Materials Science on High Performance Computers for Fusion Applications

March 31 - April 2, 2004

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

LLNL is deploying systems along three technology curves
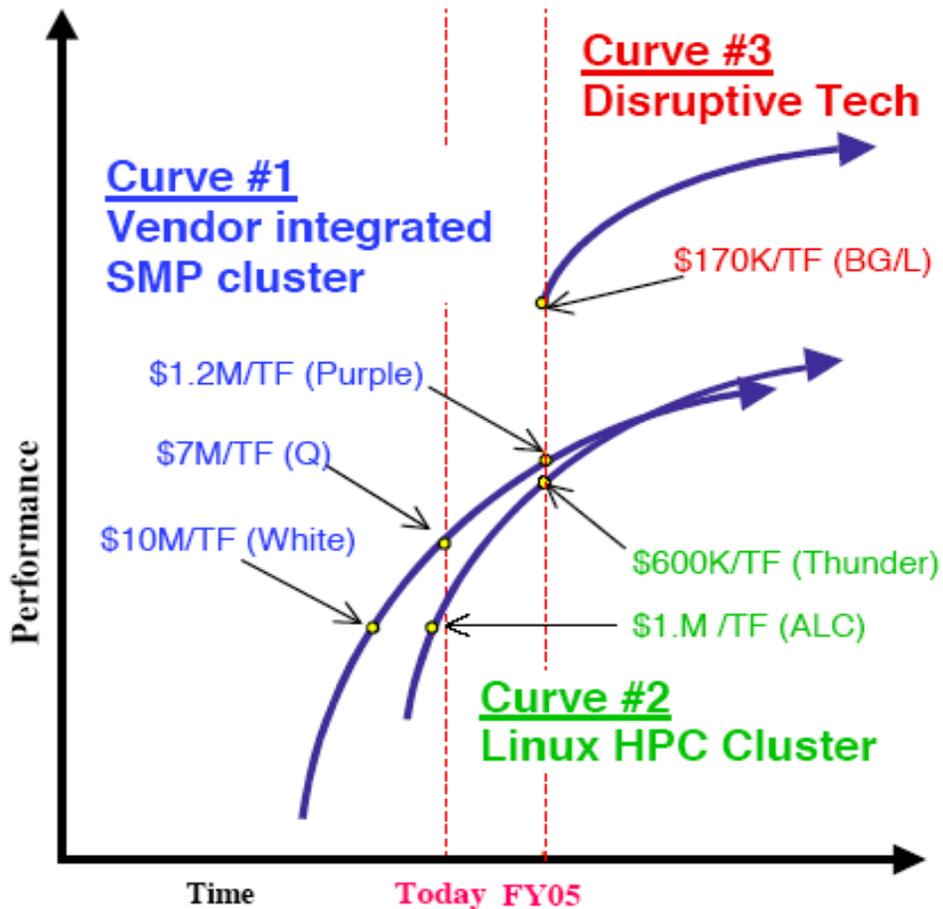
23TF Thunder
Spring 2004

1,024 nodes
4,096 process
16 TB memory
Linux software

TF BlueGene/L
2005
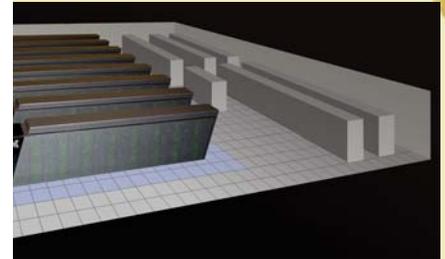
cabinets
536 nodes
1,072 processors)
TB memory
MW
0 square feet

s of computing

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

Full-Scale, High-Fidelity Simulation Codes
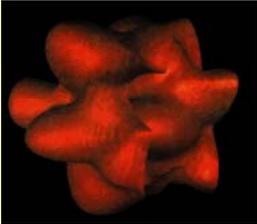
- 3D simulations
- High resolution
- Detailed physics
- Validation
- Parallel computing
- Scalable algorithms
- Mesh generation
- Visualization

Sub-grid Models / Zonal Physics

Turbulence	Materials Models
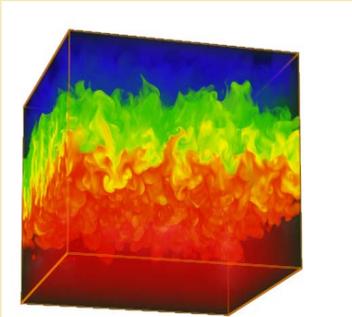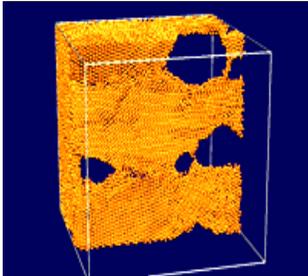
- Direct numerical simulations
- Predictive physics models
- First principle approaches

