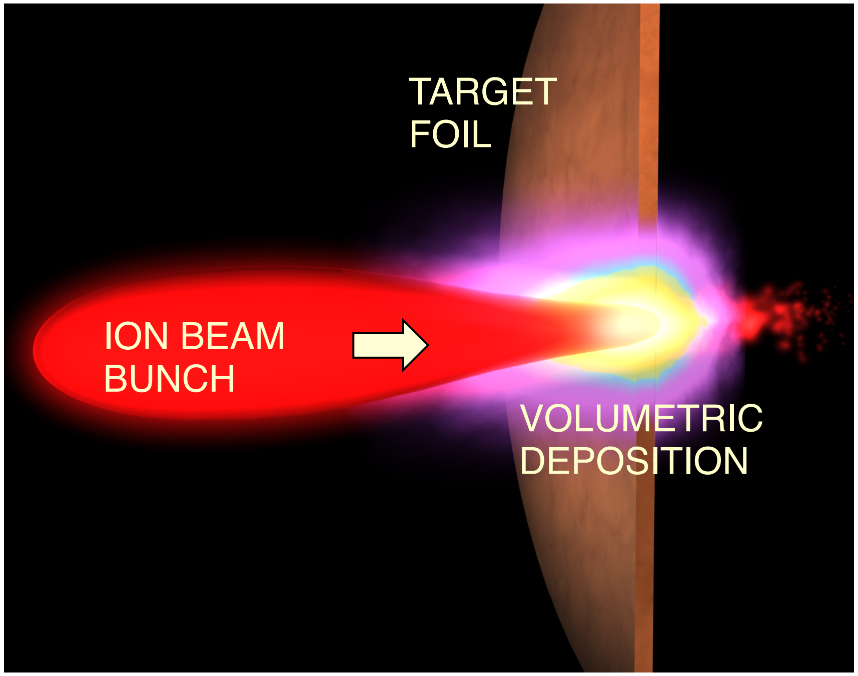
NDCX-II user facility at LBNL accelerates Li ions for warm dense matter experiments





Optimized for volumetric heating of micron-thick samples to eV temperatures within hydrodynamic expansion times

A user facility for studies of:

- **physics of ion-heated matter**
- **heavy-ion-driven ICF target physics**
- **space-charge-dominated beams**

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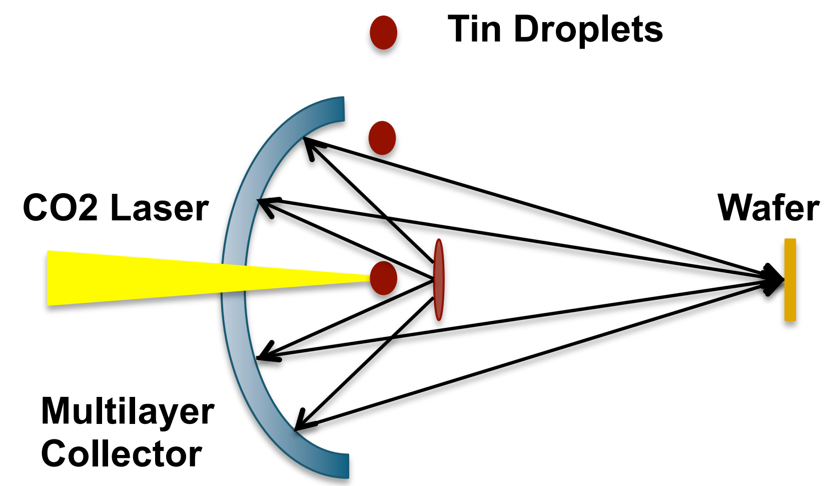
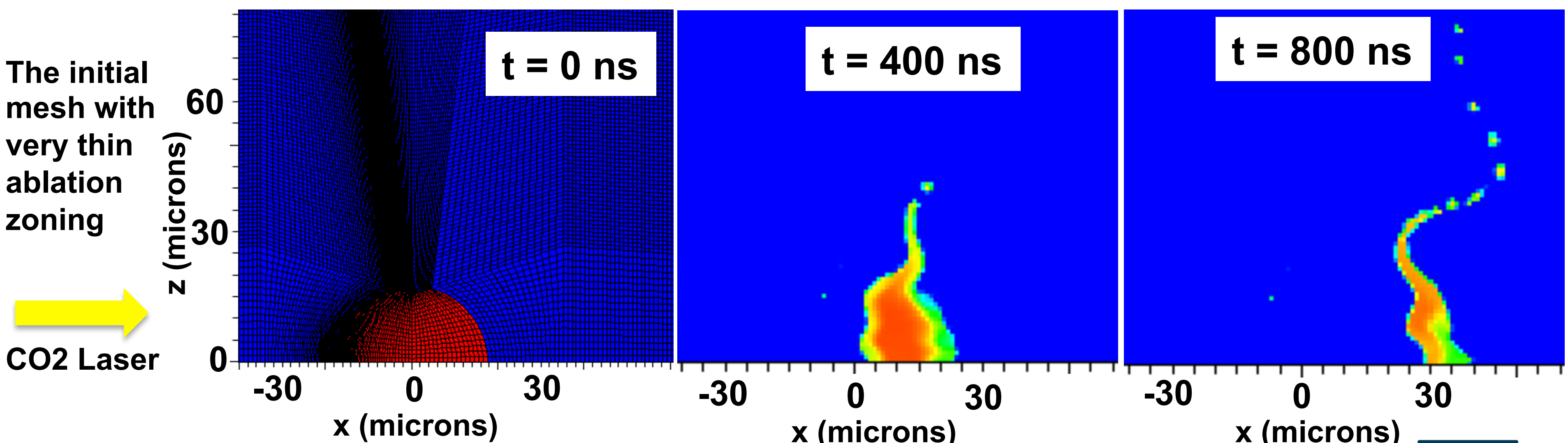
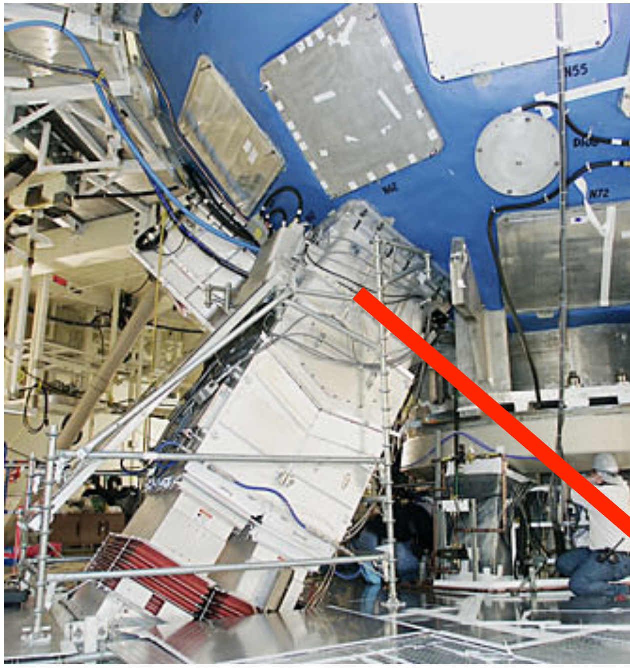
The Cymer extreme UV lithography experiment uses laser heated molten metal droplets

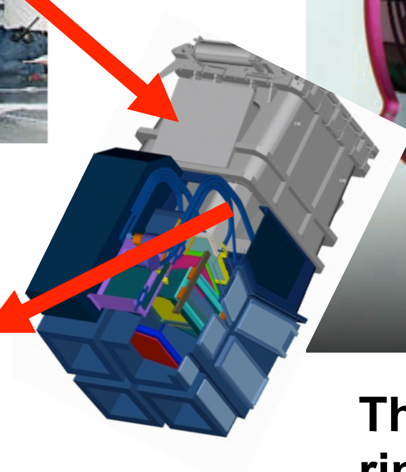


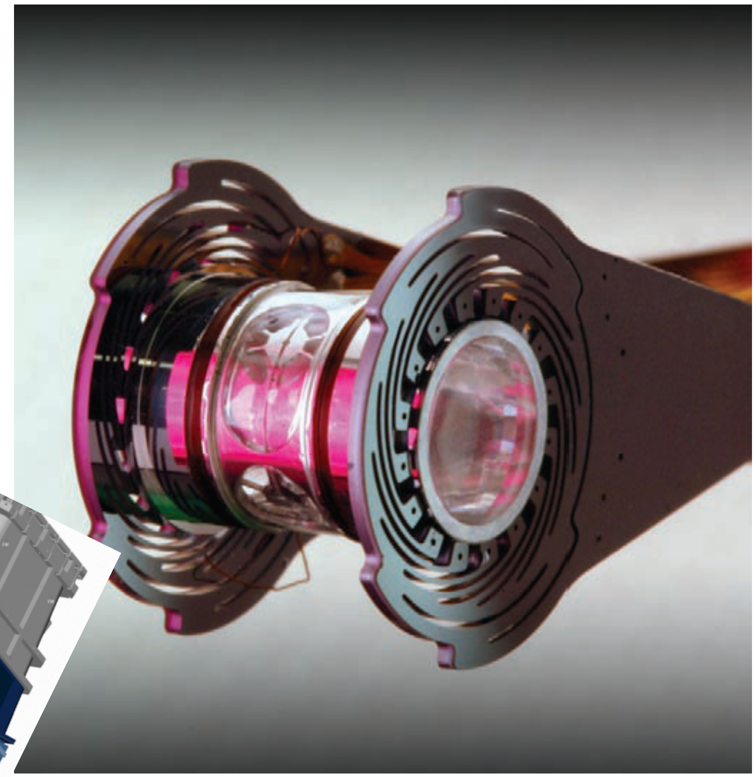
- Technique uses a prepulse to flatten droplet prior to main pulse
- At low prepulse energies, droplet is observed to oscillate (surface tension effect)
- Any misalignment requires detailed 3D simulations

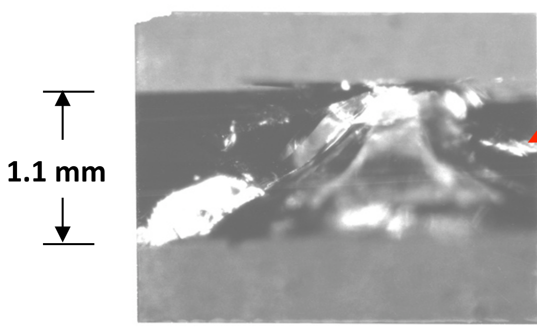


Large laser facilities, e.g., NIF and LMJ, require modeling to protect optics and diagnostics





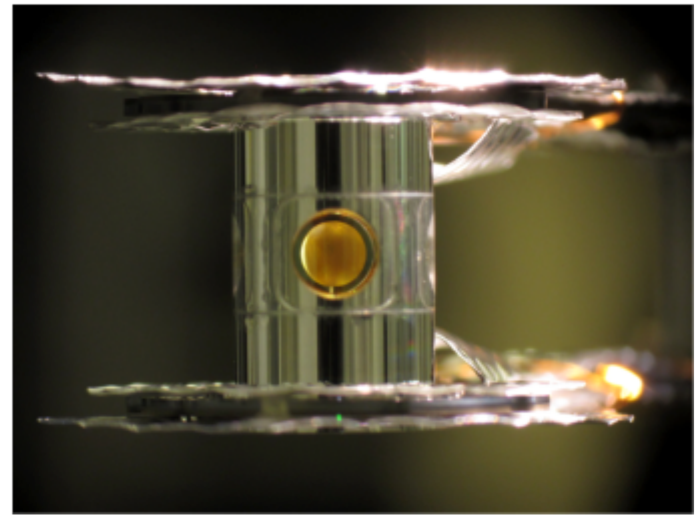




Damage to debris shields

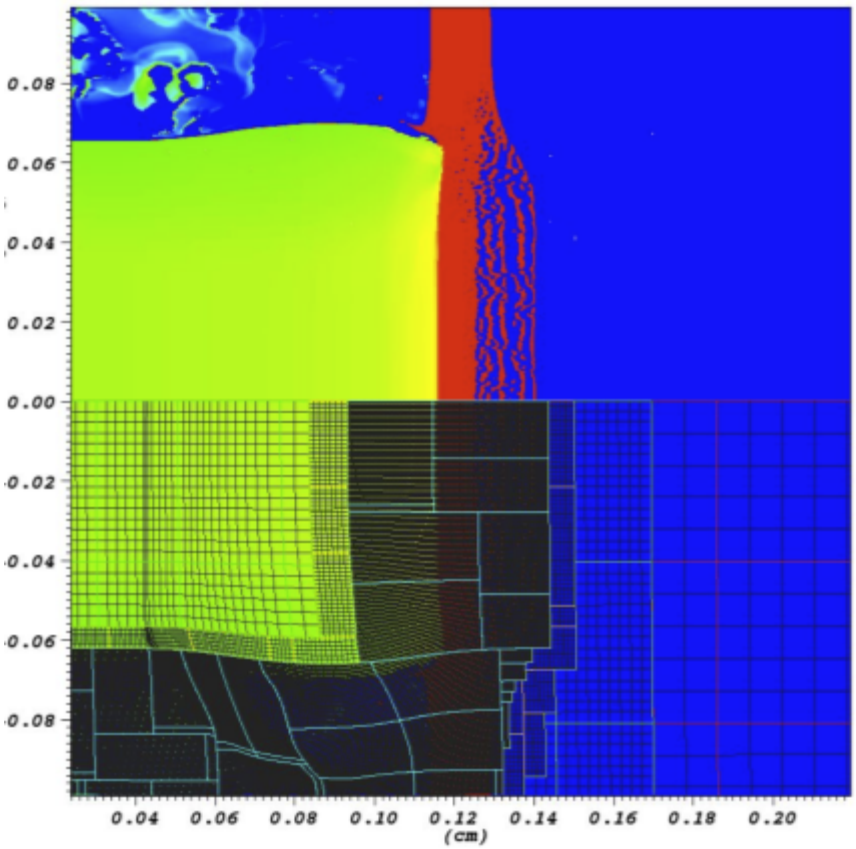
The entire target, e. g., Si cooling rings and Al casing, must be modeled

