50 years of Molecular Dynamics

Aneesur Rahman

1927-1987

- *Correlations in the Motion of Atoms in Liquid Argon*, Physical Review 136, A405-A411 (1964).
- 864 Lennard-Jones atoms on CDC 3600 computer
- 780 timesteps, 45 sec/step
- Irving Langmuir Prize - 1977
- American Physical Society (APS) Computational Prize is named in Aneesur's honor

What's new in LAMMPS

Steve Plimpton
Sandia National Labs
sjplimp@sandia.gov

4th LAMMPS User Workshop
August 2015 - Albuquerque, NM

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.
Presentation: SAND2015-6465C

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  - Stephen Foiles (Sandia)
  - Andres Jaramillo-Botero (Caltech)
  - Fabio Pavia (EPLF and Ansys, Switzerland)
  - Jim Larenztos and Brian Barnes (ARL)
  - Gary Grest (Sandia)
  - Christoph Kloss (DCS Computing, Austria)

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  - Christoph Kloss (DCS Computing, Austria)
- DOE/NNSA ASC - funding for facility/equipment rentals
- Materials Design - providing lunches!
- Scienomics - providing snacks and drinks!

Social activities

2 dinners & tram ride:

3 recreational choices:

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  2014 stats:
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- Please talk to LAMMPS developers whenever/wherever you can find us. Or just send us an email.

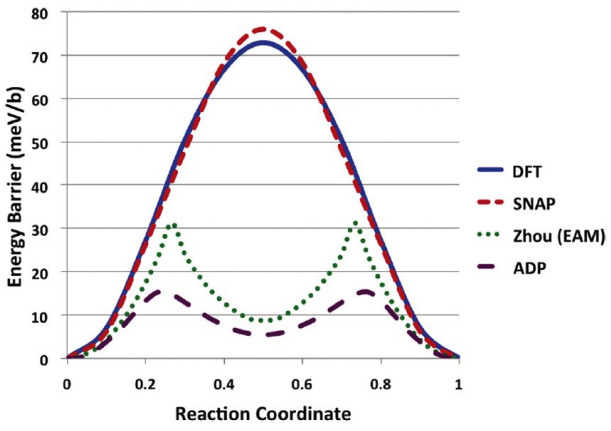
New interatomic potentials (pair styles)

- Comb3 with polarization effects
  - U Florida groups of Sinnott and Phillpot
  - metals, oxides, hydrocarbons
- Ziegler-Biersack-Littmark (ZBL)
  - Stephen Foiles and Aidan Thompson (Sandia)
  - strong short-range repulsions
  - can be added to other potentials via pair hybrid
- Peridynamics
  - Rezwanur Rahman talk (Fri 8:30 AM), UT Austin
  - new viscoelastic and elastic/plastic models
- Soft segmental repulsive potential (SRP)
  - Tim Sirk (ARL)
  - prevents bond-crossing in DPD polymer chains
- QEq charge equilibration
  - Ray Shan talk (Wed 2:15 PM), Sandia
  - matrix and damped dynamics methods via fix qeq
  - can be added to other potentials (ReaxFF,COMB,etc)
  - with coul/streitz and EAM, enables Streitz-Mintmire potential

New "quantum-accurate" potentials

- Goal is to be as good as DFT for some systems, at a fraction of the cost
- Derived from "big data" archives of DFT results

- QUIP
  - Albert Bartok (Cambridge U)
  - interface to their QUIP MD code
  - variety of potentials including GAP
- SNAP
  - Aidan Thompson talk (Thu PM breakout A1), Sandia
  - new potential for tantalum



