Materials Science on High Performance Computers for Fusion Applications

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SC/NE workshop

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Associate Director
Lawrence Livermore National Laboratory
LLNL is deploying some of the world’s most powerful computers for both classified and unclassified work.

- **100TF ASCI Purple**
  - 1,536 nodes
  - 12,288 Power5 processors
  - 50 TB memory
  - AIX software
  - Mid-2005

- **360TF BlueGene/L**
  - 64 cabinets
  - 65,536 nodes
  - (131,072 processors)
  - 32 TB memory
  - 1.5 MW
  - 2,500 square feet
  - Early 2005

- **23TF Thunder Linux cluster**
  - 1,024 nodes
  - 4,096 processors
  - 16 TB memory
  - Linux software
  - Spring 2004

LLNL will have 0.5 Petaflops of computing power by early 2005.

LLNL is deploying systems along three technology curves:
Stockpile stewardship is the mission driver for computing at LLNL

ASC’s suite of high-fidelity simulation codes is being used to answer critical questions about the stockpile

<table>
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<tr>
<th>Full-Scale, High-Fidelity Simulation Codes</th>
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<td>3D simulations</td>
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<td>High resolution</td>
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<td>Detailed physics</td>
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<td>Validation</td>
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<th>Sub-grid Models / Zonal Physics</th>
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<tr>
<td>Turbulence</td>
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<td>Materials Models</td>
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- Parallel computing
- Scalable algorithms
- Mesh generation
- Visualization
- Direct numerical simulations
- Predictive physics models
- First principle approaches

Advanced visualization facilities and LC’s hotline are part of the “total simulation environment”
Our current strategy devotes unprecedented HPC resources to unclassified, collaborative scientific exploration.

Unprecedented HPC capabilities…

- **Liquid/Vapor Interface**
  - First observation of hydrogen bonding moieties
  - 2000 CPUs, 1400000 CPU hours

- **Novel Polymer Materials**
  - First-time observation of crystallization in polymers
  - 2000 CPUs, 720000 CPU hours

- **Rayleigh-Tayler Instabilities**
  - First fully atomistic model with dynamic ICF conditions
  - 2000 CPUs, 96000 CPU hours

- **Nano-scale Fabrication**
  - Laser-matter interactions on experimentally accessible time and space
  - 2000 CPUs, 96000 CPU hours

… are being used by LLNL and its collaborators to tackle exciting new scientific challenges.
BlueGene/L is moving from design to functioning hardware and software

- First wave SSP applications
  - LLNL, LANL, SNL, Alliance codes
  - See next slide for examples

- Discussing collaborations with DOE-SC labs to create a better software environment for BG/L

180/360 TF in 2500 sq.ft.
100x higher compute density
25x greater power efficiency
20x greater cost effectiveness

Compared to recent high-end computers
LLNL is developing scalable materials science application codes that will enable breakthrough computational science for ASC and fusion materials.

MDCASK: Classical molecular dynamics code for materials science applications
μm and ns

GP & MGmol: First-Principles Molecular Dynamics for materials
nm and ps

ParaDiS: Multi-scale dislocation dynamics for studying materials under extreme conditions
mm and ms

ALE3D: Versatile multi-scale, multi-physics code for studying materials under strain
m and s

These codes represent that first suite of applications on BlueGene/L and are/will be available (subject to export control issues) for wide distribution to the scientific community.
LLNL’s multiscale materials modeling effort represents a major institutional commitment and involves a large multidisciplinary team.

Our vision is to develop and apply multiscale models to predict materials properties and performance under extreme conditions.

Successful implementation requires closely coupled experiments and models.

Multiple directorates at LLNL participate:
- DNT: Program is led by E. Chandler
- PAT: Atomic Scale ---> Microscale
- CMS: Atomic ---> Microscale ---> Mesoscale
- Eng: Mesoscale ---> Continuum

Rules for dislocation motion and multiplication

Single crystal constitutive relation

Yield surface

Continuum

ALE3D

Mesoscale

NIKE3D
LLNL’s multiscale materials modeling effort is synergistic with the needs of the fusion program.