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 …

petaFLOP/s
100,000 nodes

Q
30 teraFLOP/s

Earth Simulator
40 teraFLOP/s

LLNL BlueGene/L
360 teraFLOP/s

Thunder

MCR

LLNL Purple
100 teraFLOP/s

LLNL White (IBM)
12+ teraFLOP/s

LLNL/LANL Blue (IBM/SGI)
3+ teraFLOP/s

Sandia Red (Intel)
1+ teraFLOP/s

Peak TeraFLOP/s

Moore's Law, single processor performance

1996 1997 1998 1999 2000 2001 2002 2003 2004 2005 2010
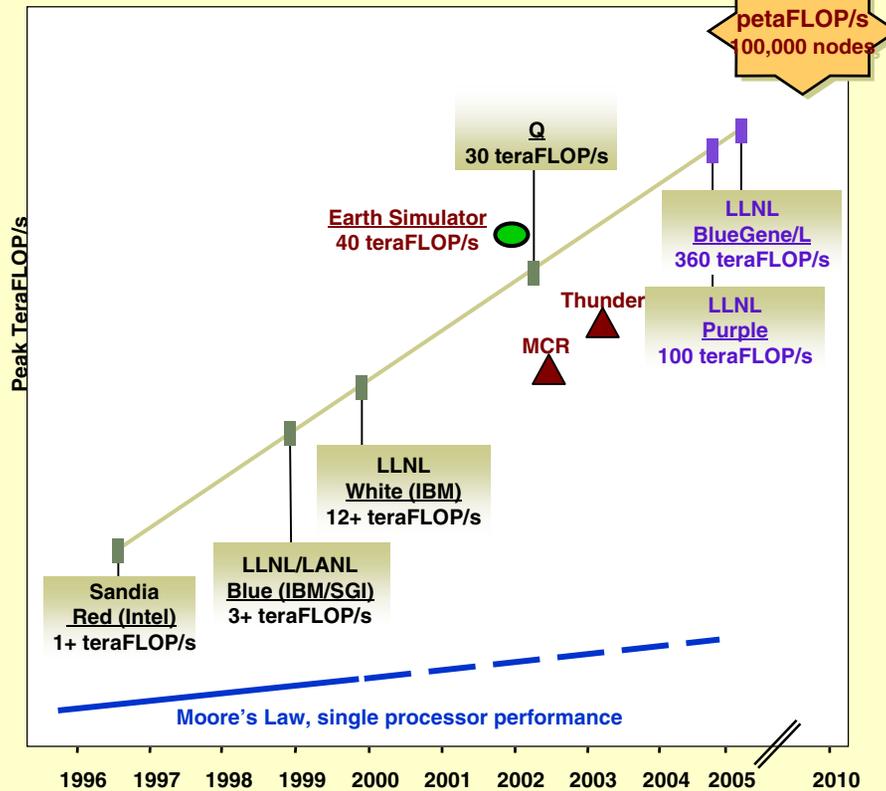
… are being used by LLNL and its collaborators to tackle exciting new scientific challenges

Scientific Breakthroughs

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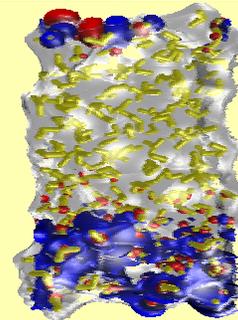
First observation of hydrogen bonding moieties
2000 CPUs, 1400000 CPU hours

Novel Polymer Materials

Experiment
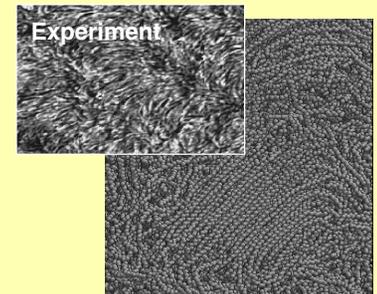
First-time observation of crystallization in polymers
2000 CPUs, 720000 CPU hours

Rayleigh-Tayler Instabilities

4 ns

6 ns
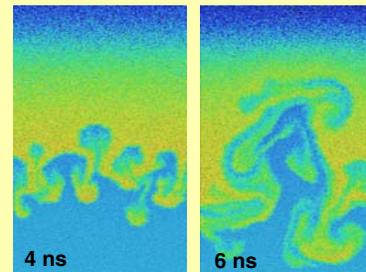
First fully atomistic model with dynamic ICF conditions
2000 CPUs, 96000 CPU hours

Nano-scale Fabrication

59 ps

170 ps
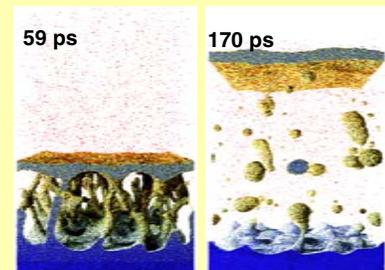
Laser-matter interactions on experimentally accessible time and space
2000 CPUs, 96000 CPU hours

