Atoms-to-Continuum (AtC) user package for LAMMPS

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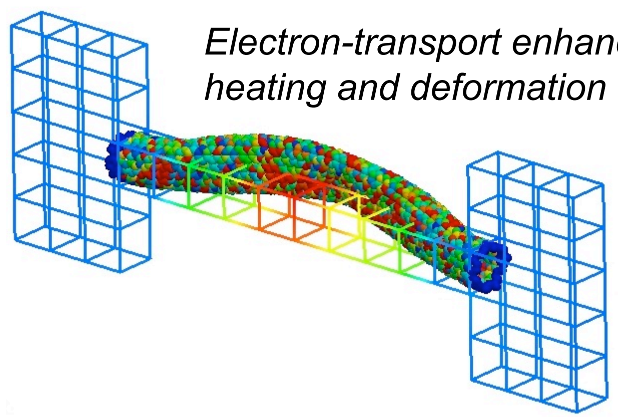
Objectives for Package

- Calculation of continuum mechanical variables from atomistic simulation data using the Hardy's Eulerian formulation and our Lagrangian formulation.
- Coupling of atomistic (MD, MS) and continuum (finite element) regions for rigorous thermal and mechanical boundary conditions.
- Coupling to emulate electronic temperature effects in metals via the two temperature model (TTM).

Compressive stress field for an atomic simulation of shock loading



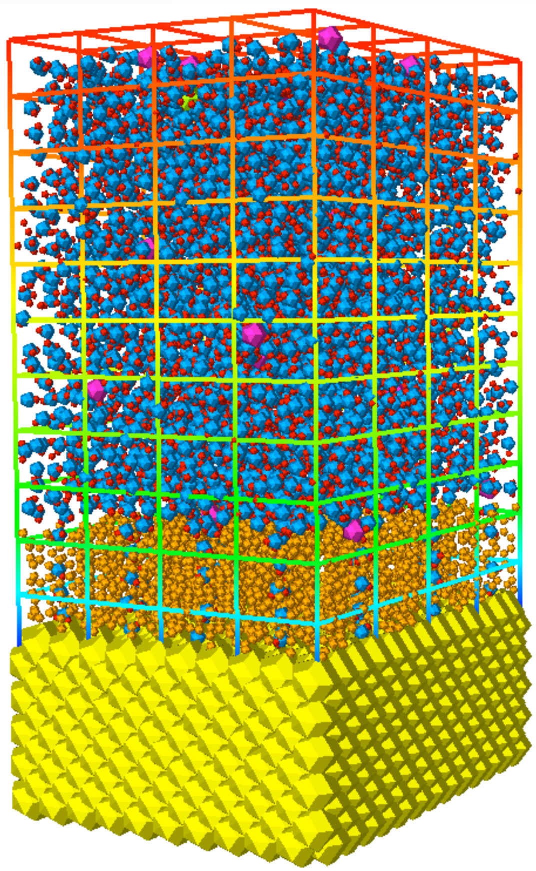
Electron-transport enhanced simulation of heating and deformation of a metallic CNT

fix atc

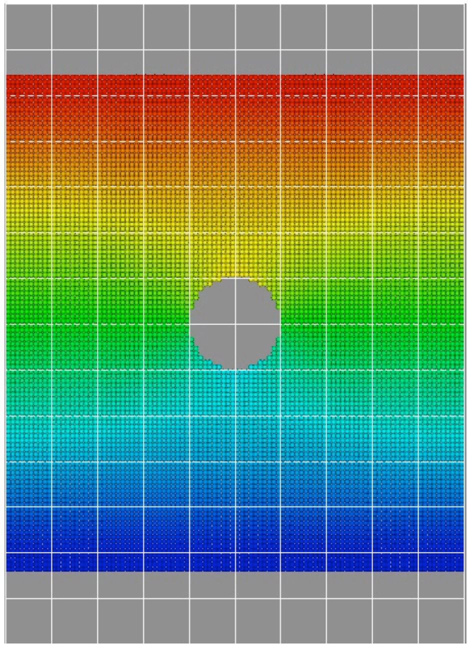
```
fix ID groupID atc type paramfile
```

