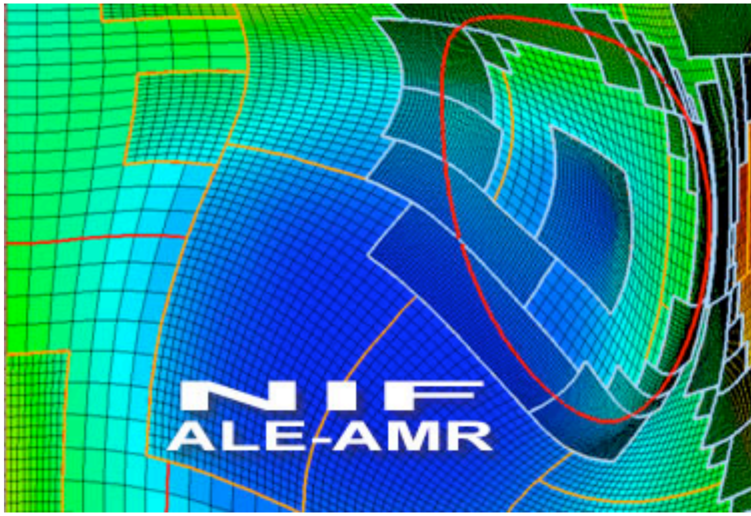


Development and Validation of a New Predictive Simulation Code using Multiscale Material Models

Alice Koniges,[1] Aaron Fisher,[1] Nathan Masters,[1] Parag Dixit,[2] Robert Anderson, [1] David Benson,[2] Brian Gunney,[1] Tom Kaiser,[1] David Eder,[1] Dan Kalantar,[1] William Brown,[1] Marc Meyers,[2] H. Jarmakani,[2] Betsy Foote[1]

[1] Lawrence Livermore National Laboratory,

[2] University of California, San Diego

Numerical methods for multi-material flows, Prague, CZ, Sept. 10 - 14, 2007

UCRL-PRES-236338

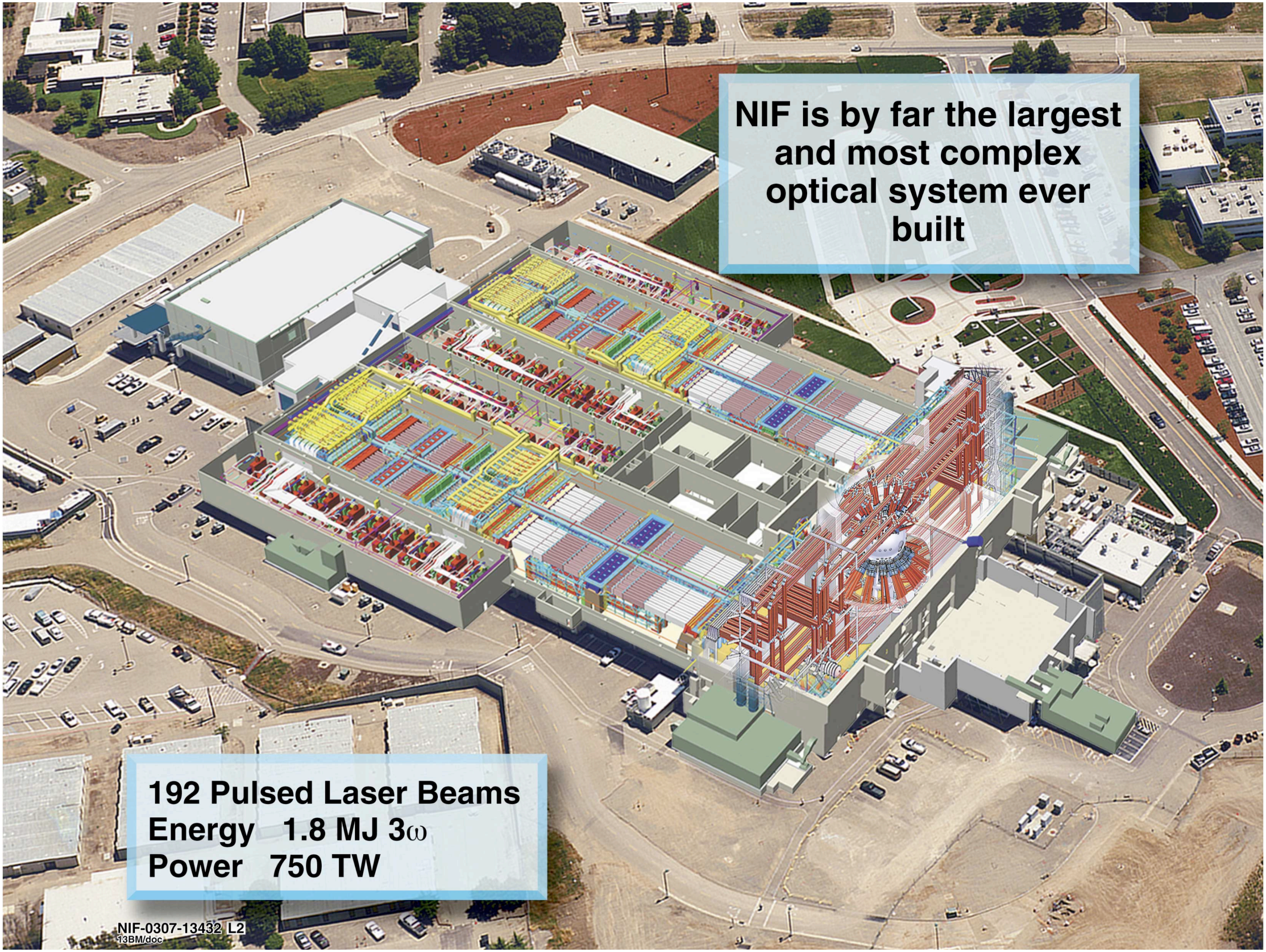
Computation Directorate

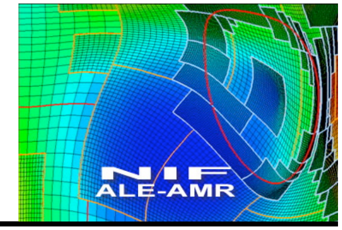
OUTLINE

- **Motivation/Application Domain**

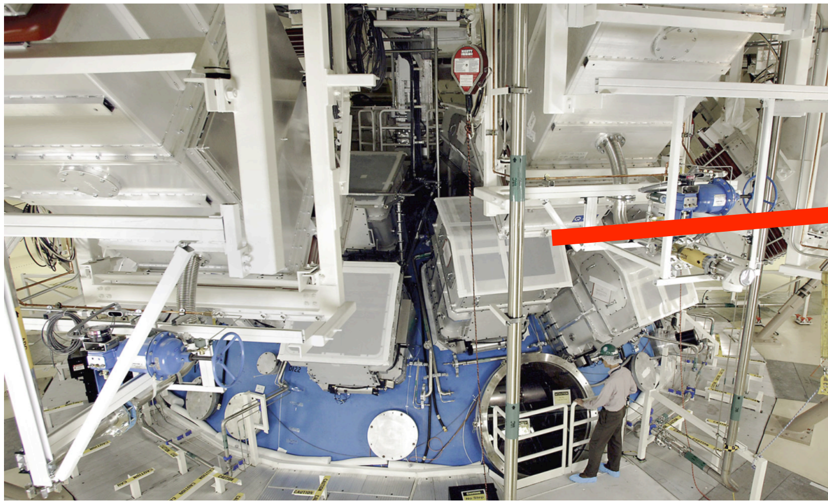
- **NIF-ALE-AMR**
  - **Basic ideas**
  - **Interface reconstruction**
  - **Hierarchical material models**
  - **Fragment modeling with void**

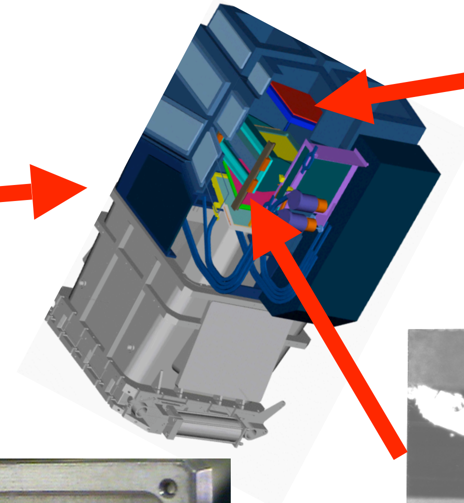
- **Team Development**


NIF is by far the largest and most complex optical system ever built
192 Pulsed Laser Beams
Energy 1.8 MJ 3ω
Power 750 TW
NIF-0307-13432_L2
13BM/doc

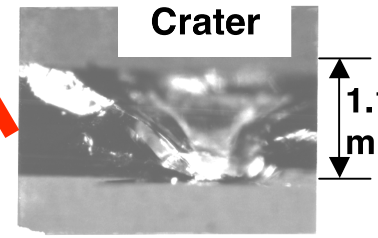


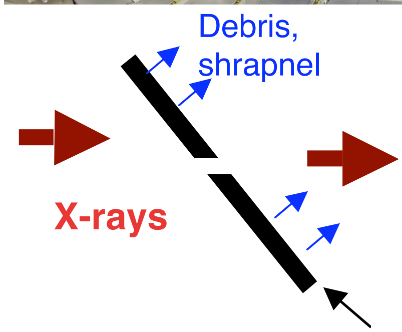
Debris and Shrapnel damage to optics and diagnostics must be mitigated

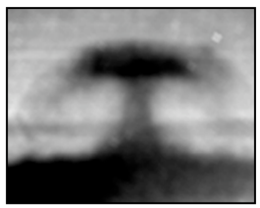


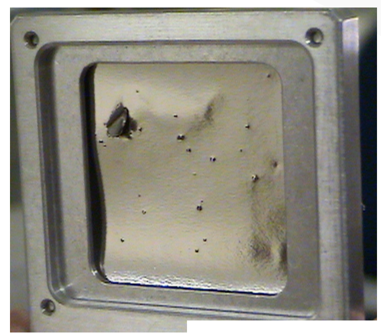


Vacuum window

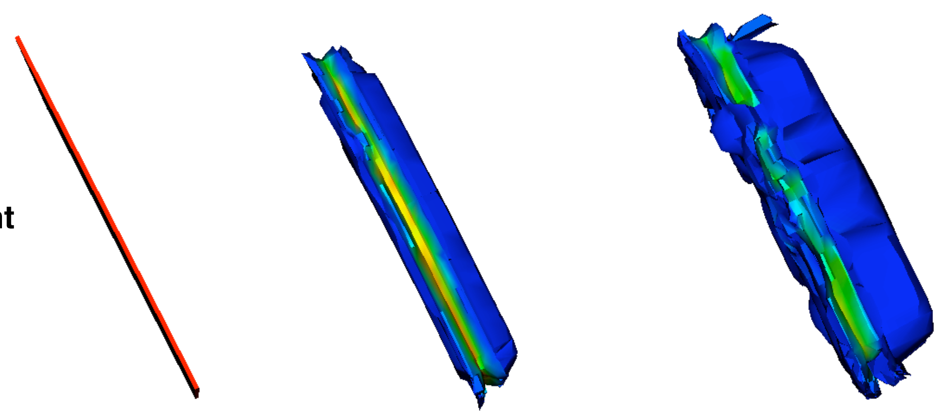








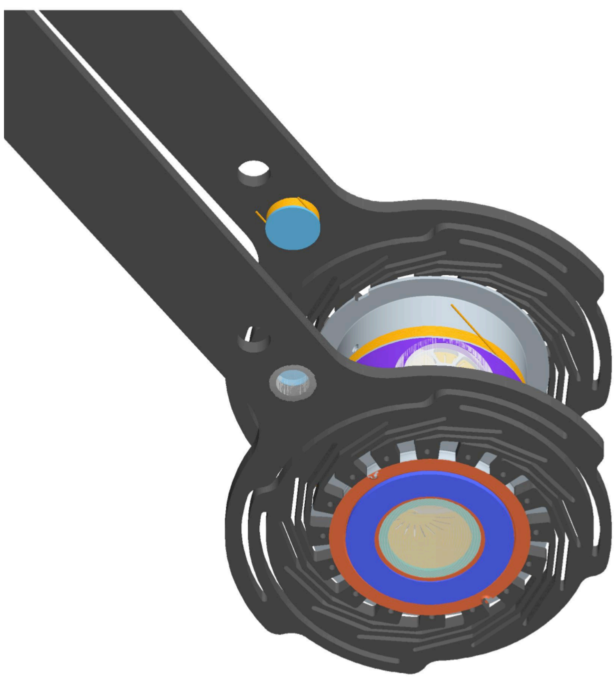
Damage prior to tilting pinhole substrate

