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Atomistic-to-Continuum Modeling for Multi-scale and Multi-physics Computations

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Stanford University

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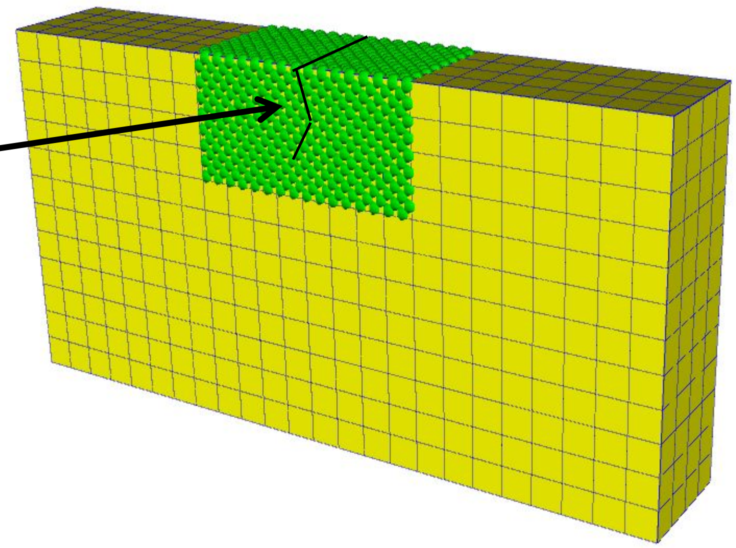
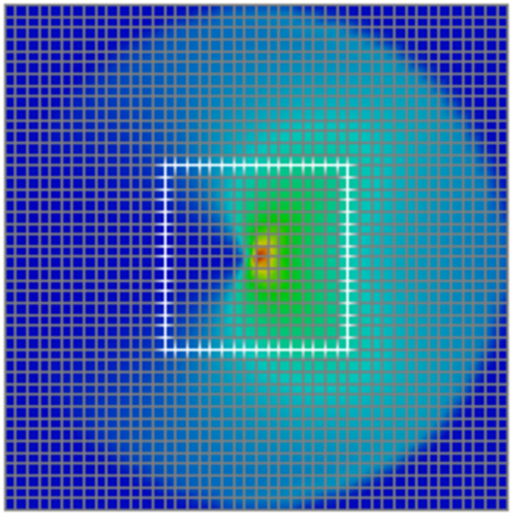
Motivation

- Provide a unified computational framework for finite element (FE) and an molecular dynamics (MD) for problems in which atomistic description of material is needed only for a localized region and the dynamical interactions between the FE and MD are important for understanding the system
  - MD cost to simulate entire system atomistically would be prohibitive
  - Dual Statement: FE constitutive models are not of sufficient fidelity for all of the system

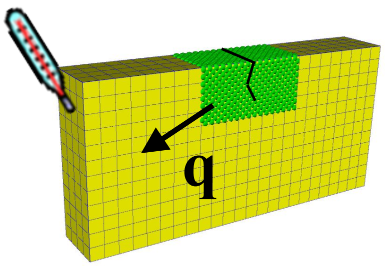


- Apply boundary conditions and sources to MD to enable engineering simulation of nanosystems analogous to FE analysis
- Enhance MD with multiphysics capabilities mediated by a FE model
  - Electron transport effects augmenting classical MD
  - Electric field modeling for long-range interactions
- Learn something!
  - On-the-fly Hardy post-processing
  - Think before you simulate



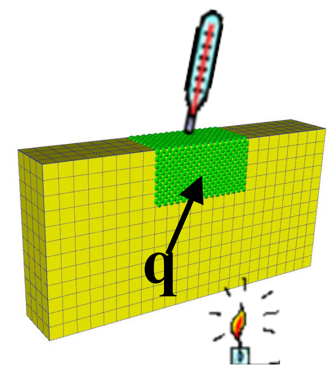
Two-Way Coupling for Heat Transfer

Goal: Coupling strategy that allows both fine-to-coarse scale heat transfer and coarse-to-fine scale heat transfer



Fine-to-coarse: Fine scale vibrational energy from the MD region should flow into the surrounding FE region and be accounted for as temperature

Coarse-to-fine: Temperature of the FE model (θ) should have an effect on the MD region, through e.g. thermal excitation of atoms



Two interdependent parts of coupling strategy:

1. Modification of finite element equation to incorporate effects of atoms on θ
2. Thermostat to enforce temperature field θ at atoms

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Continuum Heat Equation

- Heat equation with Fourier heat conduction arising from Boltzmann Transport equation for energy conservation:

$$\rho c_v \frac{\partial \theta}{\partial t}(\mathbf{x}, t) = \nabla \cdot (\kappa \nabla \theta (\mathbf{x}, t))$$

- Finite element discretization leads to a set of ODE's for the nodal temperatures

$$\theta^h(\mathbf{x}, t) = \sum_I N_I(\mathbf{x})\, \theta_I(t) \implies \mathbf{M}\dot{\theta} = \mathbf{K}\theta$$

$$M_{IJ} = \int_\Omega \rho c_v N_I N_J \, dV$$

$$K_{IJ} = \int_\Omega \kappa \nabla N_I \cdot \nabla N_J \, dV$$

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MD Temperature Definition

- We have to relate the dynamics of atoms to the nodal temperature field

Using Equipartition of Energy:

$$E^{MD} = \sum_{\alpha} \frac{1}{2} m_\alpha \left|\mathbf{v}_\alpha\right|^2 + \Phi \implies e_\alpha \approx m_\alpha \left|\mathbf{v}_\alpha\right|^2 / \Delta V_\alpha$$

- Define restriction operation: MD field → Nodal field
  - E.g. projection, averaging, shape functions…
  - One way: minimize difference between MD and continuum temperature fields

$$\min_{\theta_I} \sum_{\alpha \in \text{atoms}} \left(e_\alpha \Delta V_\alpha - \sum_{I \in \text{nodes}} \rho c_v N_{I\alpha} \theta_I \Delta V_\alpha \right)^2 \Longrightarrow \theta_I = \sum_{\alpha} \hat{N}_{I\alpha} T_\alpha$$

$$\rho \equiv \frac{m_\alpha}{\Delta V_\alpha}, \quad c_v \equiv \frac{3k_B}{m_\alpha}$$

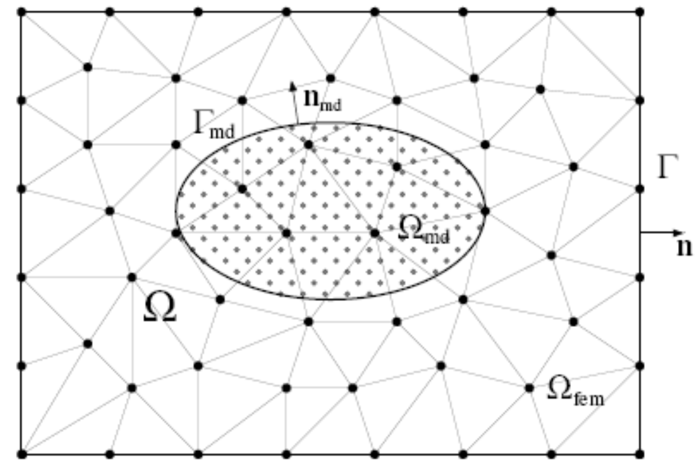
Dulong-Petit expression for heat capacity of a mono-atomic solid or dense fluid above the Debye temperature

Using row-sum lumping (localization) and atomic quadrature for mass matrix in MD region (thermodynamic consistency)

$$\hat{N}_{I\alpha} = \frac{N_{I\alpha}}{\sum_\beta N_{I\beta}}$$

$$T_\alpha = \frac{1}{3k_B} m_\alpha \left|\mathbf{v}_\alpha\right|^2$$

Derivation of Coupled FEM-MD Equations



- Apply Galerkin method to entire domain:
  - Decompose domain:

$$\int_{\Omega} N_I(\mathbf{x})\,\rho c_v \dot{\theta}^h(\mathbf{x})\; dV = \int_{\Omega_{\text{fem}}} N_I(\mathbf{x})\,\rho c_v \dot{\theta}^h(\mathbf{x})\; dV + \sum_{\alpha} N_{I\alpha}\rho c_v \dot{\theta}^h_\alpha \Delta V_\alpha$$

