Computational and modeling challenges to simulate materials under extreme conditions

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Our universe provides various regions of extreme conditions far from thermodynamic equilibrium.


http://www7.nationalacademies.org/bpa/projects_cpu_index.html

Interplanetary dust particle - Bradley et al. 1984
New experimental techniques are reaching time and length scales comparable to the ones in atomistic simulations.

Process control under extreme conditions ➔ production of new materials & comprehension of astrophysical processes.
MD limitations in materials sciences

Main Challenges:
Memory limitations +
Communication limitations

Additional problems:
Short range vs. long range potentials (how to find neighbors?), increasing complexity of potentials, I/O (including checkpointing), on the fly analysis, etc.

Pushing boundaries has led to many Gordon-Bell awards
Are we currently stagnating?

Figure by T. Germann for SPaSM (LANL)
Example: Multi-scale models of plasticity and phase diagrams are needed to predict high pressure, high strain rate plastic flow in ductile metals (Remington et al.)

Electronic scale  Atomistic scale  Microscale  Macroscale continuum

Phase boundaries vs loading rates (kinetics)

Thermal activation vs phonon drag

Hu, 2010
Henning, 2008
Pecker, 2005
Kerley, 2003
“Potential” problems: EAM potentials, phonons and elastic constants

or when, even if the PV EOS is OK, other things can go wrong

Ruestes et al., Materials Science & Engineering A 613, 390 (2014)

Good agreement with phonons at P=0 GPa, but discontinuities in elastic constants, due to splines in the potential, lead to multiple elastic fronts
**Another example: EFS Ta Potential**


- Excellent agreement with PV, equilibrium Hugoniot, **melt line**, etc.
- Elastic constants OK up to ~1 Mbar.
- **BUT**... BCC→HCP at ~69 GPa (Ravelo *et al*., SCCM-2011).

Potential validity depends strongly on type of fit, which can emphasize a certain property, temperature & pressure range, structure, etc.

Potentials are often non-transferable 😞
ncFe under pressure: plasticity + phase transition (bcc $\rightarrow$ hcp/fcc)

Potentials

Mendelev ($\sim 65$ GPa)

MEAM-p ($\sim 13$ GPa)

Ackland ($\sim 20$ GPa)

Voter ($\sim 8$ GPa)

Homogeneous compressive loading, Gunkelmann et al., PRB 86 (2012) 144111
Simulation details need to include info on BC

**Coupling to continuum?**

- PBC in (x,y), free BC with expansion (z). Langevin bath with critical damping at the sides.
- Need to re-calculate damping for each interatomic potential and bath condition.
- There are complex schemes to have impedance matching at boundaries, but none standard.
- Size has to be large enough to capture desired phenomena. Need to verify this by running simulations of different sizes: results should not change beyond certain size $L$, or they could be extrapolated versus $1/L$. 

Simulation of hot spot

- Langevin, $T=0.1$
- Mobile, NVE
- Track, $T=10$
- Fix
Large-scale MD links nano and microscales in damage induced by nanoprojectiles [C. Anders et al., PRL 108, 027601 (2012)]

$R_{\text{cluster}} = 20$ nm, 20 ps after impact, $\sim 300 \times 10^6$ atoms, 15 hours using 3,840 CPU’s in Thunder (LLNL)

Only dislocations + liquid atoms are shown
Data analysis

• On the fly and post-processing of data takes considerable time …
• Need to choose appropriate analysis tools to avoid artificial results.
• Whenever possible, carry out the analysis in parallel with domain decomposition and neighbor lists.
• Care must be taken with time averaging, thermodynamic variables.
Thermodynamics? Temperature in nano systems

Usual: \( (3/2) N k_B T = E_{\text{kin}} \)

Nano Systems: \( T_\omega = \frac{1}{k} \left[ \left( \frac{3N}{2} - 1 \right) \langle E_{\text{kin}}^{-1} \rangle_{\mu} \right]^{-1} \)