Two polarization models

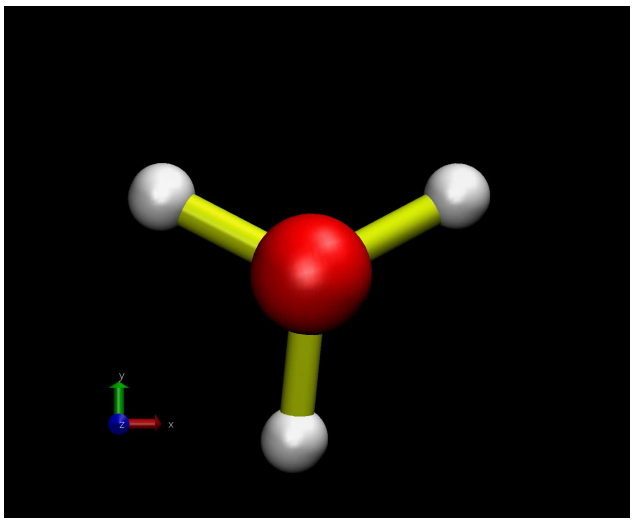
In addition to fix qeq (fluctuating charge) and COMB3 pair style ...

- Adiabatic core/shell model
  - Hendrik Heenan (Technical University of Munich)
  - CORESHELL package
  - crystalline materials
- Thermalized Drude dipole model
  - Alain Dequidt (Clermont University, France), with Julien Devemy and Agilio Padua
  - USER-DRUDE package
  - molecular systems and fluid states
- Helpful docs
  - doc/Section_howto.html: 24, 25, 26
  - doc/tutorial_drude.html

Two path-integral MD (PIMD) options

- Quantum MD via Feynman path integral method
  for quantum effects like tunneling
- One atom $\Rightarrow$ ring polymer of P quasi-beads,
  equivalent to QM partition function

- Fix pimd command
  - Chris Knight & Yuxing Peng
    (U Chicago)
  - uses multi-replica partitioning
    within LAMMPS
  - scales nicely to large systems and
    machines
- Fix ipi command
  - Michele Ceriotti (EPFL)
  - i-PI Python package performs PIMD
  - LAMMPS called as client (via
    sockets) to compute forces/energies



Acceleration packages

- Kokkos package
  - Christian Trott, Stan Moore, Ray Shan (Sandia)
  - support for GPUs, Xeon Phi, OpenMP
  - 31 pair styles, some bonded styles, no PPPM (yet)
  - Stan talk (Thu 9:30 AM)
- Intel package
  - Mike Brown talk (Wed 3:15 PM), Intel
  - support for Xeon Phi, optimization for Intel CPUs
  - 5 pair styles, no PPPM (yet)
- GPU package
  - Mike Brown and Trung Nguyen (ORNL)
  - support for GPUs
  - 43 pair styles, PPPM
- USER-OMP package
  - Axel Kohlmeyer (Temple U)
  - 103 pair styles, 29 fixes, PPPM, Verlet & rRESPA
  - most bonded styles and PPPM variants
- USER-CUDA package being deprecated for Kokkos

Working to make acceleration packages easier to use

- All packages now usable via one build command
- Example:

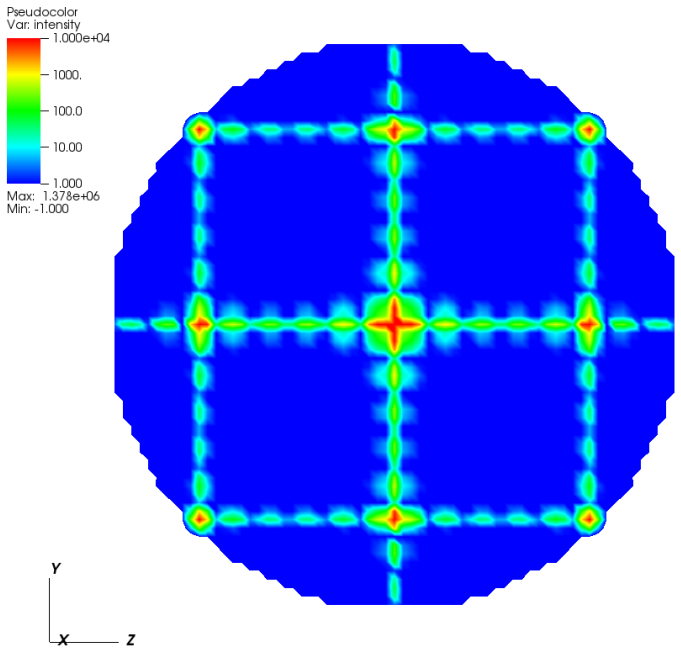
  Make.py -p gpu -gpu mode=single arch=31
  -o gpu -a lib-gpu file mpi