A 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



ALE - Arbitrary Lagrangian Eulerian
AMR - Adaptive Mesh Refinement

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

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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

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

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

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

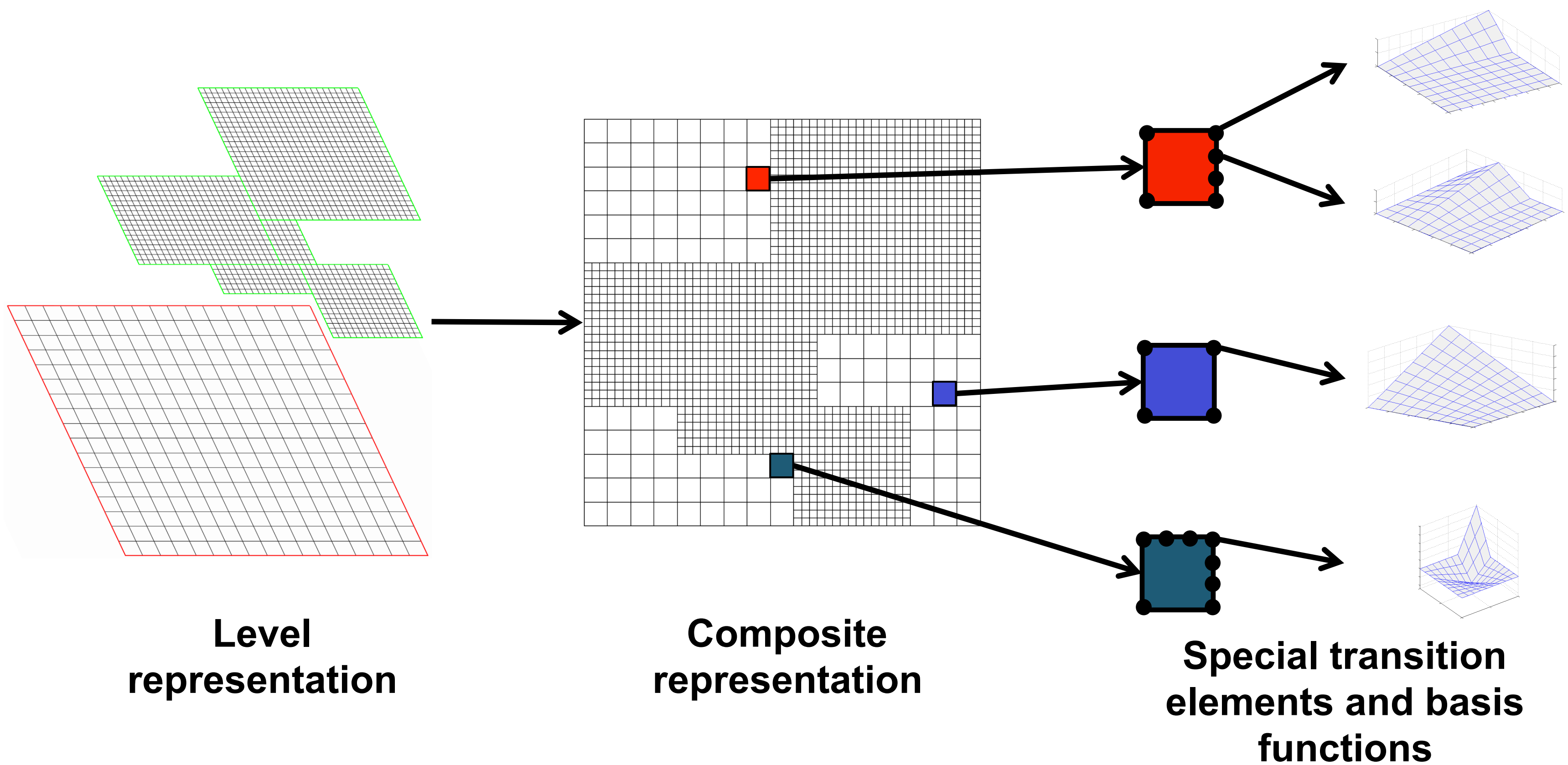
$$\alpha = \lambda \left(\frac{c}{\kappa_R} \right)$$

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

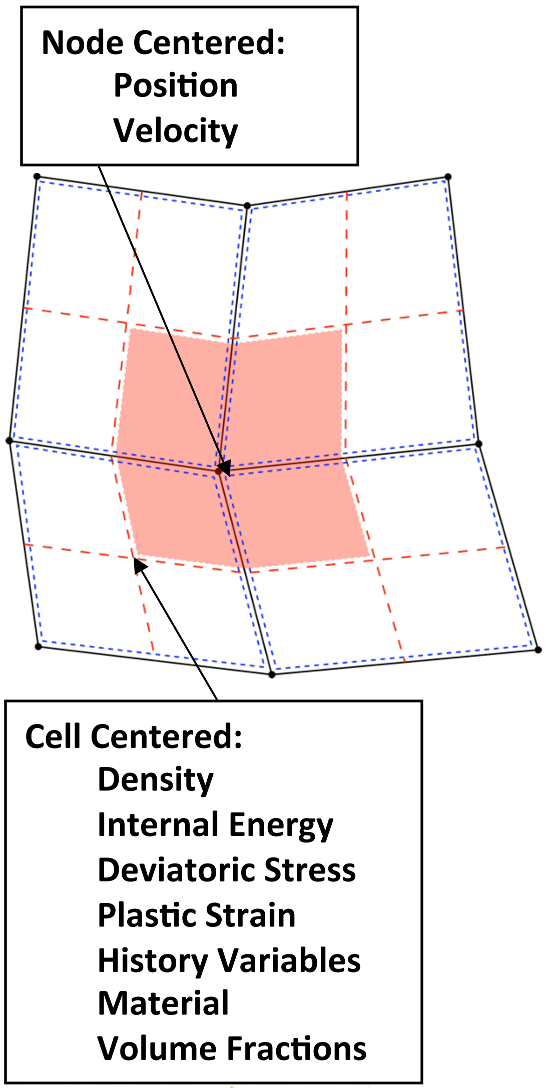
$$f = -\frac{1}{\Delta t} - \tilde{\kappa}_P B^n$$

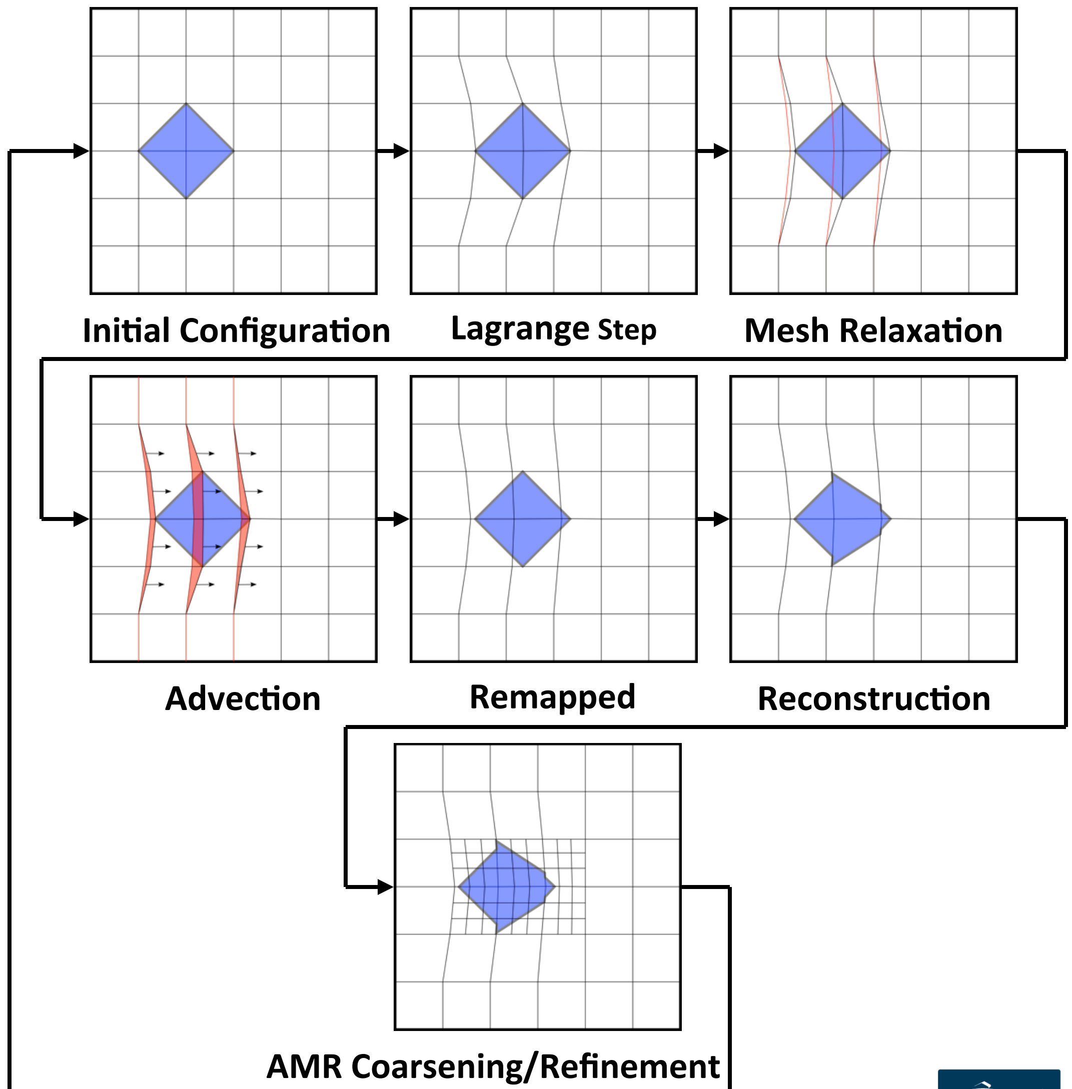
The diffusion equations are solved using Finite Element Methods accounting for AMR issues

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



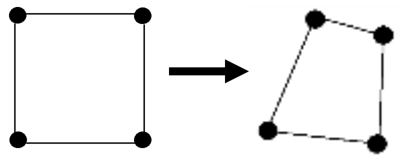
The staggered mesh Lagrange+Remap built on a structured adaptive mesh refinement framework (SAMRAI)





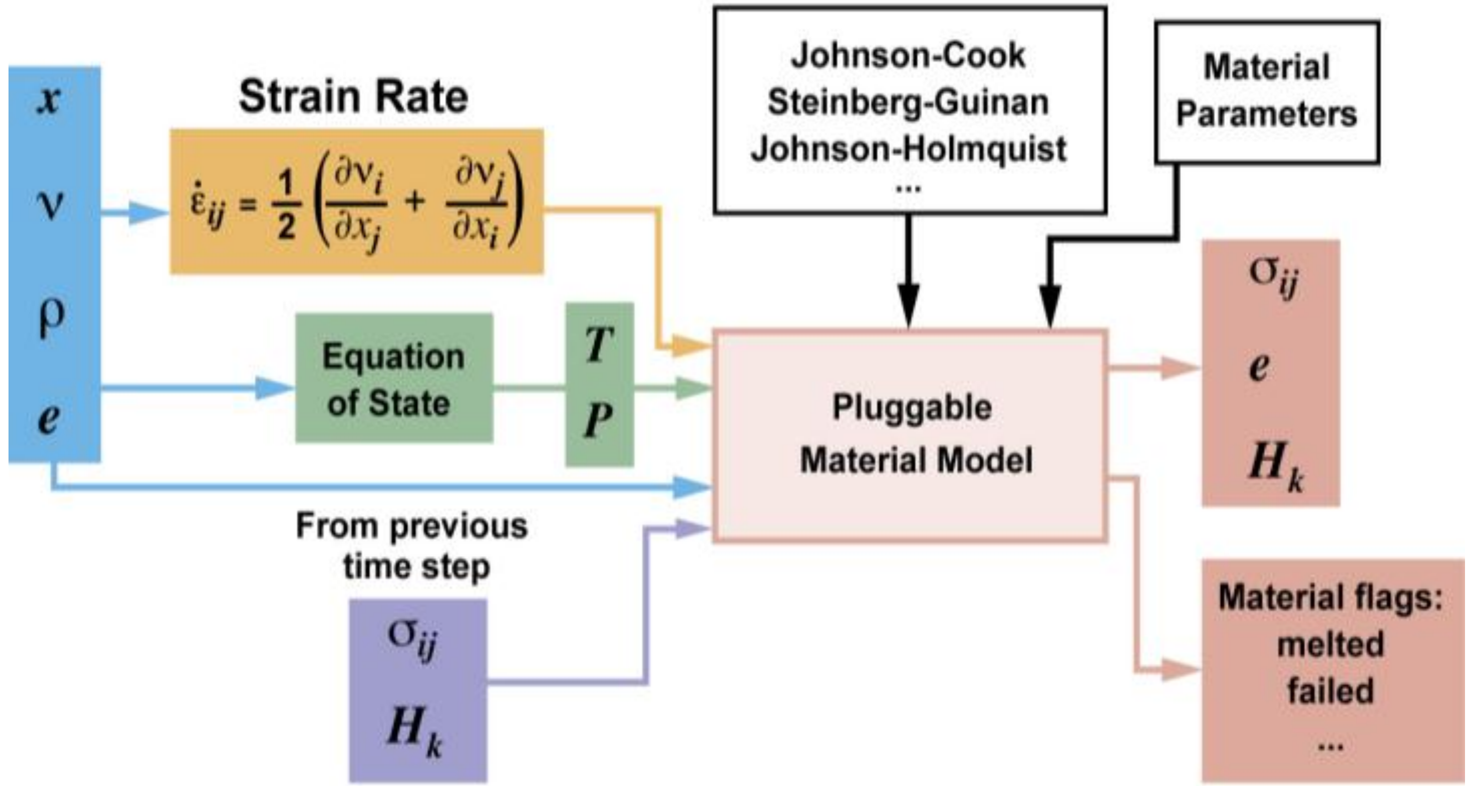
Code has a flexible framework with a new surface tension model active during the Lagrange step