Pearson et al, PRB (1985)

Correction due to non-zero flow velocity \( <v> \):

\[ E_{\text{kin}} \rightarrow (m/2) (v - <v>)^2 \]

\( E_{\text{kin}} > 0 \), but \( T = ?? \)

“Partial” \( T \)'s: \( T_{\text{rot}}, T_{\text{vib}}, T_{ij} \)
Thermodynamics?
Can we define an atomic stress tensor? Only with caveats

\[ S_{ab} = -\left[ m v_a v_b + \frac{1}{2} \sum_{n=1}^{N_p} (r_{1a} F_{1b} + r_{2a} F_{2b}) + \frac{1}{2} \sum_{n=1}^{N_b} (r_{1a} F_{1b} + r_{2a} F_{2b}) + \right. \\
\left. \frac{1}{3} \sum_{n=1}^{N_a} (r_{1a} F_{1b} + r_{2a} F_{2b} + r_{3a} F_{3b}) + \frac{1}{4} \sum_{n=1}^{N_d} (r_{1a} F_{1b} + r_{2a} F_{2b} + r_{3a} F_{3b} + r_{4a} F_{4b}) + \right. \\
\left. \frac{1}{4} \sum_{n=1}^{N_i} (r_{1a} F_{1b} + r_{2a} F_{2b} + r_{3a} F_{3b} + r_{4a} F_{4b}) + \sum_{n=1}^{N_f} r_{ia} F_{ib} \right] \]

\[ a, b = x, y, z \] Includes thermal, pair, bond, angle, dihedral, improper, and “fix”
Be careful with \( Nk_B T \) term …it should discount flow velocity in calculation of \( T \)
\[ S = \sigma V \] ➔ how do we define “atomic” volume to calculate momentum flux?

**Possible solution**: use Voronoi polyhedra

**PdH nanoclusters**. Using Voronoi or mean volume gives roughly the same results. Work with G. Bertolino, M. Ruda (Centro Atomico Bariloche), S. Ramos, E. Crespo (UN Comahue, Neuquen)

**Int. J. Hydrogen Energy (2012)**
Perfect crystals are the `spherical horse’ of atomistic simulations
(also for many model Hamiltonians)

How to make more realistic simulations? Add defects:
vacancies → voids → bubbles, interstitials, dislocation loops/lines,
grant boundaries (bi-cristals → polycrystals), impurities, etc.

Polycrystal (50 nm grain size)
(400 million atoms)
Few GB are Σ boundaries …
Not 1 dislocation but many …
Common Neighbor Analysis

- **CNA**: a parameter to measure the local disorder
- Sensitive to cutoff radius, **problems at large uniaxial strain**
- 12 nearest neighbor for perfect FCC and HCP crystals, 14 nearest neighbors for perfect BCC crystals

\[ r_{cc}^{fcc} = \frac{1}{2} \left( \frac{\sqrt{2}}{2} + 1 \right) a \approx 0.8536 a \]
\[ r_{cc}^{bcc} = \frac{1}{2} (\sqrt{2} + 1) a \approx 1.207 a \]
\[ r_{cc}^{hcp} = \frac{1}{2} \left( 1 + \sqrt{\frac{4 + 2x^2}{3}} \right) a \]


*This is done for every atom in the sample ➔ high computational cost*
Centro-Symmetry Parameter (centro)*

- **Centro-symmetry parameter** (*centro/CSP*): a parameter to measure the local disorder, particularly useful to study cubic structures. Problem at large temperatures.

\[ C = \sum_{i=1}^{6} \left| \vec{R}_i + \vec{R}_{i+6} \right|^2 \]

CSP expression for a f.c.c. unit cell

This is done for every atom in the sample ➔ high computational cost

Kelchner et al, FIG. 2, partial view. Defect structure at the first plastic yield point during indentation on Au (111), (a) view along [112], (b) rotated 45° about [111]. The colors indicate defect types as determined by the centrosymmetry parameter: partial dislocation (red), stacking fault (yellow), and surface atoms (white). Only atoms with \( P > 0.5 \) are shown.