  - Use atomic temperature:

$$\int_{\Omega_{\text{fem}}} N_I(\mathbf{x})\,\rho c_v \dot{\theta}^h(\mathbf{x})\; dV + \sum_{\alpha} N_{I\alpha}\rho c_v \dot{\theta}^h_\alpha \Delta V_\alpha = \int_{\Omega_{\text{fem}}} N_I(\mathbf{x})\,\rho c_v \dot{\theta}^h(\mathbf{x})\; dV + \sum_{\alpha} N_{I\alpha} e_\alpha \Delta V_\alpha$$

  - Apply physics:

$$\int_{\Omega_{\text{fem}}} N_I(\mathbf{x})\,\rho c_v \dot{\theta}^h(\mathbf{x})\; dV + \sum_{\alpha} N_{I\alpha}\rho c_v \dot{\theta}^h_\alpha \Delta V_\alpha = \int_{\Omega_{\text{fem}}} N_I \nabla\cdot\kappa\nabla\theta^h\, dV + 2\sum_{\alpha} N_{I\alpha}\mathbf{v}_\alpha\cdot\mathbf{f}_\alpha$$

  - Discretize:

$$\sum_J M_{IJ}\dot{\theta}_J = \sum_J K_{IJ}\theta_J + 2\sum_\alpha N_{I\alpha}\mathbf{v}_\alpha\cdot\mathbf{f}_\alpha$$

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Coupling MD Thermostat

- Effects of FEM on MD can be included by prescribing constraints relating the FE and MD dynamics:
  - Temperature constraint

$$2\sum_{\alpha} N_{I\alpha}\mathbf{v}_{\alpha}\cdot\mathbf{f}_{\alpha} - \sum_{J} M_{IJ}^{MD}\dot{\theta}_{J} = 0$$

  - Heat flux constraint

$$\sum_{\alpha} N_{I\alpha}\left(\frac{\partial\Phi}{\partial\mathbf{x}_{\alpha}}\cdot\mathbf{v}_{\alpha} + \mathbf{v}_{\alpha}\cdot\mathbf{f}_{\alpha}\right) + \int_{\Gamma_{MD}} N_{I\alpha}\mathbf{n}_{md}\cdot q^{h}\,dA = 0$$

  - Application of Gauss' principle of least constraint to atomic forces:

$$\mathbf{f}_{\alpha} = \mathbf{f}_{\alpha}^{MD} - \frac{m_{\alpha}}{2}\lambda\left(\mathbf{x}_{\alpha}\right)\mathbf{v}_{\alpha}$$

  - Variable λ is a continuum field defined on the nodes:

$$\lambda\left(\mathbf{x}_{\alpha}\right) = \sum_{I} N_{I\alpha}\lambda_{I}$$

Combined System

- Result is set of coupled FEM/MD equations

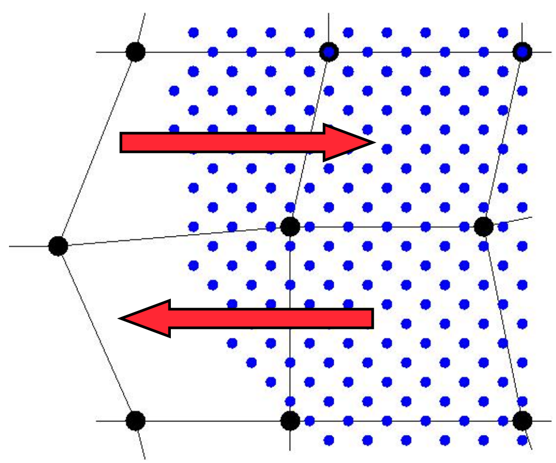
$$\sum_J M_{IJ}\dot{\theta}_J = \sum_J K_{IJ}\theta_J + 2\sum_\alpha N_{I\alpha}\mathbf{v}_\alpha \cdot \mathbf{f}_\alpha$$

$$m_\alpha \dot{\mathbf{v}}_\alpha = \mathbf{f}_\alpha^{MD} - \frac{m_\alpha}{2}\sum_I N_{I\alpha}\lambda_I \mathbf{v}_\alpha$$

Coupling parameter (temperature/flux constraint)

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

Atoms contribute to nodal heat equation



Heat at nodes affects MD energy through thermostat

Fractional Step Method for Time Integration

- Gear time integration for FE dynamics: $K_{IJ}\theta_J$
- Verlet time integration for MD dynamics: $m_\alpha \dot{\mathbf{v}}_\alpha = \mathbf{f}_\alpha^{MD}$
- Consistent update for FE-MD terms:

$$\Delta\left(N_I E_I\right) = \sum_\alpha N_{I\alpha}\left(2\Delta t \mathbf{v}_\alpha \cdot \mathbf{f}_\alpha + \Delta t^2 m_\alpha^{-1} \mathbf{f}_\alpha \cdot \mathbf{f}_\alpha\right)$$

- Exact constraint enforcement applied after other time updates using the fractional step method

$$\Delta t \sum_\alpha N_I^\alpha k_\alpha \sum_{\mathcal{J}} N_J^\alpha \lambda_J - \frac{\Delta t^2}{4} \sum_\alpha N_I^\alpha k_\alpha \left(\sum_J N_J^\alpha \lambda_J\right)\left(\sum_K N_K^\alpha \lambda_K\right) = \mathrm{RHS}$$

- Can eliminate energy loss/gain in coupling

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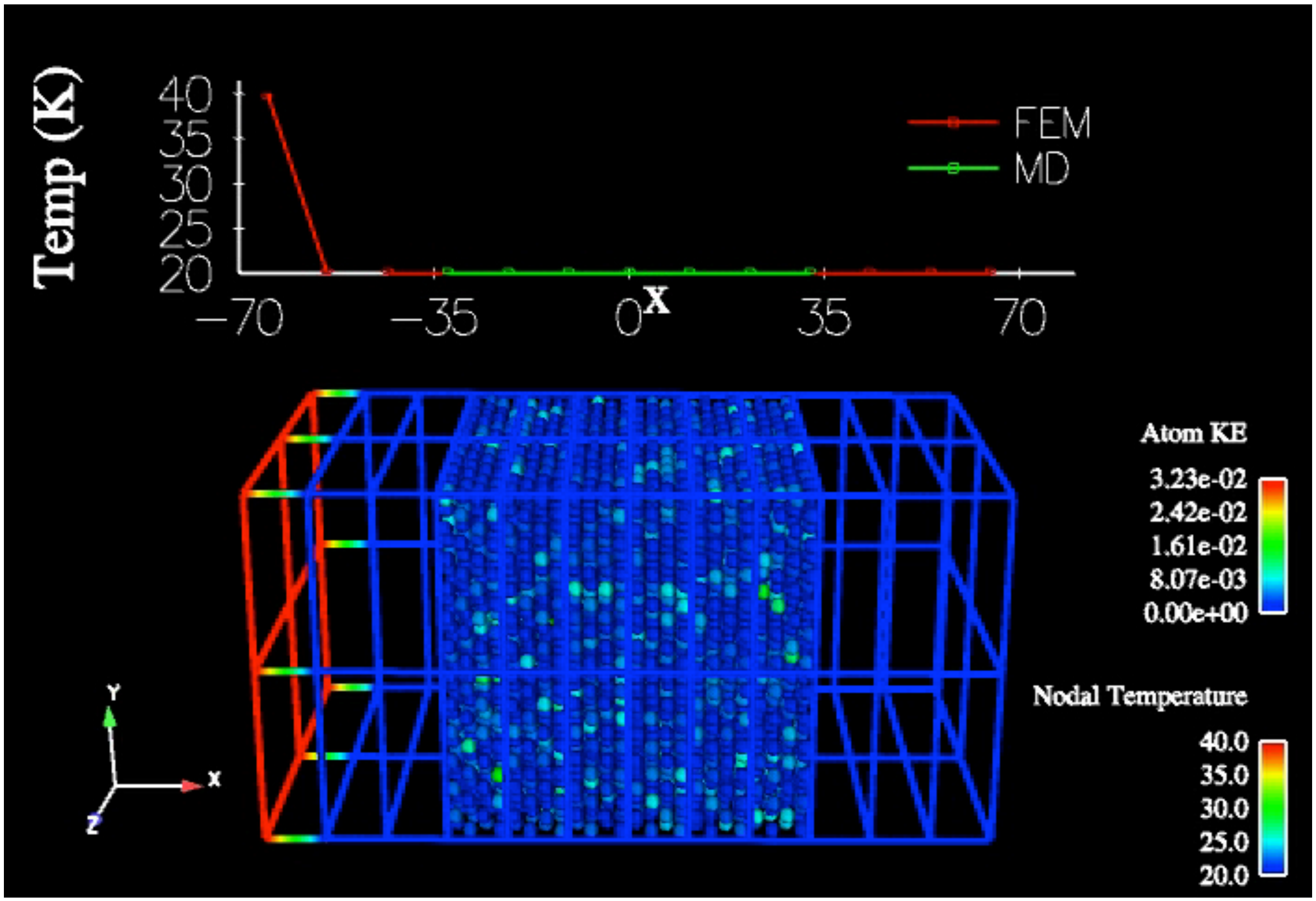
Coupled System