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**
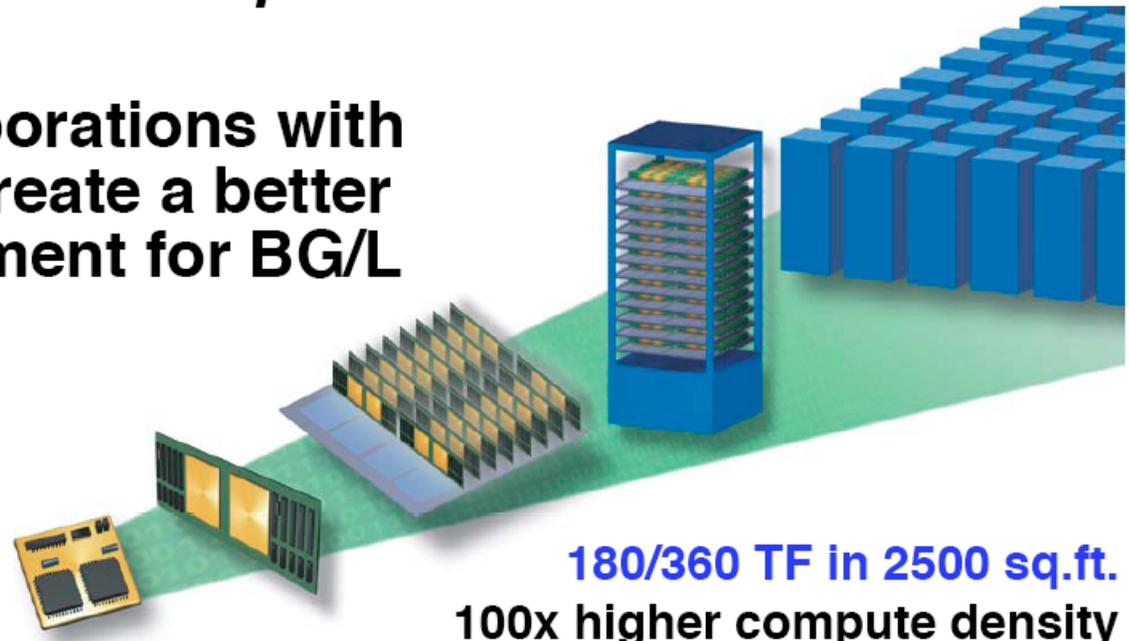
180/360 TF in 2500 sq.ft.
100x higher compute density
25x greater power efficiency
20x greater cost effectiveness
compared to recent high-end computers

LLNL is developing scalable materials science application codes that will enable breakthrough computational science for ASC and fusion materials
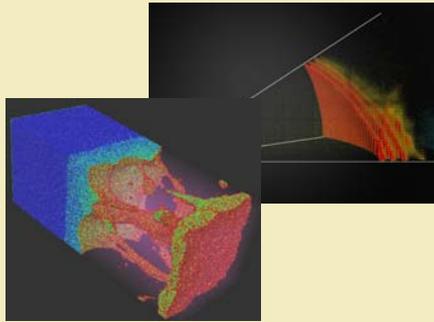
MDCASK: Classical molecular dynamics code for materials science applications

μm and ns

GP & MGmol: First-Principles Molecular Dynamics for materials

nm and ps
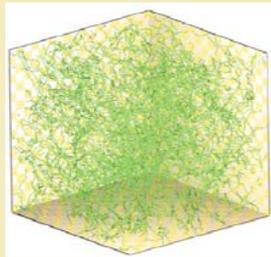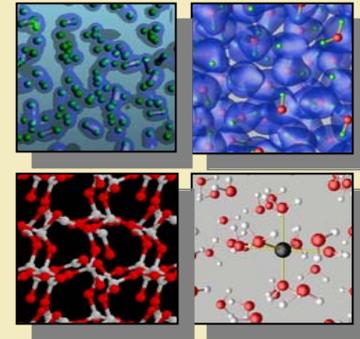
ParaDiS: Multi-scale dislocation dynamics for studying materials under extreme conditions

mm and ms

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

m and s
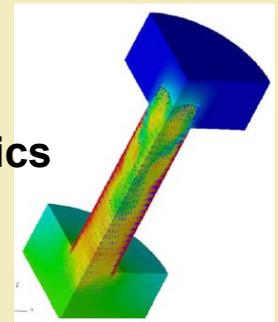
These codes represent that first suite of applications on BlueGene/L and are/will be available (subject to export control issues) for wide distribution to the scientific community

LLNL's multiscale materials modeling effort represent 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

Continuum

Yield surface

Mesoscale

ALE3D

Single crystal constitutive relation

NIKE3D

Microscale

Rules for dislocation motion and multiplication

Dislocation Dynamics

Atomic Scale

Molecular Statics and Dynamics

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

Successful implementation requires closely coupled experiments and models

LLNL's multiscale materials modeling effort is synergistic with the needs of the fusion program