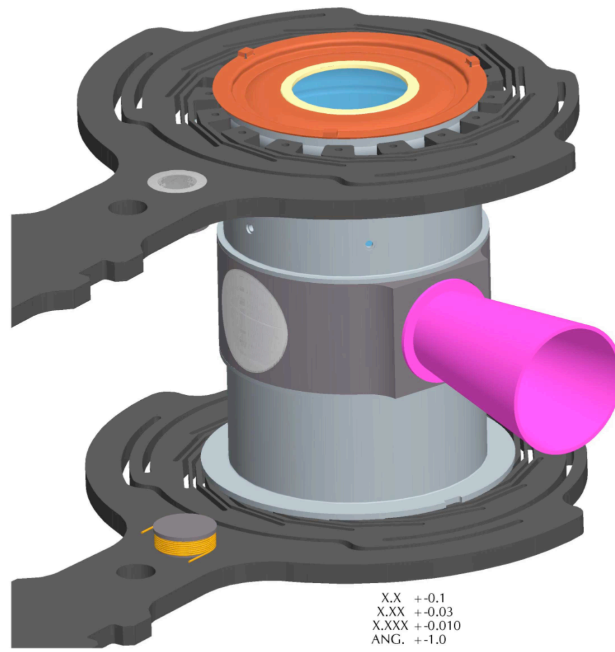


Already on NEL, simulations were important for mitigating diagnostic damage

Time progression of 3D foil simulation (density isosurfaces) shows Ta blow-off in normal direction

Calculations must include the entire target structure, focus is outside the hohlraum

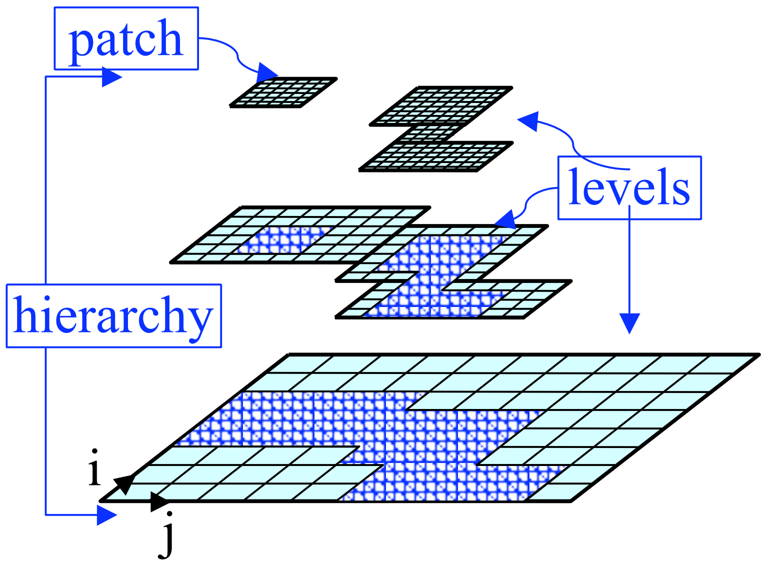




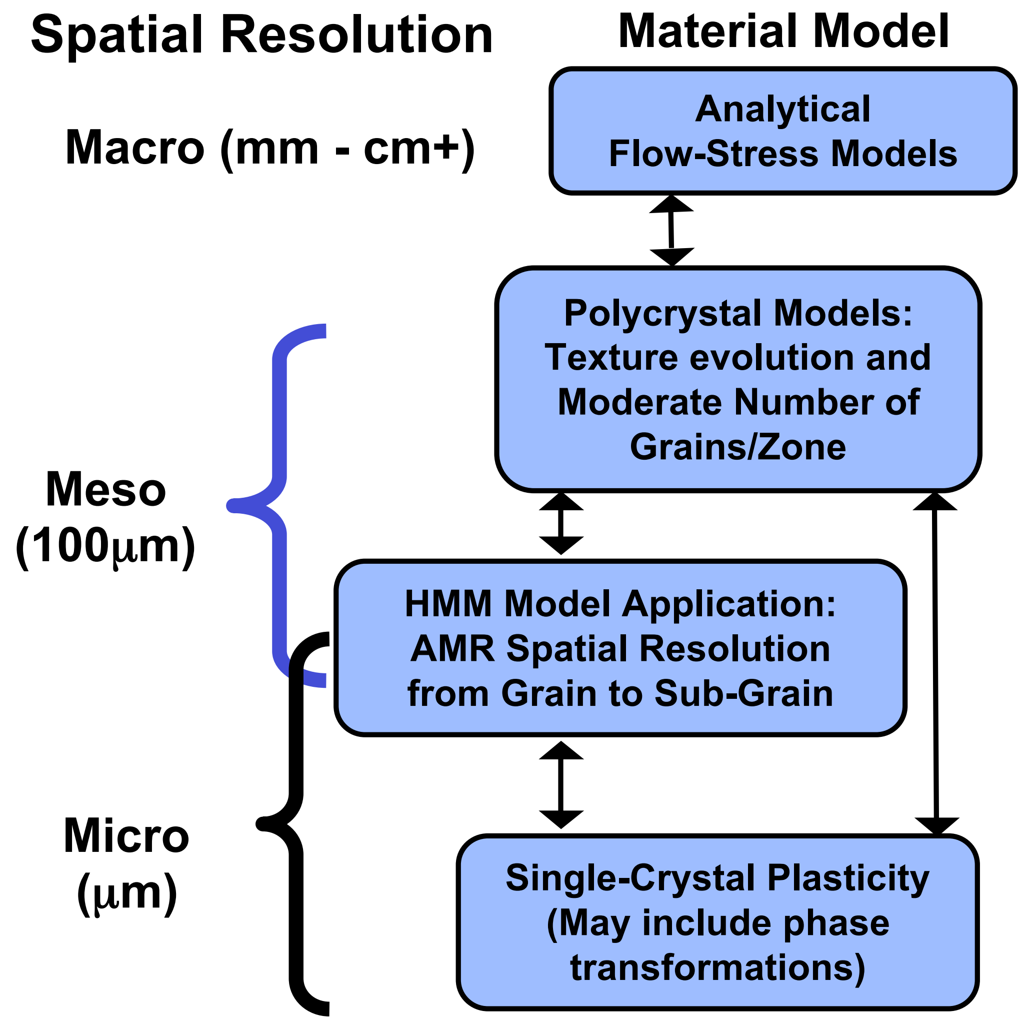
Al Outer Cone on Keyhole target

Sample 96 Beam Campaign Targets

Model has ALE and Adaptive Mesh Refinement and hierarchical material models (HMM)



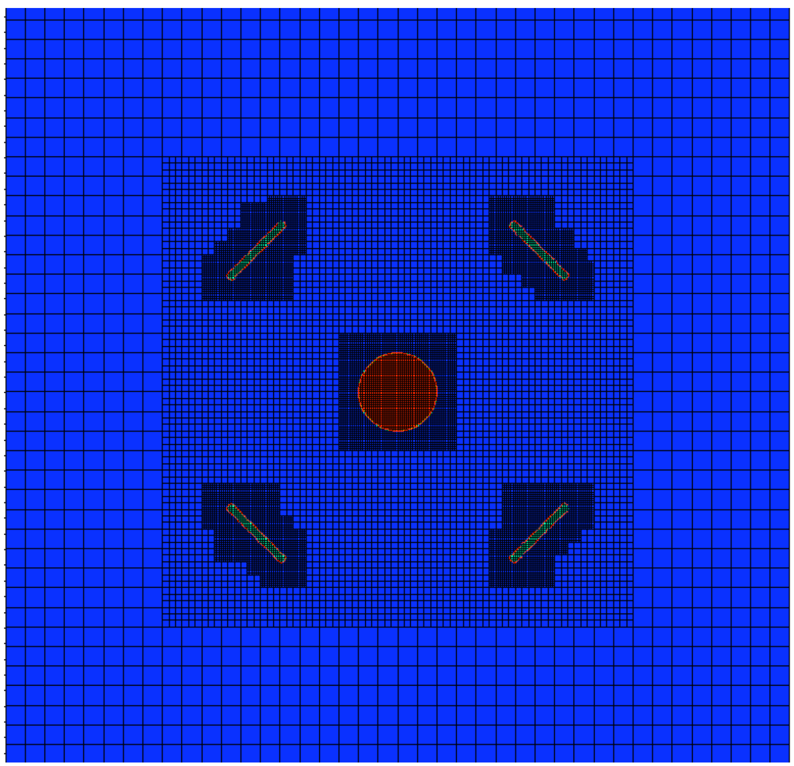
ALE + Stuctured AMR



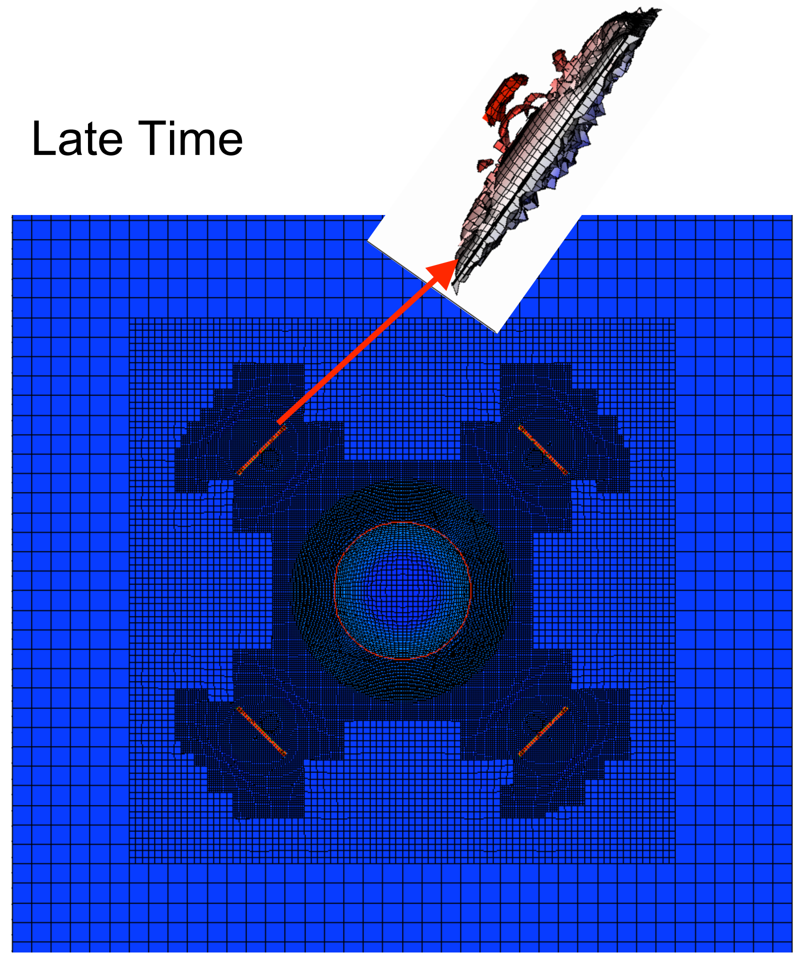
Adaptive mesh capability is crucial for large range of scales and also enables HMM*

- **Simulated target configuration with 4 shields surrounding energy source**

Early Time



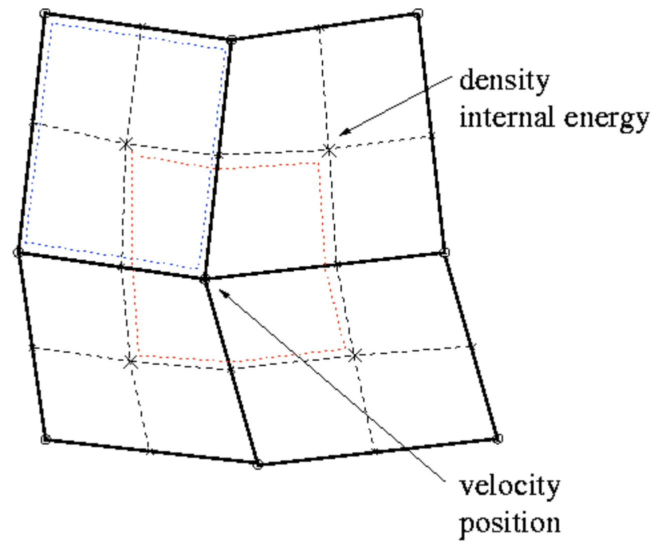
Late Time



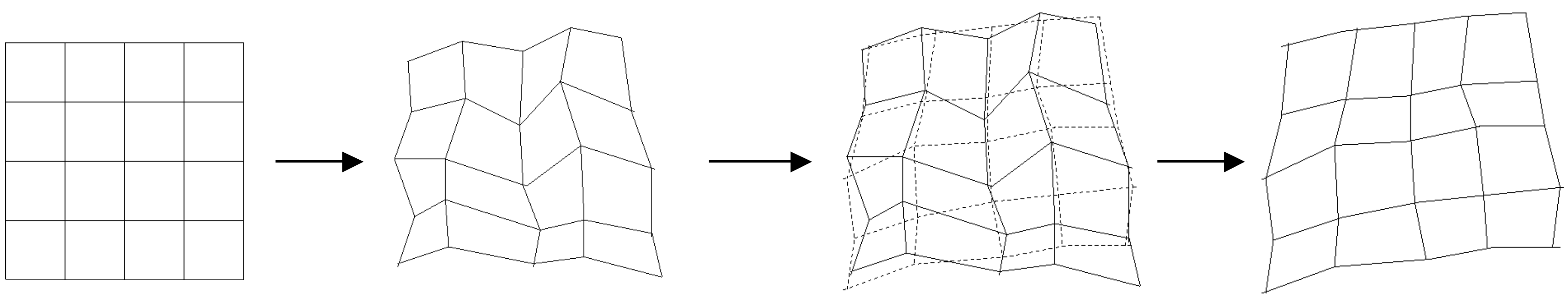
***HMM = Hierarchical Material Model**

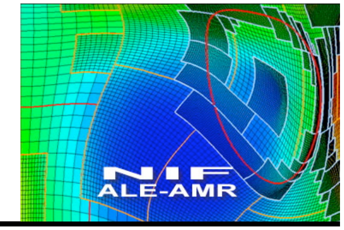
The ALE+AMR structure is due to a methodology developed by Anderson and Pember