DXA (Dislocation eXtraction Algorithm)

Stepwise conversion of atomistic dislocation cores into a geometric line representation.

(a) Atomistic input data.
(b) Bonds between disordered atoms.
(c) Interface mesh.
(d) Smoothed output.

Changes in DXA parameters can have large effect on results

Modified DXA + ParaView

Atomistic simulation of the mechanical properties of a nanoporous b.c.c. metal *

ParaView visualization of the results provided by DXA for a nanoporous Ta sample subjected to a $10^9$/s uniaxial compressive strain rate at an 8% strain. Preprocessed sample has 1.9 million atoms.

Run: 3 days in 32 cores
Analysis of each snapshot: 10 min run on AMD M520 + 4Gb RAM (dual core)

CNA analysis takes about 1/3 of the total analysis time

* Ruestes et al., Scripta Materialia (2012)
Can we obtain dislocation densities?

- Rough estimate of total dislocation density calculated from the number of atoms with CNA not BCC, and dividing by n (2-10) to account for cross-section of dislocation cores.
- Mobile dislocation densities calculated from plastic heating* [A. Higginbotham et al., JAP (2011)].

Can we compare our results with experiments?

After relaxation to P=0. Possibly, because long-term recovery of the microstructure in bcc samples should have minor effects on total density. Note the absence of twins in the recovered sample, which can be checked with X-ray diffraction.

Analytical GND model shows good agreement with MD

Ruestes et al., Mod. Sim. Mat. Sci. (2013)
ncTa: twinning (CAT+OIM sim) and dislocations (DXA)
E. Hanhn (UCSD), D. Tramontina (U.N. Cuyo), T. Germann (LANL)

Experiment:
No twins for Ta d~70 nm
Lu et al. MSE A (2013)

MD: d~5-30 nm

Inverse Hall-Petch for twinning

Hall-Petch for twinning

FCC: exp + model by Zhu et al.
J. Mater Sci (2013) 48, 4467

23 nm (Ni)
Simulated X-Ray diffraction (use cufftw)


**Twin detection in bcc metals:** Suggit et al, Phys. Rev. B (2013)

**Fe phase change:** Gunkelmann et al, Phys. Rev. B (2014)

**Experimental geometry:** 50 × 50 mm film, placed 30 mm in transmission, 8.05 keV (Cu Kα) X-rays, perpendicular to the film.
“Reaction-diffusion equation” to obtain initial foam

D. Schwen, A. Caro (LANL), D. Farkas (Va Tech)


Plasma exposed W-C surface
Takamura et al., Plasma and Fusion Research 1, 51 (2006)

Uses Cahn-Hilliard Equation, to generate 3D foam. OpenCL code by Schwen needs modifications for future research

Bringa et al, NanoLetters (2012)
Loading of high porosity ncAu foams (2-15 nm filaments)
Carlos Ruestes, UNCuyo

70% porosity foam
Elastic and plastic behavior

GBs


Porosity Model

Loading: “realistic” foam includes full dislocations in addition to SFs and twins. New porosity evolution model.

Porous samples simulated by granular mechanics

**Compaction wave for impact against hard wall**
Ringl *et al.*, PRE 91, 042205 (2015)

Granular mechanics of grain-surface collisions
Ringl *et al.*, PRE 86, 061313 (2012)
PRE KALEIDOSCOPE

Granular mechanics of nano-grain collisions

New granular friction scheme implemented for GPUs by E. Millan
GRANULAR simulations Benchmarks in GPU (extension of USER-CUDA)

GPU version by E.N. Millán
Code submitted to LAMMPS repository

The 7.5e4 curve represents the results obtained in C. Ringl (2012).

