Overview of the Atoms-to-Continuum Package for LAMMPS

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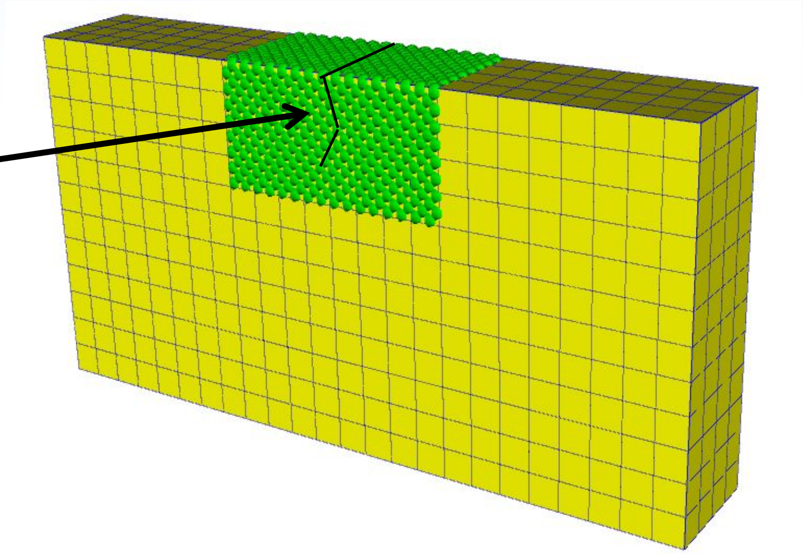
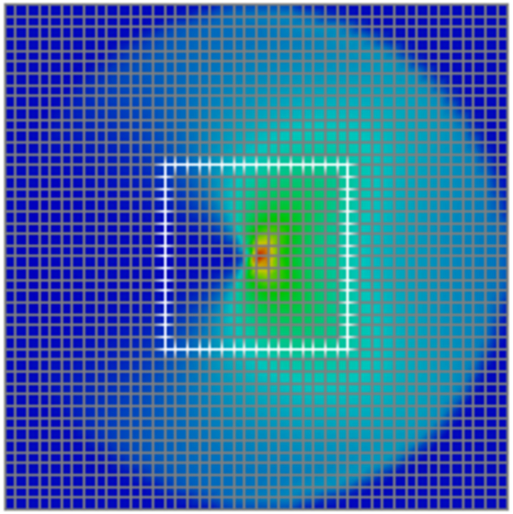
Motivation



- 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



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Getting Started with the atc Package

- The atc package is a standard user package in LAMMPS
- It is built as a library from the `/USER/atc` directory
- Several example makefiles are included
  - We have built and tested on on various flavors of Linux and MacOS
- You will need to have the blas and lapack libraries installed to support the matrix operations used by the code
- In the LAMMPS `src` directory type `make yes-atc` to link with the package
  - The `Makefile.user` should then have the appropriate libraries for linking
- The standard LAMMPS makefiles will work without modification
- See `/USER/atc/README` for more information
- Now you're ready to do some damage!

The atc fix

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

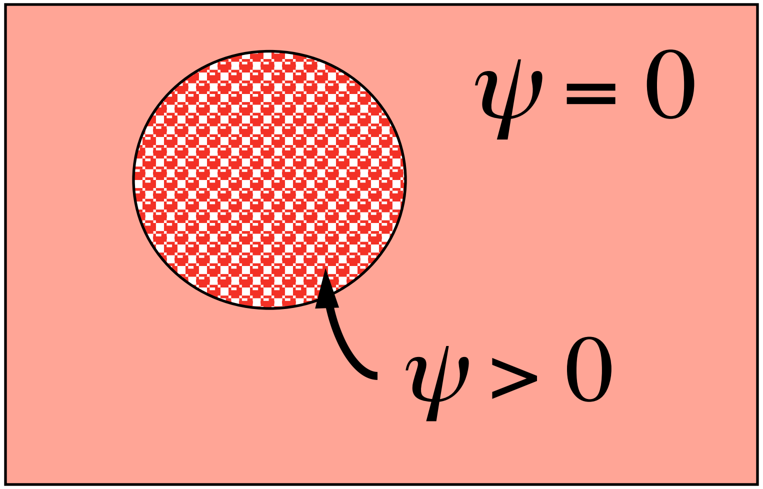
- ID, groupID documented in the fix command
  - In coupled simulations, groupID is for the internal atoms (but we'll get to that)
- type = **thermal** or **two_temperature** or **hardy**
  - **thermal** = coupling atoms with a finite element temperature field for multiscale modeling or applying boundary conditions
  - **two_temperature** = coupling atoms with a finite element electron temperature field for energy exchange
    - Also allows all capabilities of thermal
    - Distinct from fix ttm by P. Crozier
  - **hardy** = Hardy on-the-fly post-processing of atomistic quantities to a continuum field
- paramfile = file with FE material parameters
  - Not specified for hardy
  - Values not used for boundary condition problems

Hardy On-The-Fly Post-Processing

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

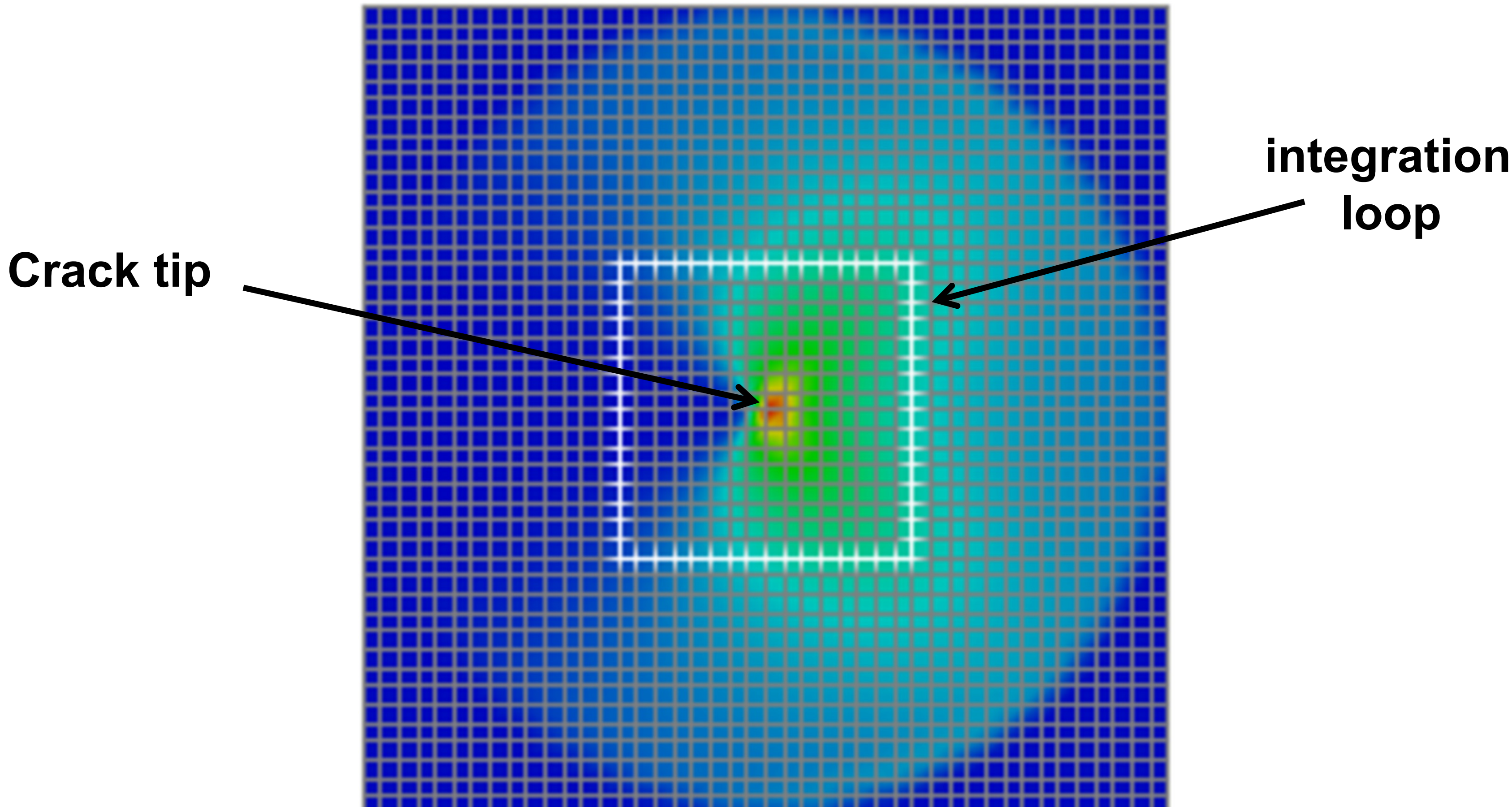
$$\mathbf{P}(\mathbf{X},t) = -\frac{1}{2}\sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N}\mathbf{f}^{\alpha\beta}\otimes\mathbf{X}^{\alpha\beta}B^{\alpha\beta}(\mathbf{X})$$

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



Example 1: Hardy Post-Processing

- Objective: calculate the Eshelby stress over various loops surrounding a crack tip



Example 1: Hardy Post-Processing

```
# …instantiate the atc fix
region     SYSTEM block -10 10 -10 10 0 3
group      internal region SYSTEM
fix        AtC internal atc hardy
fix_modify AtC mesh create 10 10 1 box p f p
fix_modify AtC transfer fields none
fix_modify AtC transfer fields add density energy
               temperature stress displacement
fix_modify AtC fields add eshelby_stress
               transformed_stress
fix_modify AtC gradients add displacement
fix_modify AtC set reference_potential_energy
fix_modify AtC output eshelby_staticFE 1 text
               binary tensor_components
```

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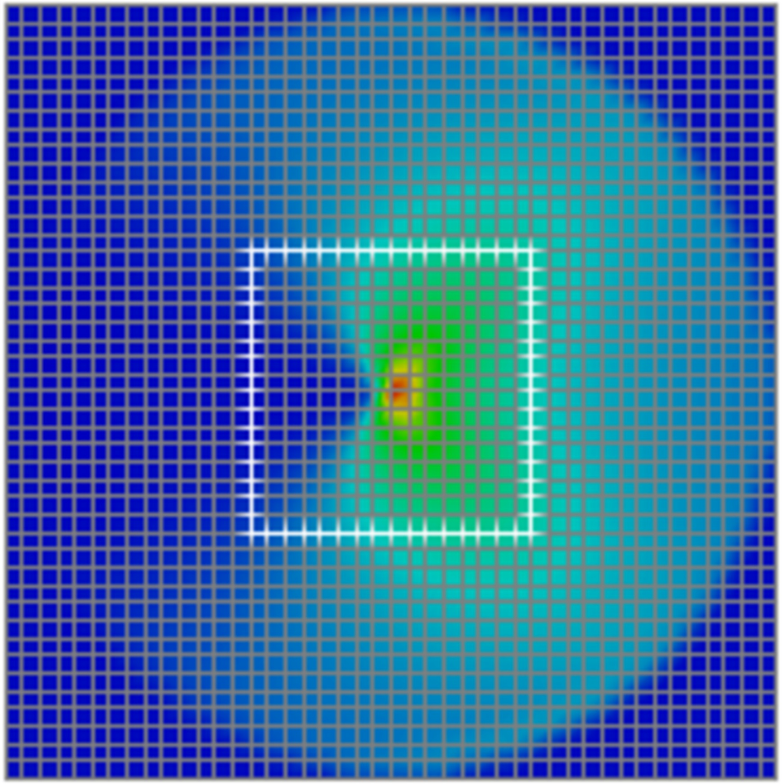
Example 1: Hardy Post-Processing