Distance (m)						
Years — Performance						
Minutes — Constitutive properties						
Milliseconds — Microstructure evolution / Alloy phase stability						
Microseconds — Cascade aging and solute re-distribution						
Nanoseconds — Defects and defect/plasma interactions						
Femtoseconds — Electronic structure, plasma physics						
10^{-10}	10^{-9}	10^{-8}	10^{-6}	10^{-2}	1	
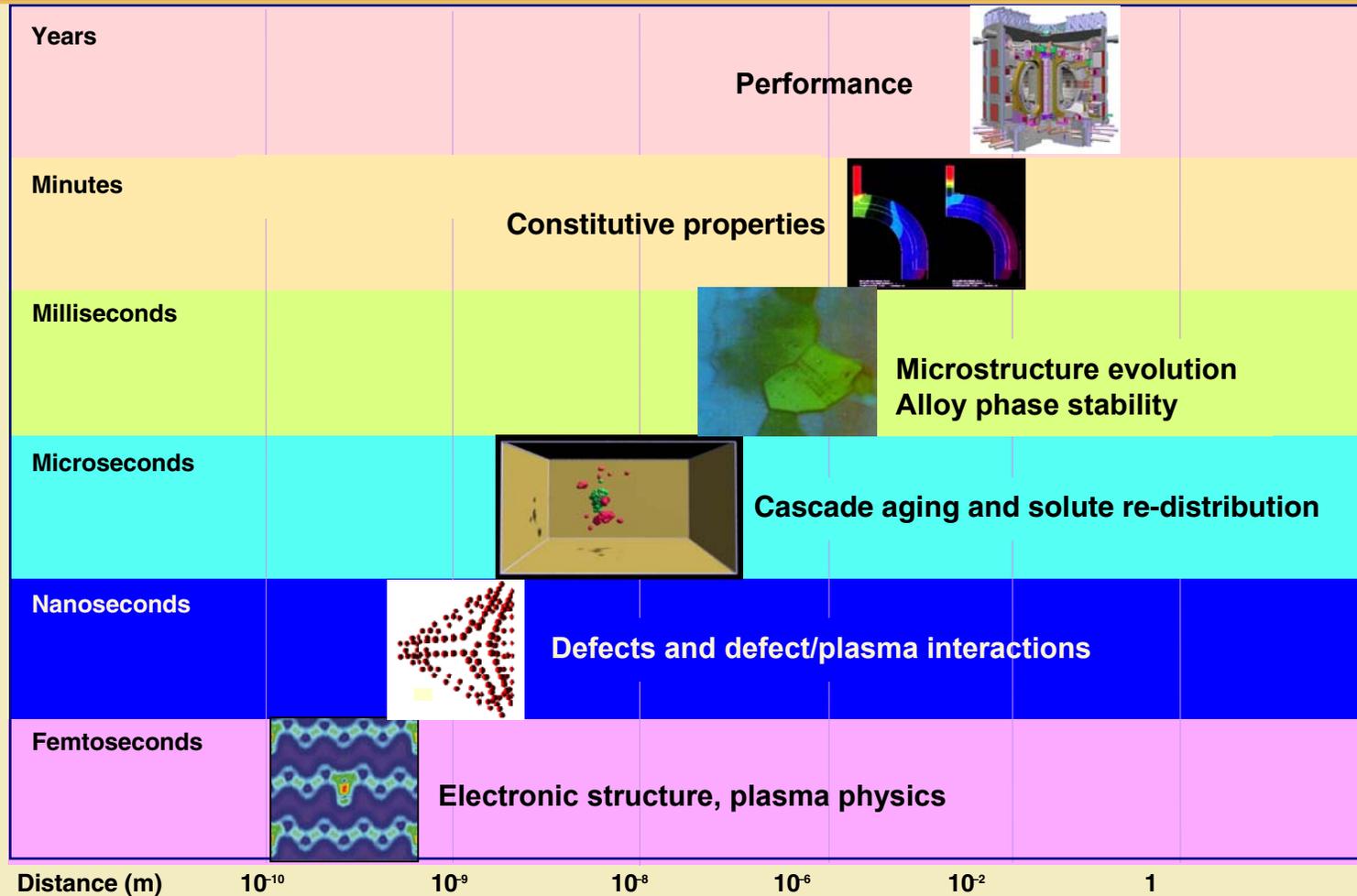
Goal: an integrated multi-scale simulation environment for designing and predicting the performance of fusion materials

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

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

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

3D DD simulations represent the link between atomistic simulations and macroscopic continuum codes

3D Dislocation Dynamics ≈ 10-100 μm

Numerical infrastructure

Initial dislocation structure

10-100 μm
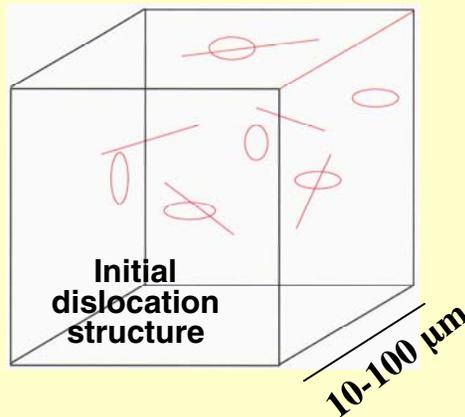
- **Discretization**
- **Time step**
- **Long range stress fields (parallel computing)**
- **Boundary conditions**

+

Dislocation physics issues

- **Motion**
  — Kink nucleation
  — Kink mobility
  — Cross slip
- **Interaction with other dislocations**
  — Junction
  — Dipole
  — Jogs
- **Grain boundary**

Simulation prediction
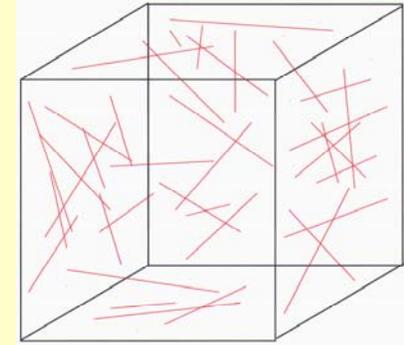
- **Dislocation structures**

σ

ε
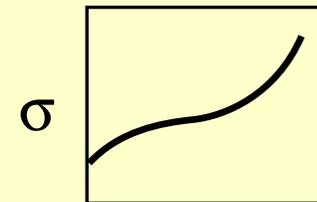
- **Single crystal strength properties**

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

a)

b)

