SAND2013-5808C

12th U.S. National Congress on Computational Mechanics

Raleigh, NC. July 22-25, 2013

# Simulating localized heating due to electron flow in molecular dynamics

REESE JONES, JEREMY TEMPLETON

*Sandia National Laboratory, Livermore, CA 94551-0969, USA*

This work was funded by the Laboratory Directed Research and Development program at Sandia National Laboratories and its support is gratefully acknowledged. *Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-ACO4-94AL85000.*

# MOTIVATION

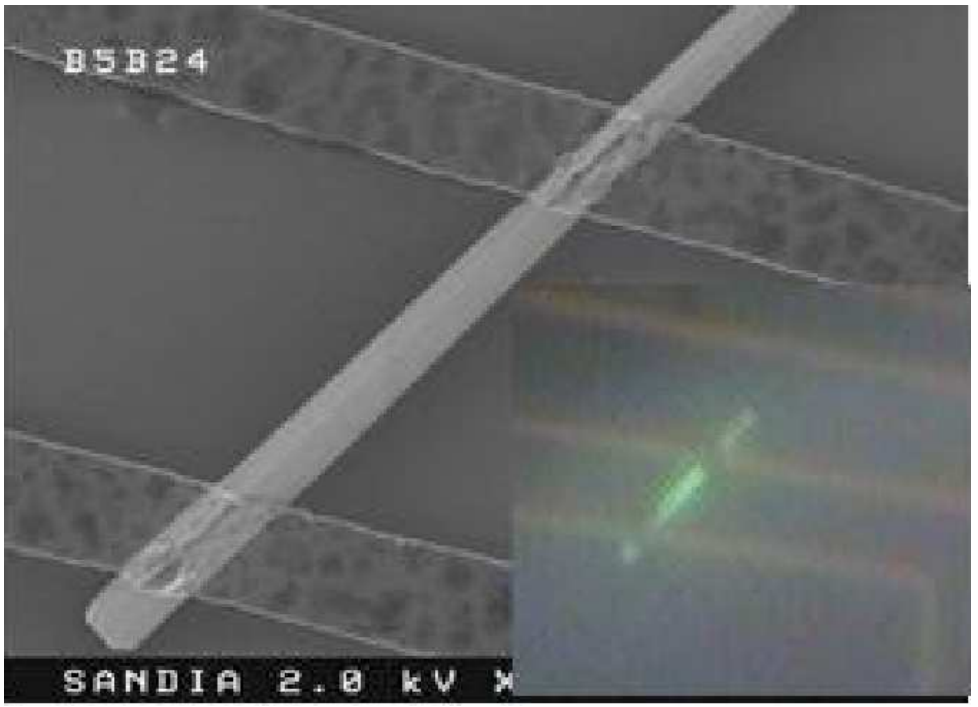
Problem: Molecular dynamics gives an explicit representation of defects and phonon modes but is missing physics associated with electrons and electron-mediated transport

| Material | thermal conductivity [W/K-m] | | | heat capacity [J/K-kg] | | | Debye T [K] | e-p coupling [W/K-m$^3$] |
|---|---|---|---|---|---|---|---|---|
| Cu | 401 | 11.2 | 244 | 385 | 394 | 10.8 | 345 | $2.6 \times 10^{17}$ |
| Si | 148 | 120 | 0.02 | 705 | 888 | 0.0002 | 645 | $1.0 \times 10^{11}$ |

Approach: use Boltzmann transport/hydrodynamic PDE models of electron transport instead of (coherent) quantuum mechanics for nm-size simulations [IVANOV & ZHIGELI,2004]

Outline:

- Two temperature PDE
- Phenomenology
- Atom-continuum
- Algorithm
- Simulations
- Future work




GaN nanowire [TALIN, SNL]
(inset PL under power)

# TWO TEMPERATURE MODEL

The balance of energy, with no significant deformation,
i.e. “rate of storage = conduction + generation” :

$$\dot{\epsilon} = -\boldsymbol{\nabla} \cdot \mathbf{q} + r$$

results from the 2nd moment of the Boltzmann transport equation.

Two empirical temperatures and carriers of energy :

$$\begin{aligned} \dot{\epsilon} &= c_e \dot{\theta}_e + c_p \dot{\theta}_p \\ \mathbf{q} &= -k_e \boldsymbol{\nabla} \theta_e - k_p \boldsymbol{\nabla} \theta_p \end{aligned}$$

where $\theta_e$ is the electron temperature and $\theta_p$ is the phonon temperature.

The TTM is two coupled, diffusive systems [KAGANOV,1956] in local form:

$$c_e \dot{\theta}_e = \boldsymbol{\nabla} \cdot (k_e \boldsymbol{\nabla} \theta_e) - g(\theta_e - \theta_p) + r_e$$

$$\boxed{c_p \dot{\theta}_p = \boldsymbol{\nabla} \cdot (k_p \boldsymbol{\nabla} \theta_p)} + g(\theta_e - \theta_p)$$

where $c$: heat capacity (per volume), $k$: conductivity, each per carrier;
and $g$: electron-phonon exchange, which are all temperature dependent.

In its simplest form, the TTM is linear.

The external source term (for the electron system) typically comes from a laser pulse or an electric field ($r_e = -\mathbf{J}_e \cdot \Psi_{\mathbf{x}} \sim \frac{1}{\text{Vol}} IV$).

# TIME & LENGTH-SCALES

A uniform exchange solution (no $x$-dependence) gives a timescale $\tau_{ep} = \frac{c_e c_p}{g(c_e+c_p)}$ :

$$\begin{aligned} \theta_e - \theta_p &= (\theta_e - \theta_p)_{t=0} \exp\left(-\frac{t}{\tau_{ep}}\right) \\ c_e\theta_e + c_p\theta_p &= (c_e\theta_e + c_p\theta_p)_{t=0} \end{aligned}$$

The temperature difference follows a simple exponential decay & the total energy $\epsilon$ is constant.

A static solution (no $t$-dependence) gives a length-scale $\ell_{ep} = \sqrt{\frac{k_e k_p}{g(k_e+k_p)}}$ :

$$\theta_e - \theta_p = (\theta_e - \theta_p)_{x=0} + \Big((\theta_e - \theta_p)_{x=L} - (\theta_e - \theta_p)_{x=0}\Big) \exp\left(\frac{L-x}{\ell_{ep}}\right) \frac{\exp\left(\frac{2x}{\ell_{ep}}\right) - 1}{\exp\left(\frac{2L}{\ell_{ep}}\right) - 1}$$

$$k_e\theta_e + k_p\theta_p = (k_e\theta_e + k_p\theta_p)_{x=0} + \Big((k_e\theta_e + k_p\theta_p)_{x=L} - (k_e\theta_e + k_p\theta_p)_{x=0}\Big) \frac{x}{L}$$

The temperature difference is again exponential & the conductivity-weighted sum $k_e\theta_e + k_p\theta_p$ is linear in space.

# PHENOMENOLOGY

The coupled PDEs have three timescales:

- phonon diffusion

$$\tau_p = \frac{L^2 c_e}{k_e}$$

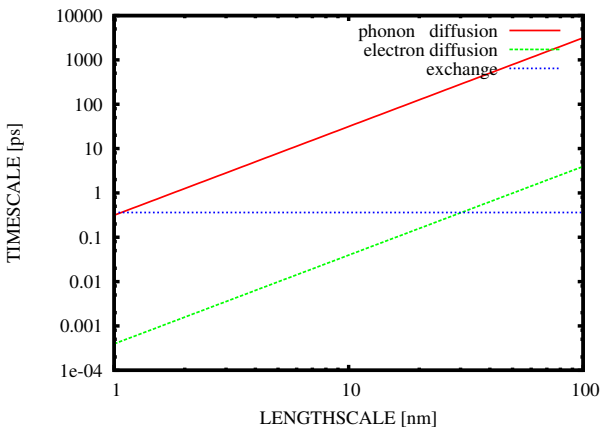
- electron diffusion

$$\tau_e = \frac{L^2 c_p}{k_p}$$

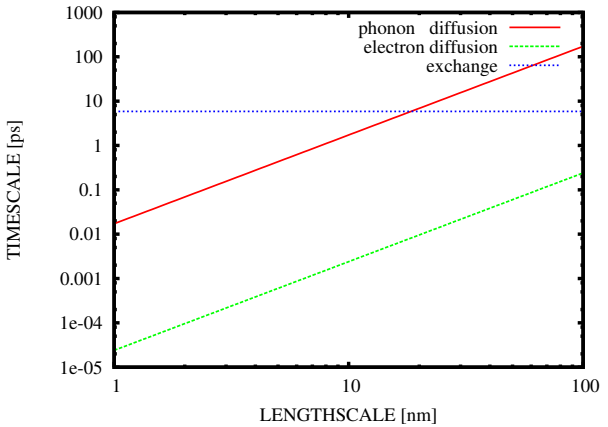
- electron-phonon exchange

$$\tau_{ep} = \frac{c_e c_p}{g(c_e + c_p)}$$

copper




silicon




For $L = 10\,nm$:

| Material | phonon diffusion | electron diffusion | exchange | lengthscale |
|---|---|---|---|---|
| Cu | 31 ps | 0.04 ps | 0.36 ps | 6.41 nm |
| Si | 1.7 ps | 0.002 ps | 5.8 ps | 494 nm |

# PHENOMENOLOGY

The coupled PDEs have three timescales:

- phonon diffusion

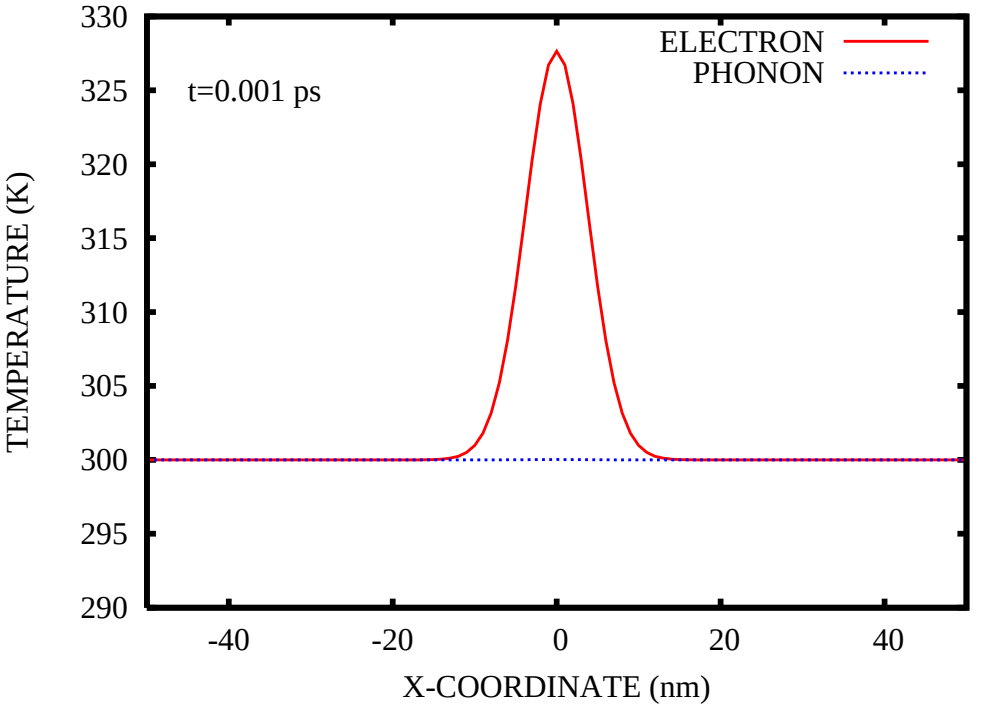
$$\tau_p = \frac{L^2 c_e}{k_e}$$

- electron diffusion

$$\tau_e = \frac{L^2 c_p}{k_p}$$

- electron-phonon exchange

$$\tau_{ep} = \frac{c_e c_p}{g(c_e + c_p)}$$




initial Gaussian pulse to electron system
& uniform phonon temperature

For $L = 10\,nm$:

| Material | phonon diffusion | electron diffusion | exchange | lengthscale |
|---|---|---|---|---|
| Cu | 31 ps | 0.04 ps | 0.36 ps | 6.41 nm |
| Si | 1.7 ps | 0.002 ps | 5.8 ps | 494 nm |

# PHENOMENOLOGY

The coupled PDEs have three timescales:

- phonon diffusion

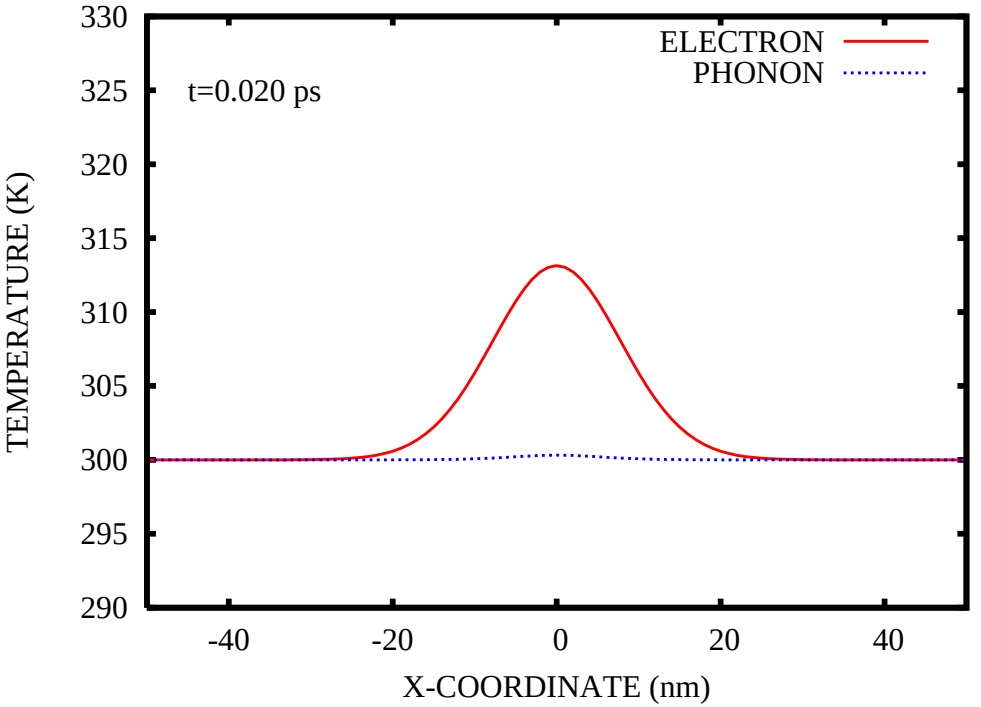
$$\tau_p = \frac{L^2 c_e}{k_e}$$

- electron diffusion

$$\tau_e = \frac{L^2 c_p}{k_p}$$

- electron-phonon exchange

$$\tau_{ep} = \frac{c_e c_p}{g(c_e + c_p)}$$




fast electron diffusion and exchange

For $L = 10\,nm$:

| Material | phonon diffusion | electron diffusion | exchange | lengthscale |
|---|---|---|---|---|
| Cu | 31 ps | 0.04 ps | 0.36 ps | 6.41 nm |
| Si | 1.7 ps | 0.002 ps | 5.8 ps | 494 nm |

