

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

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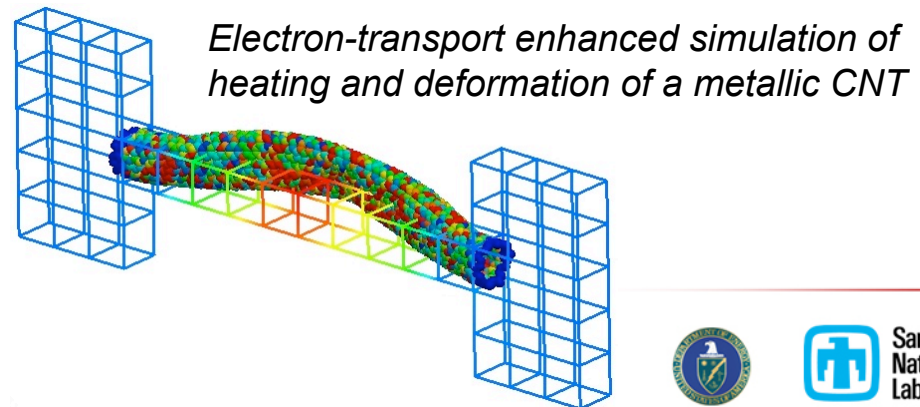


Objectives for Package

- 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



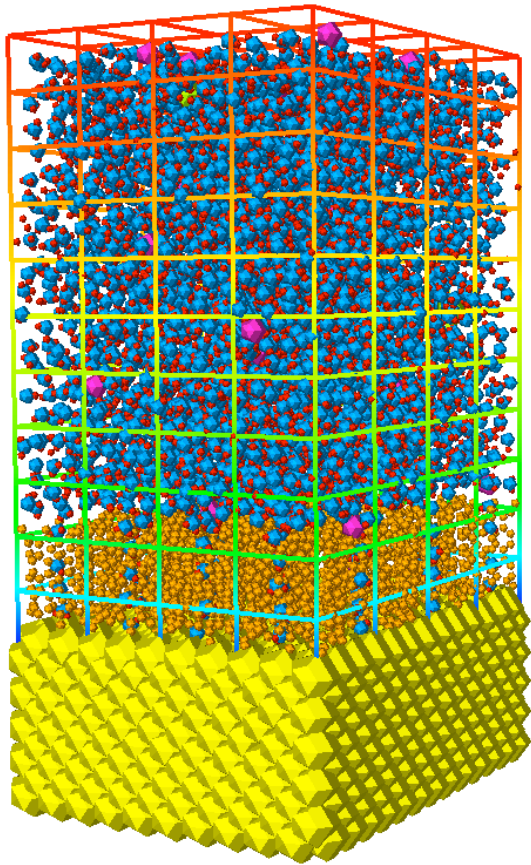
fix atc

`fix ID groupID atc type paramfile`

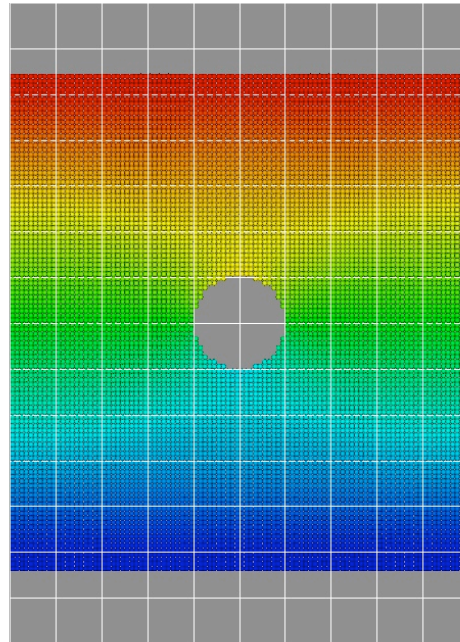
- ID, group-ID are documented in fix command
- type = *thermal* or *two_temperature* or *hardy*
 - *thermal* = thermal coupling with field: temperature
 - *two_temperature* = electron-phonon coupling with field, temperature and electron_temperature
 - *hardy* = Hardy on-the-fly post-processing
- paramfile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



