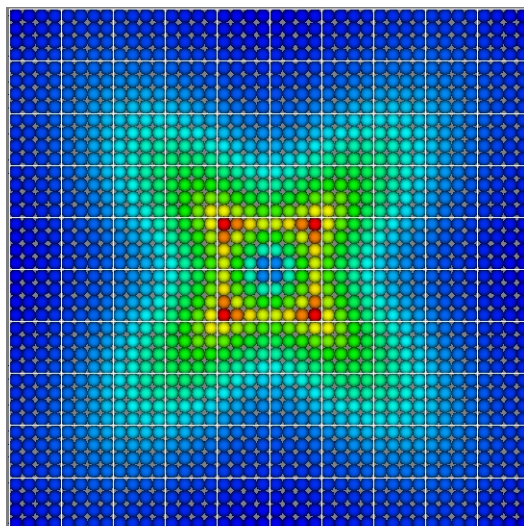


LAMMPS Workshop, Albuquerque, CA

August 7-8, 2013

Atom-to-Continuum (AtC) package for LAMMPS

aka paid advertising



Reese Jones,

Jeremy Templeton,

Jonathan Zimmerman

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.

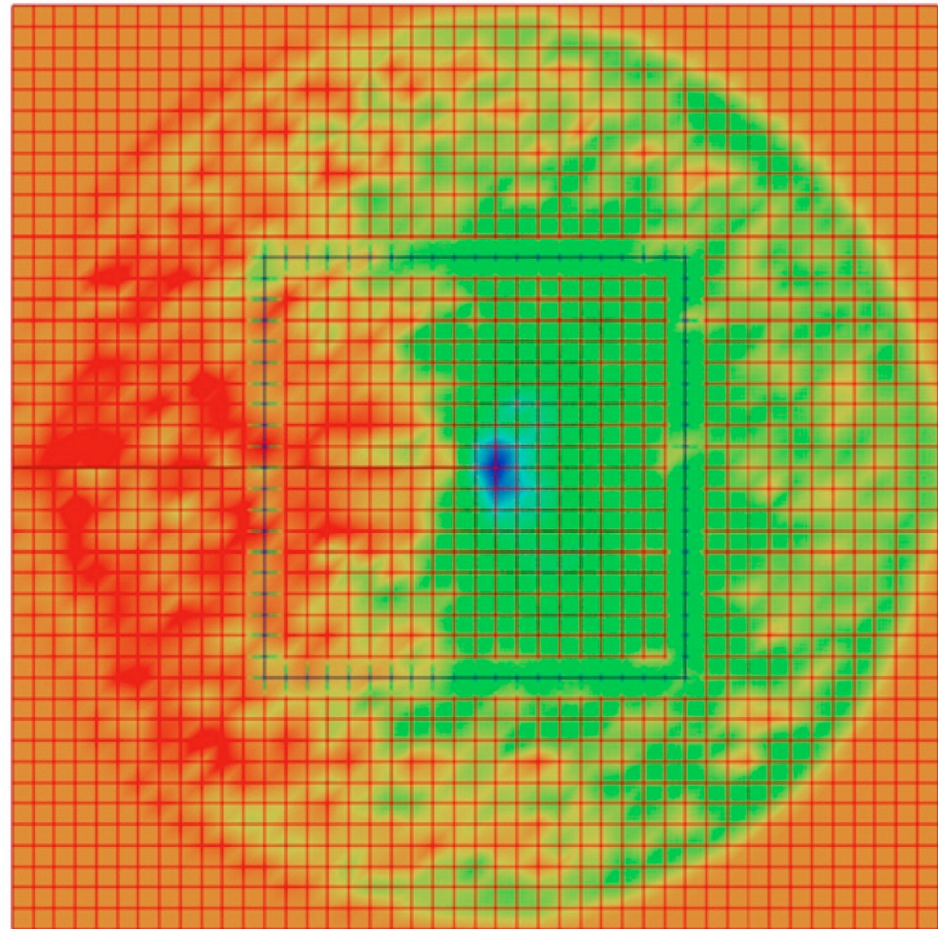


Sandia
National
Laboratories

Overview

- Objectives
- History
- Capabilities
- Examples
- Software
- Contacts
- Publications

Please ask questions



Stress field around crack at finite temperature



Objectives

- **Estimation** of continuum fields from atomistic simulation data using the consistent coarse-graining techniques. $A \rightarrow C$ *i.e. dots to rainbows*



