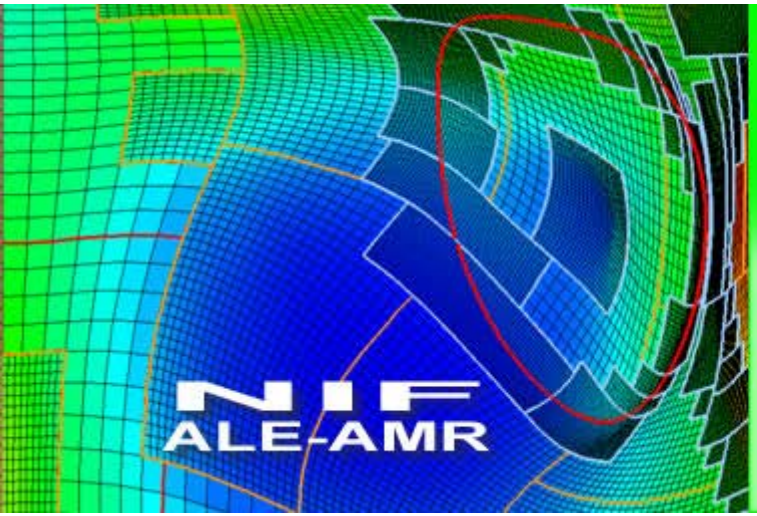


The Development of a New Predictive Simulation Code

Alice Koniges

Lawrence Livermore National Laboratory

Salishan Conference on High Speed Computing:

Confidence in HPC Predictive Simulations

April 23 - 26, 2007

Gleneden Beach, Oregon

This work was performed under the auspices of the U.S. Department of Energy by the University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

UCRL-PRES-230114

Acknowledgments

NIF-ALE-AMR Development Team:

Robert Anderson, David Benson,[1] Parag Dixit,[1] Aaron Fisher,

Brian Gunney, Tom Kaiser, Alice Koniges, Nathan Masters

LLNL V&V Tools

Tapestry: Shawn Dawson

Validation Experiments:

Jim Andrew, David Eder, Dan Kalantar, Mike Tobin

Data Analysis:

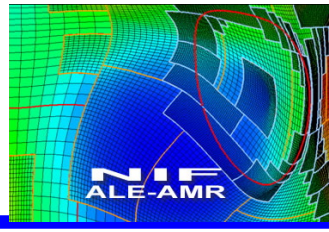
William Brown, Marc Meyers,[1] H. Jarmakani[1]

Visualization:

Betsy Foote

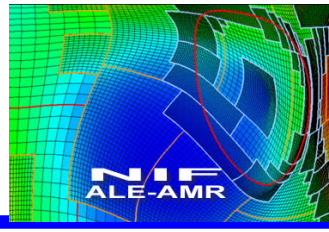
[1] University of CA, San Diego

OUTLINE



- New frontiers in application codes
  - NIF-ALE-AMR and what we need to predict
- Team development methods
- Tools and methods for verification
- Is the science right?
  - Designing experiments for validation

Advances in computer architecture and algorithms are exposing new simulation areas

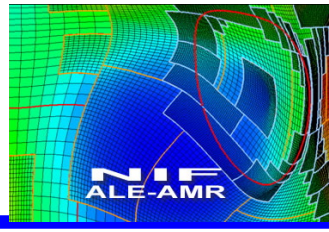


- **Realistic simulations of biological processes and biological systems from diseases and components like the heart to full-body simulations**
- **Packaging, design and manufacturing studies for optimizing industrial engineering**
- **Applied nanoscience up to mesoscale for the complete design of multicomponent electronic systems**
- **New simulation code NIF-ALE-AMR falls in this category. It is an area previously modeled with phenomological data and experimental intuition**

Prediction: the new “grand challenges” will include simulating non-traditional (and sometimes “everyday”) phenomena, not just the traditional simulation areas like climate, fusion, combustion, turbulence, etc.

3D with no 2D analogue

A new arena for predictive simulations in high-powered laser systems

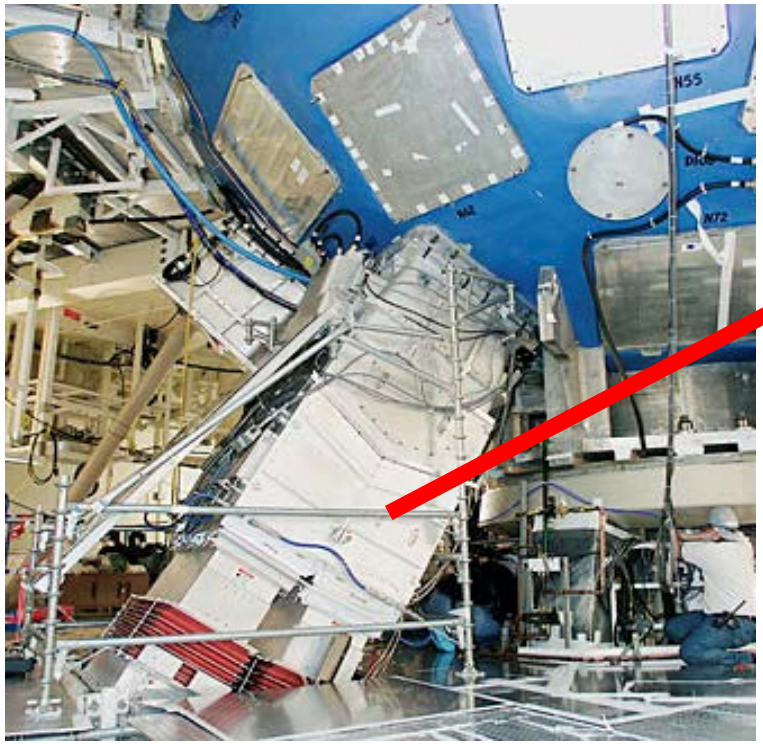


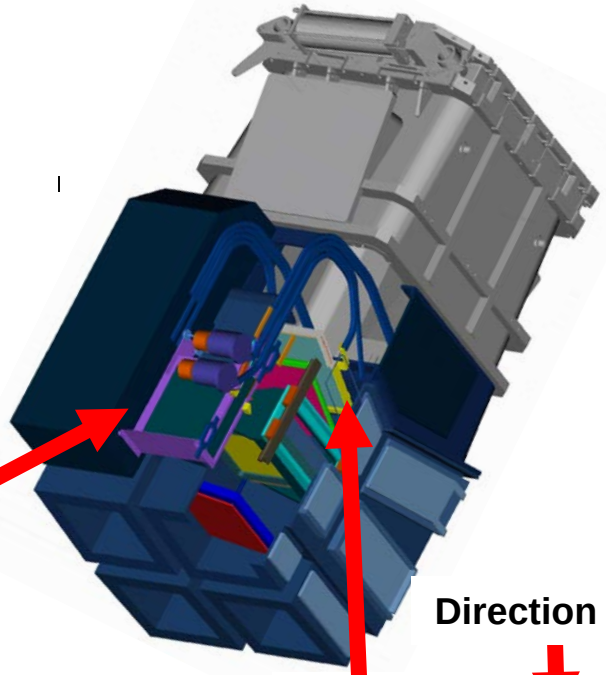
NIF
Early Light
4 Beam
Experiments

"1/2 NIF"
Or 96 beams
Starting
Next summer

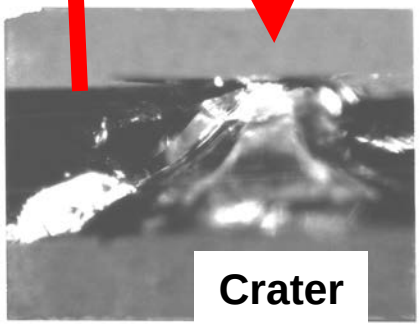
Goal: Protection of Optics and Diagnostics