Effective Plastic Strain (%)
0.634649
0.550029
0.465409
0.380789
0.296169
0.21155
0.12693
0.0423099
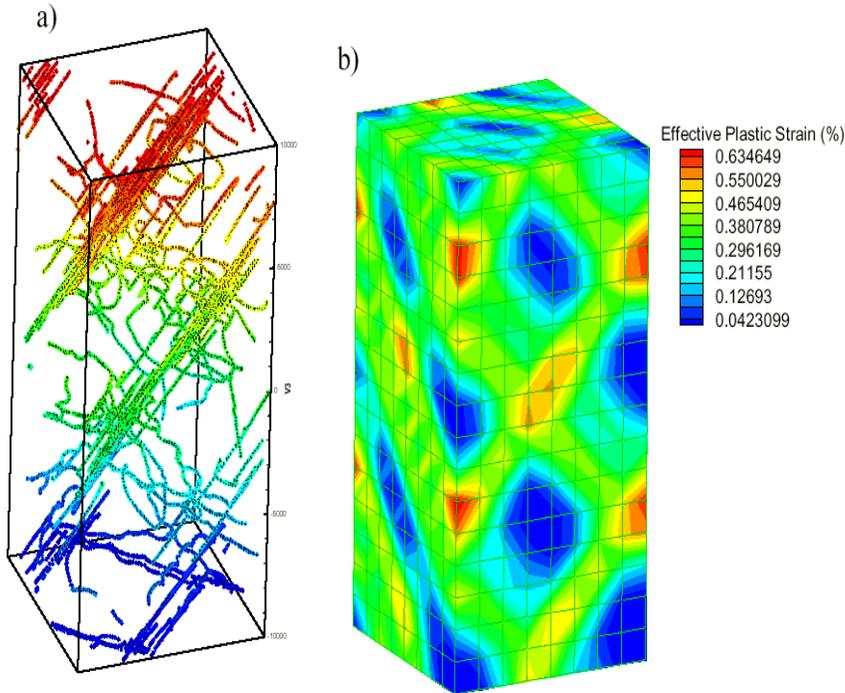
	Number of segments	Plastic strain
What we need	$N_s > 10^6$	$\varepsilon^P > 10\%$
What we had	$N_s < 10^4$	. $\varepsilon^P \sim 0.1\%$