- Use same input script with any package:
- Example:

  mpirun -np 48 -ppn 12 lmp_gpu -sf gpu -pk gpu 2
  -in in.script

USER-DIFFRACTION package

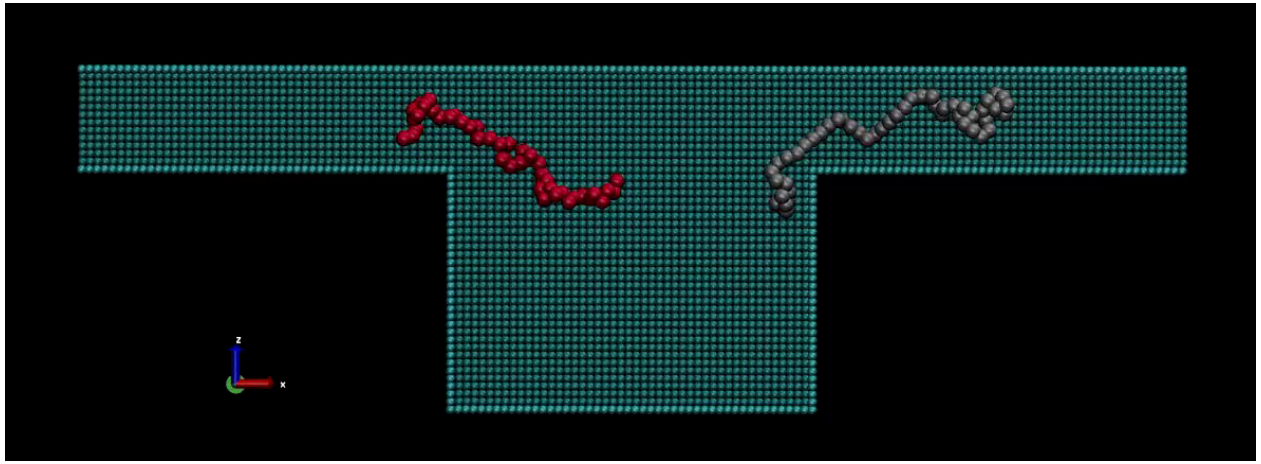
- Shawn Coleman talk (Thu 9:45 AM), ARL
- Compute X-ray and electron diffraction patterns
- Bulk Ni example:



VisIt package for visualization

USER-LB package for Lattice-Boltzmann

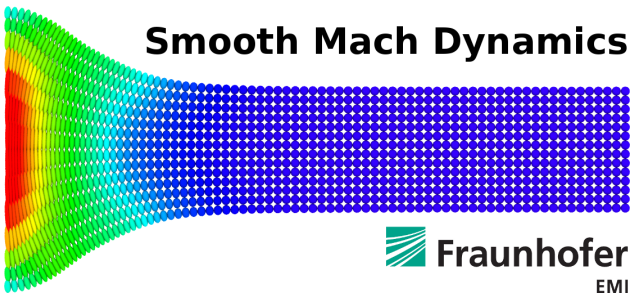
- Colin Denisston group (U Western Ontario)
- Venkat Bala poster (Fri 10:30 AM), UWO
- Particles in background Lattice-Bolztmann fluid
- MD particles influenced by hydrodynamic forces