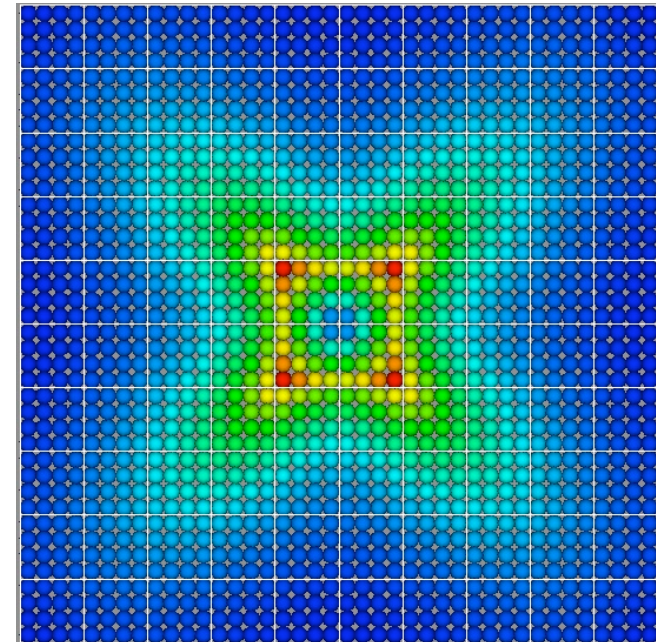
The atc picture: mesh, box and atoms



*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
```

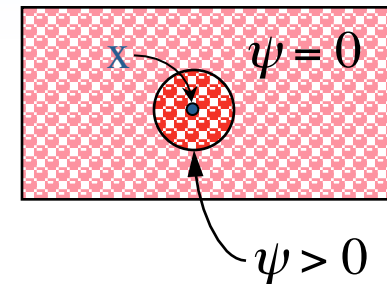
```
fix_modify AtC transfer fields none
```

```
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

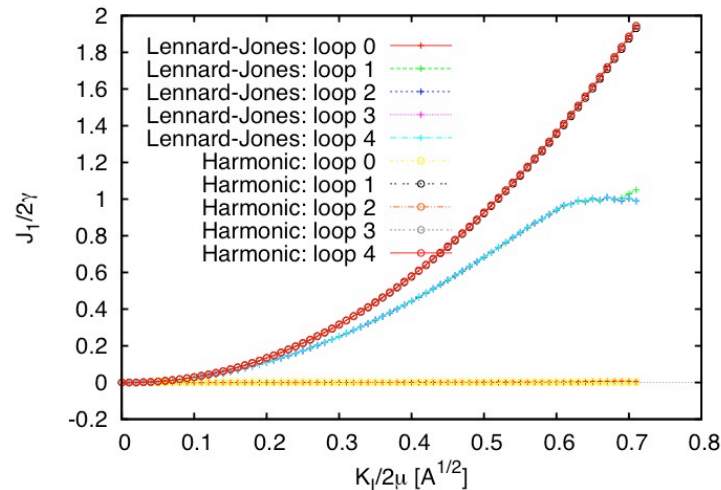
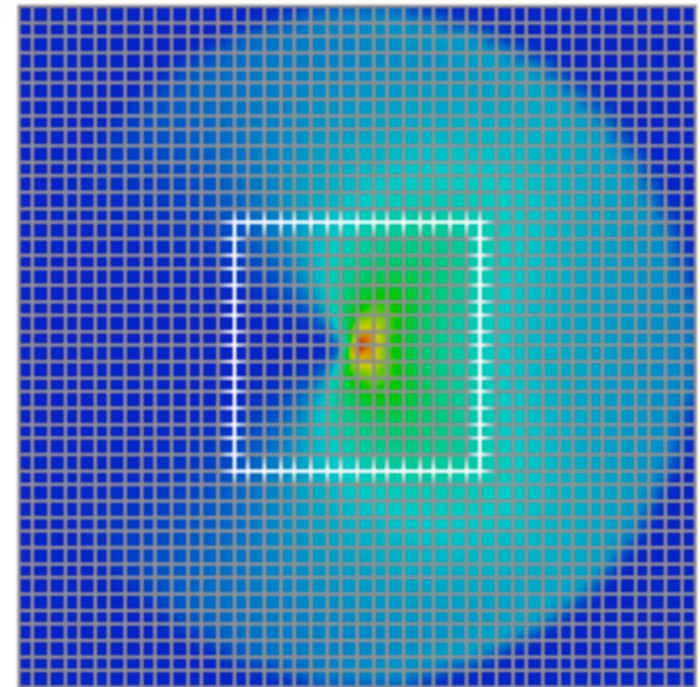
```
fix_modify AtC transfer output  
fix_modify AtC transfer atomic_output  
fix_modify AtC mesh output
```