- Create integration loops surrounding the crack tip to compare the line integral invariants with theory

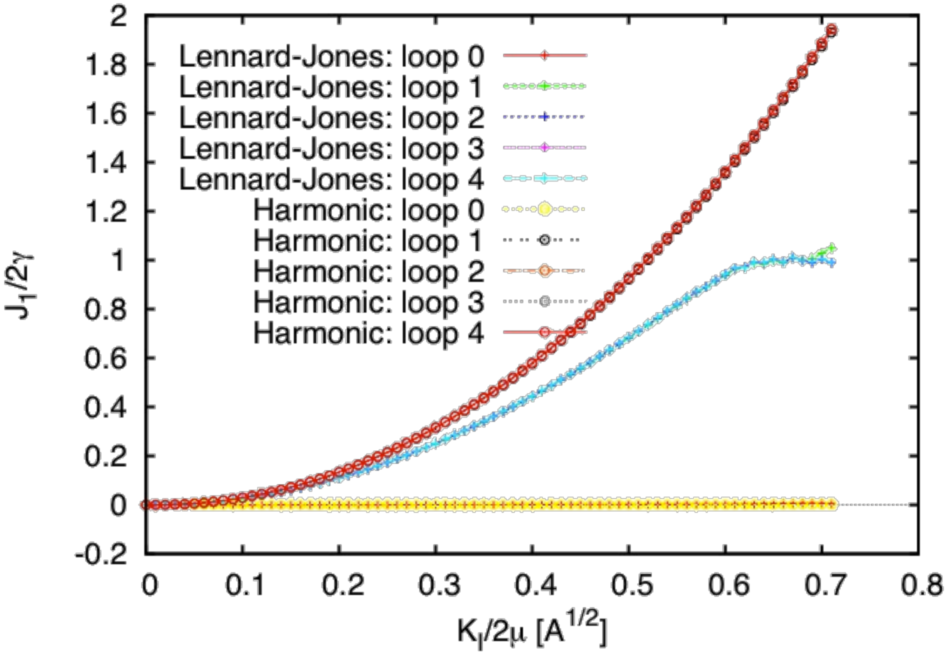
```
#... make concentric loops around the crack tip
fix_modify AtC mesh create_faceset loop0 box -6  0
               6 10 -INF INF outward
fix_modify AtC boundary_integral eshelby_stress
               faceset loop0
fix_modify AtC boundary_integral stress
               faceset loop0
fix_modify AtC boundary_integral energy
               faceset loop0
#... define other loops
#... run minimization steps
```

Example 1: Hardy Post-Processing



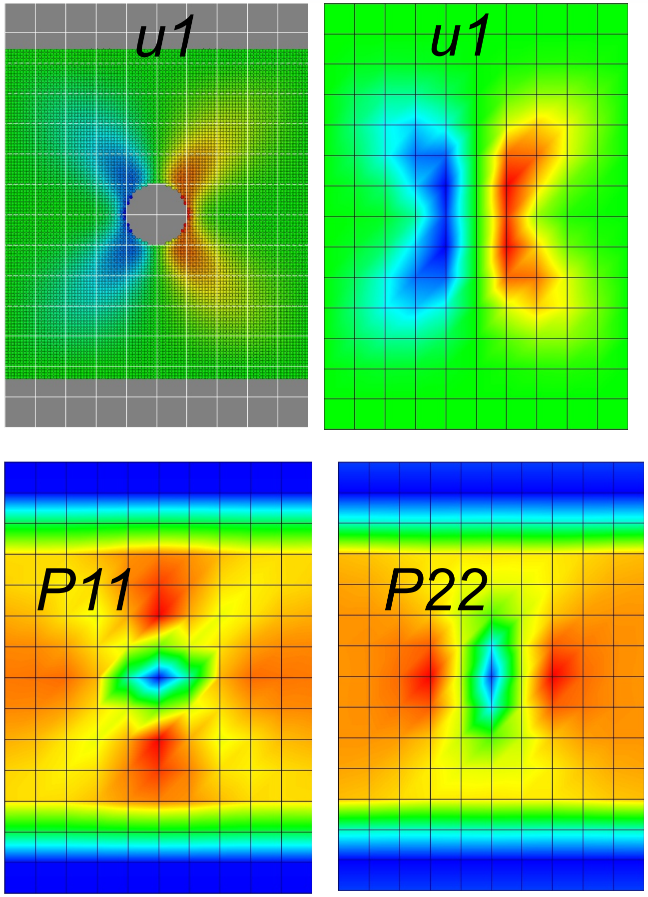
Coarse-grained atomic stress field

J-integral values over various contours

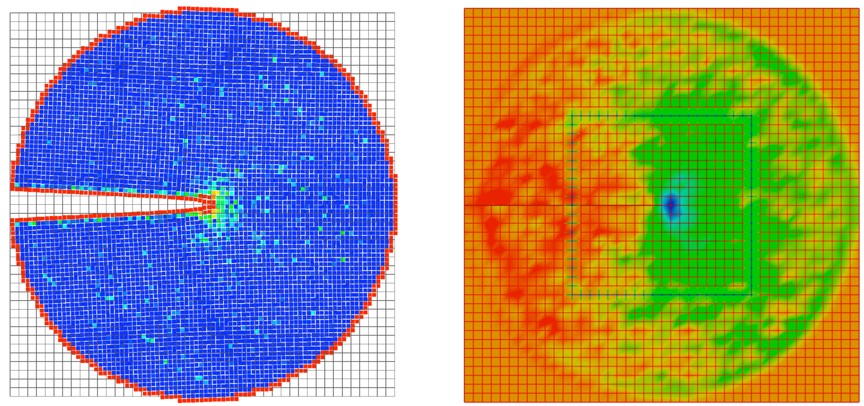


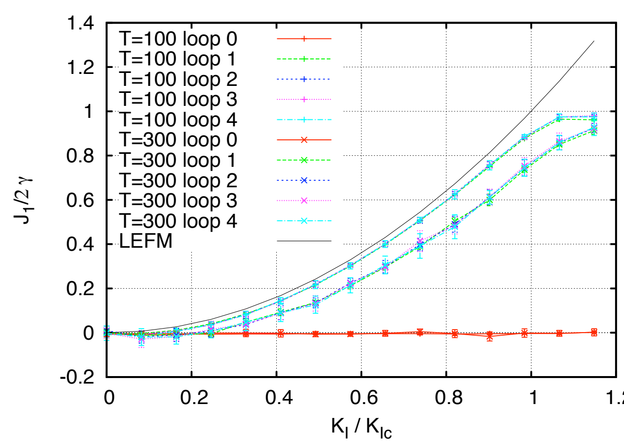
Examples of Hardy Post-Processing

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

- **Result is set of coupled FEM/MD equations**

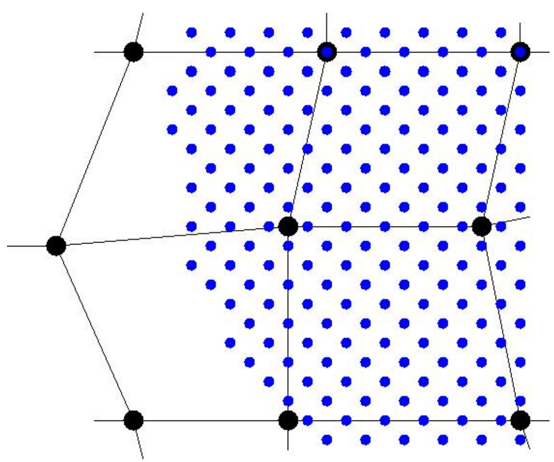
$$\sum_J M_{IJ}\dot{\theta}_J = \sum_J K_{IJ}\theta_J + 2\sum_\alpha N_{I\alpha}\mathbf{v}_\alpha \cdot \mathbf{f}_\alpha$$

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

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

Example 2: Fixed Temperature Boundaries

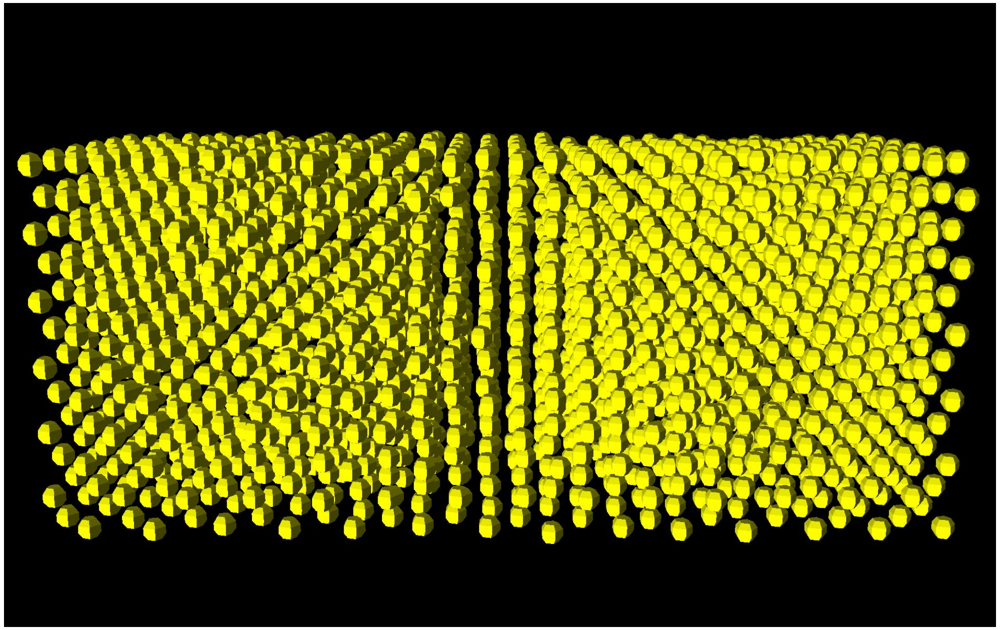
- Goal: Compute the thermal conductivity of a specimen
- Set up the problem like a finite element model

1) Mesh
    - Define the geometry of the problem
    - Specify fineness/coarseness of the discretization
2) Initial Conditions
    - Starting state of the problem
    - Can be equilibrium or non-equilibrium
3) Boundary conditions
    - Fixed temperature locations
    - Heat fluxes at each end
4) Source terms
    - Energy added to the system at specific locations
5) Time integration and numerical methods
    - Includes time filtering to smooth fluctuations