- ID, group-ID are documented in fix command
- type = *thermal* or *two_temperature* or *hardy*
  - *thermal* = thermal coupling with field: temperature
  - *two_temperature* = electron-phonon coupling with field, temperature and electron_temperature
  - *hardy* = Hardy on-the-fly post-processing
- paramfile = file with material parameters (not specified for *hardy* type)

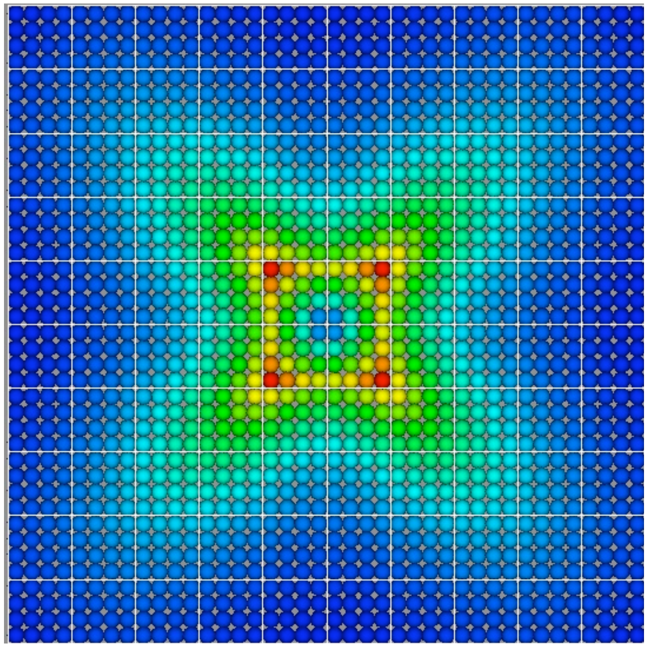
The atc picture: mesh, box and atoms



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



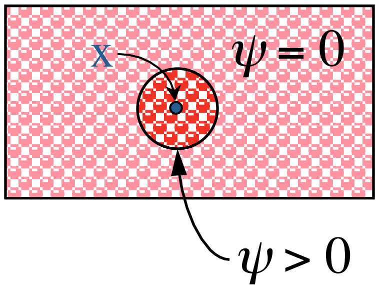
Circular hole in plate: mesh overlaps exactly with box, but atom region is subset



Elastic inclusion problem: mesh overlaps exactly with box and atoms

Hardy on-the-fly post-processing

Hardy (*Journal of Chemical Physics*, 1982)
Zimmerman *et al*. (*MSMSE*, 2004)
Zimmerman *et al.* (*Journal of Computational Physics*, 2010)




```
# …create and initialize the MD system
fix AtC internal atc hardy
fix_modify AtC fem create mesh 1 1 1 box p p p
fix_modify AtC atom_element_map eulerian 100
fix_modify AtC transfer fields none
fix_modify AtC transfer fields add density energy
  stress temperature
fix_modify AtC transfer output nvtFE 100 text
run 1000
```

