

# Two-temperature Nonequilibrium Molecular Dynamics Simulator

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*A User's Guide*

## Introduction

The **Two-temperature Nonequilibrium Molecular Dynamics Simulator** is a C/C++ based software powered by the LAMMPS Molecular Dynamics Simulator<sup>1</sup> and the RAPPTURE<sup>2</sup> (Rapid Application Infrastructure). First-time users on MD simulation can conduct the two-temperature non-equilibrium molecular dynamic simulation by launching this tool (*tmmmd*) on nanoHUB.org. It has an illustrative graphical interface which simplifies the data input process. The tool can post processing output data such as calculating the interfacial thermal resistance of heterojunctions or thermal conductivity of homogeneous structures. Users can obtain useful results including the electron and phonon temperature profile, temperature/pressure evolution history, and the interfacial thermal resistance, etc. Before move on to the features and technical details of this tool, let's take a brief look at three terminologies firmly related to our tool.

## What is nanoHUB?

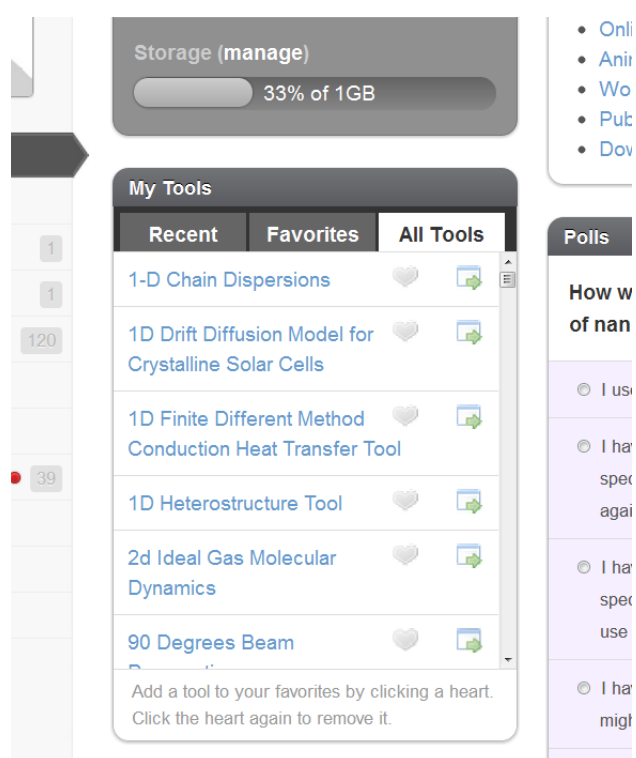
nanoHUB is a science and engineering gateway comprising community produced by Network for Computational Nanotechnology(NCN). NCN is a multi-university initiative of eight member institutions including Purdue University, the University of California at Berkeley, the University of Illinois at Urbana-Champaign, Massachusetts Institute of Technology, the Molecular Foundry at Lawrence Berkeley National Laboratory, Norfolk State

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<sup>1</sup> <http://lammps.sandia.gov/>

<sup>2</sup> <https://nanohub.org/infrastructure/rappture/>

University, Northwestern University, and the University of Texas at El Paso. It contributed resources for nanotechnology simulation tools, educational applications and professional networking. The official website for nanoHUB is <https://nanohub.org>. Users can access our tool by logging into nanoHUB, where first-time users are required to create an account (free) and then load our two-temperature non-equilibrium MD simulation tool (*tmmmd*) from the All Tools list as shown below. A faster way may be using the “searching” function and using two-temperature, or MD, as keywords.



## What is RAPPTURE?

RAPPTURE (Rapid application infrastructure) is a toolkit for developing powerful scientific applications provided by NCN nanoFORGE. The RAPPTURE graphical user interface objects are described in Extensible Markup Language (XML). The underlying simulator can be written in C/C++, Fortan, MATLAB/Octave, R, Java, Perl, Python, or Tcl. In our tool, C/C++ and Python languages have been used. RAPPTURE also makes it easier to put a friendly and interactive user interface on existing simulation applications such as LAMMPS.

## **What is LAMMPS?**

LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) is a classical molecular dynamics open source code distributed by Sandia National Laboratories. It can be used to model micro/nano scale systems. Our Two-Temperature Non-equilibrium Molecular Dynamics Simulation tool is powered by LAMMPS version 19-JUL-11 with some additional customized functions (the `fix_mttm` command for two-temperature nonequilibrium molecular dynamics simulation).