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

$d\sigma/d\varepsilon \sim \mu/300 = $ **0.43 GPa**

$d\sigma/d\varepsilon \sim \mu/10 = $ **13 GPa**

stress – strain
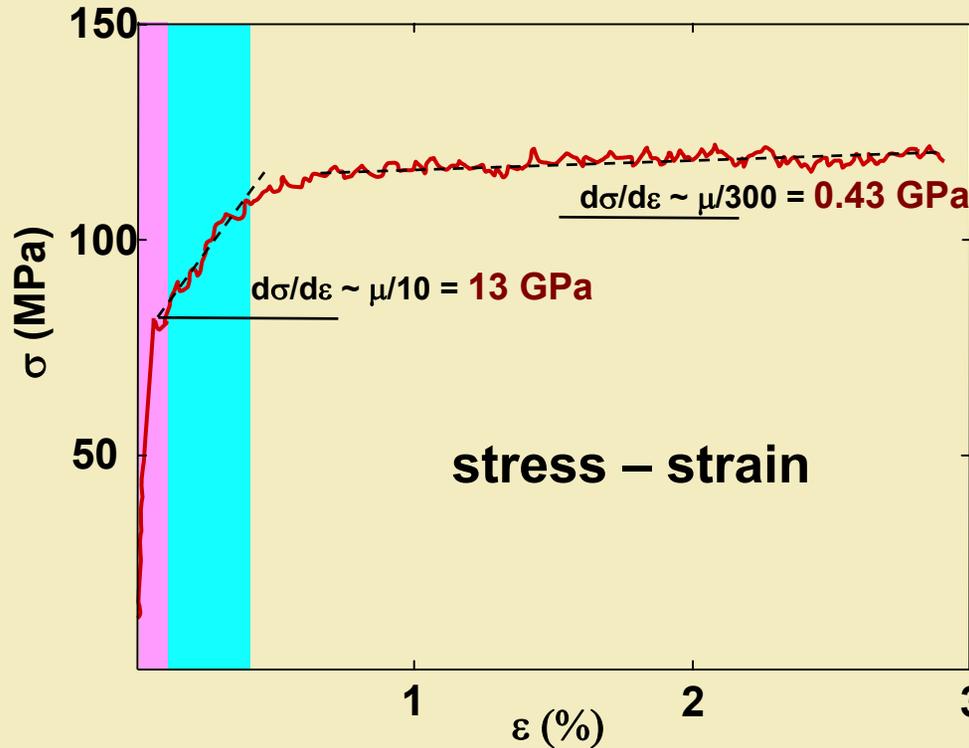
Experimental Data

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

~0.5 GPa

~20 GPa

Simulation by M. Tang
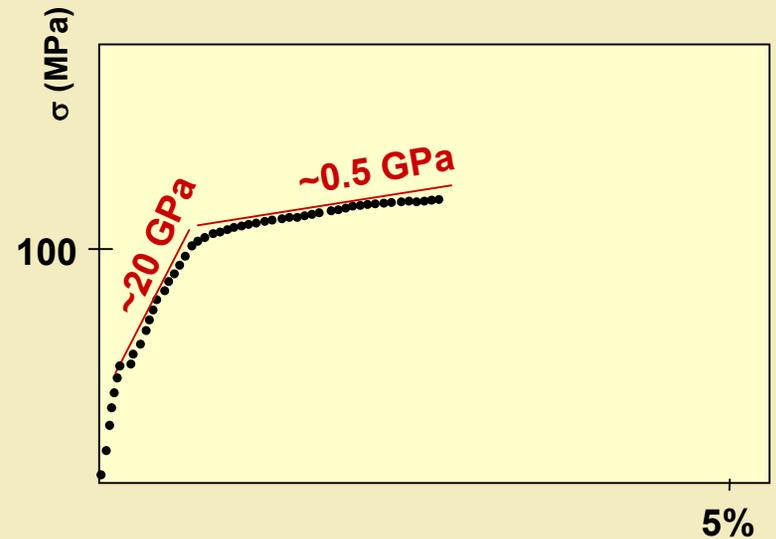
Two weeks on a 512 CPUs of SP3 machine

We are carrying out statistical analysis of evolving dislocation configurations to investigate the development of dislocation patterns

dislocation density evolution

Evidence of dynamic recovery in stage II
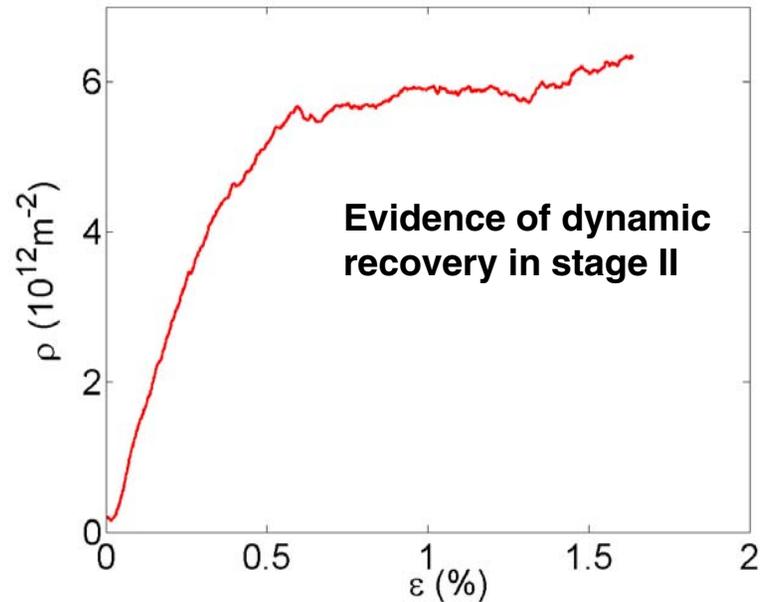
Dislocation pair distribution function in (11-1) plane of fcc Ni
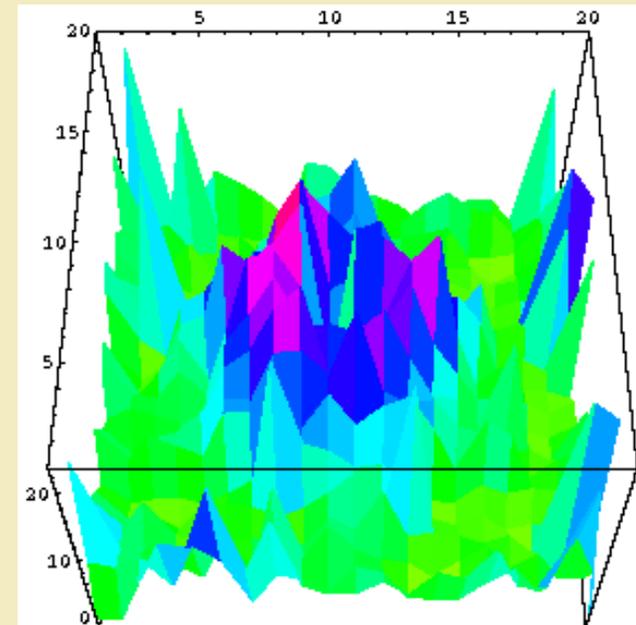
We continue to improve the current code and will release it in stages - ParaDiS – Parallel Dislocation Simulator

Ongoing Work

- **Port growing model on a growing machine – Blue Gene/L challenge**
- **Elastic anisotropy: at no additional computational cost**
- **Free surfaces: non-singular treatment of threading dislocations + FEM**
- **Ability to handle climb**
- **More stable and efficient integrators: implicit, semi-implicit**
- **Langevin dislocation dynamics**
- **Interaction with radiation defects**
- **Interaction and co-evolution with alloy microstructure - combining phase fields and DD**

The goal is to make 3D-DD routine

- **A single hero DD simulation to 10% plastic strain now will take three weeks on a 2,000 CPU**

- **A series of standard simulations should take < 3 days on 512 CPU**

- **Routine simulations of the same size should take < 8 hrs on 512 CPU**

- **Stage 1:** Limited release (in process) source code to collaborators
- **Stage 2:** Unlimited release of source code through OUP website (later in 2004/2005)

V. Bulatov and W. Cai "*Computer Simulations of Dislocations*" (Oxford University Press, 2004)

We are investigating new directions to couple alloy and dislocation microstructure evolution under irradiation conditions