Example 2: Fixed Temperature Boundaries

- Instantiation of the AtC fix and creation of the mesh

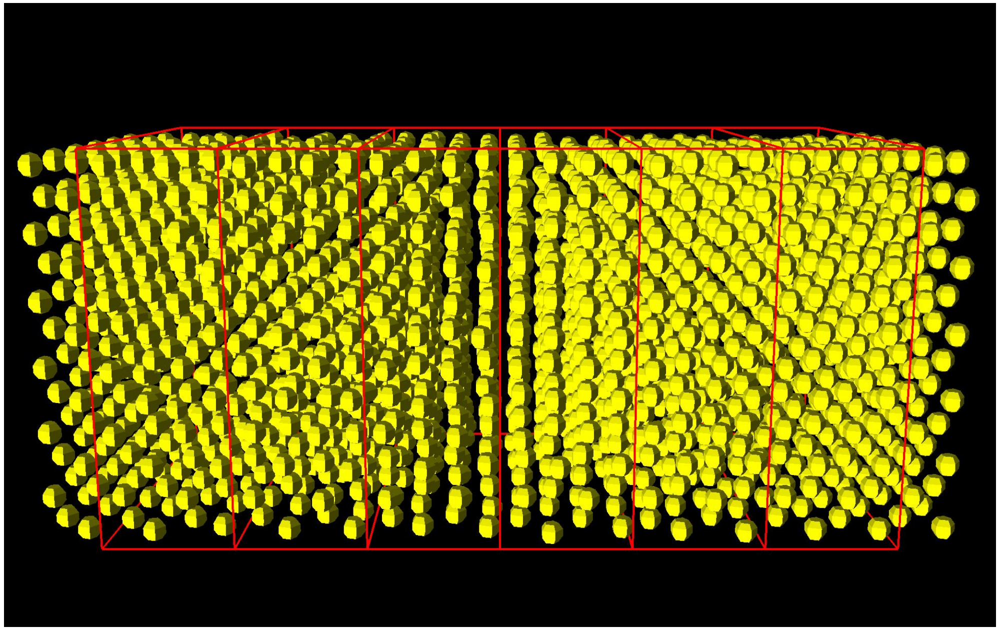
```
region      mdInternal block -6 6 -3 3 -3 3
group       internal region mdInternal
```



Example 2: Fixed Temperature Boundaries

- Instantiation of the AtC fix and creation of the mesh

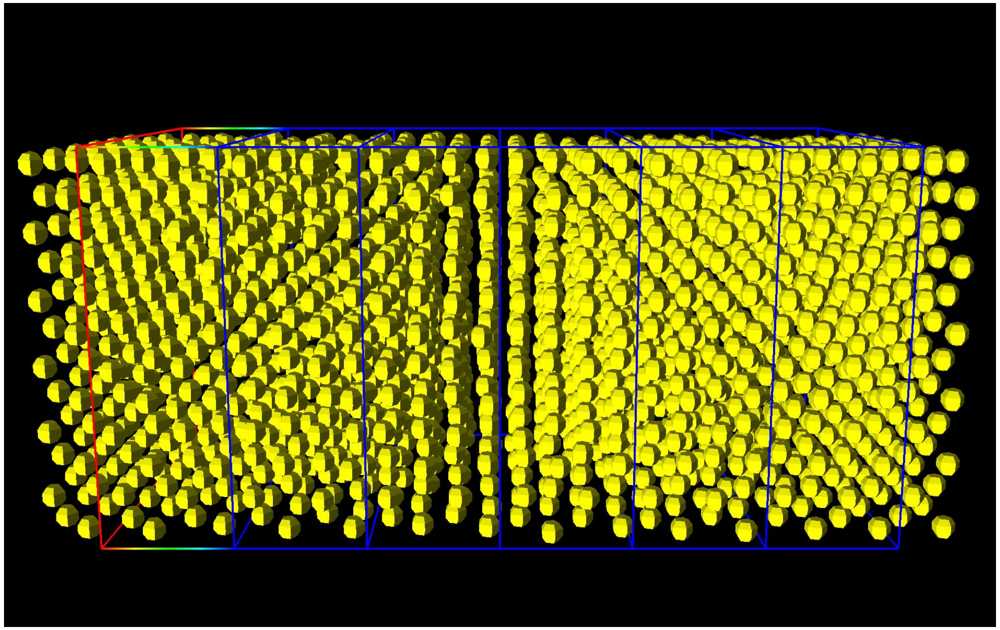
```
region      mdInternal block -6 6 -3 3 -3 3
group       internal region mdInternal
fix         AtC internal atc thermal Ar_thermal.mat
fix_modify AtC mesh create 6 1 1 mdInternal f p p
```



Example 2: Fixed Temperature Boundaries

- Add needed groups to the mesh

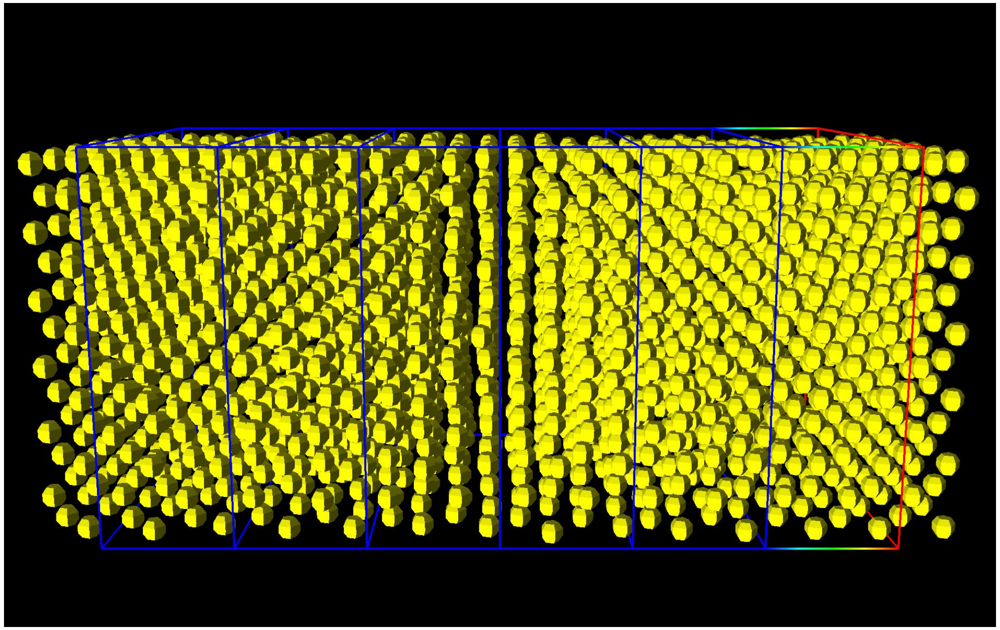
```
fix_modify AtC mesh create_faceset lbndy box -6.0
               16.0 -INF INF -INF INF outward
fix_modify AtC mesh create_nodeset lbc -6.1 -5.9
               -INF INF -INF INF
```



Example 2: Fixed Temperature Boundaries

- Add needed groups to the mesh

```
fix_modify AtC mesh create_faceset lbndy box -6.0
               16.0 -INF INF -INF INF outward
fix_modify AtC mesh create_nodeset lbc -6.1 -5.9
               -INF INF -INF INF
fix_modify AtC mesh create_nodeset rbc  5.9  6.1
               -INF INF -INF INF
```



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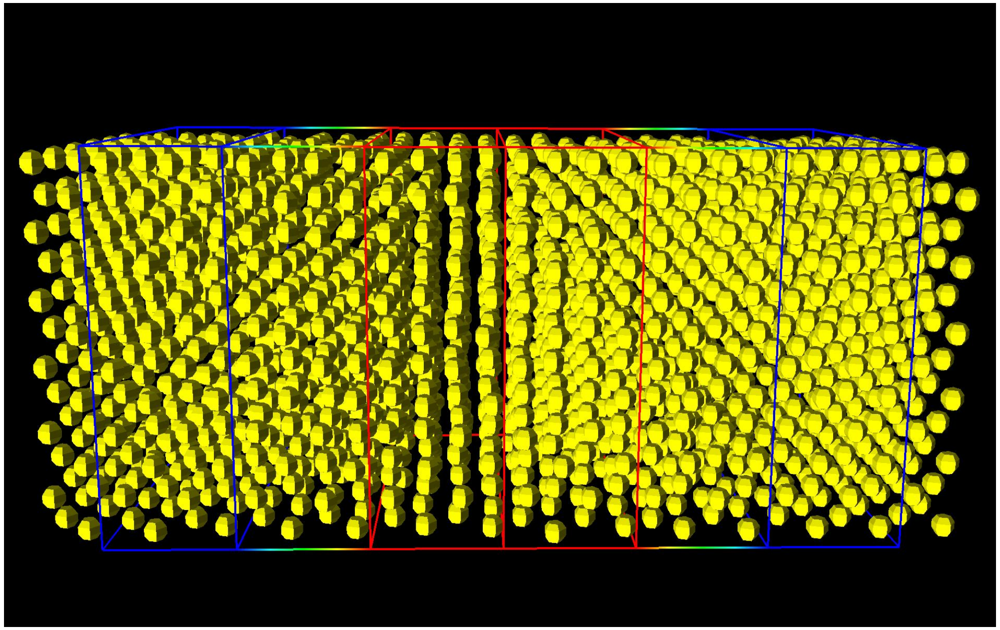
Example 2: Fixed Temperature Boundaries

- Add needed groups to the mesh

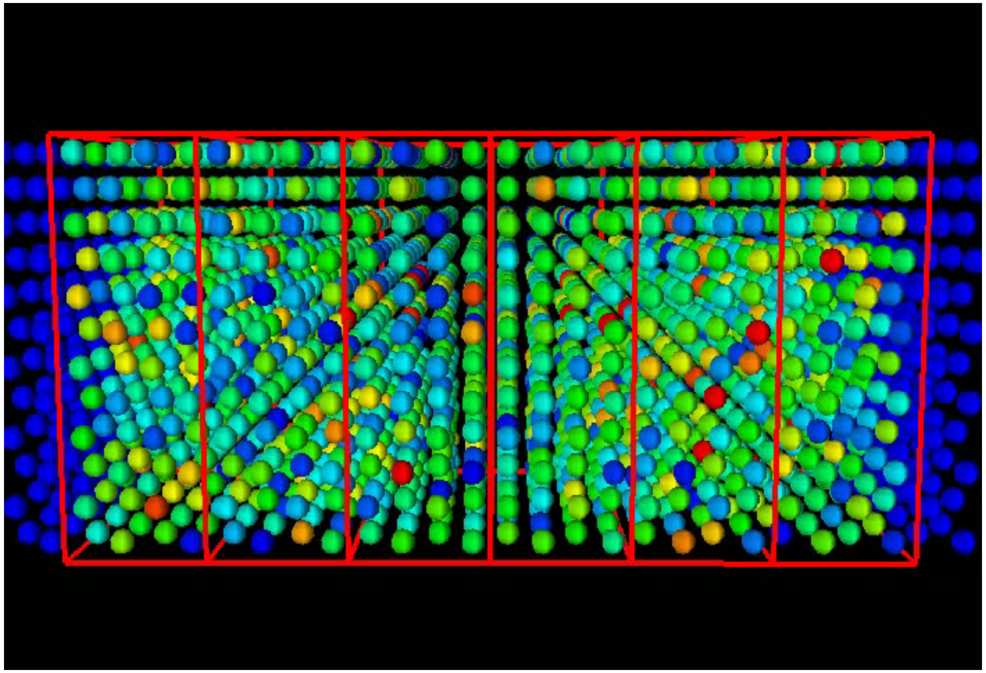
```
fix_modify AtC mesh create_faceset lbndy box -6.0
               16.0 -INF INF -INF INF outward
fix_modify AtC mesh create_nodeset lbc -6.1 -5.9
               -INF INF -INF INF
fix_modify AtC mesh create_nodeset rbc  5.9  6.1
               -INF INF -INF INF
fix_modify AtC mesh create_elementset mid -2.1 2.1
               -INF INF -INF INF
```