Compressive stress field for an atomic simulation of shock loading

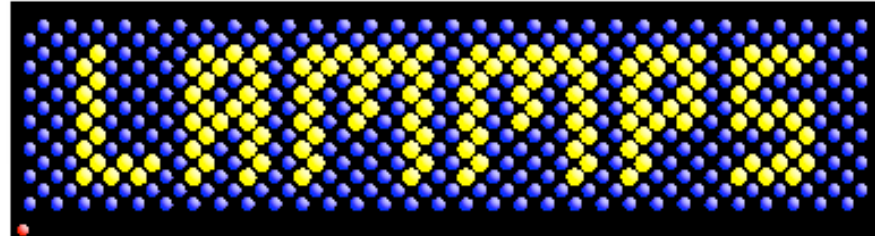
- **Coupling** of static and dynamic atomistic and finite element regions for rigorous thermal, mechanical, electrostatic & charge and mass transport simulations. $A \leftrightarrow C$ *... and back again*



History

- LeHoucq LDRD, Greg Wagner, Reese Jones, and later Jeremy Templeton:

Thermal coupling in WARP

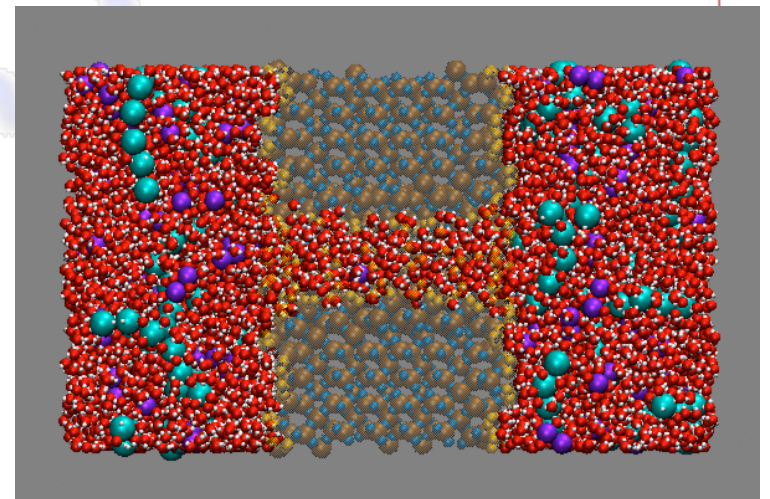


- Transition to LAMMPS
- Decisions about Matrix/Lin. Alg., FE library
- Expanding to have a Hardy capability (transition from Paradyn & Jon from Fortran → C++)
- Electron transport LDRD (Jones)
- J-integral ESRF (Jones)
- Ionic Fluids LDRD (Templeton)
- Dislocation/Plasticity ESRF (Zimmerman)



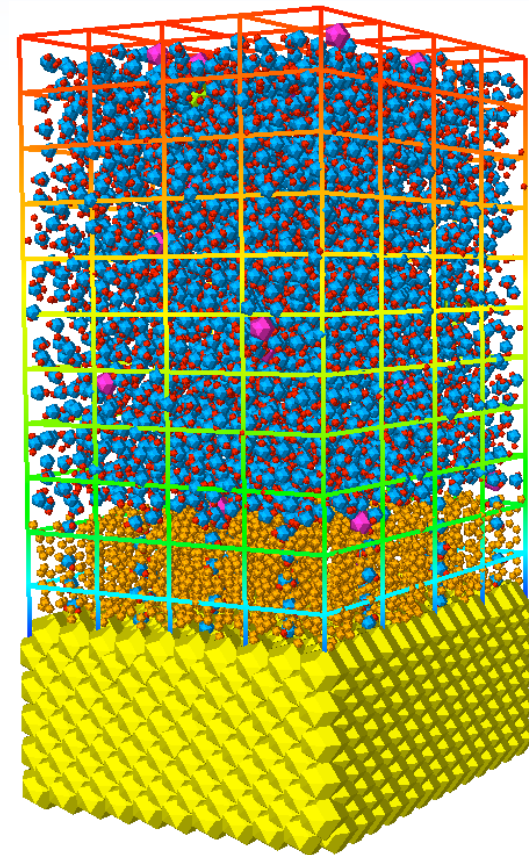
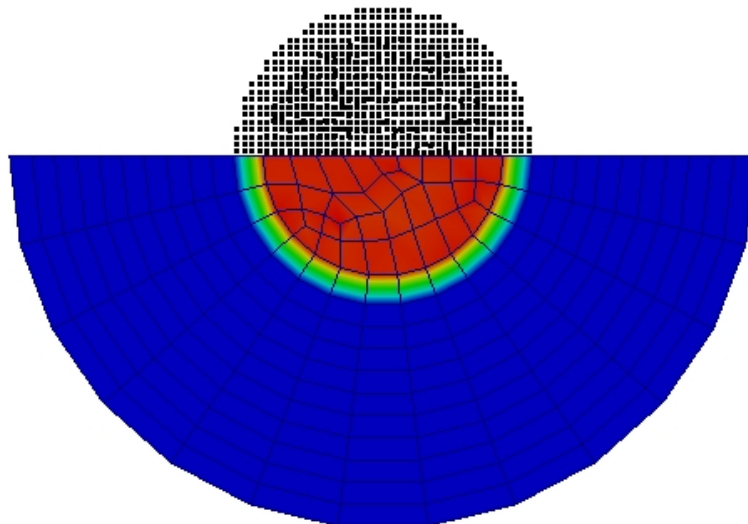
Capabilities

