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

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Objectives for User Package

- **Calculation of continuum mechanical variables from atomistic simulation data using the Hardy's Eulerian formulation and our Lagrangian formulation.**
- **Coupling of atomistic (molecular statics / dynamics) 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).**

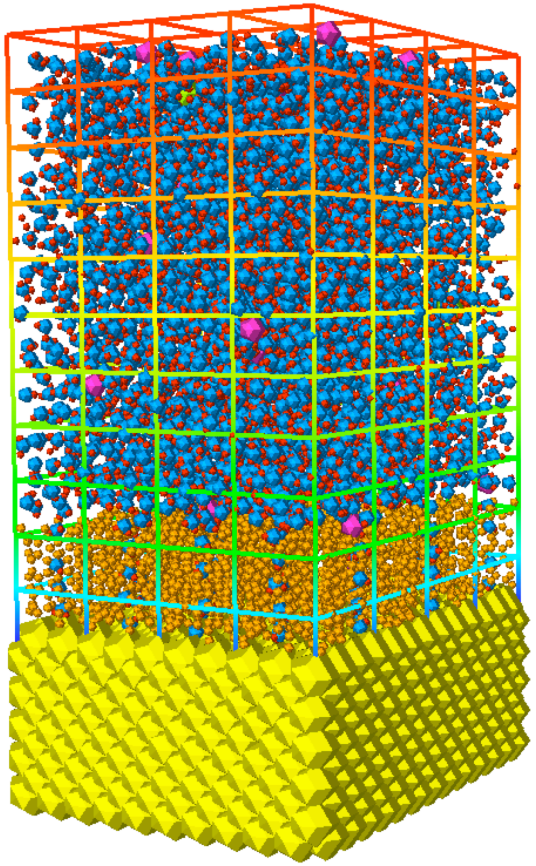
fix atc

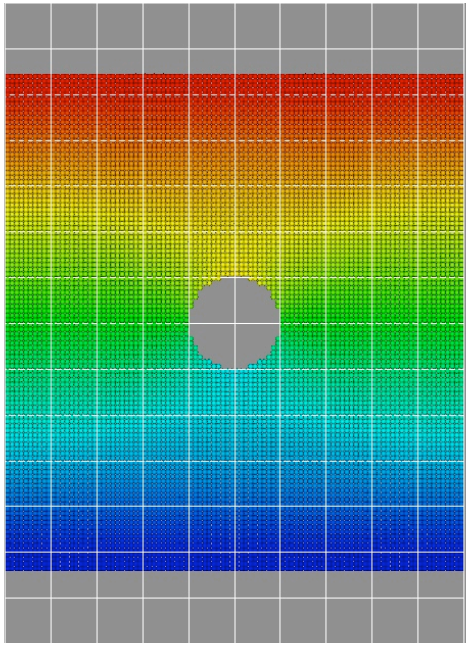
```
fix ID groupID atc type paramfile
```

- 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)