<table>
<thead>
<tr>
<th>Distance (m)</th>
<th>Femtoseconds</th>
<th>Nanoseconds</th>
<th>Microseconds</th>
<th>Milliseconds</th>
<th>Minutes</th>
<th>Years</th>
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<tbody>
<tr>
<td></td>
<td>Electronic structure, plasma physics</td>
<td>Defects and defect/plasma interactions</td>
<td>Cascade aging and solute re-distribution</td>
<td>Microstructure evolution</td>
<td>Constitutive properties</td>
<td>Performance</td>
</tr>
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</table>

- **Defects and defect/plasma interactions**
- **Cascade aging and solute re-distribution**
- **Microstructure evolution**
- **Constitutive properties**
- **Performance**

**Goal:** an integrated multi-scale simulation environment for designing and predicting the performance of fusion materials.
Development of MDCASK for atomistic simulations of displacement cascades was initiated at LLNL in 1989 with funding from OFES

Today, MDCASK is used across the world for myriad applications
3D DD simulations represent the link between atomistic simulations and macroscopic continuum codes.

### 3D Dislocation Dynamics ≈ 10-100 µm

<table>
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<tr>
<th>Numerical infrastructure</th>
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<tr>
<td>Initial dislocation structure</td>
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<tr>
<td>10-100 µm</td>
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</table>

- Discretization
- Time step
- Long range stress fields (parallel computing)
- Boundary conditions

<table>
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<tr>
<th>Dislocation physics issues</th>
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</table>
- Motion
  - Kink nucleation
  - Kink mobility
  - Cross slip
- Interaction with other dislocations
  - Junction
  - Dipole
  - Jogs
- Grain boundary

### Simulation prediction

- Dislocation structures
- Single crystal strength properties

Several groups have successfully applied 3D DD to interesting materials science problems, including radiation damage.
However, on January 2001 we were two orders of magnitude from the desired target performance.

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<tr>
<th></th>
<th>Number of segments</th>
<th>Plastic strain</th>
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<tbody>
<tr>
<td><strong>What we need</strong></td>
<td>$N_s &gt; 10^6$</td>
<td>$\varepsilon^p &gt; 10%$</td>
</tr>
<tr>
<td><strong>What we had</strong></td>
<td>$N_s &lt; 10^4$</td>
<td>$\varepsilon^p \sim 0.1%$</td>
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</tbody>
</table>

Lessons learned from existing parallel DD implementations:
- "French" DD code: parallel code slower (!) than sequential
- *micro3d* (WSU): improvement but poor scalability
- *paranoid* (IBM): better but far from target performance

We decided to write a new parallel 3D DD code - PARADIS
Teaming with computer scientists has resulted in an efficient solution to domain decomposition and load balancing issues for 3D DD.

| Scalability | Dynamic load balance |

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

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

Code is scalable up to 1500 CPUs thus far.
Load balancing efficiency at 80% up to 1,500 CPU.
Current simulations on 512 CPUs are reaching a few % strain and provide direct comparison to experimental data.

Computed stress-strain curve:

\[
\frac{d\sigma}{d\varepsilon} \sim \frac{\mu}{10} = 13 \text{ GPa}
\]

\[
\frac{d\sigma}{d\varepsilon} \sim \frac{\mu}{300} = 0.43 \text{ GPa}
\]

Experimental Data:

R. W. Evans (1977)
Molybdenum
001 compression at RT

\(~\sigma = 20 \text{ GPa} \quad ~\varepsilon = 0.5 \text{ GPa}~\)

Simulation by M. Tang

Two weeks on a 512 CPUs of SP3 machine
We are carrying out statistical analysis of evolving dislocation configurations to investigate the development of dislocation patterns.