- Transfer/Coarse graining, fields: mass & charge density, displacement, velocity, stress, concentration, Eshelby stress, Cauchy-Born stress, temperature, potential energy, heat flux, electric potential, dipole moment, dislocation density, gradients, rates, contour & boundary integrals,
- Coupling: mass, charge, diffusion, mechanical/momentum, energy/thermal, thermo-mechanical, two temperature, drift diffusion, Schrodinger-Poisson, ...
- Arbitrary hex & tet meshes, library of kernel estimators and time filters
- Parallel, object oriented, extensible, benchmarked nightly with ~100 benchmarks, 80k+ lines of code



Examples

- Atoms, lattices, interatomic potentials
- Mesh, elements, constitutive surrogates
- Extrinsic fields & physics, e.g. electrons, electric field
- Filters: spatial estimators and temporal filters

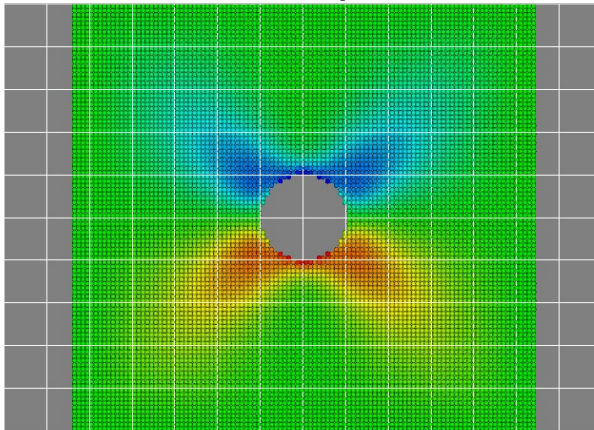


*Saltwater-electrode-CNT
system: mesh overlaps exactly
with water-CNT atom region*

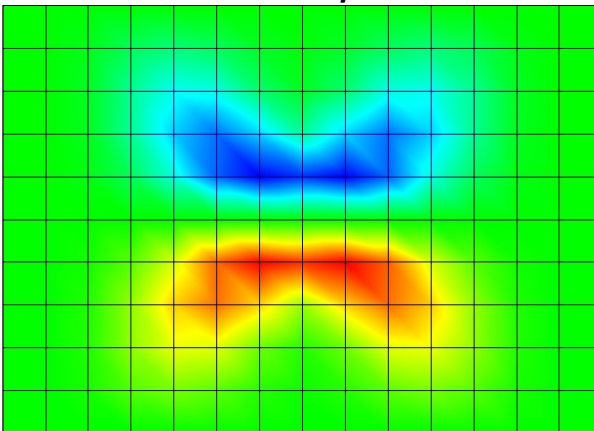


Example: Tensile stretching of a circular hole

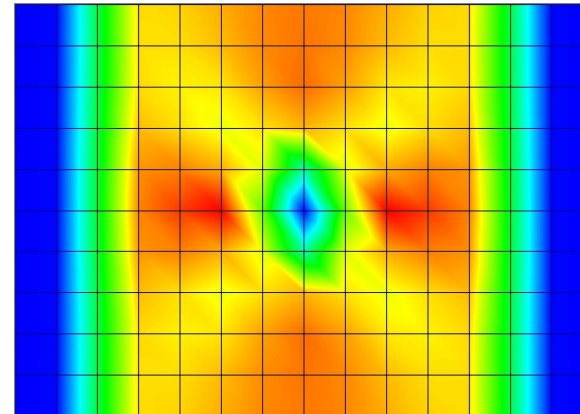
*Atoms colored by
horizontal displacement*