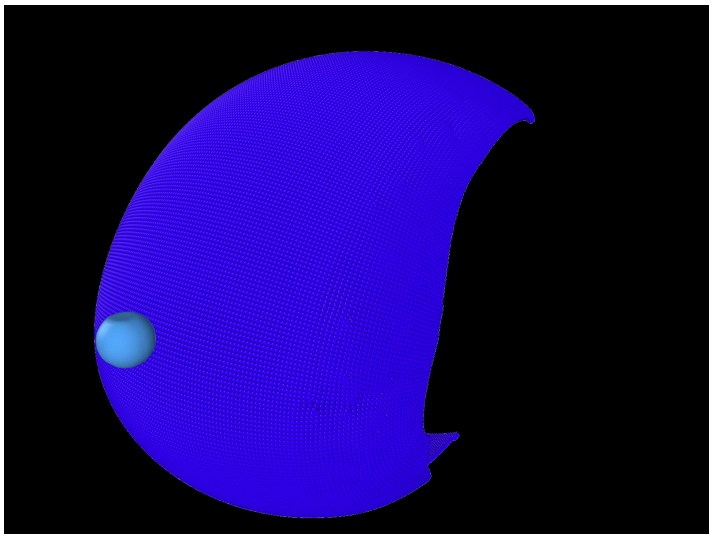


- Biopolymer filtration, Phys Rev Lett 112, 118301 (2014)
- GPU version for LB now available (contact Colin)

USER-SMD package = SPH for solids

- Georg Ganzenmueller (Ernst Mach Institute, Germany)
- Stable, quadratic convergence, various material models





Other new user packages

- USER-FEP package
  - Agilio Padua (Universite Blaise Pascal Clermont-Ferrand)
  - free-energy perturbation with soft potentials
  - fix adapt/fep command and several pair styles
- USER-QMMM package
  - Axel Kohlmeyer (Temple U)
  - couple LAMMPS with DFT using Quantum Espresso
  - LAMMPS performs MD algorithm, BC, constraints, etc
  - QE called to compute QM forces (subset of atoms and procs)
  - could be generalized to other DFT codes
- USER-QTB package
  - Yuan Shen, Tingting Qi, and Evan Reed (Stanford)
  - quantum nuclear effects (low temperatures, heat capacity)
  - fix qtb and fix qbmsst commands

Monte Carlo options

MC only, or MC moves interspersed with MD
Paul Crozier (Sandia), Aidan Thompson talk (Fri 9:15 AM)

- Fix gcmc command
  - Atomic/molecular insertions/deletions, rotate, displace
  - Supports all pair styles, KSpace
  - Local or global energy evaluation
- Fix atom/swap command
  - Metropolis MC for surface relaxation
  - Swaps atom types, displaces atoms
- Fix tfmc command
  - Kristof Bal (U Antwerp, Belgium)
  - Force-biasing to enable longer timescales
  - E.g. chemical vapor deposition onto surface

Molecule template files

- New molecule command reads molecule template file
  - coords, atom types, bond topology (angles, dihedrals, etc)
  - center of mass, moment of inertia
    for overlapping finite-size particles
- Input to other commands:
  - create_atoms (with molecules)
  - molecule insertion: fix gcmc, fix deposit, fix pour
  - fix rigid/small
- See doc/molecule.html for details

Invoke Python code from your input script

In addition to Python scripts calling LAMMPS ...