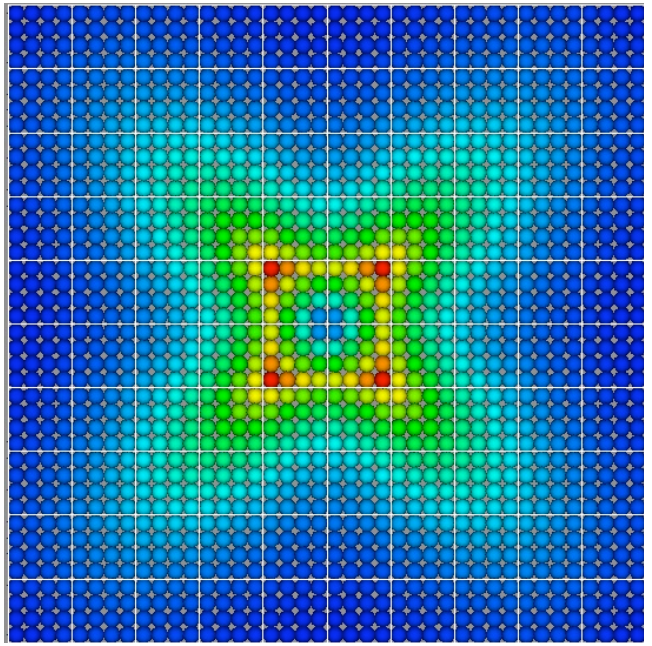
The atc picture: mesh, box and atoms

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

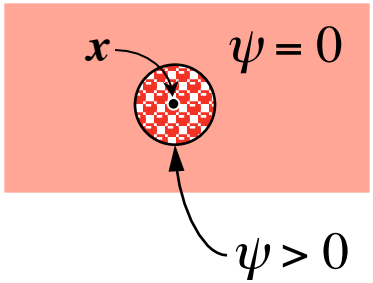


Elastic inclusion problem: mesh overlaps exactly with box and atoms

Hardy on-the-fly post-processing

$$\boldsymbol{\sigma}(\mathbf{x},t) = -\left\{\frac{1}{2}\sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N}\mathbf{x}^{\alpha\beta}\otimes\mathbf{f}^{\alpha\beta}B^{\alpha\beta}(\mathbf{x}) + \sum_{\alpha=1}^{N}m^{\alpha}\hat{\mathbf{v}}^{\alpha}\otimes\hat{\mathbf{v}}^{\alpha}\psi(\mathbf{x}^{\alpha}-\mathbf{x})\right\}$$

$$\mathbf{P}(\mathbf{X},t) = -\frac{1}{2}\sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N}\mathbf{f}^{\alpha\beta}\otimes\mathbf{X}^{\alpha\beta}B^{\alpha\beta}(\mathbf{X})$$



$$\mathbf{q}(\mathbf{x},t) = -\sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N}\frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}}\frac{\partial\phi_{\beta}}{\partial x^{\alpha\beta}}\left(\mathbf{x}^{\alpha\beta}\cdot\hat{\mathbf{v}}^{\alpha}\right)B^{\alpha\beta}(\mathbf{x}) + \sum_{\alpha=1}^{N}\left\{\frac{1}{2}m^{\alpha}\left(\hat{v}^{\alpha}\right)^{2}+\phi^{\alpha}\right\}\hat{\mathbf{v}}^{\alpha}\psi(\mathbf{x}^{\alpha}-\mathbf{x})$$

```
# …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
```

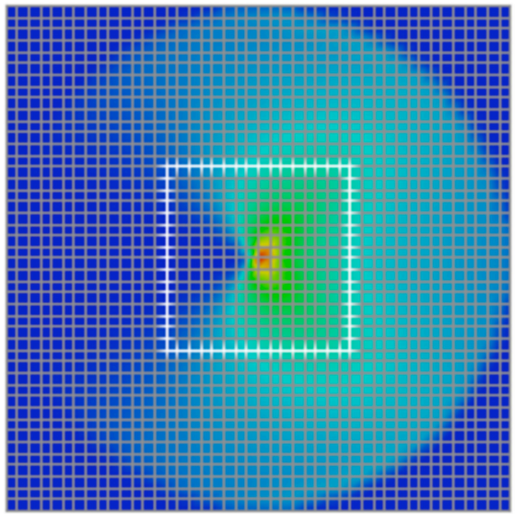
Output: text and EnSight

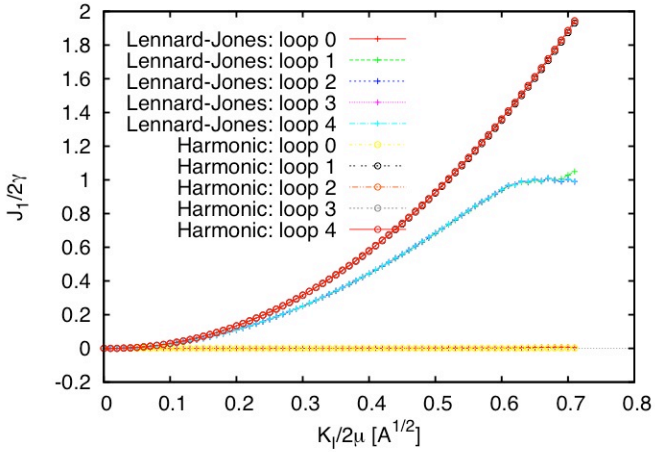
```
fix_modify AtC transfer output
fix_modify AtC transfer atomic_output
fix_modify AtC mesh output
```

Common fix_modify commands for atc-hardy

Computation of fields:

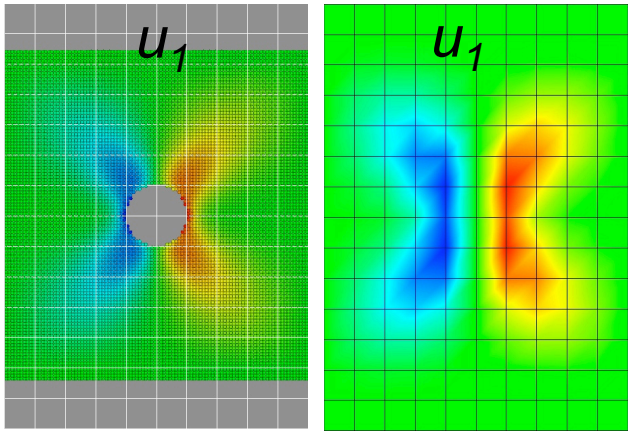
```
fix_modify AtC transfer fields
fix_modify AtC transfer gradients
fix_modify AtC transfer rates
fix_modify AtC transfer computes
fix_modify AtC transfer on_the_fly
fix_modify AtC boundary_integral
fix_modify AtC contour_integral
```

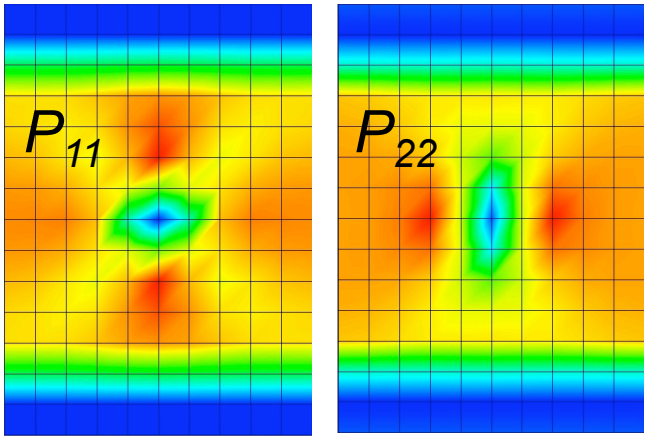




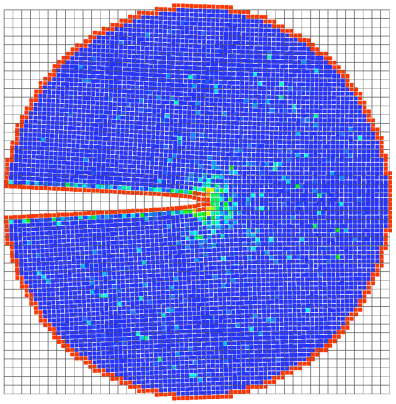
Examples of using atc-hardy

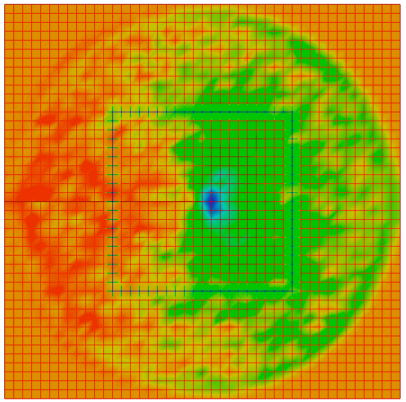
Tensile stretching of plate with circular hole

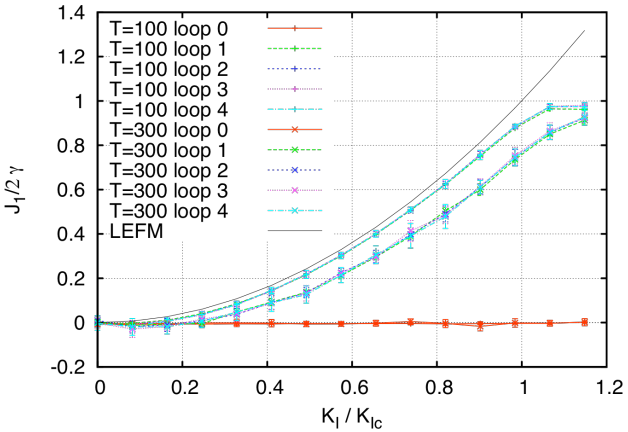




Compressive stress field for an atomic simulation of shock loading







Calculation of local values of atomic potential energy, Eshelby tensor, and J-integral at finite temperature