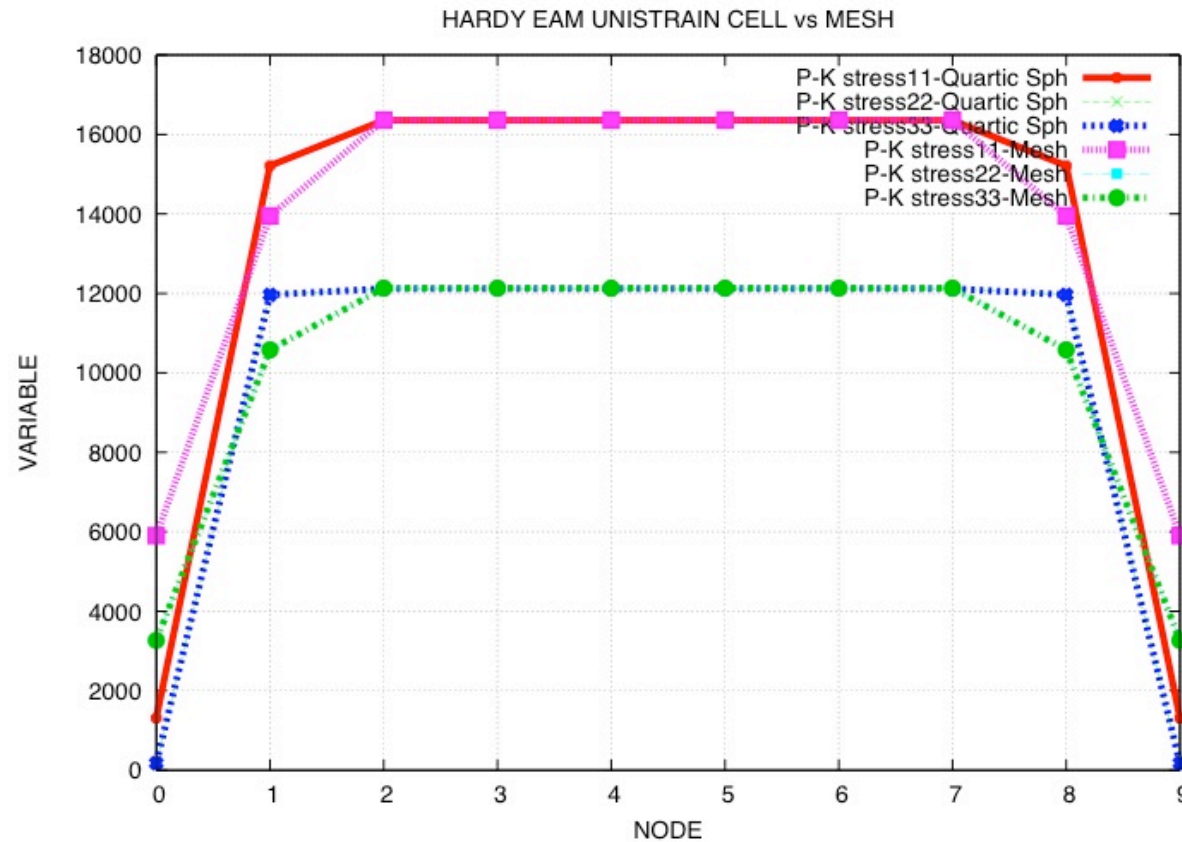
Common fix_modify commands for atc-hardy