ALE approach is due to Wilkins ("HEMP") -uses a moving staggered mesh and a three step computational cycle on a structured grid with staggered variables



- **Time step: Lagrange + Grid Relax + Remap**



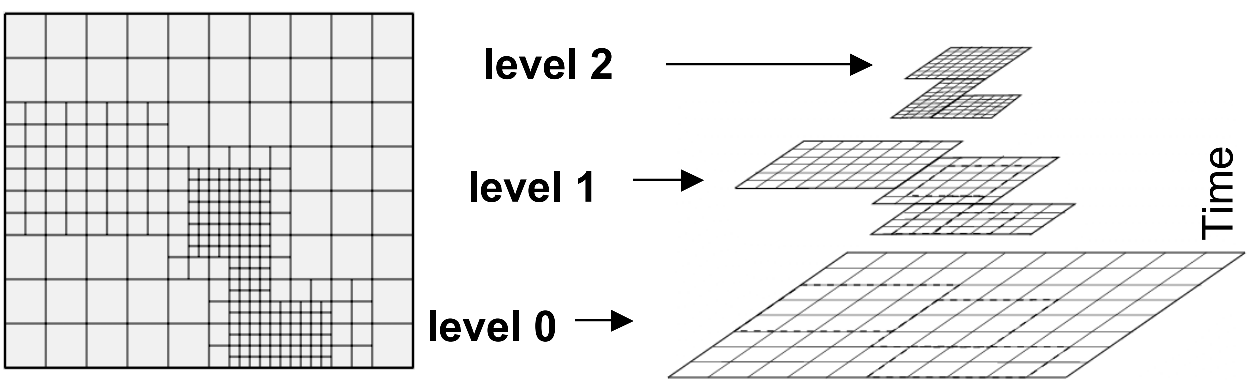


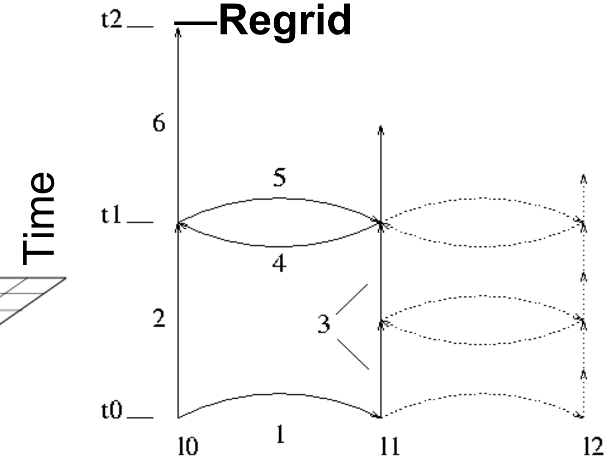
Anderson and Pember designed a strategy for incorporating the AMR into ALE codes

- **Single-level methods + Interlevel transfer operators + hierarchy advance algorithms**
- **An added benefit is that the NIF-ALE-AMR code is automatically scalable based on its underlying use of the SAMRAI adaptive mesh refinement framework**
- **Another benefit is that we are able to use different material models at different levels**

•Hierarchy time step:
- **—Advance coarse level**
- **—Advance fine level**
- **—Synchronize levels**
- **—Regrid**

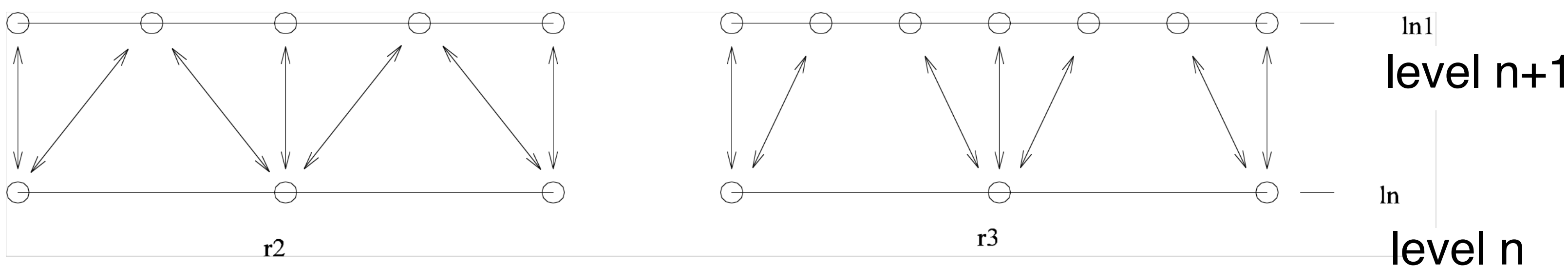
•Spatial refinement





Levels of Spatial Refinement

Refinement is unlimited, but practically we keep ~ 3-4 levels. Ratio of 3 required for invertibility

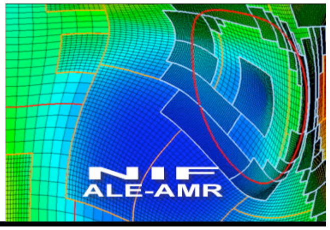


r = 2 r = 3

A $1{:}r^d$ logical correspondence between *both* cell and nodal quantities is only possible with *odd* refinement ratios.

This makes invertible pairs of operators simple to construct.

Use of SAMRAI Library yields a scalable code and hides details of MPI and optimization

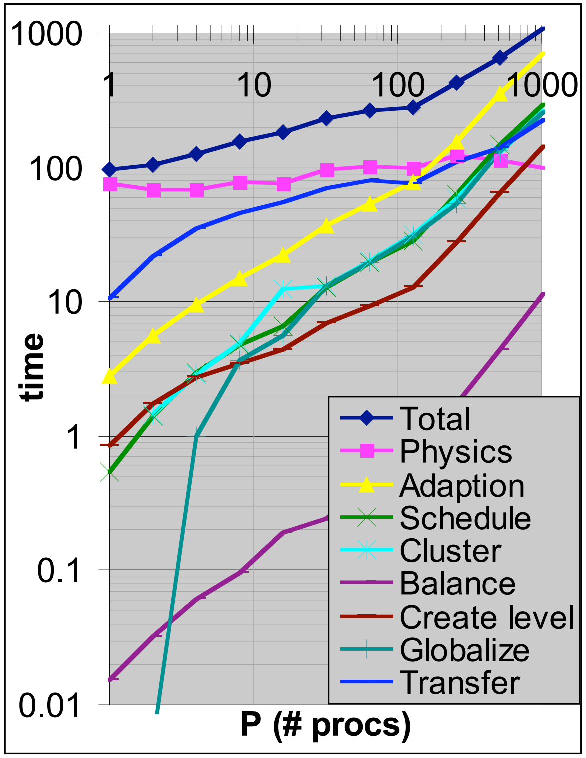


OLD Algorithm inefficiencies:

- **Acquiring/storing global mesh description**
- **Operations and loops on global meta data**

Many algorithms scaling like O(N).

All algorithms require global mesh description

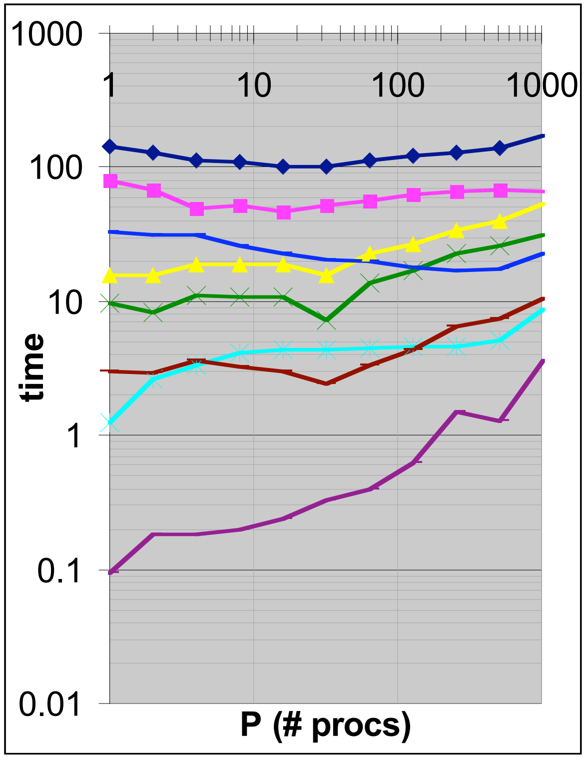


Most NEW algorithms scale close to ideal (N/P)

Rises in curves are due to

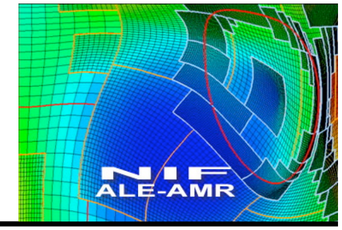
- **Initializing long arrays**
- **Sequentializing patch indices**

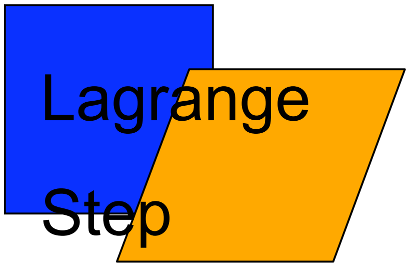
Physics scales really well -- so adding more physics tends to increase scalability

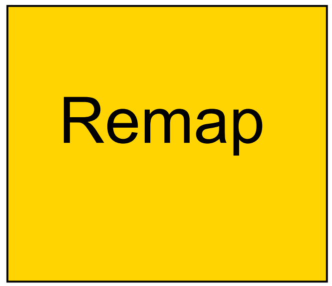


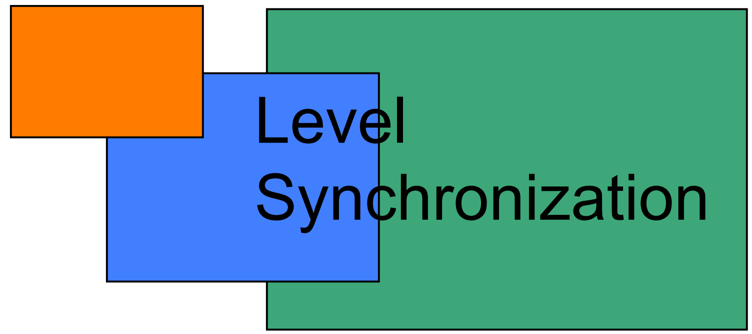
See e.g., Gunney, et. al., “Parallel Clustering Algorithms for Structured AMR”, J. Parallel and Distributed Computing, in press.

NIF's ALE-AMR has sub-scale physics and fragmentation models for anisotropic materials





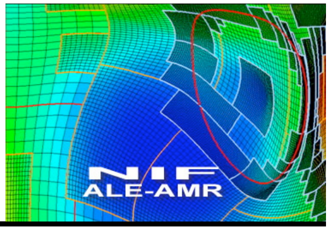




- **Advance all levels (Lagrangian)**
- **Determine new mesh configuration: Relaxed (ALE) or Original (Eulerian)**
- **Remap (Advection) to new mesh**
- **Synchronize levels and Coarsen/Refine (Regrid) as necessary**

- **Determine new volume fractions, evaluate stress, accelerations, material failure, etc. Weight by bulk modulus/shear modulus as needed. Important for e.g., problems with air/solid interfaces.**
- **Consider material topology in advection**
- **Reconstruct appropriate material interfaces during coarsening and refinement**

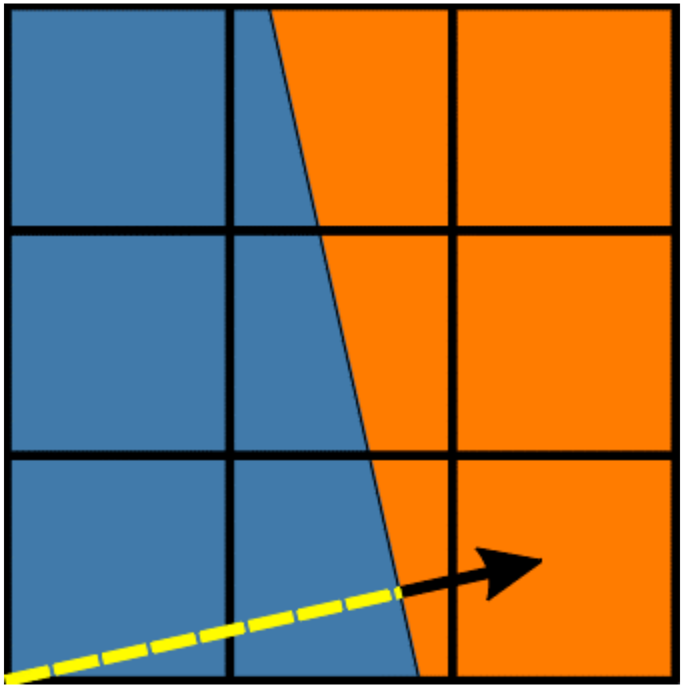
AMR: Coarsening is easy, Refinement requires explicit interface reconstruction



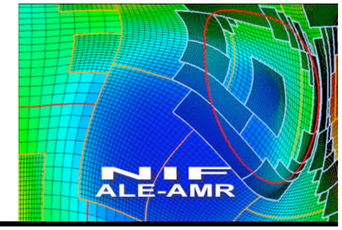
- **Sum of volume fractions**

$$V_f^c = \sum_i V_{f,i}^f V_i^f \Big/ \sum_i V_i^f$$

- **Orientation uses Vf ' s of neighboring cells**
- **Solve for location of interface**
- **Assign refined Vf ' s**

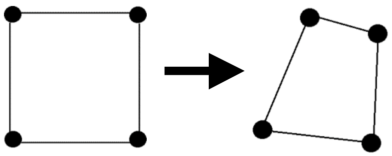


For details, see Masters, et al., IFSA Proceedings 2007.