- 1D bar with embedded MD region (~7000 atoms)
- FEM nodes fixed hot/cold at left/right ends
- Temperature coupling method



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Coupled System

- 1D bar with embedded MD region (~7000 atoms)
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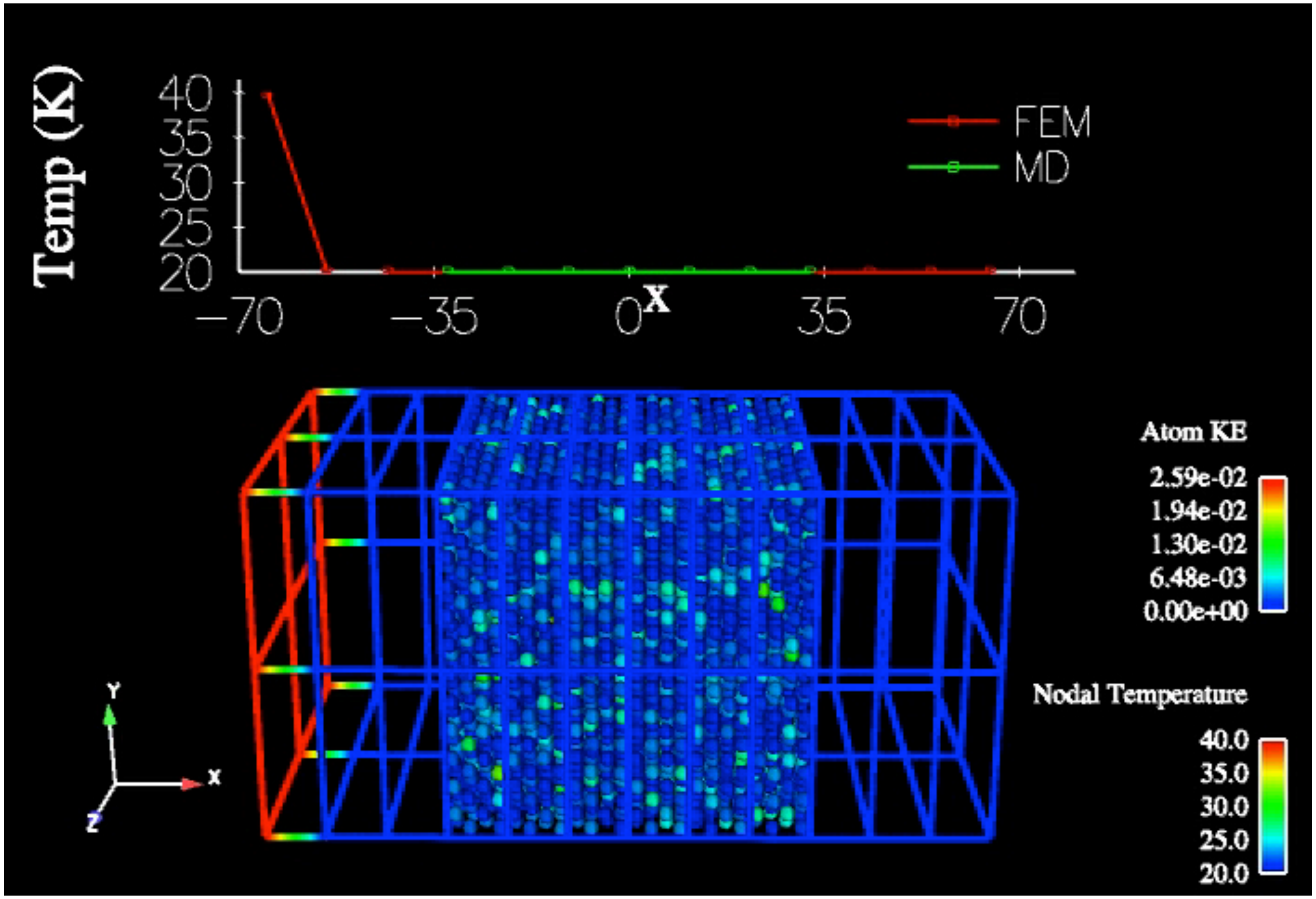

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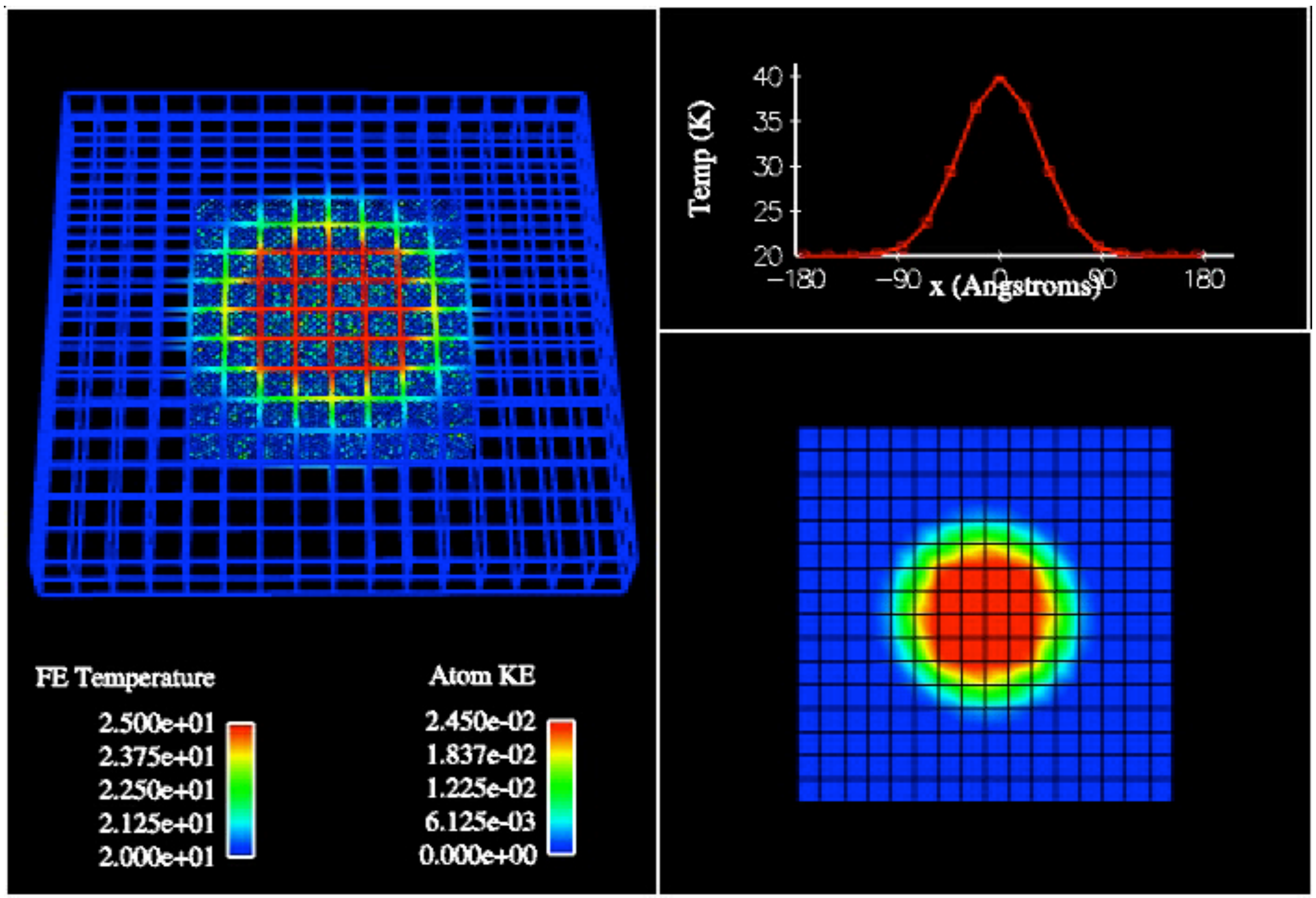
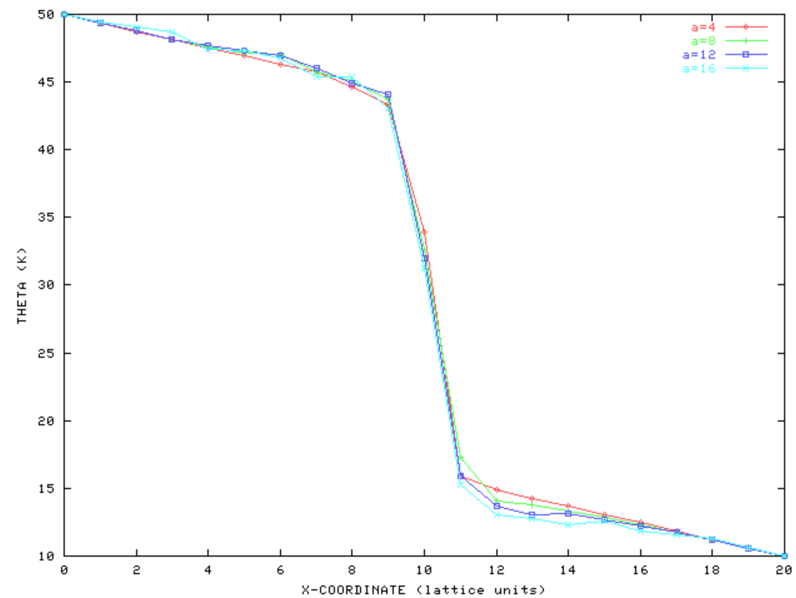
2D Diffusion Problem