## **Features**

The **Two-temperature Non-equilibrium Molecular Dynamics Simulator** is totally web based. No installation is needed. With an interactive GUI, this tool reduces the complexity of the LAMMPS MD simulation progress, which shortens the learning curve for MD learners. New users can conduct the Two-temperature Non-equilibrium Molecular Dynamics Method on several different systems, e.g., pure copper system, silicon-copper system, carbon nanotube-copper system, graphene-copper system, etc. There are also four build-in examples which are recommended to first time users to try before using their own structures.

The whole simulation process is mainly divided into three phases: input phase, LAMMPS running phase and output phase. In the input phase, users can tune the simulation environment by modifying input parameters directly on the RAPPTURE GUI. In the LAMMPS running phase, the customized LAMMPS is running in the `ncn-hub@coates` server remotely. In the output phase, the users can check and download the results.

## **Input parameters**

The input parameters are categorized into five groups:

- Lattice Structure

- Dimension Parameters
- Thermal Control
- Step Parameters
- TTM Parameters

Users can modify the input parameters in each category by clicking the corresponding tabs. Parameter specificity is listed in the table below:

**Table 1: Input Parameters**

TAB LABEL	INPUT PARAMETER LABEL	UNIT	DESCRIPTIONS
Lattice Structure	Input coordinate file or examples	N/A	Upload or choose the build-in input coordinate files by a drop-down list. Note that metal should always be placed on the right side, and nonmetal on the left side in coordinate file.
	Element choice	N/A	Choose the corresponding input elements.
	Input coordinate file	N/A	Display the uploaded or build-in input coordinate file. Modifications can also be made here. (Please follow the format of the example coordinate files if you want to create your own.)
	Cross-sectional area	Å <sup>2</sup>	The cross-sectional area of the free system
Dimension parameters	fx_min	Å	The x coordinate of the left edge of the free system
	fx_max	Å	The x coordinate of the right edge of the free system
	X_interface	Å	X coordinate of the interface. Note that this value should equal to fx_min for the Pure copper case. This might be useful for studying the thermal rectification effect, if any.
	Cold/Hot region choice	N/A	Determine Cold/Hot region on which side of the system, which might be useful for studying thermal rectification effects.
	W_cold	Å	Width of the cold bath
	W_hot	Å	Width of the hot bath
Thermal Control	Average temperature	Kelvin	The average temperature of the whole system
	Heat current	eV/ps	The heat current flowing through

			the system.
Step Parameters	Number of NPT steps	N/A	The simulation steps for NPT stage which relax the system to the desired temperature
	Time step interval	ps	The time interval between steps
	Number of NVE steps	N/A	The simulation steps for NVE stage which is for data production after system reaches steady state.
TTM Parameters	Enable TTM?	N/A	Enable the TTM-MD function by checking this; or only conventional phononic MD is conducted.
	Electronic Thermal Conductivity	eV/(ps·Å·K)	Thermal conductivity of electrons
	Electron-phonon coupling factor	g/(mol·ps)	Friction coefficient due to electron-phonon interactions; its relation to the more commonly used electron-phonon coupling constant, $G$ , can be found in detail in <i>D M Duffy and A M Rutherford, J. Phys.: Condens. Matter, 19, 016207-016218 (2007)</i>
	Number of finite element nodes in the x direction	N/A	Discussions on appropriate choice of this parameter can be found in <i>Yan Wang, Xiulin Ruan, and Ajit K. Roy, Phys. Rev. B 85, 205311 (2012)</i>

## Outputs

Three figures are plotted after the customized LAMMPS generates output files and the post-processing codes finish their work: the temperature profile, and the temperature and pressure evolution history.

In the temperature profile, total system temperature is represented by scattered blue points. Best fit lines are generated based on the central parts of the scatter plots. Electron temperatures are shown as scattered red symbols when the TTM-MD function is enabled. The temperature and pressure evolution show the temperature and pressure variations during the NPT stage. The estimated interfacial thermal resistance of the Si-Cu and CNT-Cu systems and the estimated thermal conductivity of the pure Cu are calculated and output. All these outputs mentioned above can be viewed and downloaded by selecting them from the drop down menu. We highly recommend the users downloading the temperature profiles `ls450.tempdist` and `ls450out.txt` to

extrapolate for the interfacial temperature drop and calculate the interfacial thermal resistance on their own.

