Enabling Physics insight with Multidimensional Computer Simulations

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SC14 Panel
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Mathematics + Algorithms for a new Multiphysics Simulation Code applied to large experiments
History: Predictive calculations needed for optics and diagnostics protection on NIF
Problem: Traditional ALE codes complicated and crashed for late-time simulations
Led a project to design a new 3D multimaterial ALE + AMR code including substantial new physics

- 3D ALE hydrodynamics
- AMR (use 3X refinement)
  - With 6 levels, vol ratio $10^7$ to 1
- Multi-Material (interface reconstruction)
- Anisotropic stress tensor
- Tabulated EOS and opacities
- Material failure with history
- Laser ray trace and deposition
- Ion deposition
- Thermal conduction
- Radiation diffusion
- 2D Axisymmetric capability
- AMR with 3X in only 1 direction
- Surface tension

ALE-AMR is an open science code that runs at various computing centers including NERSC and has no export control restrictions
Multimaterial ALE + AMR; including anisotropic stress tensor

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0
\]

Continuity equation

\[
\rho \frac{\partial \vec{v}}{\partial t} = \nabla p + \nabla \cdot \Sigma' + \rho \vec{b}
\]

Equations of motion

\[
\rho \frac{\partial e}{\partial t} + p \nabla \cdot \vec{v} = 0
\]

PdV work

\[
\sum^{n+1} = f(\Sigma^n, \rho, e, \vec{v}, p, T, \vec{h})
\]

Material Stress Update

\[
\begin{align*}
p &= p(\rho, e) \\
T &= T(\rho, e)
\end{align*}
\]

EOS tables
Various gas laws

Radiation Diffusion added via an operator splitting method
ALE-AMR was used to model the late time properties of HEDLP targets shot for National Ignition Campaign (450 M$ per year, 4B$ to construct)

Materials at end of laser pulse

Time = 220 ns

Patch boundaries shown

Refinement Levels

-0
-1
-2
-3
-4
-5
Multimaterial interface reconstruction + AMR allows fast and accurate modeling of complex targets.
Molten Al in a Keyhole wedge simulation expands and drops in density in a divergent velocity field

Need to estimate droplet sizes in divergent velocity fields motivated effort on surface tension
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.

X-rays 6 J/cm²

Density (g/cm³)

Prefilter  Sample

0.2 µs

0.6 µs

1.0 µs

1.2 µs

1.4 µs

Redesigned Sample Holder

X-rays & Debris wind at ~30 km/s

~300 m/s
Some stuff about me

- 1st Woman to get a PhD in Applied Mathematics at Princeton
- Approximately 100 Papers and 1000 Citations
- PI on a few million dollars of research grants
- Raised 3 Kids, have a physicist spouse (34 years)
- Worked part time a bit – but don’t tell anyone 😊
- Had 9 post-docs in last 6 years
- Try to make time to – ride my horse, do an occasional sprint triathlon, play piccolo
Leader/PI, Petascale Initiative in Computational Science and Engineering

<table>
<thead>
<tr>
<th>Project:</th>
<th>Post Doc</th>
<th>Start Date</th>
<th>Education (PhD)</th>
</tr>
</thead>
<tbody>
<tr>
<td>EFRC: Q-Chem parallelization and GPU Optimization</td>
<td>J Kim</td>
<td>Oct-09</td>
<td>Univ. IL Urbana-Champaign</td>
</tr>
<tr>
<td>Fusion: GTS for ITER-Scale; Programming Models</td>
<td>R Preissl</td>
<td>Feb-10</td>
<td>J. Kepler Univ. (Austria)</td>
</tr>
<tr>
<td>Multiphase Flow in Porous Media for Carbon Sequestration</td>
<td>K Fagnan</td>
<td>Mar-10</td>
<td>Univ. of Washington</td>
</tr>
<tr>
<td>Modeling for Next Generation Advanced Light Source</td>
<td>B Austin</td>
<td>Jun-10</td>
<td>UC Berkeley</td>
</tr>
<tr>
<td>Advanced Light Source and Geophysical Imaging with GPU's</td>
<td>F Maia</td>
<td>Jul-10</td>
<td>Uppsala Univ. (Sweden)</td>
</tr>
<tr>
<td>Benchmarking and Optimization of Energy-Related Applications</td>
<td>P Narayanan</td>
<td>Sep-10</td>
<td>Univ. of Maryland</td>
</tr>
<tr>
<td>ARRA-funded LBL NDCX-II modeling with ALE-AMR</td>
<td>W Liu</td>
<td>Jan-11</td>
<td>UC Los Angeles</td>
</tr>
<tr>
<td>Linear Solvers and Hybrid Programming</td>
<td>X Yuan</td>
<td>Mar-11</td>
<td>Columbia University</td>
</tr>
<tr>
<td>Poission Solver for Nano-Control EFRC</td>
<td>C Kavouklis</td>
<td>Jun-11</td>
<td>Univ. of Texas Austin</td>
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</tbody>
</table>
Teaching, mentoring, recruiting and public outreach

Program Committees

IEEE Cluster 2015
Sep. 8-11, Chicago, IL, USA
Working in the community

- Scientific Programming
  - Guest Editor
- Computational Science and Engineering
  - Invited Lead-off chapter
- International Journal of High Performance Computing
  - Associate Editor
SUMMARY: While pseudo-spectral methods have been popular in the early PIC codes, the finite-difference time-domain method has become dominant with the rise of massively parallel computing owing to its locality advantage that lends to message passing that is limited to neighboring processors. Recently, a novel parallelization strategy was proposed [1] that takes advantage of the local nature of Maxwell equations that has the potential to combine pseudo-spectral accuracy with finite-difference favorable parallel scaling. In this talk, we will present the latest developments in the implementation of spectral-based solvers in Warp and discuss our latest findings.

FDTD converges to PSTD when order goes to infinity and PSATD when time step goes to zero.

Flexible order of accuracy and subcycling of time steps enable control of locality

Ultimate flexibility is provided by runtime auto-tuning of order of accuracy vs locality and multi-level concurrency for a given architecture

Context

Novel Parallelization Concept

Flexible order of accuracy for FDTD allows order to machine precision

PSATD enables extreme accuracy in space and time while preserving locality

Strong scaling of Warp’s spectral PIC solver on a test problem of a 4,096x4,096 2-D plasma with periodic boundary conditions and 64 macroparticles/cell

Strong scaling of the Parallel Pseudo-Spectral Solver based on domain decompositions vs. A global domain FFT on NERSC’s Hopper

Performance variability for different runs of the solvers in Warp on Hopper and Edison. Performance plots are relative to the best runtime per configuration.

SOLVERS (see Poster) AND THIS SESSION:

THANKS TONY DRUMMOND