Combination of Phase-Field and Dislocation Dynamics
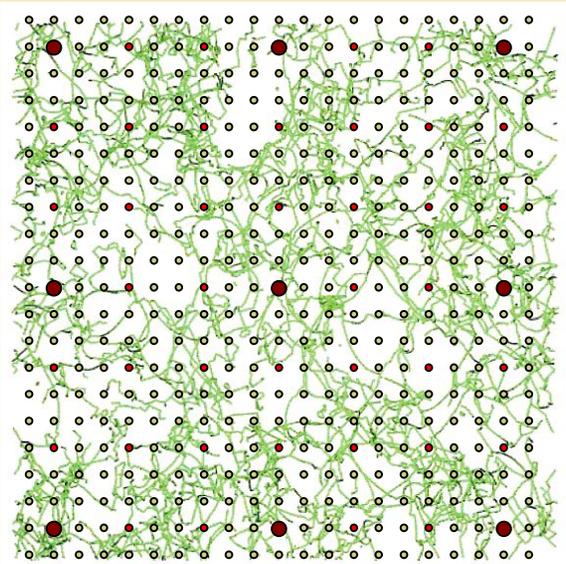
- PFM and DD are complimentary methods

- 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

Detailed crystal model

 • **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**
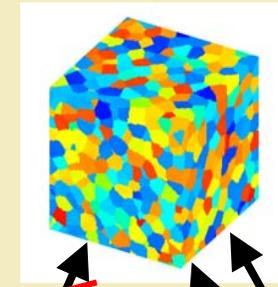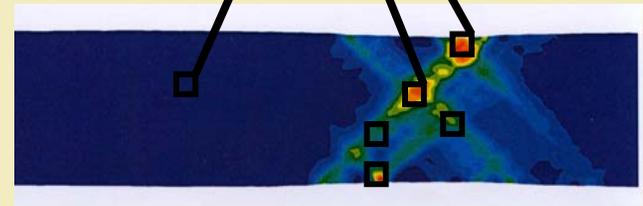
Run detailed model only where things are happening

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

Tokamak magnetic fusion device   Simulated edge-plasma region

edge plasma
core region
X-point
divertor plate
Vertical position
Major radius

C. Whole edge plasma region
Edge plasma code

B. Near-surface plasma sheath
Neutral/plasma Monte Carlo

A. Solid plate - carbon, W, etc
Molecular dynamics and surface Monte Carlo
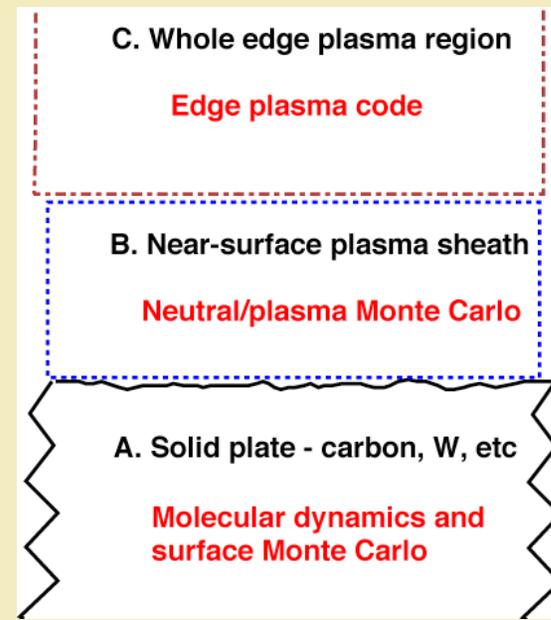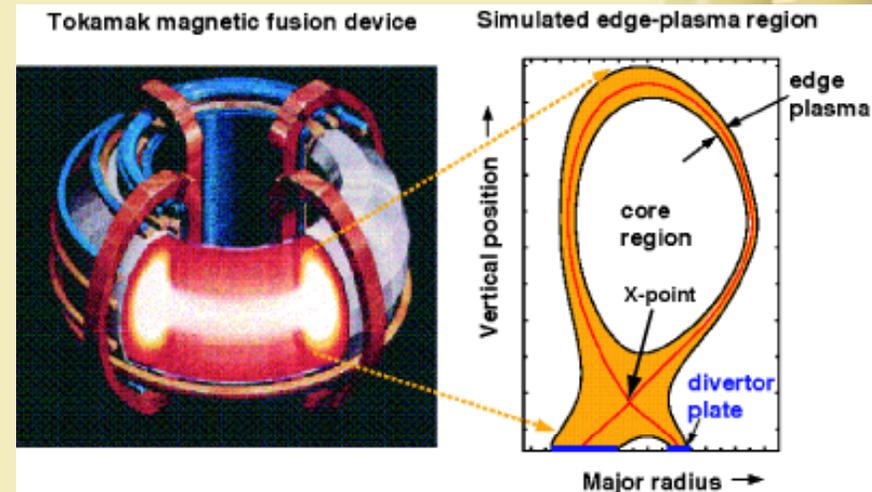
Two-way coupling

Experimental validation is essential - we are developing new ultrafast e⁻ and x-ray diagnostics of materials under extreme conditions

New ultrafast electron microscopy

Unique user experimental capabilities

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

pulse generator

Nd: YAG laser
266 nm
7 ns

treating laser
7 ns / 532 nm
100 fs / 620 nm

voltage step generator

trigger unit → PC

Point x-ray source

Shock wave driver
(laser or x-ray)