# PHENOMENOLOGY

The coupled PDEs have three timescales:

- phonon diffusion

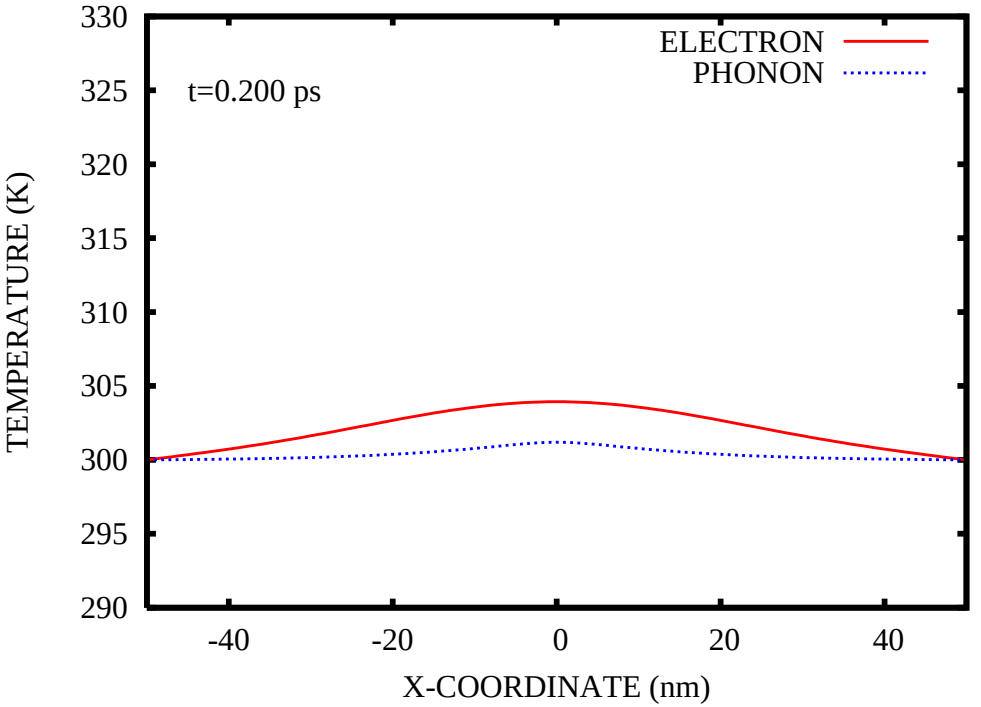
$$\tau_p = \frac{L^2 c_e}{k_e}$$

- electron diffusion

$$\tau_e = \frac{L^2 c_p}{k_p}$$

- electron-phonon exchange

$$\tau_{ep} = \frac{c_e c_p}{g(c_e + c_p)}$$




phonon profile more localized than electron

For $L = 10\,nm$:

| Material | phonon diffusion | electron diffusion | exchange | lengthscale |
|---|---|---|---|---|
| Cu | 31 ps | 0.04 ps | 0.36 ps | 6.41 nm |
| Si | 1.7 ps | 0.002 ps | 5.8 ps | 494 nm |

# PHENOMENOLOGY

The coupled PDEs have three timescales:

- phonon diffusion

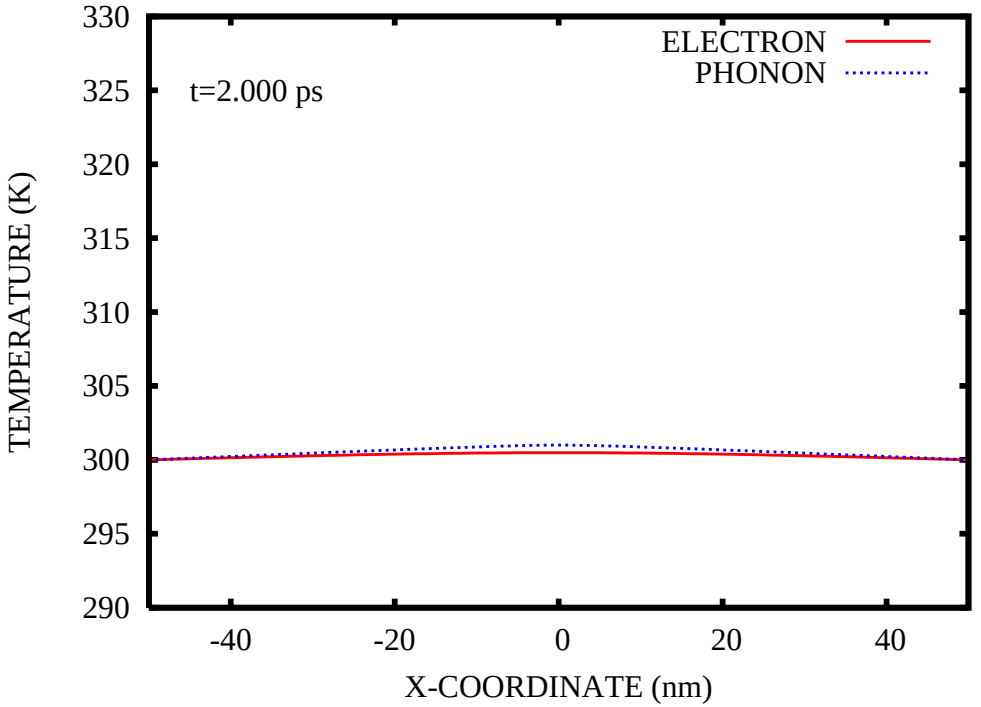
$$\tau_p = \frac{L^2 c_e}{k_e}$$

- electron diffusion

$$\tau_e = \frac{L^2 c_p}{k_p}$$

- electron-phonon exchange

$$\tau_{ep} = \frac{c_e c_p}{g(c_e + c_p)}$$

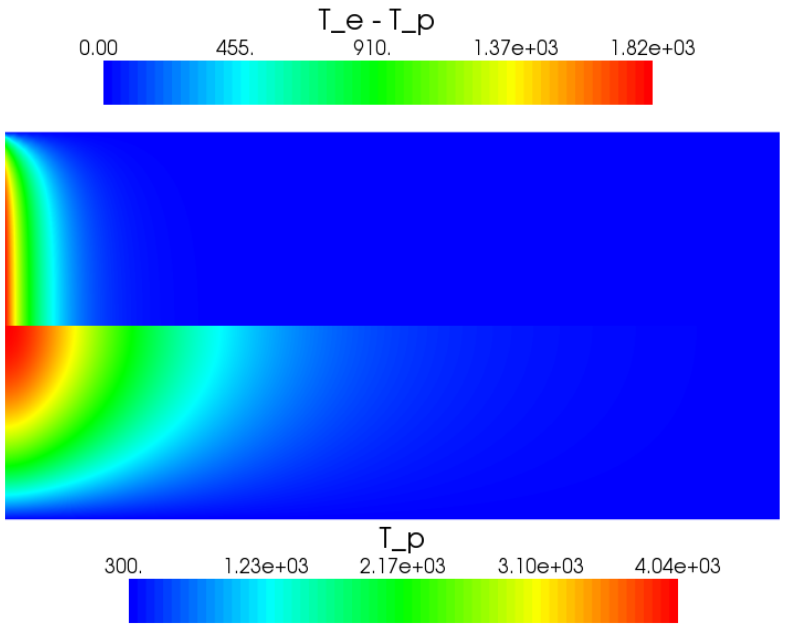


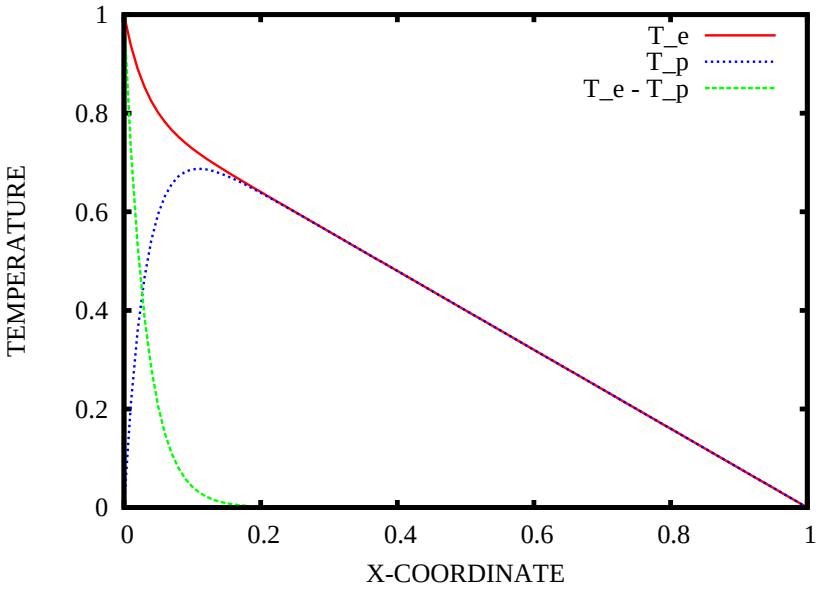

near equilibrium : $\theta_e \approx \theta_p$

For $L = 10\,nm$:

| Material | phonon diffusion | electron diffusion | exchange | lengthscale |
|---|---|---|---|---|
| Cu | 31 ps | 0.04 ps | 0.36 ps | 6.41 nm |
| Si | 1.7 ps | 0.002 ps | 5.8 ps | 494 nm |

# BOUNDARY LAYERS




- injection of "hot" electrons simulation: at all boundaries except the left $\theta_e = \theta_p$ and on the left a flux $\mathbf{q}_e > 0$ is prescribed for the electron temperature.

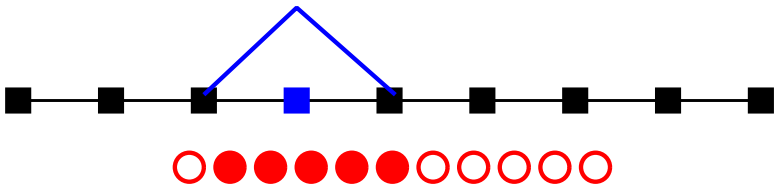
- the boundary layer scales with $\sqrt{\frac{1}{g}}$ and the coupling coefficient is proportional to the (electron) carrier concentration $\approx 10^{-12} m^3$

- boundary layers where electrons are out-of-equilibrium with the phonons affect device performance and possibly can be exploited

# MD/FE COUPLING

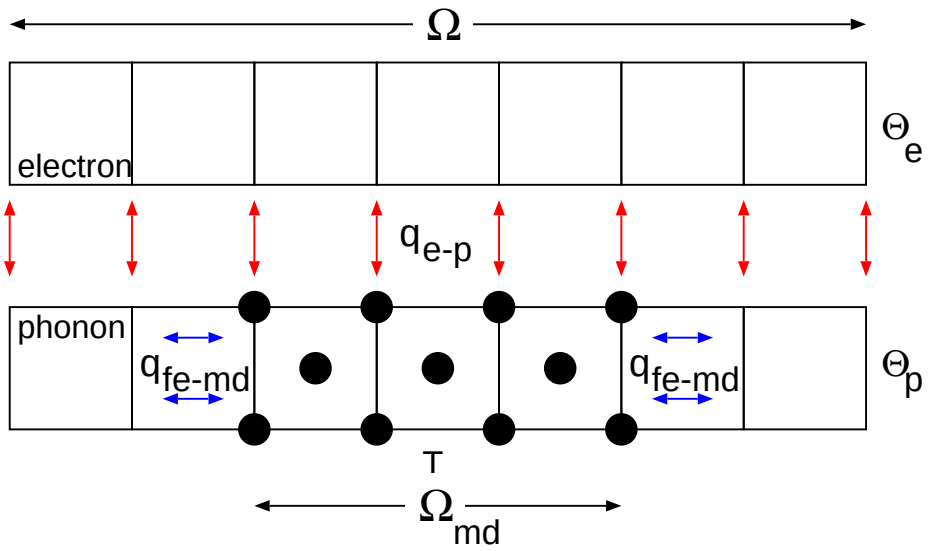
- Operators for coarsening/upscaling of fine-scale model (MD) information, e.g. a coarse-scale temperature can be defined

$$T_I \equiv \sum_{I,\alpha} \frac{m_\alpha}{3\kappa_B} \tilde{N}_{I\alpha} \langle \mathbf{v}_\alpha \cdot \mathbf{v}_\alpha \rangle$$



by averaging atomic velocities to get a corresponding continuum field

- Coarse-scale governing equations which are "consistent" surrogates for the fine-scale model in regions where:
  - atomic detail is not needed (e.g. far away from a lattice defect)
  - information is missing (e.g. electron transport).




- Fine-scale control algorithms, e.g. MD thermostats, which enable coarse-scale information to "condition" the small scale solutions so that they interact/follow the coarse-scale behavior

# ENERGY BALANCE

For a closed system, the total energy should be conserved:

$$\dot{E} = \langle \dot{E}_{md} \rangle + \dot{E}_{fe} = 0$$

where $\langle \bullet \rangle$ represents a time average.

The energy of the electron & phonon FE systems changes due to exchange with each other and with the MD system

$$\begin{aligned}
\dot{E}_{fe} &= \int_{\Omega \setminus \Omega_{\text{md}}} \boldsymbol{\nabla} \cdot \mathbf{q}_p \, dV + \int_{\Omega} \boldsymbol{\nabla} \cdot \mathbf{q}_e \, dV + \int_{\Omega \setminus \Omega_{\text{md}}} g\big(\theta_e - \theta_p\big) \, dV - \int_{\Omega} g\big(\theta_e - \theta_p\big) \, dV \\
&= \int_{\partial(\Omega \setminus \Omega_{\text{md}})} \mathbf{n} \cdot \mathbf{q}_p \, dA + \int_{\partial \Omega} \mathbf{n} \cdot \mathbf{q}_e \, dA + \int_{\Omega_{\text{md}}} g\big(\theta_e - \theta_p\big) \, dV
\end{aligned}$$

The energy of the MD system only changes due to a thermostat force

$$\dot{E}_{md} = \dot{K} + \dot{\Phi} = \sum_{\alpha} \big( m_\alpha \mathbf{v}_\alpha \cdot \dot{\mathbf{v}}_\alpha + \partial_{\mathbf{x}_\alpha} \Phi \cdot \mathbf{v}_\alpha \big) = \sum_{\alpha} \mathbf{f}^{\lambda}_{\alpha} \cdot \mathbf{v}_\alpha$$

We postulate a local balance on the FE-scale (for an isolated system):

$$\dot{E}_I = \sum_{\alpha} N_{I\alpha} \langle \mathbf{f}^{\lambda}_{\alpha} \cdot \mathbf{v}_\alpha \rangle + \int_{\partial(\Omega \setminus \Omega_{\text{md}})} N_I \, \mathbf{n} \cdot \mathbf{q}_p \, dA + \int_{\Omega_{\text{md}}} N_I \, g\big(\theta_e - \theta_p\big) \, dV = 0$$

i.e. “thermostat power + FE/MD boundary conduction + exchange to MD = zero”

Here $N_I$ is the shape function associated with node $I$ and $N_{I\alpha}$ is the shape function evaluated at $\mathbf{x}_\alpha$. This leads to (a) thermostat & (b) temperature evolution equations

# LOCAL THERMOSTAT

Just like for the Hoover thermostat [EVANS,1983], Gauss's principle of least constraint can be used to derive the thermostat

$$\min_{\dot{\mathbf{v}}_\alpha} \frac{1}{2} \sum_\alpha m_\alpha \|\dot{\mathbf{v}}_\alpha - \dot{\mathbf{v}}_\alpha^*\|^2 + \sum_I \lambda_I \dot{E}_I$$

where $\dot{\mathbf{v}}_\alpha^* = \frac{1}{m_\alpha}\mathbf{f}_\alpha$ are the unconstrained accelerations and $\lambda_I$ are Lagrange multipliers.