Example 2: Fixed Temperature Boundaries

- Initial conditions set through a combination of LAMMPS and AtC commands to construct and equilibrate the lattice

```
velocity   internal create 40. 87287 mom yes
fix_modify AtC  fix temperature all 20.
fix_modify AtC  control thermal rescale 10
fix_modify AtC  output BCex_eqFE 100 text binary
run 1000
```



Example 2: Fixed Temperature Boundaries

- Time integration, filtering, constitutive models and numerical methods

```
fix_modify      AtC  filter type exponential
fix_modify      AtC  filter scale 1000.0
fix_modify      AtC  filter on
fix_modify      AtC  internal_quadrature off
fix_modify      AtC  unfix temperature all

# Ar_thermal.mat file
material Ar
 heat_flux linear
  conductivity .00000000168
 end
end
```

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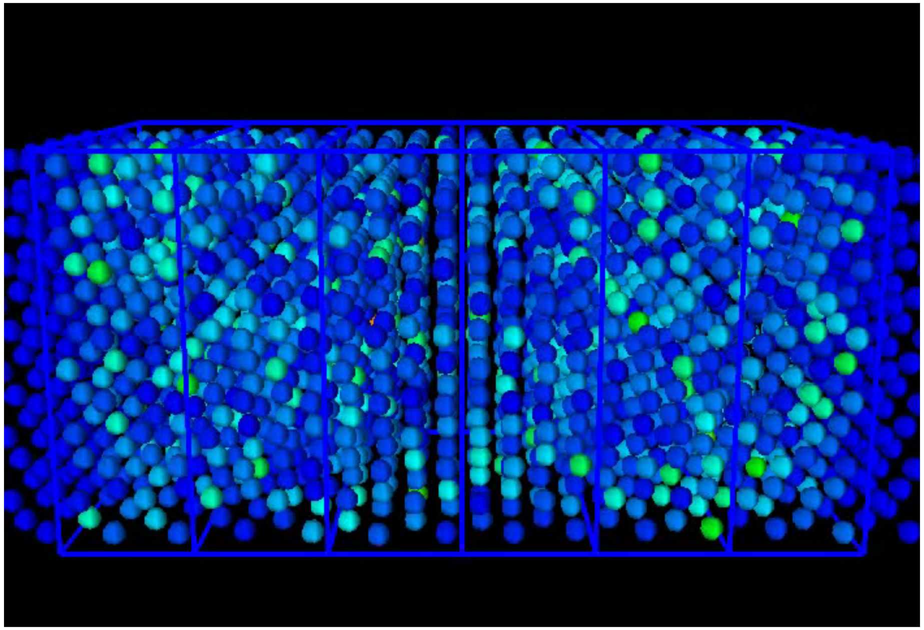
Example 2: Fixed Temperature Boundaries

- Define boundary conditions on nodesets

```
fix_modify AtC  fix temperature lbc temporal_ramp
                20. 40. 25000.
reset_timestep  0
fix_modify      AtC  reset_time
fix_modify AtC  fix temperature rbc 20.
fix_modify AtC  control thermal flux no_boundary
run             10000
```



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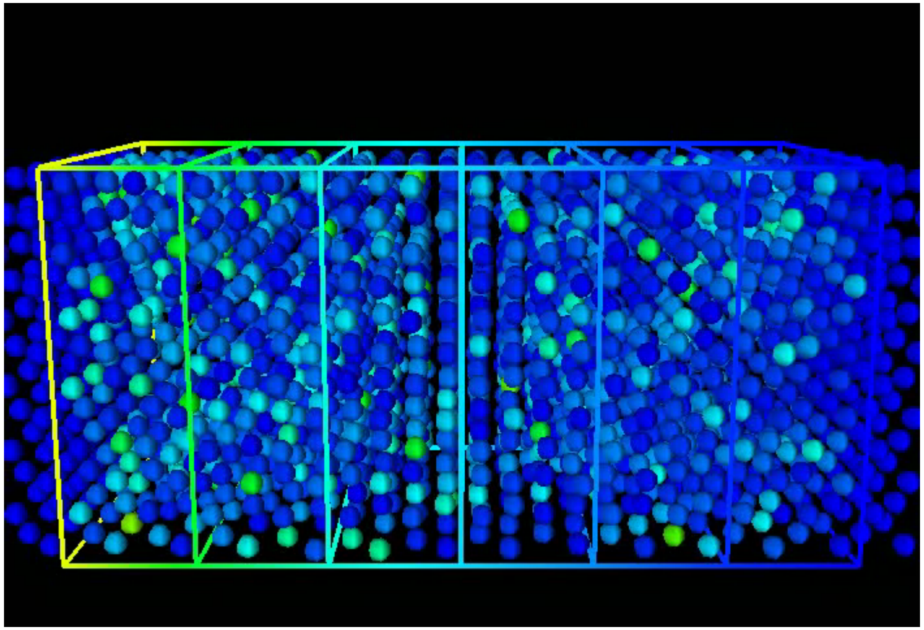
Example 2: Fixed Temperature Boundaries

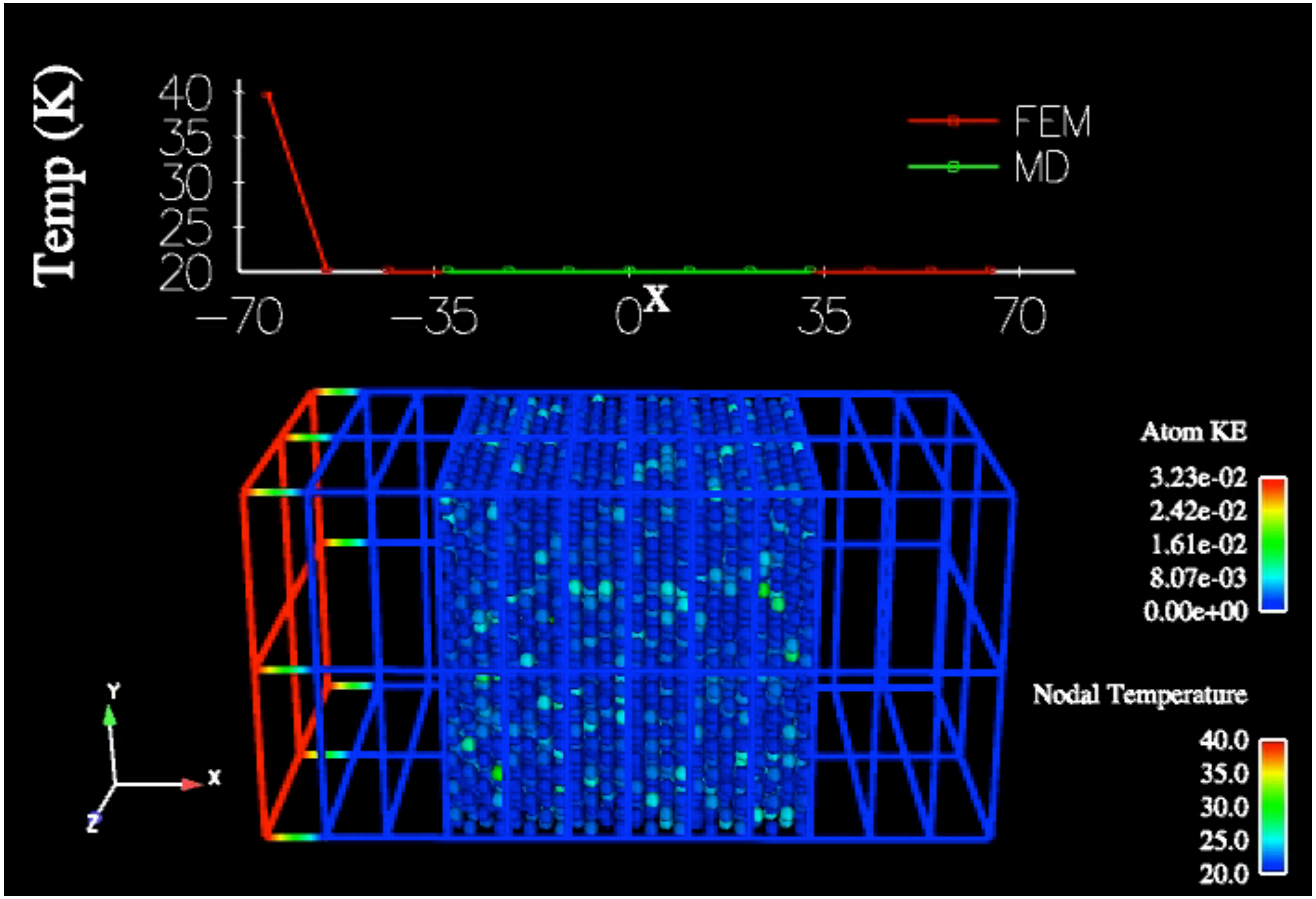
- Apply source terms and boundary fluxes

```
fix_modify AtC  unfix temperature lbc
fix_modify AtC  fix_flux temperature lbndy
                0.0000000001
fix_modify AtC  source temperature mid 0.0000000001
reset_timestep  0
fix_modify      AtC  reset_time
run             10000
```