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
```

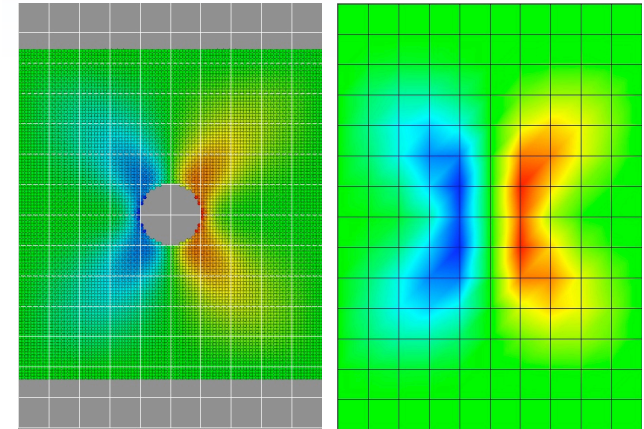


Examples of using atc-hardy



eam_unistrain_qsphere

*Uniaxial stretching of homogeneous bar,
1D elements*

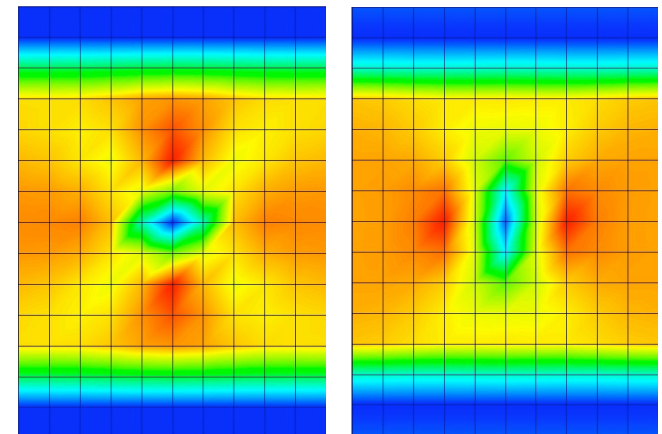


U_1

*Tensile stretching of
plate with circular hole*

P_{11}

P_{22}



Thermal coupling using atc

- Coupled FEM/MD equations