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Thermal coupling using atc

- **Coupled FEM/MD equations**

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

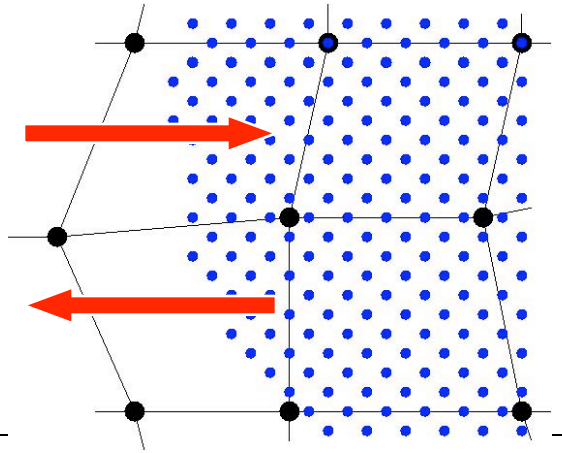
$$m_\alpha \dot{\mathbf{v}}_\alpha = -\frac{\partial U}{\partial \mathbf{x}_\alpha} - \sum_I N_{I\alpha}\lambda_I \mathbf{v}_\alpha$$

Coupling parameter (temperature/flux constraint)

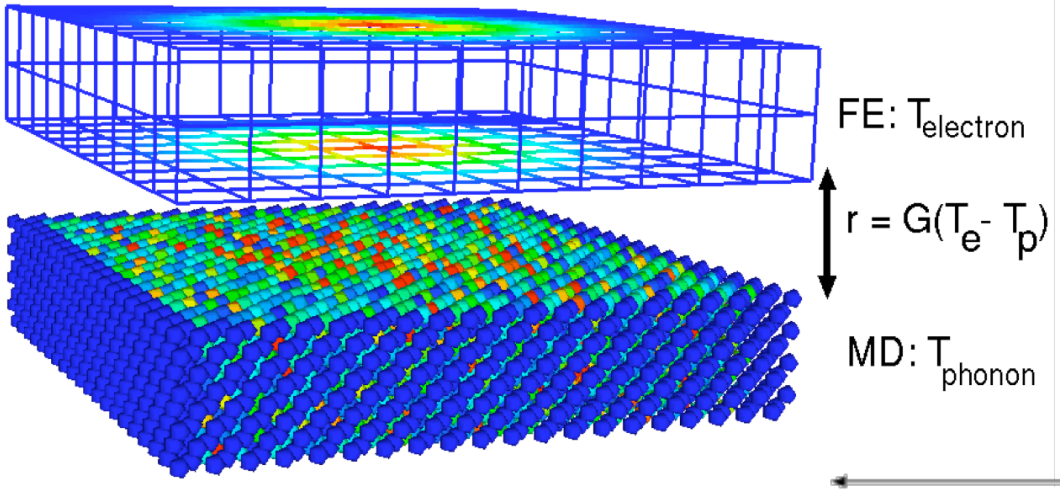
Atoms contribute to nodal heat equation

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

Heat at nodes affects MD energy through thermostat



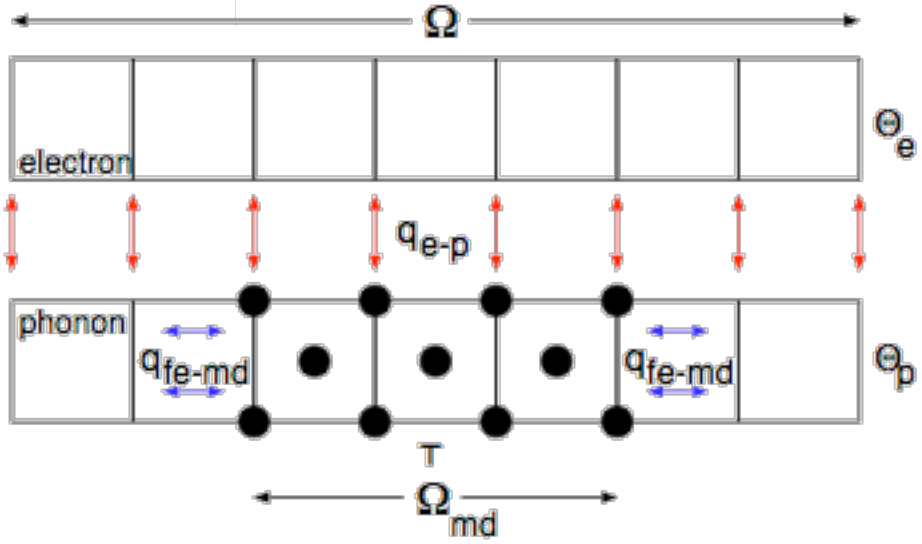
Two-Temperature coupling using atc



Explicit representation of phonons by MD

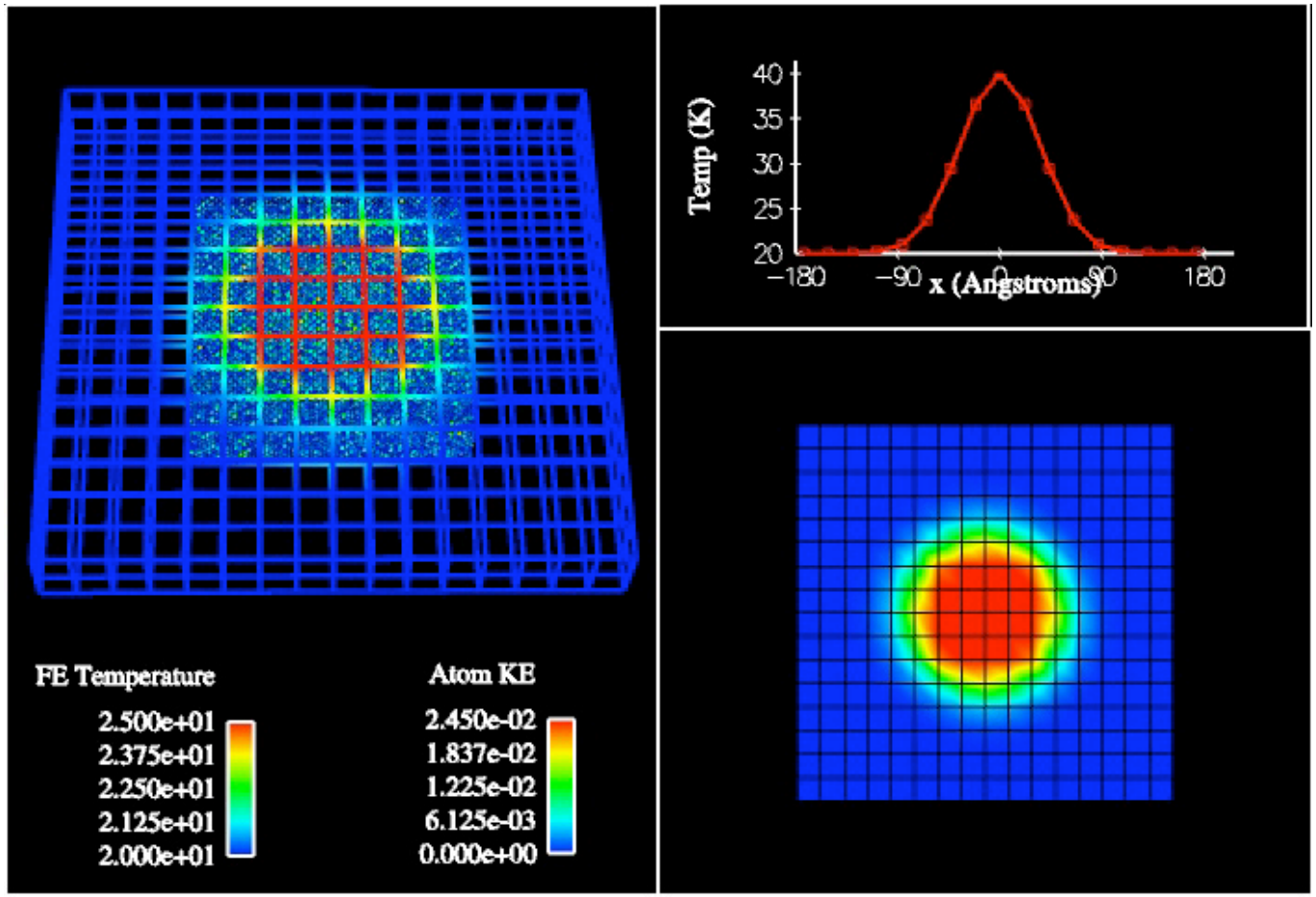
Electron effects solved for on overlaid mesh