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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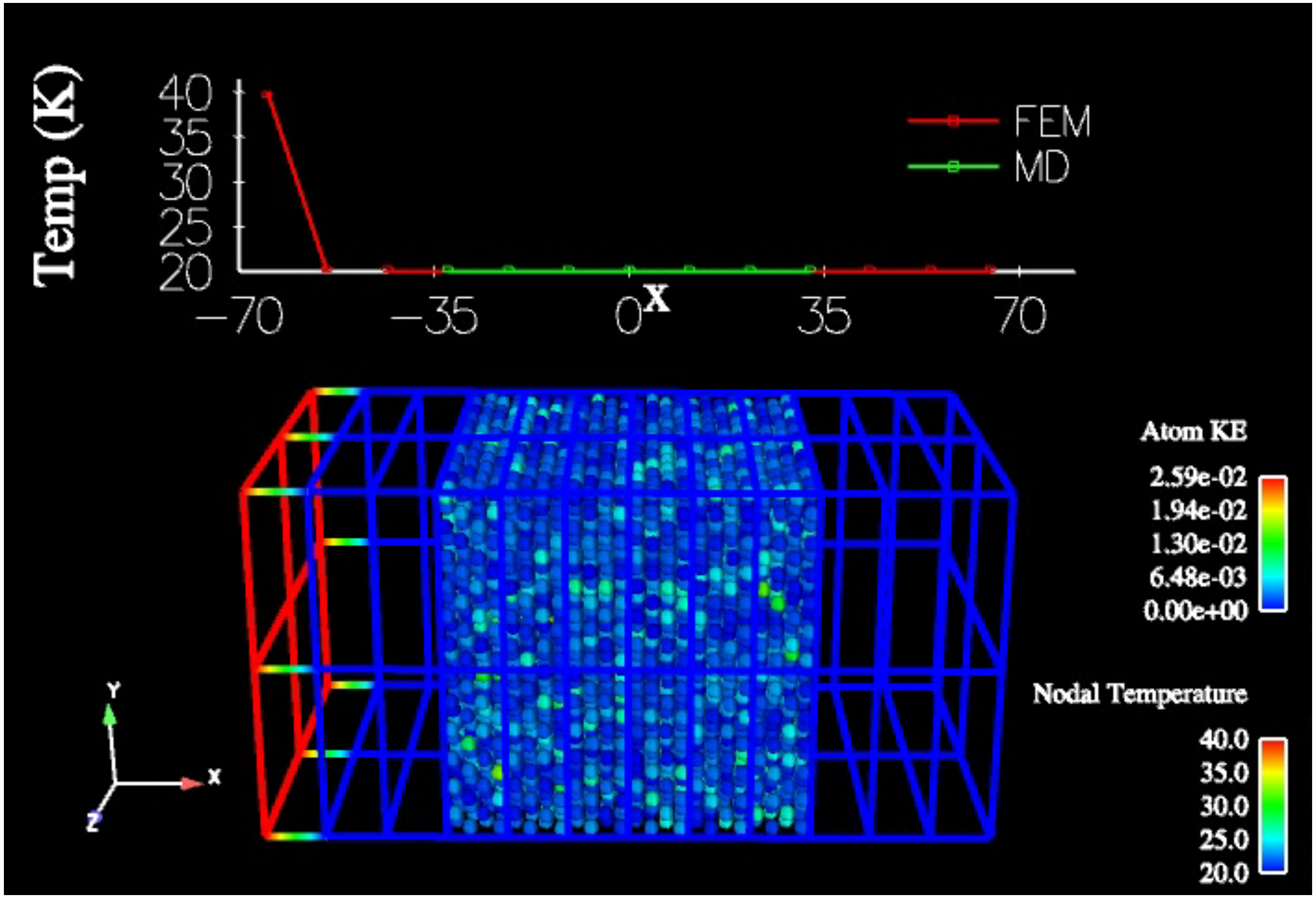
Coupled System

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



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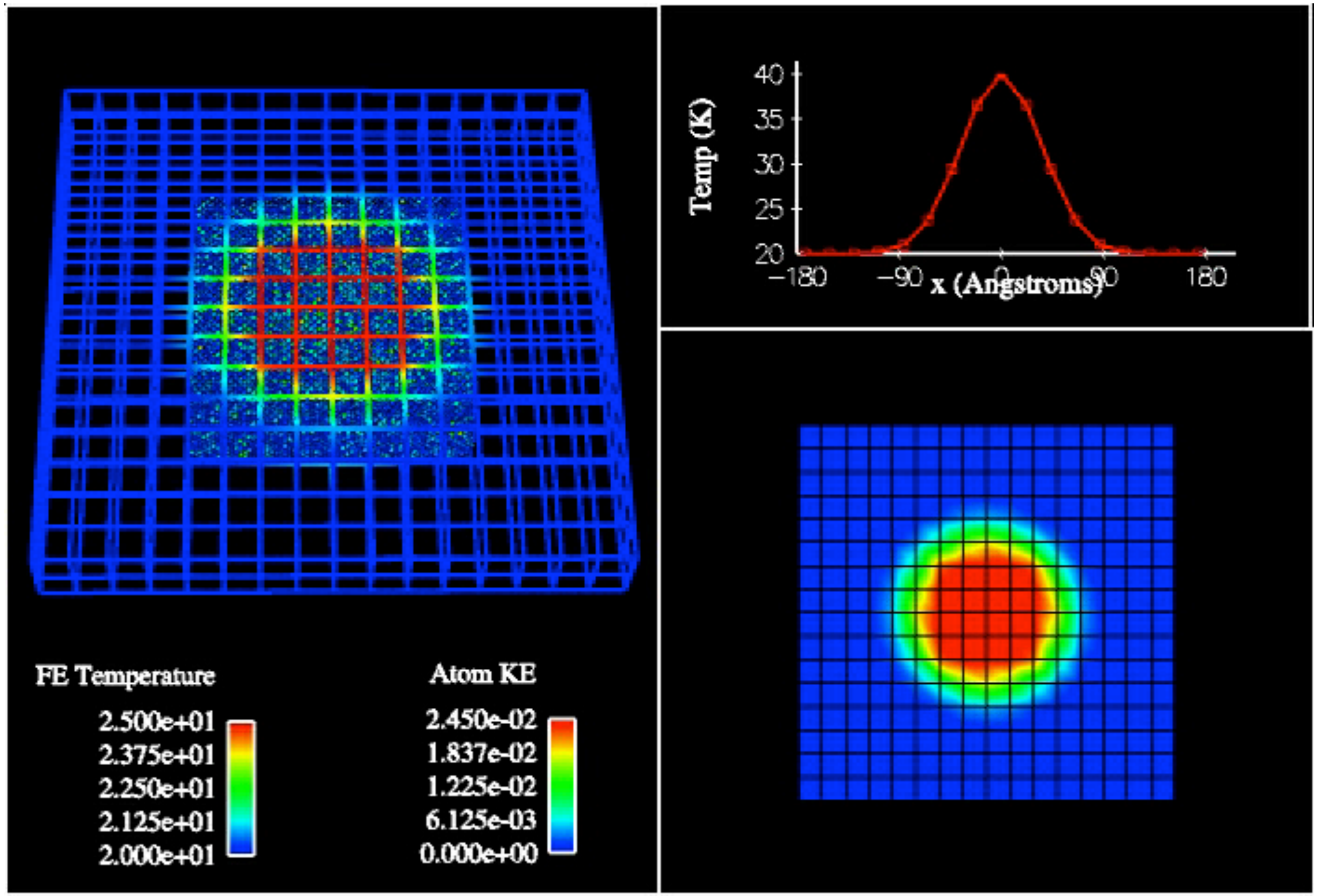
2D Diffusion Problem

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



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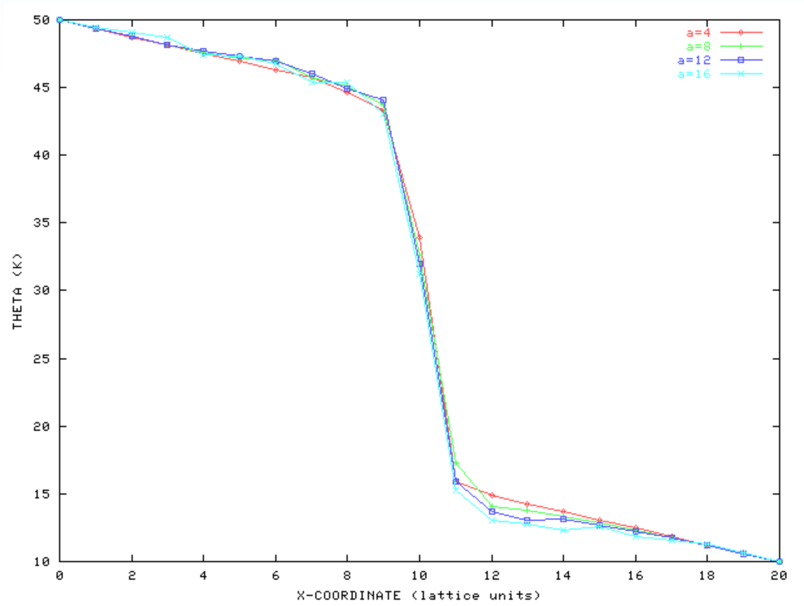
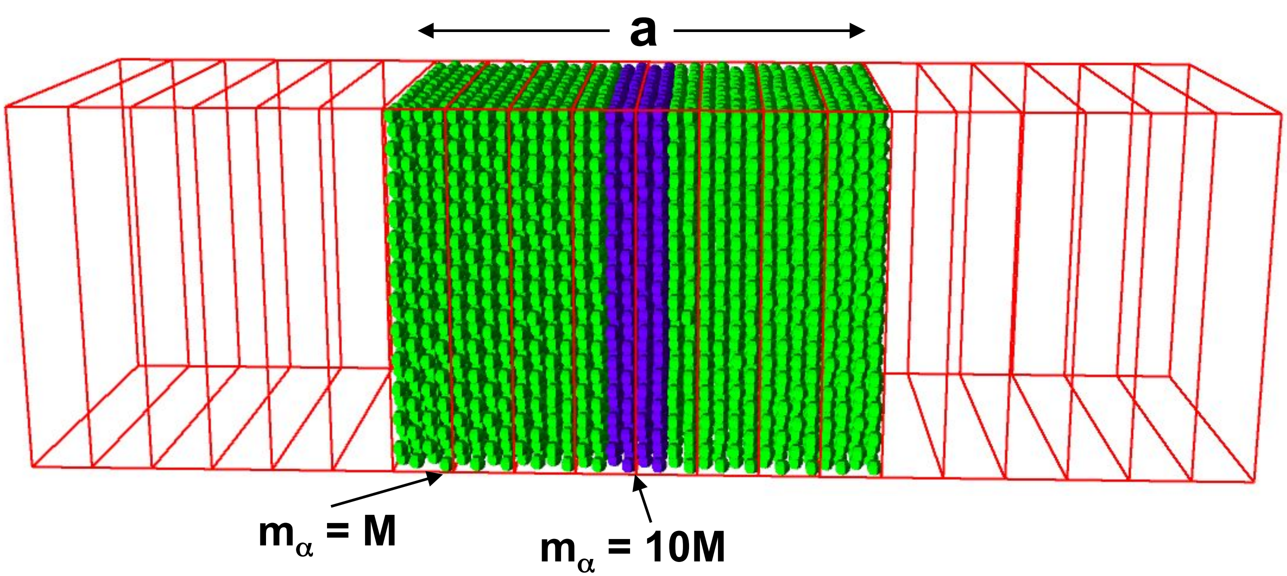
Effects of Imperfections on Conductivity