Lagrange Step



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

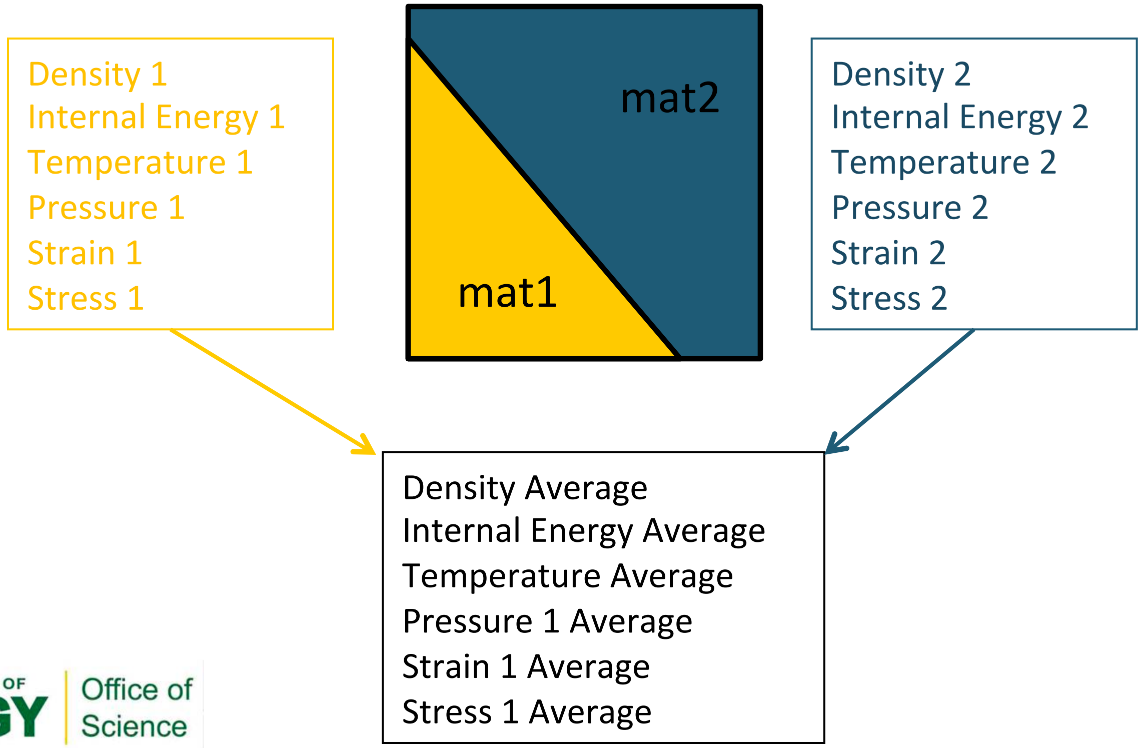
Post-Lagrange Material Update



Relax/Remap Split Physics

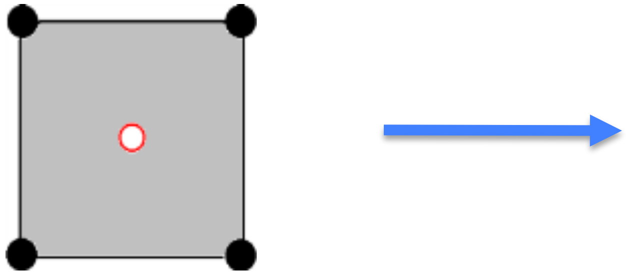
Mixed cells

- 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

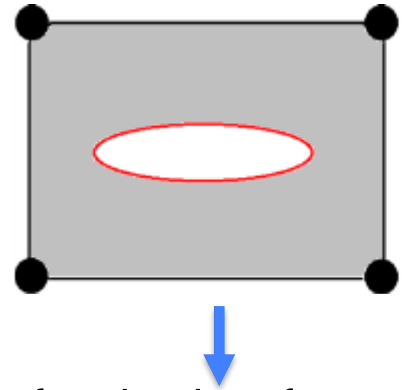


Solid fragmentation obtained using a void insertion model plus interface reconstruction

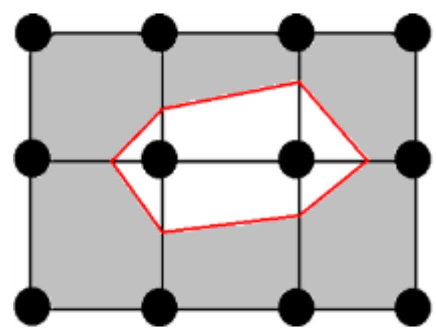
Upon failure a small volume fraction of void is introduced into the cell

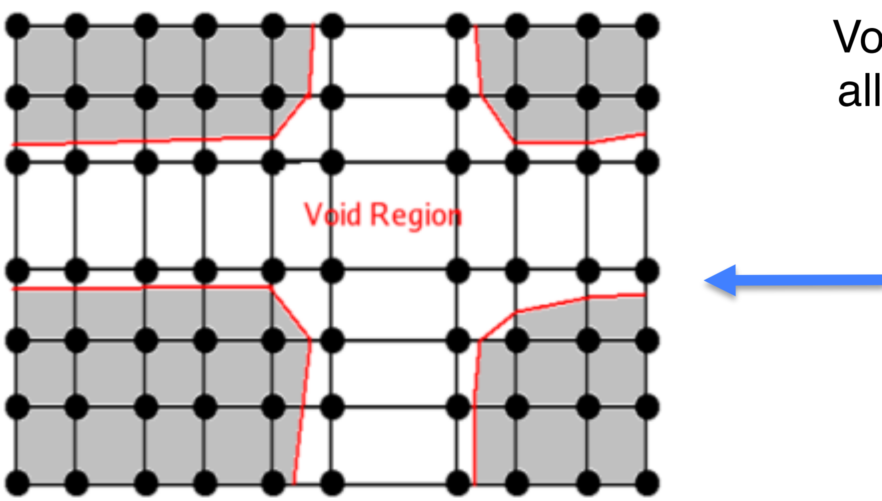


If the cell continues to grow the void enlarges to meet that growth

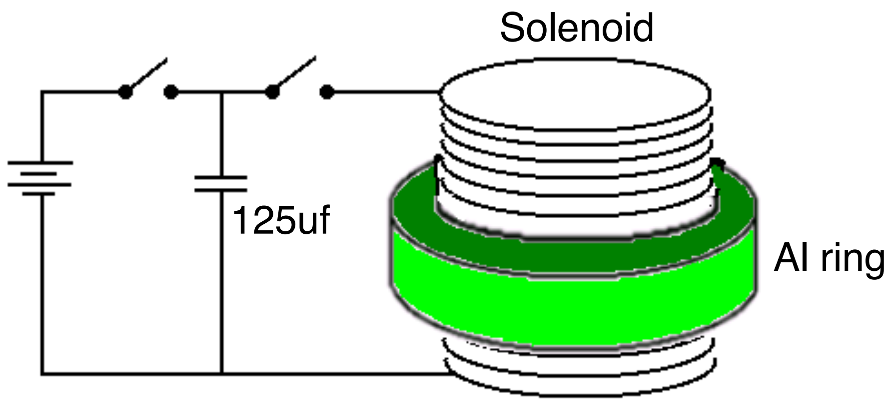


Volume fraction interface reconstruction allows voids to coalesce to form cracks

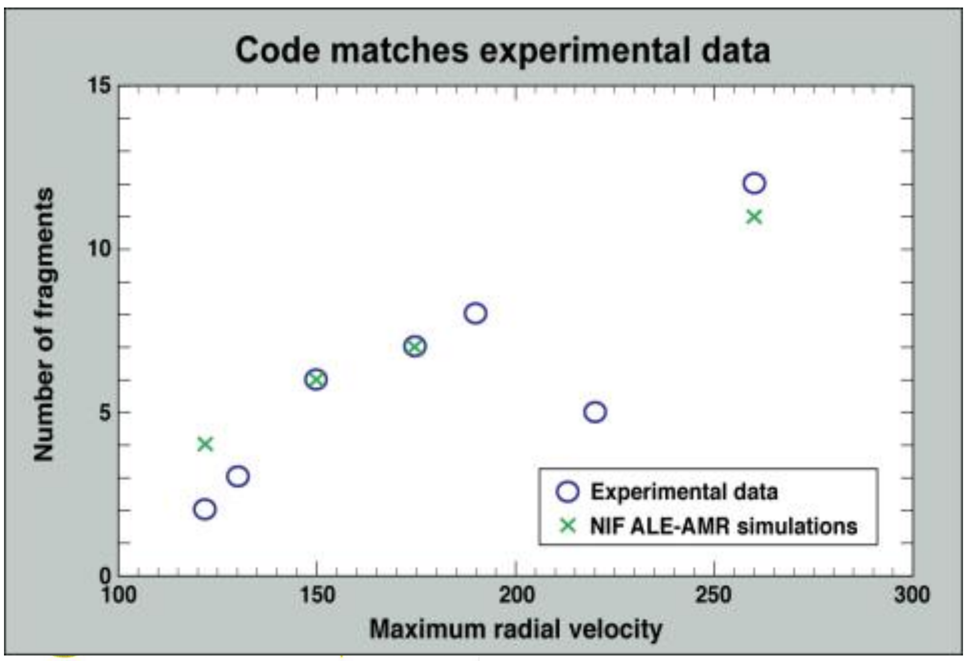




Fragmentation modeling validated against expanding ring experiment



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



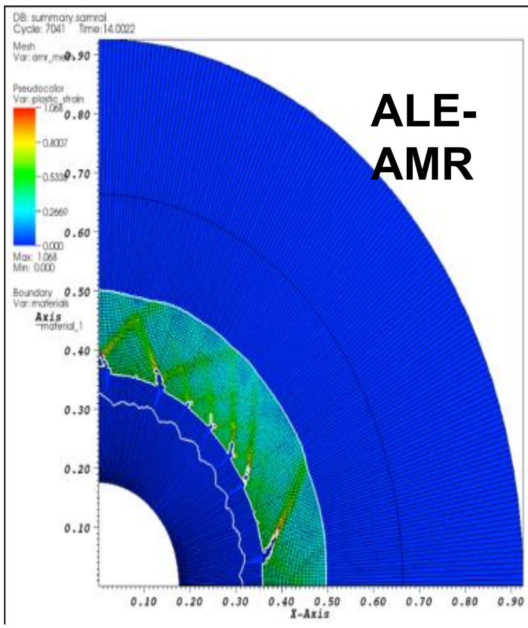
ALE-AMR simulations

- 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

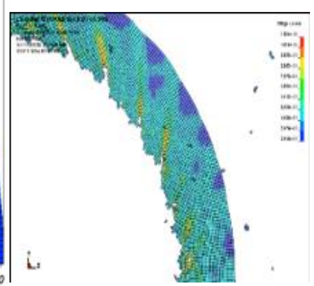
M. Altynova, X. Hu, and G. Daehn: Increased Ductility in High Velocity Electromagnetic Ring Expansion, Metall. Material Trans. A, 27A, p1837-1844, (1996)

Benchmarking using other codes and test problems

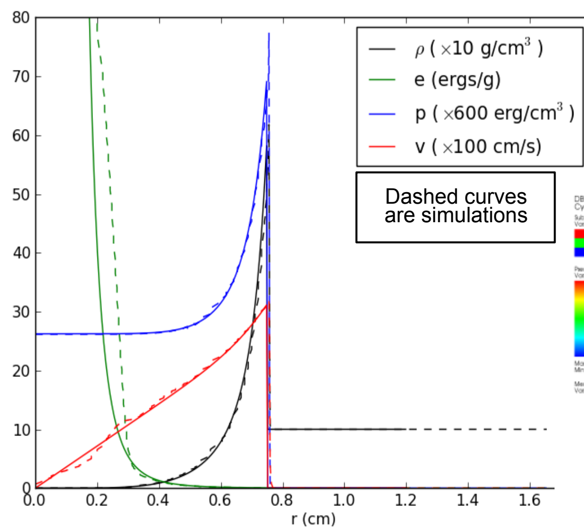


- 4-mm ring made of Al6061 surrounded by void
- Johnson-Cook strength and damage models

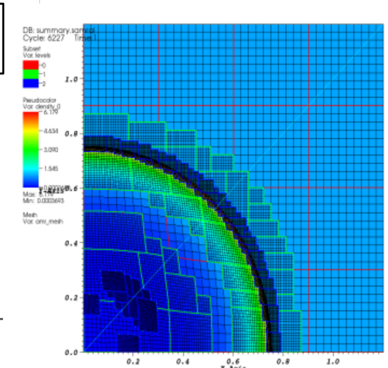
LS-DYNA



Plastic strain comparison



ALE-AMR ALE mode (3 level 360x360)



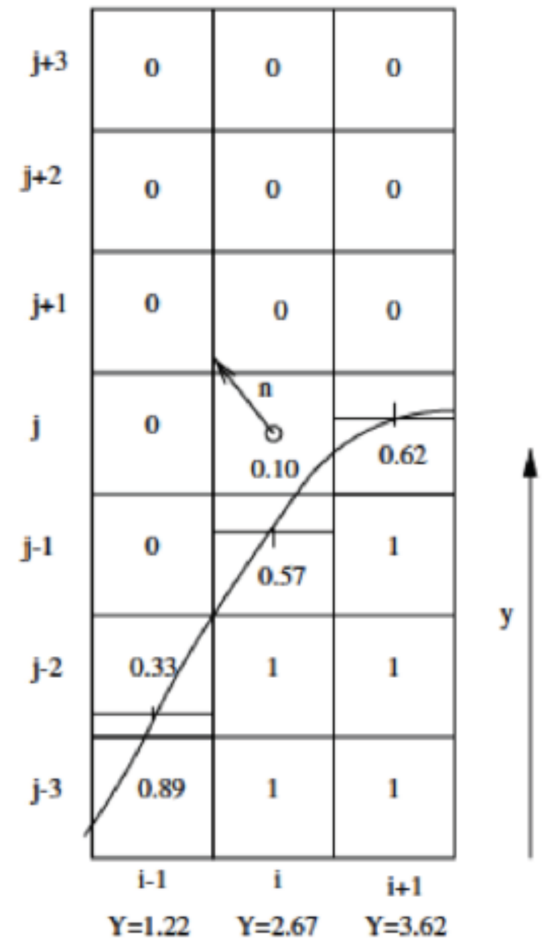
Surface tension calculation is adopted from the height function method using volume fractions