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

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

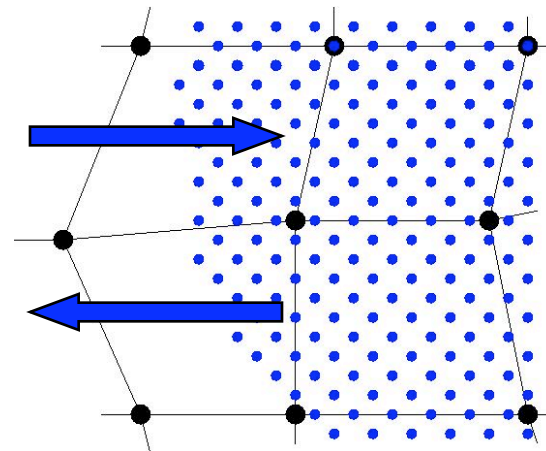
Coupling parameter
(temperature/flux constraint)



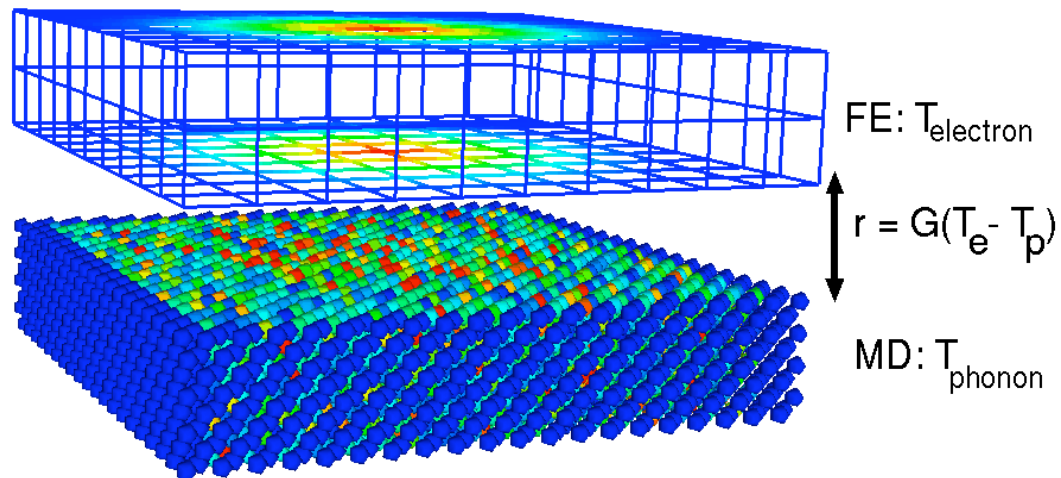
Atoms contribute to nodal heat equation

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

Heat at nodes affects MD energy through thermostat