Failure implementation can use a variety of models including Johnson - Cook

Deformation from Lagrange step



Compute Strain rates

$$\dot{\varepsilon}_{ij} = \frac{1}{2}\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right)$$

Compute Stress with Johnson-Cook Model

$$\sigma = [A + B(\varepsilon^p)^n][1 + C\ln(\dot{\varepsilon}^p)][1 - (\frac{T - T_{room}}{T_{melt} - T_{room}})]$$

Accumulate Damage with Johnson-Cook Failure Strain model

$$\varepsilon^f = [d_1 + d_2 e^{d_3\sigma^p/\sigma^e}][1 + d_4\ln(\dot{\varepsilon}^p)][1 + d_5(\frac{T - T_{room}}{T_{melt} - T_{room}})]$$

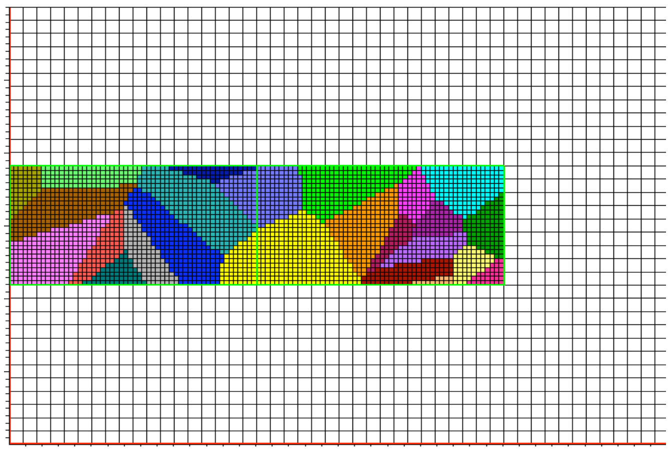
$$D = \sum \frac{\Delta\varepsilon^p}{\varepsilon^f}$$

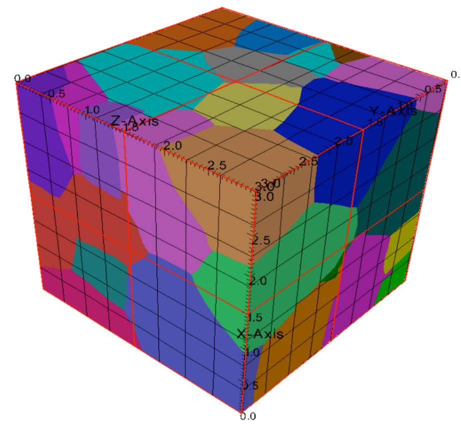
For D>1 material in cell fails

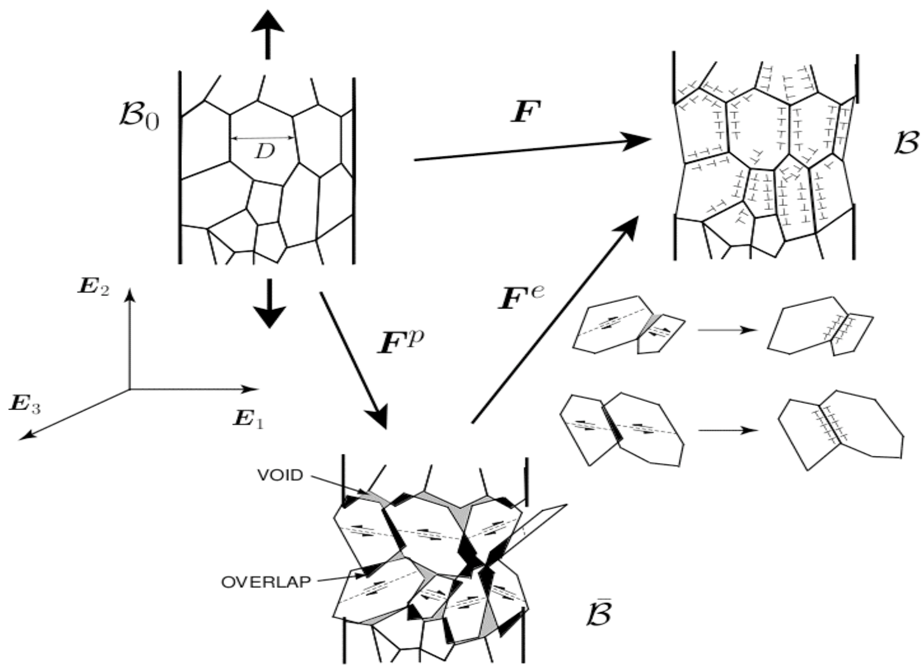
For details, see Fisher, et al., IFSA Proceedings 2007.

With AMR/HMM at finest scales we can introduce anisotropic models like single and polycrystals

Polycrystal Model on bar test problem with AMR mesh



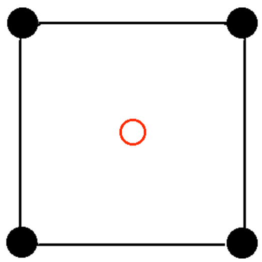




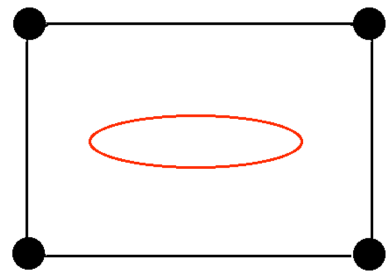
- **Voronoi method to generate polycrystals within AMR infrastructur is implemented**
  - **Set up the voronoi polycrystals a the finest level.**
  - **Johnson-Cook model is run at levels 0 and 1 and the Single Crystal Plasticity is at level 2.**

Part of the failure model allows fragment formation

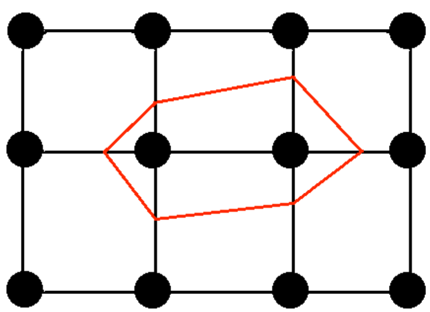
Upon failure a small volume fraction of void is introduced into the cell



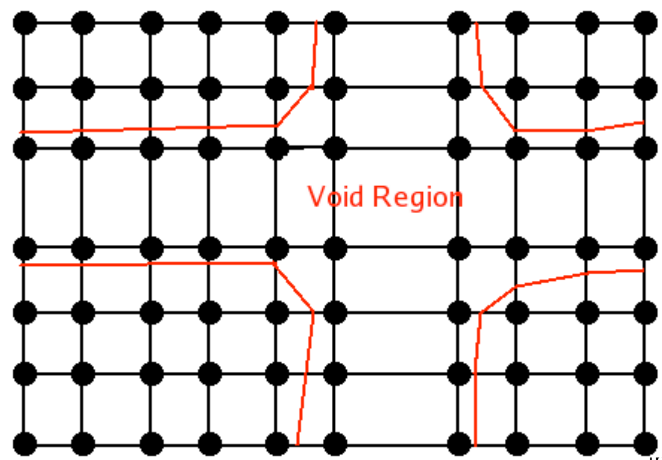
If the cell continues to grow the void enlarges to meet that growth



Volume fraction interface reconstruction allows voids to coalesce to form cracks



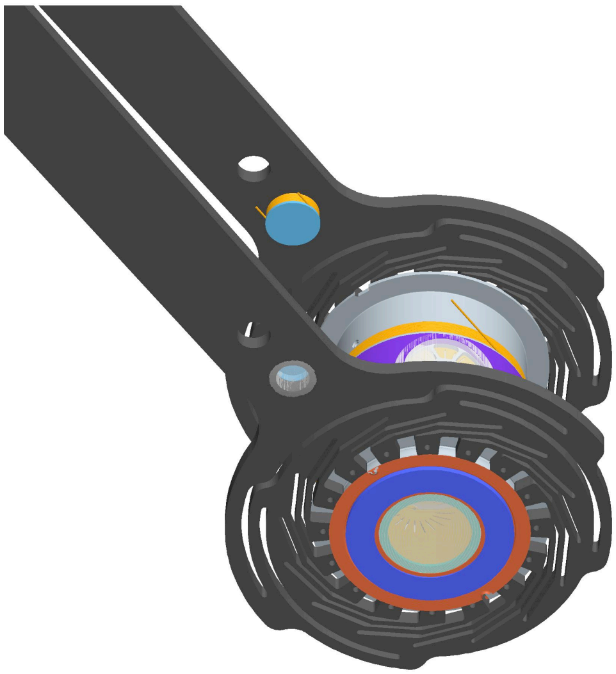
Cracks can grow large enough to span across cells allowing fragment formation

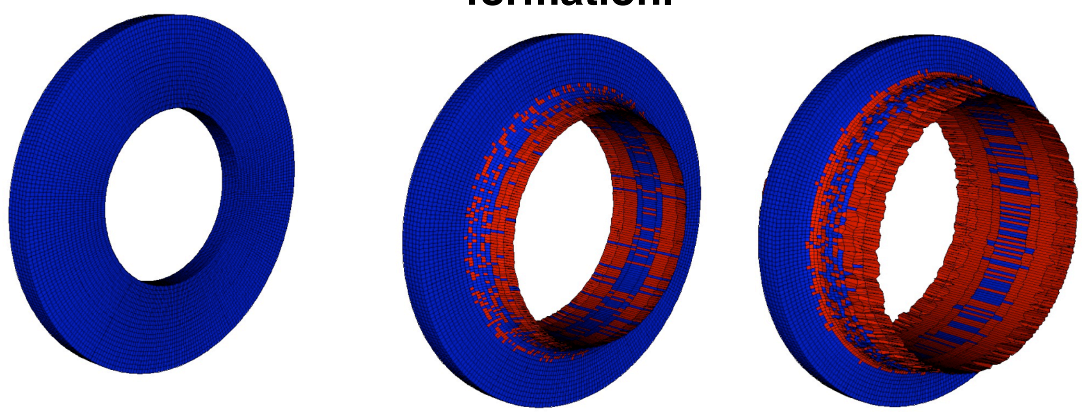


All calculations should include the entire target structure, focus is outside the hohlraum

Johnson-Cook model fragment size prediction of NIF target cooling rings

Low resolution scoping simulation shows direction of fragment blow off. High resolution simulation on next slide shows fragment formation.