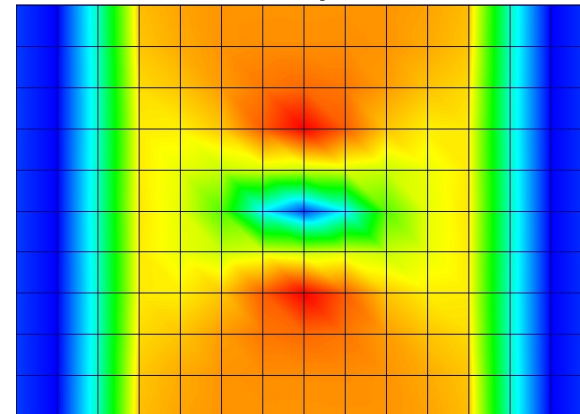
*Mesh colored by
horizontal displacement*



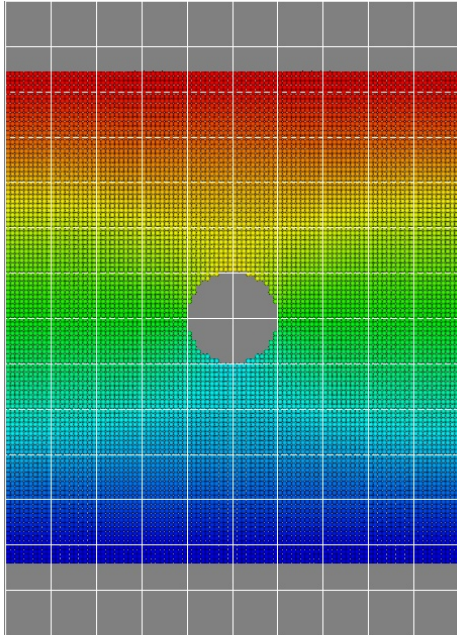
*1st Piola-Kirchoff stress,
11 component*



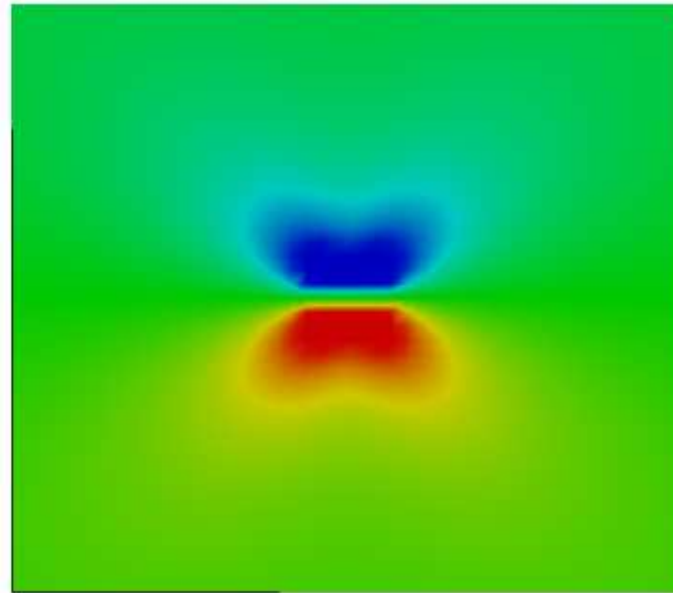
*1st Piola-Kirchoff stress,
22 component*



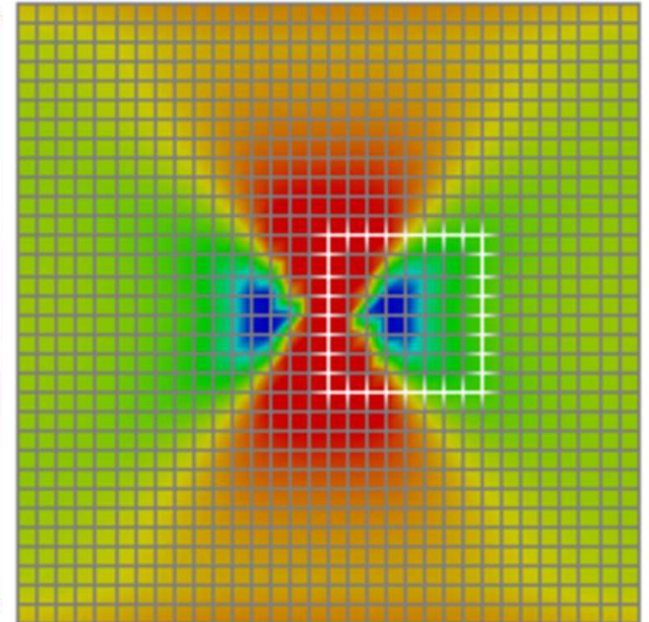
Example: Stress estimation



Circular hole in plate: mesh overlaps exactly with box, but atom region is subset