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 $\kappa = 2h_1 (1 + h_2{}^2)^{-1.5}$

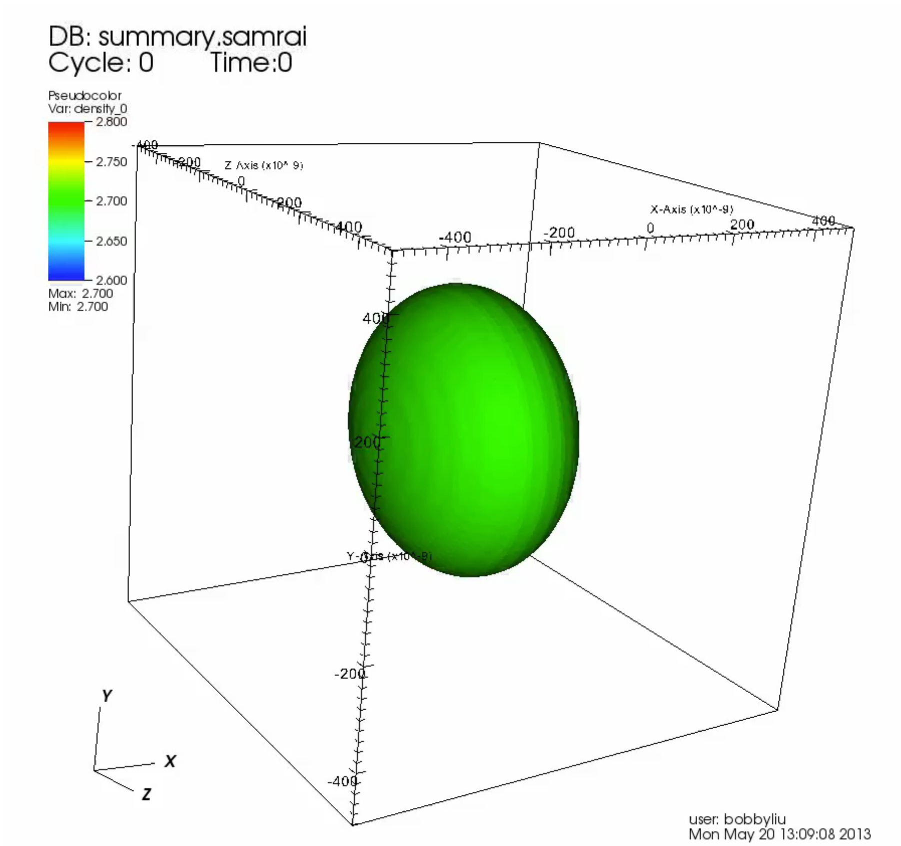
The curvature and normal are calculated in cells but the force like velocity are nodal so cell curvature is averaged to get node value



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

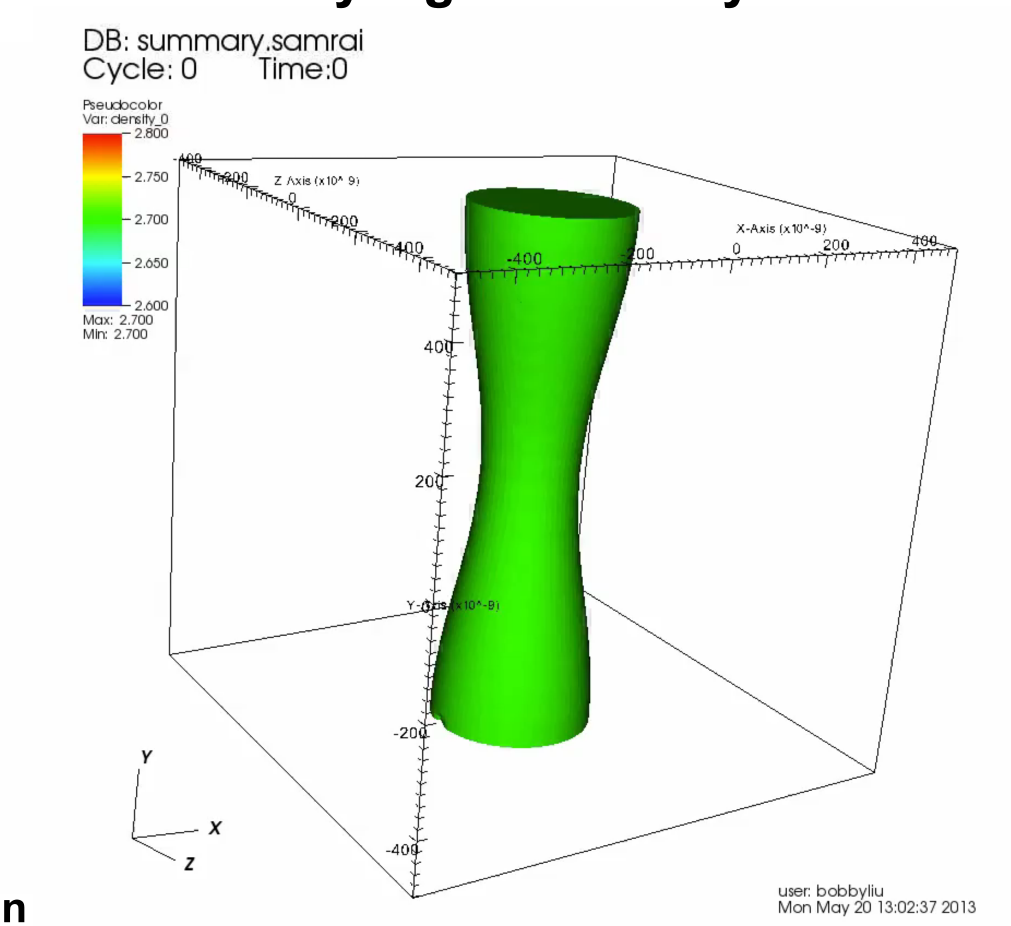
We have validated the surface tension model using different test cases with analytic solutions

Ellipsoid oscillation



Level of damping depends on the surrounding material

Rayleigh instability



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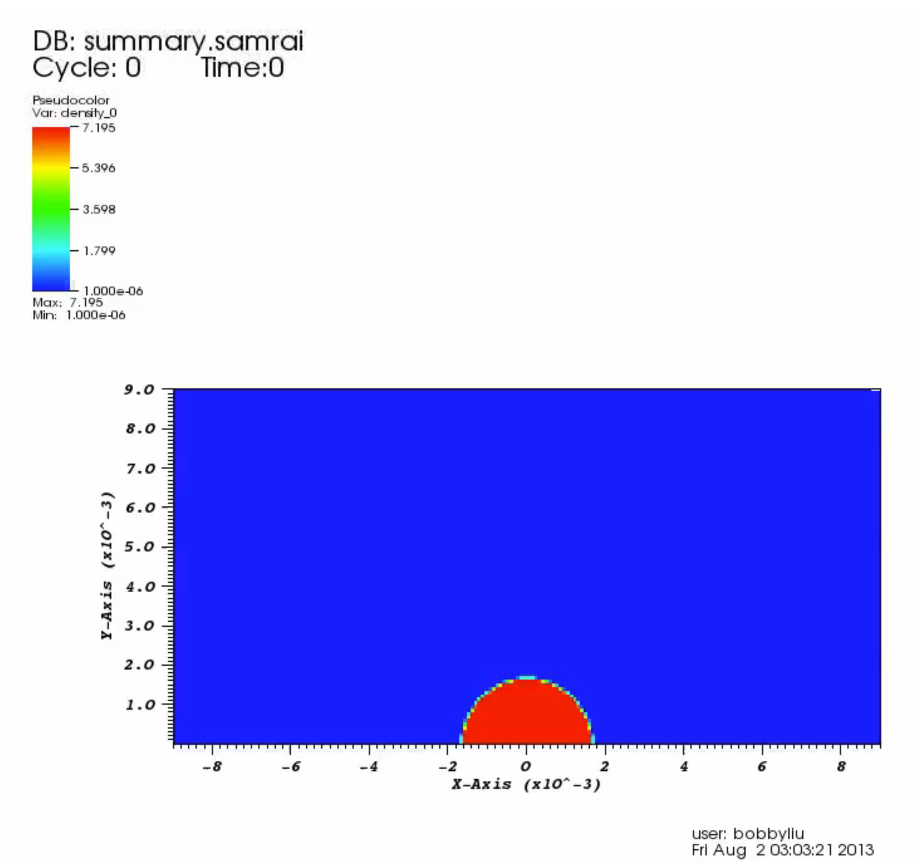
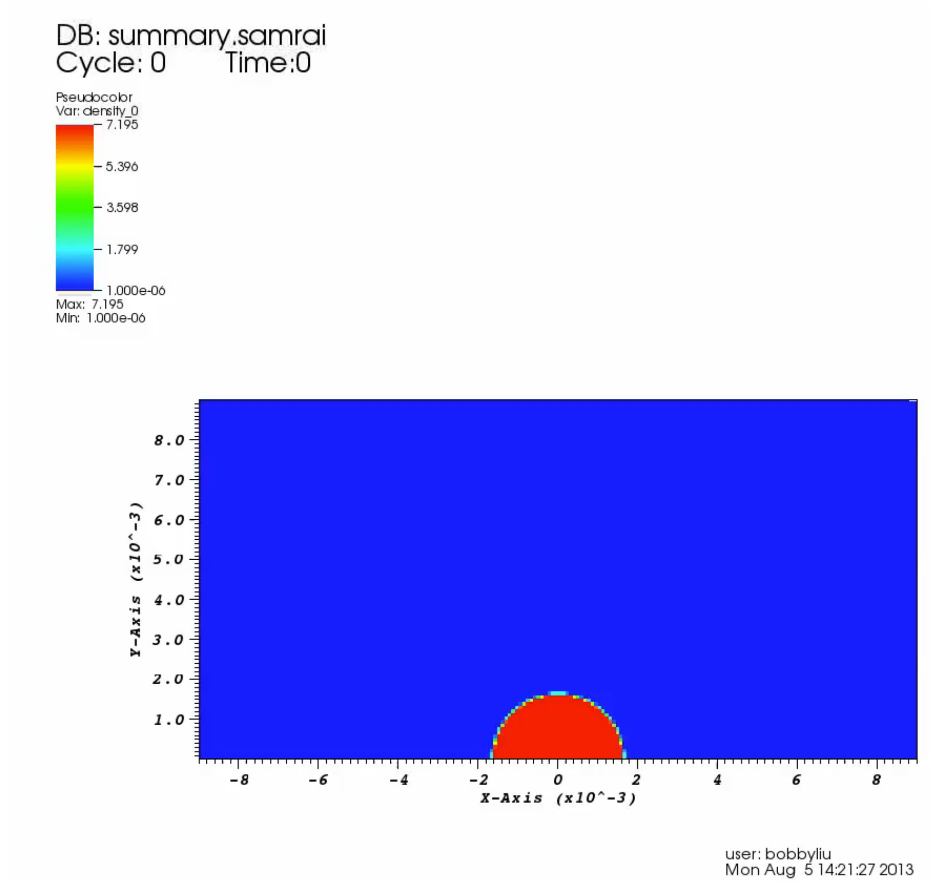
We are exploring different ways to define the liquid vapor interface in the simulations

Without surface tension



With surface tension



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These simulations use a simple density criteria to define interface