Common fix_modify commands for atc-hardy

Setup:

```
fix_modify AtC fem create mesh
fix_modify AtC transfer internal
```

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
fix_modify AtC transfer atomic_output
fix_modify AtC mesh output
```

Common fix_modify commands for atc-hardy

Computation of fields:

fix_modify AtC transfer **fields**

fix_modify AtC transfer **gradients**

fix_modify AtC transfer rates

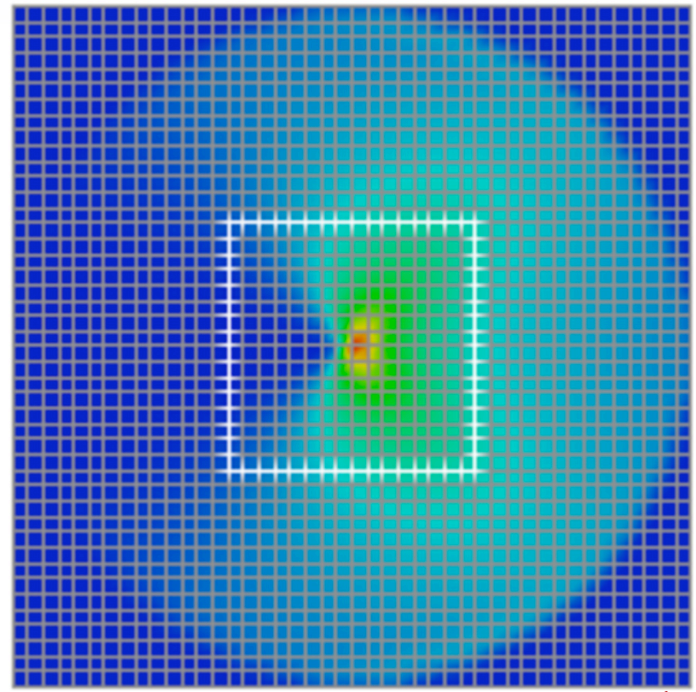