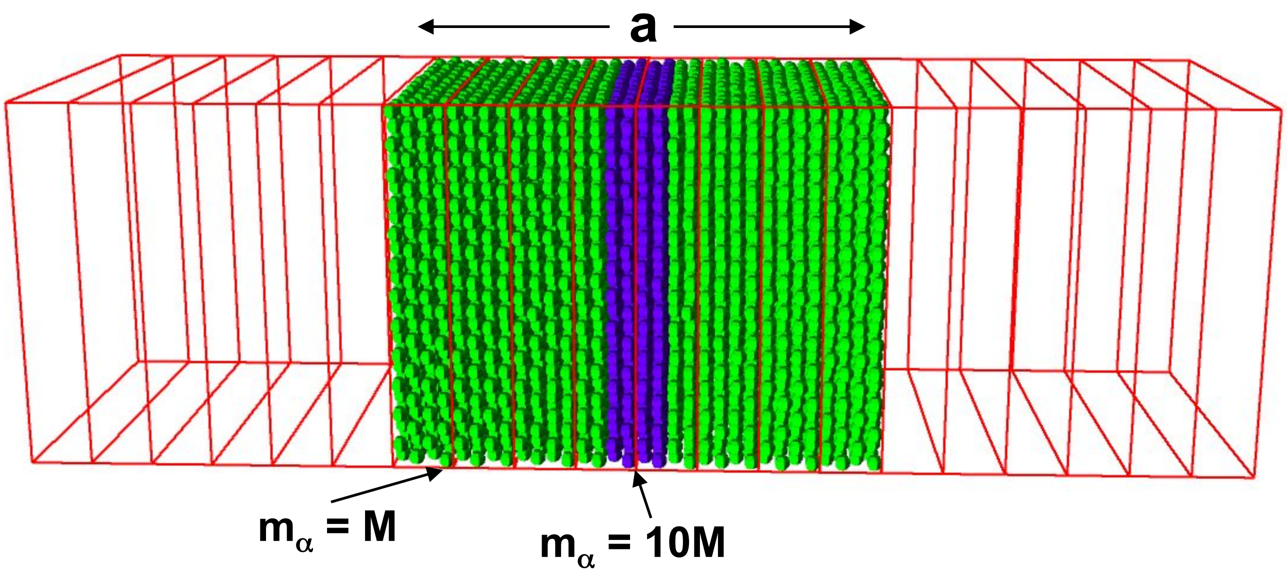
- Plate with embedded MD region (~33,000 atoms)
- Initialized to temperature field with gaussian profile
- Adiabatic boundary conditions at edges



Effects of Imperfections on Conductivity

- Center layers of atoms given 10x mass of surroundings
  - Acoustic mismatch leads to inherent resistance in center layer
- Results are fairly insensitive to size of MD region





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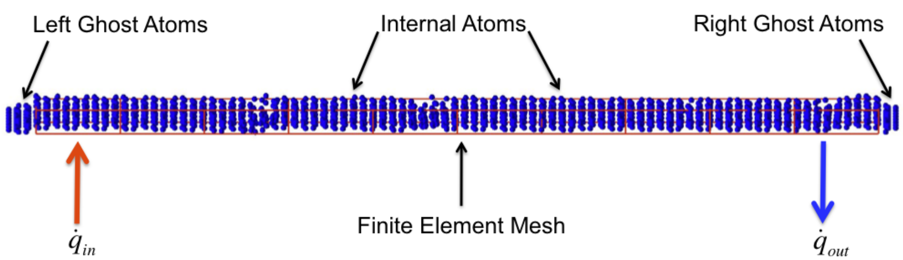
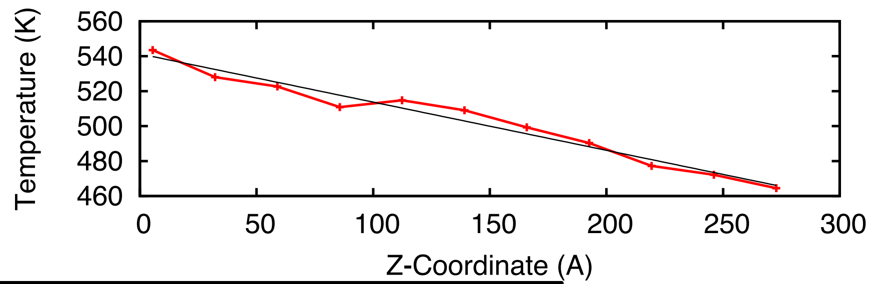
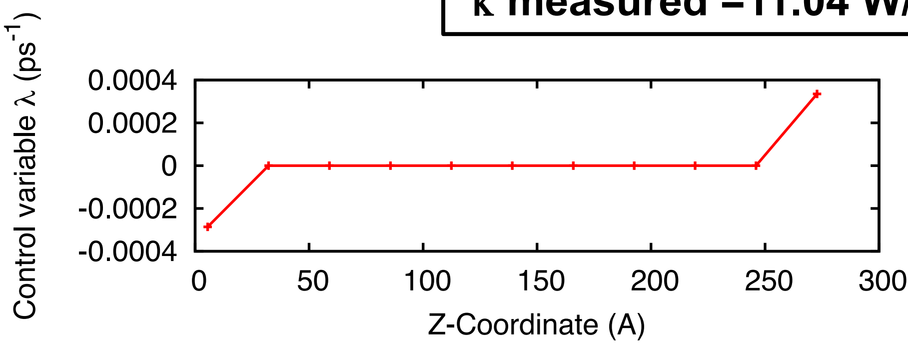
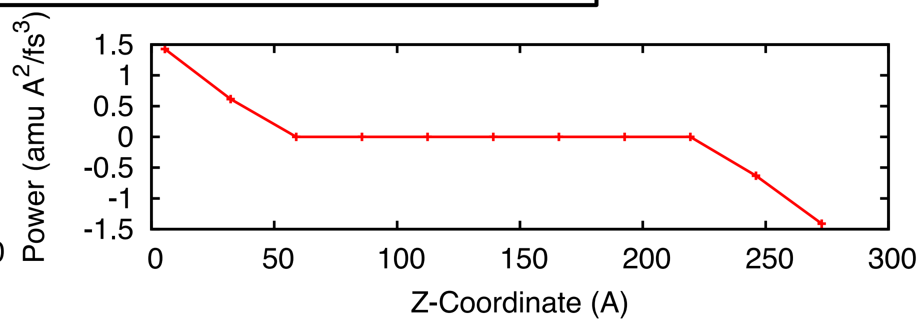
Thermal Conductivity Calculations using AtC Boundary Conditions





