Reproducing MD simulations in

Thermal transport in SiGe superlattice thin films and nanowires: Effects of specimen and periodic lengths

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The paper

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Thermal transport in SiGe superlattice thin films and nanowires: Effects of specimen and periodic lengths

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We compute the thermal conductivity of superlattice (SL) thin films and nanowires for various SL periods and total specimen lengths using nonequilibrium molecular dynamics. Both types of materials exhibit similar behaviors with respect to SL period but the thermal conductivity of the thin films exhibits a significantly higher sensitivity to the specimen length. Notably, the thermal conductivity of SL thin films is smaller than those of the corresponding nanowires for specimen lengths below approximately 35 nm. These results arise from the complex dependence of the conductivities of the interfaces and the SL components on the specimen size and period. These trends and observations are explained using a simple phonon model that builds on the relationship between the cumulative thermal conductivity and the phonon wavelength.

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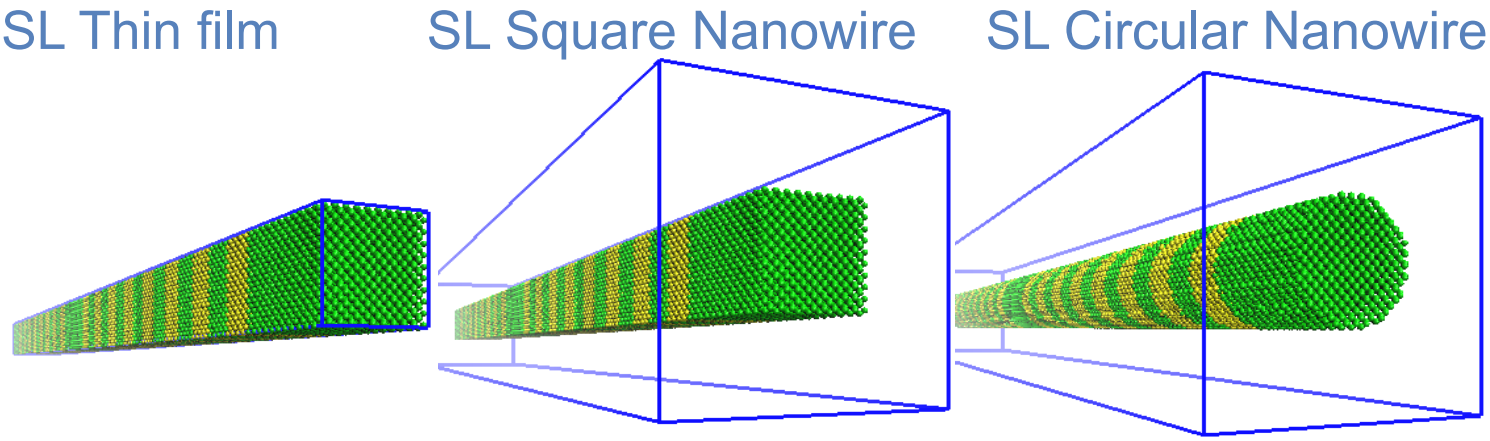
Key results

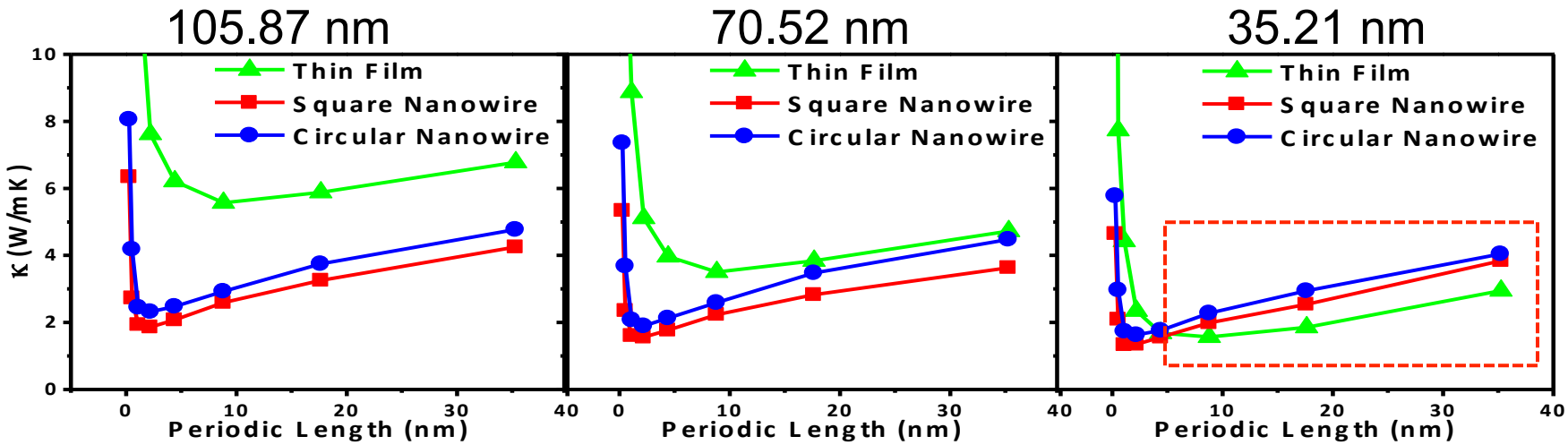
Studied thermal transport on various semiconductor superlattices



- Thin film and nanowire configurations
- Focused on how characteristic sizes affect thermal transport
  - Superlattice period
  - Total specimen length