- New python command defines a Python function
  - Function can be in-lined in input script or in a file
  - Pass LAMMPS variables to Python, values returned
  - Associate function with python-style variable
  - Python function invoked whenever variable is evaluated
    - Immediate in input script (parameter for command)
    - Every N steps during a simulation when fix requests it
  - Function can callback into LAMMPS (e.g. grab atom coords)
- Why?
  - Make input script into a real programming language:
    complex looping, branching, etc
  - Compute values more complex than LAMMPS variables allow
  - Easier way to add functionality than C++ coding
    - assuming it's not a time-critical operation
- See doc/Section_python.html for details

New chunk commands

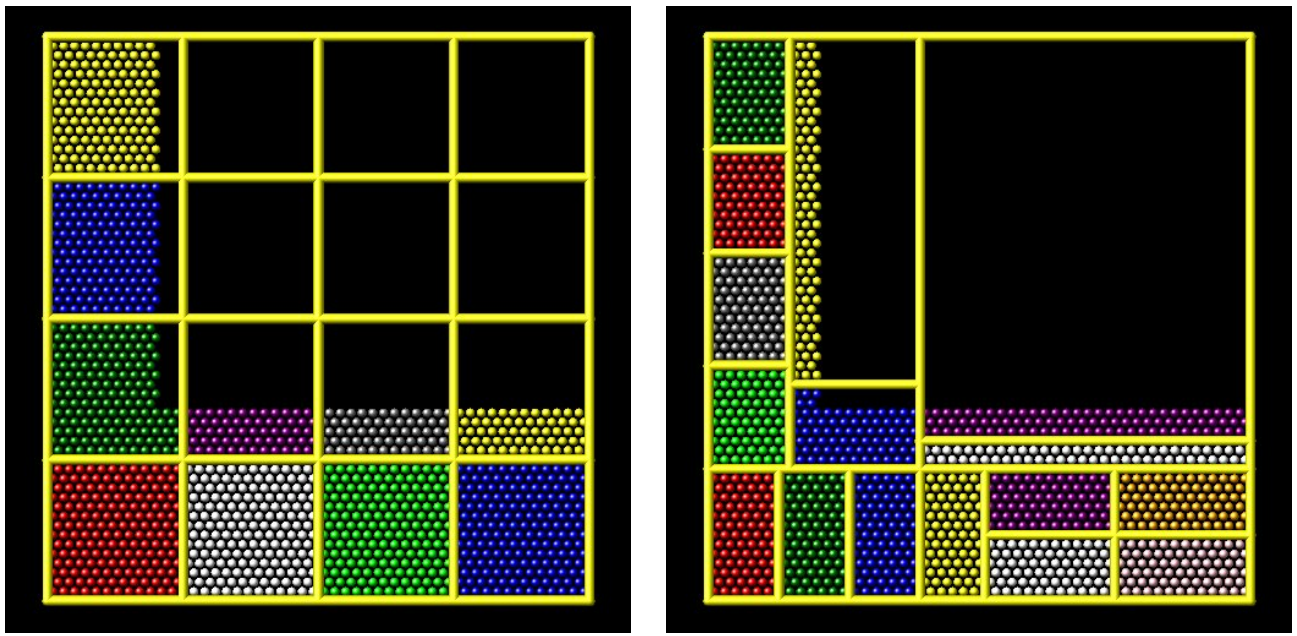
- General way to compute quantities for subsets of atoms
- Chunk = atoms in spatial bin, molecule, same atom type, etc
- More generally, chunks can be set by any atom property, output of per-atom compute or atom-style variable
  - atoms in local clusters
  - atoms within velocity windows
  - atoms with similar potential energy
  - atoms with same local defect structure
- Compute chunk/atom assigns chunk ID to each atom
  - one-time or dynamically (e.g. as clusters change)
- Compute */chunk commands calculate per-chunk values
  - count, sum of atom property, COM, MSD, etc
- Fix ave/chunk time averages & outputs per-chunk values
- See doc/Section howto 23 for overview

Miscellaneous input/output enhancements

- Read_data command
  - can now be used multiple times
  - allows building of system, component by component
  - e.g. substrate, adsorbed molecule, solvent
- Write_data command
  - write out a data file for current configuration
  - replaces old restart2data program
- MPIIO package for parallel I/O
  - Paul Coffman (IBM)
  - read/write of dump and restart files