fix_modify AtC transfer **computes**

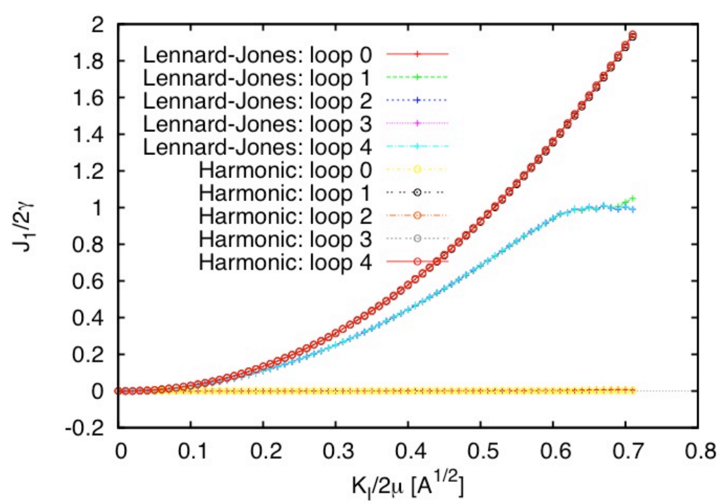
fix_modify AtC set

fix_modify AtC transfer **on_the_fly**

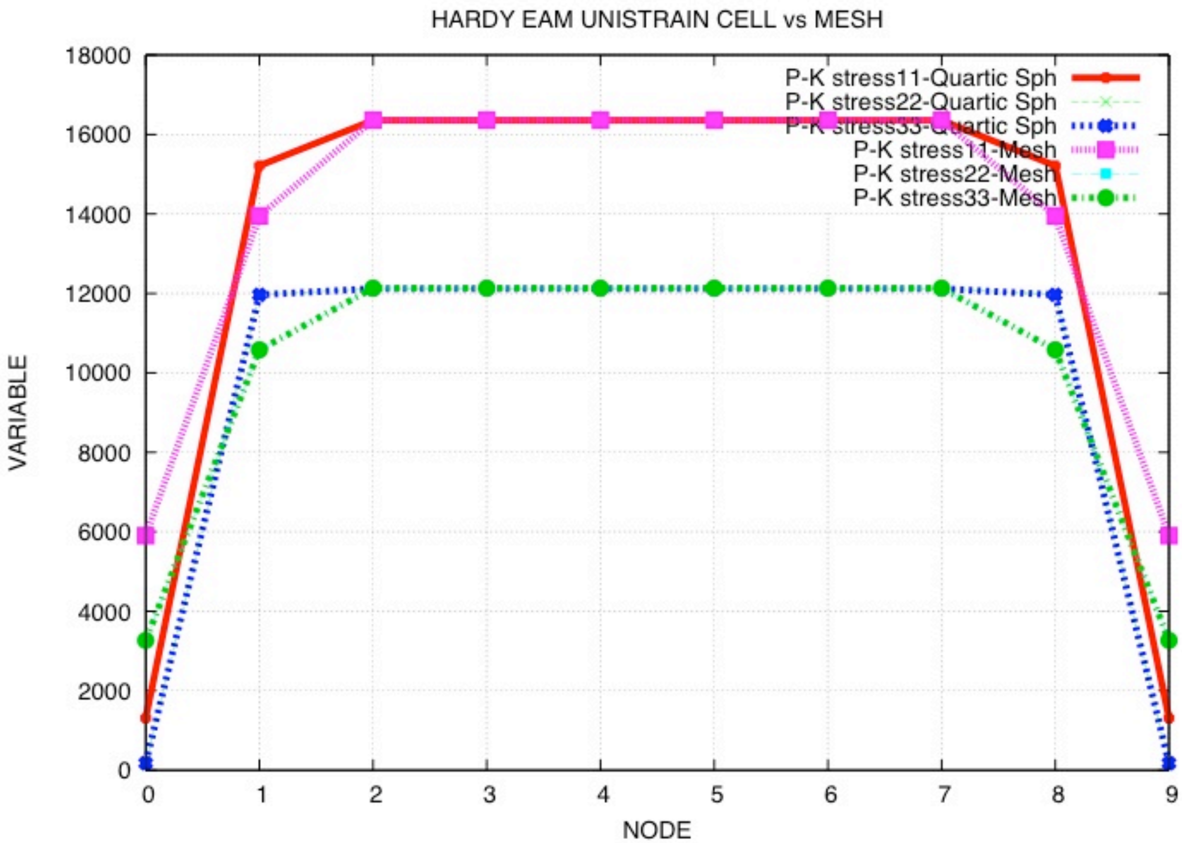
fix_modify AtC boundary_integral

fix_modify AtC **contour_integral**



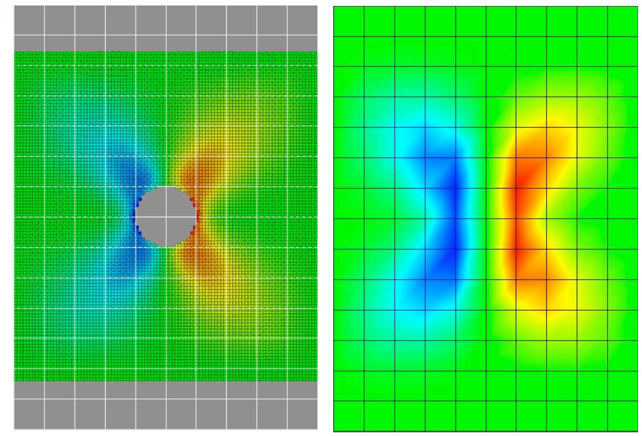


Examples of using atc-hardy



eam_unistrain_qsphere

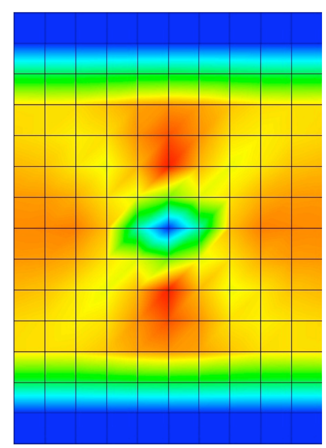
Uniaxial stretching of homogeneous bar, 1D elements