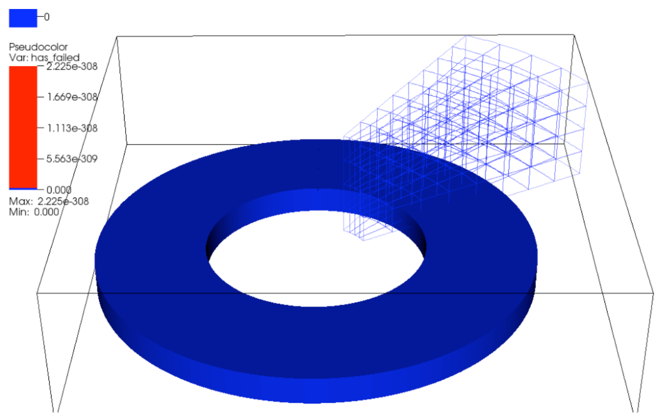
t = 0 μs | **t = 0.5 μs** | **t = 1 μs**

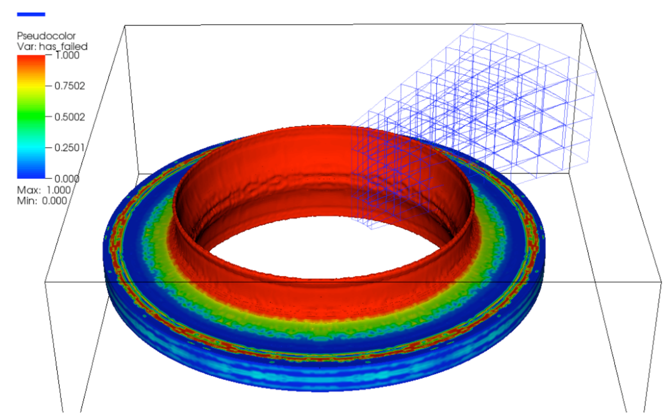
Target

R_{inner} = 2 mm
R_{outer} = 4 mm
Width = 0.5 mm

Red indicates failure

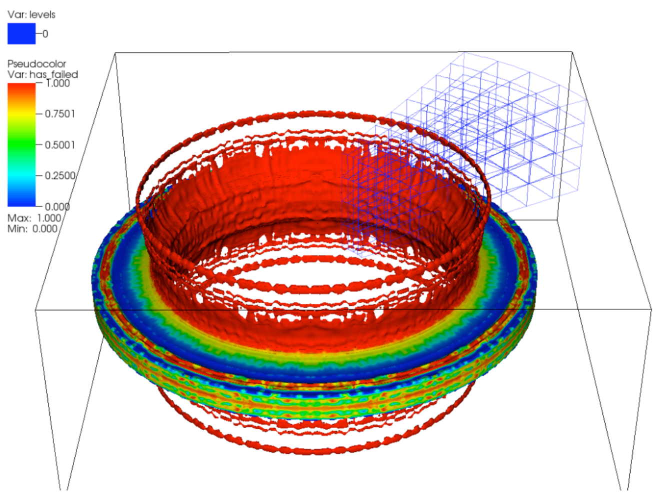
Cooling Ring Fragmentation Simulation shows spall-ring formation and predicts fragment size

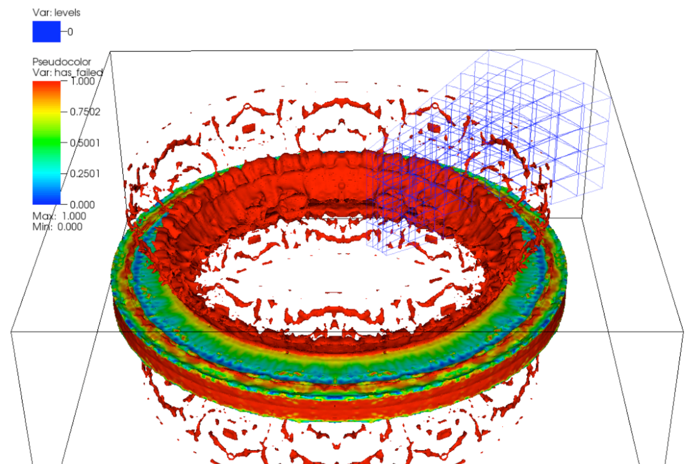




Blue boxes show computational domain and initial parallel processor decomposition (128 Procs) -- one domain per cube

Color Bar denotes percentage of failure in a zone: blue -- no failure, red: zone completely failed





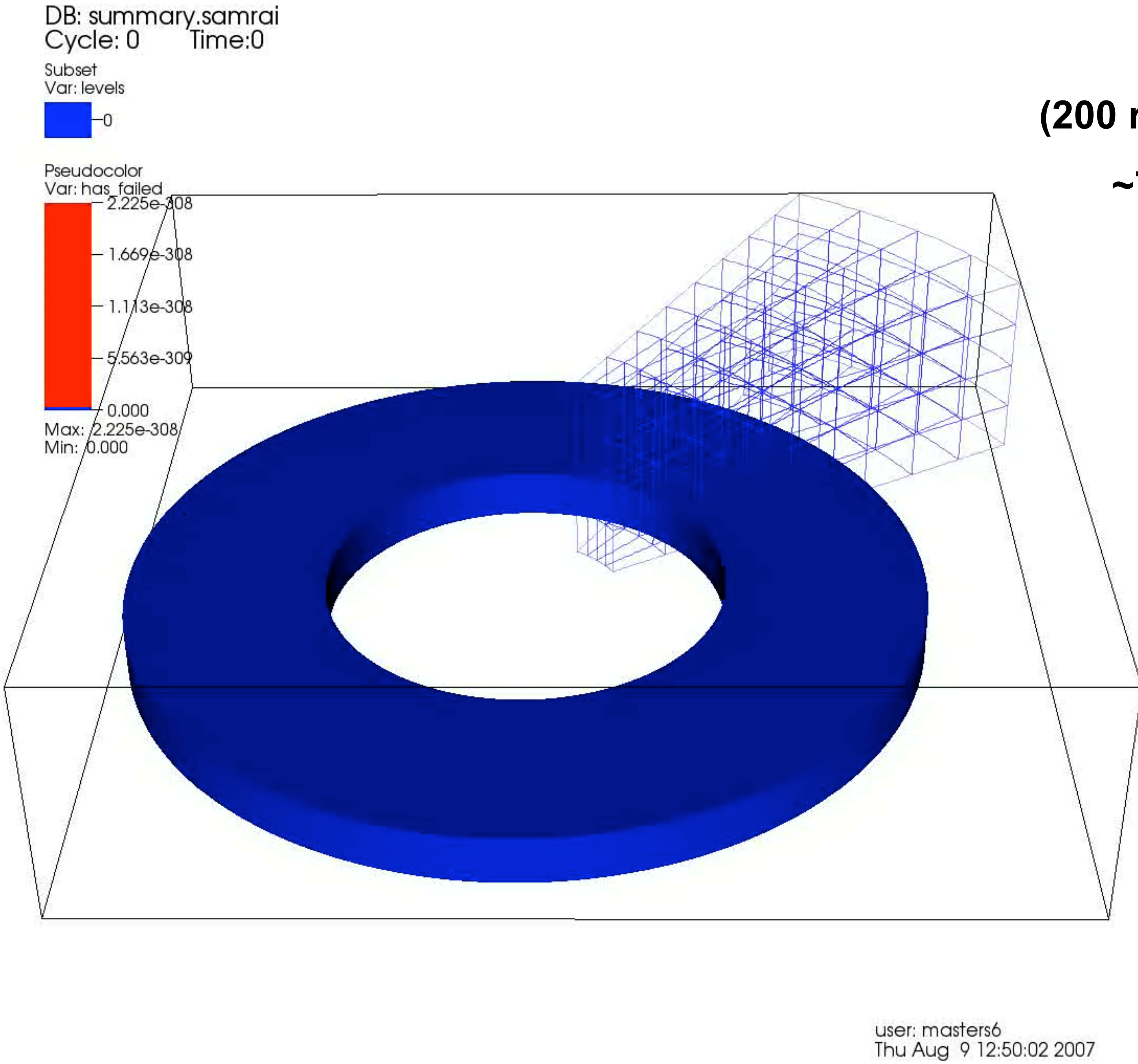
The ring disintegrates into spall planes or rings that disperse along the hohlraum axis. Because the zones have failed, the fragments get smaller as they propagate outward. No large chunks are formed -- contrast with upcoming copper notch simulation on upcoming slides.

128 Procs

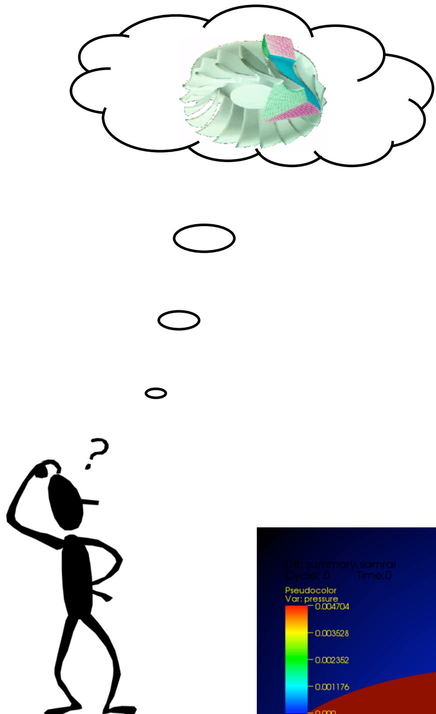
960,000 zones

(200 radial, 60 theta, 80 z)

~7500 zones/proc



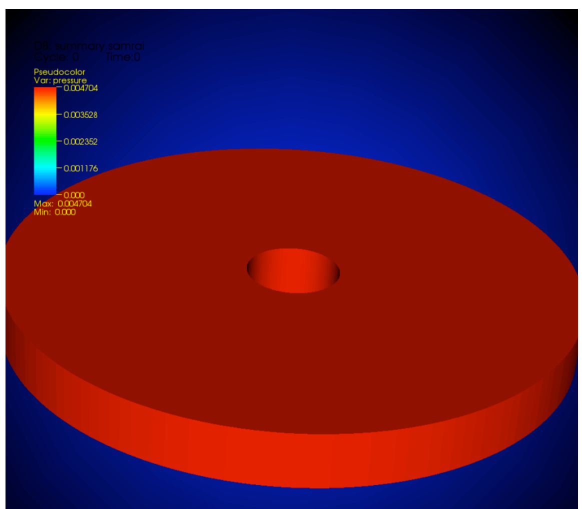
Problem: Copper cooling rings causing damage on Omega