The Euler-Lagrange equations can be solved for $\lambda_I$

$$\begin{aligned} 0 &= m_\alpha \dot{\mathbf{v}}_\alpha - \mathbf{f}_\alpha + \sum_I N_{I\alpha} \lambda_I m_\alpha \mathbf{v}_\alpha \\ 0 &= \dot{E}_I \end{aligned}$$

The result is a thermostat velocity-drag force that is interpolated on the FE basis & acts on $\mathbf{v}_\alpha$

$$\mathbf{f}_\alpha^\lambda = -\frac{1}{2} \sum_I N_{I\alpha} \lambda_I \mathbf{v}_\alpha$$

in effect a coarse-scale force acting on fine-scale kinematics.

# CONCURRENT COUPLING ALGORITHM

temperature evolution equations:

$$\Big(\int_\Omega N_I N_J dV\Big)\dot{\theta}^e_J = \sum_{J\in\mathcal{N}}\Big(-\int_\Omega \frac{k_e}{c_e}\nabla N_I\cdot\nabla N_J\, dV\,\theta^e_J - \int_\Omega \frac{g}{c_p} N_I N_J\, dV\,(\theta^e_J-\theta^p_J) + \int_{\Gamma_q}\frac{k_e}{c_e}N_I\mathbf{n}\cdot\nabla N_J\, dV\,\theta^e_J\Big)$$

$$\Big(\int_\Omega N_I N_J dV\Big)\dot{\theta}^p_J = \sum_{J\in\mathcal{N}}\Big(-\int_{\Omega\setminus\Omega_{\text{md}}}\frac{k_p}{c_p}\nabla N_I\cdot\nabla N_J dV\theta^p_J + \int_{\Omega\setminus\Omega_{\text{md}}}\frac{g}{c_p}N_I N_J\, dA\,(\theta^e_J-\theta^p_J) + \int_{\Gamma_q\cup\partial\Omega_{\text{md}}}\frac{k_p}{c_p}N_I\mathbf{n}\cdot\nabla N_J\, dV\,\theta^p_J\Big) + \frac{2}{3\kappa_B}\sum_{\alpha\in\mathcal{A}} N_{I\alpha}\Delta V_\alpha\left\langle \mathbf{v}_\alpha\cdot\Big(\mathbf{f}^\lambda_\alpha - \partial_{\mathbf{x}_\alpha}\Phi\Big)\right\rangle$$

thermostat:

$$\dot{\mathbf{v}}_\alpha = -\frac{1}{m_\alpha}\partial_{\mathbf{x}_\alpha}\Phi - \frac{1}{2}\sum_I N_{I\alpha}\lambda_I\mathbf{v}_\alpha$$

$$\sum_J N_{I\alpha}(m_\alpha\mathbf{v}_\alpha\cdot\mathbf{v}_\alpha)N_{J\alpha}\,\lambda_J = -\int_{\Omega_{\text{md}}} N_I\, g(\theta^e-\theta^p+\tau(\dot{\theta}^e-\dot{\theta}^p))\,dV - \int_{\partial\Omega_{\text{md}}} N_I\mathbf{n}\cdot k_p\nabla(\theta^p+\tau\dot{\theta}^p)\,dA$$

# TIME INTEGRATION

- FE temperature evolution equations:

$$\dot{\theta}^e_J = F^e_J(\theta^e_J, \theta^p_J)$$
$$\dot{\theta}^p_J = F^p_J(\theta^p_J, \theta^e_J) + M_J(\mathbf{x}_\alpha, \mathbf{v}_\alpha, \lambda_\alpha)$$

- MD thermostat:

$$\dot{\mathbf{v}}_\alpha = \mathbf{f}_\alpha(\mathbf{x}_\alpha) + \mathbf{f}^\lambda_\alpha(\mathbf{v}_\alpha, \lambda_\alpha)$$

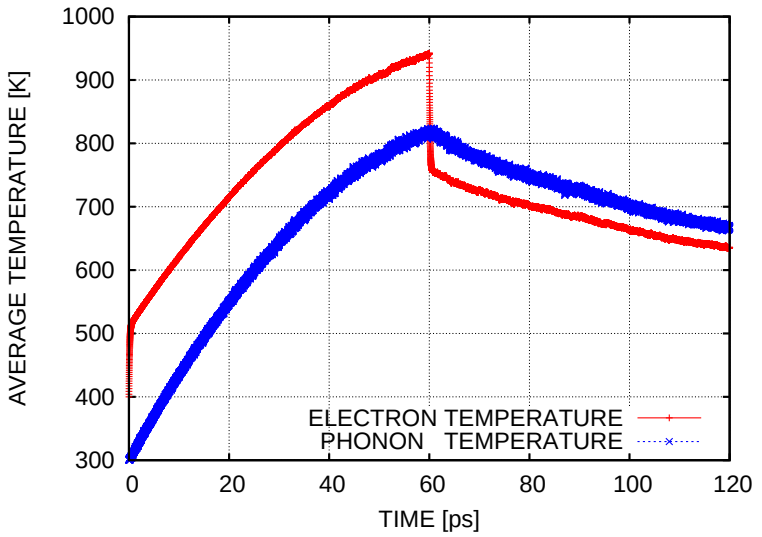
To accommodate fast timescales, & the structure of an MD code (LAMMPS) we use a mixture of integration schemes. For one time step:

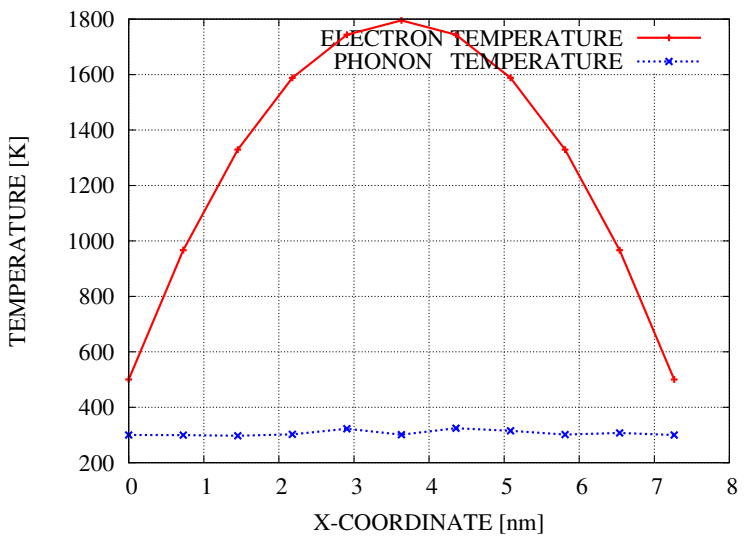
1. Apply the thermostat by solving for $\lambda$ and integrating $\dot{\mathbf{v}} = \mathbf{f}^\lambda$ with Verlet
2. Phonon: Gear predictor for $\theta^p = \theta^p(\dot{\theta}^p, \ddot{\theta}^p)$ and Verlet for $\dot{\theta}^p = M$
3. Electron: either implicit backwards Euler or subcycled forward Euler for $\dot{\theta}^e = F^e$
4. First Verlet half step for $\dot{\mathbf{v}} = \mathbf{f}$ and update $\mathbf{x}$ and $\mathbf{f}$
5. Second Verlet half step for $\dot{\mathbf{v}} = \mathbf{f}$
6. Apply the thermostat by solving for $\lambda$ and integrating $\dot{\mathbf{v}} = \mathbf{f}^\lambda$ with Verlet
7. Phonon: Gear corrector for $\dot{\theta}^p = F^p$ and Verlet for $\dot{\theta}^p = M$

# JOULE HEATING

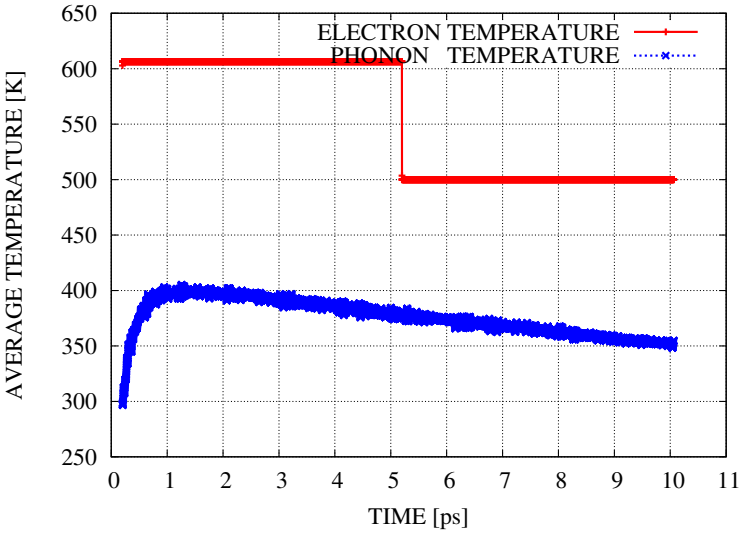
Nanowires 20 cells long, electron system heated with a uniform source

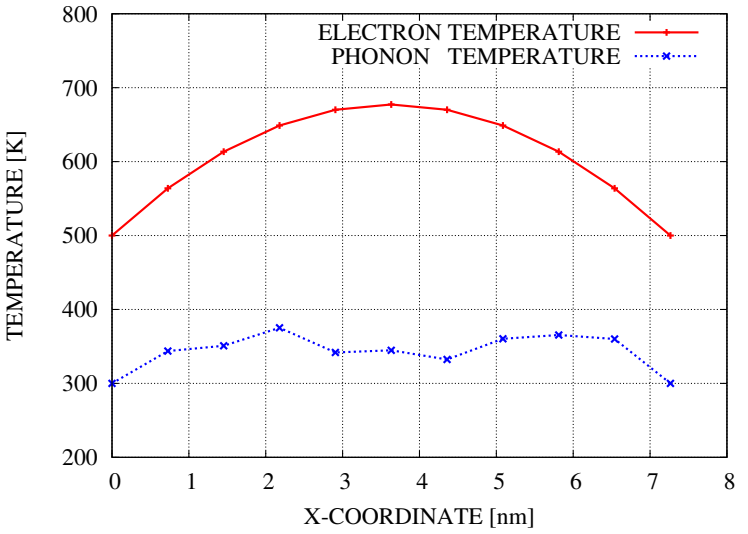
## Copper




## Silicon

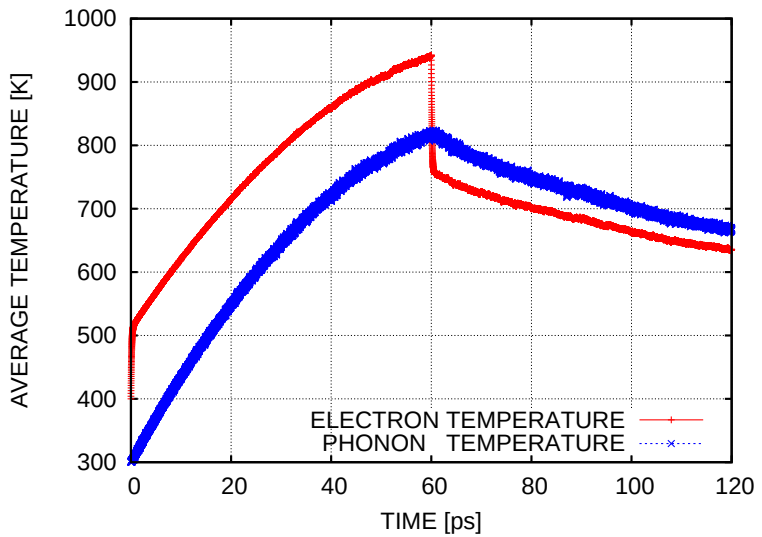


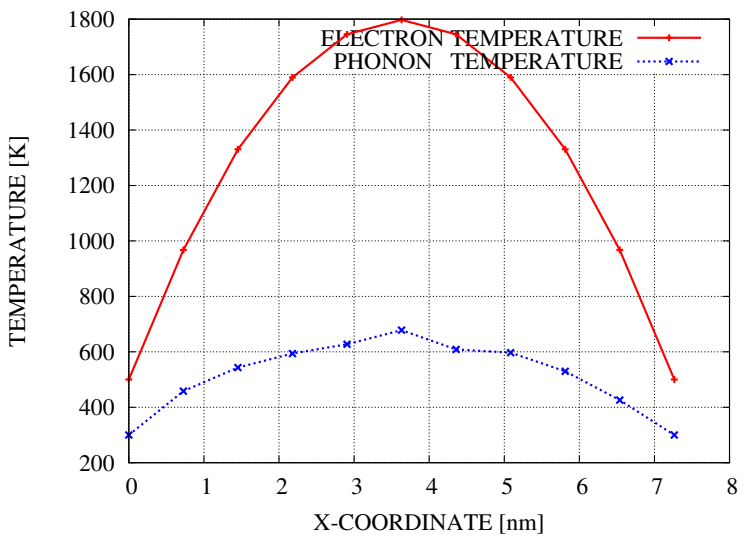



# JOULE HEATING

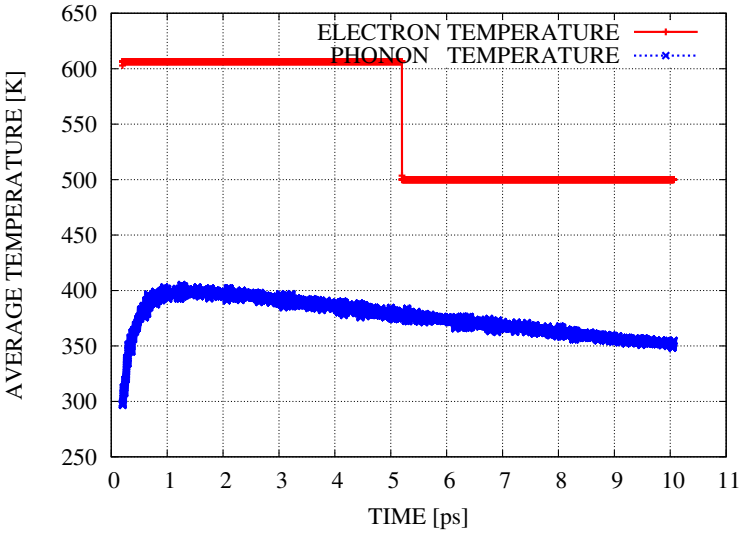
Nanowires 20 cells long, electron system heated with a uniform source