- 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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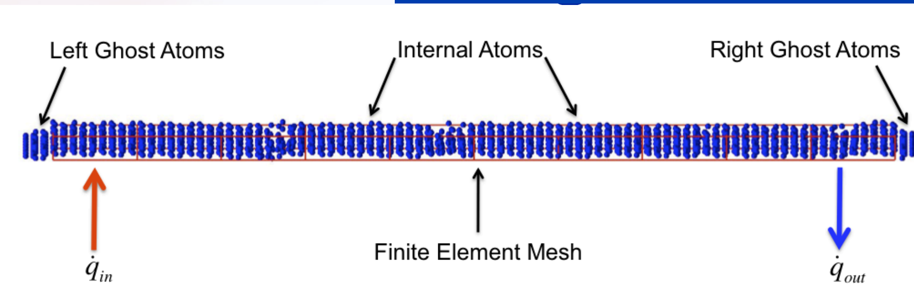
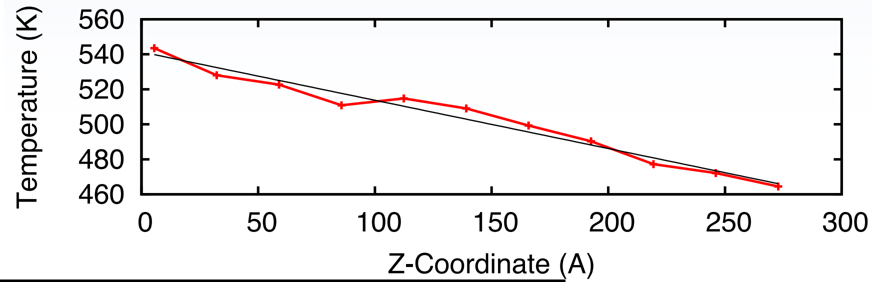
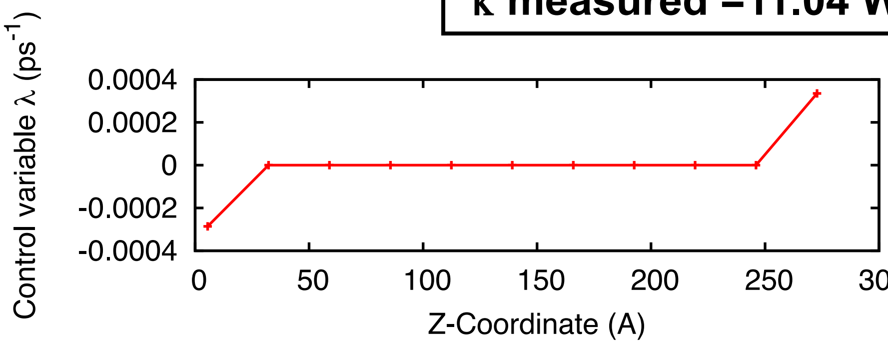
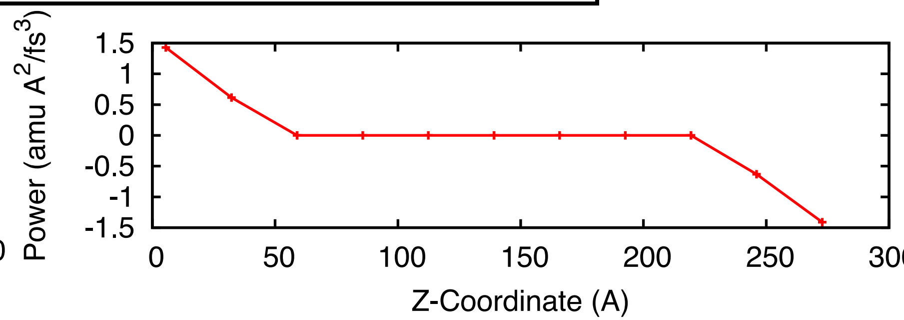
Thermal Conductivity Calculations using AtC Boundary Conditions

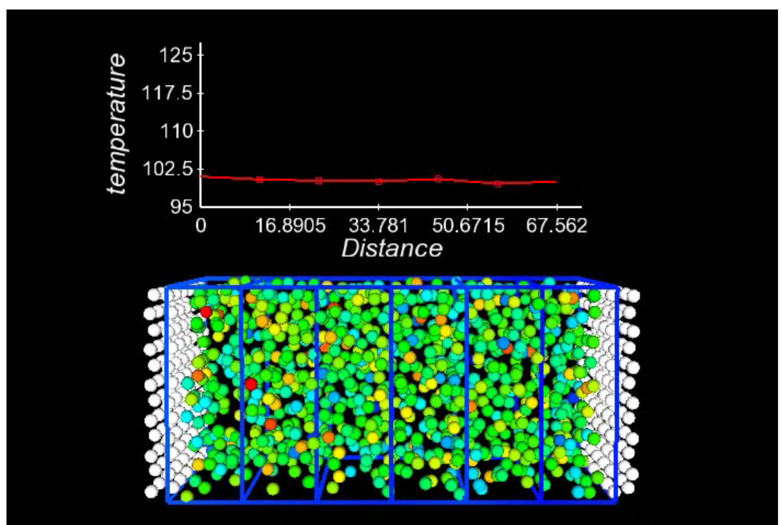




κ measured =11.04 W/mK, κ theory = 12.01 W/mK







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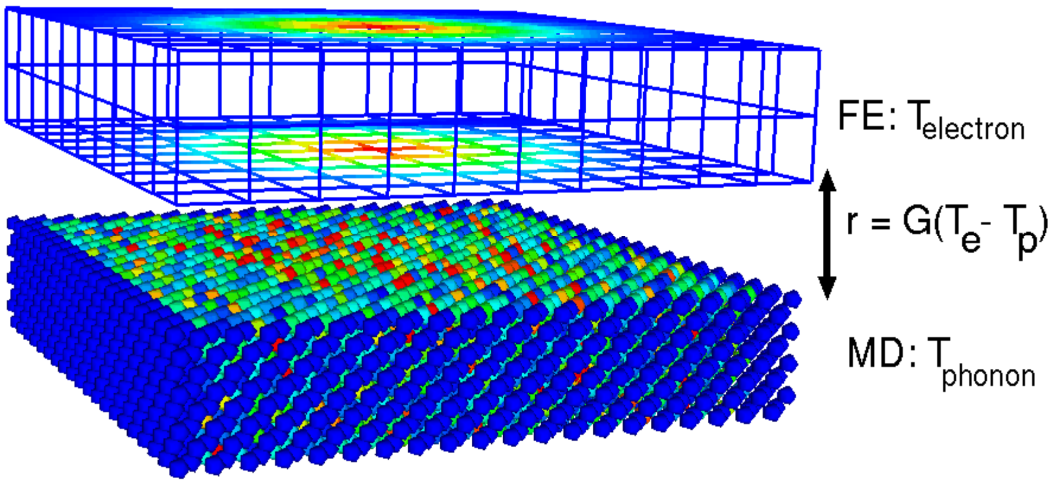
Extrinsic Physics Modeling

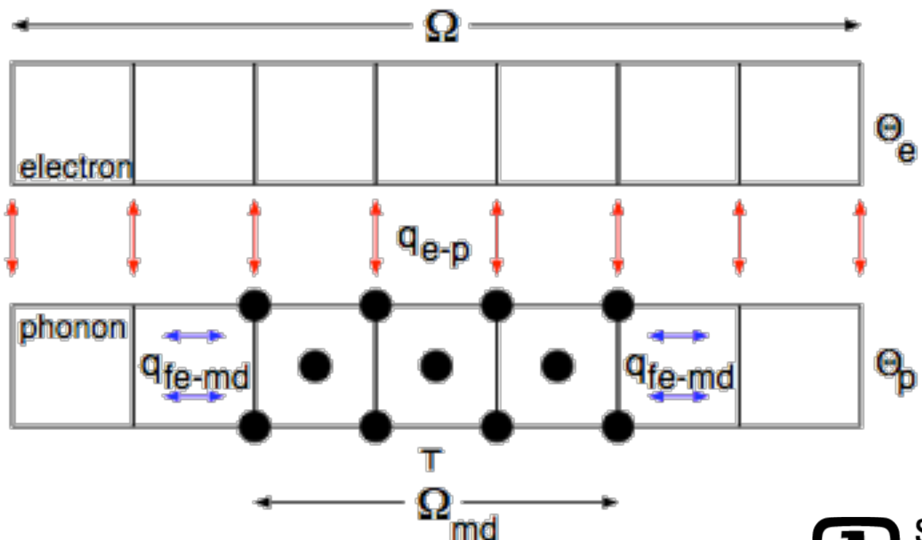
- MD explicitly represents atomic motions with great accuracy
  - Balistic phonon propagation
  - Defects
  - Nanostructures
- MD does not capture many other important physics
  - Electric fields
  - Energy carriers
  - Electrons
- Represent additional physics in a continuum model
- Use coupling techniques 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

Coupled Two-Temperature Approach



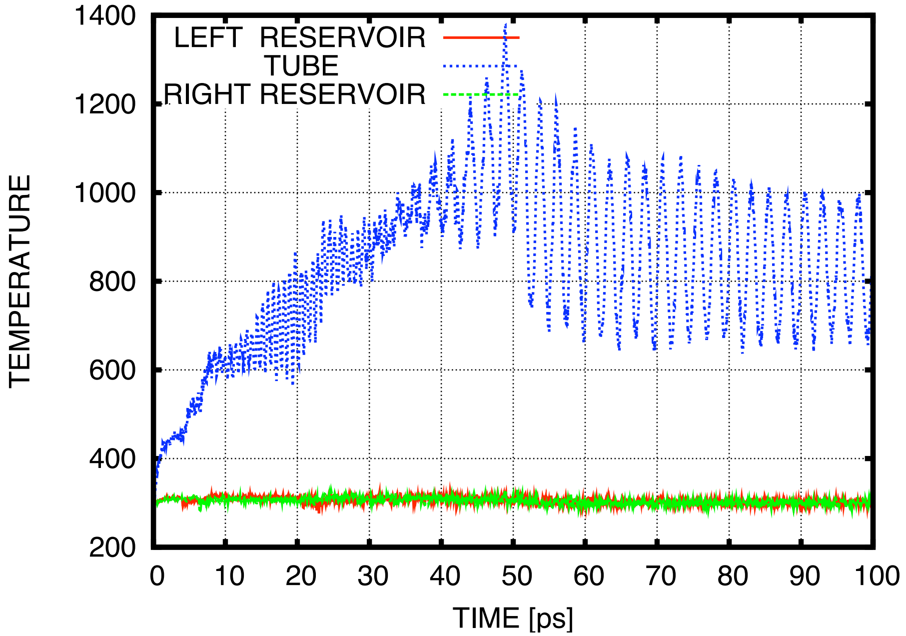
Explicit representation of phonons by MD, Electron effects solved for on overlaid mesh