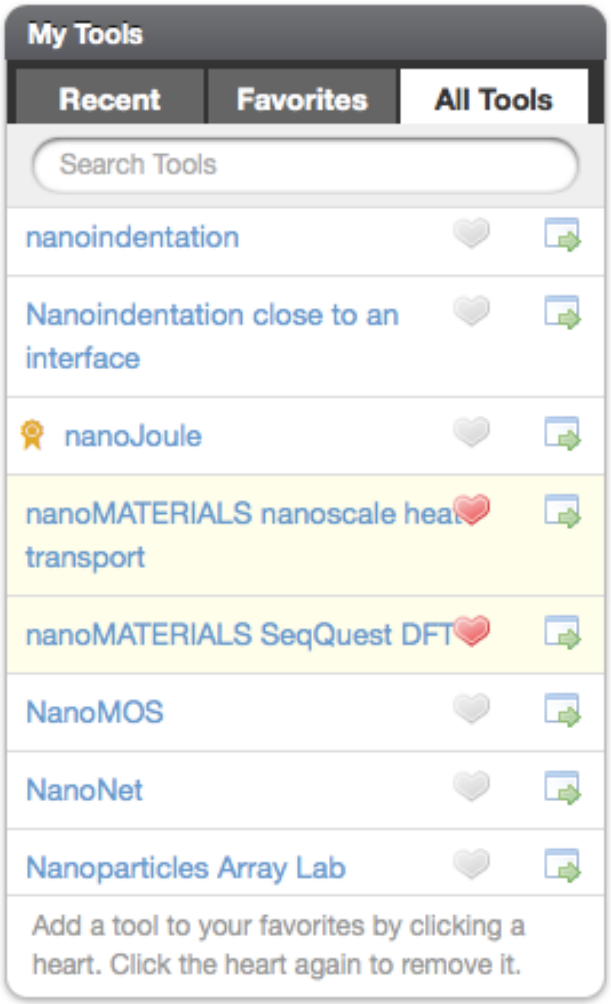
Key results

Thermal conductivity vs. superlattice period for three specimen lengths



- Thermal conductivity decreases with decreasing period until it reaches a minimum, further reduction leads to an increase in thermal conductivity – this is well known
- For long specimens thermal conductivity of wires is smaller than thin films – this is expected due to surface scattering
- Reducing specimen length reduces thermal conductivity – also well known – but the decrease in thin film is much more marked -> key result of the paper
- For short specimens thermal conductivity of thin films is predicted to be smaller than that of nanowires – surprising & interesting

The simulation tool



From the tools menu launch "nanoMATERIALS nanoscale heat transport"

About the tool:

Build nanoscale semiconductor samples and heterostructures and compute their thermal transport using MD

Learn more about MD:

- nanoHUB-U course "Atoms to Materials" https://nanohub.org/courses/FATM
- https://nanohub.org/topics/MD