Debris Shields as Main Line Defense



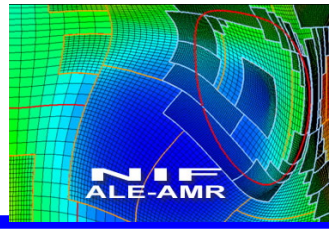


Direction of Impact

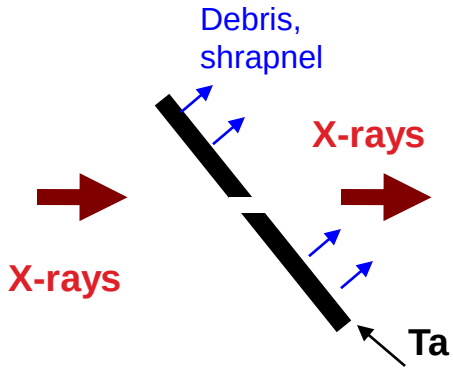


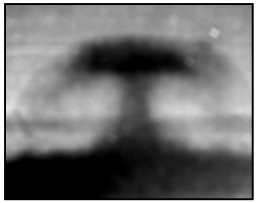
1.1 mm

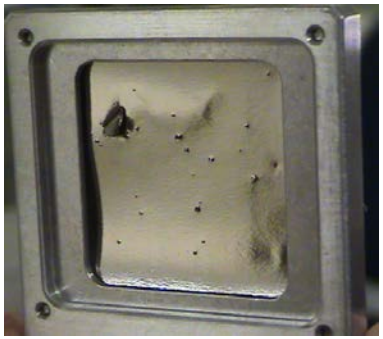
Numerical simulations show how to mitigate damage from debris and shrapnel



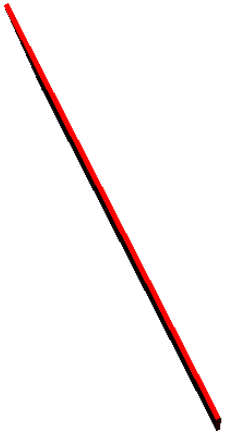
NIF Early Light Diagnostic Damage

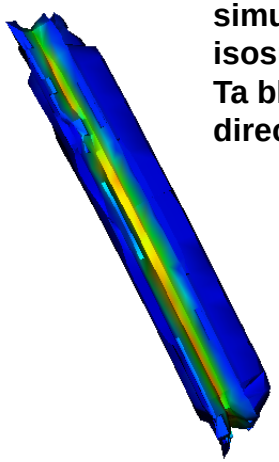




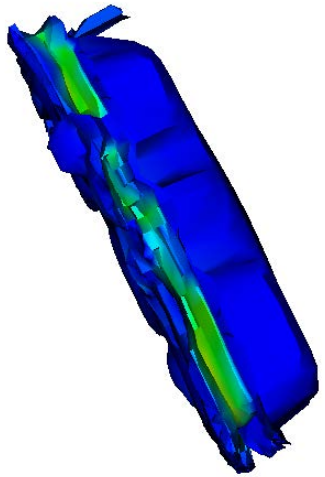


Damage prior to tilting pinhole substrate



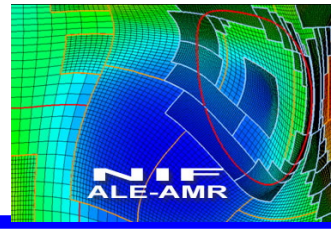


Time progression of 3D foil simulation (density isosurfaces) shows Ta blow-off in normal direction

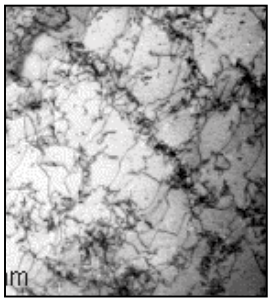


Tilted pinhole directs debris and shrapnel away from diagnostic filter. Tilt concept (Eder) & Omega experiments (Robey, Blue, et al.)