Unshocked

Shocked

Shock compression

Lattice planes

Crystal

CLS

GeV   FFTB
       <100 fs

RF Gun

Existing Linac

Bunch Compressor 1

Bunch Compressor 2

- Dynamic Transmission Microscope (DTEM): photocathode to produce pulse

- Inter-frame times 10

- Streaking capability
  - Image mode, Diffraction mode

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
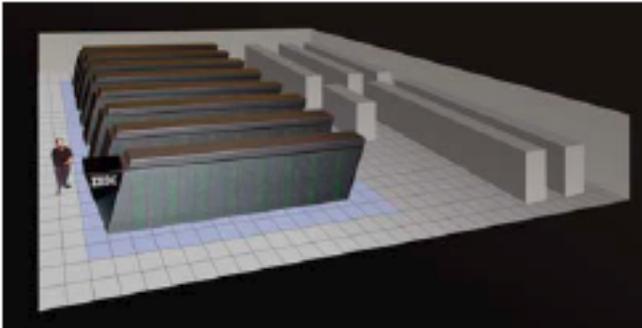
Computational materials science group of Vasily Bulatov's

and neurons

… 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

Pair potential Molecular Dynamics

Density Functional Theory Band structure of solids

-40

Many body potentials

Ab initio Molecular dynamics

-20

M-EAM/MGPT Angular Forces

Ab Initio **Order N**

-10

Bond Order Potentials

Tight Binding/ DMFT

t_0
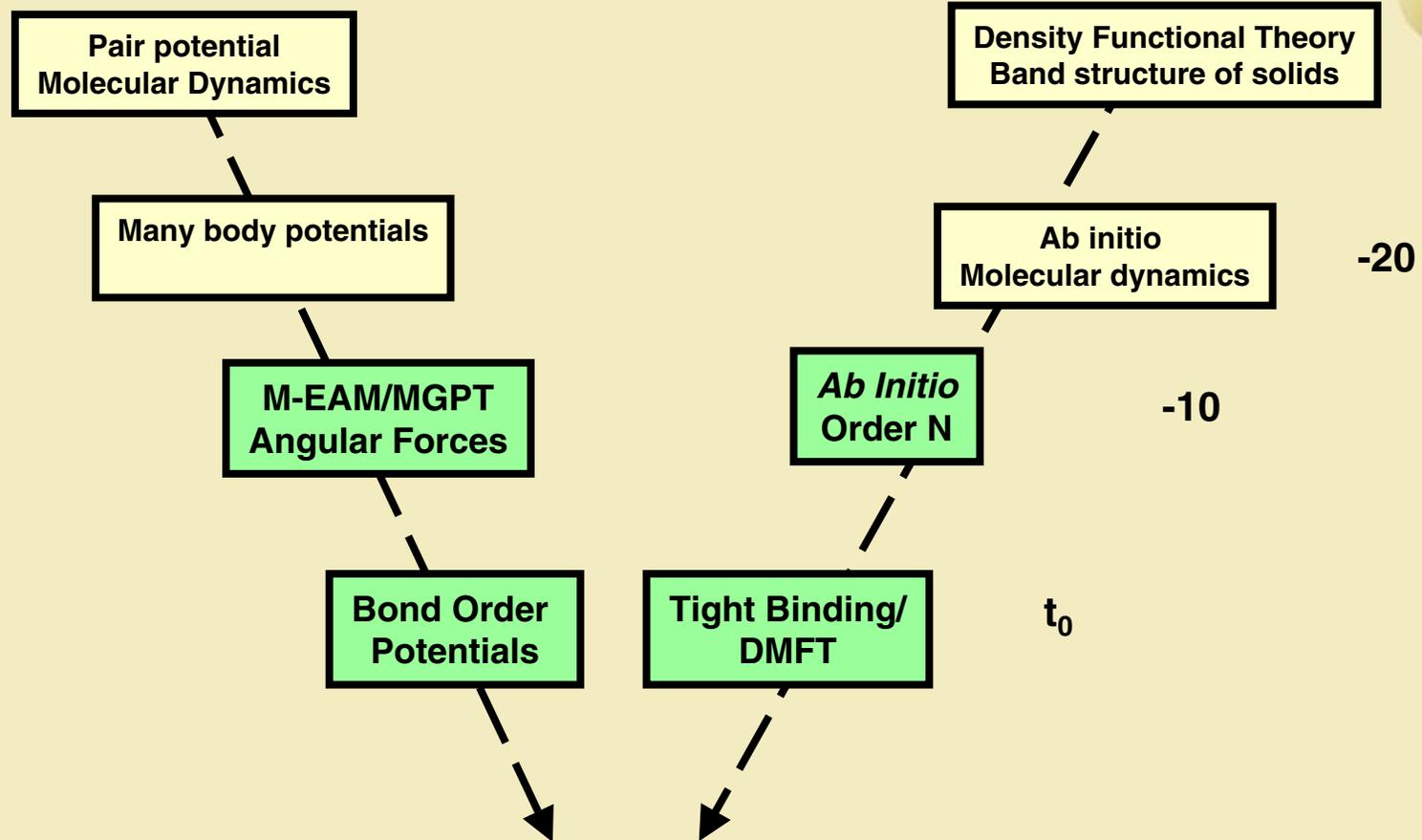
Future atomistic models must incorporate *ab initio* physics in a tractable manner