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



Example of using atc-thermal

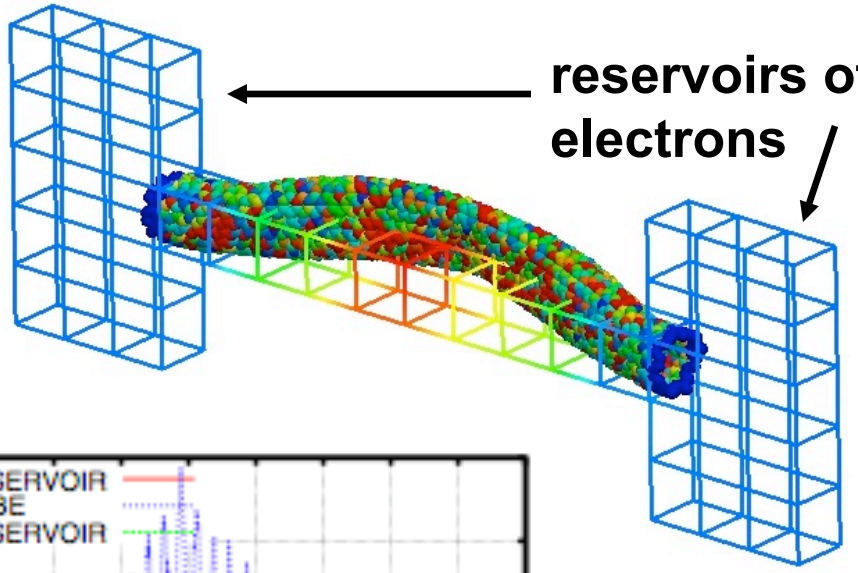
2D diffusion problem



- 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

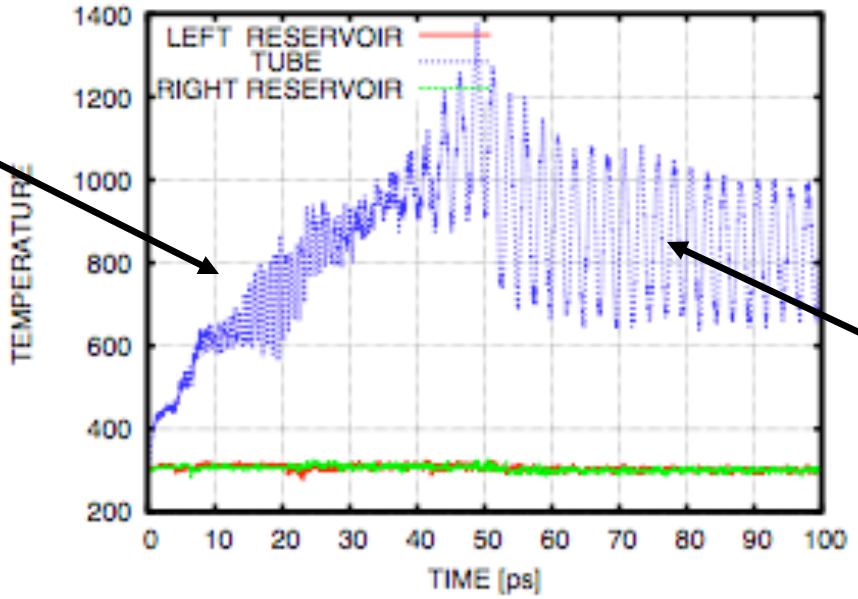
Joule heating in nanodevices



reservoirs of hot electrons

CNT used as a nanowire

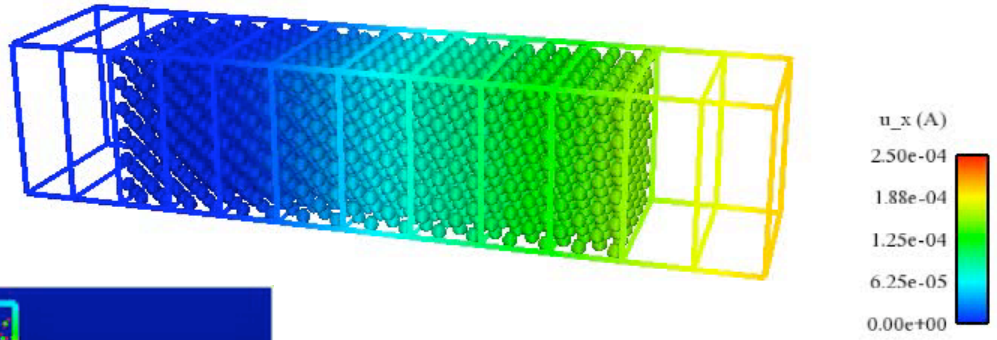
CNT heating through exchange with electrons