Predictive capability includes multi-scale model with adaptive mesh refinement

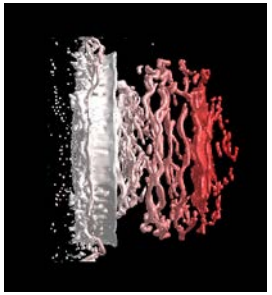


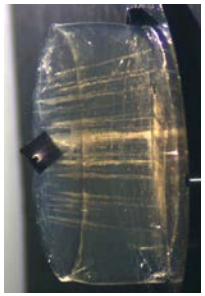
Dedicated Experimental Validation



Initial characterization of thin tantalum pinhole

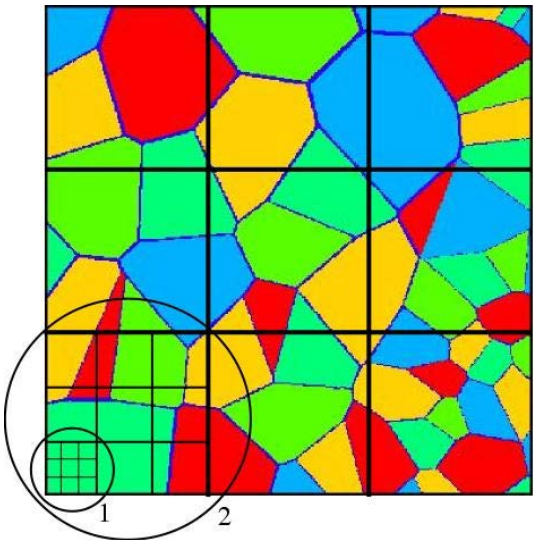
Laser Input



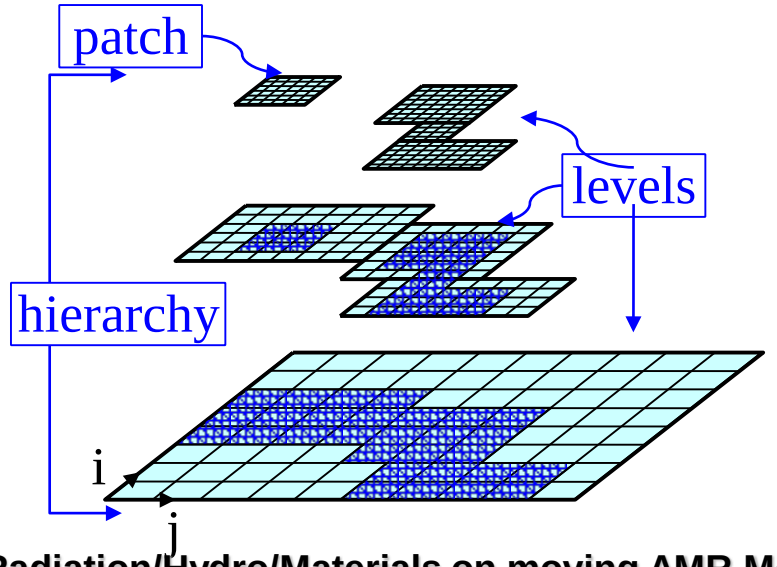


Recovery experiment -- fragments captured in aerogel

Residual characterization to show grain structure

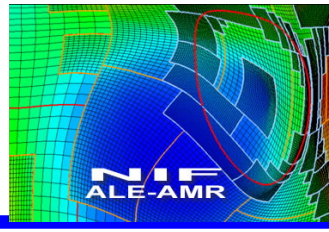


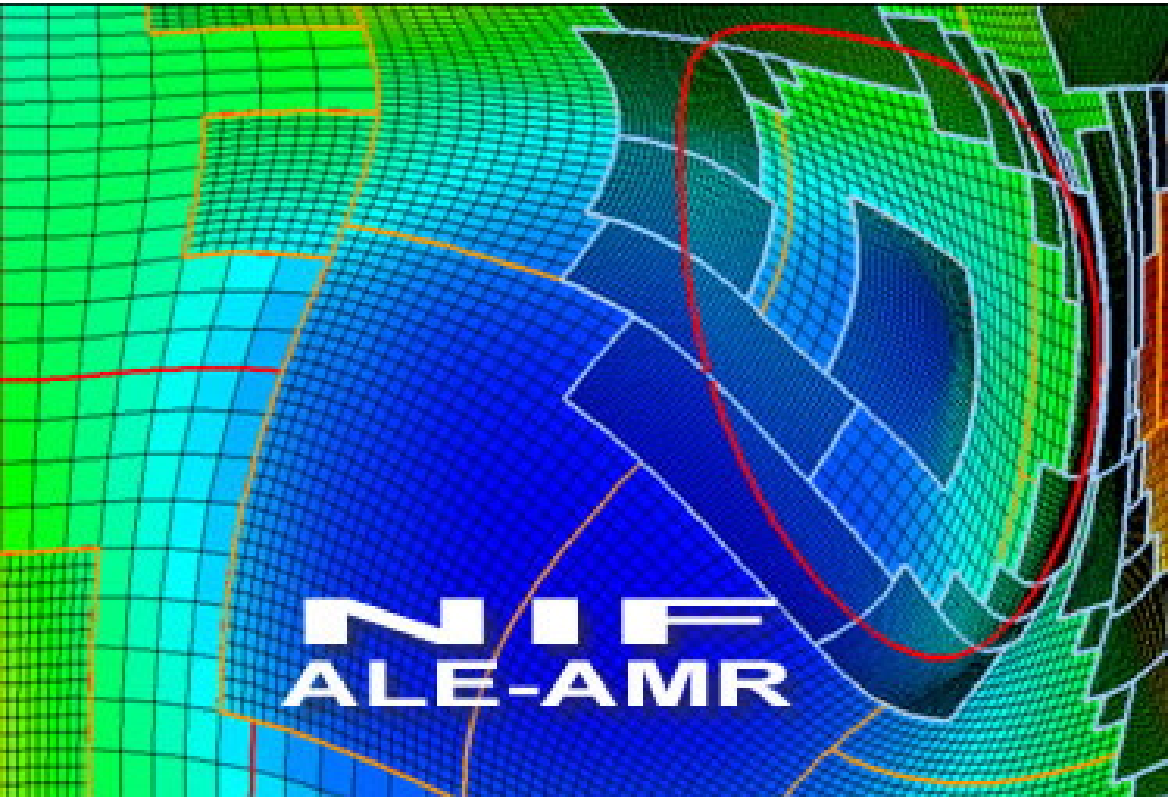
Multiscale Hierarchical Material Model (HMM)

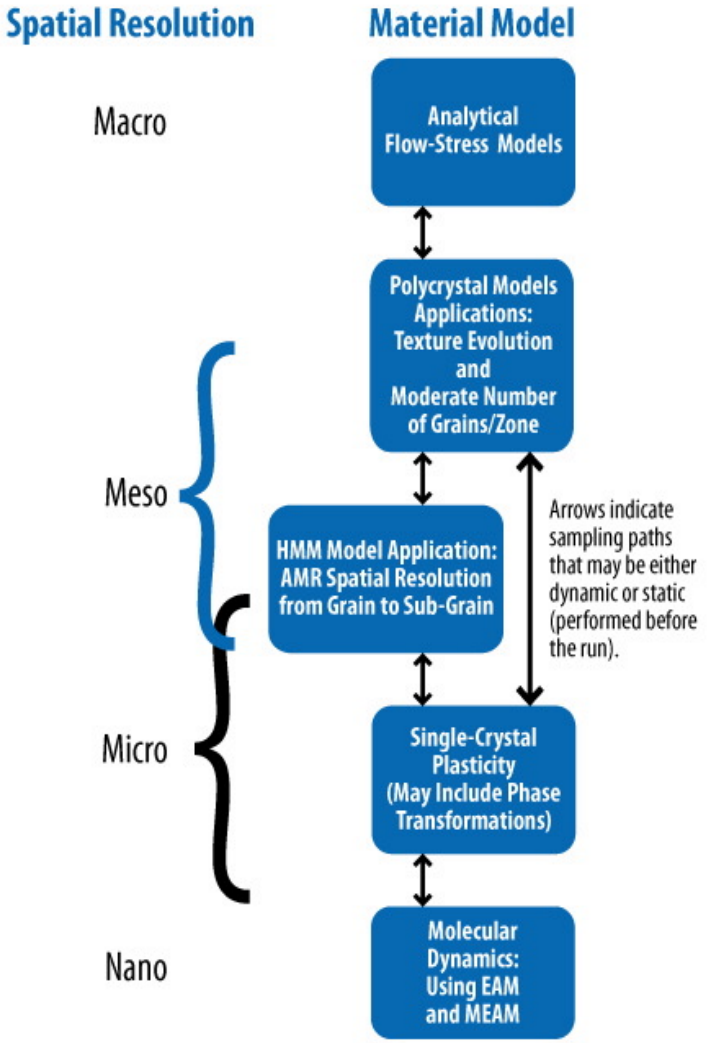


Radiation/Hydro/Materials on moving AMR Mesh

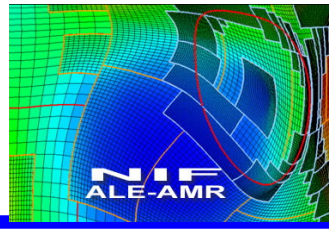
We use an adaptive and moving mesh, allowing different models at different levels (multiscale)





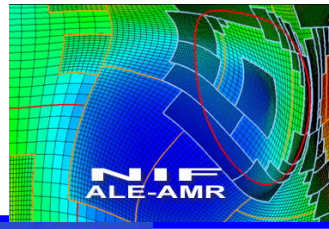


OUTLINE



- New frontiers in scientific application codes
  - NIF-ALE-AMR and what we need to predict
- Team development methods
- Tools and methods for verification
- Is the science right?
  - Designing experiments for validation
- Thoughts on the future needs of validation studies

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



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

(13:15:31) coder1: I added that support to the command language (Commandfile.C)
(13:15:51) cleverguy: You didn't touch the Strength class though, did you?
(13:15:57) coder1: No
(13:17:45) cleverguy: I enabled strength for thinplate, and it took much much longer to run.
(13:18:56) developer2: STRENGTH does calculations for every lookup, so it is more expensive, but I'm not sure it should be "much much" more expensive.
(13:19:44) cleverguy: I think it also uses more iterations. Doublechecking.
(13:23:30) cleverguy: Yeah, thinplate has air and titanium. Seems to be fine if I used strength for titanium (but different time steps size and fewer steps needed).
(14:39:01) newbie1: Out of curiosity, does anyone use Eclipse CDT or any other IDE around here?
(10:20:24) cleverguy: want to give aleamr permission on /usr/casc/aleamr/zeus-local/boost* ?
(10:21:13) coder1: yeah
(10:24:31) coder1: Does it work for you now?
(10:25:00) cleverguy: checking by compiling
(10:38:28) developer2: regarding dt above, that big drop is quite possible because dt is controlled by sound speed, which is presumably much higher in Ti

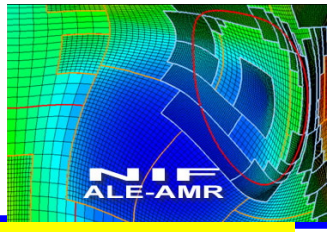
(SEE NEXT SLIDE FOR BLOW-UP)

…

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.

Sample Jabber Dialogue



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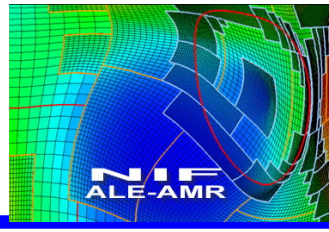
Team Development Approach - 2: TiddlyWiki provides an easy collective document



TiddlyWiki

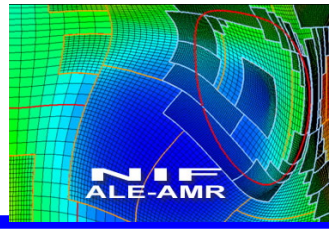
a reusable non-linear personal web notebook

- **Wiki**
  - **enables documents to be written collectively (co-authoring) in a simple markup language using a web browser**
  - **A single page in a wiki is referred to as a "wiki page"**
  - **entire body of pages, which are usually highly interconnected via hyperlinks, is called "the wiki"**
  - **An easy-to-use, easy-to-write data base**

- **TiddlyWiki**
  - **Microcontent WikiWikiWeb**
  - **Written in HTML, CSS[1] and JavaScript**
  - **Runs on any modern browser without needing any ServerSide logic**
  - **Allows anyone to create personal self contained hypertext documents that can be posted to any webserver, sent by email or kept on a USB thumb drive**
  - **written by Jeremy Ruston**

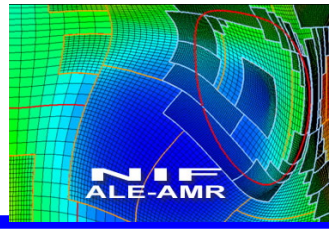
[1]CascadingStyleSheets

ALE-AMR-Notebook TiddlyWiki goes here



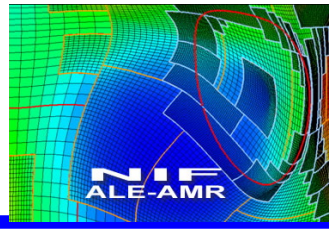
- **Link to file:///Users/admin/wiki.html**

OUTLINE



- New frontiers in scientific application codes
  - NIF-ALE-AMR and what we need to predict
- Team development methods
- **Tools and methods for verification**
- **Is the science right?**
  - **Designing experiments for validation**

Anatomy of a new simulation code



SAMRAI
Structured Adaptive Mesh Refinement Application Infrastructure

Subversion support from COLLABNET.