**CPU:** AMD Phenom x6 1055t 2.8GHz
**GPU:** NVIDIA Tesla c2050

**AVG speedup**
GPU vs 1 CPU core = 7x
GPU vs 6 CPU core = 2.95x

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Granular benchmarks in small clusters

Granular simulation with the GranularEasy pair style, with $4.48\times10^6$ grains and 1000 steps, for 1-64 processes, in Mendieta and ICB-ITIC clusters. Various NVIDIA GPUs are tested: C2050, C2075 and M2090.

Tesla c2050 GPU $\sim$ 16 CPU cores ICB-ITIC cluster.

Mendieta Tesla M2090 GPUs best performance using 4 GPUs in two cluster nodes. speedup of $\sim4.2 \times$ against the best CPU result (ICB-ITIC cluster with 16 CPU cores).

Elongated box, too much communication
COMPLEXITY in cluster collisions

Parameters:
✓ Velocity (v)
✓ Impact parameter (x)
✓ Radius (d/2)
✓ Structure
✓ Orientation of the lattice

“Numerical” experiments using LAMMPS: parameter sweep for cluster collisions

Need to sweep over relative orientation, velocity, R, etc. (1e6 sims)

**Goal:** reduce the total wall-clock time of multiples jobs executing parallel processes both in the CPU and GPU.

**Ad-hoc strategy:** split jobs bewteen CPU&GPU. Could be improved further with other job scheduling tools.

**Different parallel modes considered:**
- Process parametric study on multicore CPU workstation using OpenMPI.
- Process parametric study on the GPU.
- Hybrid studies: RUBY script to assign workload both to CPU and GPU according to predefined strategy. MPI plus Dynamic or Static load balancing.
- Only up to 10 simultaneous jobs in single GPU, due to memory limitations.
Plasticity threshold in grain-grain impacts

Granular models typically assume lack of plasticity


GPU + CPUs to run ~1,000,000 independent MD simulations

Future (?) of MD

• **Sample size:** in 10 years, ~tens of μm, but most simulations still sub-μm.

• More/better **hybrid codes** to extend time and length scales: MD+MC, MD+kMC, MD+DD, MD+continuum, MD+BCA, MD+TB, MD+CPMD, MD+QMMM. Examples in LAMMPS ...

• **Time scale problem:** new algorithms to extend time scale and simulate thermal evolution.

• Better description of **electronic effects** by:
  
  I) Physics + Chemistry + Biology ➔ “reactive” potentials that are accurate and efficient for full periodic table. Need reactive potentials which work for radiation (ZBL) and high P.

  II) coupling to CPMD, tight-binding, etc. (TDDFT?)

  III) TTM, Ehrenfest dynamics, inclusion of magnetic effects, etc.

**Major roadblocks (need brave volunteers!)**

• Computers are becoming faster and larger, but algorithms for **long range potentials** (biology & oxides), ab-initio and continuum simulations typically do not scale well beyond couple thousand CPUs ➔ expect better results within the next 10 years.

• No set recipes to build **better potentials**, specially if chemistry (reactive potentials) or electronic effects (charge transfer, potentials for excited states, etc.) are involved.

• Nobody knows yet what to do to efficiently solve the time scale problem beyond some relatively simple model problems.

• **Data mining and viz** for TBs datasets? Open source simulated X-ray and TEM imaging (talk)
Summary: there are many opportunities for MD


• New hardware: better (faster/greener/cheaper) processors, connectivity, memory and disk access; MD-tailored machines (MD-GRAPE-4, Anton, etc.); GPUs, Phi, MICs, hybrid architectures (GPU/CPU); cloud computing, etc.

• Experiments going micro-nano/ns-ps ➔ same as MD

• Can go micron-size, but still have to connect to mm-m scale ➔ novel approaches needed, including smart sampling, concurrent coupling, dynamic/adaptive load balancing/refining for heterogeneous systems, asynchronous simulations, etc.

• Need better and cheaper reactive potentials to handle non-equilibrium scenarios

• Need human resources with mix of hardware, software & science expertise.
That’s all folks!!

SiMAF: Simulations in Materials Science, Astrophysics, and Physics

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