**Dislocation density evolution**

![Graph showing dislocation density evolution](image)

- Evidence of dynamic recovery in stage II

**Dislocation pair distribution function in (11-1) plane of fcc Ni**

![3D plot showing dislocation pair distribution](image)
We continue to improve the current code and will release it in stages - ParaDiS – Parallel Dislocation Simulator

<table>
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<tr>
<th>Ongoing Work</th>
<th>The goal is to make 3D-DD routine</th>
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<tbody>
<tr>
<td>• Port growing model on a growing machine – Blue Gene/L challenge</td>
<td>• A single hero DD simulation to 10% plastic strain now will take three weeks on a 2,000 CPU</td>
</tr>
<tr>
<td>• Elastic anisotropy: at no additional computational cost</td>
<td>• A series of standard simulations should take &lt; 3 days on 512 CPU</td>
</tr>
<tr>
<td>• Free surfaces: non-singular treatment of threading dislocations + FEM</td>
<td>• Routine simulations of the same size should take &lt; 8 hrs on 512 CPU</td>
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<tr>
<td>• Ability to handle climb</td>
<td>• Stage 1: Limited release (in process) source code to collaborators</td>
</tr>
<tr>
<td>• More stable and efficient integrators: implicit, semi-implicit</td>
<td>• Stage 2: Unlimited release of source code through OUP website (later in 2004/2005)</td>
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<tr>
<td>• Langevin dislocation dynamics</td>
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<tr>
<td>• Interaction with radiation defects</td>
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<tr>
<td>• Interaction and co-evolution with alloy microstructure - combining phase fields and DD</td>
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We are investigating new directions to couple alloy and dislocation microstructure evolution under irradiation conditions.

Combination of Phase-Field and Dislocation Dynamics

- PFM and DD are complimentary methods
- PFM was shown to be capable of handling alloy microstructures well
- PFM can be extended to handle radiation defect microstructure
- The goal is to combine DD with PFM so that the former handles the dislocations while the latter handles the alloy and rad. defect microstructures
- Understanding and accurate prediction of co-evolution of these three microstructure is key
LLNL is exploring a “Petascale Simulation Initiative” to develop concurrent multiscale-multiphysics modeling platforms

“Smart” multiscale algorithms
Selective/adaptive sampling
On-the-flight self learning algorithms

- Infrastructure and protocols for linking up heterogeneous applications (such as ALE3D and DD)
- “equationless” integration where the larger scale model “inquires” on the fly with the low scale model how it should behave
- “inquiry” data can be tabulated for re-use in the future, if and when states of some material points appear close to the ones already sampled

The goal is a general simulation framework for multiscale simulations that links heterogeneous models and codes to predict defect and alloy microstructure evolution under irradiation
We have launched an initiative in plasma-material interactions to couple plasma and materials models.

- Edge-plasma characteristics strongly affect fusion performance.
- For the hot edge of ITER, three issues are key:
  - edge-plasma temperature
  - impurity influx from sputtering
  - tritium co-deposition with carbon
- Our LDRD project is focused on a complete model:
  - developing a new 5D kinetic plasma code
  - extending MD calculations for carbon sputtering
  - integrating plasma/surface components

Goal is a fully coupled edge-plasma and material spattering/transport code.
Experimental validation is essential - we are developing new ultrafast e- and x-ray diagnostics of materials under extreme conditions.

- Inter-frame times 10 ns.
- Streaking capability — Image mode, Diffraction mode.

Real time diffraction with short x-ray and electron pulses allows experiments on the time scale of the physics of deformation.

Experiments will allow precise validation of various components of multiscale modeling methodology.
The Livermore effort benefits from a unique combination of silicon and neurons …

Silicon …

360TF BlueGene/L Early 2005

and neurons

Computational materials science group of Vasily Bulatov’s

... to develop physics-based multiscale modeling tools for designing and predicting the performance of strongly driven materials
Most atomistic simulations today do not describe complex alloys or microstructures.

Future atomistic models must incorporate *ab initio* physics in a tractable manner.