TiddlyWiki
a reusable non-linear personal web notebook

VisIt

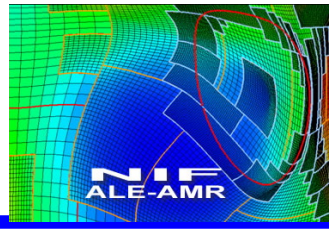
The HDF Group

hypre
high performance preconditioners

Modern HPC codes rely on a variety libraries and tools in addition to including multi- physics or engineering packages

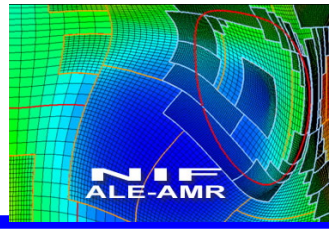
boost
C++ LIBRARIES

Verification Basics



- **Build Tests**
  - **The multitude of libraries means that daily (nightly) builds are necessary**
  - **Build tests automatically check code out of repository**
  - **Specify systems of interest**
  - **Usually finds errors in configuration, not our code**
- **Smoke Tests**
  - **Designed to see if things are working in general without necessarily verifying correctness -- a few iterations of various problems**
- **Unit Tests**
  - **Tests that examine smaller units of code for correctness**

For verification, there is a choice between simple developmental approach and tools



- **Low-key approach:**
  - **Cron script, automatic email, html file, daily checking**
- **Sophisticated Production Tools**
  - **LLNL's Shawn Larson has developed Tapestry** (next slides)
    - **MPI parallel application**
    - **Batch and interactive**
    - **Tests spanning multiple codes**
    - **Multiple test suites support**
    - **And many more features**
- **Open Source Options like Trac integrate other objects**
    - *** wiki pages**
    - *** tickets**
    - *** changesets**
    - *** reports**
    - **etc.**

Code Testing

2007, March 07

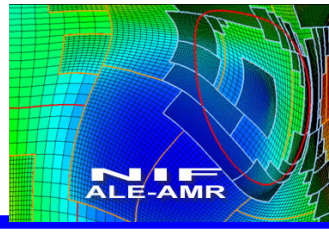
TAPESTRY
Shawn Dawson

Past Results		
Year	**Month**	**Date**
2007	March	1 . 2 . 5 . 6 . 7 . 8 . 9 .
	February	5 . 12 . 19 .
	January	1 . 8 . 15 . 22 . 29 .

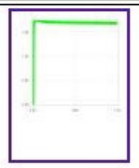
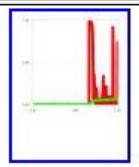
chaos_3_x86_elan3

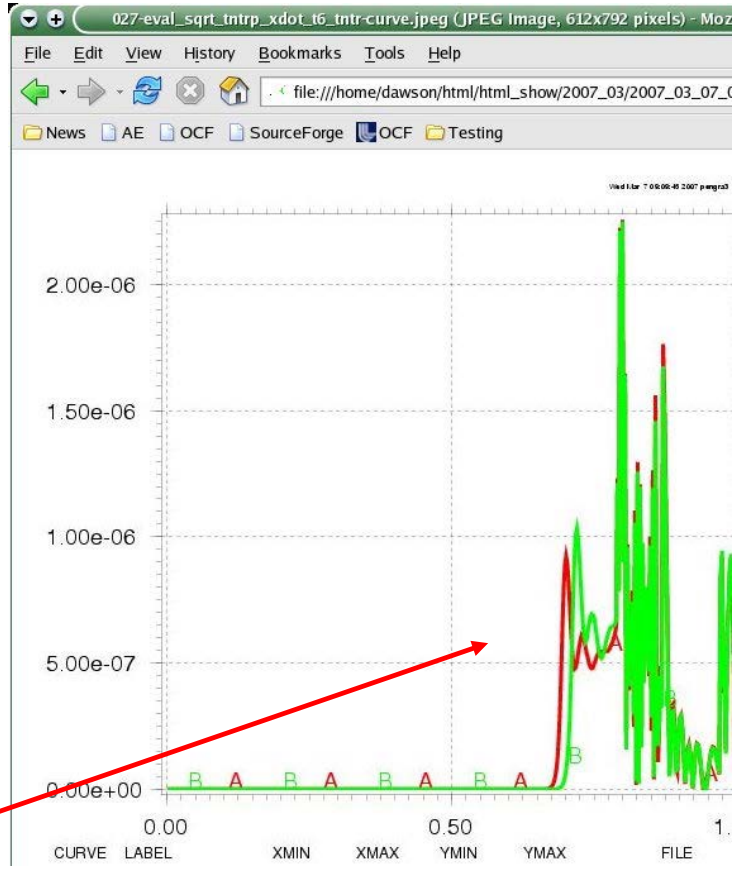
Machine	Code Task	Result	Finish Time	Task Log Links & Reports	Test Artifacts
machine3	verification test	23 batch jobs submitted	2007/03/07 06:30:49	View Test Run Log	
machine3	verification report Code Version : 1.13.248 IOLib Version : 4.5.1 Library4 Version : 1.0.38 PAPI Version : 196608 Library3 Version : 7.23 Library1 Version : 4.9.$Revision: 733 $ Thu Feb 8 14:26:18 PST 2007 Another Library : YES - Version 20060613 Library2 Version : L 1.8.2b $Date: 2003/10/22 23:46:36 $ Compiled: Mar 7 2007 01:17:31	failures curve diffs in report 05 Deck.2d Deck.1d deck.cyl deck.sph.2d deck3 deck4	2007/03/07 09:16:11	View Report Generation Log View Curves Summary Report (03) View Curves Detail Report (04) View Curves Pass / Fail Report (05) View Simple Pass Fail Report (log)	☐ Deck.2d ☐ Deck.1d ☐ deck.cyl ☐ deck.sph.2d ☐ deck3

Curve differences are automatically plotted and can be enlarged in Tapestry

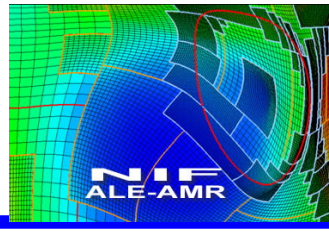


Large Image HTML	Link to large image HTML - contains embedded large images
System	chaos_3_x86_elan3
Report Date	2007, March 07
Baseline Code Version	Code Version : 1.13.225
New Code Version	Code Version : 1.13.248
Test Runtime	5 minutes
Test Case	Deck.1d
test step 1	Deck.1d
Version.baseline	Version.baseline
Version.current	Version.current
ultra.curves	ultra.curves
ultra.curves.baseline	ultra.curves.baseline

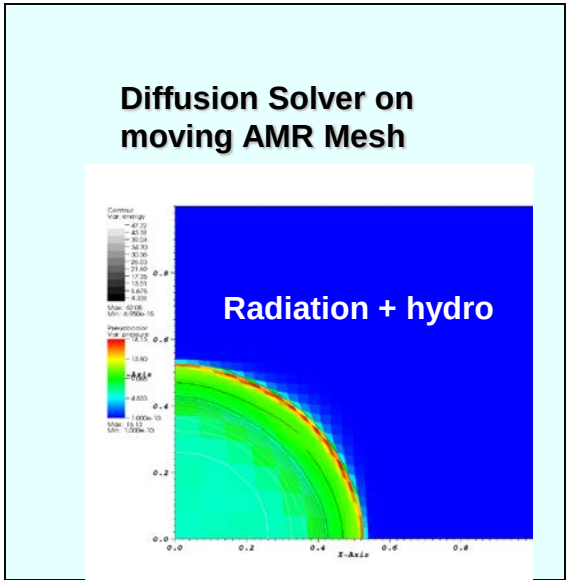
Curve Description	Code Curves A = New Curve B = Baseline Curve	Diff-Measure Curves C = Fractional Difference D = Average Fractional Difference
Curve 007 : reg1ke_vs_time		
Curve 027 : eval_sqrt_tntrp_xdot_t6_tntr		