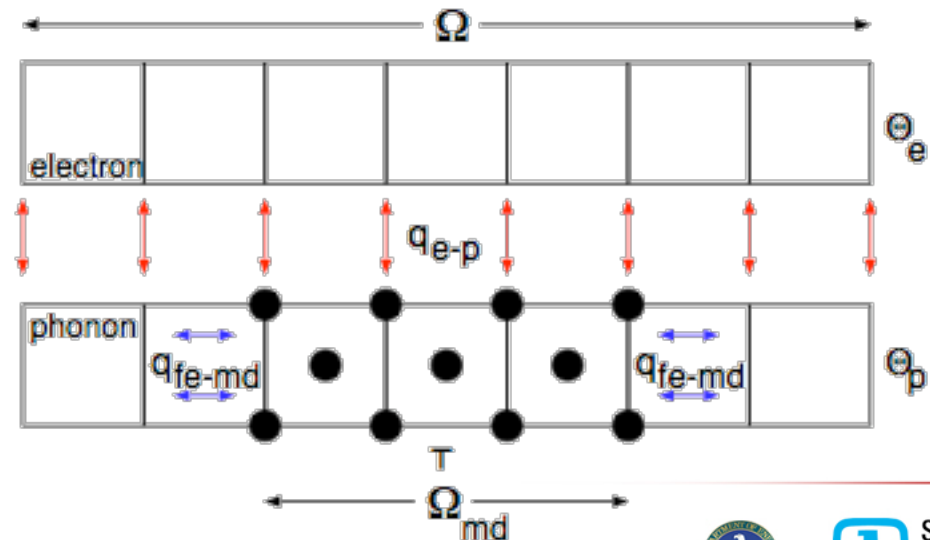
Two-Temperature coupling using atc



Explicit representation
of phonons by MD

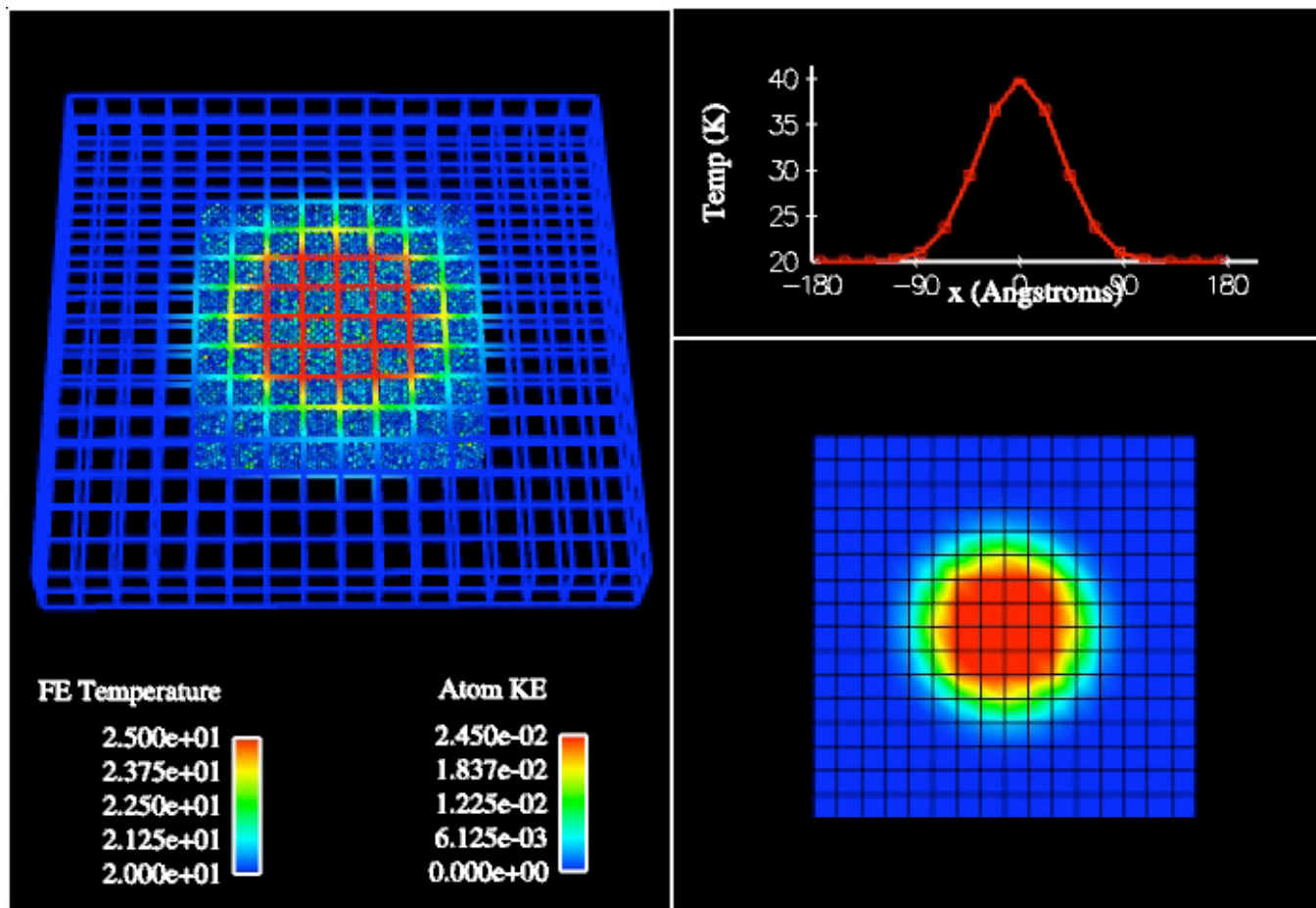
Electron effects solved
for on overlaid mesh

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



Example of using atc-thermal

2D diffusion problem

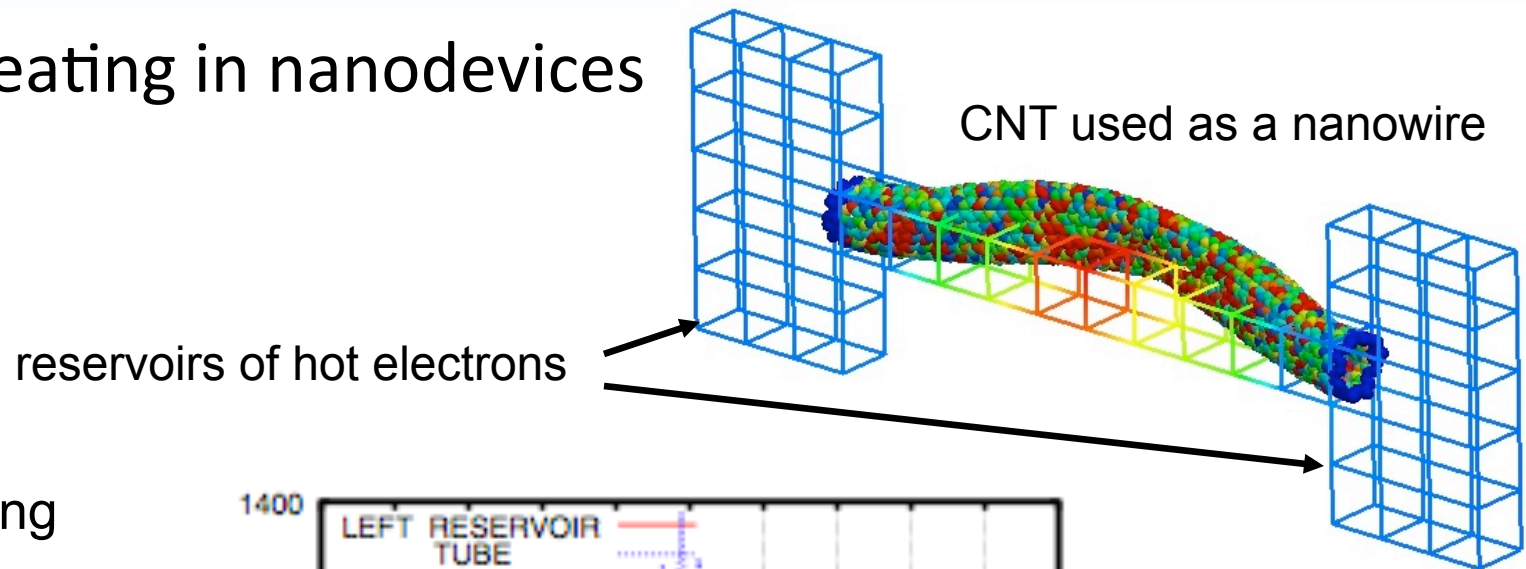


- Plate with embedded MD region (~33,000 atoms)