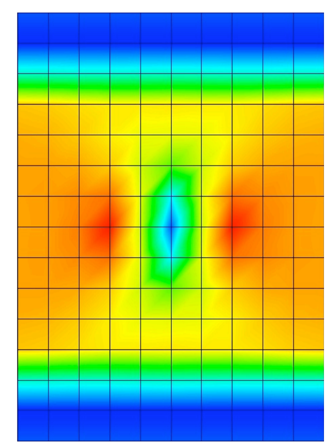
u_1

Tensile stretching of plate with circular hole

P_{11}



P_{22}



Thermal coupling using atc

- Coupled FEM/MD equations

$$\sum_J M_{IJ}\dot{\theta}_J = \frac{2}{3k_B}\sum_\alpha N_{I\alpha}\left(\mathbf{v}_\alpha \cdot \mathbf{f}_\alpha\right)\Delta V_\alpha + \sum_J K_{IJ}^{fem}\theta_J$$

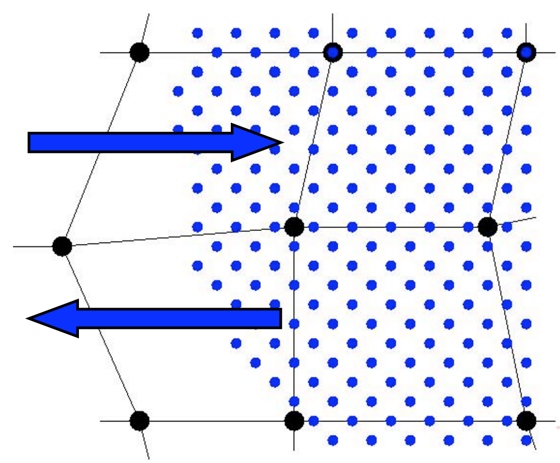
$$m_\alpha \dot{\mathbf{v}}_\alpha = -\frac{\partial U}{\partial \mathbf{x}_\alpha} - \sum_I N_{I\alpha}\lambda_I \mathbf{v}_\alpha$$