Load-balancing via RCB

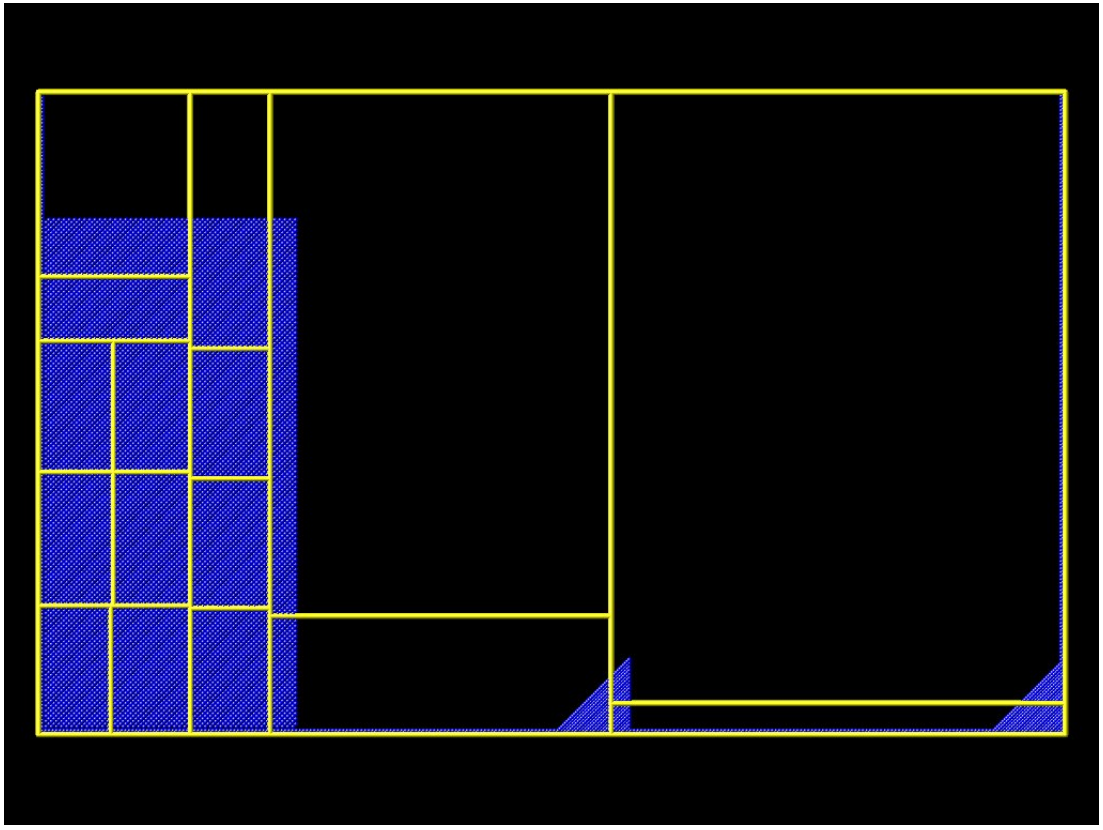
- RCB = recursive coordinate bisectioning
- Assigns same number of (weighted) atoms per processor
- See balance and fix balance commands
- Often needed for coarse-grained models
  - DPD, SPH, Peridynamics, granular, etc



- Worked to reduce comm with 26 neighbors to 6+ (for 3d)

Load-balancing examples for soft and hard materials

2d SPH "water" flowing over a dam
Georg Ganzenmueller (Ernst Mach Institute, Germany)