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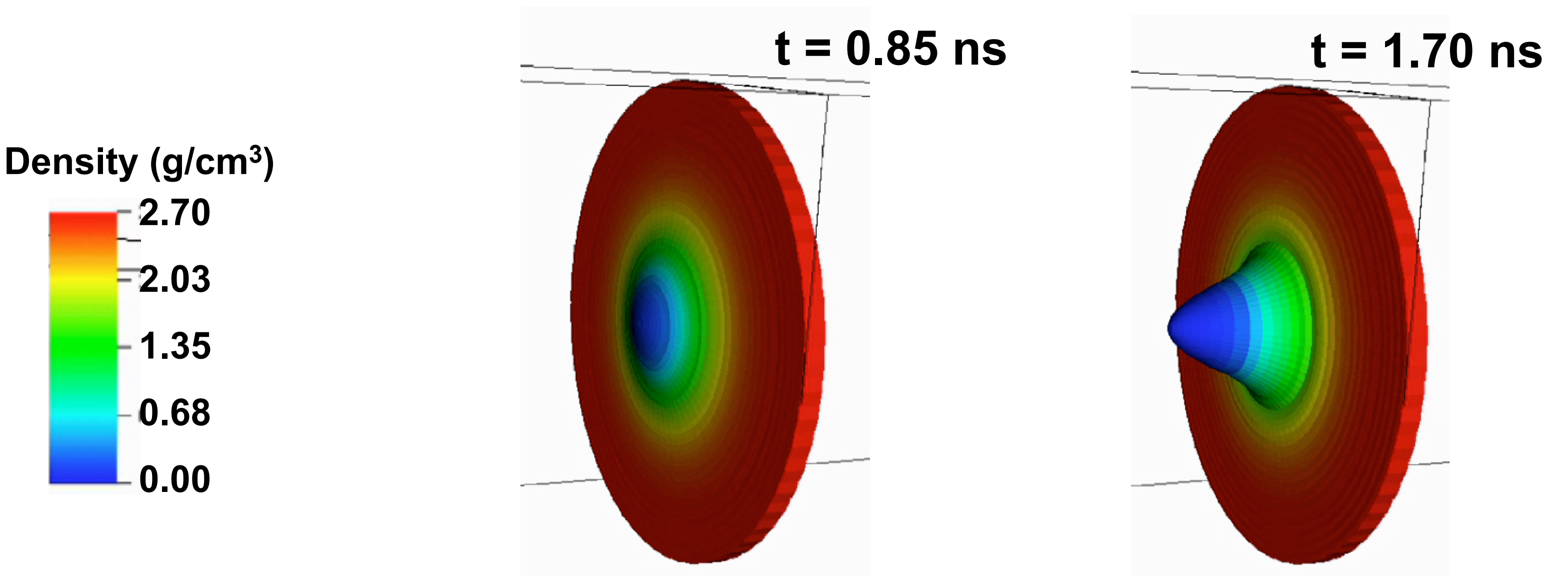
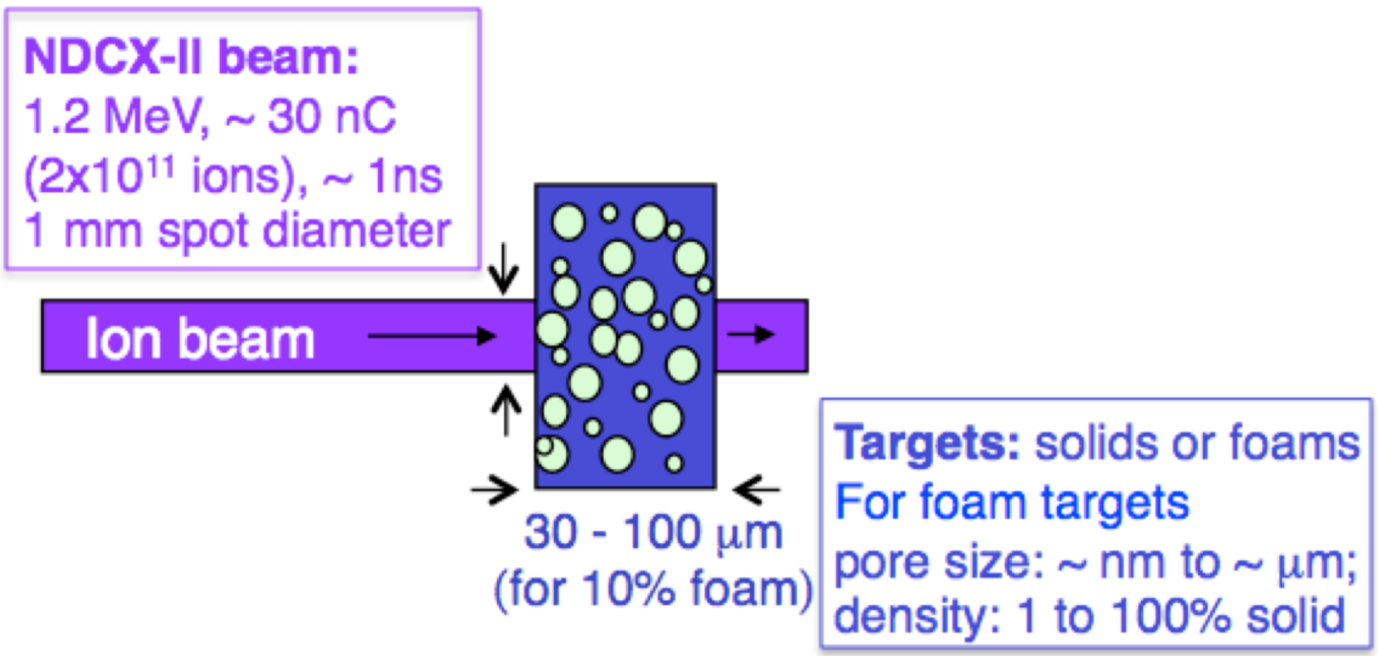
ALE-AMR being used to design future NDCX II experiments with sub ns high-energy pulses



- 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

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**



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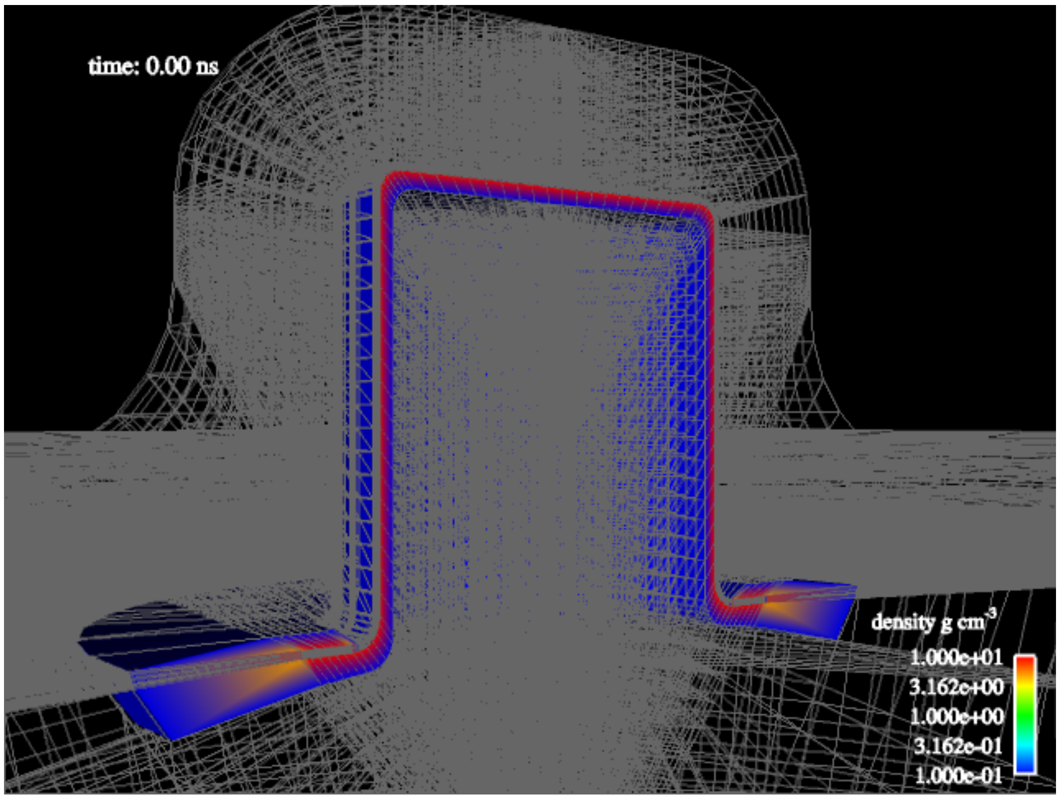
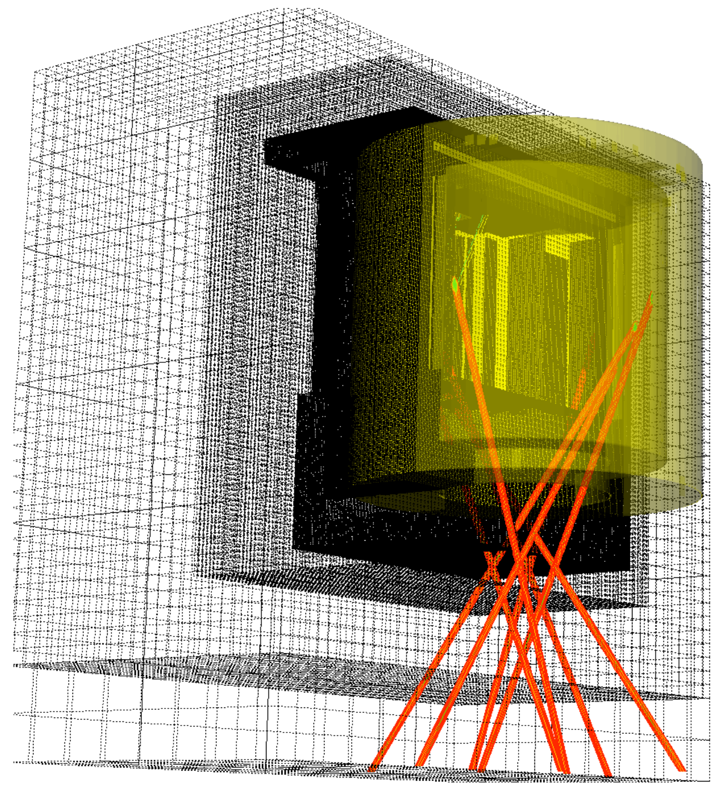
Problem: Traditional ALE codes (like Hydra) complicated mesh and tangled for late-time

Traditional ALE

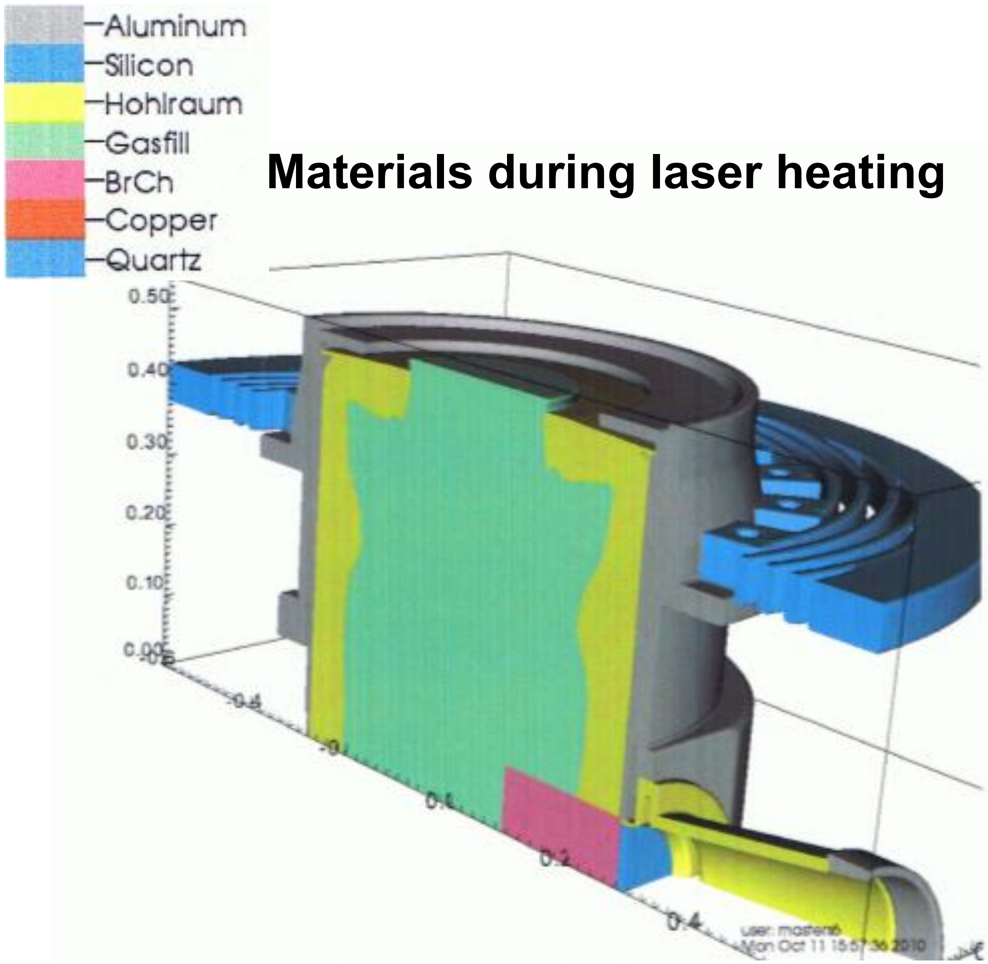
Newly Designed ALE-AMR



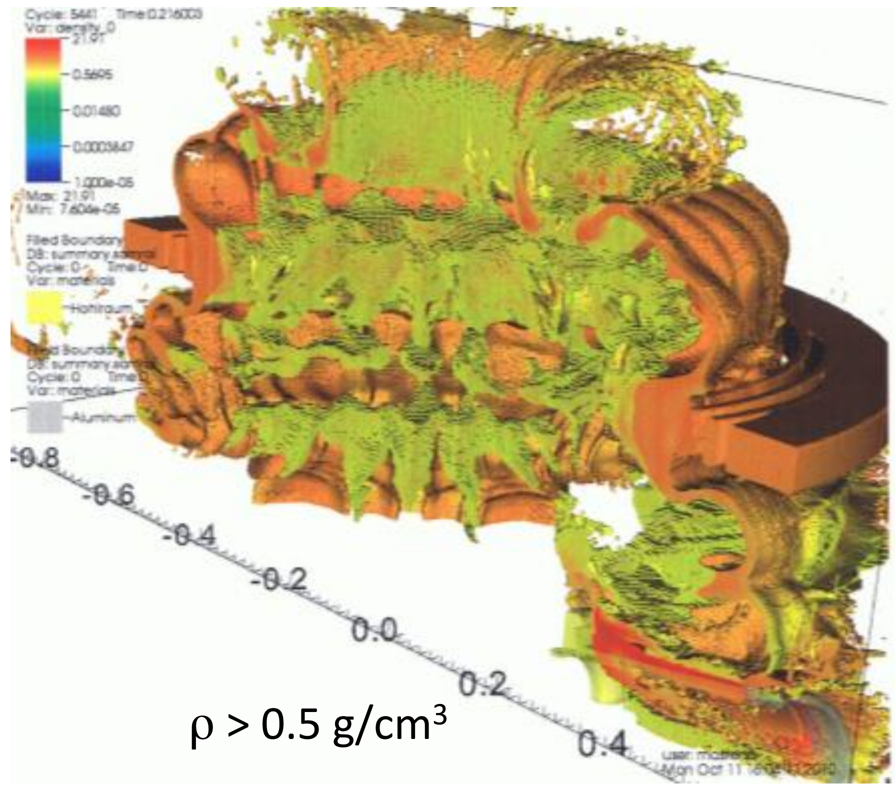


ALE-AMR was developed initially for late-time whole-target (not just hohlraum) NIF simulations