κ measured =11.04 W/mK, κ theory = 12.01 W/mK





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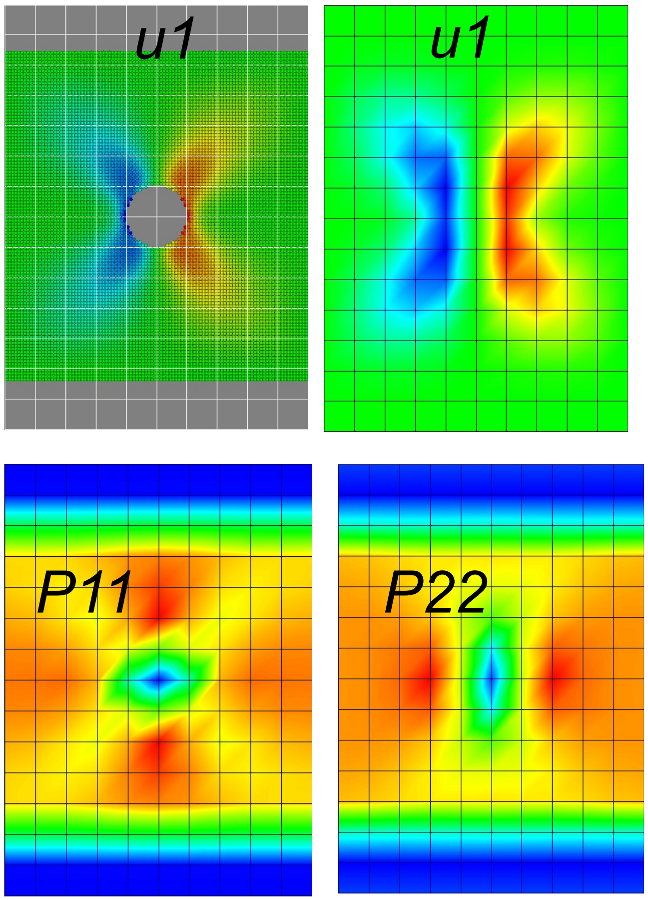
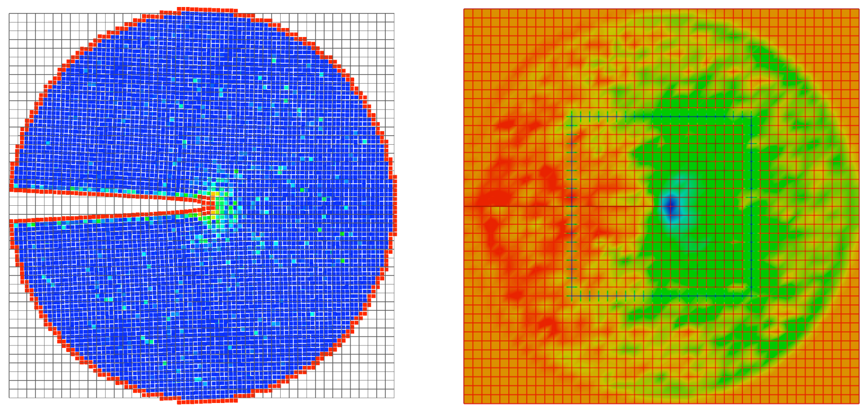
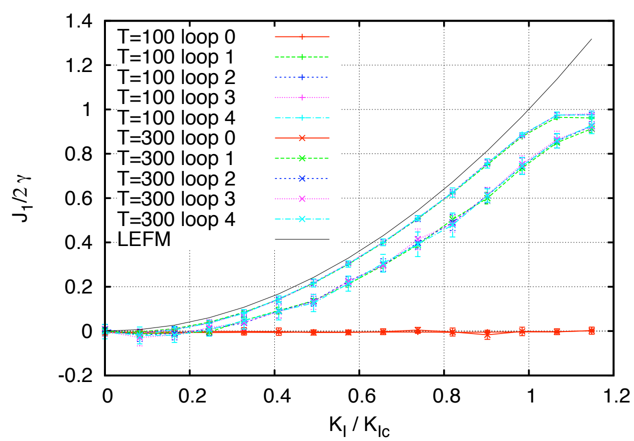
Hardy Analysis

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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Extrinsic Physics Modeling

- MD explicitly represents atomic motions with great accuracy
  - Balistic phonon propagation
  - Defects
  - Nanostructures
- MD does not capture many other important physics
  - Electric fields
  - Energy carriers
  - Electrons
- Represent additional physics in a continuum model
- Use coupling techniques developed in thermal work to interface the two disparate types of physics descriptions
- Examples underway: electron temperature, consistent electric fields, energy carrier density, full "fluidic" description of unrepresented particles

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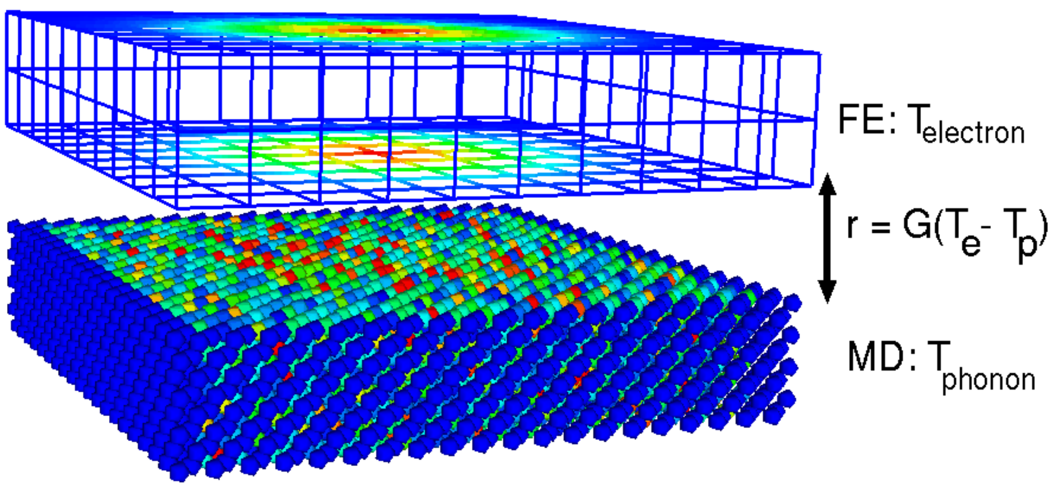
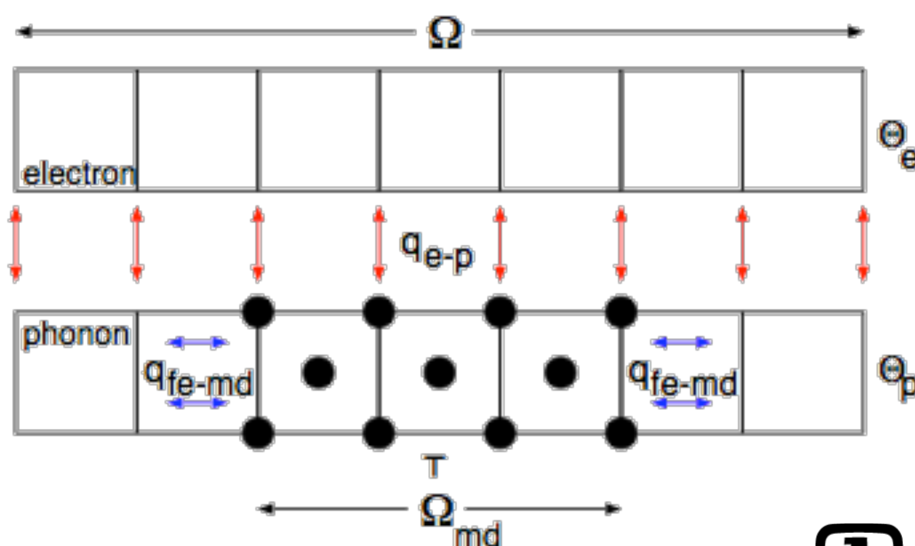
Coupled Two-Temperature Approach