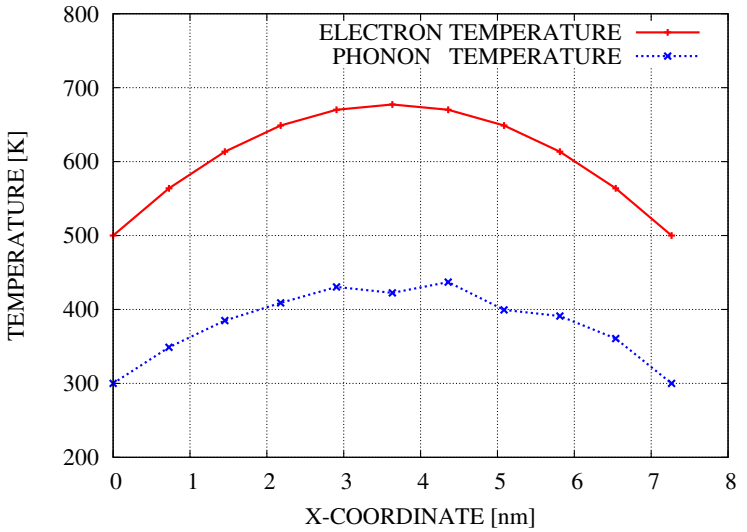
## Copper




## Silicon

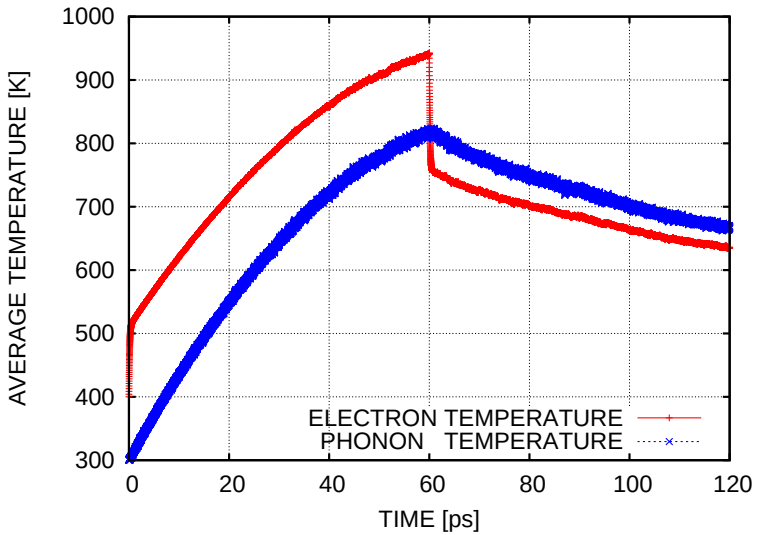


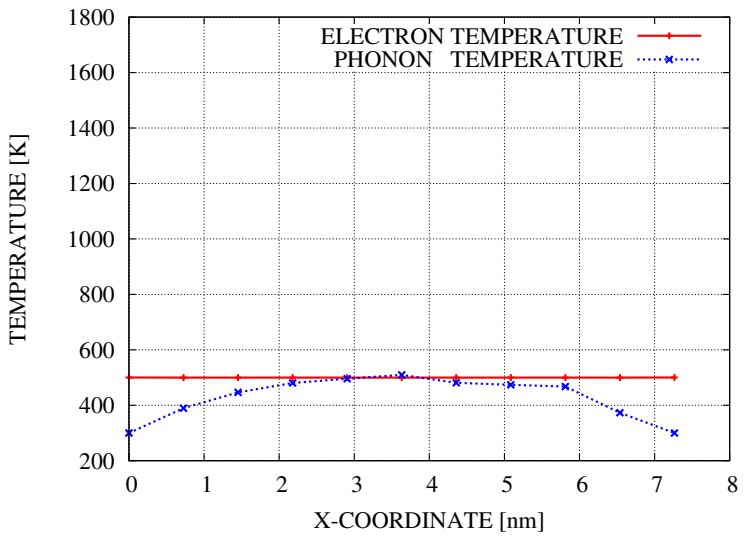



# JOULE HEATING

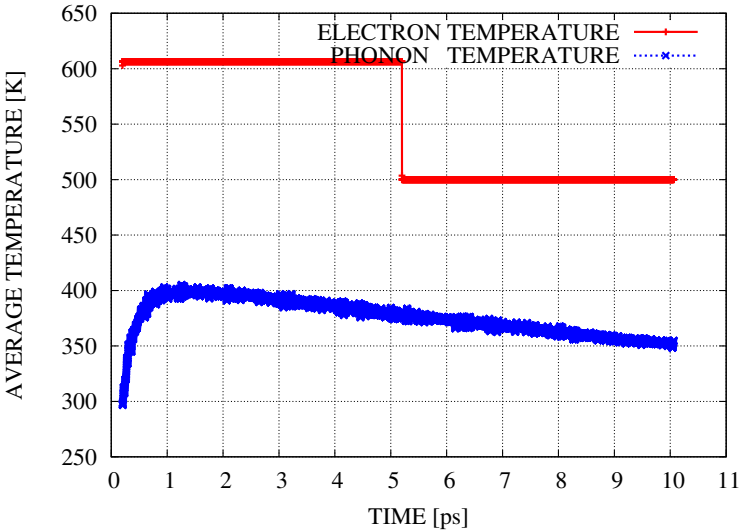
Nanowires 20 cells long, electron system heated with a uniform source

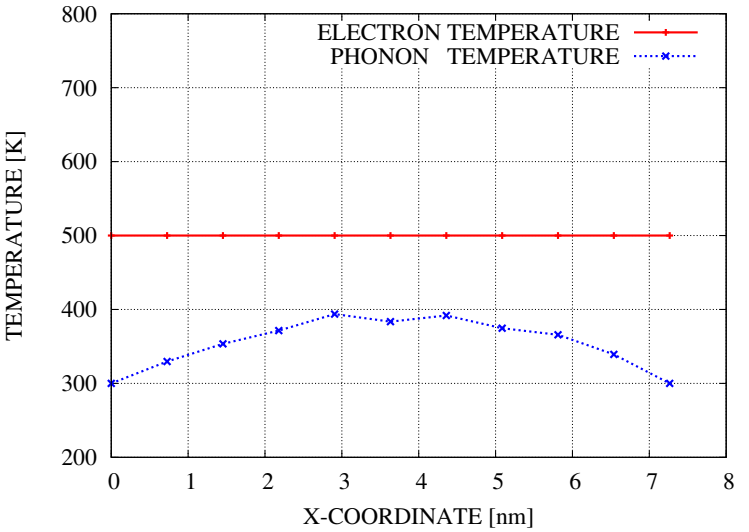
## Copper



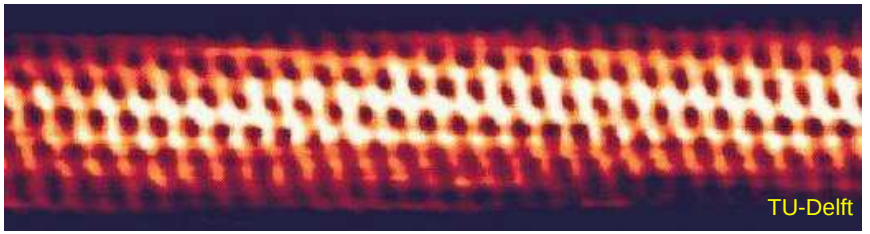



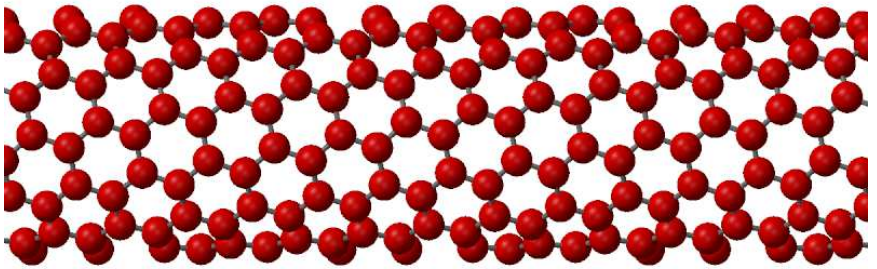

## Silicon

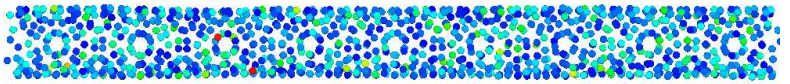


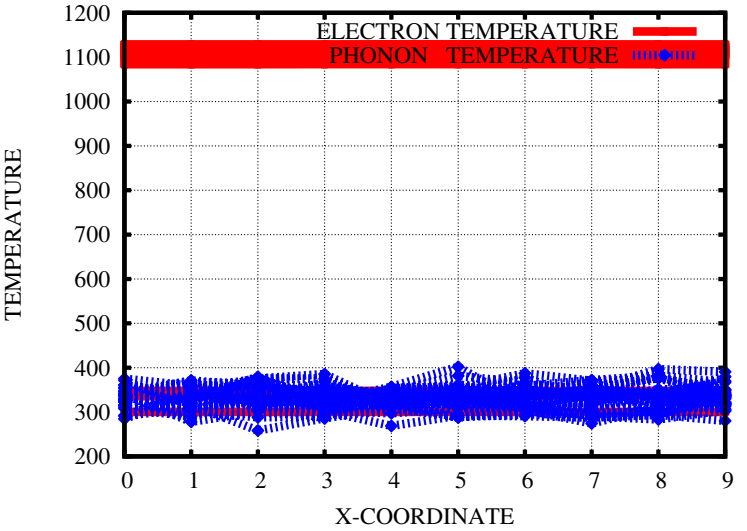



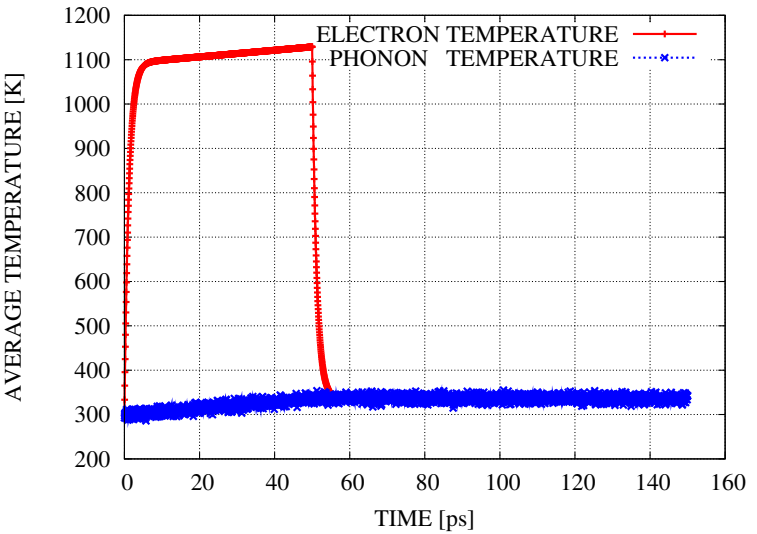
# CARBON NANOTUBE







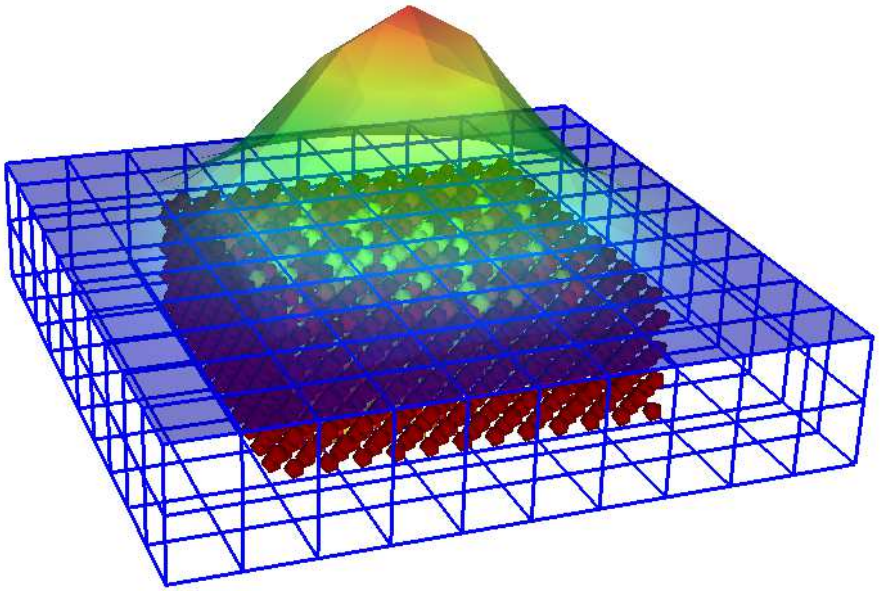

- CNT heated with a localized source but the electron conductivity sufficiently high to flatten temperature profile
- fast rise in electron temperature, followed by slower (linear) rise that matches the phonon temperature rise
- phonon temperature "noisy" due to small number of atoms under each node's support

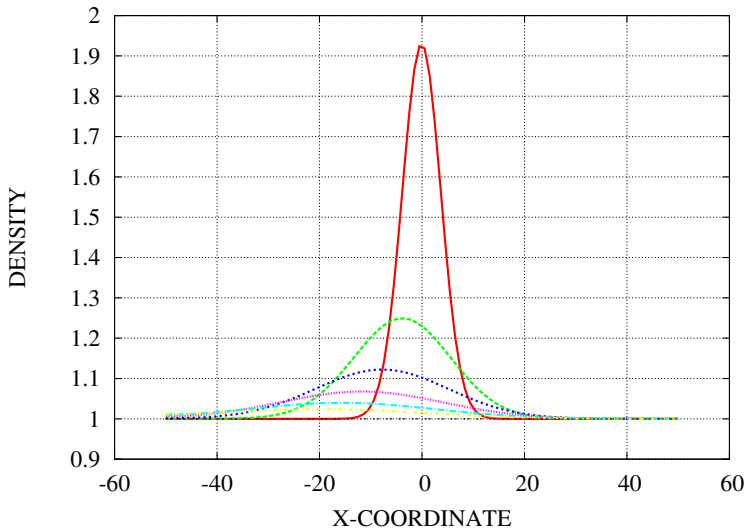
| conductivity [W/K-m] | | capacity [J/K-kg] | | e-p coupling [W/K-m$^3$] |
|---|---|---|---|---|
| 100 | 24.4 | 415 | 0.46 | $0.9 \times 10^{14}$ |

# CURRENT WORK

Work-to-date shows the utility of the method in enhancing nonequilibrium MD, but there are many remaining issues to consider, including:

- Boundary conditions for the two temperatures
- Non-linear temperature effects: $c_e(\theta_e)$ & $g(\theta_e - \theta_p)$
- Defects : effects on electrons, phonons and exchange
- Electron conservation & momentum equations



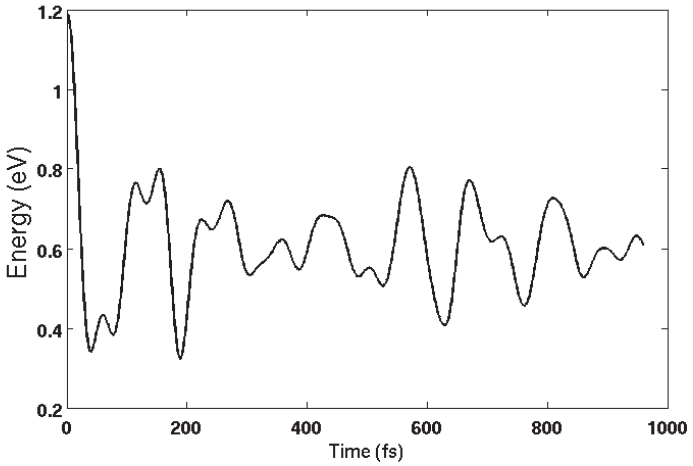



Haynes-Shockley experiment showing drift & diffusion

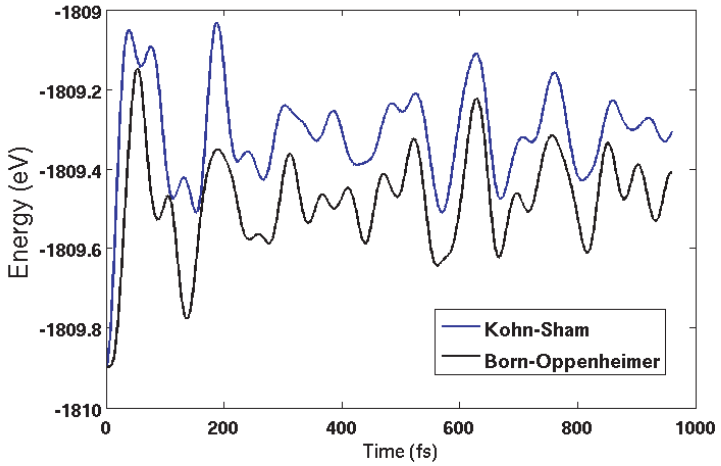
contact : rjones@sandia.gov

# ADDITIONAL SLIDES

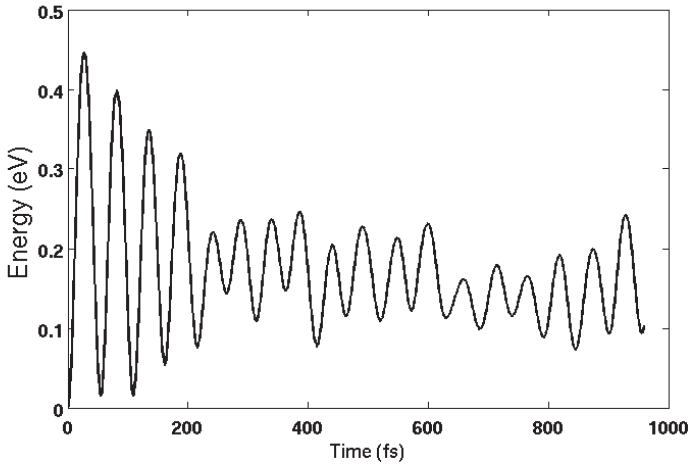
# TIME DEPENDENT DENSITY FUNCTIONAL ESTIMATION




kinetic energy of nuclei




TDDFT calculates the transients in the electron density and atomic motion, thus directly simulating the exchange of energy

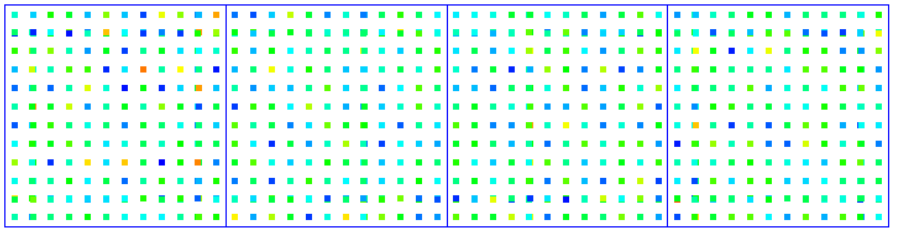


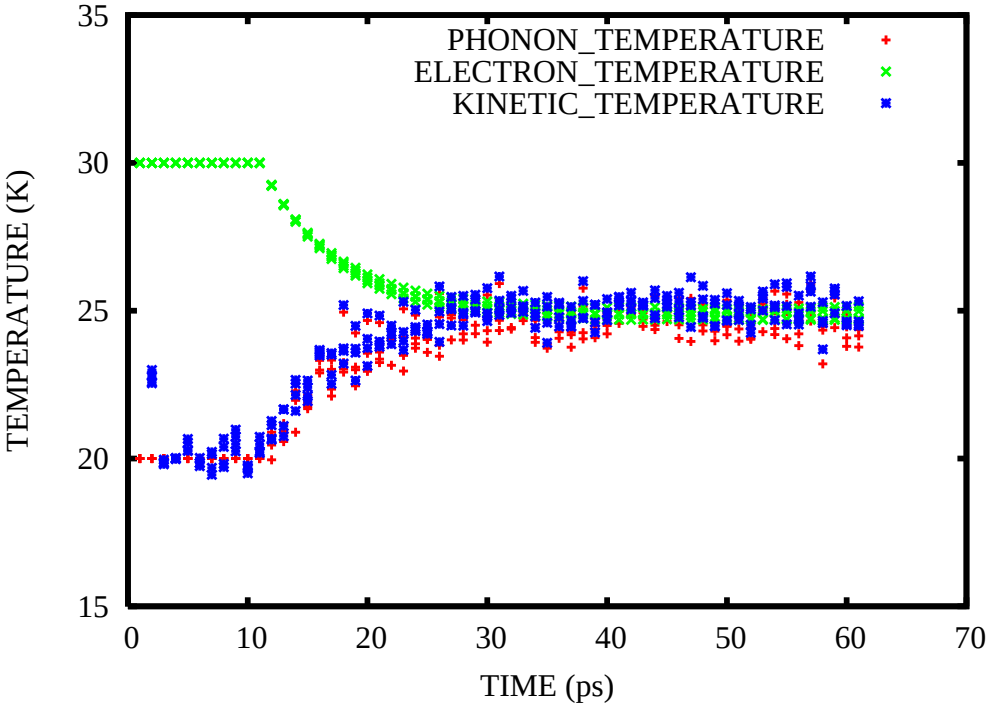

kinetic energy of electrons

# EXAMPLE: UNIFORM EXCHANGE

A simple simulation to test consistency with the two temperature model, $\Omega = \Omega_{md}$:

- code : LAMMPS [PLIMPTON]
- material : 3D (solid) Argon, Lennard-Jones pair potential lattice size $\ell = 5.405\,\mathring{A}$ at $30\,K$
- system size $(24 \times 6 \times 6)\ell$ with periodic boundary conditions
- MD thermalization for $10.000\,ps$
- exchange timescale $\tau_{\text{e-p}} = 3.2ps$
- same heat capacity & conductivity for electron system as the phonon system (temperature independent)



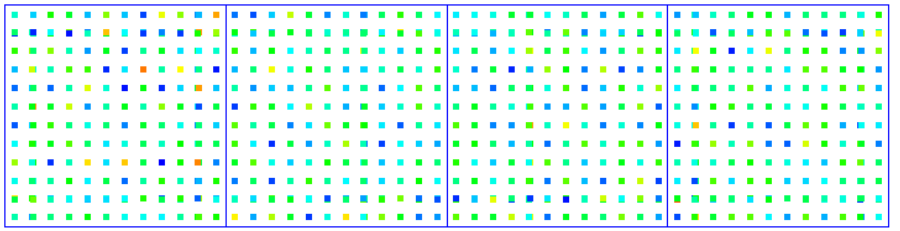



no filtering

# EXAMPLE: UNIFORM EXCHANGE

A simple simulation to test consistency with the two temperature model, $\Omega = \Omega_{md}$:

- code : LAMMPS [PLIMPTON]



- material : 3D (solid) Argon, Lennard-Jones pair potential lattice size $\ell = 5.405\,\mathring{A}$ at $30\,K$

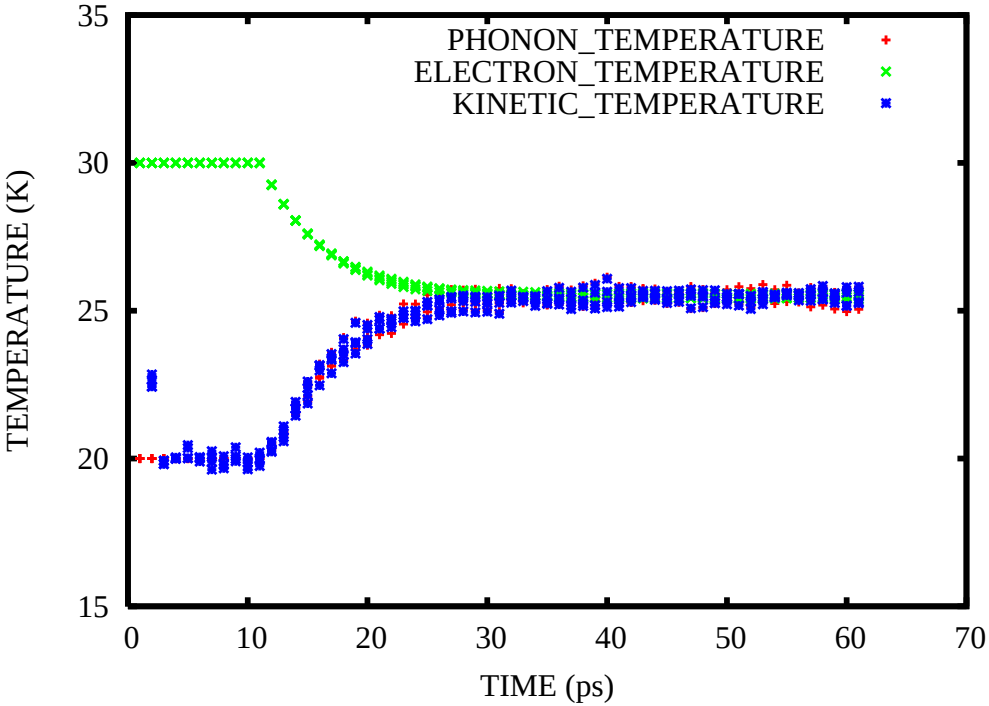
- system size $(24 \times 6 \times 6)\ell$ with periodic boundary conditions

- MD thermalization for $10.000\,ps$

- exchange timescale $\tau_{\text{e-p}} = 3.2ps$

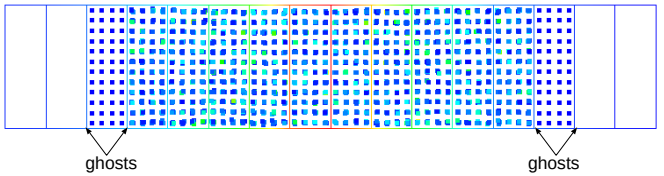
- same heat capacity & conductivity for electron system as the phonon system (temperature independent)

- given statistical fluctuations, filtering is consistent with the chosen continuum heat transfer model & does not change observables

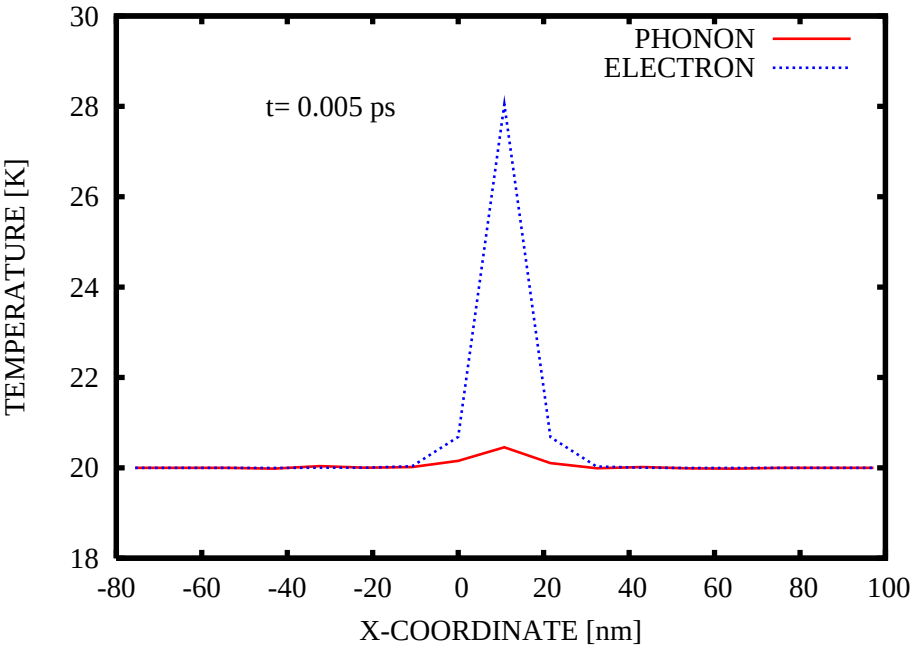


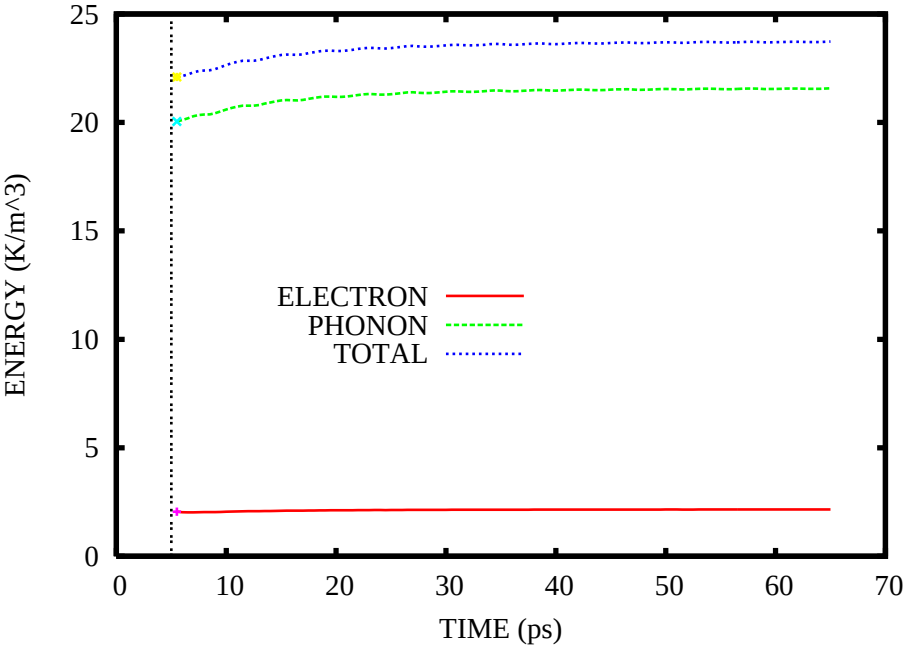

filter $\tau = 0.500\,ps$

# EXAMPLE: "NANOWIRE"

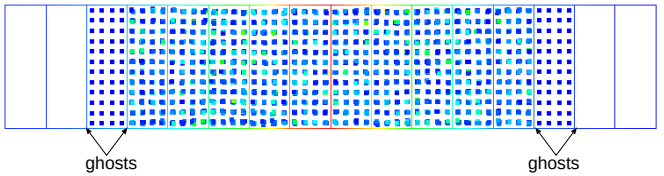



- Lennard-Jones Argon $(32\times8\times8)\ell$
- Internal FE/MD boundaries padded with zero displacement, zero temperature ghost atoms
- Gaussian initial electron temperature to emulate laser heating
- Heat capacity $c_e = \frac{1}{10}c_p$
- Adiabatic FE boundary conditions
- Weak FE-scale energy conservation (but exact total energy conservation) since $\theta_p$ is tied to kinetic energy in $\Omega_{md}$ and total energy in $\Omega \setminus \Omega_{md}$