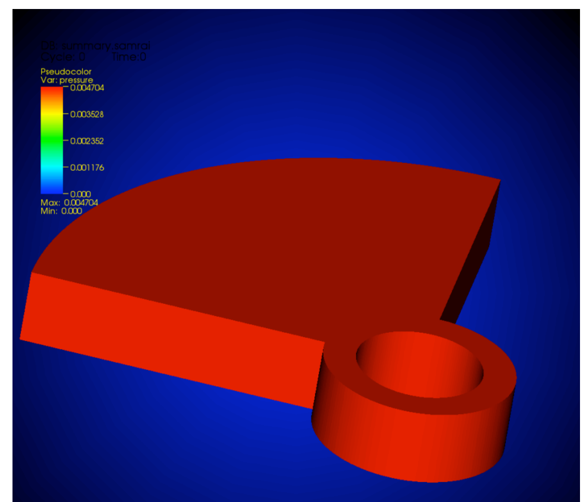
Full Ring and Notched Ring Designs

Possibly more damage with Notched Ring

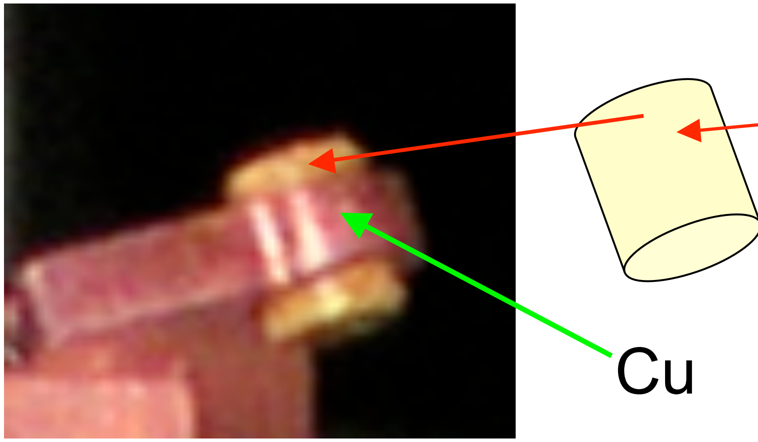
Explanation: Simulation



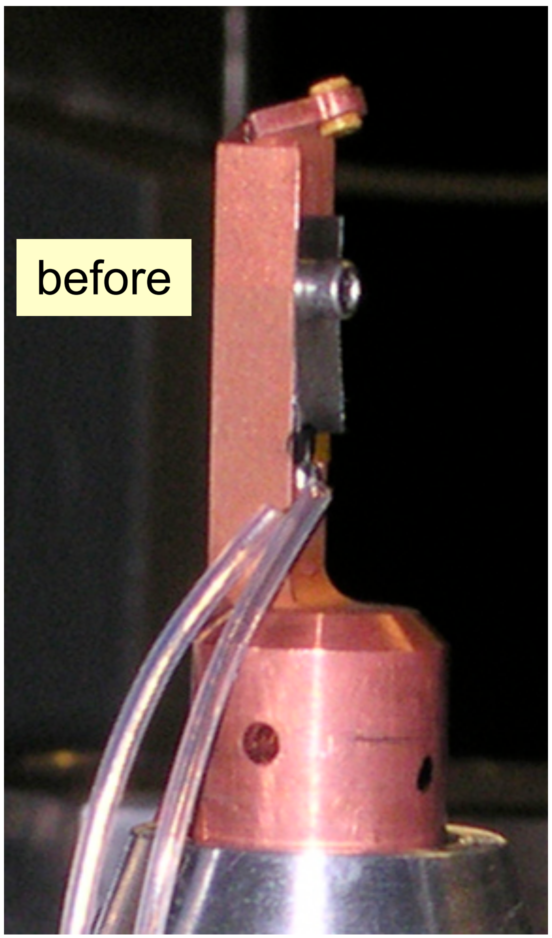
Full Ring



Notched Ring



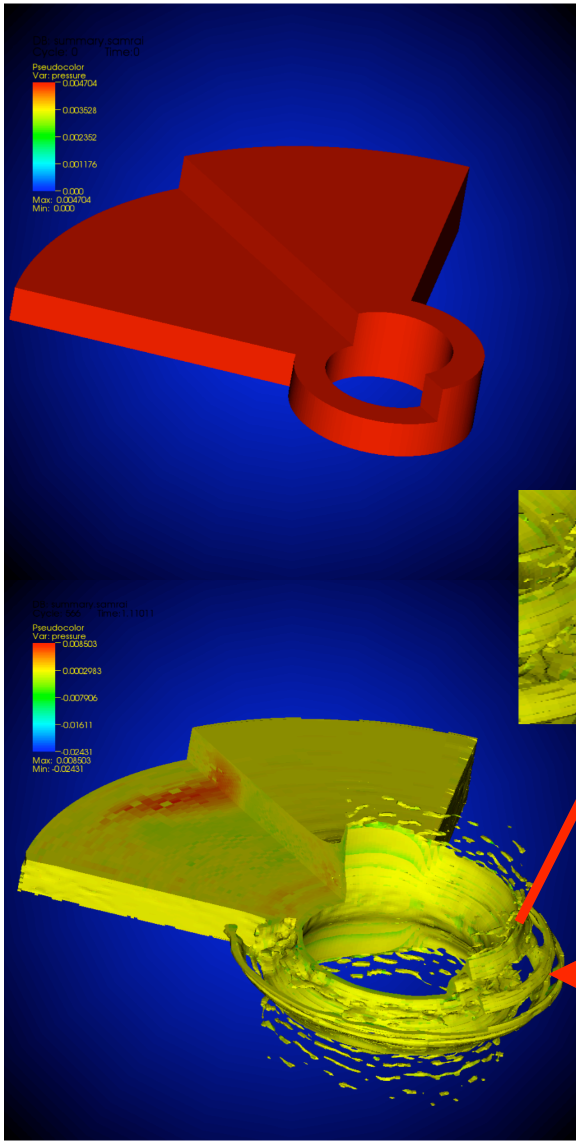
Hohlraum surrounded by Cu notched cooling ring structure rendered 10 debris shields inoperable on Omega.

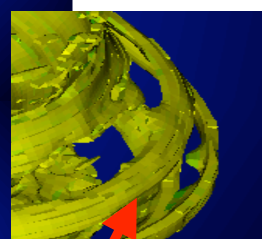


- 10 debris shields were damaged to the point that the scattered light caused them to fail transmission specifications
- 1 of these debris shields, 5 mm thick, had a chip that went through the entire thickness
- loss in transmission from these 3 shots was on average 3% over all 60 debris shields
- To put this in perspective we normally see ~6% loss over a full month

Simulations explain why this was not a good solution to debris problem.

Simulation explains that notched ring breaks into larger pieces instead of small spall planes/rings

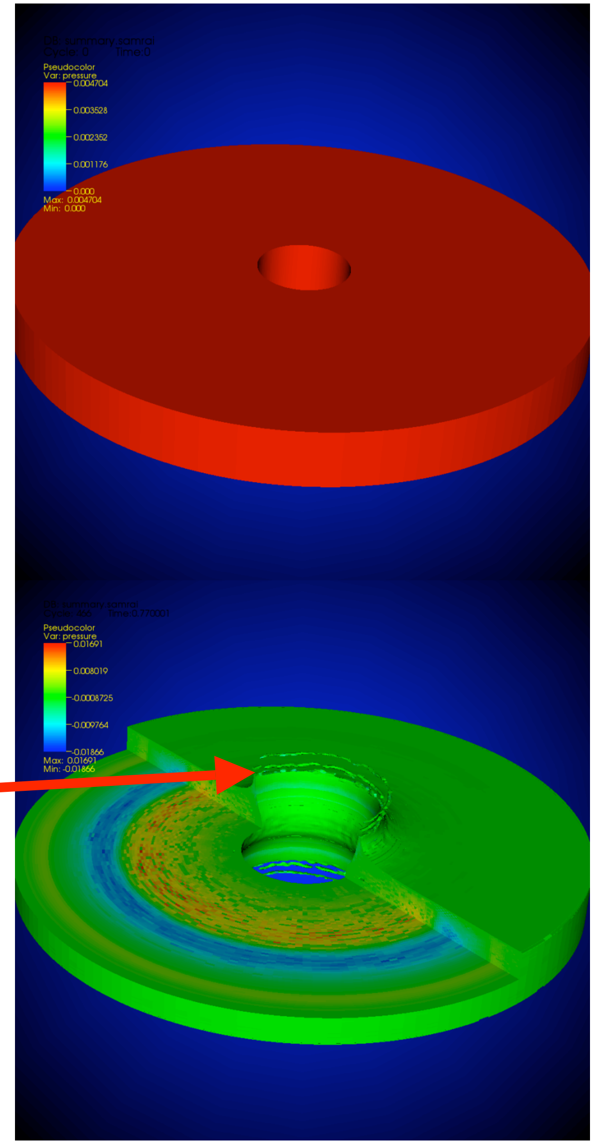




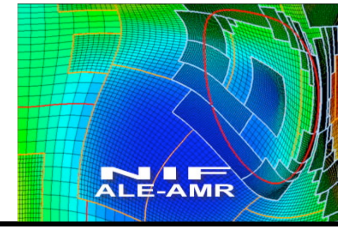
Note: "step" in target is not physical -- just to show interior of simulation.

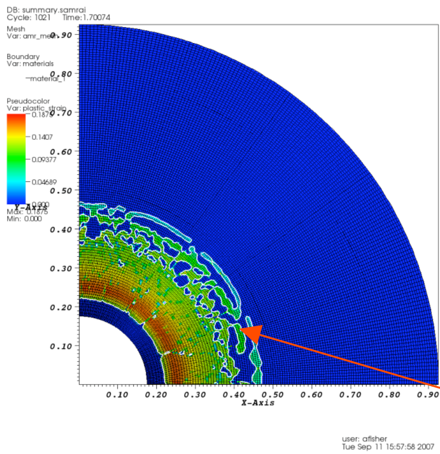
FORMATION OF SMALL SPALL PLANES

FORMATION OF LARGE DAMAGING PIECES IN THIS REGION



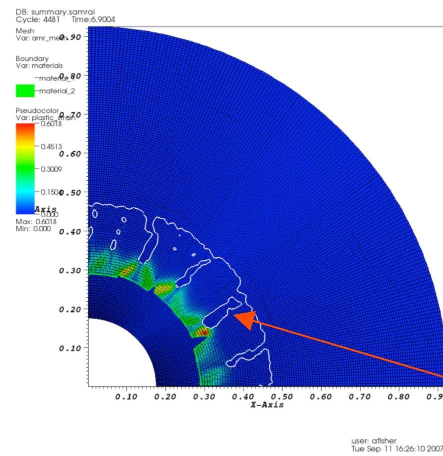
Verification involves comparison with LS-DYNA. Different loading yields different behaviors.





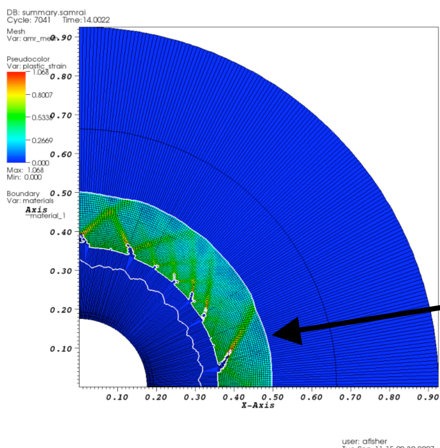
- ALE-AMR
- Eulerian
- impulsive loading
- w/ tensile failure
- mix fracture

Due to impulsive loading

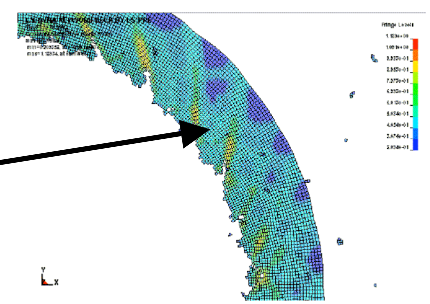


- ALE-AMR
- Eulerian
- pressure loading
- w/ tensile failure
- mix fracture

Tensile failures



- ALE-AMR
- Lagrangian
- pressure loading
- no tensile failure
- cell fracture



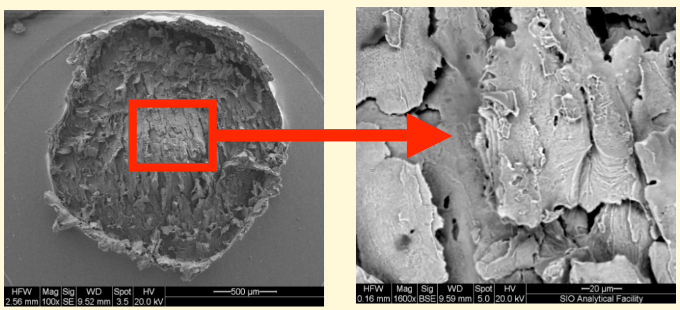
- LS-DYNA
- Lagrangian
- pressure loading
- no tensile failure
- cell fracture

Pressurized void loading (less impulsive) gives a good match to LS-DYNA.

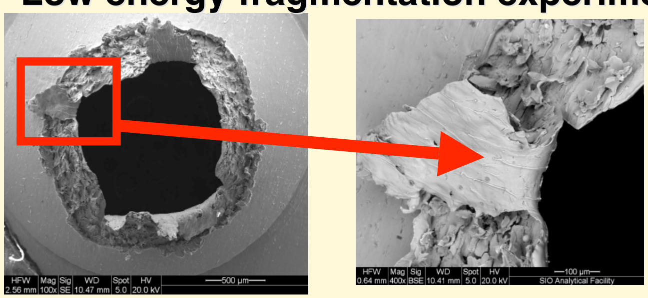
ICF experiment is a more impulsive load from the expanding hohlraum.

Analysis of dedicated laser fragmentation experiments on Janus is in progress

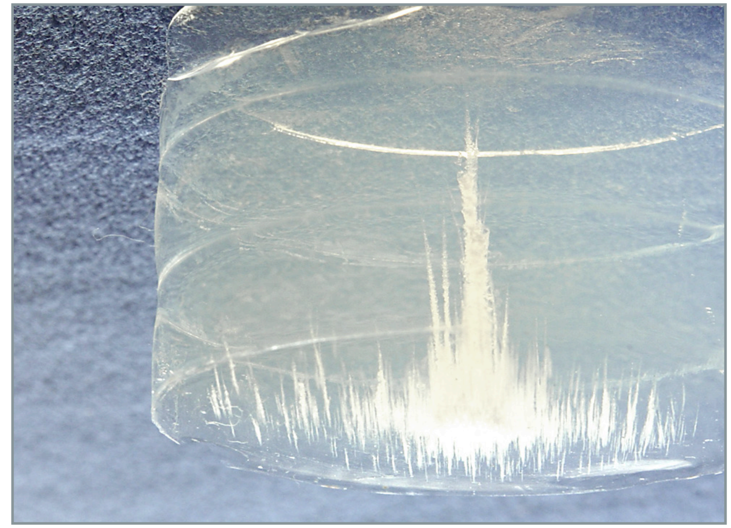
Since targets are small (~1 cm), size scale of targets is within a few orders of magnitude of the microstructure (grain sizes ~ 10 microns)

