# Monte Carlo Solution of the Boltzmann Transport Equation

Ryan Deskins and Anter El-Azab

Department of Scientific Computing, Florida State University, Tallahassee, FL USA

## Abstract

Heat conduction can be classically described by Fourier's law which is a diffusion equation. These types of equations can be thought of as describing average properties of a random walk of many particles. When describing heat conduction, the considered 'particles' are electrons in metals and phonons in ionic crystals.. However, when the number of collisions of heat carriers becomes Low, a diffusion equation is no longer valid.

The Boltzmann transport equation ( BTE) can be used to model both the diffusion regime (when the number of heat carrier collisions is high) and the ballistic regime (when the number of collisions is low). The BTE is an evolution equation of a distribution function which gives the number of particles in an elementary volume in phase space. The BTE describes the distribution function in space and time as influenced by advection, external forces, and 'particle' collisions.

We present a computational model for solving the BTE for phonons through Monte Carlo. In the model we use the relaxation time approximation. In this approximation the full BTE is simplified by assigning time-scales to each scattering mechanism associated with phonon interactions. Currently, only phonon-phonon interactions are modeled. Including boundary and impurity scatterings, however, would be a simple extension. With this model we successfully reproduce the Ballistic regime of phonon transport in silicon. In this case, the simulation correctly predicts a uniform temperature profile once steady-state is achieved.

## Relaxation Time Approximation

The full Boltzmann equation reads:

$$\frac{\partial f}{\partial t} + \vec{v}_g \cdot \nabla f = \left[\frac{\partial f}{\partial t}\right]_{scat} = \sum_{\vec{K}'} [\phi(\vec{K}',\vec{K})f(\vec{K}') - \phi(\vec{K},\vec{K}')f(\vec{K})]$$

$f(\vec{r},\vec{K},t)$  Distribution function   $\vec{v}_g = \nabla_K \omega$  Group velocity

$\phi(\vec{K}',\vec{K})$  Scattering rate from state K to state K'

The difficulty of solving the full Boltzmann equation is the scattering term on the RHS. To formulate the RHS exactly in the Monte Carlo would mean to not only track all phonon states but also to compare each state with all other states on every time step. This is not possible even with modern Computers. Instead we make the so called relaxation time approximation. Here we assign a total relaxation time to each phonon to encapsulate all phonon scattering. This can include phonon-phonon scattering, phonon-boundary scattering, and phonon-defect scattering.

$$\left[\frac{\partial f}{\partial t}\right]_{scat} = \frac{f - f_0}{\tau} \longrightarrow f - f_0 = \exp(-t/\tau)$$

To combine all scattering mechanisms into a single, total relaxation time for a given phonon, we employ Mathiessen's Rule. This assumes that each scattering mechanism behaves independently of all others and yields

$$\tau^{-1} = \tau_N^{-1} + \tau_U^{-1} + \tau_{impurity}^{-1} + \ldots$$

## Lattice Vibrations and Phonon Modeling

Phonon Occupation # (Bose-Einstein)   $\langle n \rangle = \frac{1}{\exp\left(\frac{\hbar\omega}{k_b T}\right) - 1}$

Total Vibrational Energy   $E = \sum_p \sum_{\vec{K}} \left(\langle n \rangle + \frac{1}{2}\right)\hbar\omega \longrightarrow E = \sum_p \int_\omega \left(\langle n \rangle + \frac{1}{2}\right)\hbar\omega D_p(\omega) g_p d\omega$

Density of States   $D(\omega) = \frac{VK^2}{2\pi^2}\frac{dK}{d\omega} = \frac{VK^2}{2\pi^2 v_g}$

## Monte Carlo Model

### Initialization

**– Create Sub-Volumes**
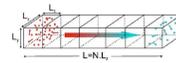


Set local temperature for each cell

Time step is chosen such that the fastest phonons are not allowed to traverse an entire cell during a single step.

**– Use energy equation to get phonon numbers for each cell.**

$$N = V \sum_{p=TA,LA} \sum_{b=1}^{N_b} \left(\frac{1}{\exp\left(\frac{\hbar\omega_{b,p}}{k_B T}\right) - 1}\right)\frac{K_{b,p}^2}{2\pi^2 v_{g b,p}} g_p d\omega$$

This number is usually too large to simulate computationally, and so we define a scaling factor:

$$N' = \frac{N}{W}$$

N' is the number of phonos that we will track in the simulation. Each simulated phonon is then representative of W number of actual phonons.

**– Determine Polarization**

$$P_{LA}(\omega_i) = \frac{N_{LA}(\omega_i)}{N_{LA}(\omega_i) + N_{TA}(\omega_i)}$$

A random number then determines each phonon's branch.