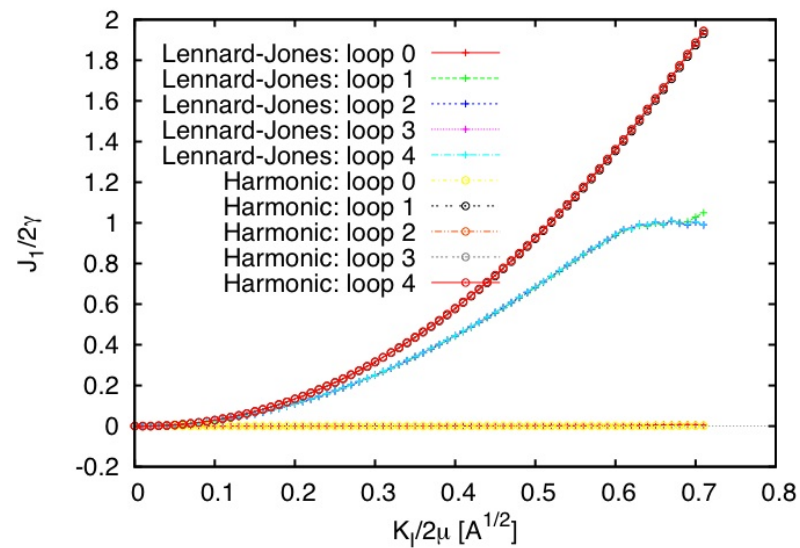
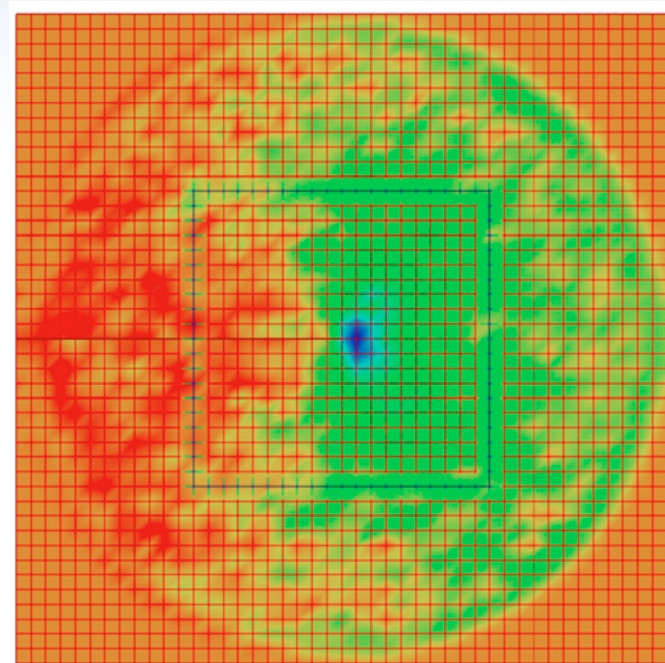
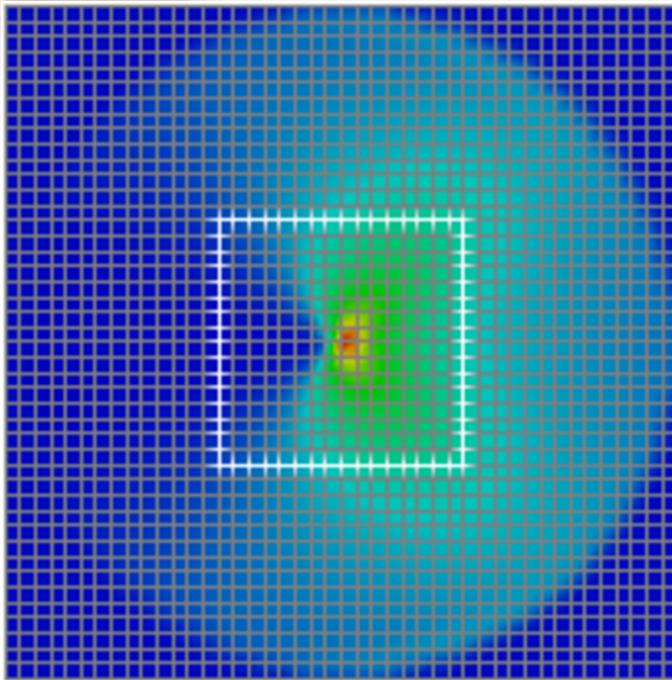
Stress around an atomistic edge dislocation