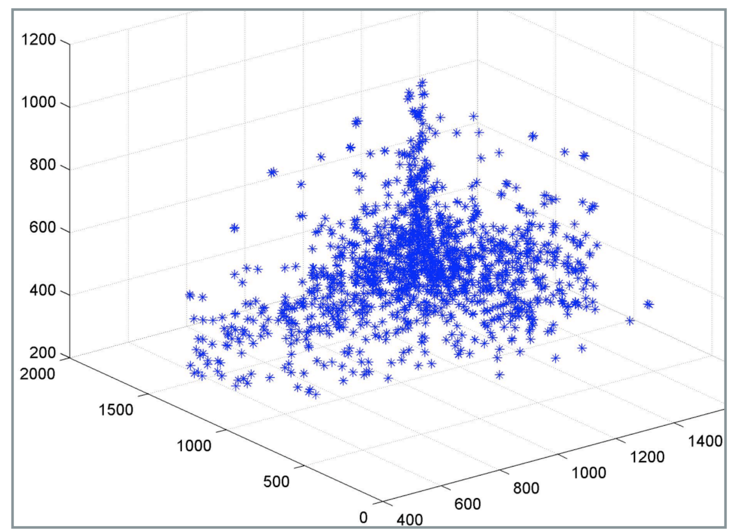


Low energy fragmentation experiment



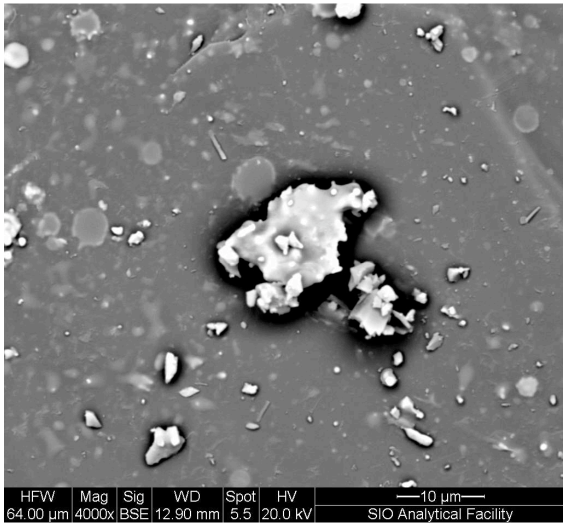
High energy fragmentation experiment

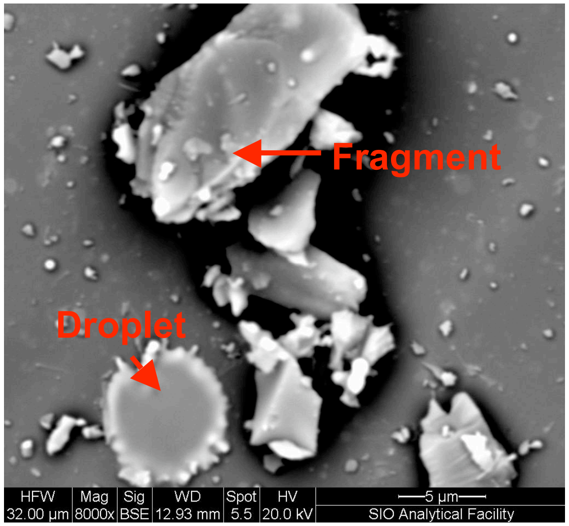


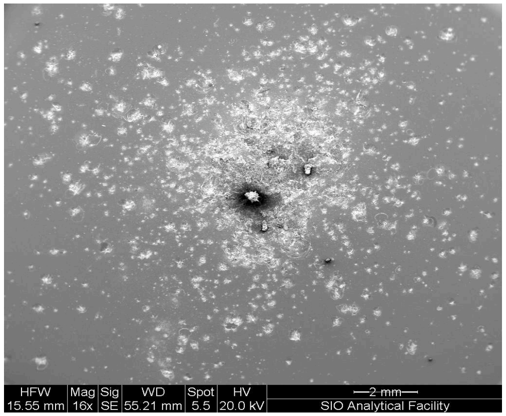


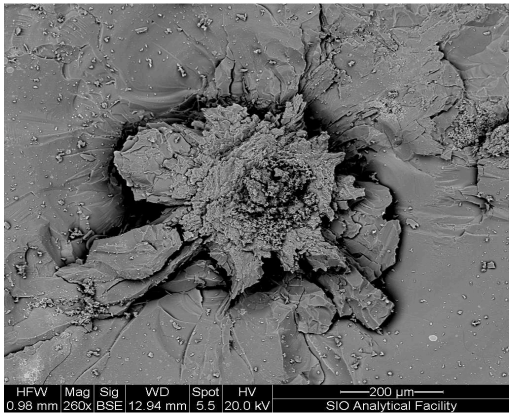
The scale of targets provides a unique test bed for multi-scale simulations

Janus shots on glass are analyzed to distinguish fragments and liquid debris







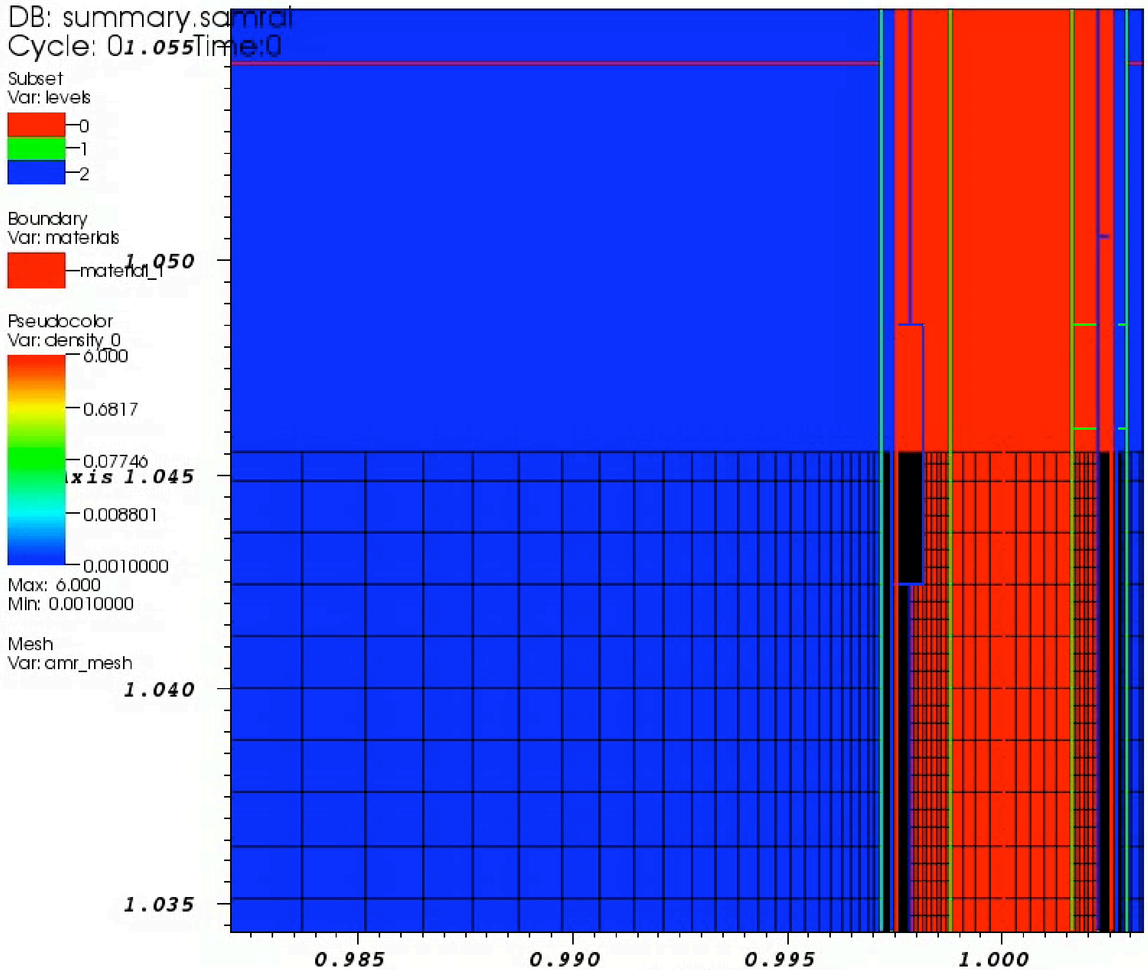


Validation includes predicting state from glass (liquid/solid) as well as statistical comparison of fragment sizes and velocities from aerogel collection

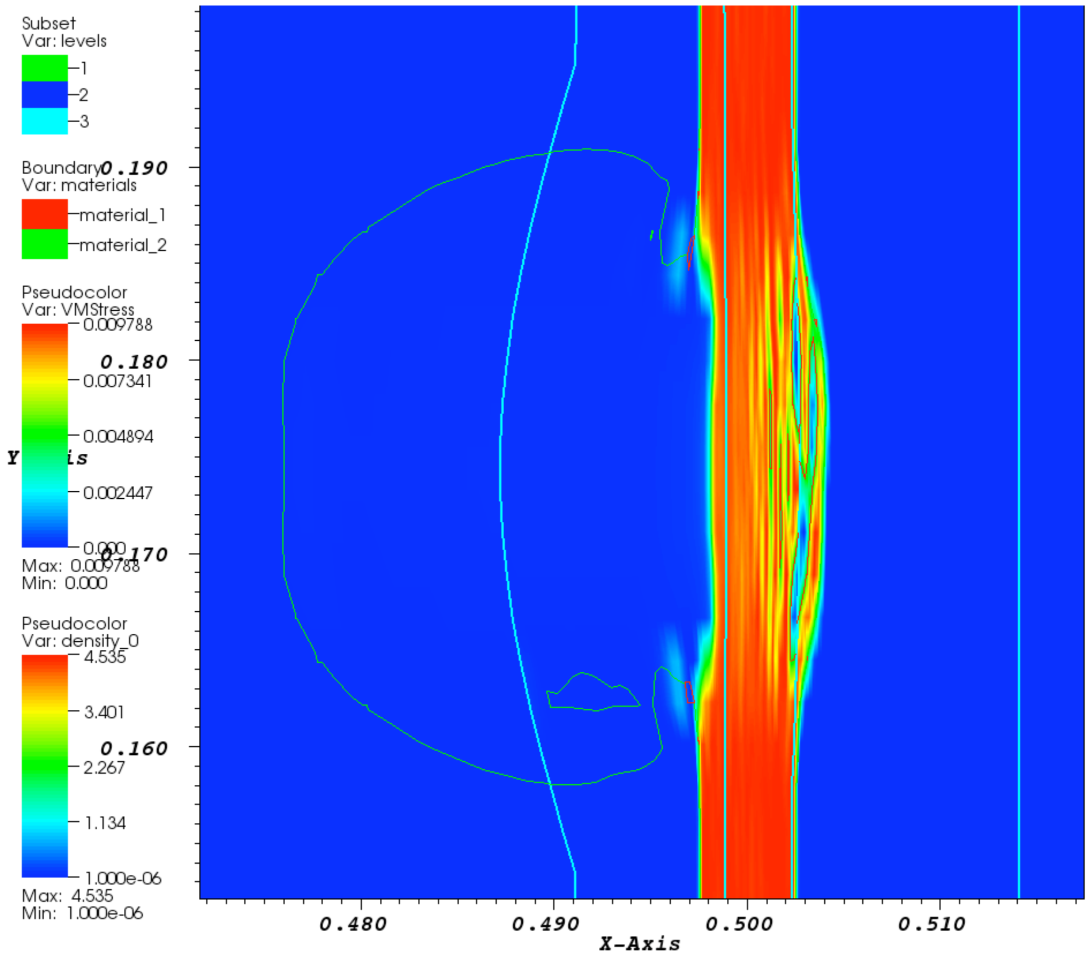
Upcoming Janus shots will have specially-made large single crystal vanadium to vary input to crystal plasticity model

Thin plate problem shows levels of refinement

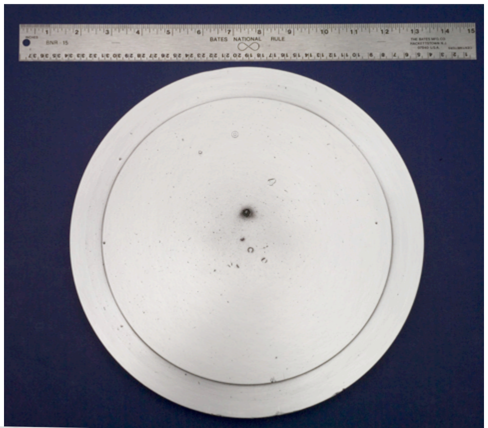
- **Shooting very thin foils puts us close to the microstructural level.**
- **Problem is taxing for any code. Ability to run both Lagrangian and adaptively meshing Eulerian is critical**

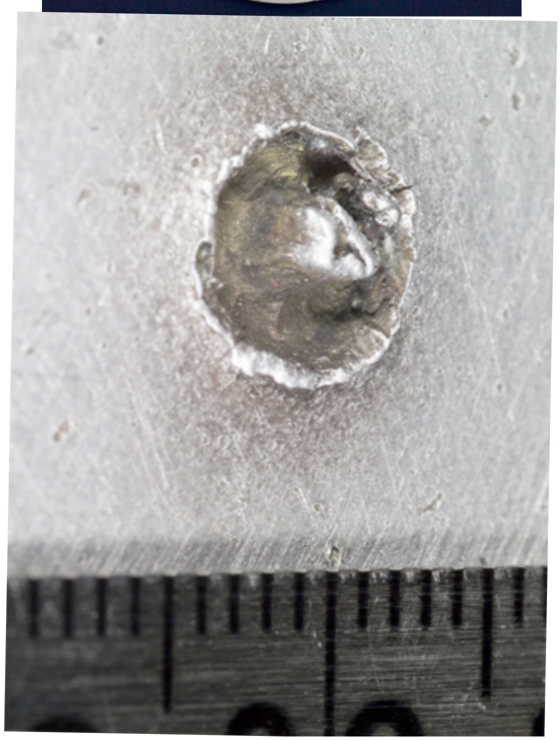


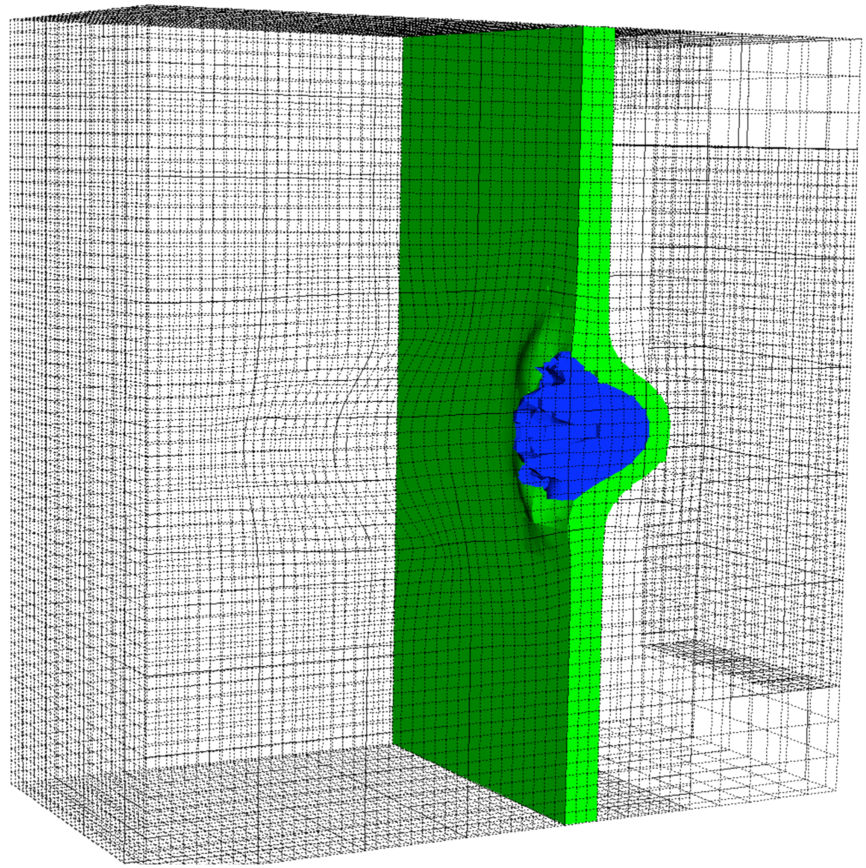
Simulations shows spall off back plane that creates fragments for experimental validation



