Multi-Physics Plasma Modeling for a Range of Applications on HPC Platforms

Alice Koniges[1], David Eder[2], Aaron Fisher[2], Wangyi Lui[1], Nathan Masters[2], John Barnard[2]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA, USA [2]Lawrence Livermore National Laboratory, Livermore, CA, USA

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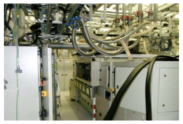
ized Drift Compression Experiment (NDCX-II)

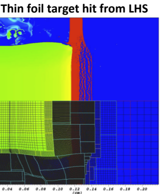

CYMER EUV Lithography System


National Ignition Facility (NIF) - USA


Laser Mega Joule (LMJ) - France

A large range of facilities can benefit from multi-physics plasma modeling

Thin foil target hit from LHS


E - Arbitrary Lagrangian Eulerian
IR - Adaptive Mesh Refinement

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

- 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

Basic equations in ALE-AMR

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

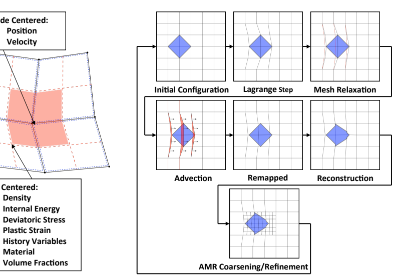
$$\rho\frac{D\vec{U}}{Dt} = \frac{1}{\rho}\nabla\cdot\boldsymbol{\sigma} = \frac{1}{\rho}\sigma_{ij,j}$$

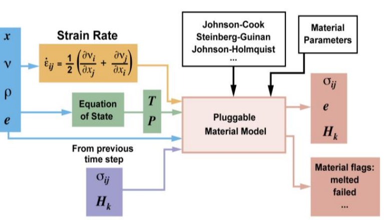
$$\frac{De}{Dt} = \frac{1}{\rho}V\mathbf{s}:\dot{\boldsymbol{\epsilon}} - P\dot{V} + \frac{1}{\rho}W_{sources} = \frac{1}{\rho}V\left(s_{ij}\dot{\epsilon}_{ij}\right) - P\dot{V} + \frac{1}{\rho}W_{sources}$$

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

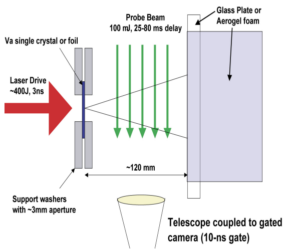
is the total stress tensor (surface tension enters here), s is the deviatoric stress, and $\dot{\epsilon}$ is the strain rate tensor with

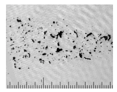
$$s_{ij} = \sigma_{ij} + P\delta_{ij} \quad\text{and}\quad \dot{\epsilon}_{ij} = \frac{1}{2}\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right).$$

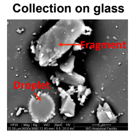


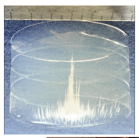


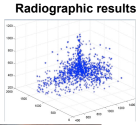
Fragmentation model uses void insertion and Model validated with experiments at Jupiter Laser Facility

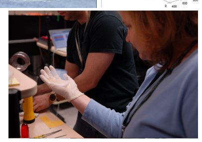



Collection on glass

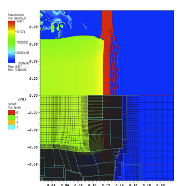



Radiographic results





Simulation with spall



Code is used to model ion beam experiments at NDCX-II

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

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

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

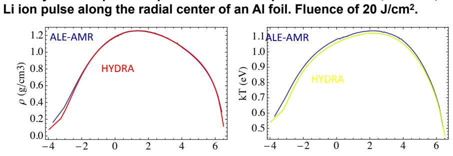
$$\Lambda_B = 2m_e c^2\beta^2/\bar{I}$$

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

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

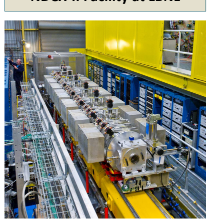
$$R = 2(\log\gamma) - \beta^2$$

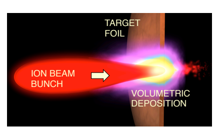
Density and temperature profiles at the completion of the 1 ns, 2.8 MeV, Li ion pulse along the radial center of an Al foil. Fluence of 20 J/cm².