Coupling parameter (temperature/flux constraint)

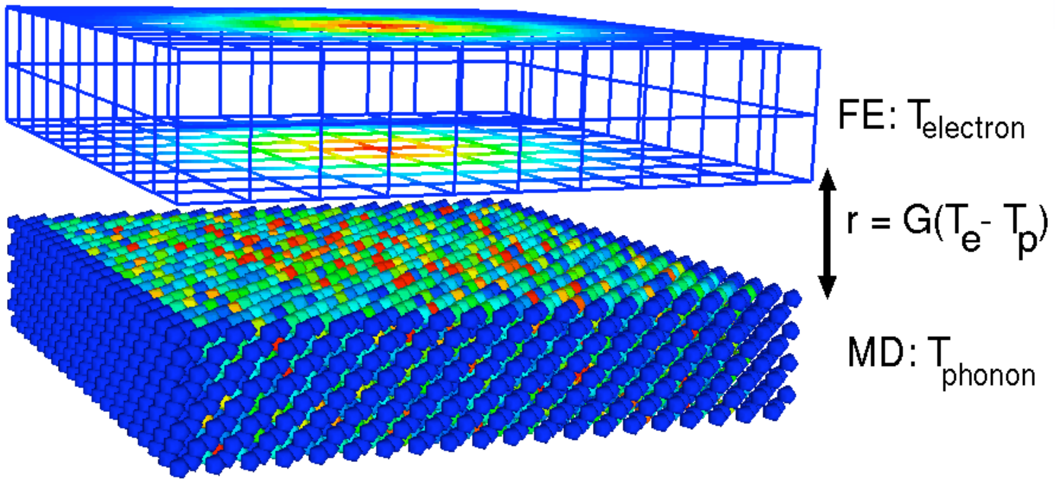
Atoms contribute to nodal heat equation

- Combined MD/FEM system has two-way coupling:

Heat at nodes affects MD energy through thermostat



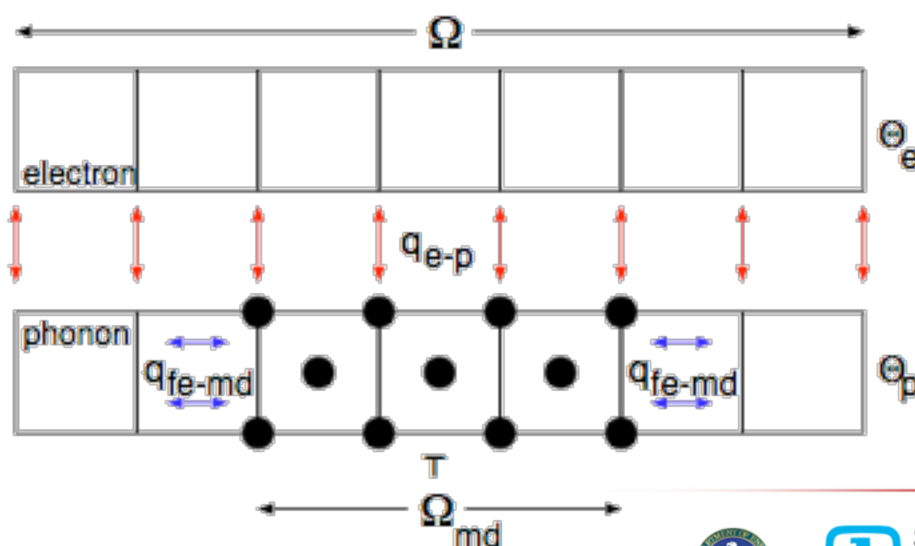
Two-Temperature coupling using atc



Explicit representation of phonons by MD

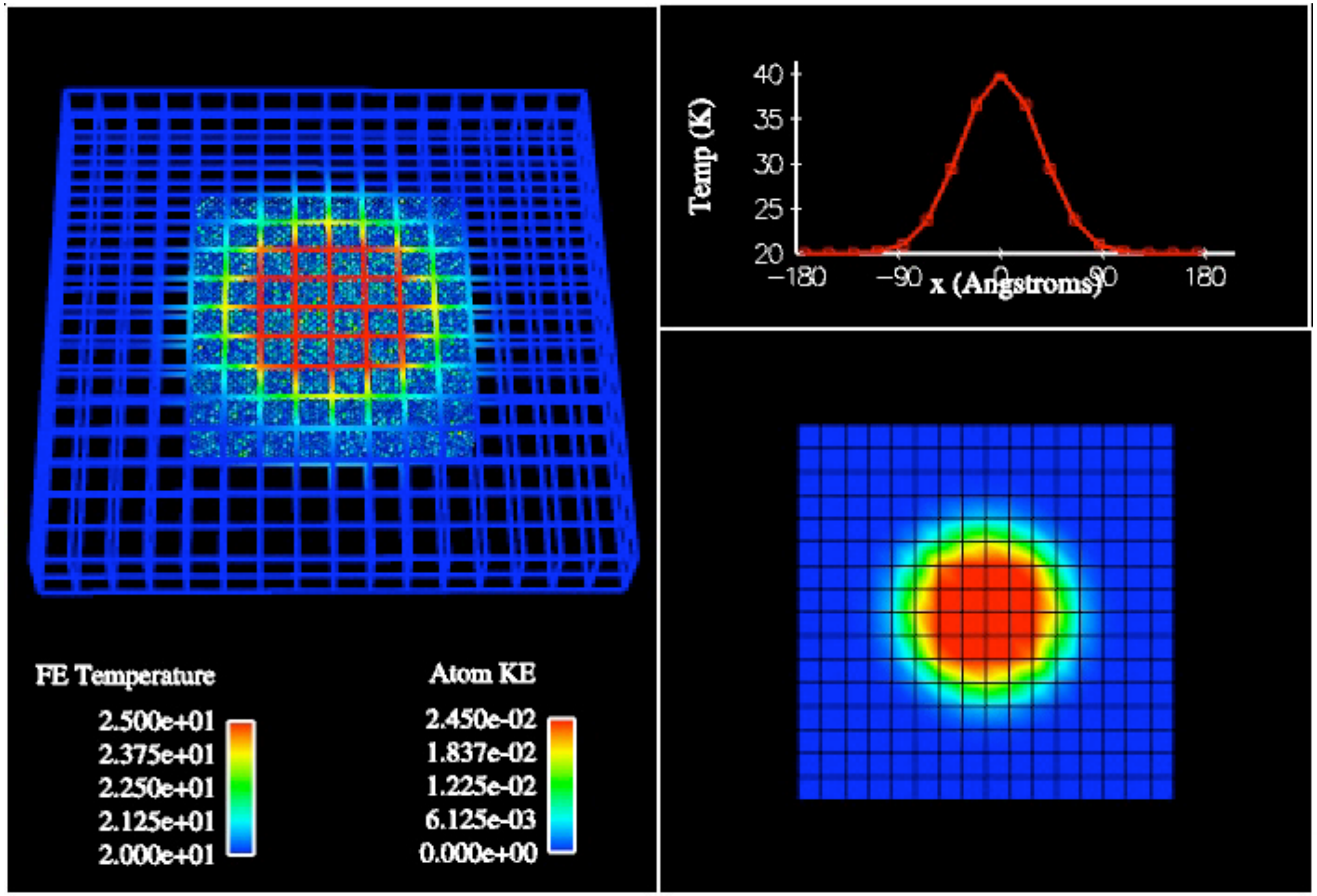