Materials during laser heating



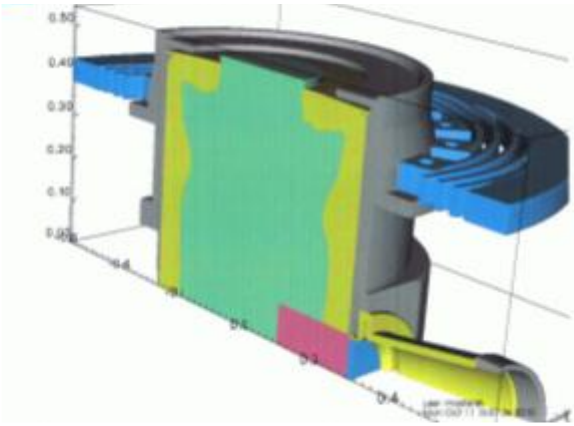
Threshold density at 220 ns



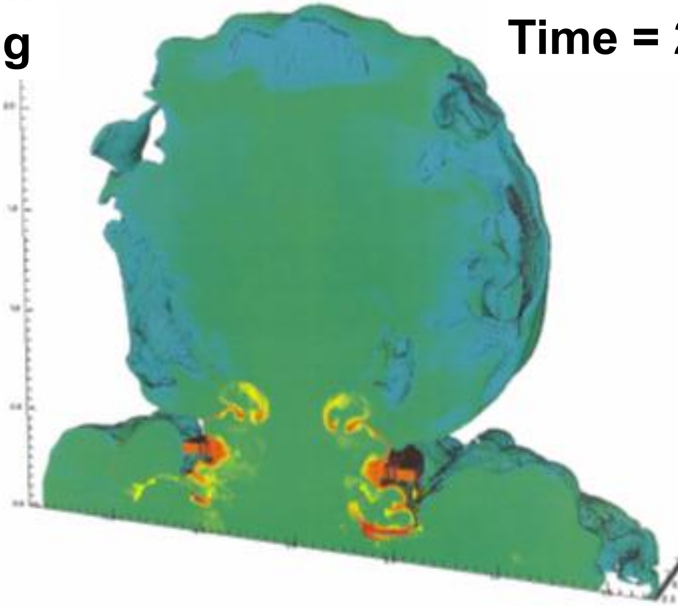
D. C. Eder, A. C. Fisher, A. E. Koniges, and N. D. Masters, "Modeling Debris and Shrapnel Generation in ICF Experiments," to appear in Nuclear Fusion (2013)

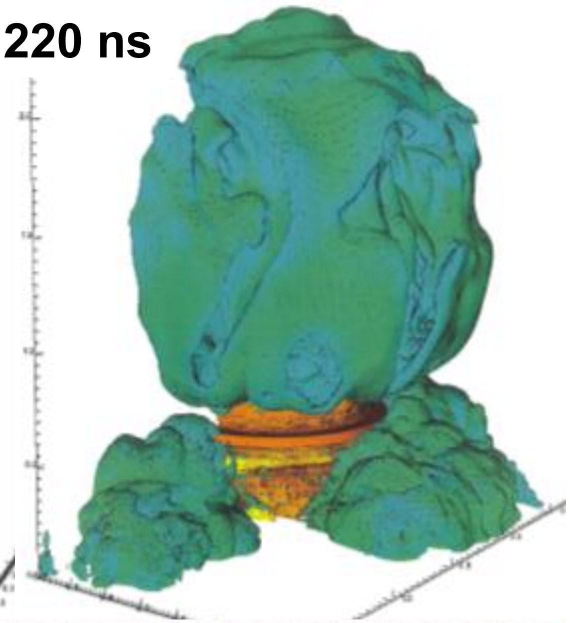
The use of AMR with six levels of refinement is critical to model plasma plume expansion

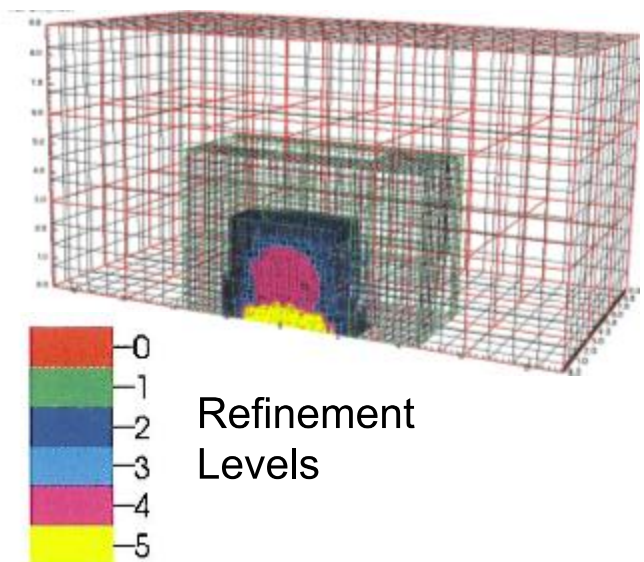
Materials during laser heating



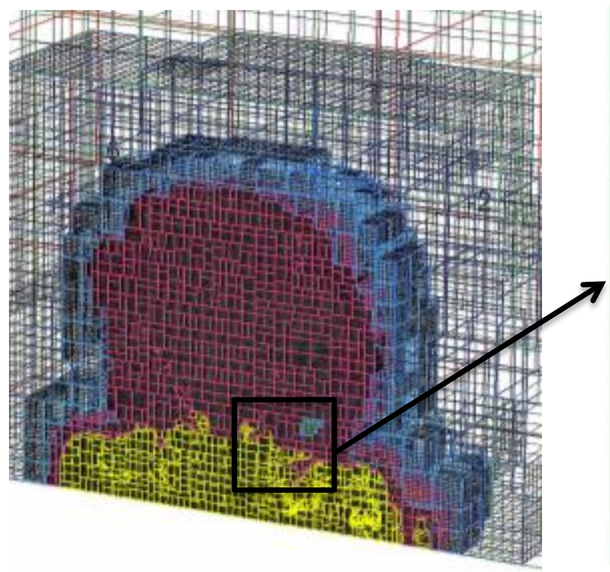
Time = 220 ns

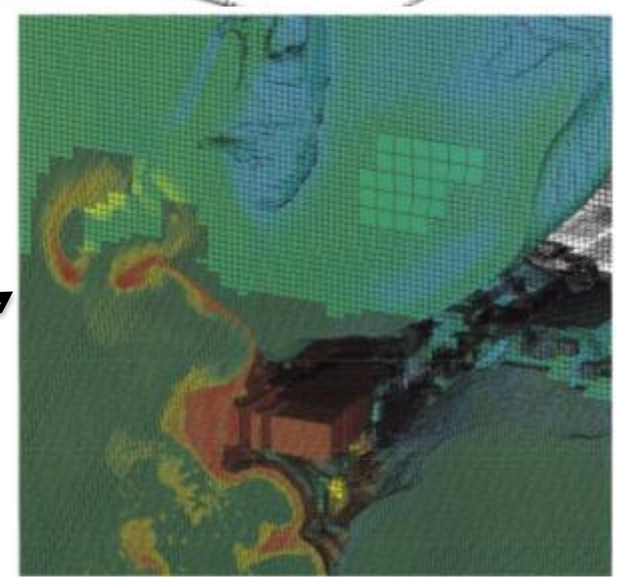






Refinement Levels





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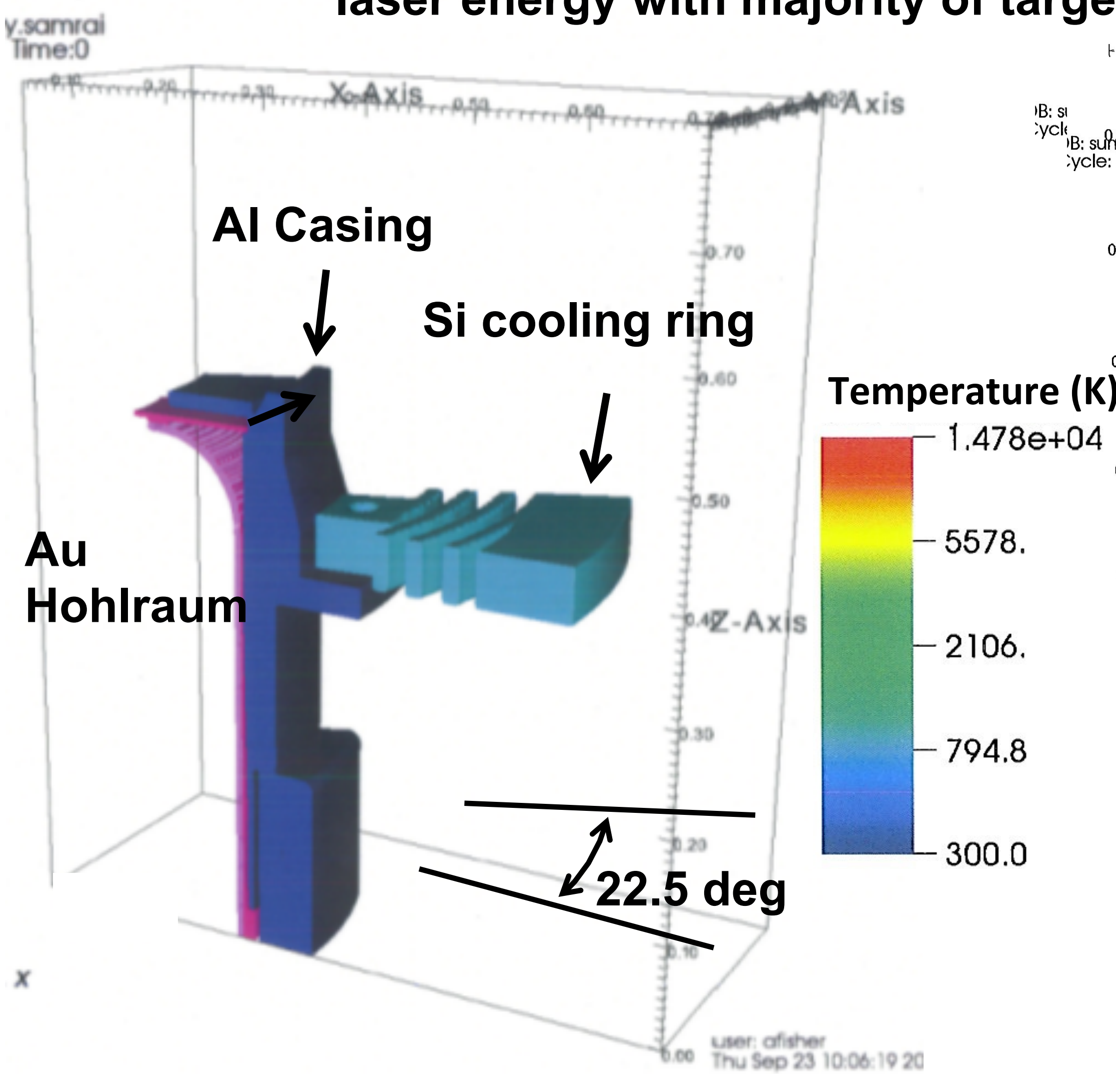
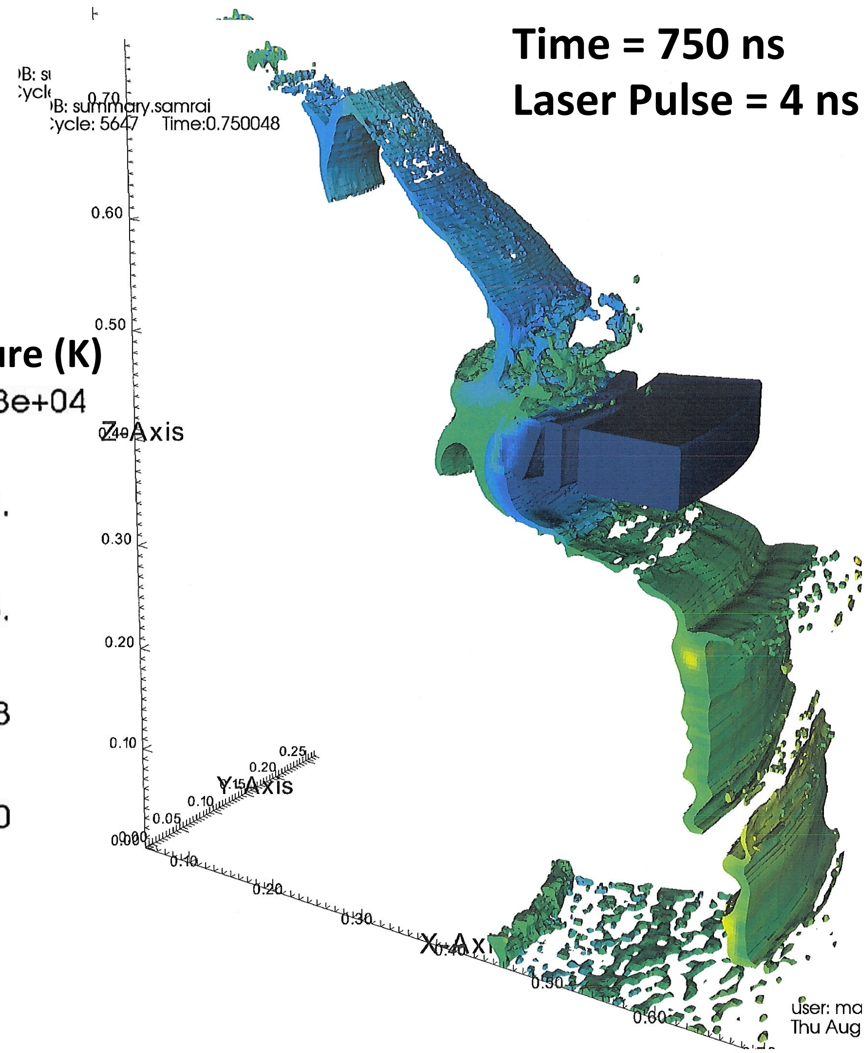
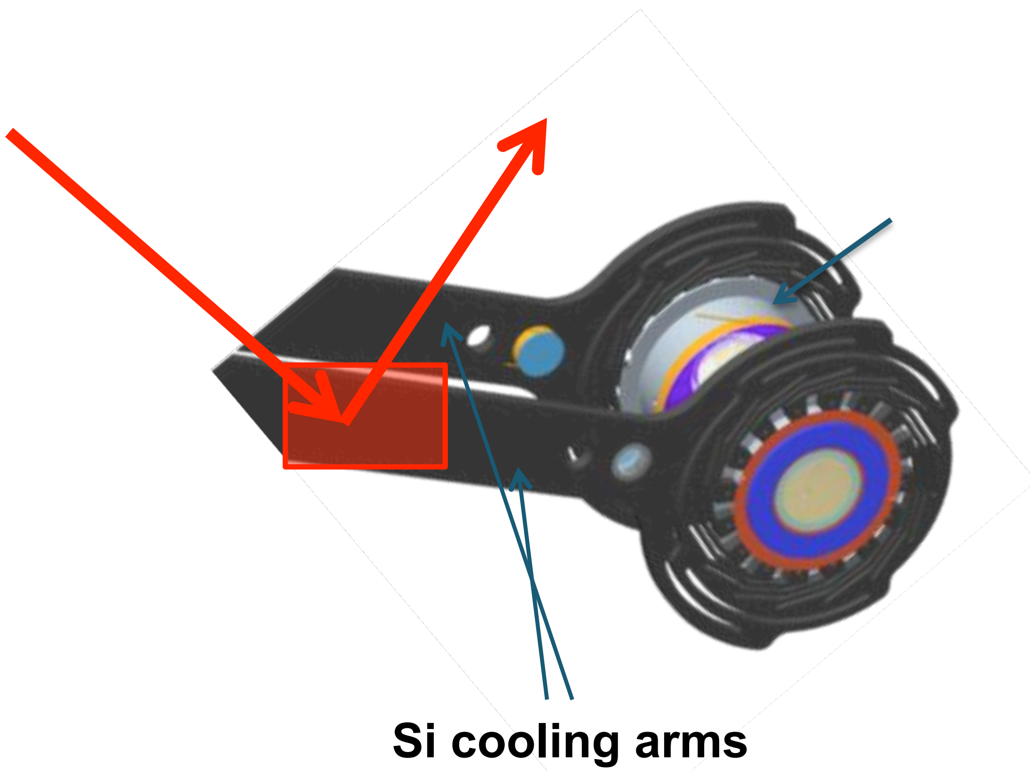
Sample NIF target where fragmentation modeling is needed for protection of optics and diagnostics