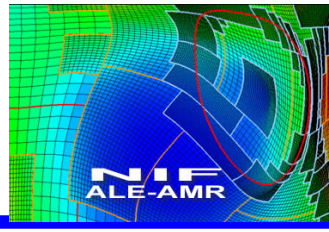
Standard code-correctness tests are applied first, but these are limited in breadth



- Simple, published and/or analytic problems can pinpoint problems with code physics/design
  - Sedov blast wave
  - Mousseau diffusion
- A large number of different gridding possibilities should give “similar” but not identical results
  - With AMR
    - How many levels
    - Refinement criteria
  - With advection
  - Quantifying “similar” is a big issue

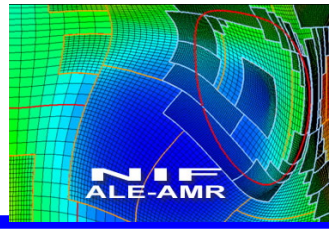


OUTLINE



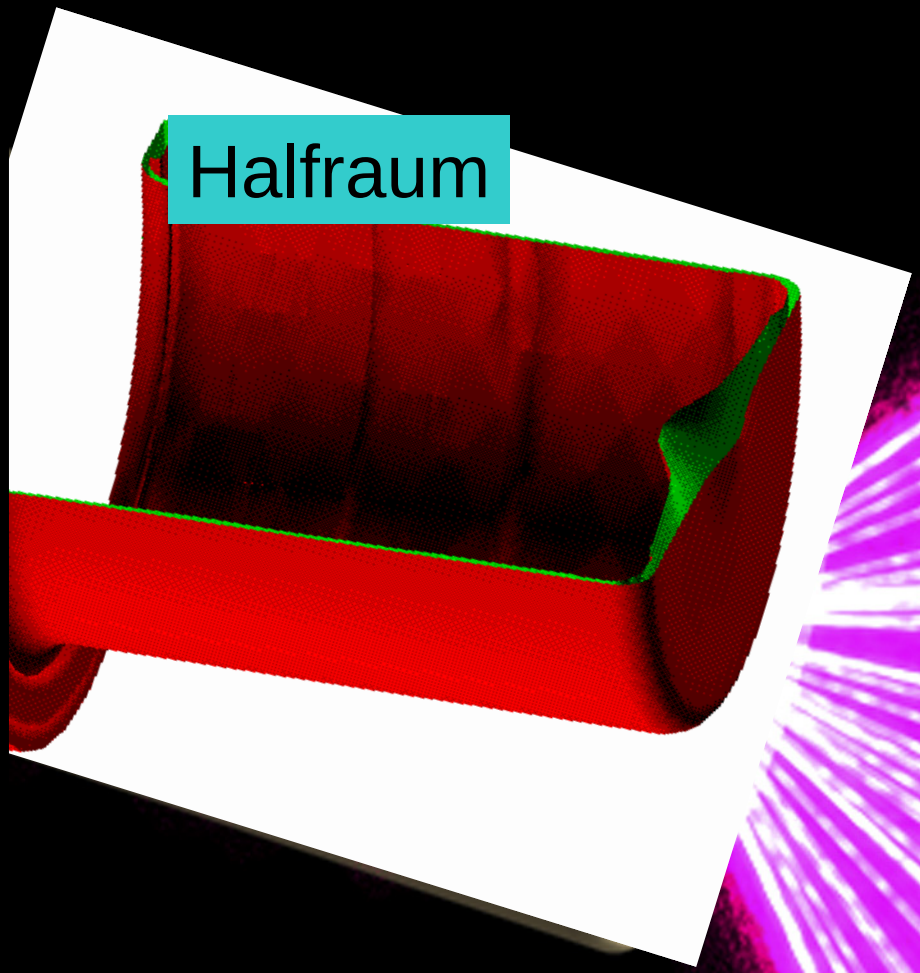
- New frontiers in scientific application codes
  - NIF-ALE-AMR and what we need to predict
- Team development methods
- Tools and methods for verification
- **Is the science right?**
  - **Designing experiments for validation**

We have designed several dedicated experiments for benchmarking debris/shrapnel



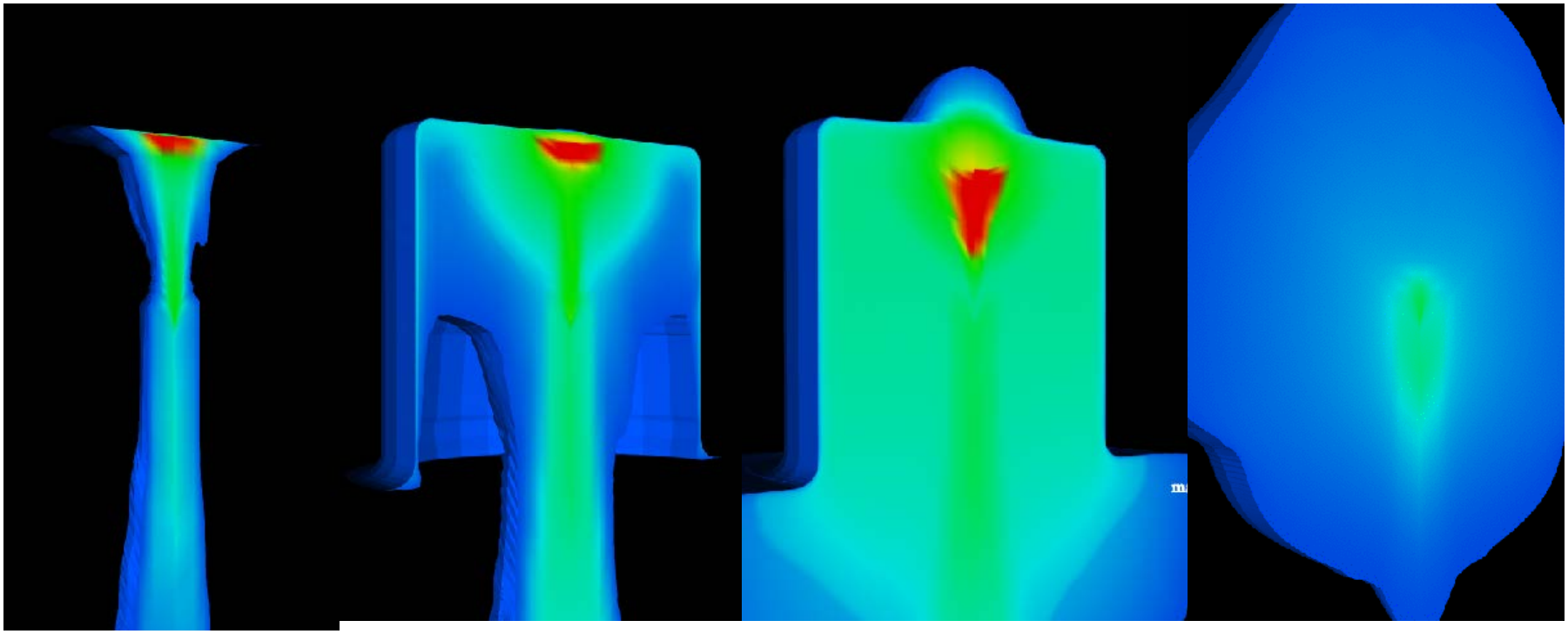
- Three dimensional codes with relevant tests are extremely difficult to reduce to a single curve or number for comparison
  - Contrast this, e.g., to an icf capsule simulation where the yield is a single critical number
- Halfraum Experiment
- Ring Fragmentation
- Thin Plate Experiments