Electron effects solved for on overlaid mesh

Energy exchange handled though thermostats as in the thermal-only problem



Example of using atc-thermal

2D diffusion problem

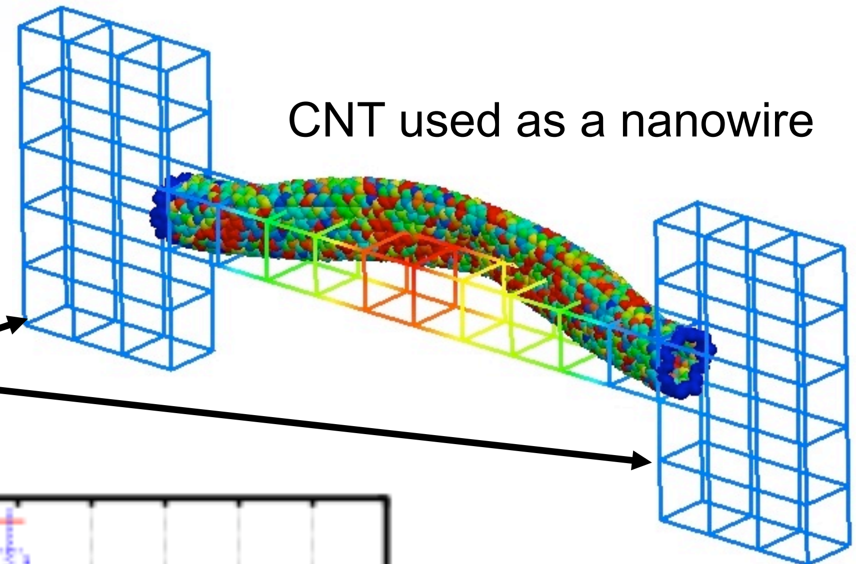


- Plate with embedded MD region (~33,000 atoms)
- Initialized to temperature field with gaussian profile
- Adiabatic boundary conditions at edges

Example of using atc-two_temperature

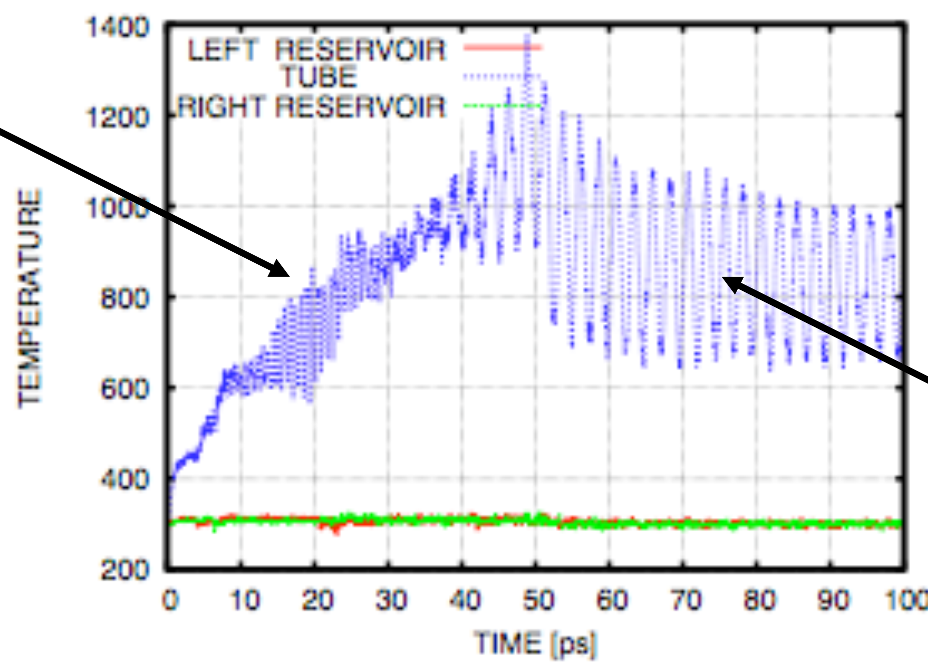
Joule heating in nanodevices