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



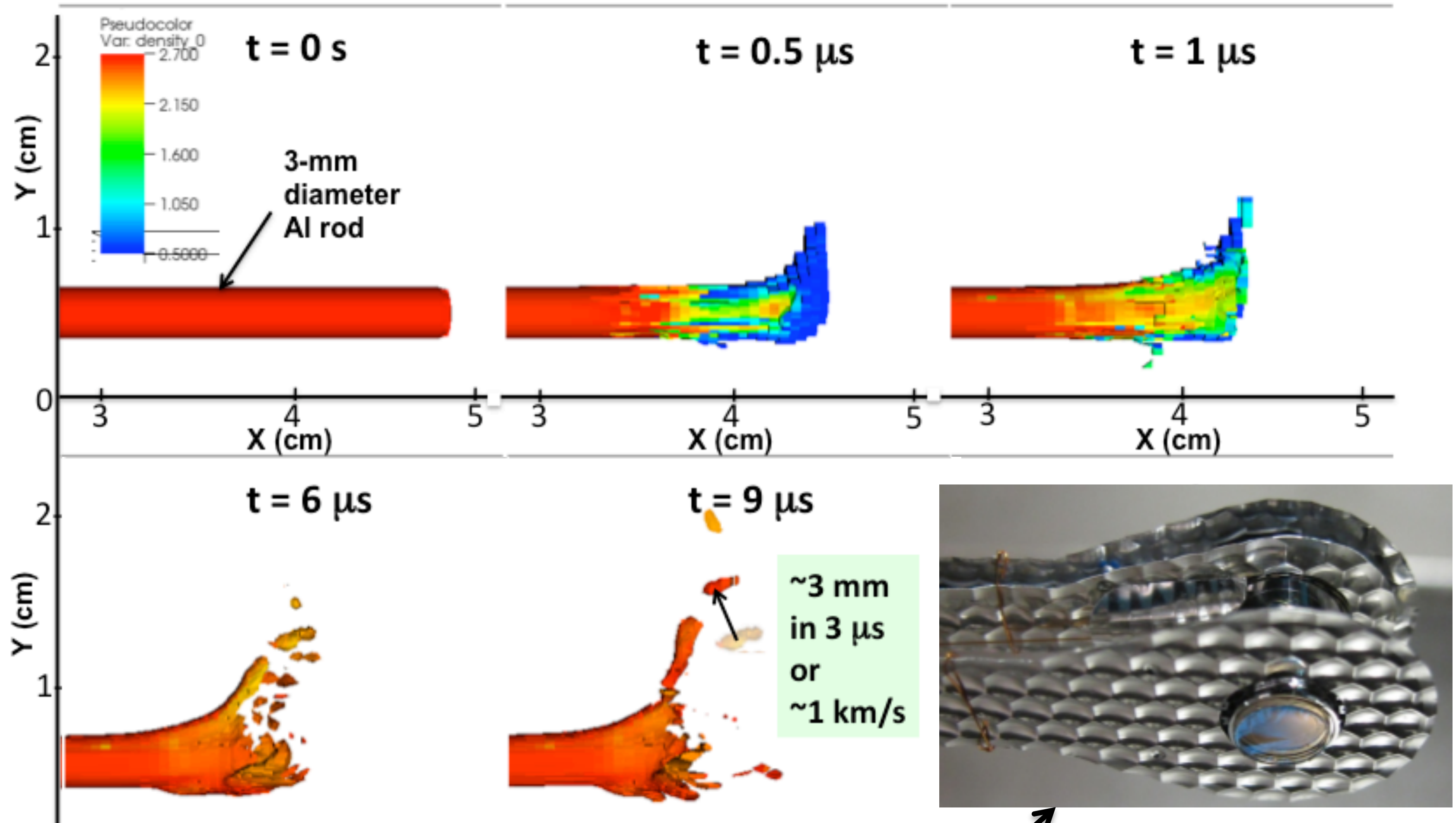


Code instrumental in redesign of several experimental configurations to meet safety/performance standards



- 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

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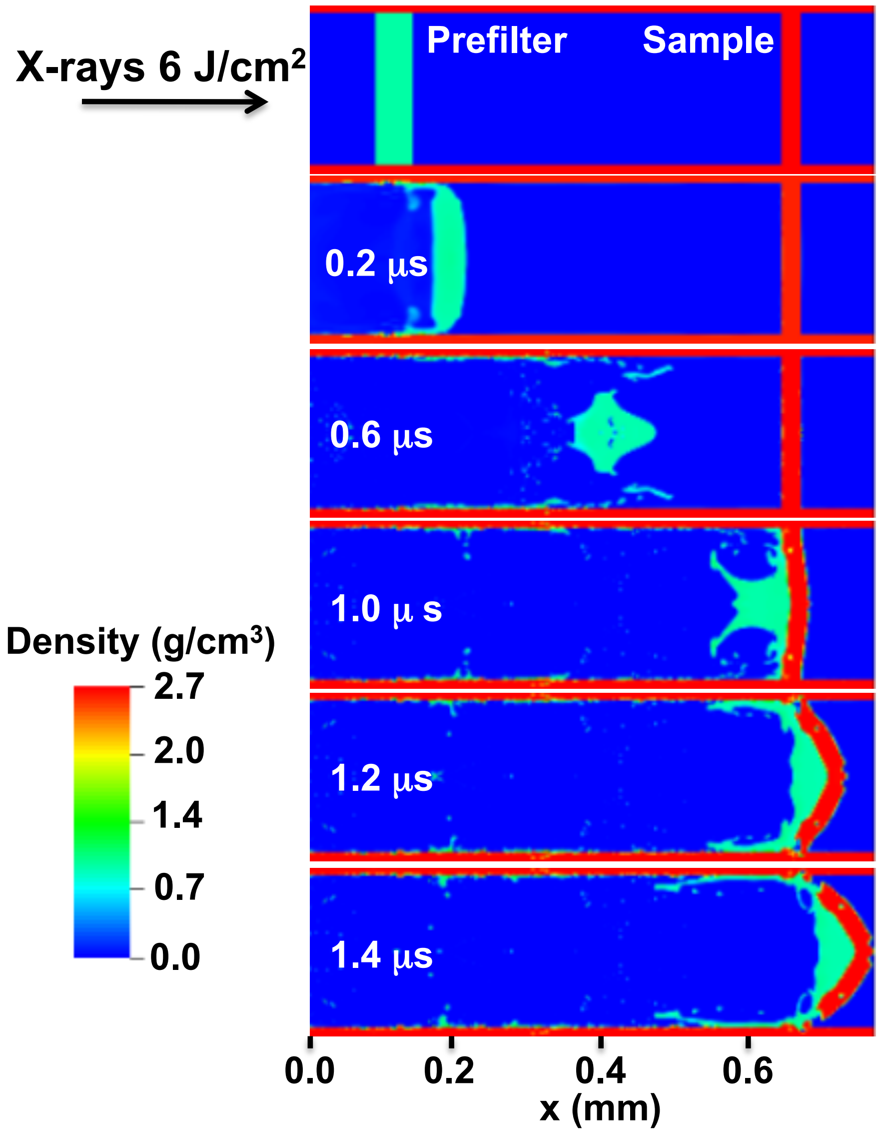
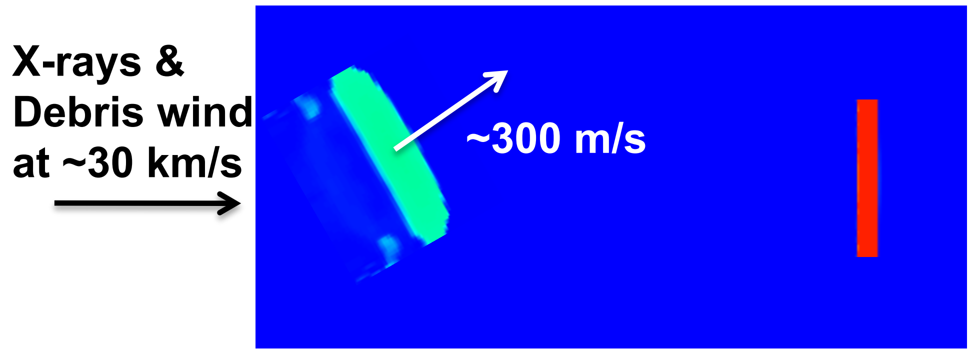
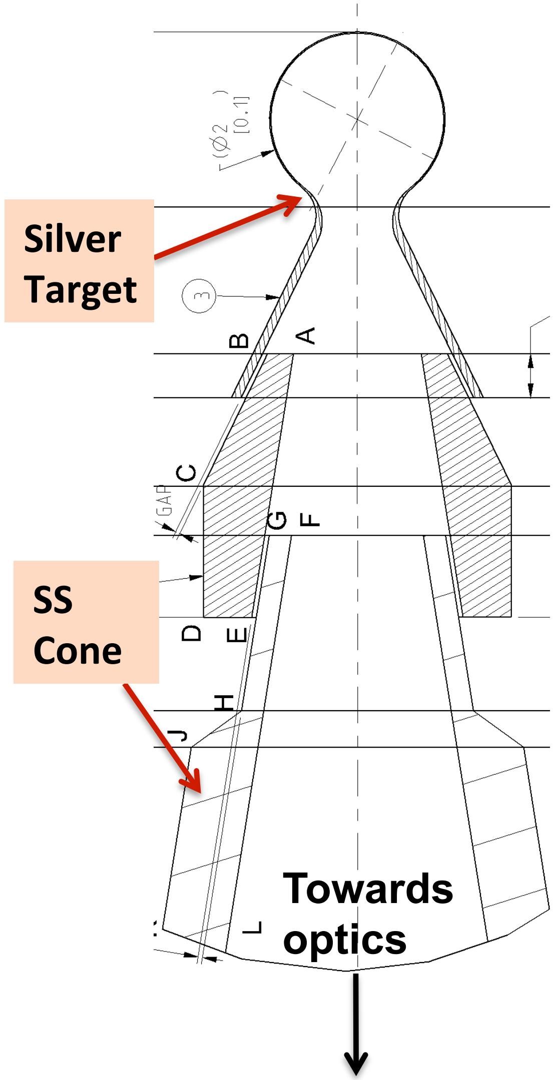
Simulations showed that x-ray loading in initial design damaged thin samples and tilted redesign protects samples from x-rays and fast debris wind from target