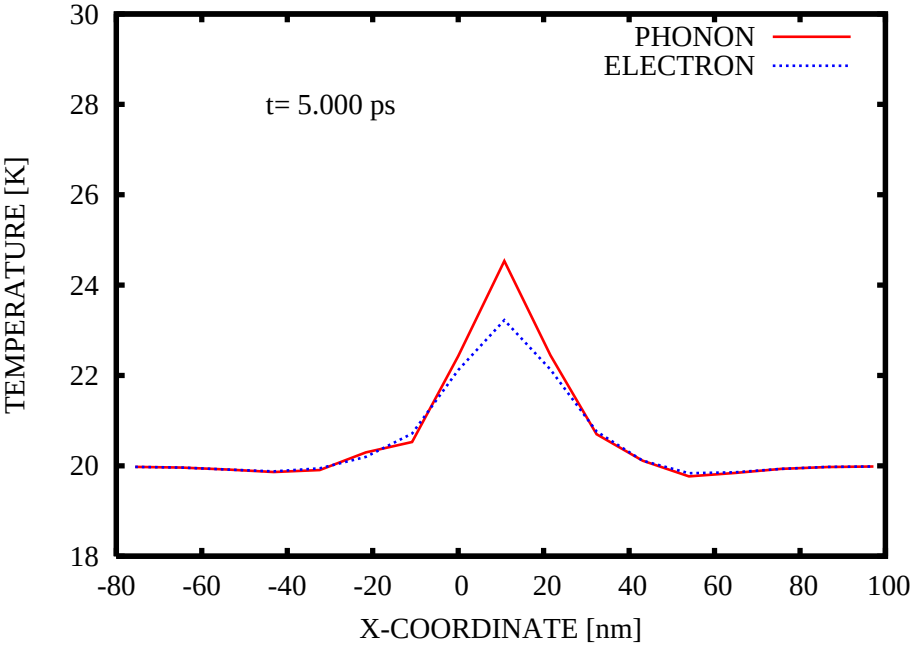


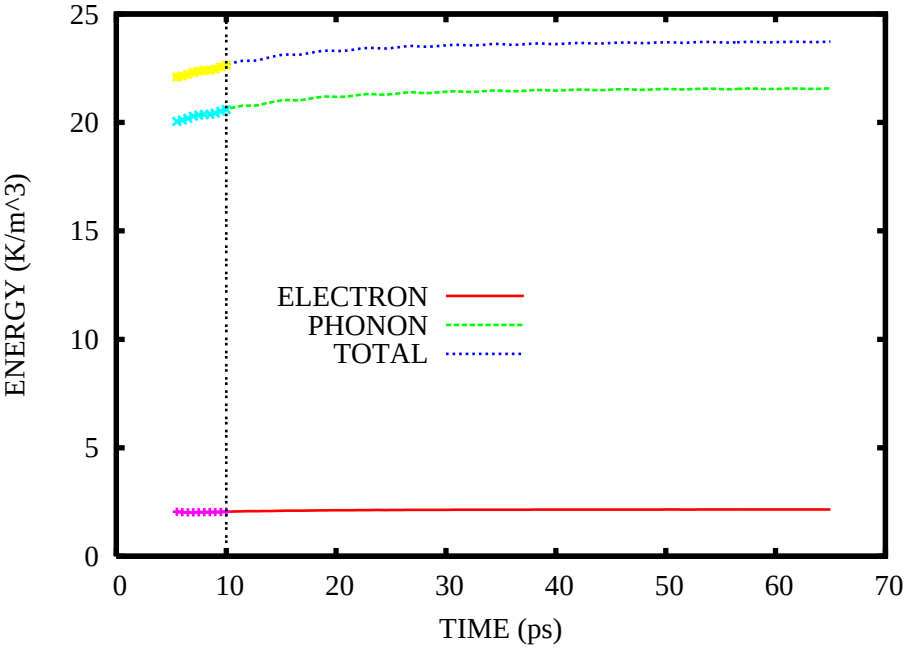



# EXAMPLE: "NANOWIRE"

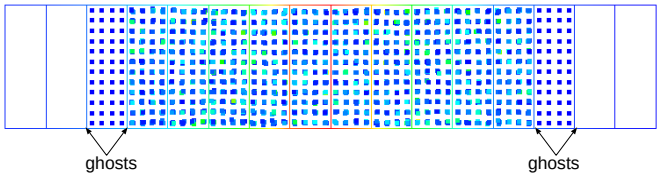



- Lennard-Jones Argon $(32\times8\times8)\ell$
- Internal FE/MD boundaries padded with zero displacement, zero temperature ghost atoms
- Gaussian initial electron temperature to emulate laser heating
- Heat capacity $c_e = \frac{1}{10}c_p$
- Adiabatic FE boundary conditions
- Weak FE-scale energy conservation (but exact total energy conservation) since $\theta_p$ is tied to kinetic energy in $\Omega_{md}$ and total energy in $\Omega \setminus \Omega_{md}$

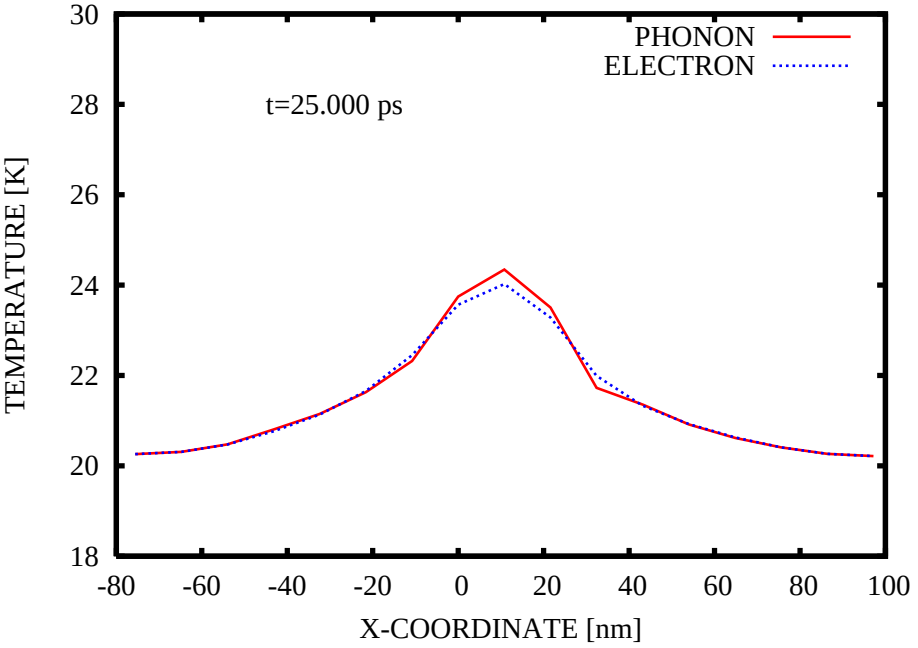


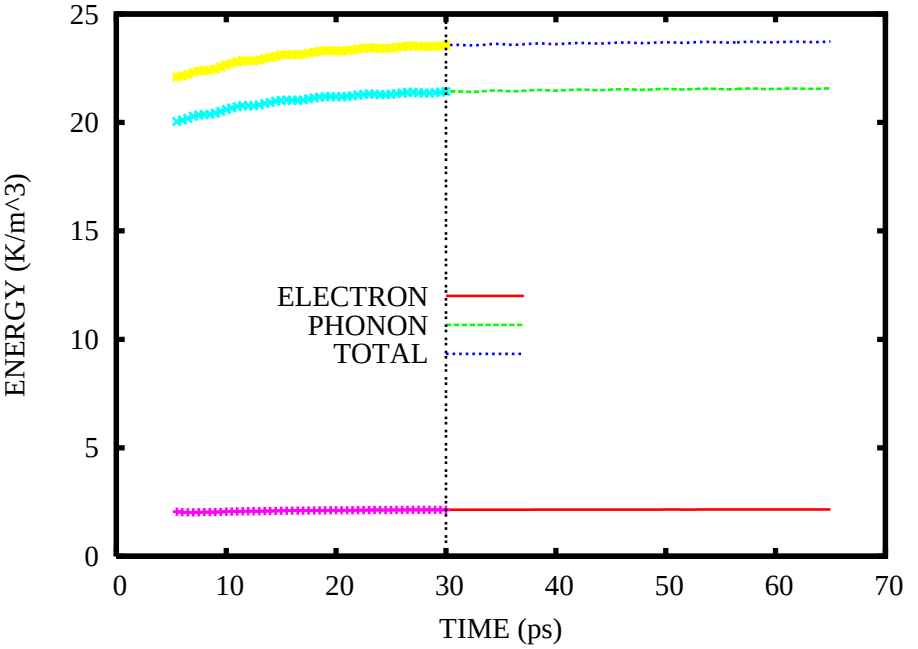



# EXAMPLE: "NANOWIRE"

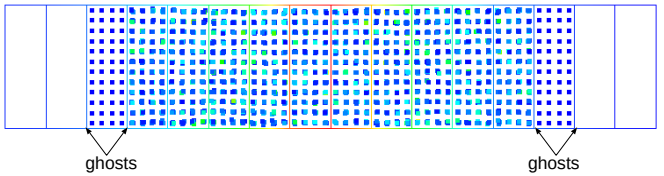



- Lennard-Jones Argon $(32\times8\times8)\ell$
- Internal FE/MD boundaries padded with zero displacement, zero temperature ghost atoms
- Gaussian initial electron temperature to emulate laser heating
- Heat capacity $c_e = \frac{1}{10}c_p$
- Adiabatic FE boundary conditions
- Weak FE-scale energy conservation (but exact total energy conservation) since $\theta_p$ is tied to kinetic energy in $\Omega_{md}$ and total energy in $\Omega \setminus \Omega_{md}$

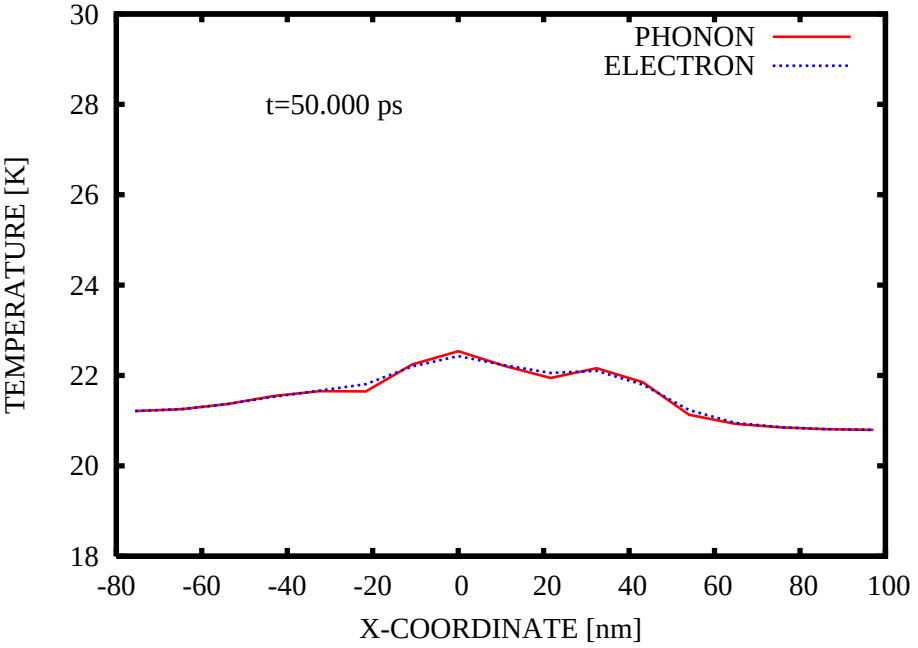


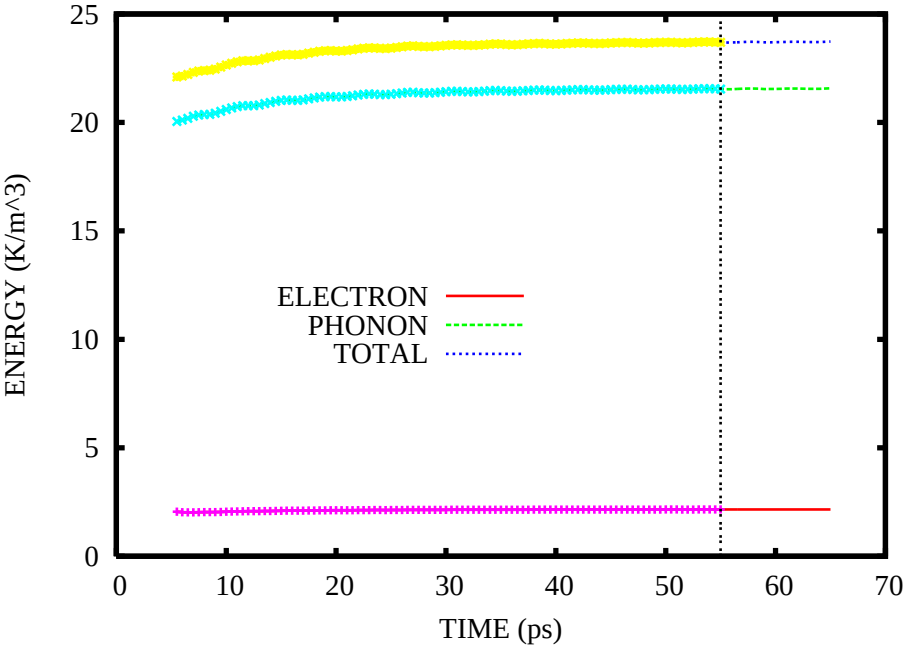



# EXAMPLE: "NANOWIRE"

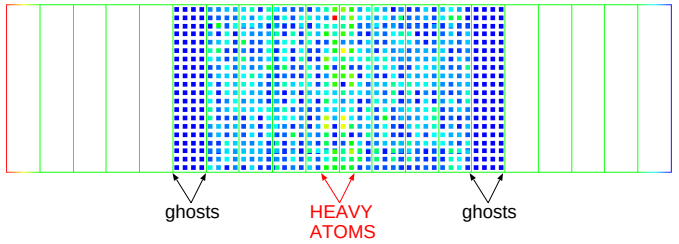



- Lennard-Jones Argon $(32\times8\times8)\ell$
- Internal FE/MD boundaries padded with zero displacement, zero temperature ghost atoms
- Gaussian initial electron temperature to emulate laser heating
- Heat capacity $c_e = \frac{1}{10}c_p$
- Adiabatic FE boundary conditions
- Weak FE-scale energy conservation (but exact total energy conservation) since $\theta_p$ is tied to kinetic energy in $\Omega_{md}$ and total energy in $\Omega \setminus \Omega_{md}$