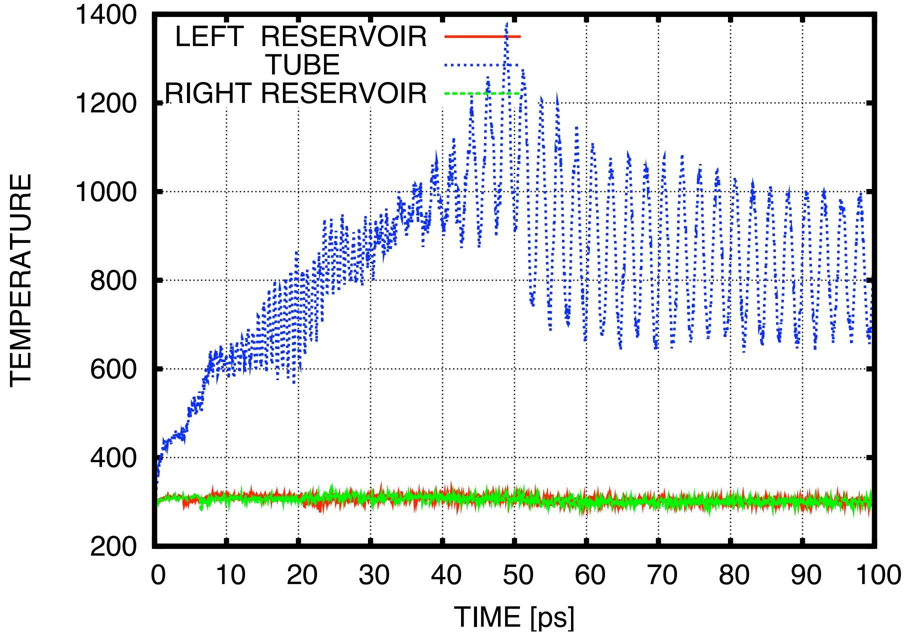
Explicit representation of phonons by MD, Electron effects solved for on overlaid mesh

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

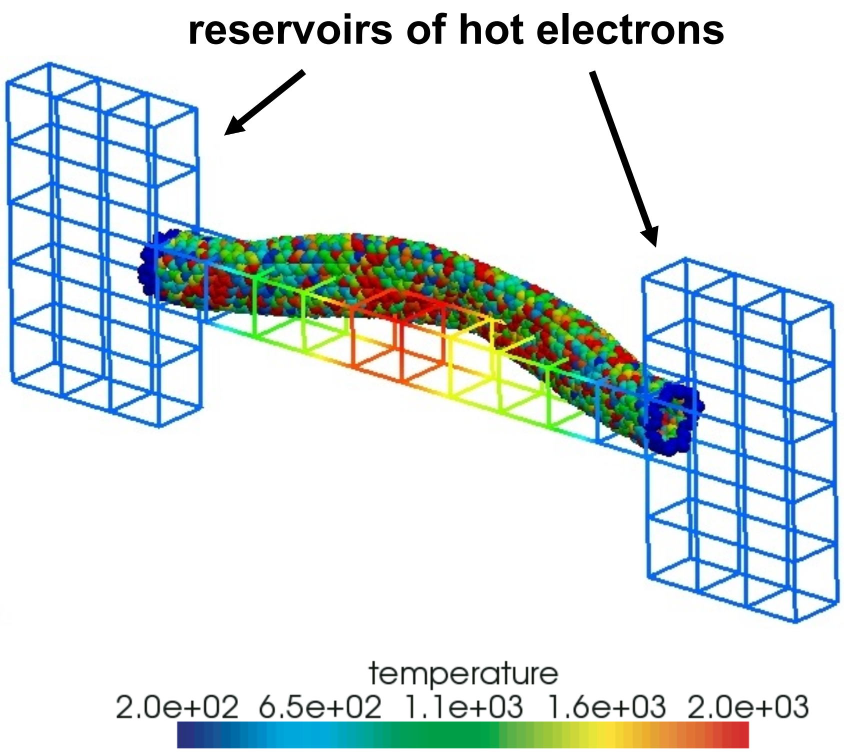


Laser heating of a metallic CNT

- eMD can be used to model heating and thermal-induced vibration in nanostructures that possess a metallic character of thermal conduction, e.g. (8,8) armchair CNT.



Evolution of average temperatures of CNT and reservoirs



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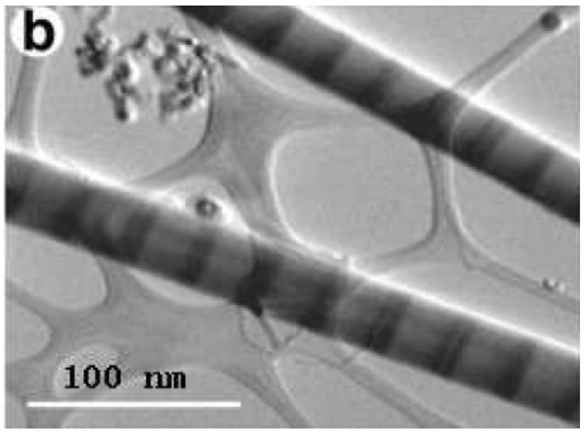
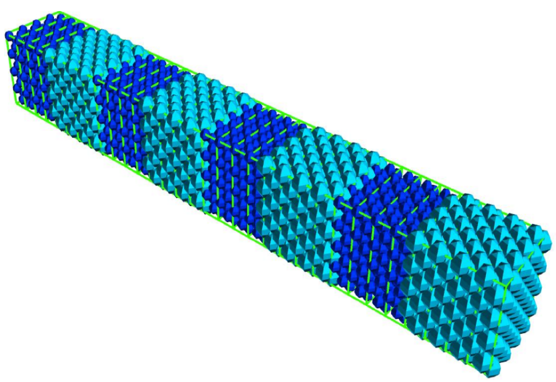
Ge/Si superlattice nanowires

- Our method captures the retarded phonon transmission observed for Ge/Si superlattice nanowires with application to thermoelectrics





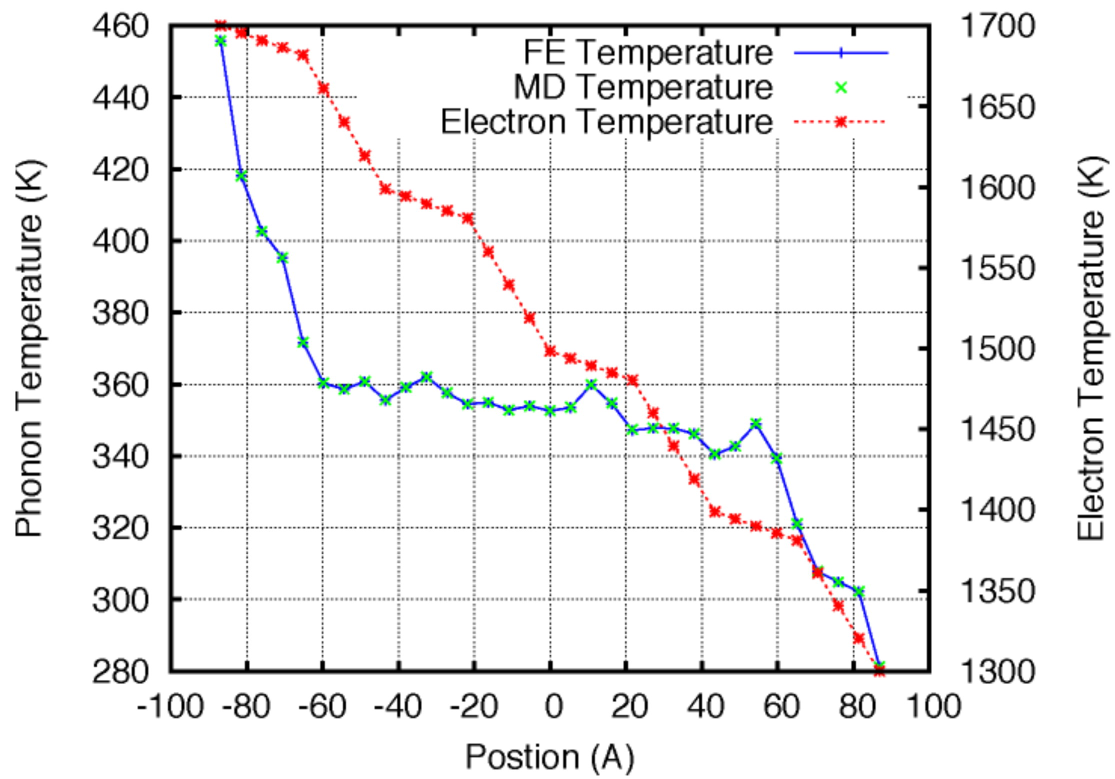
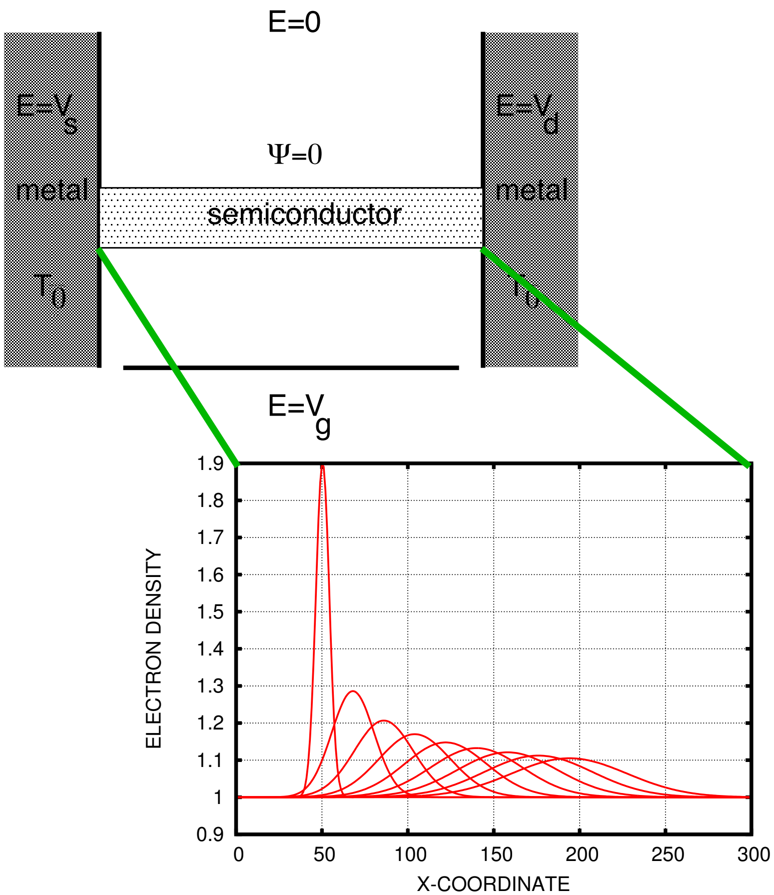