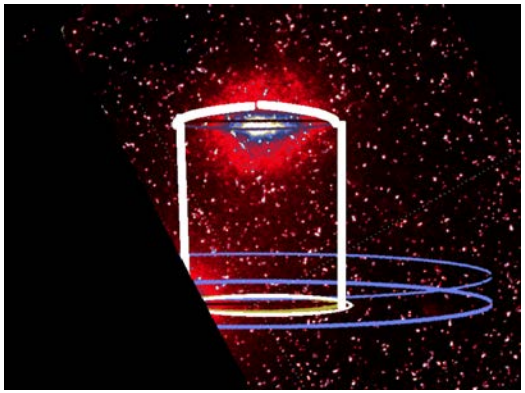
Hohlraum

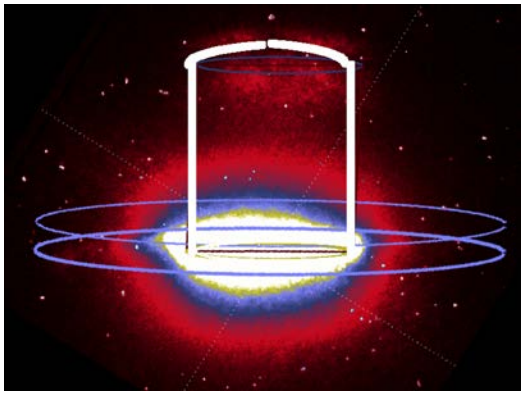


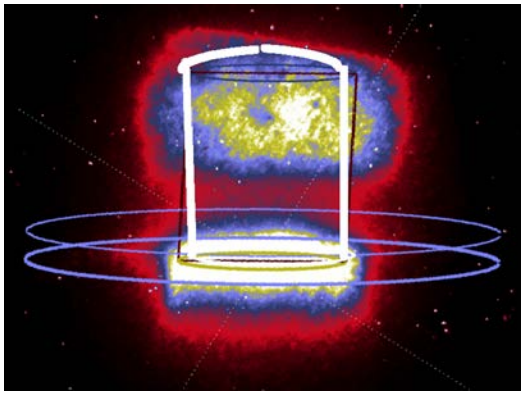
Comparison of NIF Eary Light data with 3D simulations-

Experiment: M. Schneider, et al.

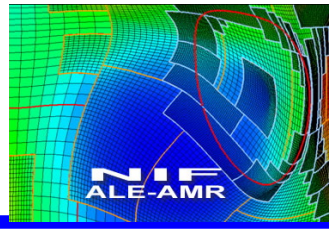


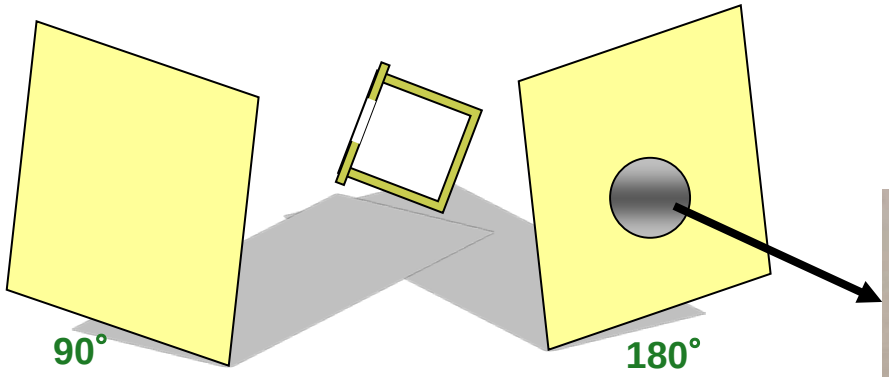




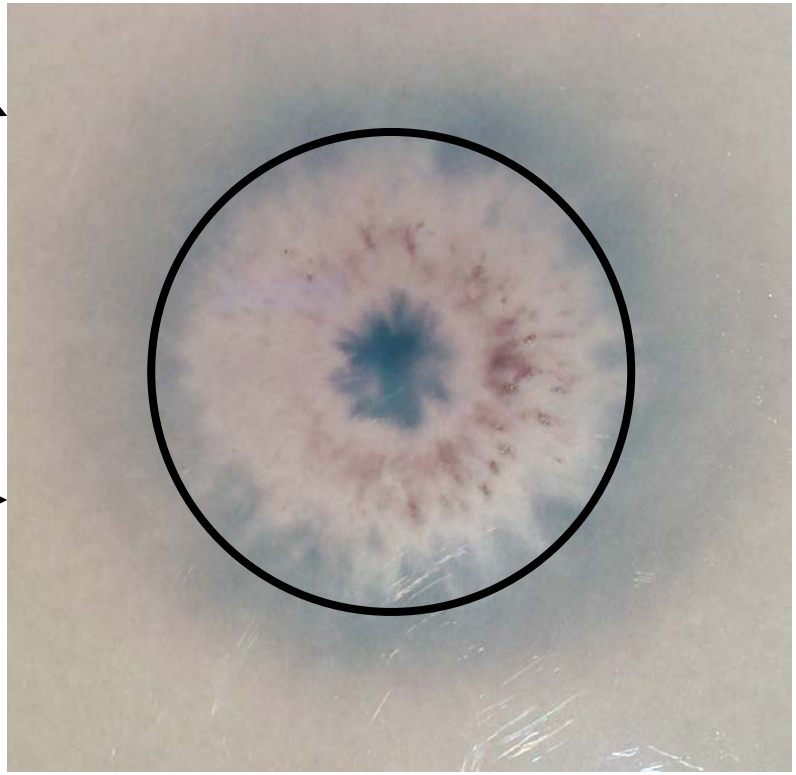


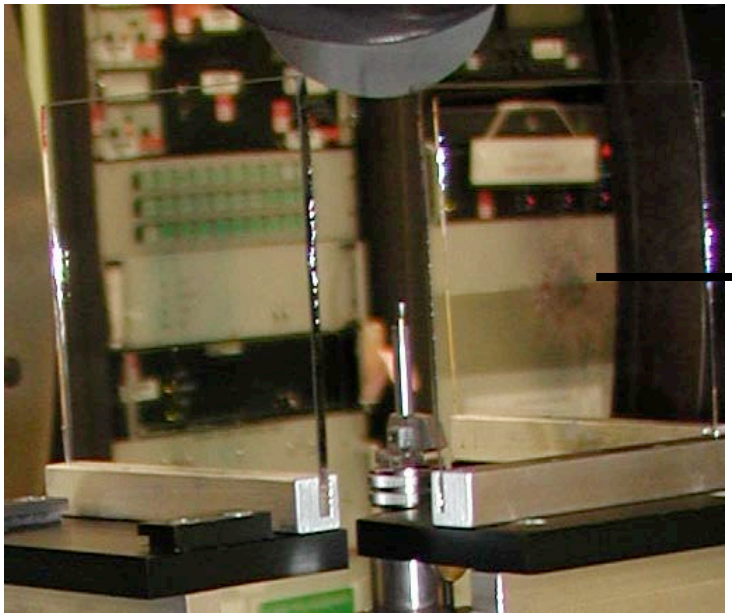
Benchmarking Simulations: On Helen at AWE, glass plates collect gold debris (experiment by J. Andrew)