# EXAMPLE: "GRAIN BOUNDARY"

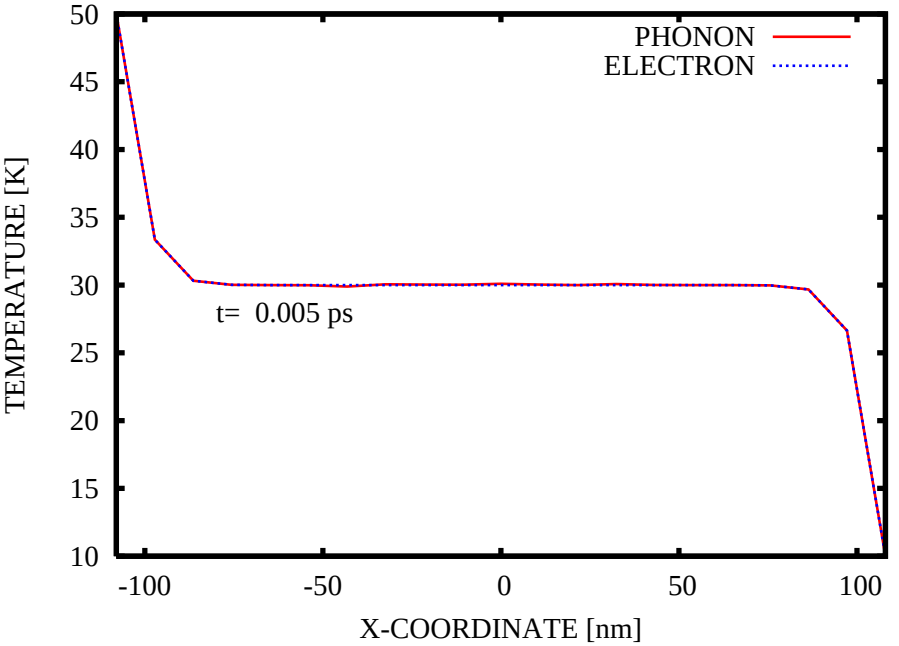


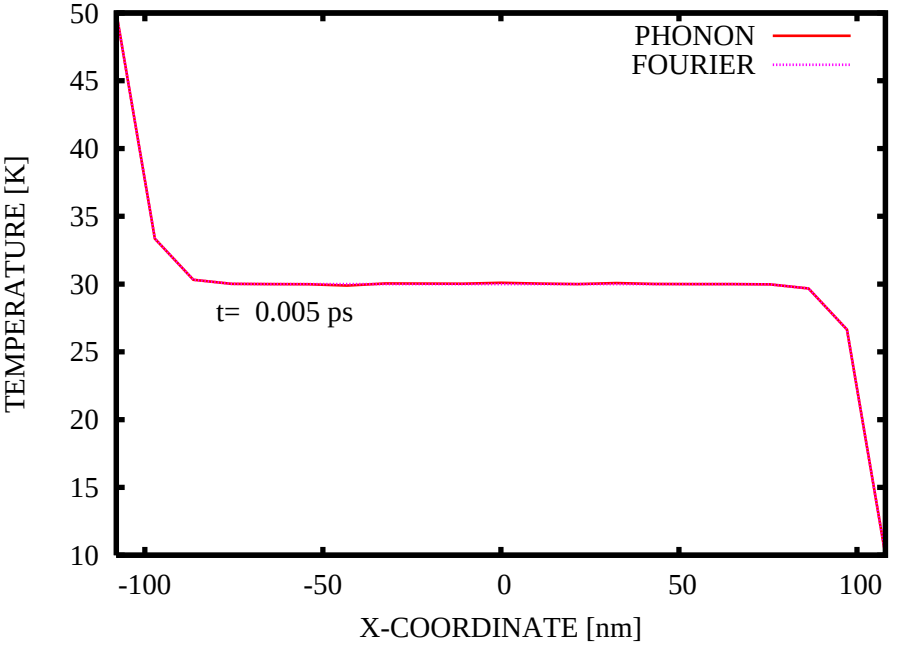

- L-J Argon $(40 \times 10 \times 10)\ell$

- Acoustic mismatch created with atomic masses equal to $10m_\alpha$ in a $2\ell$ wide region in the center

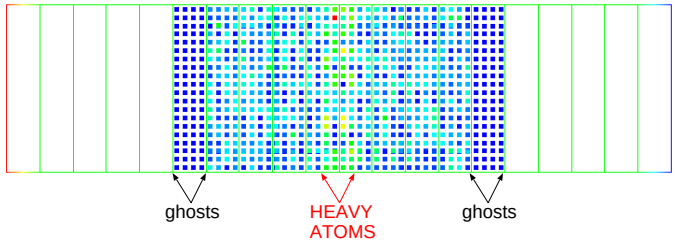
- MD thermalized to $30K$ and at $t = 0$ FE temperature boundary condition prescribed $50K$ on the left and $10K$ on the right

- Coupled system, assuming defect is transparent to the electron system, has similar transient behavior to phonon-only system but electron-phonon exchange minimizes the Kapitza resistance at steady state



# EXAMPLE: "GRAIN BOUNDARY"

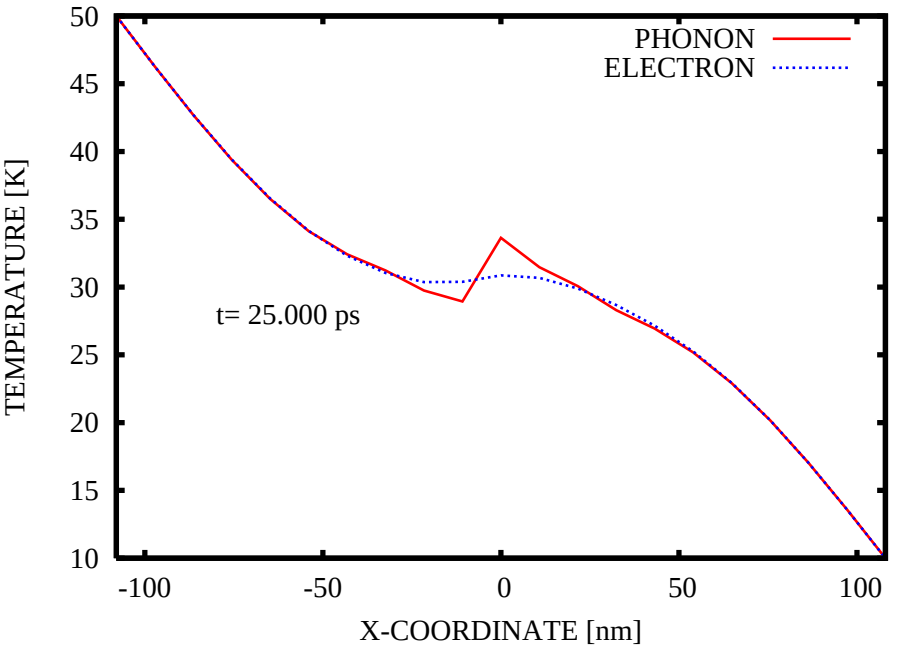


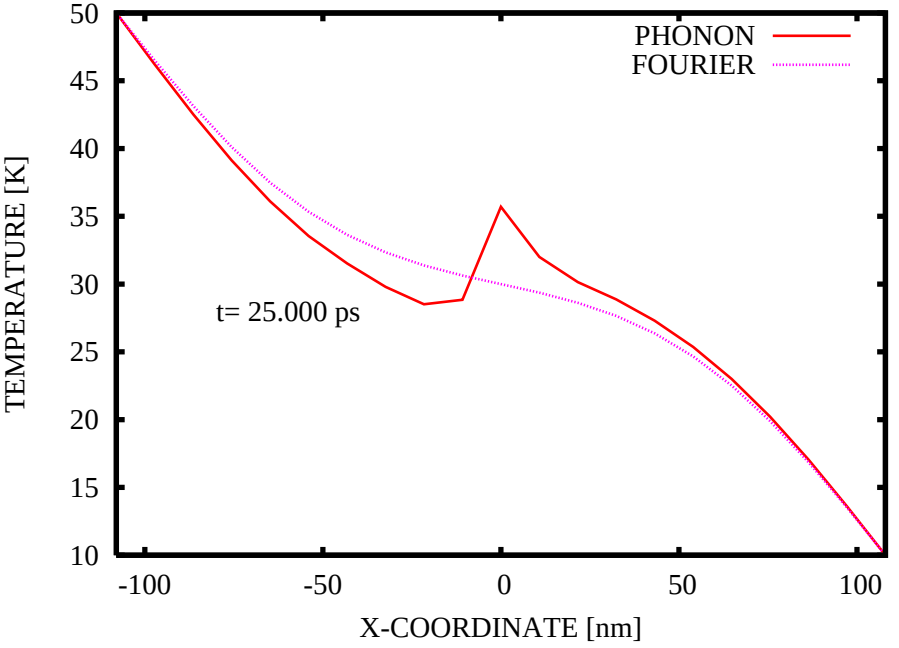

- L-J Argon $(40 \times 10 \times 10)\ell$

- Acoustic mismatch created with atomic masses equal to $10m_\alpha$ in a $2\ell$ wide region in the center

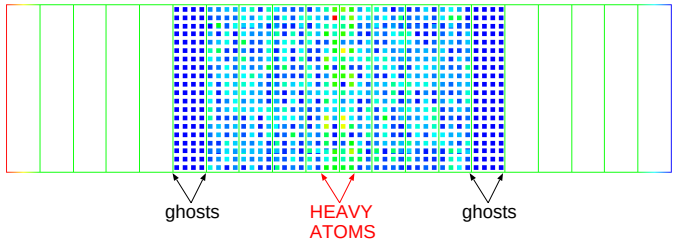
- MD thermalized to $30K$ and at $t = 0$ FE temperature boundary condition prescribed $50K$ on the left and $10K$ on the right

- Coupled system, assuming defect is transparent to the electron system, has similar transient behavior to phonon-only system but electron-phonon exchange minimizes the Kapitza resistance at steady state



# EXAMPLE: "GRAIN BOUNDARY"

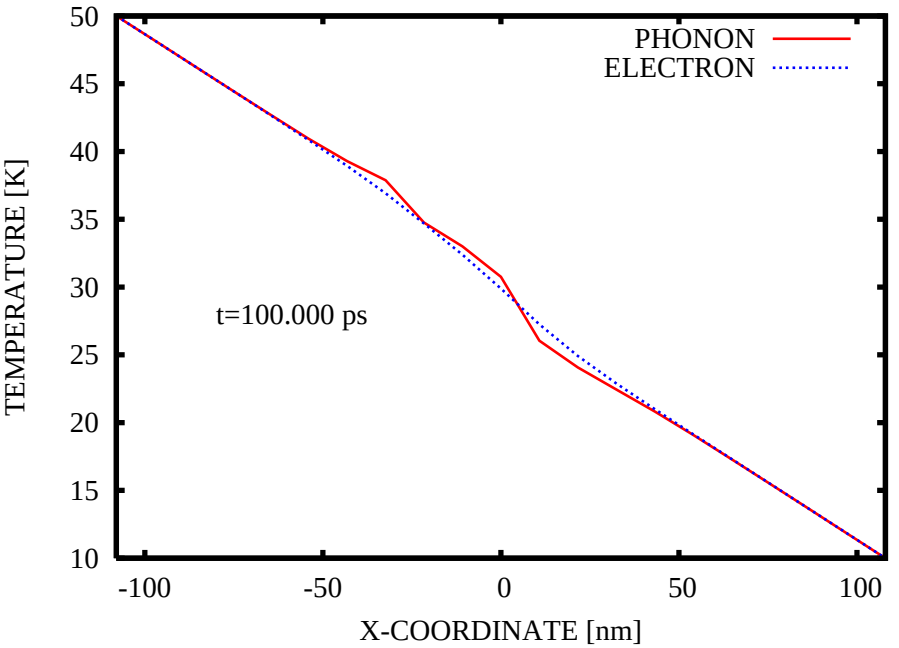


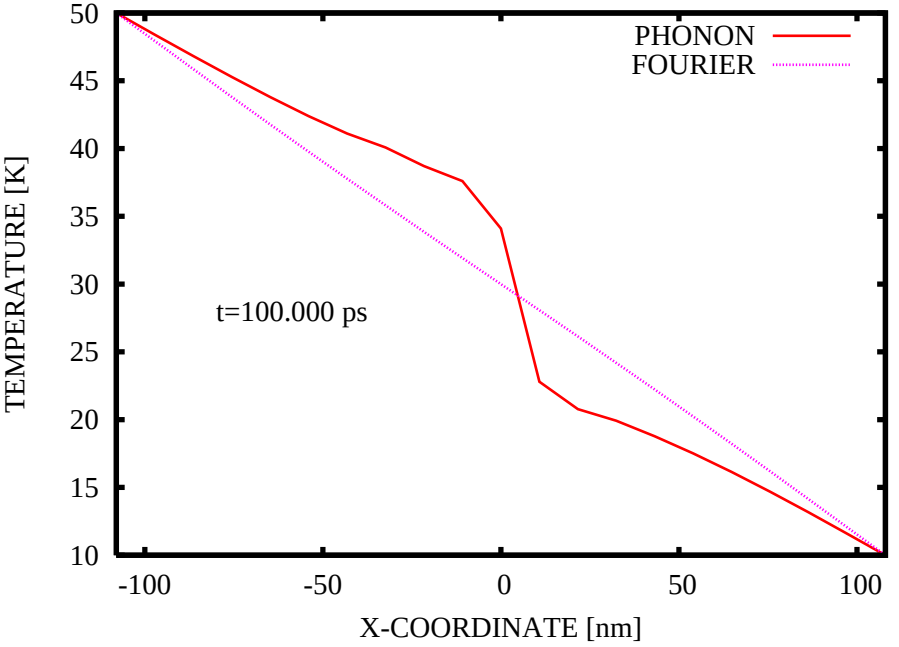

- L-J Argon $(40 \times 10 \times 10)\ell$

- Acoustic mismatch created with atomic masses equal to $10m_\alpha$ in a $2\ell$ wide region in the center