- Initialized to temperature field with gaussian profile
- Adiabatic boundary conditions at edges

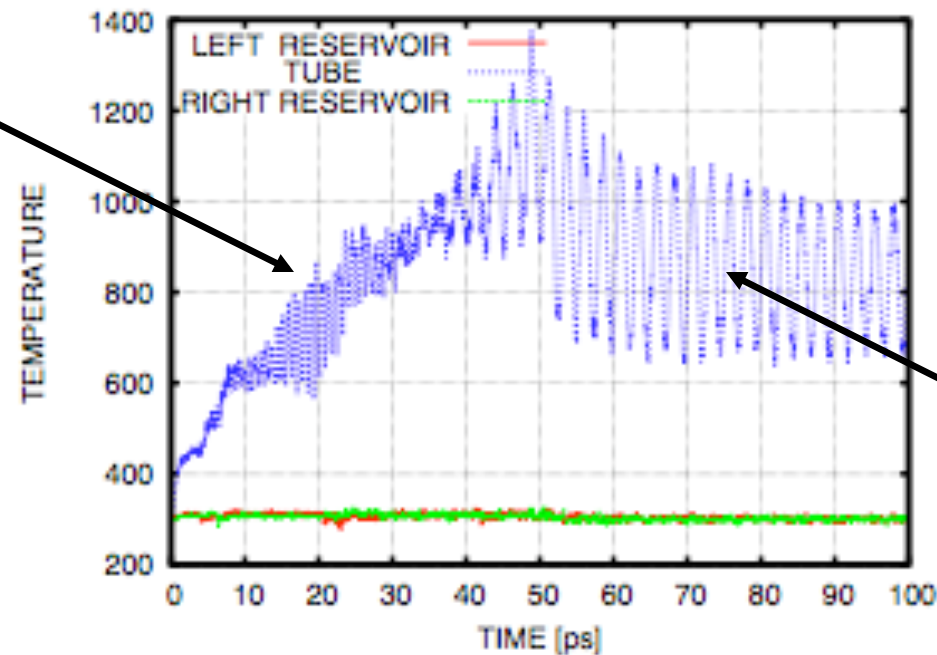


Example of using atc-two_temperature

Joule heating in nanodevices



CNT heating
through
exchange with
electrons

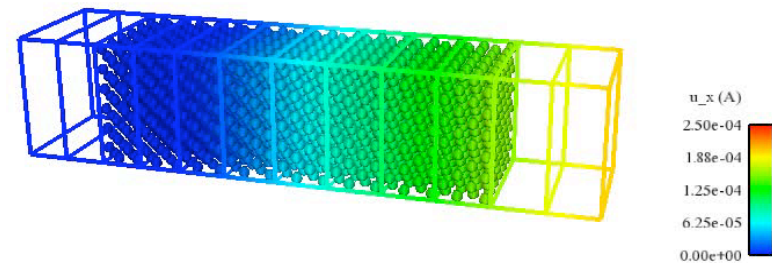


Thermal-
induced
mechanical
oscillations



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