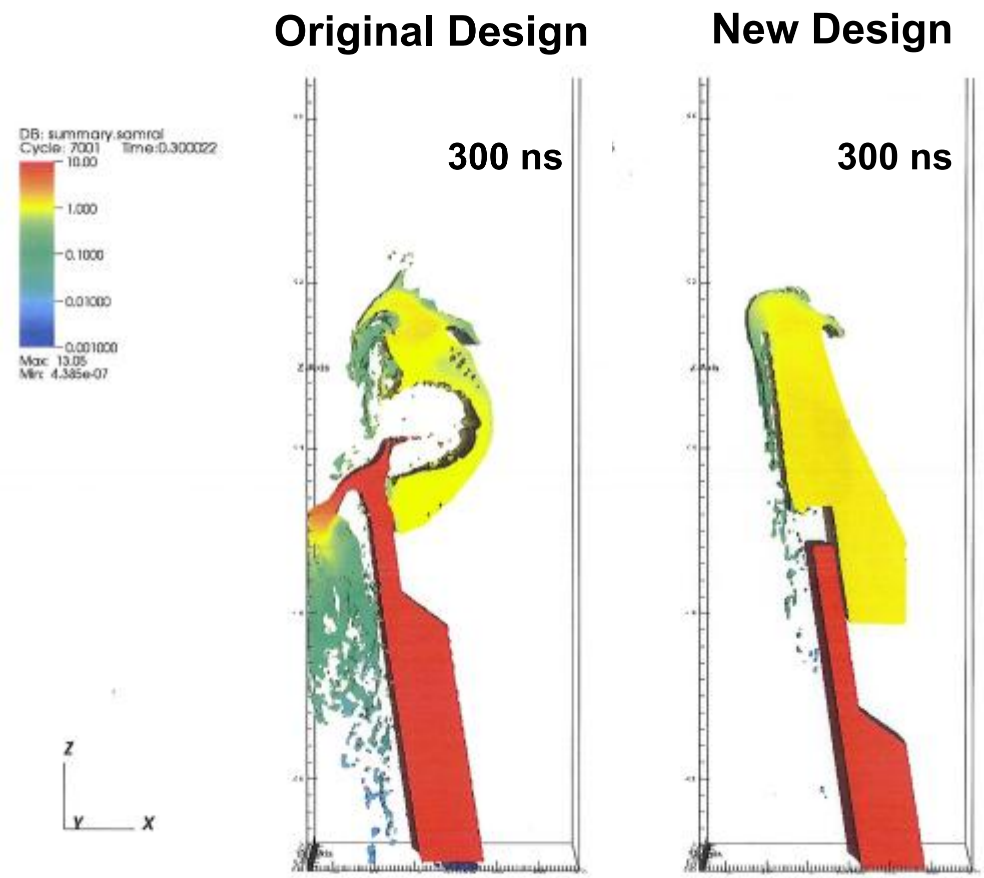




Redesigned Sample Holder

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



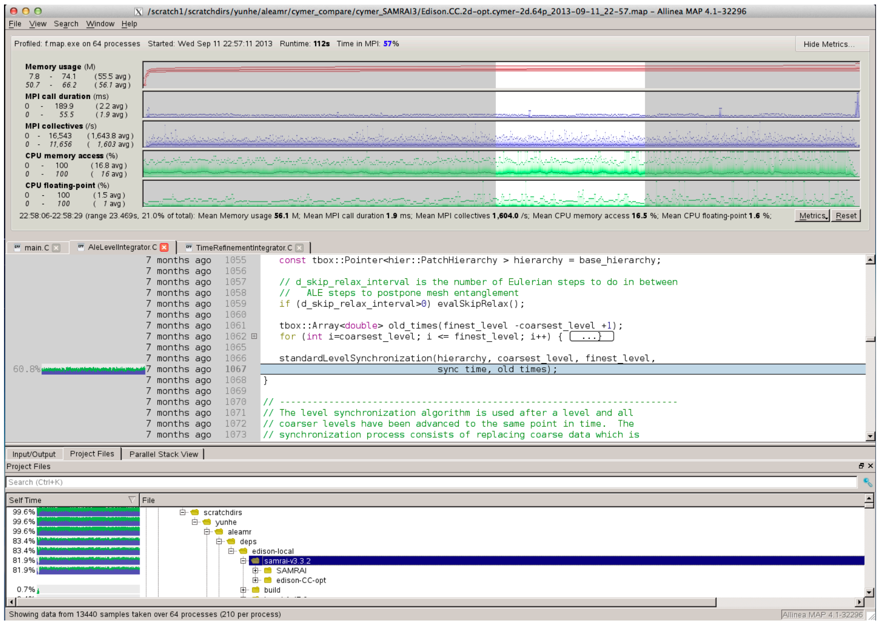


Code recently ported to new Edison

- Cray XC30
- 2.4 Pflops peak
- 124,800 compute cores
- 332 TB memory
- Ivy Bridge Processor at 2.4GHz
- Cray Aries interconnect (8 GB/s MPI bandwidth)
- ~2X faster/core than Hopper

Additional information and scaling results under NDA

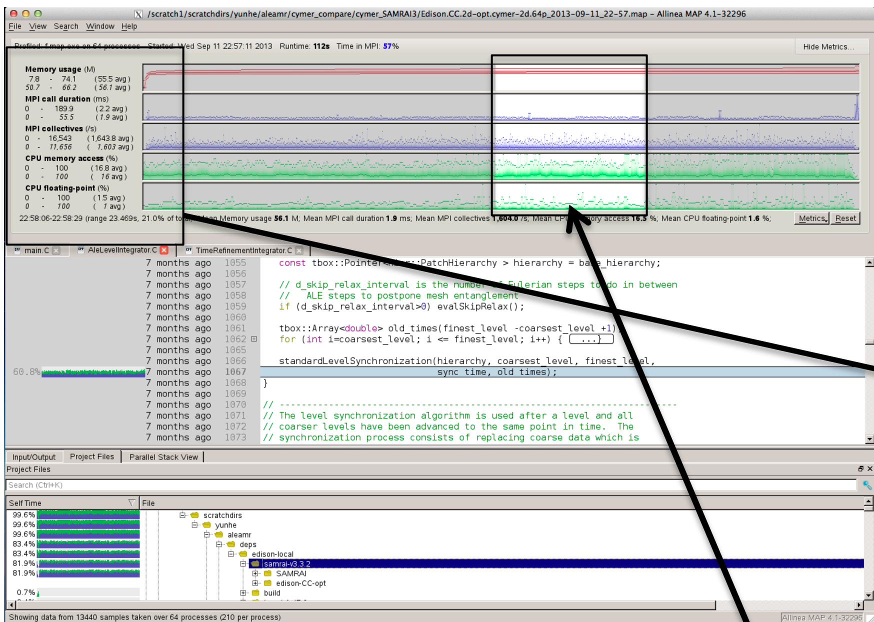
Sample MAP performance analysis on Edison

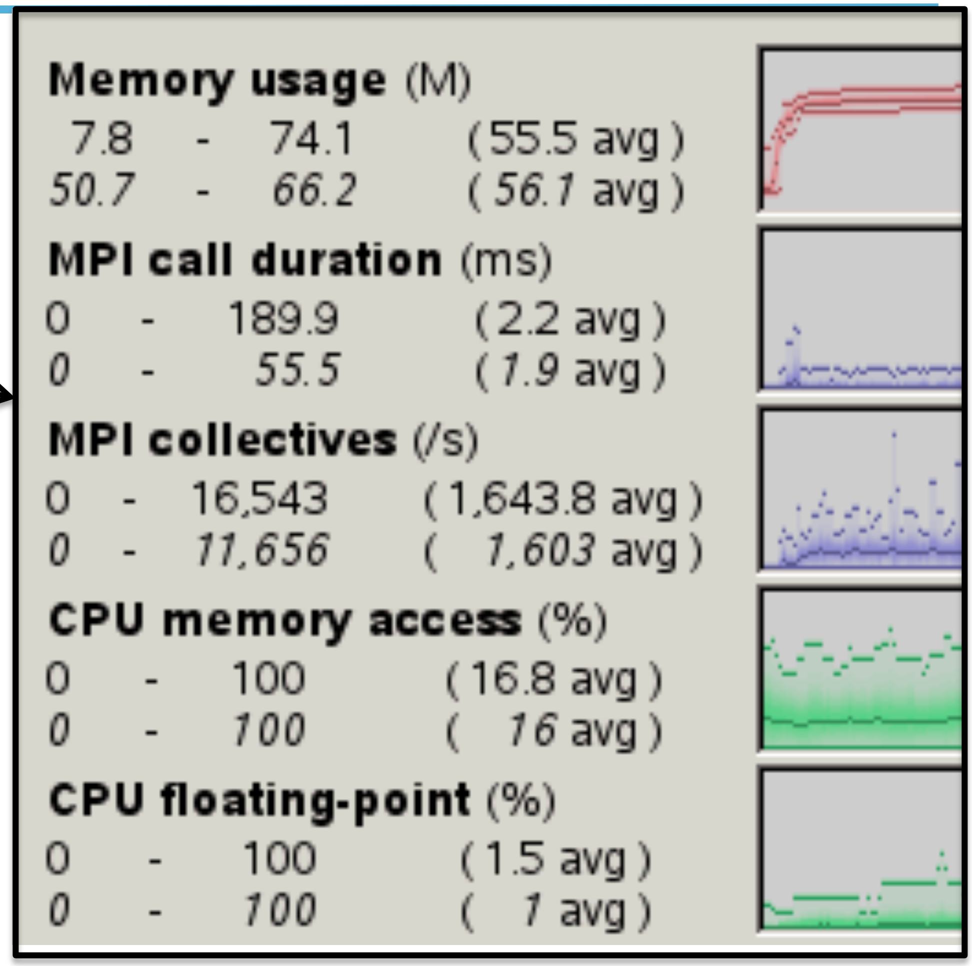


Screen capture of MAP window with memory usage, MPI calls, etc. as a function of time shown along the top

- **Large multiphysics codes like ALE-AMR have complex make/build scripts to load a significant number of supporting libraries**
- **It is important that performance analysis tools can work in this environment and can be accessed in a relatively painless manner**
- **MAP developed by Allinea is available on Edison**

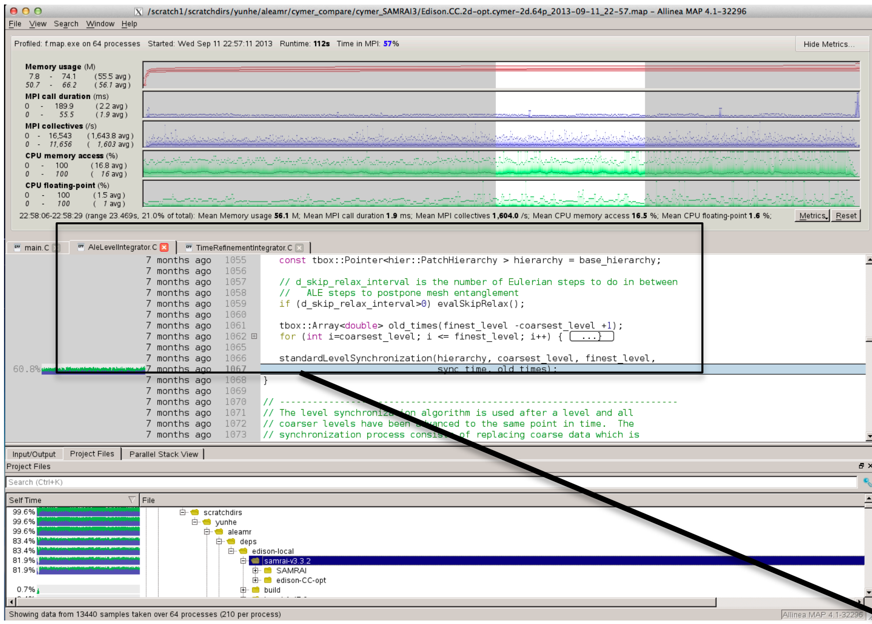
Sample MAP performance analysis on Edison

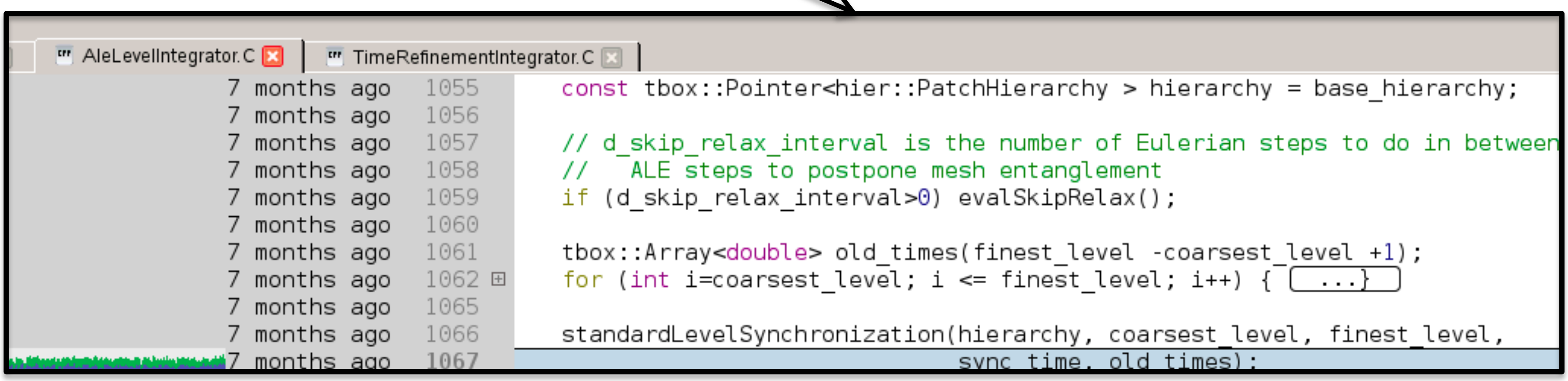




For a particular time interval Δt one can evaluate code behavior

Sample MAP performance analysis on Edison





The source code associated with the the majority of communication or computation also can be displayed

Code performance, e.g., time spent in communication, is problem dependent for multiphysics applications

- **Decreasing domain size in strong scaling studies with increasing number of cores is common cause for increased communication**
- **Code performance/behavior can also depend on problem type**
  - **Cymer problem with tabular EOS has a 2X difference in ratio of communication to computation compared to shock physics problem**
- **Integration of multiple physics packages makes code optimization difficult**
- **However, doing "full physics" with same code/grid/domain, etc., generally gives much higher accuracy than code coupling**

Summary

- Advanced multi-material rad/hydro/materials code developed for NIF is continuing use on a variety of problems
  - NIF Optics and Diagnostics
  - LMJ (France) new experiments
  - NDCX Warm Dense Matter
  - Cymer Laser-heated droplets
- Uses combination of ALE with AMR unlike traditional ICF simulation codes
- New models for surface tension are being integrated/studied
- Code runs on variety of HPC platforms, currently being optimized for NERSC Edison (Cray Cascade)