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

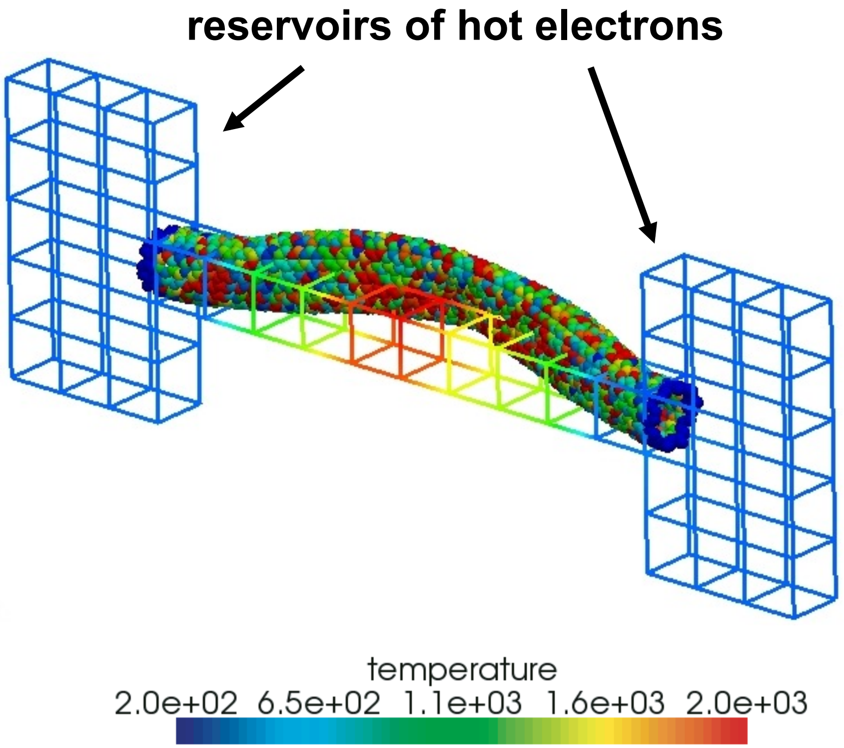


Electron Heating of a metallic CNT

- 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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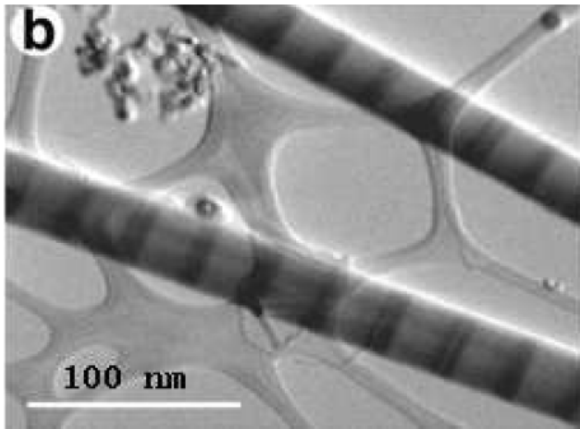
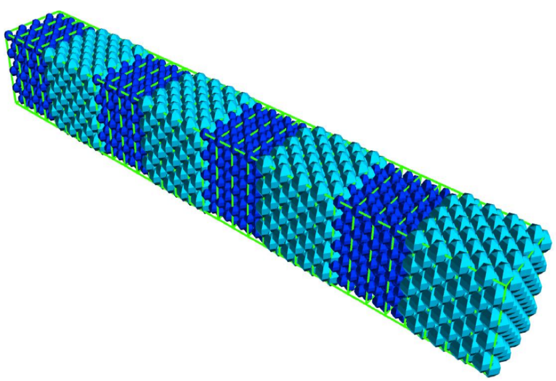
Ge/Si superlattice nanowires

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





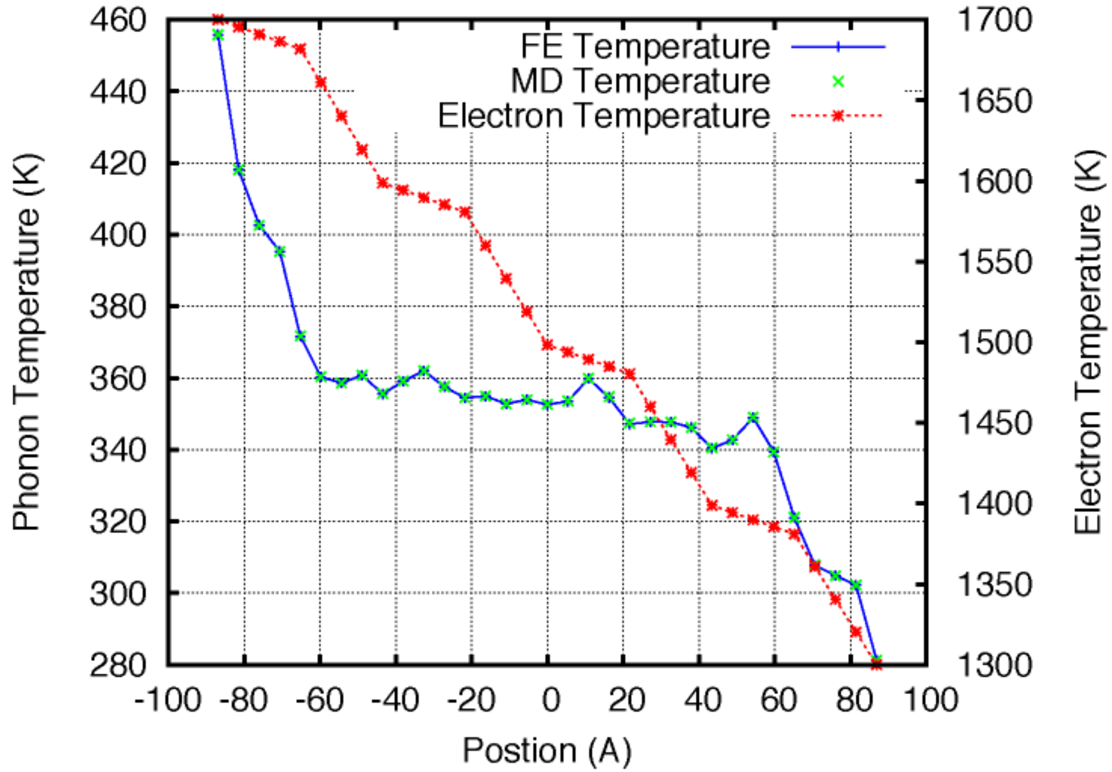


Figure 8: Temperature profiles in the superlattice

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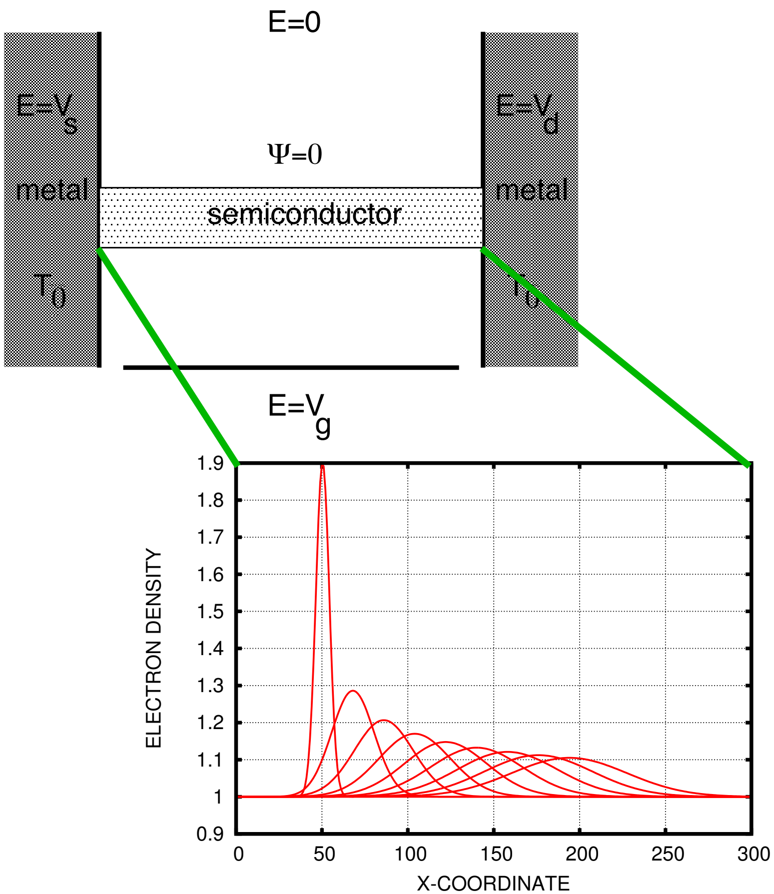
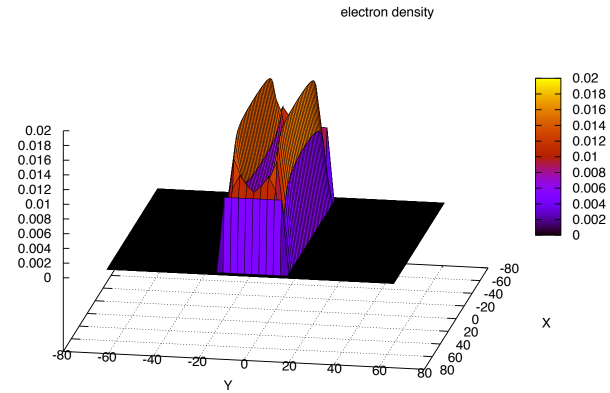
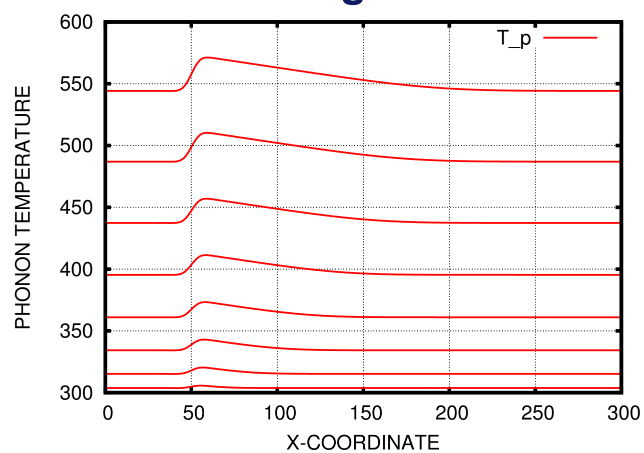
Metallic and Semi-Conductor Powered Nanodevices