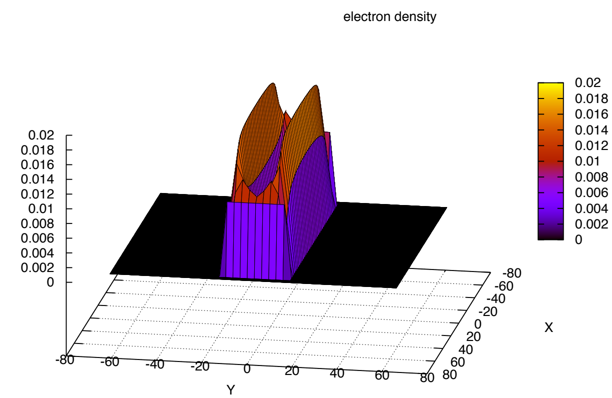
Figure 8: Temperature profiles in the superlattice

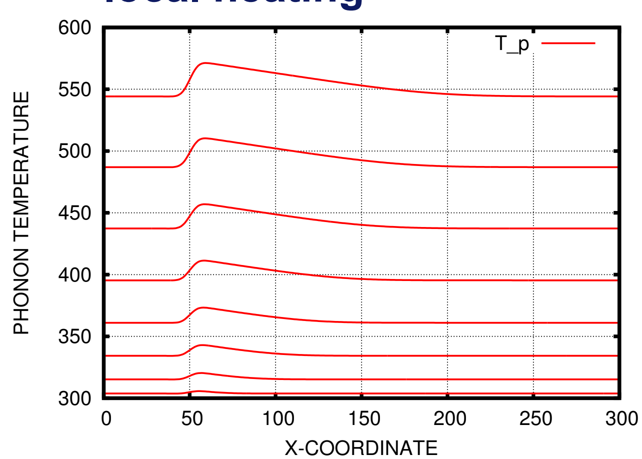
Metallic and Semi-Conductor Powered Nanodevices

- Drift-diffusion models can be used to study powered nanowires and the interaction between current and heating



Quantum effects in nanowires give rise to spatially varying electron density and local heating





Electron pulse gives rise to uniform and local heating

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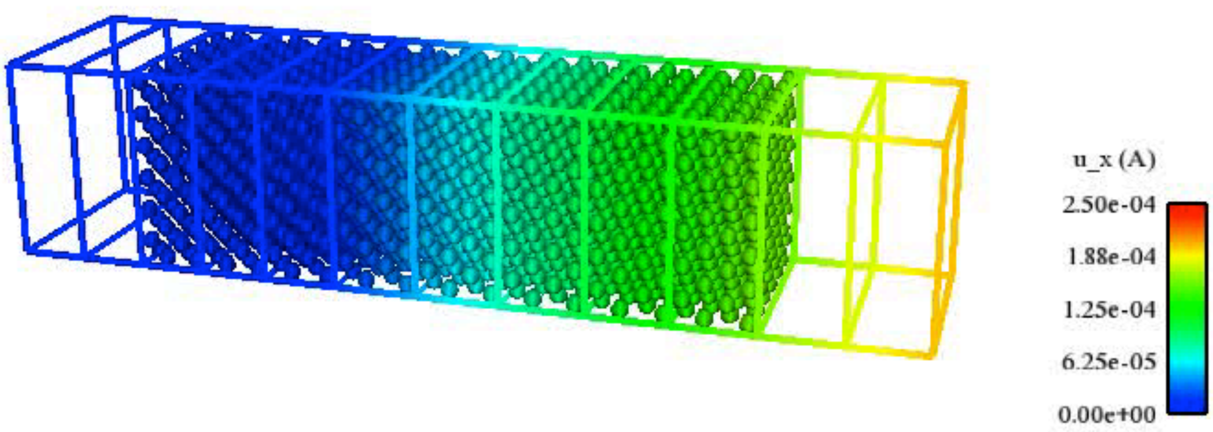
Other Physical Models: Elasticity

- Many types of physics problems can use the same mathematical and algorithmic structure
- Elasticity dynamics of a bar at the nano-scale:



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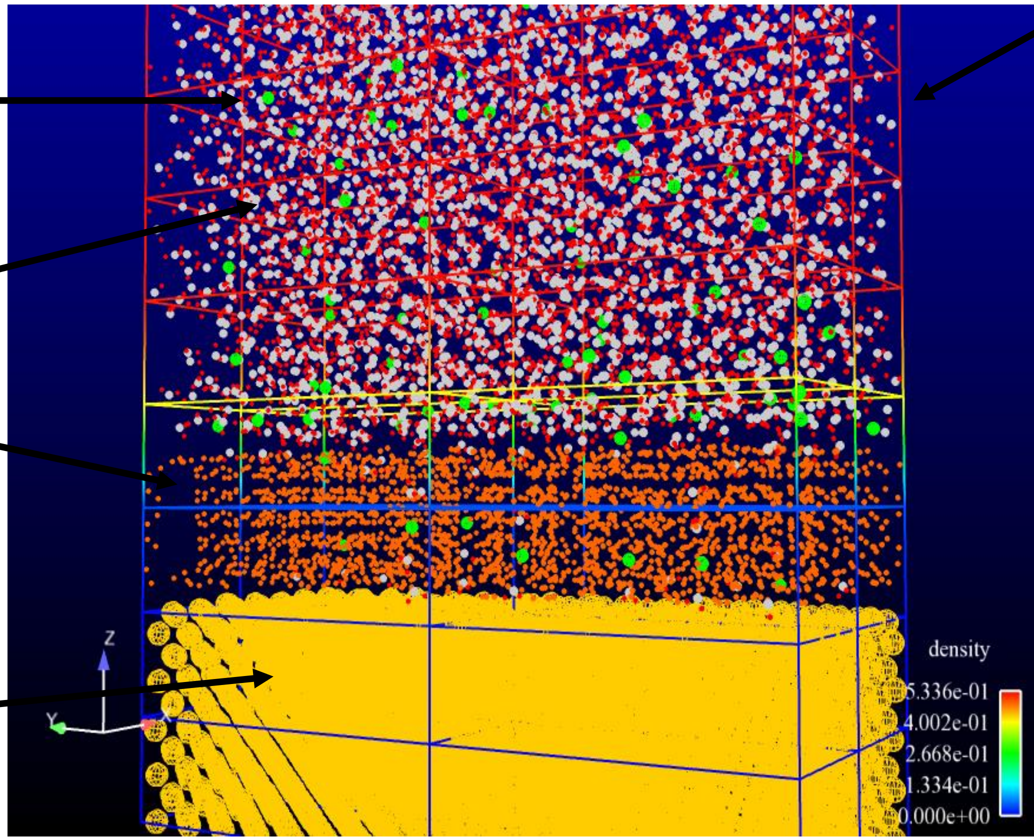
AtC Model for Long-range Electrostatics