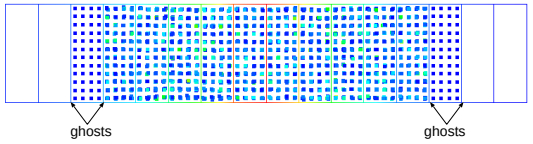
- MD thermalized to $30K$ and at $t = 0$ FE temperature boundary condition prescribed $50K$ on the left and $10K$ on the right

- Coupled system, assuming defect is transparent to the electron system, has similar transient behavior to phonon-only system but electron-phonon exchange minimizes the Kapitza resistance at steady state



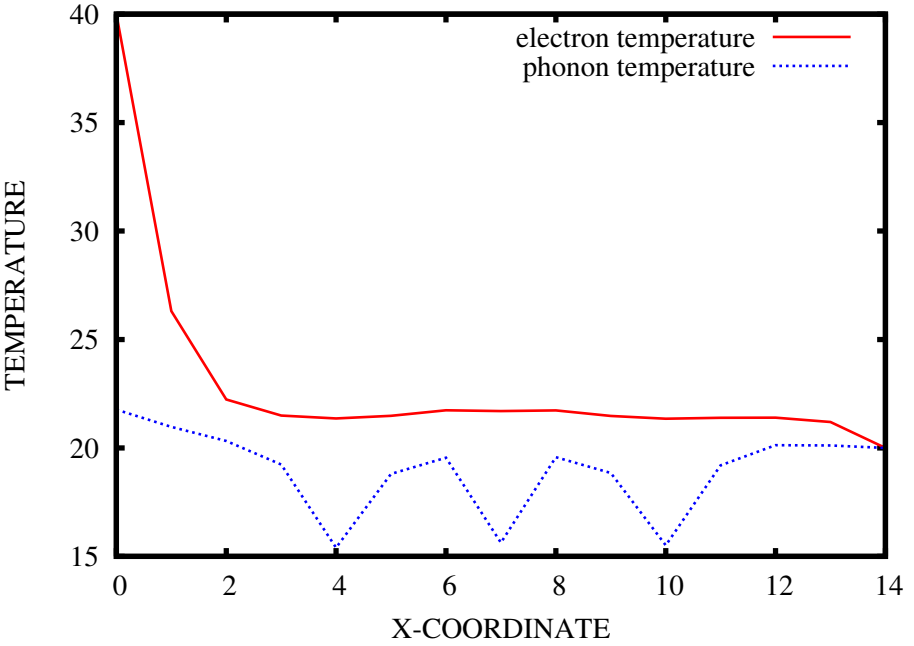
# EXAMPLE: "JOULE HEATING"

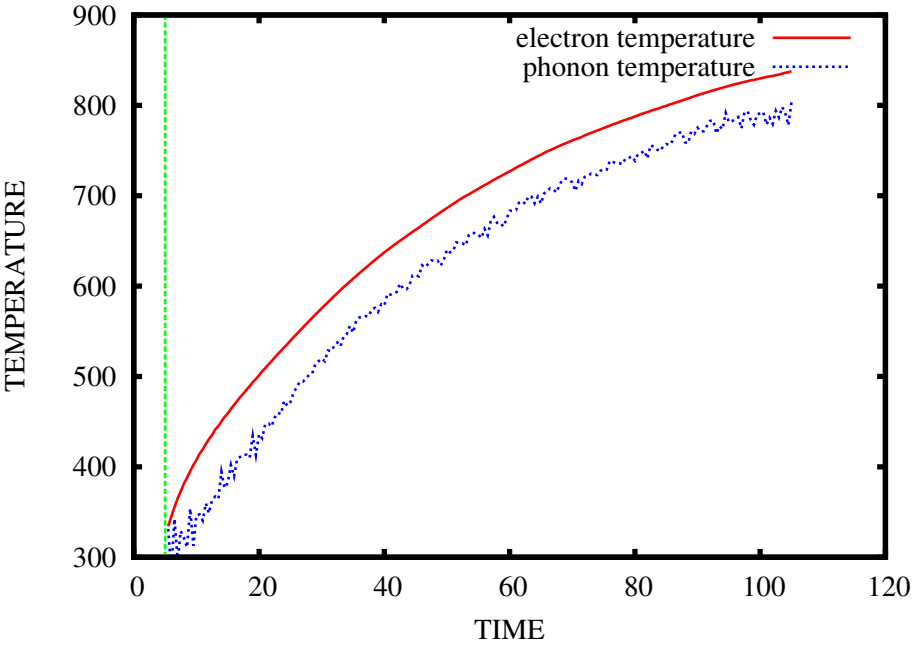



- L-J Argon $(40 \times 10 \times 10)\ell$

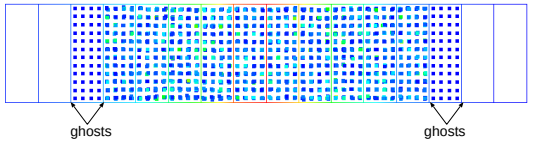
- MD thermalized to $20K$ and at $t = 0$ FE temperature boundary condition prescribed $40K$ on the left and $20K$ on the right to simulate "hot" electrons coming in from the left

- the electrons are given a source of heat that represents the effects of an external electric field



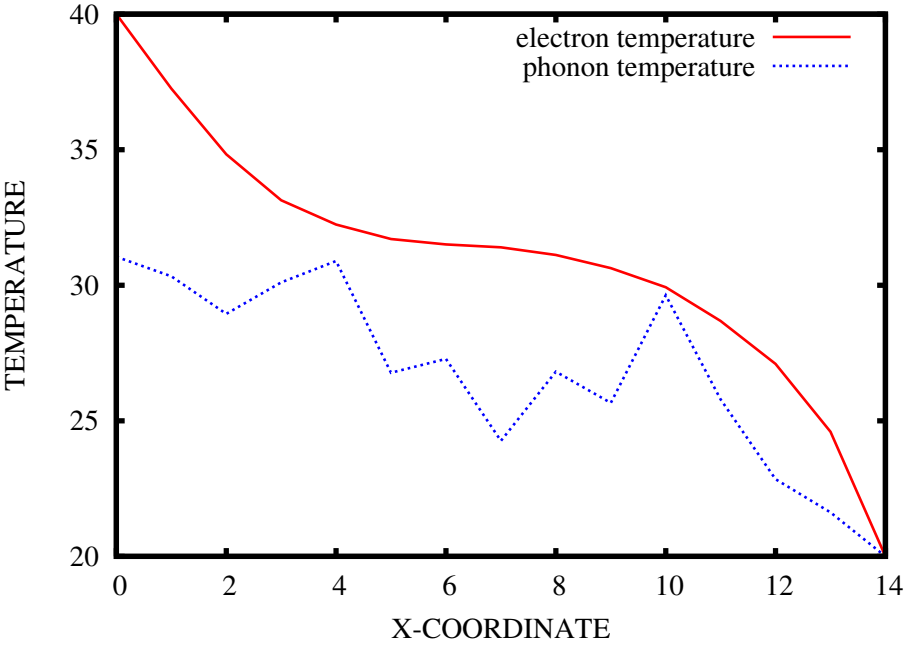
# EXAMPLE: "JOULE HEATING"

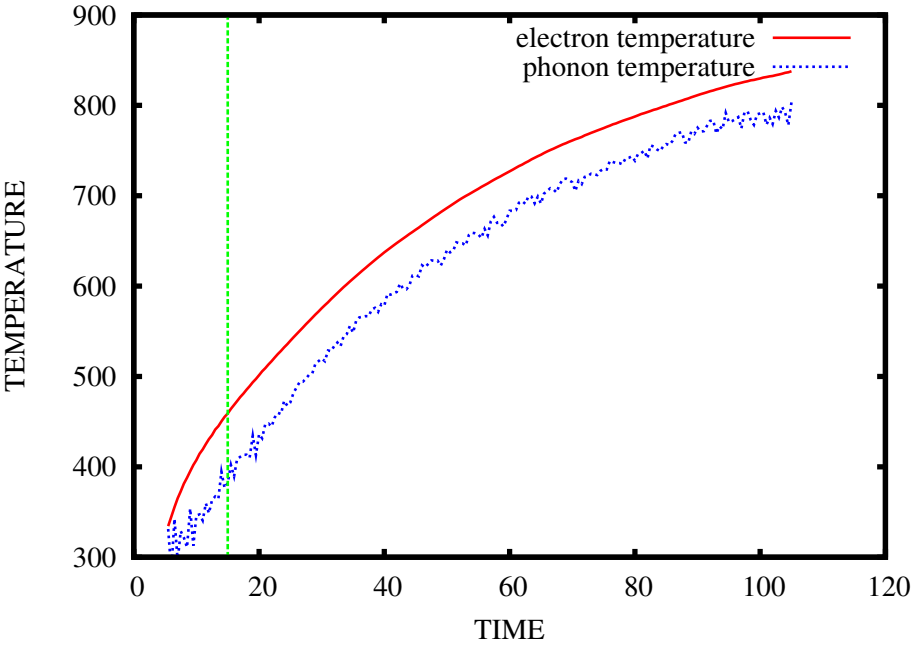



- L-J Argon $(40 \times 10 \times 10)\ell$

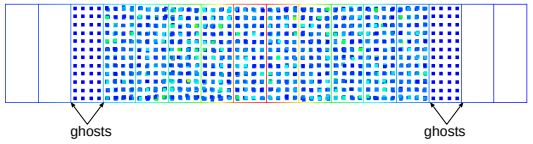
- MD thermalized to $20K$ and at $t = 0$ FE temperature boundary condition prescribed $40K$ on the left and $20K$ on the right to simulate "hot" electrons coming in from the left

- the electrons are given a source of heat that represents the effects of an external electric field



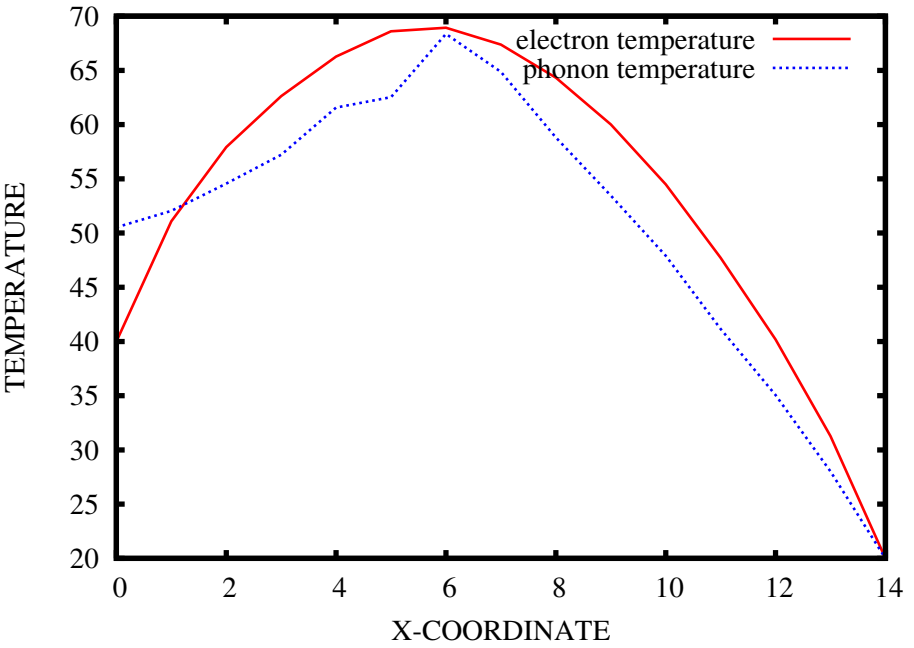
# EXAMPLE: "JOULE HEATING"

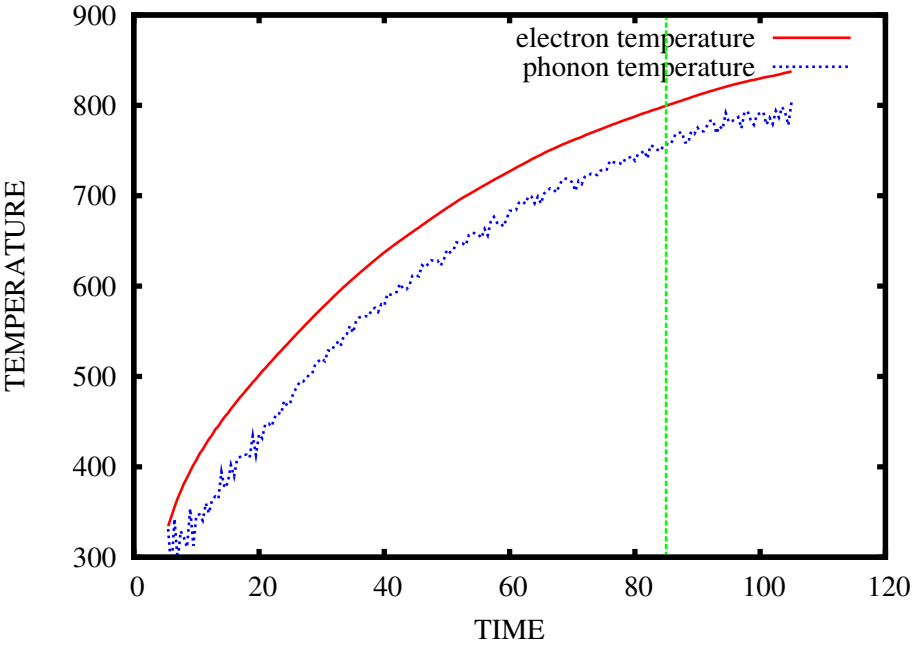



- L-J Argon $(40 \times 10 \times 10)\ell$

- MD thermalized to $20K$ and at $t = 0$ FE temperature boundary condition prescribed $40K$ on the left and $20K$ on the right to simulate "hot" electrons coming in from the left

- the electrons are given a source of heat that represents the effects of an external electric field



# MOTIVATION

Models of electron-mediated energy transport:

- coherent transport where wave-like nature and phase electrons is important : ab initio quantum mechanical simulation is needed at small scales (also limited to small systems).
- incoherent transport where electrons can be treated a particles : Boltzmann equation

$$f_{,t} + \boldsymbol{\nabla}_{\mathbf{x}} f \cdot \mathbf{v} + \frac{1}{m} \boldsymbol{\nabla}_{\mathbf{v}} f \cdot \mathbf{F} = s$$

where the distribution $f$ depends on an enormous number of variables $\{\mathbf{x}_i, \mathbf{v}_i\}$. Also the scattering/source term $s$ is very hard to prescribe.

A number of reductions exist:

- Two temperature model (TTM) which comes from the 2nd moment : energy
- Hydrodynamic model HDM (first 3 moments : density, momentum & energy)
- Drift-Diffusion model (DDM) which is a simplification of HDM commonly used in device simulation