and thermal transport

- nanoHUB-U course "Atoms to Materials" https://nanohub.org/courses/FATM

What we will do

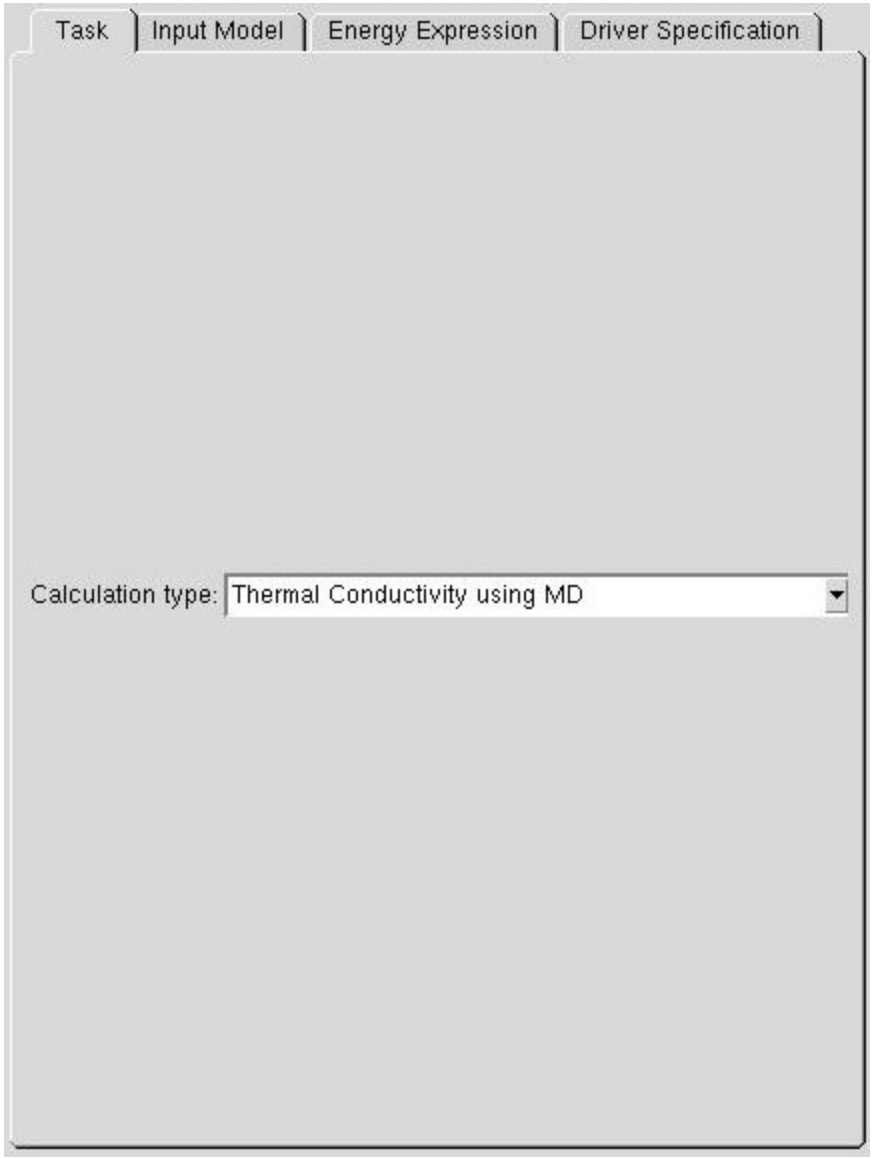
Objective

Build heterostructures and compute their thermal conductivity

Approach

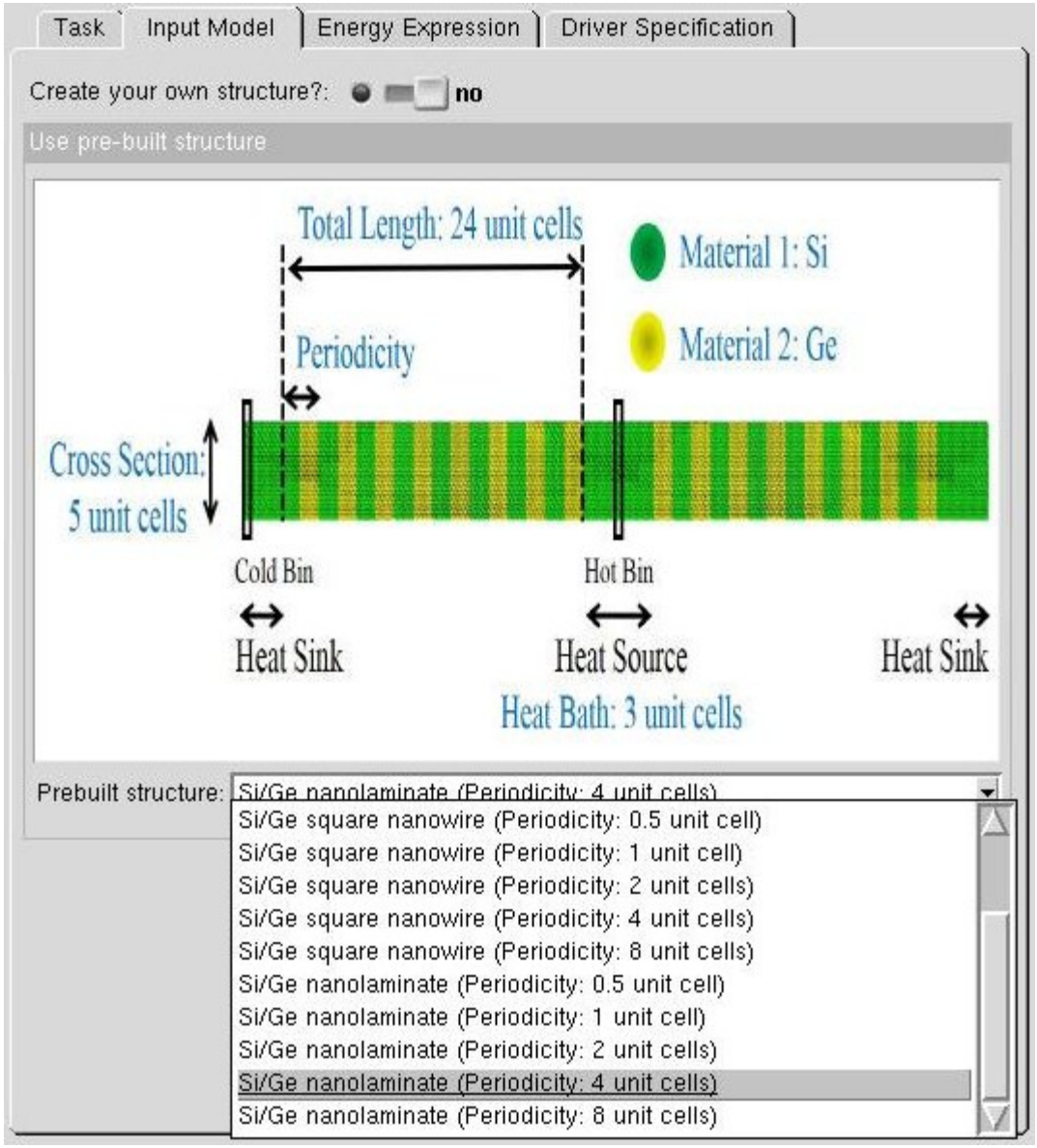
- Thermal conduction using MD simulations in LAMMPS
  - http://lammps.sandia.gov
- Use a method by Müller-Plathe to compute thermal conductivity
  - F. Müller-Plathe, J. Chem. Phys. 106, 6082 (1997).

Setting up the simulation



The default calculation type is set to thermal conductivity, so move on to the “Input Model” tab

Setting up the simulation

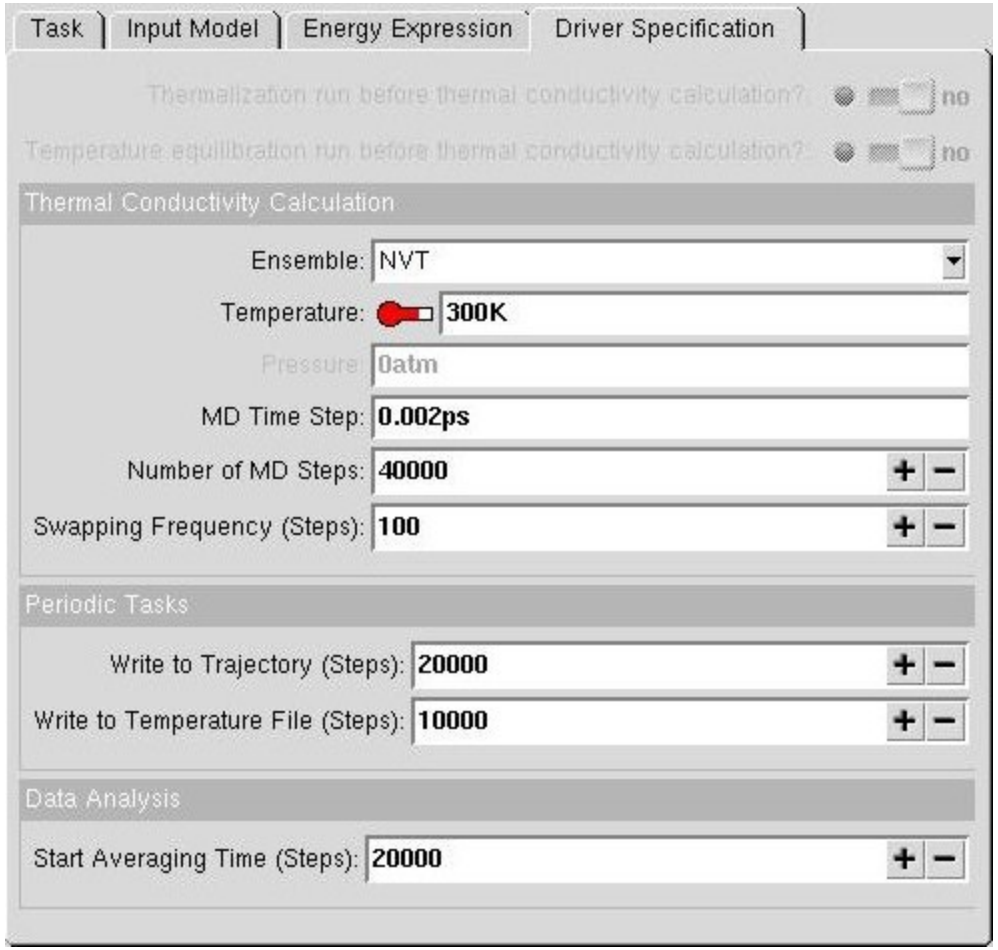


The tool supplies prebuilt structures for square nanowire and nanolaminate simulations