Impact damage simulations were done to validate interface reconstruction and physics

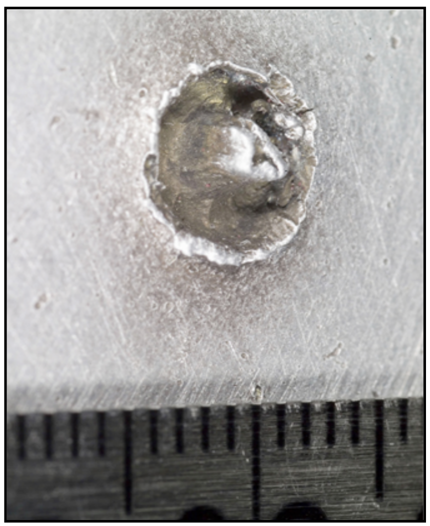


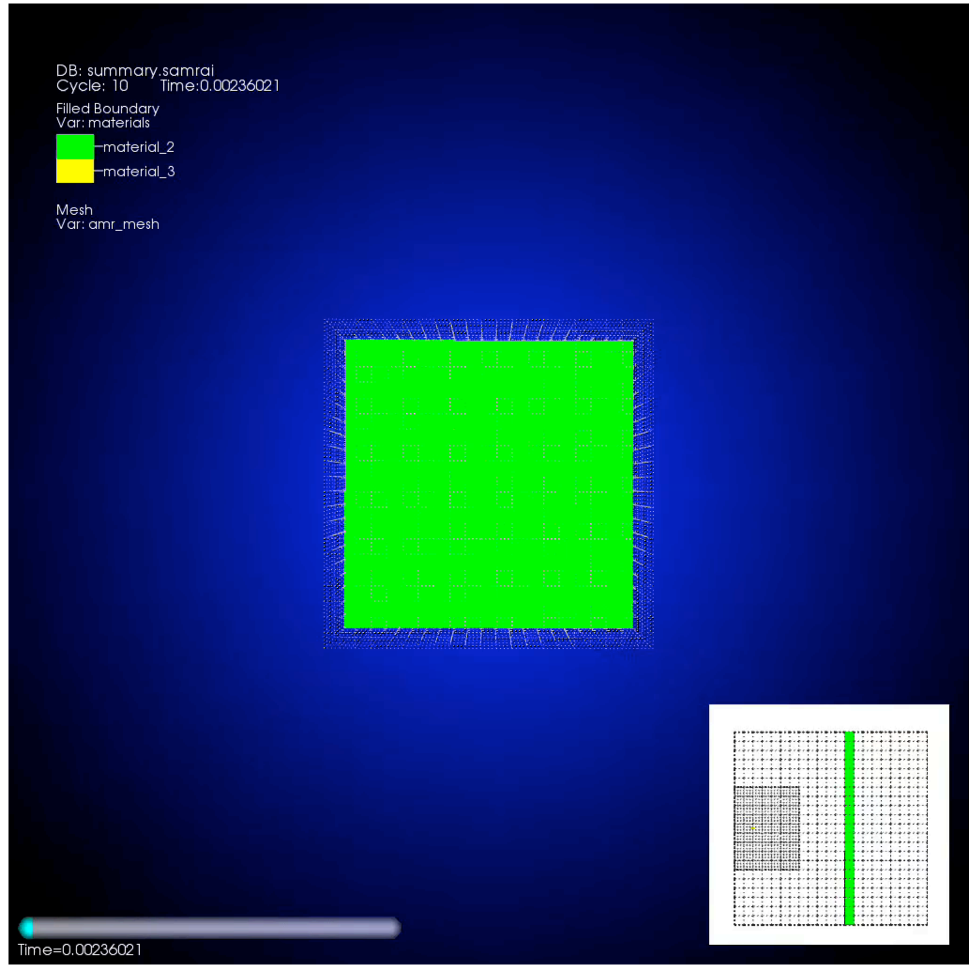




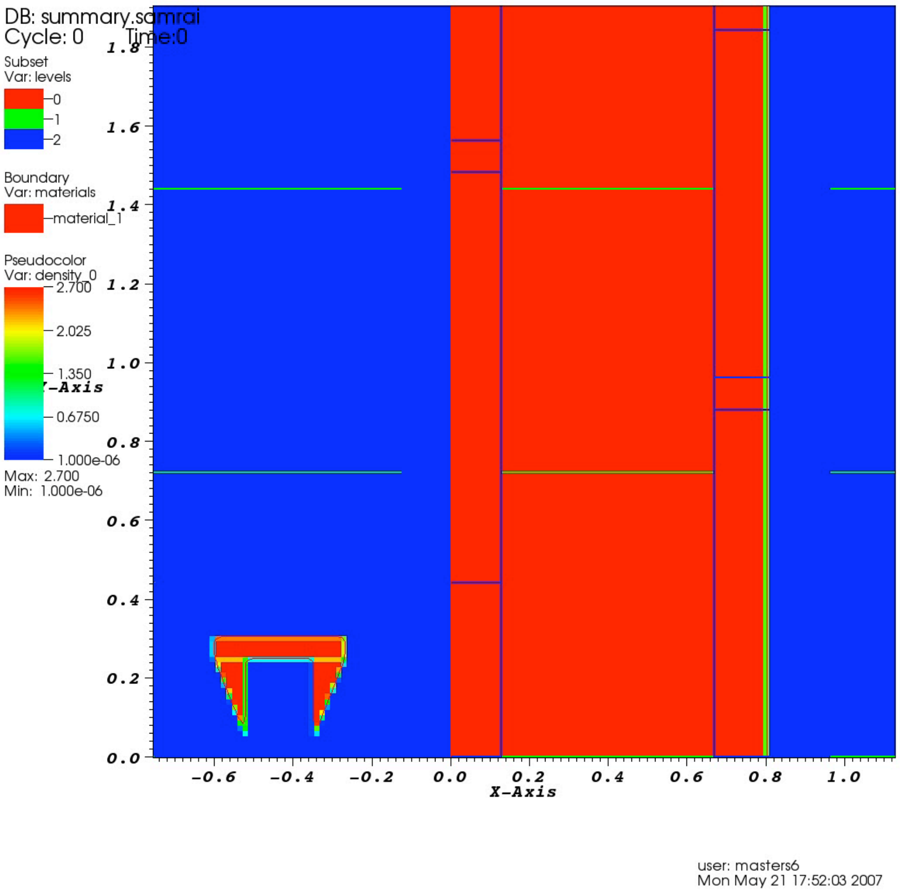
Simulation of OMEGA flapper plate damage

Early Movie of projectile simulation

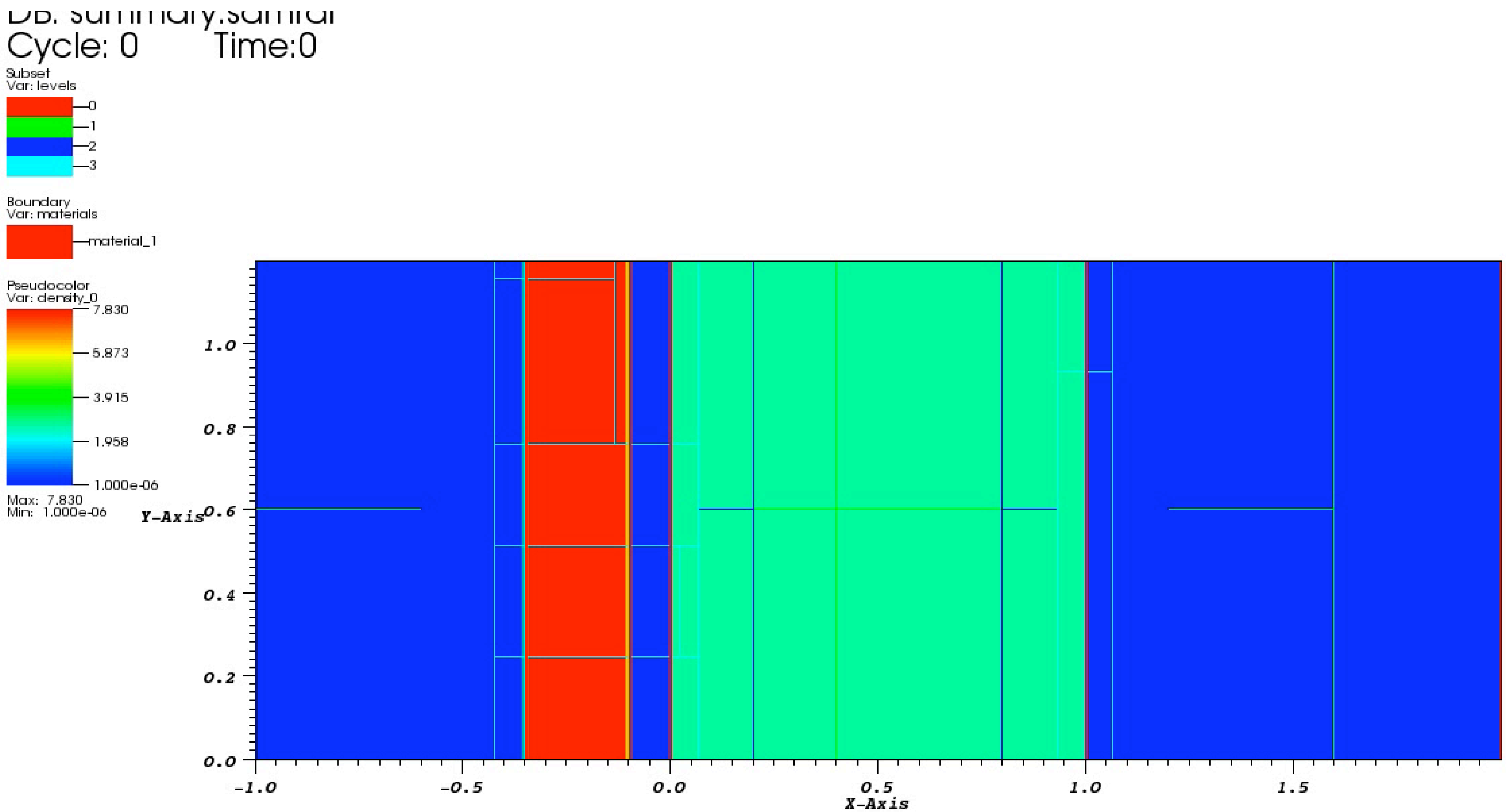




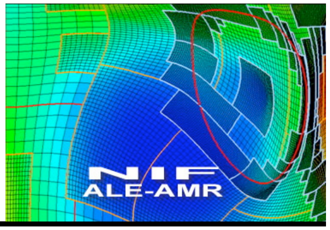
Object (halfraum) launched towards a steel plate shows fragment formation -- first simulation with fragmentation model



Flyer Plate three material simulation



Team Development Approach: text messaging allows modern developers to work together



- **Text messaging takes over**
  - **Probably single most-used resource in cutting development time**

Example chat dialogue was shown in talk.

Chat Room Security

•LLNL internal chat does not work from offsite unless you set up an SSH tunnel to the server.
•Not all rooms are "public"; a user must be invited before they can successfully join a room.
•There may be more rooms in existence than what you see: rooms may be defined to be invisible.

Summary

- We have developed a new code for analysis of NIF chamber debris and shrapnel
- NIF ALE-AMR uses a combination of Arbitrary Lagrangian Eulerian algorithms and Adaptive Mesh Refinement
- AMR allows us to use different material models at different levels -- in progress
- Most issues related to implementing interface reconstruction and fragmentation models have been resolved
- We are continuing testing/verification/validation, while doing calculations for upcoming NIF shots

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