CNT used as a nanowire



reservoirs of hot electrons

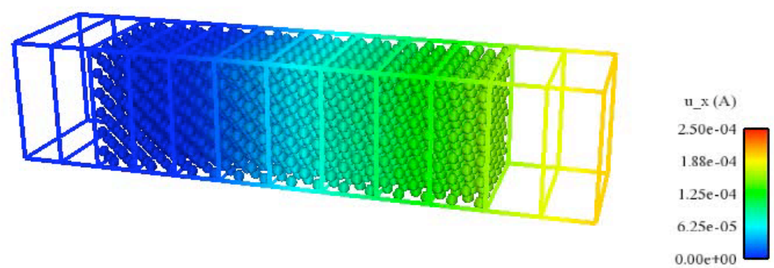
CNT heating through exchange with electrons

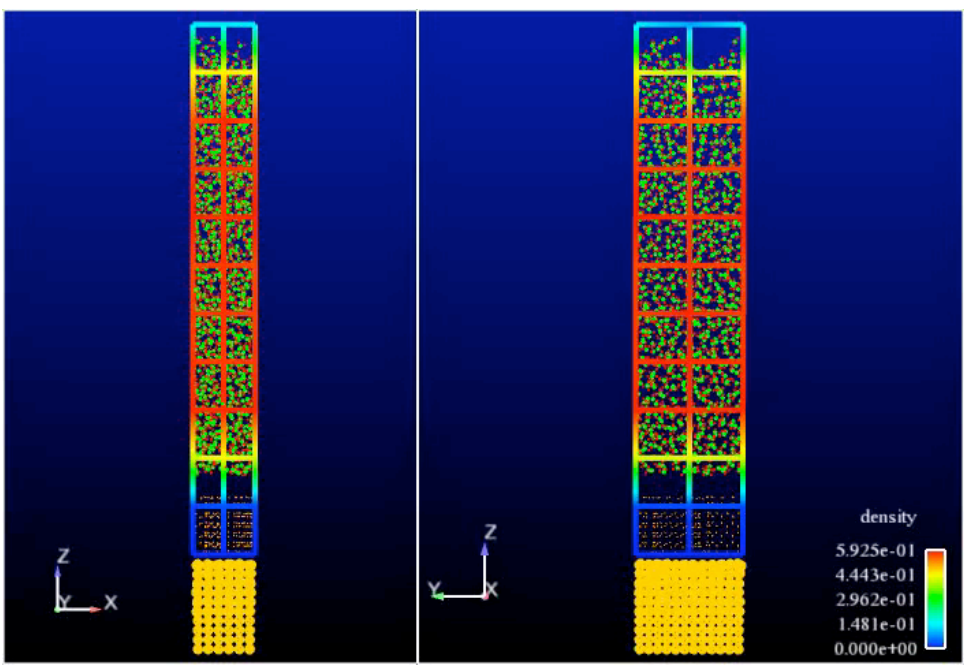


Thermal-induced mechanical oscillations

Future work: other physical models

- Elasto-dynamic response at the nano-scale





- Fluidic species transport
  - Transport of saltwater into NTs
  - Energy storage devices
  - Long-range electrostatic interactions on FE mesh