Each prebuilt structure has the same specimen length (29.32 nm) but varies in periodicity

Running one simulation for each prebuilt structures will generate the data needed to plot thermal conductivity vs. periodic length

Setting up the simulation



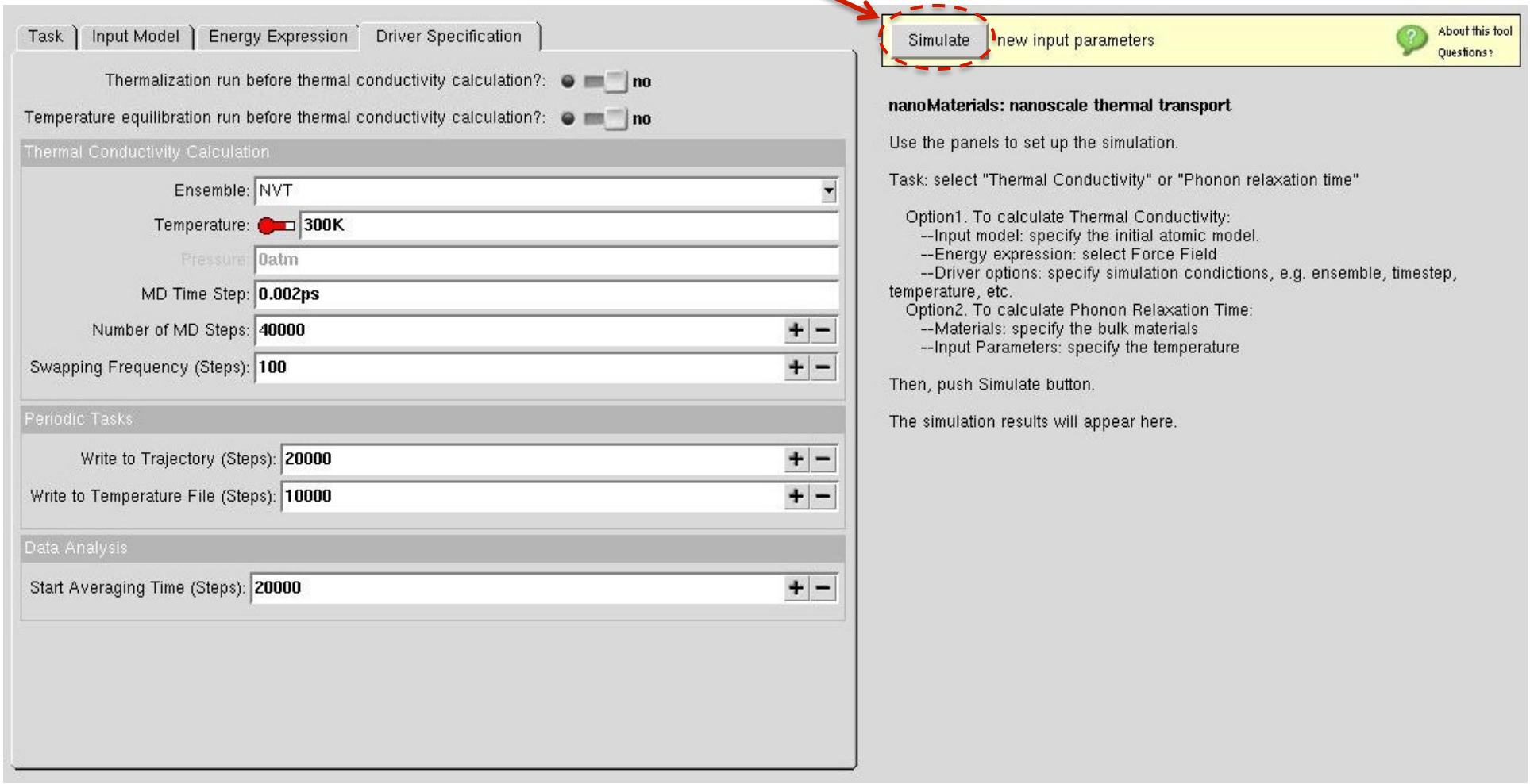
The “Energy Expression” tab can be skipped as it only shows the use of the Stillinger-Weber interatomic potential

The “Driver Specification” tab lists MD simulation parameters that can be adjusted if desired, but can be left as is

For improved results, increase the “Number of MD Steps” to 100,000 and set the “Start Averaging Time” to 50,000. This will give the give the specimen more time to reach steady-state and increase the amount of averaging points, but at the cost of a longer simulation