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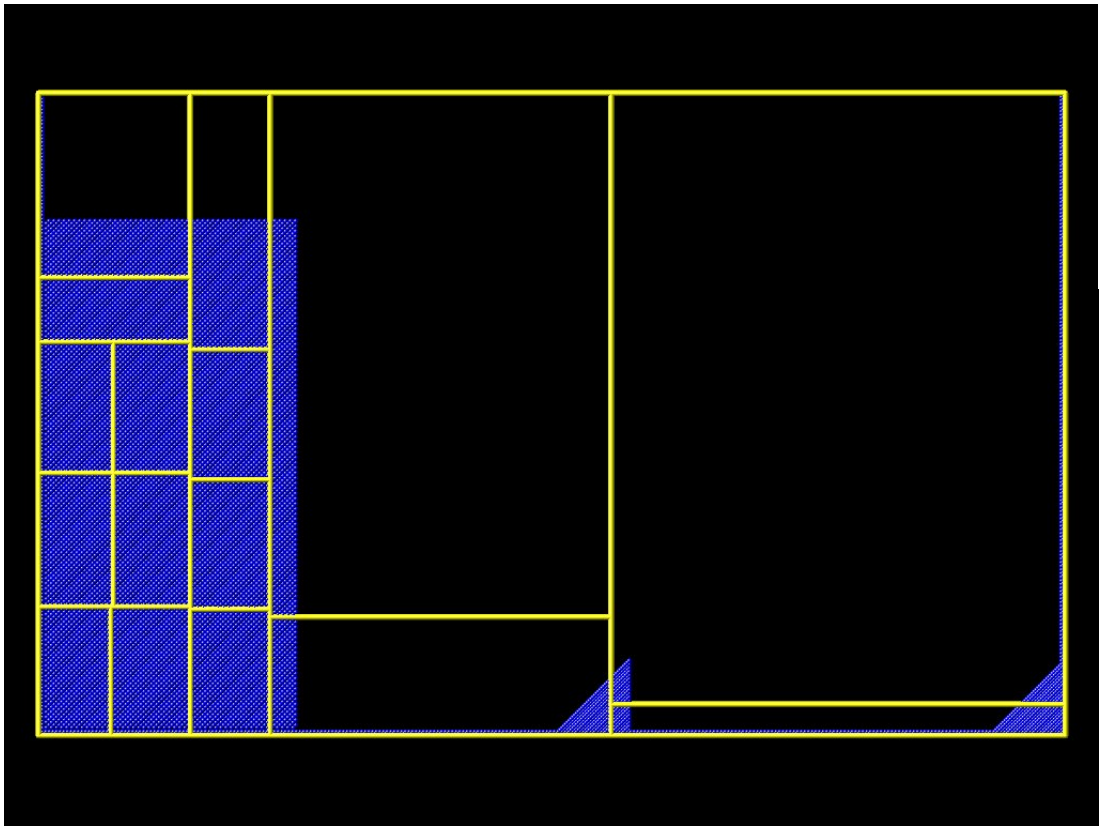

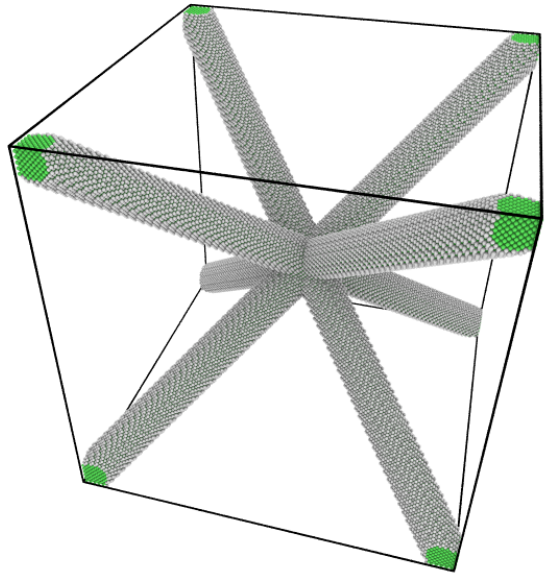

Atomic microlattice of metal struts
Alex Stukowski (Tech Univ Darmstadt)

- star imbalance = 18x
- 13x speed-up for 21M atoms on 16K cores

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