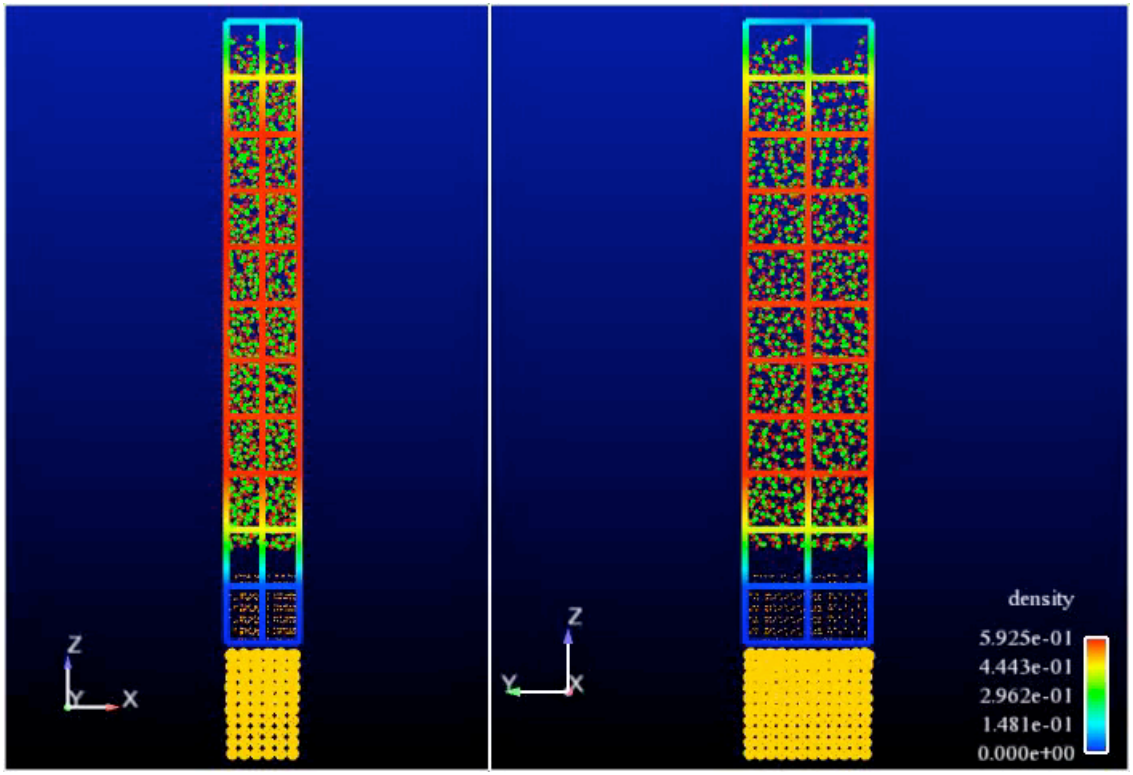


Thermal-induced mechanical oscillations

Future efforts

- **Elasto-dynamic response at the nano-scale**





- **Fluidic species transport**
  - **Transport of saltwater in nanotubes**
  - **Energy storage devices**
  - **Long-range electrostatic interactions on FE mesh**

Concluding Remarks

- **References:**
  - **atc-hardy**
    - **Zimmerman, Jones and Templeton, *J. Comput. Phys.* (2010)**
    - **Jones and Zimmerman, *J. Mech. Phys. Solids* (2010)**
    - **Jones *et al.*, *J. Phys.: Condens. Matter* (2010)**
  - **atc-thermal**
    - **Wagner *et al.*, *Comp. Meth. Appl. Mech. Eng.* (2008)**
    - **Templeton, Jones and Wagner, Model. Simul. Mater. Sci. Eng (2010)**
  - **atc-two temperature**
    - **Jones *et al.*, *Intl. J. Numer. Meth. Eng.* (2010)**
- **Simulations performed with LAMMPS MD code:**

  http://lammps.sandia.gov

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