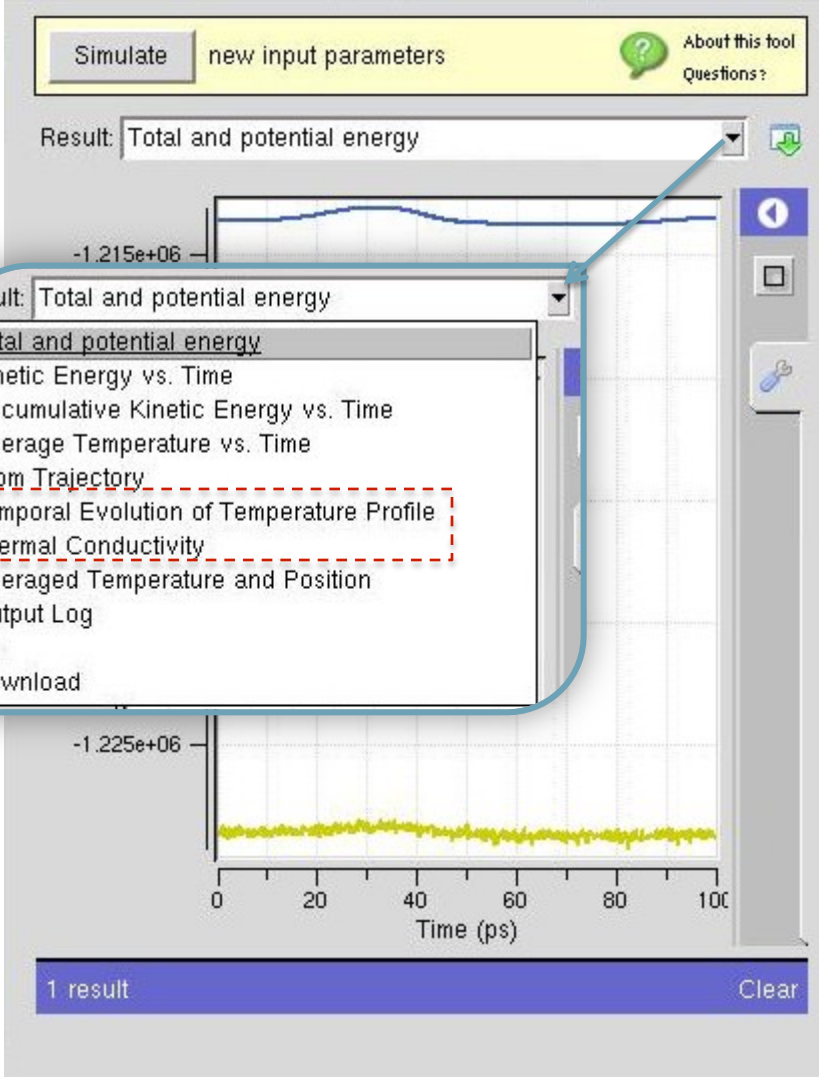
Running the simulation

Click “Simulate” to begin the simulation



Allow for 1-4 hours for the simulation to run

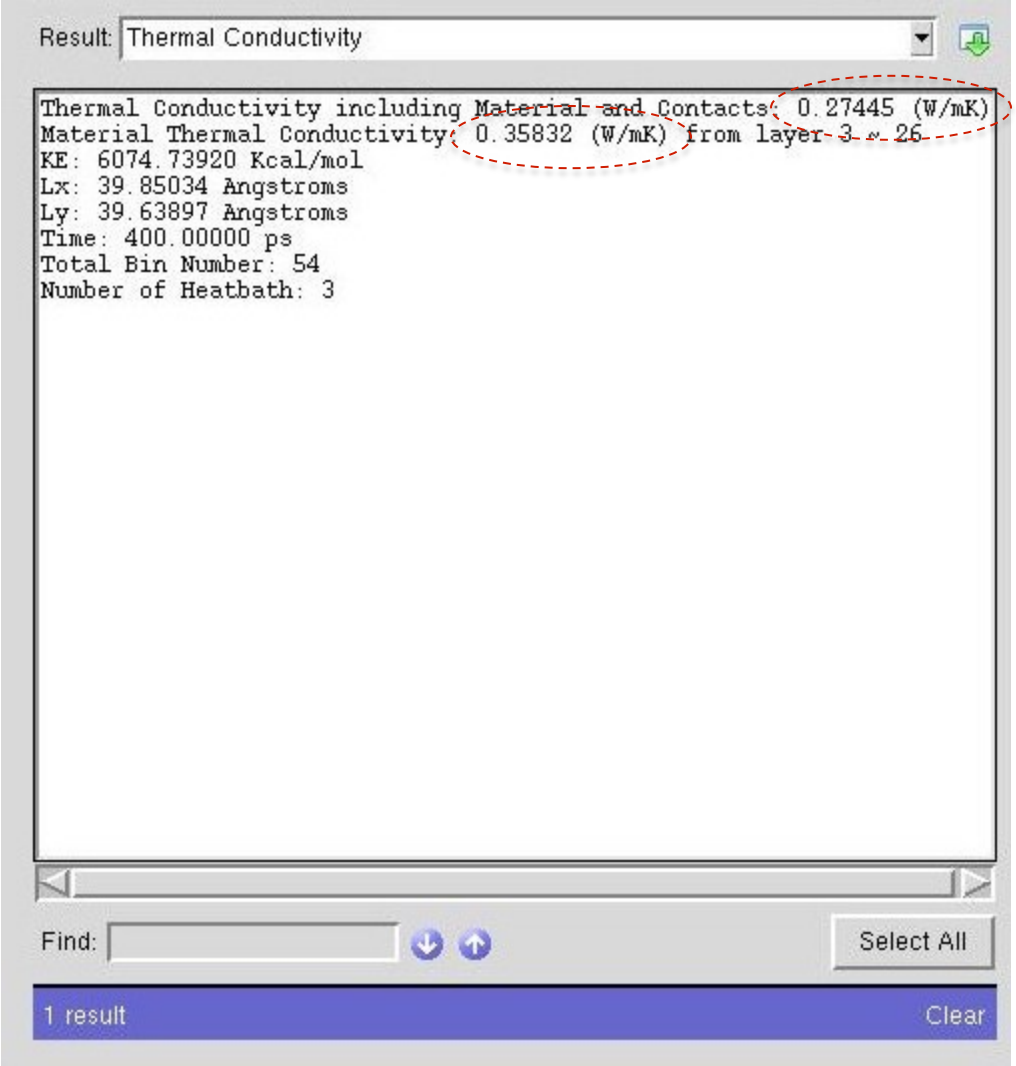
Viewing the output



Once the simulation finishes, the simulation results panel will appear

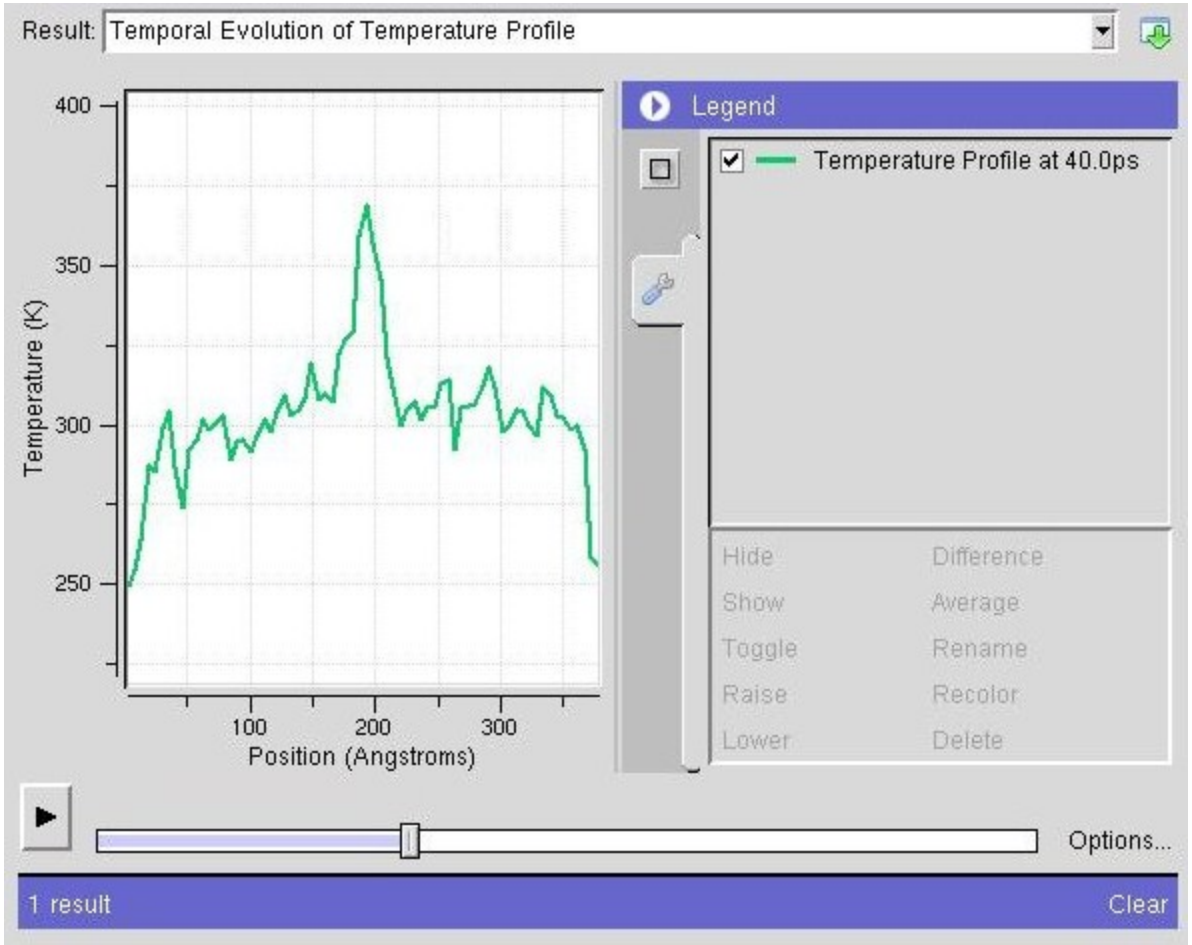
The “Thermal Conductivity” page contains the results of interest, and the “Temporal Evolution of Temperature Profile” page is useful to view

Viewing the output



The “Thermal Conductivity” page gives the κ values for the material with contacts and for just the material