Eshelby stress around a finite crack

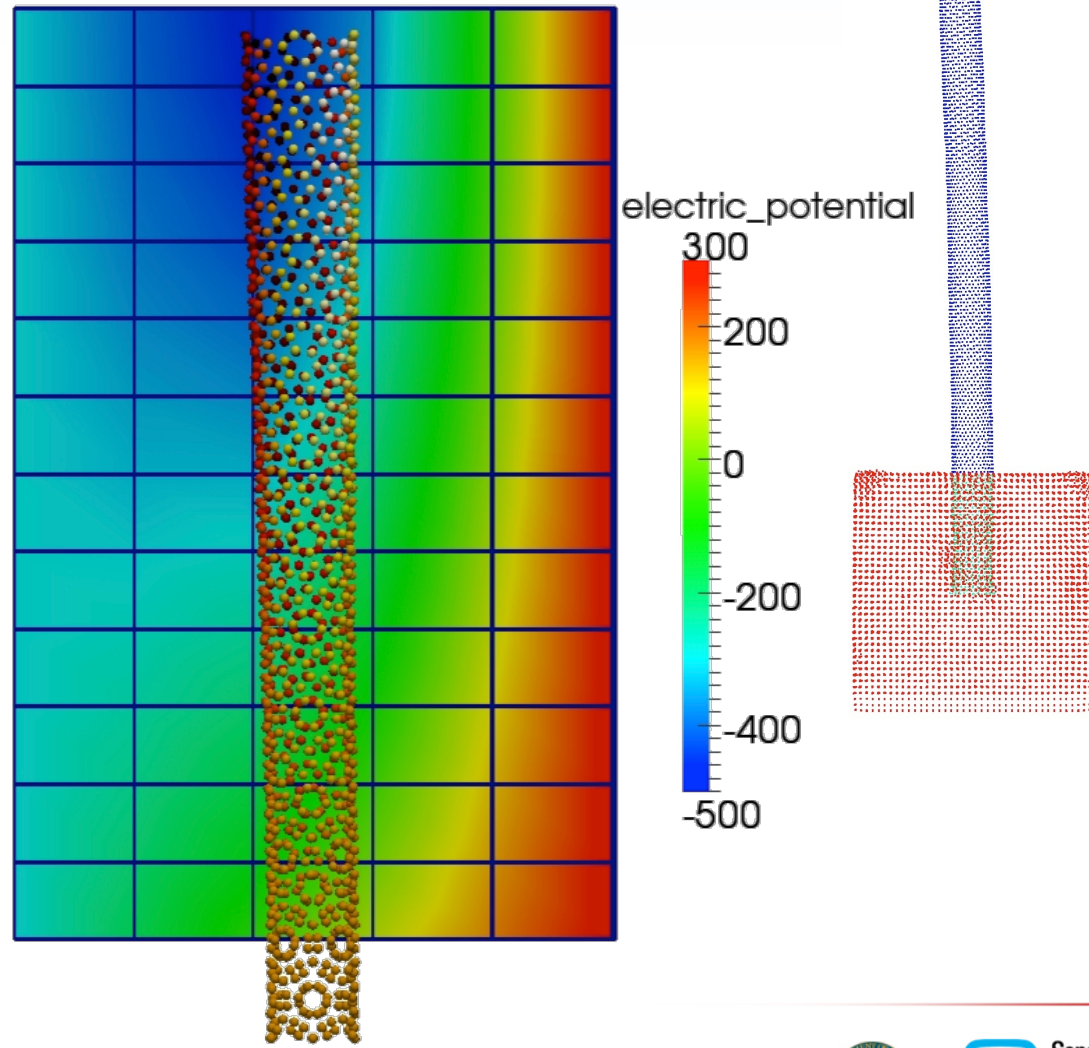


Example: J-integral calculation

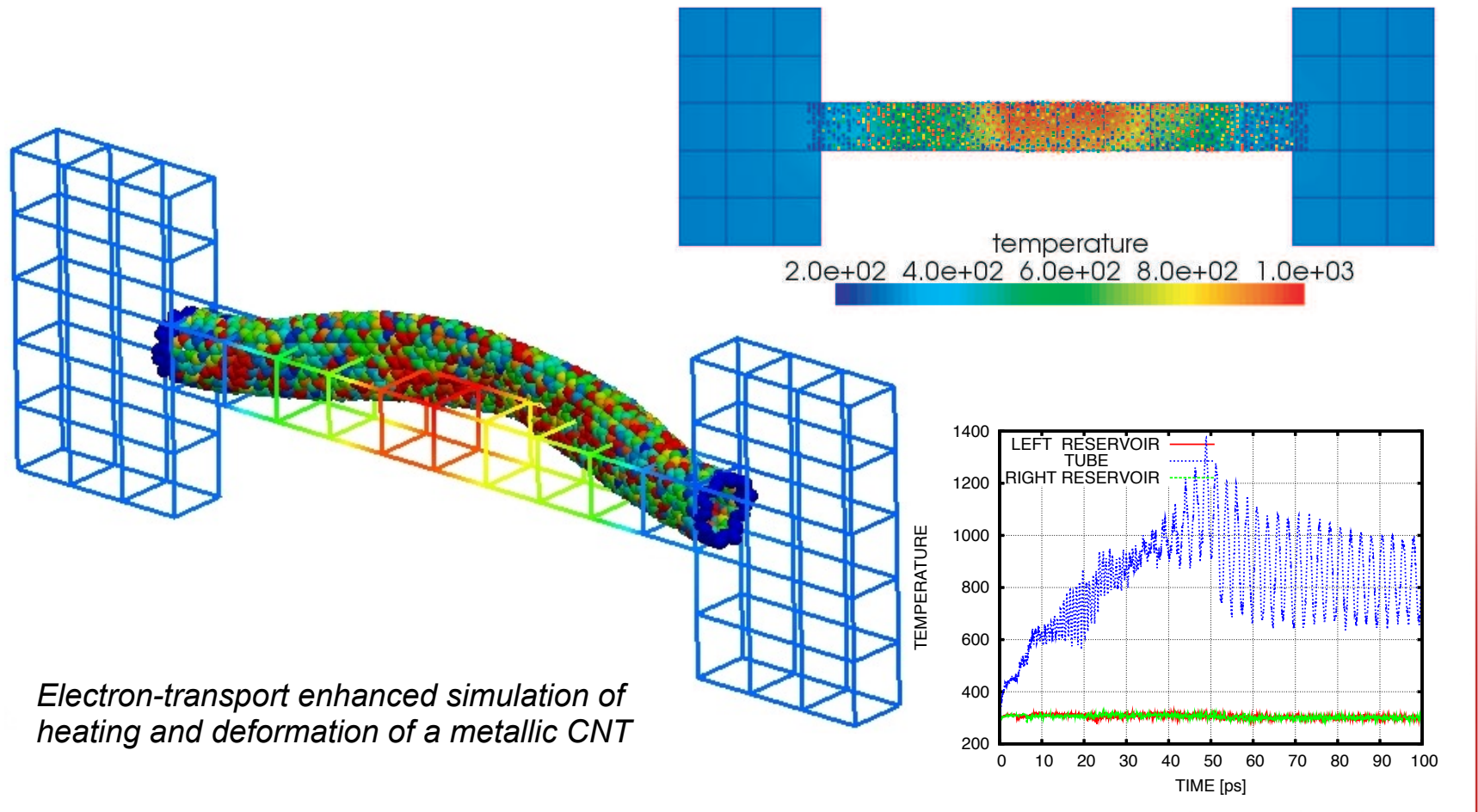


Example: Electrostatics

- *Surrogate model of electron density*
- *Electrons segregate to tip*
- *Potential drop across short axis*
- *Mutual repulsion opens tip*
- *Net charge causes net tip displacement*
- *CNT anchored in a warm substrate*



Example: Electron transport



Electron-transport enhanced simulation of heating and deformation of a metallic CNT



Software & Contacts

- Publically available at:

<http://lammps.sandia.gov/download.html>

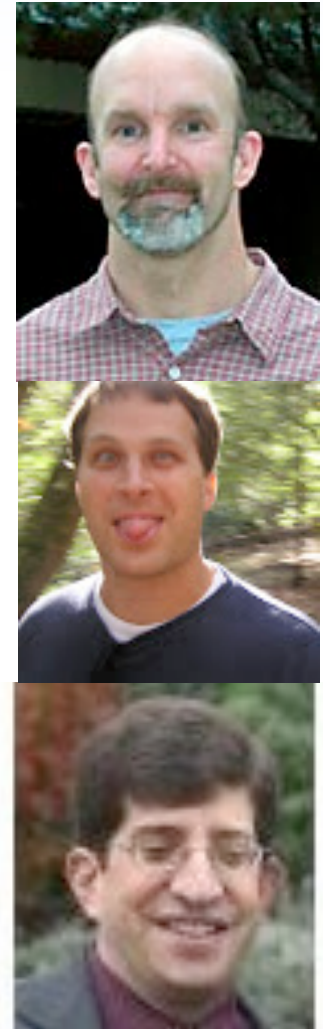
S.J. Plimpton, A. Thompson, P. Crozier

- Development version available through:

Reese Jones rjones@sandia.gov

Jeremy Templeton jatempl@sandia.gov

Jon Zimmerman jzimmer@sandia.gov



Careful what you put on the web



Software & Contacts

- Publically available at:

<http://lammps.sandia.gov/download.html>

S.J. Plimpton, A. Thompson, P. Crozier

- Development version available through:

Reese Jones rjones@sandia.gov

Jeremy Templeton jatempl@sandia.gov

Jon Zimmerman jzimmer@sandia.gov



Syntax examples

Setup:

```
fix AtC ATOMS atc hardy  
fix AtC ATOMS atc thermal Ar_thermal.dat  
fix_modify AtC fem create mesh
```

Control and time filtering:

```
fix_modify AtC transfer filter  
fix_modify AtC transfer filter scale  
fix_modify AtC transfer atom_element_map  
fix_modify AtC transfer neighbor_reset_frequency  
fix_modify AtC transfer kernel
```

Output: text and EnSight

```
fix_modify AtC transfer output 10 binary  
fix_modify AtC mesh output
```



Publications

- K. K. Mandadapu, R. E. Jones, J. A. Zimmerman, **On the microscopic definitions of the dislocation density tensor**. Mathematics and Mechanics of Solids, 2013
- F. Rizzi, R. E. Jones, B. J. Debusschere, O. M. Knio. **Uncertainty quantification in MD simulations of concentration driven ionic flow through a silica nanopore**. Part I: sensitivity to physical parameters of the pore. J. Chem. Phys., 2013
- J. A. Zimmerman, and R. E. Jones. **The application of an atomistic J-integral to a ductile crack**. J. Phys.-Cond.Mat., 25(15):155402, 2013
- R. E. Jones, J. A. Templeton, and T. W. Rebold. **Simulated real-time detection of a small molecule on a carbon nanotube cantilever**. J. Comp. Theo. NanoSci., 8:1364–1384, 2011.
- J. A. Templeton, R. E. Jones, J. W. Lee, J. A. Zimmerman, and B. M. Wong. **A long-range electric field solver for molecular dynamics based on atomistic-to-continuum modeling**. J. Chem. Theo. Comp., 7(6):1736–1749, 2011.
- R. E. Jones, J. A. Zimmerman, J. Oswald, and T. Belytschko. **An atomistic J- integral at finite temperature based on Hardy estimates of continuum fields**. J. Phys. Cond. Mat., 23:015002, 2010.
- J. A. Templeton, R. E. Jones, and G. J. Wagner. **Application of a field-based method to spatially varying thermal transport problems in molecular dynamics**. Mod. Sim. Mat. Sci. Eng., 18:085007, 2010.
- R. E. Jones and J. A. Zimmerman. **The construction and application of an atomistic J-integral via Hardy estimates of continuum fields**. J. Mech. Phys. Solids, 58:1318–1337, 2010.
- R. E. Jones, J. A. Templeton, G. J. Wagner, D. Olmsted, and Nomand A. Modine. **Electron transport enhanced molecular dynamics for metals and semi-metals**. Int. J. Num. Meth. Engin., 83(8-9):940–967, 2010.
- R. E. Jones and C. J. Kimmer. **Efficient non-reflecting boundary condition constructed via optimization of damped layers**. Phys. Rev. B, 81(9):094301, 2010.
- J. A. Zimmerman, R. E. Jones, and J. A. Templeton. **A material frame approach for evaluating continuum variables in atomistic simulations**. J. Comp. Phys., 229:2364–2389, 2010.
- G. J. Wagner, R. E. Jones, J. A. Templeton, and M. L. Parks. **An atomistic-to-continuum coupling method for heat transfer in solids**. Comp. Meth. Appl. Mech. Eng., 197(41-42):3351–3365, 2008