Target emissions on 180° glass form ring pattern

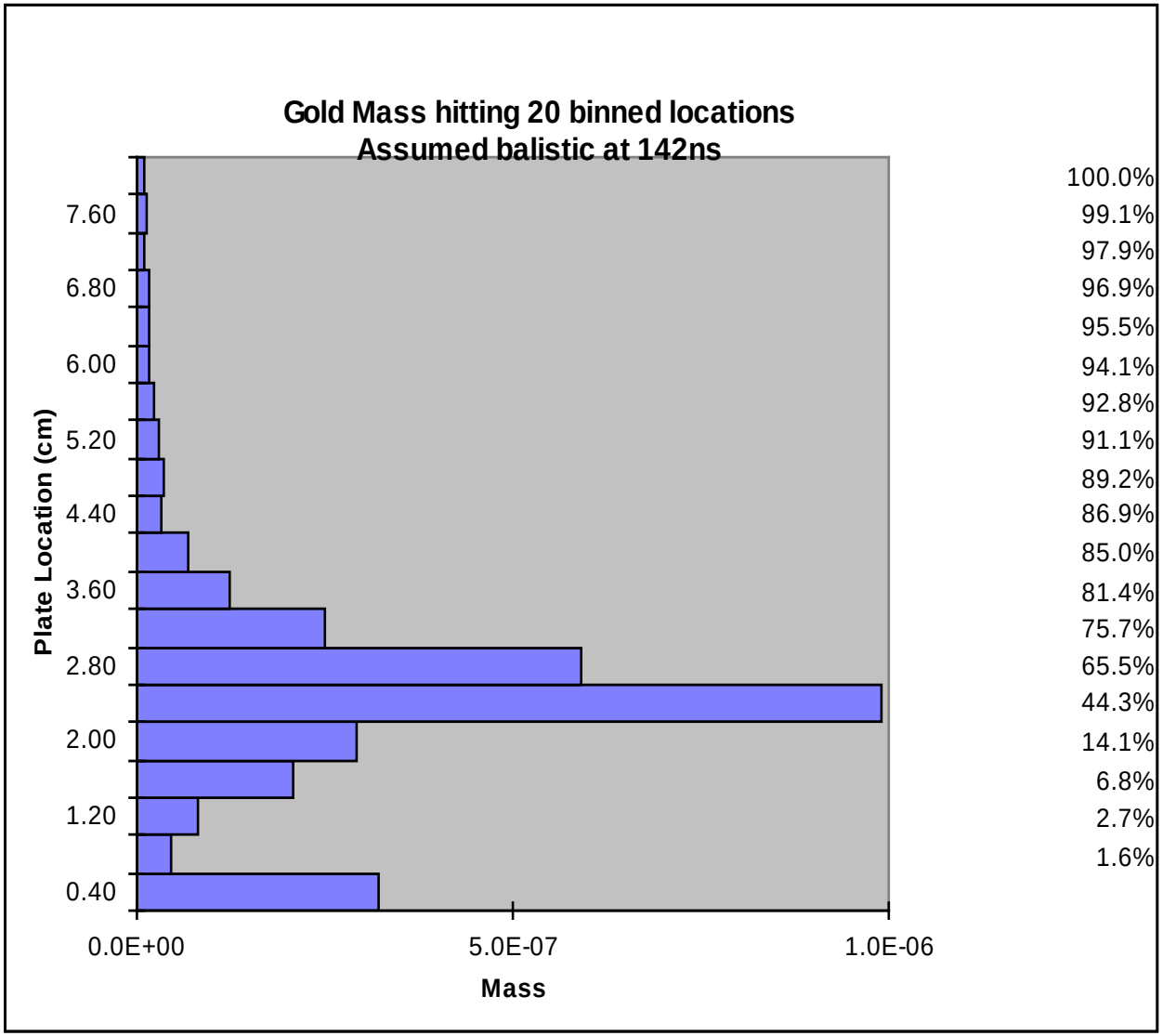




Standoff distance 8cm

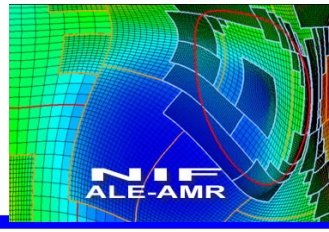
Most mass contained in ring (r ~ 3 cm)
In agreement with simulation

Simulations and data agree on the expansion of the debris from halfraum



Predict 80% of the mass is contained in the rings below 3 cm

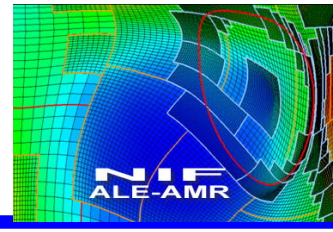
For fragmentation validation, there are some classic experiments with expanding rings



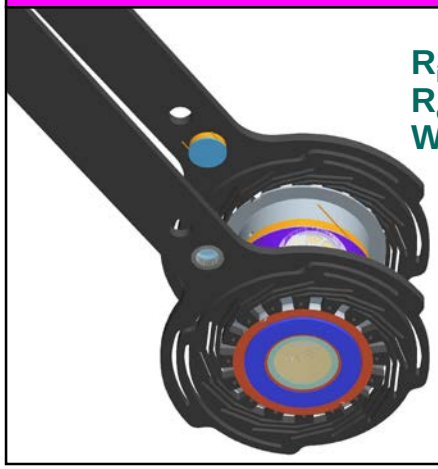
- **E-M Forces are used to force ring to expand with various velocities**
- **Ring breaks into differing numbers of pieces depending on velocity**
- **Comparision is somewhat subjective because of random seeding**
- **As is typical of 3D, visualization uncovered errors in code (too much regularity was fault of overlapping bc's)**

QuickTime™ and a
YUV420 codec decompressor
are needed to see this picture.

Actual NIF experiments will also provide a benchmarking data base

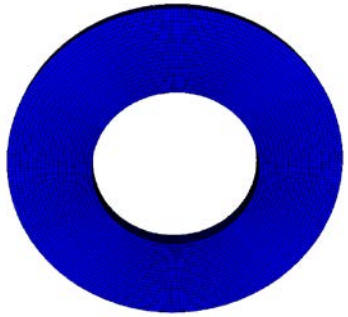


Cooling Rings Fragmentation Simulation

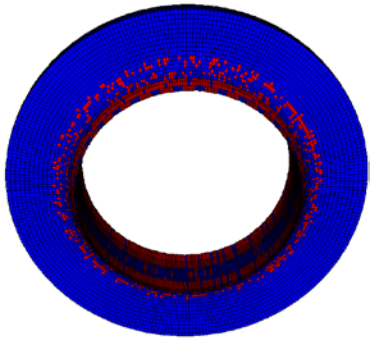


R_{inner} = 2 mm
R_{outer} = 4 mm
Width = 0.5 mm

QuickTime™ and a
None decompressor
are needed to see this picture.

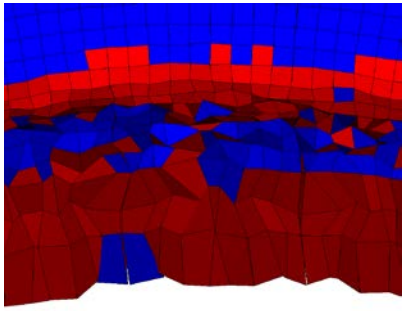


t = 0 μs



t = 0.5 μs

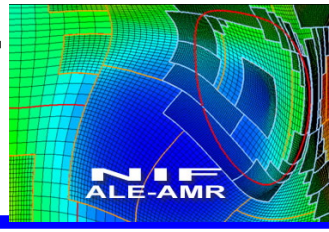
Red Indicates Failure



t = 1 μs

Close-up
of fragments
(~.1 mm or smaller)

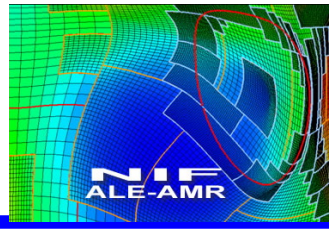
We are have dedicated shots on the Janus Laser at LLNL to capture fragments in aerogel



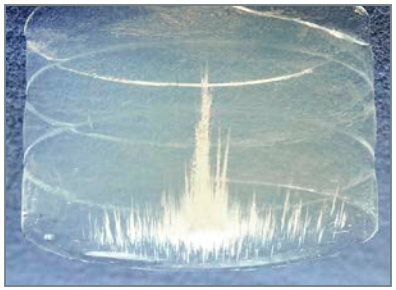
- **Shooting very thin foils puts us close to the microstructural level.**
- **Problem is taxing for any code. Ability to run both Lagrangian and adaptively meshing Eulerian is critial**