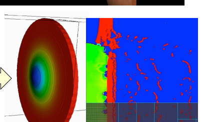


The Hydra source is not open, which limits the ability to add new packages, e.g., AMR, surface tension, fragmentation models, and new multiphysics

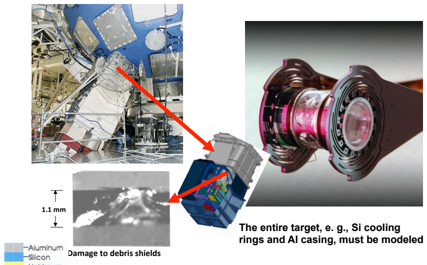
NDCX-II Facility at LBNL



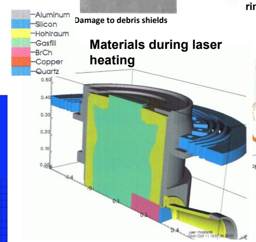



ALE-AMR simulations

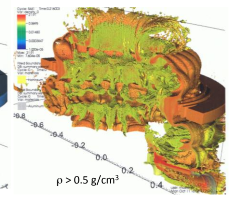
Large laser facilities, e.g., NIF and LMJ, require modeling to protect optics and diagnostics



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

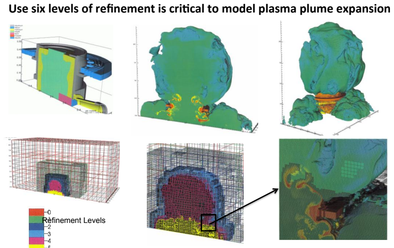


Materials during laser heating

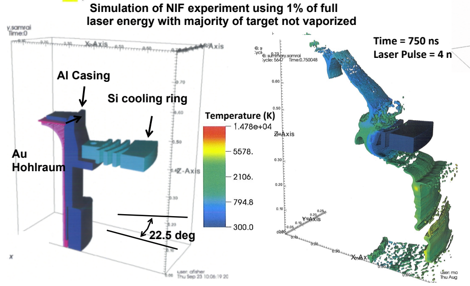


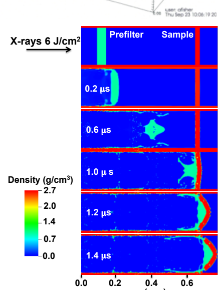
Threshold density at 220 ns

Use six levels of refinement is critical to model plasma plume expansion



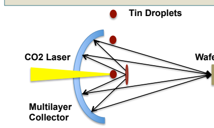
Simulation of NIF experiment using 1% of full laser energy with majority of target not vaporized





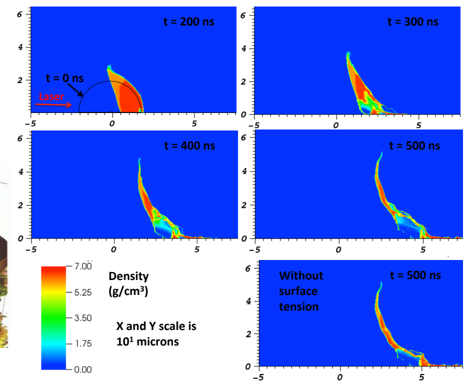
Redesigned Sample Holder

ALE-AMR used to model extreme UV lithography experiment using laser heated molten metal droplets

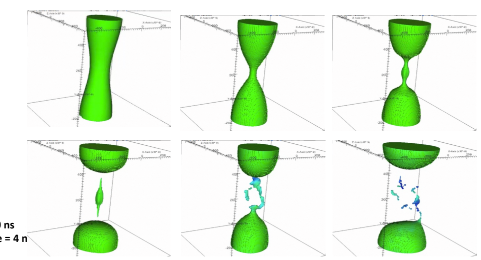


Use a prepulse to flatten droplet prior to main pulse

At low prepulse energies, droplet is observed to oscillate (surface tension effect)