Viewing the output



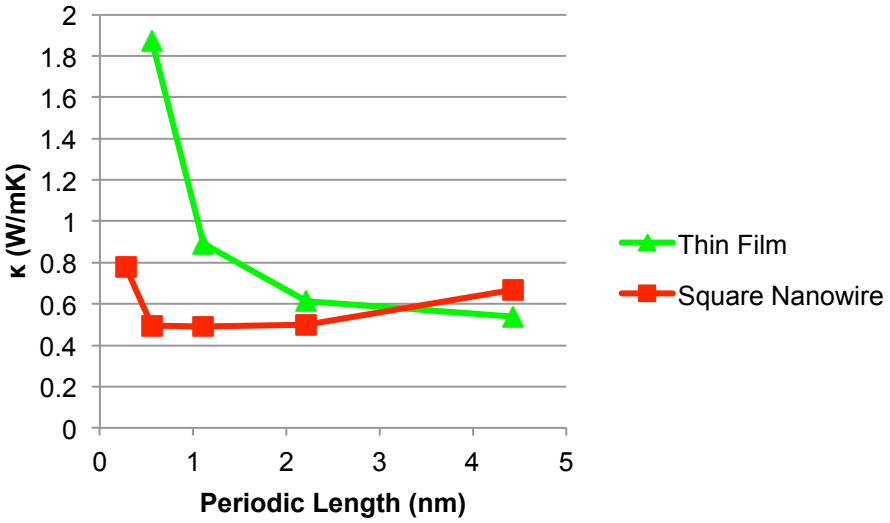
The “Temporal Evolution of Temperature Profile” page depicts the temperature profile of the specimen at periodic timesteps, which can be set as one of the simulation parameters. The slider at the bottom is used to cycle through the profiles

Looking at the temperature profiles reveals when the specimen reaches steady-state within the simulation

Analyzing the data

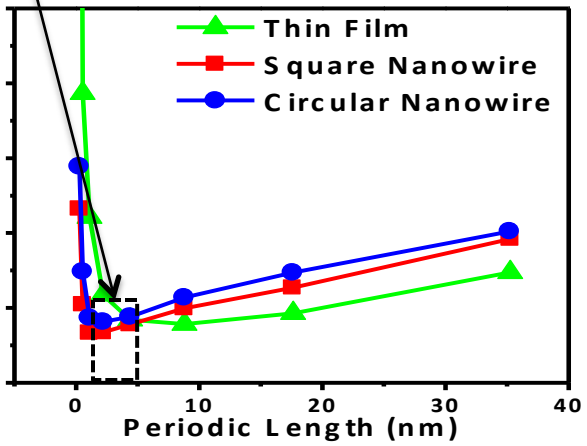
By collecting and mapping the thermal conductivities for each of the prebuilt structures, the following curves are generated:

29.32 nm



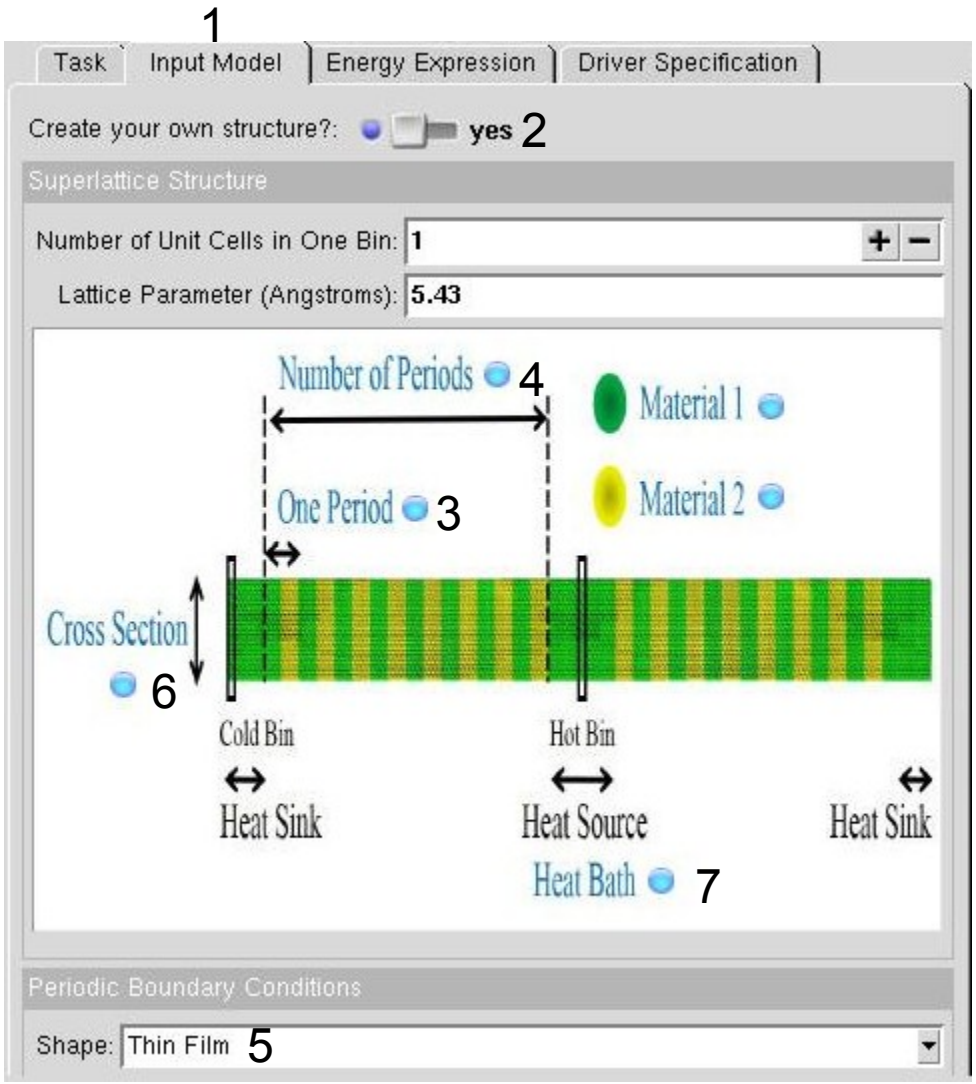
These results correspond to this portion of the graph provided in the paper

35.21 nm



Similar behavior of the two curves is clearly seen, as the thin film thermal conductivity becomes greater than the square nanowire thermal conductivity at lower periodic lengths

Creating additional structures



To simulate longer SiGe structures, as used in the paper, go back to the "Input Model" tab (1) and click "Create your own structure" (2)

Use the "One Period" hotspot (3) to define the number of bins of each material per period

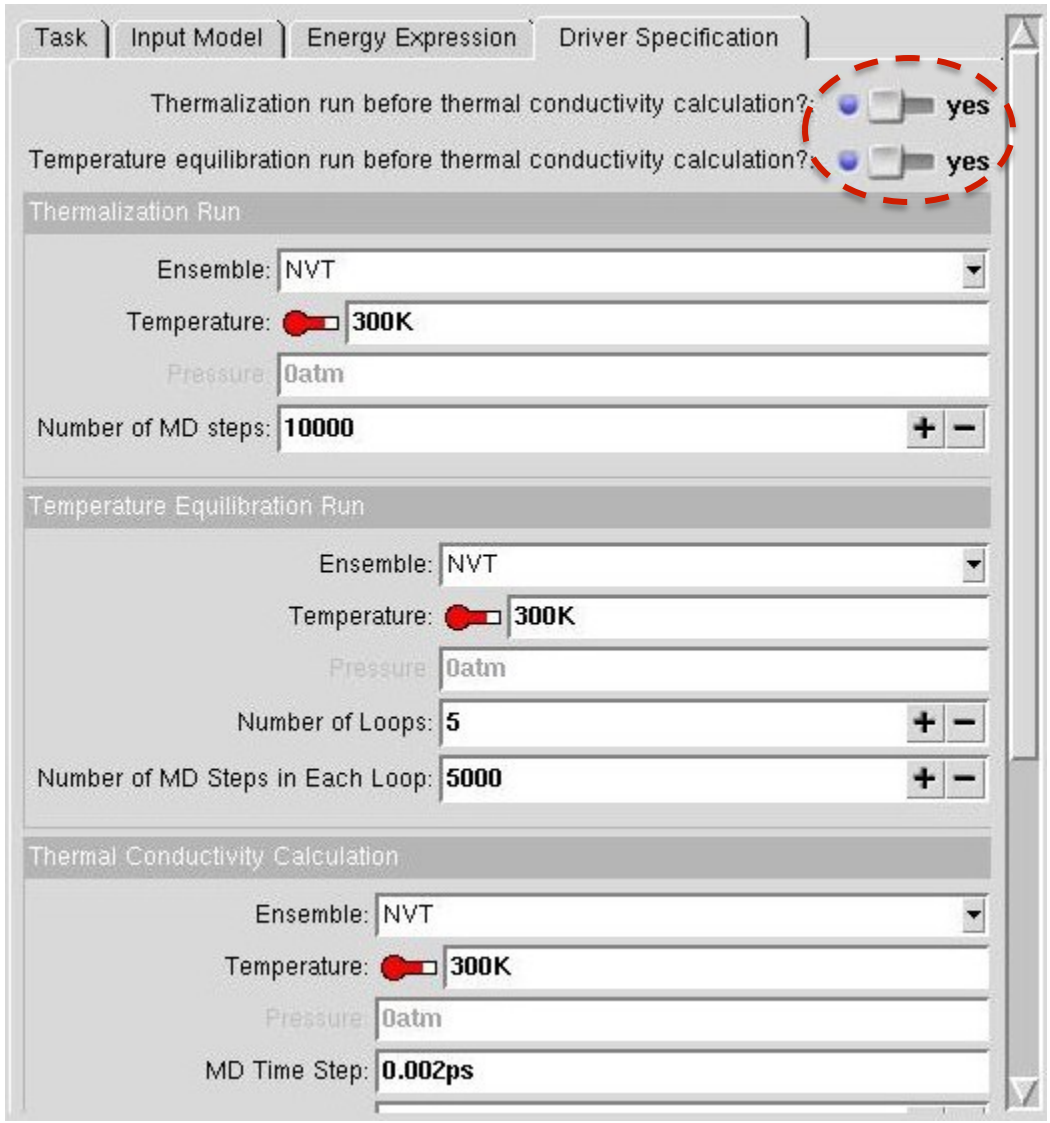
Use the "Number of Periods" hotspot (4) to adjust the total length of the structure