**– Calculate velocities from a quadratic fit to experimental dispersion data.**
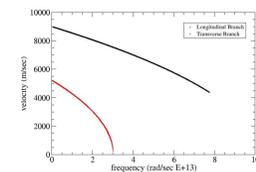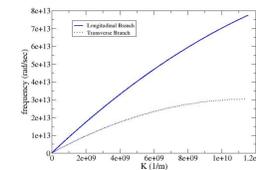




**– Sample directions randomly across a sphere and positions within each cell.**

### Stepping in Time

**– Phonon Drift**

$$\vec{r}_{new} = \vec{r}_{old} + \vec{v}_g \Delta t$$

We treat the first and last cells as blackbodies. Any phonons drifting into these cells are deleted from the simulation. The first and last cells are then initialized again to the hot and cold temperatures.

Currently we specularly reflect phonons from all other boundaries to obtain results that can be compared to bulk data.

Size effects can be simulated by implementing diffuse reflections at the boundaries.

**– Calculate Cell Temperatures**

$$E_T = \sum_{n=1}^{N'} W \hbar\omega_{n,c}$$

Invert energy equation to get a pseudo-temperature for each cell.

These temperatures are then used to calculate the three-phonon relaxation times.

**– Phonon Scattering**

Calculate the total relaxation time for each phonons prescribed by Holland (2).

$$P_{NU} = 1 - \exp(-\Delta t/\tau_{NU})$$

$\tau_{NU}^{-1} = B_L \omega^2 T^3$   Longitudinal

$\tau_N^{-1} = B_{TN} \omega T^4$   Transverse

$$\tau_U^{-1} = \begin{cases} 0 & \omega < \omega_{1/2} \\ B_{TU}\omega^2/\sinh\left(\frac{\hbar\omega}{k_B T}\right) & \omega > \omega_{1/2} \end{cases}$$

Below are the total relaxation times for each branch at 100K as function of phonon frequency.
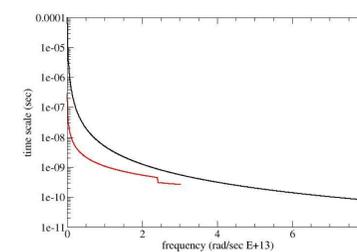


### Stepping in Time Cont.

If a phonon scatters, it's state is completely reset as defined in the initialization process. The only difference being that a new distribution function must be used to resample frequencies.

The modified distribution function for resampling frequencies was prescribed by Lacroix et.al. (1) and ensures that Kirchhoff's law (creation balances destruction) is obeyed.

$$F(\tilde{T}) = \frac{\sum_{j=1}^{i} N_j(\tilde{T})}{\sum_{j=1}^{N_i} N_j(\tilde{T})} \longrightarrow F_{scat}(\tilde{T}) = \frac{\sum_{j=1}^{i} N_j(\tilde{T}) \times P_{scat\,j}}{\sum_{j=1}^{N_i} N_j(\tilde{T}) \times P_{scat\,j}}$$



**– Store Relevant Data**

**– Step in time**

## Results and Discussion
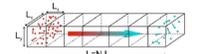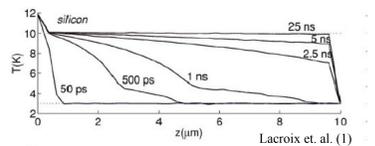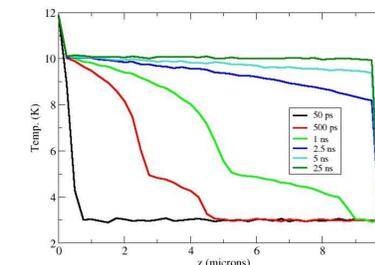




We are currently testing our model against results obtained by Lacroix et. al. (1). Above we compare results of a low temperature simulation for silicon. Here the hot and cold cells are held at 11.88K and 3K respectively, and we plot the temperature evolution along the z-axis with time. At 10K there are essentially no phonon scatterings and we achieve a pure ballistic simulation. A steady-state temperature of 10K is reached throughout the simulated geometry as seen by Lacroix.

As we move to higher temperatures, phonon-phonon scatterings become more frequent. During a room temperature simulation, roughly half the phonons will scatter within a 5 ps time interval. Here, ensuring that the system conserves energy during the scattering process is crucial in obtaining correct results. With the current code, our system tends to lose energy as phonon energies are redistributed according to the F_scat function defined above. We are currently investigating this issue.

After resolving the issue with energy conservation, we plan to model a pure UO2 crystal and eventually model UO2 with varoius crystal defects. Here optical phonons will need to be included since their group velocities are much higher than those found in silicon.

## References

1. D. Lacroix, C. Joulain, and D. Lemonnier, Phys. Rev. B 72, 064305 (2005)

2. M. Holland, Phys. Rev. 132, 2461 (1963)