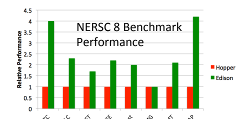
Surface tension model based on volume fractions was validated with analytic test cases



Multi-Physics Code Available for Collaborations

- Plasma wall interactions for magnetic fusion devices
- Modeling of ion beam experiments
- Fragmentation of materials
- Surface tension effects for molten material

Cray XC30 with Intel Ivy Bridge 12-core process Aries interconnect with Dragonfly topology

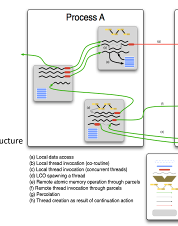


Edison is very s to Hopper, but 2-5 times the performance p on most codes

	Hopper	Edison
Peak Flops (PF)	1.29	2.4
CPU cores	152,408	124,800
Frequency (GHz)	2.1	2.4
Memory (TB) Total / Per-node	217 / 32	333 / 64
Memory BW* (TB/s)	331	530.4
Memory BW/ node* (GB/s)	52	102
Filesystem	2 PB 70 GB/s	6.4 PB 140 GB/s
Peak Bisection BW (TB/s)	5.1	11.0
Sq ft	1956	1200
Power (MW Linpack)	2.91	1.9

New algorithms should work in concert with n exascale operating systems: ParalleX Execution M

- Lightweight multi-threading
  - Divides work into smaller tasks
  - Increases concurrency
- Message-driven computation
  - Move work to data
  - Keeps work local, stops blocking
- Constraint-based synchronization
  - Declarative criteria for work
  - Event driven
  - Eliminates global barriers
- Data-directed execution
  - Merger of flow control & data structure
- Shared name space
  - Global address space
  - Simplifies random gathers



Thomas Sterling, et al. IU and XPI

HPX and Related Application Development

- Explore app development alternative to "traditional MPI+X".
- Question: Can a qualitatively different approach (Parallex-ba
  - Exploit untapped and new parallelism?
  - Improve expressability?
  - Improve productivity?
  - Get us to Exascale and beyond?
- Broad sampling of app domains & algorithms:
  - Plasma physics, Many-body & particle-in-cell (PIC)
  - Nuclear engineering & finite volume/eigensolvers.
  - Shock physics & finite element/explicit time integration.
  - Computational mechanics & implicit sparse solvers.
- Full team effort involving app designers, XPRESS team, HPX ParalleX developers, and compiler and tools developers

Some recent ALE-AMR Publications:

Alice Koniges, Nathan Masters, Aaron Fisher, David Eder, Wangyi Liu, Robert Anderson, David Benson, and Andrea Bertozzi, "Multi-Material ALE with AMR for Modeling Hot Plasmas and Cold Fragmenting Materials", Invited for special issue of Plasma Science and Technology (in review), 2014

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

Alice Koniges, Wangyi Liu, Steven Lidia, Thomas Schenkel, John Barnard, Alex Friedman, David Eder, Aaron Fisher, and Nathan Masters, "Advanced Target Effe Modeling for Ion Accelerators and other High-Energy-Density Experiments", 8th International Conference on Inertial Fusion Sciences & Application (in review),

Alice Koniges, Wangyi Liu, John Barnard, Alex Friedman, Grant Logan, David Eder, Aaron Fisher, Nathan Masters, and Andrea Bertozzi, "Modeling warm dense experiments using the 3D ALE-AMR code and the move toward exascale computing", EPJ Web of Conferences 59, 09006, 2013,

D.C. Eder, A.C. Fisher, A.E. Koniges and N.D. Masters, "Modelling debris and shrapnel generation in inertial confinement fusion experiments", Nuclear Fusion 5 113037, 2013,