Use the "Shape" option (5) at the bottom is the option to choose between thin film (nanolaminate) and square nanowire structures

The "Cross Section" (6) and "Heat Bath" hotspots can also be adjusted if desired (7)

Specimen length = 2 x (number of periods x periodic length + length of heat bath)

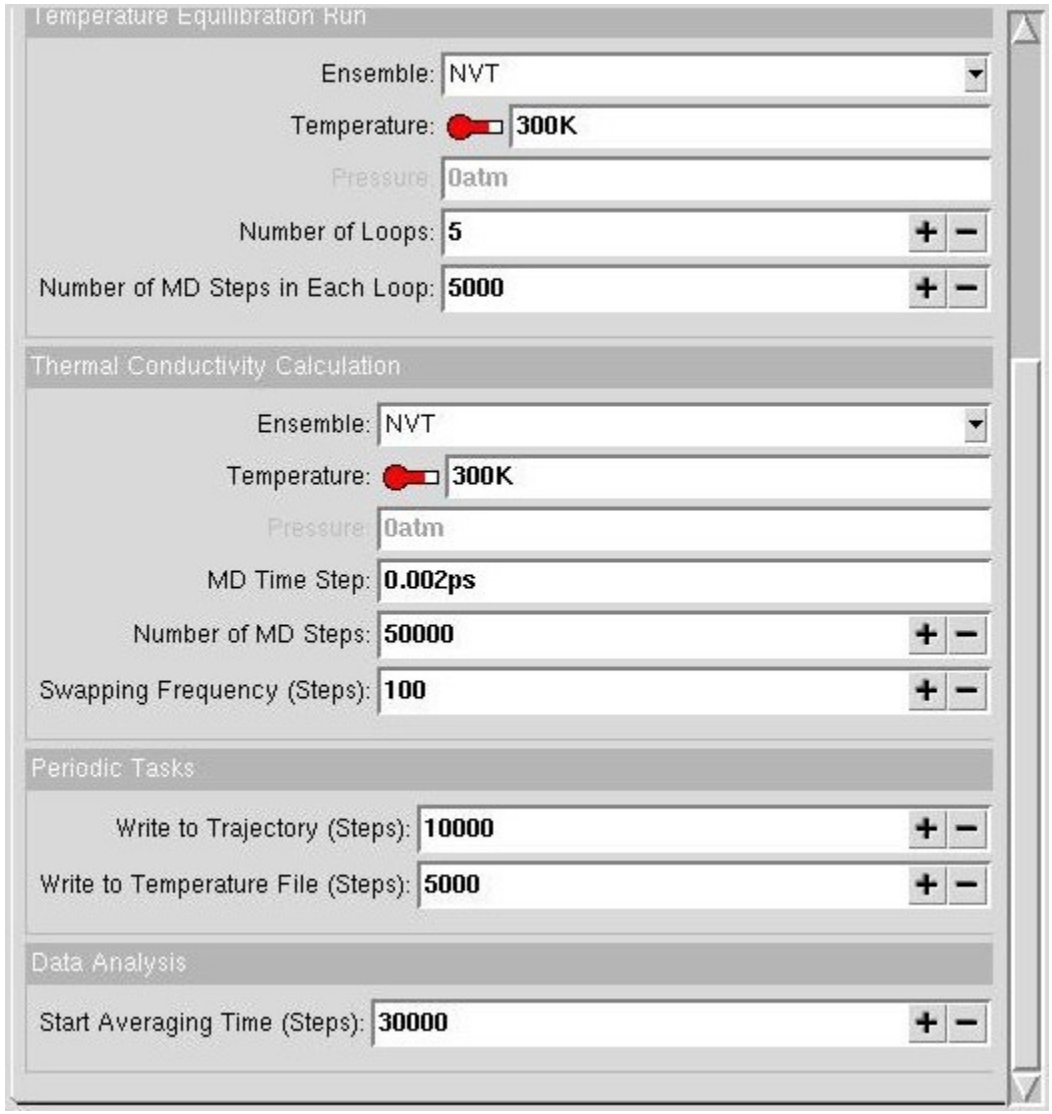
Simulating created structures



Unlike the prebuilt structures, every newly generated structure needs to undergo thermalization and temperature equilibration as part of the simulation, so these options should be switched to 'yes' under the "Driver Specification" Tab

The default parameters for thermalization and temperature equilibration need only be adjusted if desired

Simulating created structures



The remaining simulations parameters can be left at their default value, or can be adjusted for improved, but longer, simulations

The “Start Averaging Time” needs to be sufficiently large for the specimen to reach steady-state before averaging begins (> 40ps)

The “Number of MD Steps” needs to be sufficiently larger than the “Start Averaging Time” to generate a large number of data points (usually at least 40ps greater)

Once the parameters are set, begin the simulation.