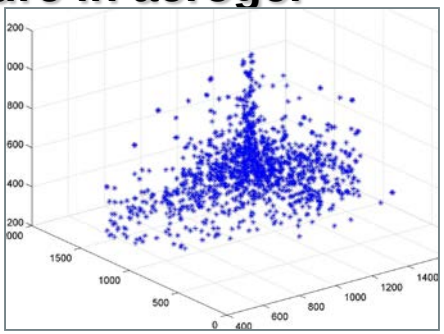
MP4 Movie
Plays here

We are implementing a complex set of material models at different AMR levels

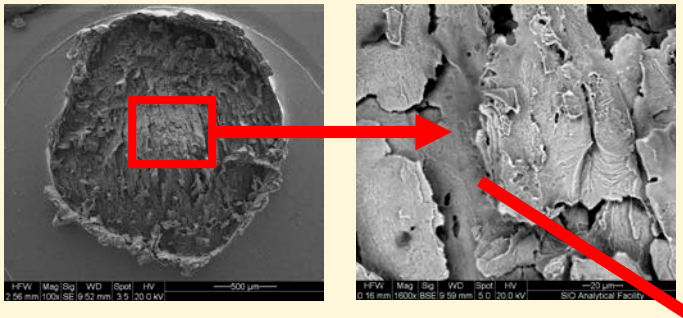


Fragment capture in aerogel

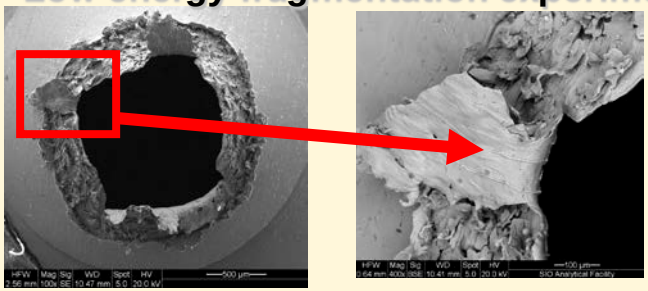




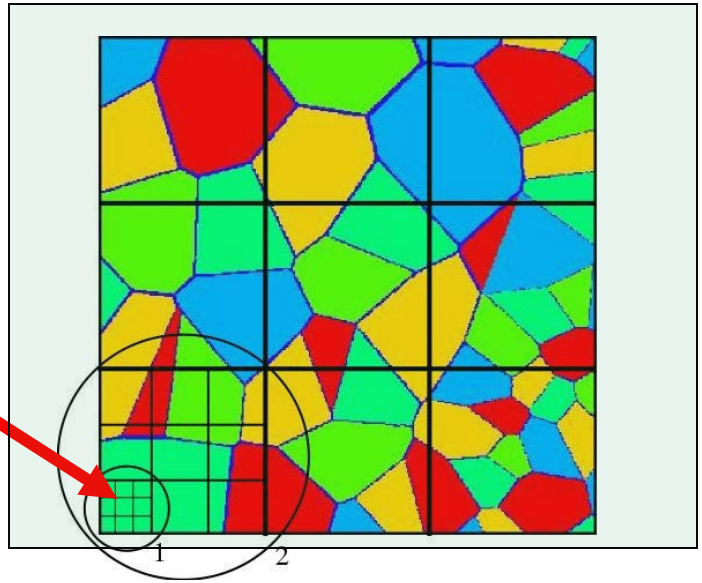
Hierarchical Material Model (HMM) with Voronoi Construction representing grain structure



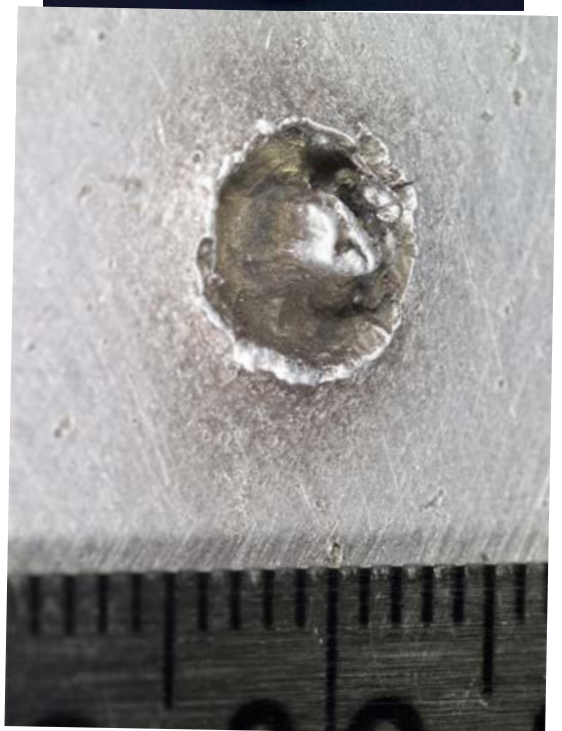
Low energy fragmentation experiment

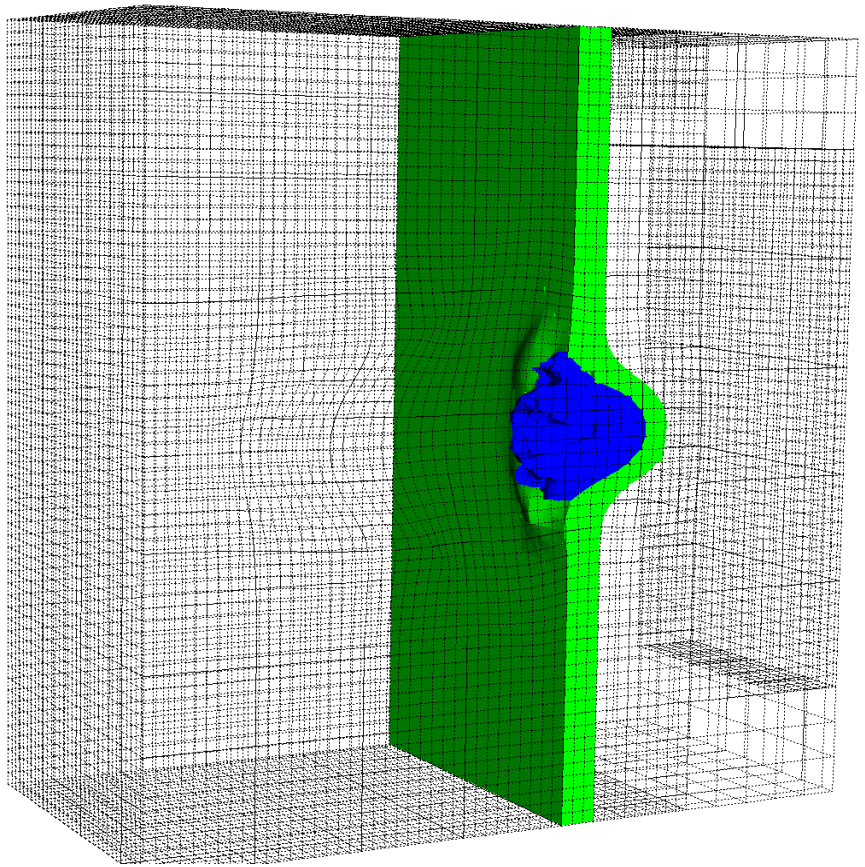


High energy fragmentation experiment



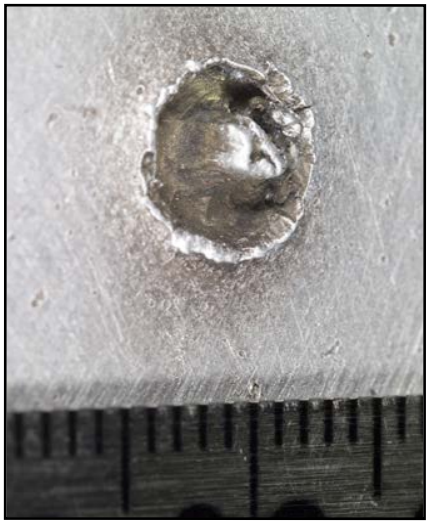
The “it looks right” test is useful for 3D





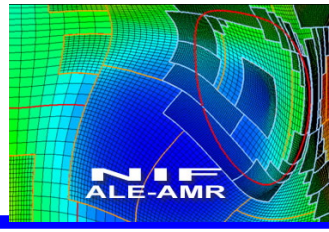
Simulation of OMEGA flapper plate damage

Movie of projectile simulation



QuickTime™ and a
H.264 decompressor
are needed to see this picture.

Summary



- Development of a new predictive simulation code is enhanced and accelerated by team tools
  - Chat room
  - Wiki
- V&V tools (with emphasis on verification) are available
  - Differing needs for large efforts/mature codes and smaller developmental projects
- Predict: lots of new 3 D simulation codes in areas we have not tried to model in the last century
  - The validation part of V&V is very difficult in this 3D regime
  - Dedicated experiments, cameras, other tools helpful