- 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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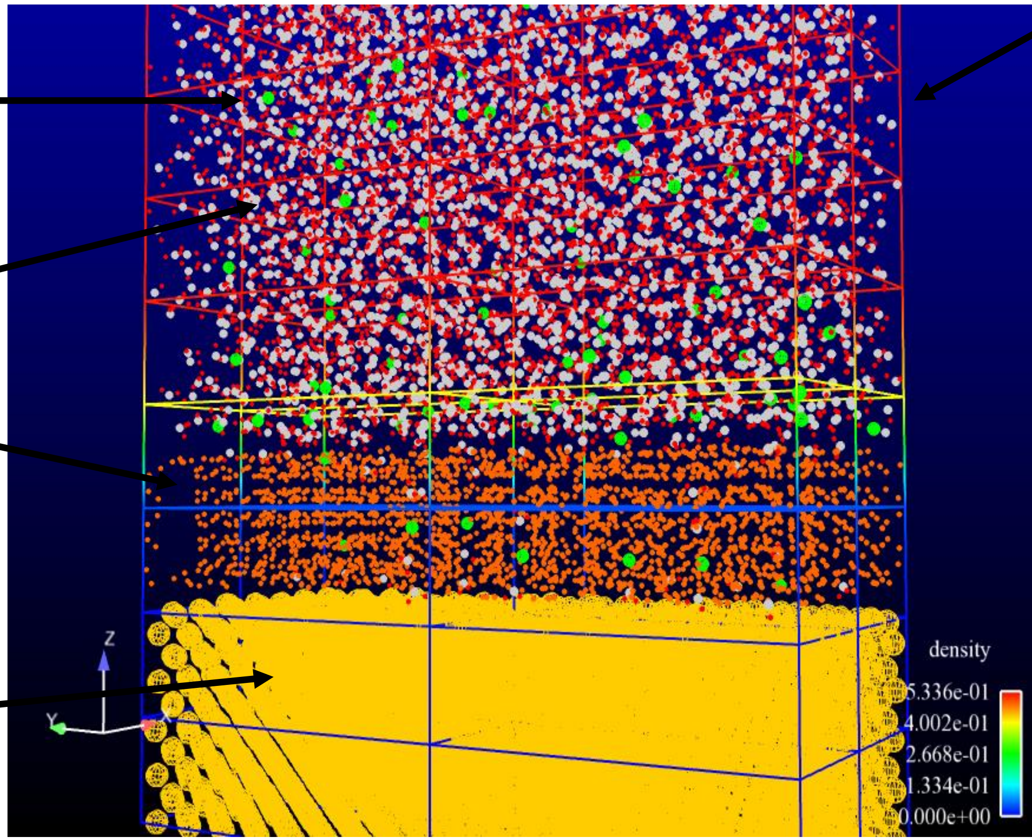
AtC Model for Long-range Electrostatics

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

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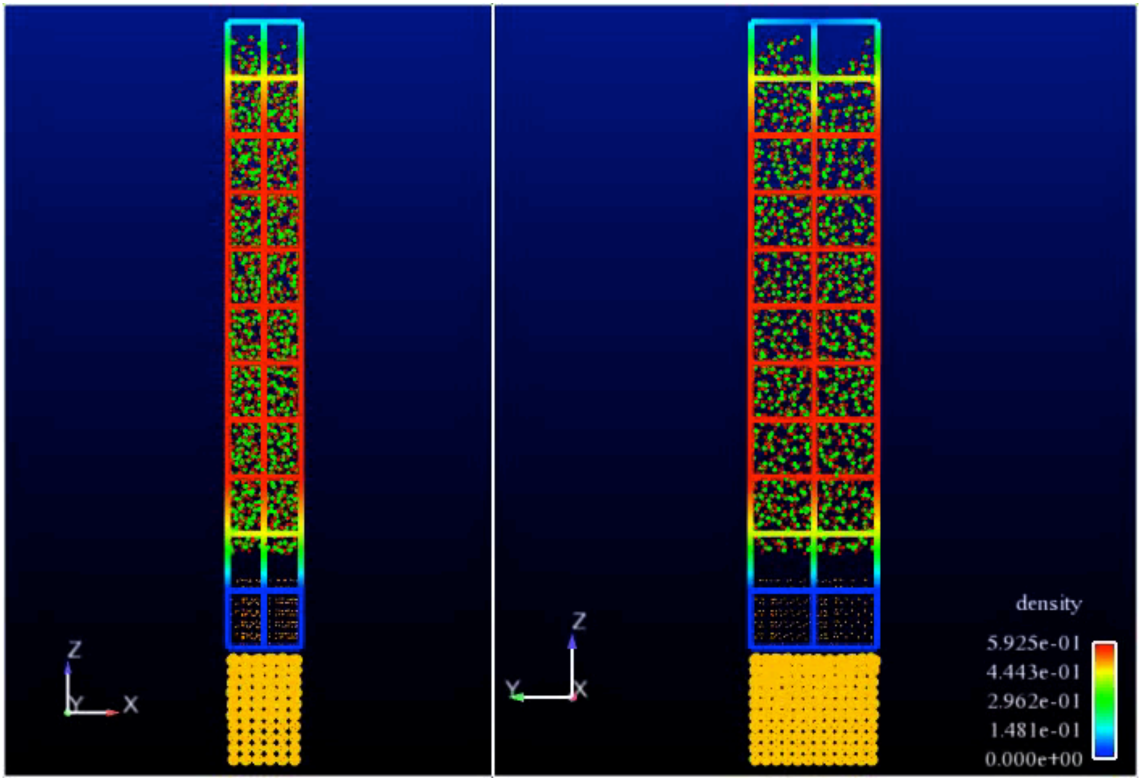
Other Physical Models: Fluidic Species Transport

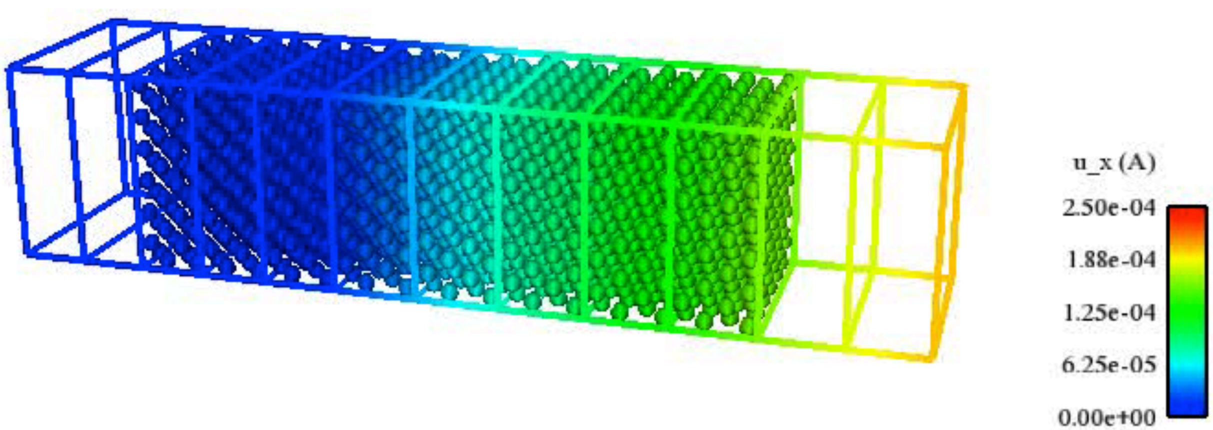
- Define coupling in Eulerian frame rather than Lagrangian
- Track individual species to understand particle agglomeration and diffusion
- Example problem: transport of saltwater into nanotubes



- Future work: energy storage devices

Other Physical Models: 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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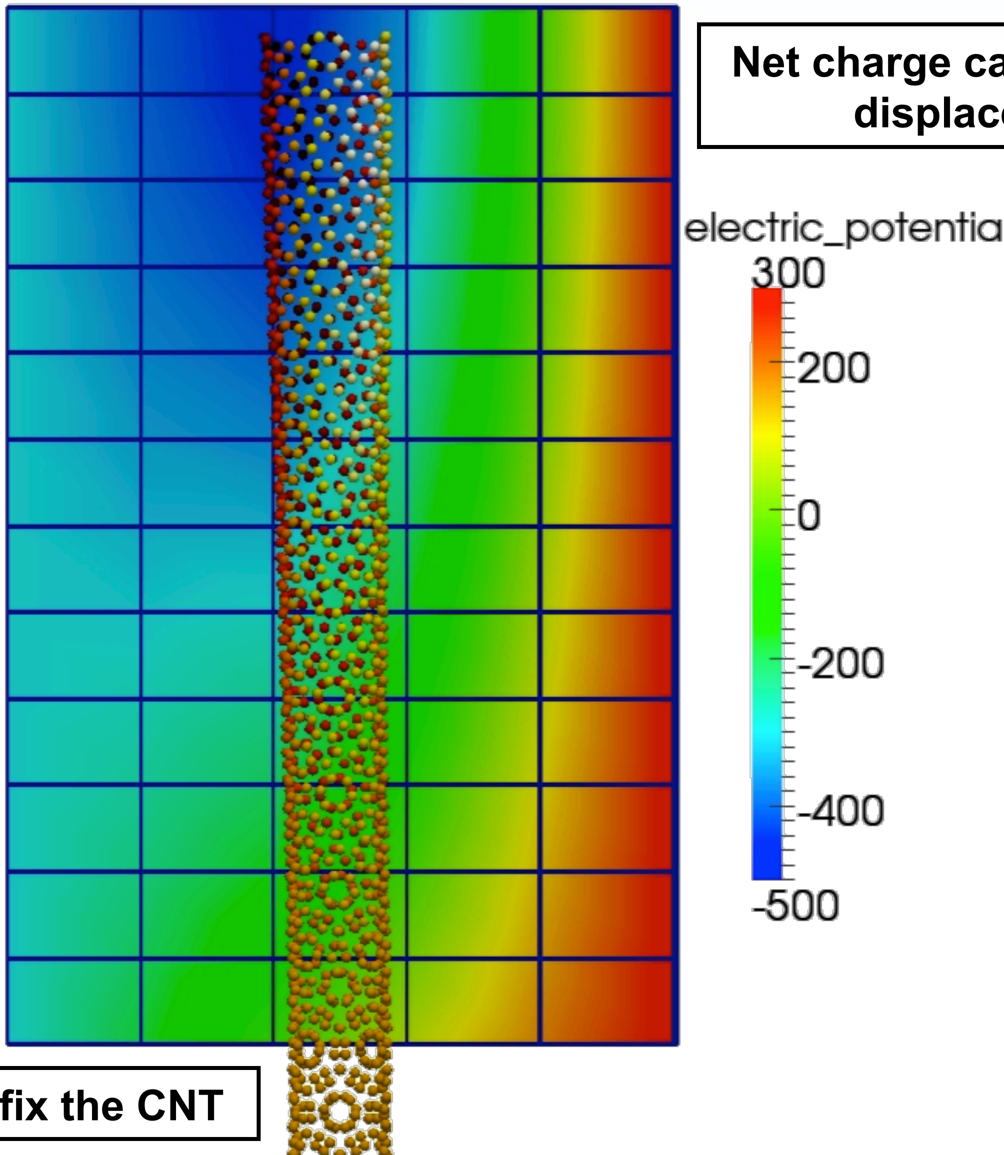
Other Physical Models: Electrostatics

Potential drop across short axis

Mutual repulsion opens tip

Net charge causes net tip displacement

Electrons segregate to tip



Atoms anchored to fix the CNT

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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)
- **Coming soon**
  - Long-range electrostatics (Templeton *et al., J. Chem. Theor. Comput.* (2011))
  - Drift-diffusion modeling, Elasticity, Eulerian frame coupling
- **Package documentation can be found at:**

http://lammps.sandia.gov

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