Ions

Water

CNT Channels

Gold Electrode

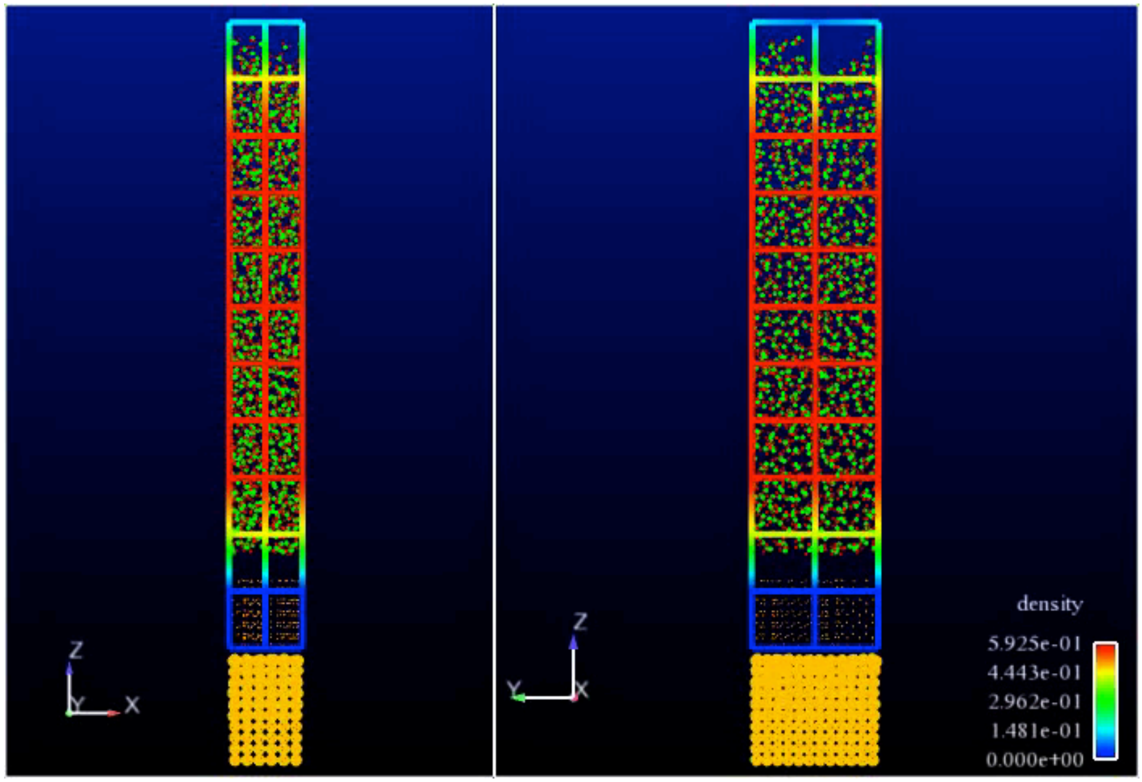


FE Mesh Enables

1. Coarse-scaling MD for increased physical understanding
2. Solves for electric field with
   a) Upscale FE source terms
   b) Downscale MD electric forces

Other Physical Models: Fluidic Species Transport

- Define coupling in Eulerian frame rather than Lagrangian
- Track individual species to understand particle agglomeration and diffusion
- Example problem: transport of saltwater into nanotubes



- Future work: energy storage devices

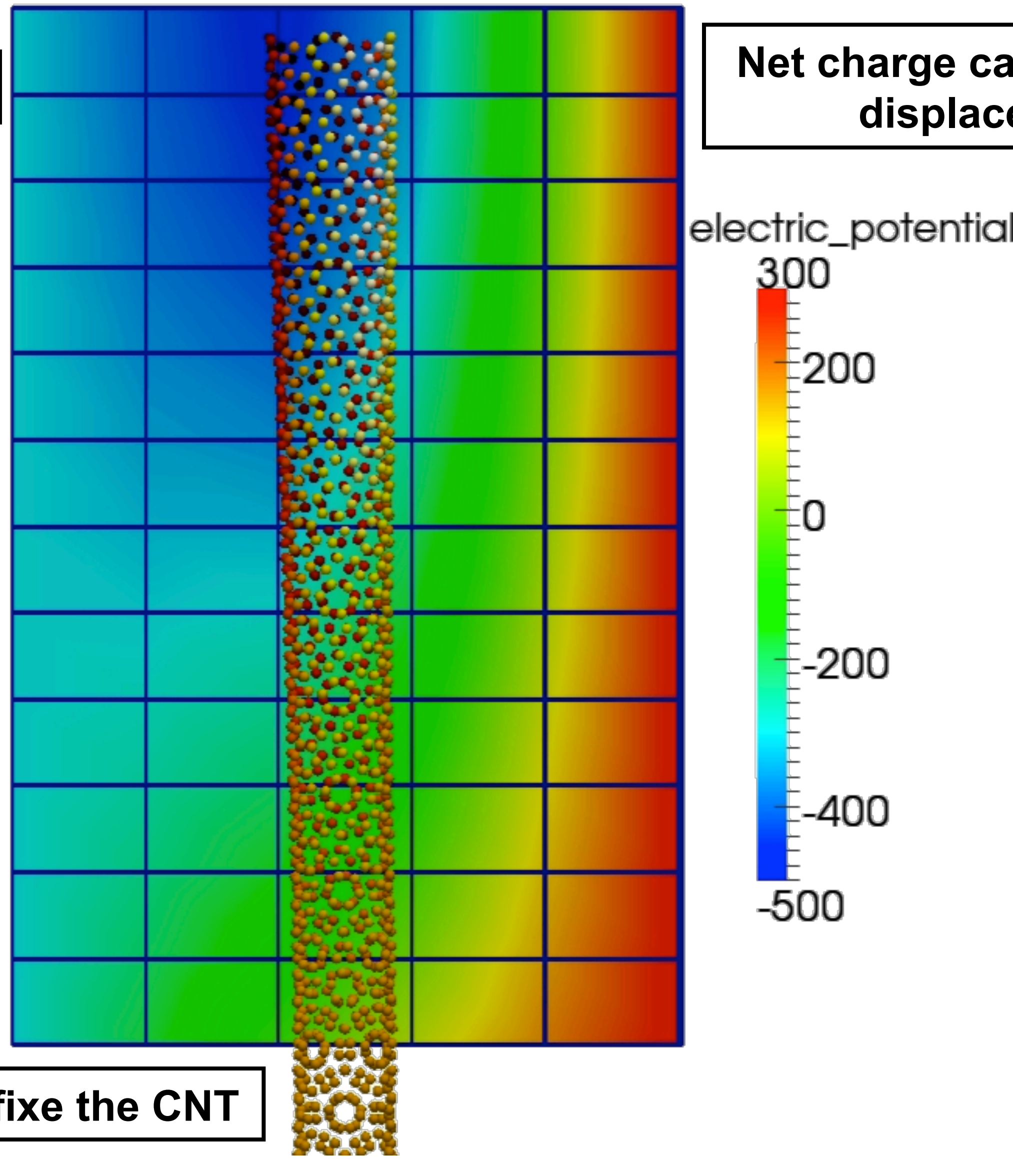
Other Physical Models: Electrostatics

Potential drop across short axis

Mutual repulsion opens tip

Net charge causes net tip displacement

Electrons segregate to tip



Atoms anchored to fixe the CNT

References

- **Thermal coupling**
  - Wagner *et al.*, *Comp. Meth. Appl. Mech. Eng.* (2008)
  - Templeton, Jones, & Wagner, *Model. Simul. Mater. Sci. Eng* (2010)
- **Hardy post-processing**
  - Zimmerman, Jones, & Templeton, *J. Comp. Phys.* (2010)
  - Jones & Zimmerman, *J. Mech. Phys. Solids* (2010)
  - Jones *et al., Phys. Condens. Matter* (2010)
- **Two-temperature modeling**
  - Jones *et al., Int'l J. Numer. Meth. Eng.* (2010)
- **Long-range electrostatics**
  - Templeton *et al., J. Comput. Theor. Chem.* (in press)

Simulations performed with LAMMPS MD code:

http://lammps.sandia.gov

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