## Default Simulation Results

- **Pure Cu case**

Figure 4 is the temperature profile (temperature vs. x-axis output plot) for the example homogeneous copper system. The default input values are:

Average temperature = 300 K

Heat Current = 2.4 eV/ps

NPT steps = 20000

Time step interval = 0.0008 ps

NVE steps = 100000

Electronic Thermal Conductivity = 0.05 eV/(ps · Å · K)

Electron-phonon coupling constant = 8 g/(mol · ps)

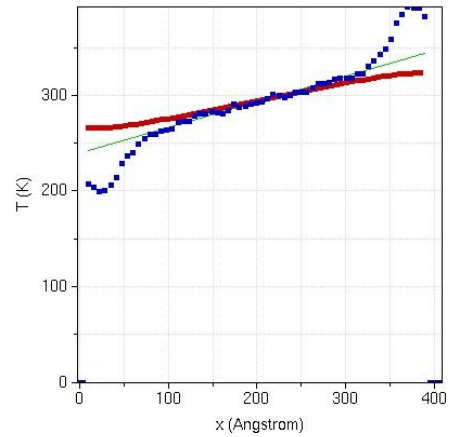


Figure 4: The output temperature profile for pure copper system

The electron-phonon non-equilibrium (temperature gap between the between the blue scatters and red scatters) can be seen at the boundaries. It is worth noting that the heat baths are only for phonons, while electrons are closed to the environment except having interactions with phonons when the TTM simulation is enabled. That's why the electron temperature at the two ends is different from phonon's.

- **Si-Cu (LJ) case**

The example silicon-copper system steady state profile is shown in Figure 5 with the default input values:

Average temperature = 450 K

Heat Current = 0.6 eV/ps

NPT steps = 30000

Time step interval = 0.0005 ps

NVE steps = 100000

Electronic Thermal Conductivity = 0.01  
eV/(ps · Å · K)

Electron-phonon coupling constant = 4.6904 g/(mol · ps)

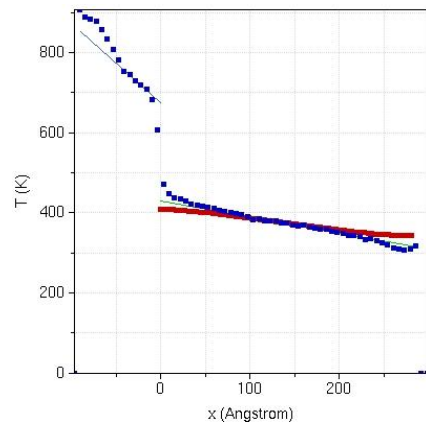


Figure 5: The output temperature profile for

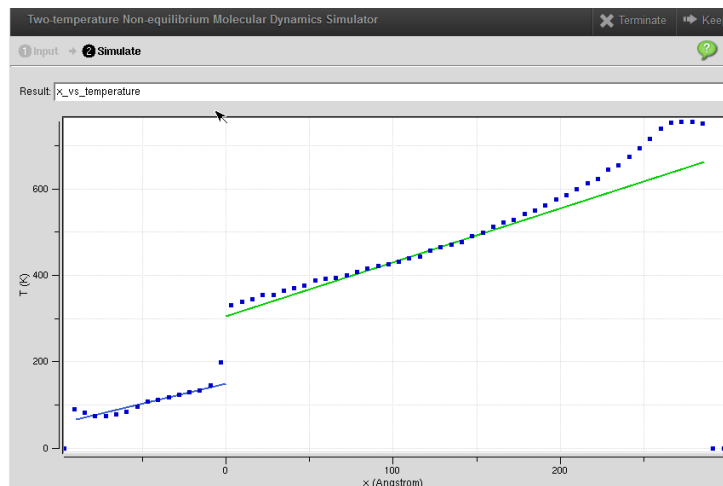
There's a temperature jump at silicon-copper interface. The electron-phonon non-equilibrium can also be found in regions adjacent to the interface on the metal side. There are analytical discussions on this electron-phonon non-equilibrium region, which is called cooling length, and can be found in detail in *Yan Wang, Xiulin Ruan, and Ajit K. Roy, Phys. Rev. B 85, 205311 (2012)*<sup>[4]</sup>

- **Si-Cu (LJ) case: effect of including electrons in the two-temperature model**

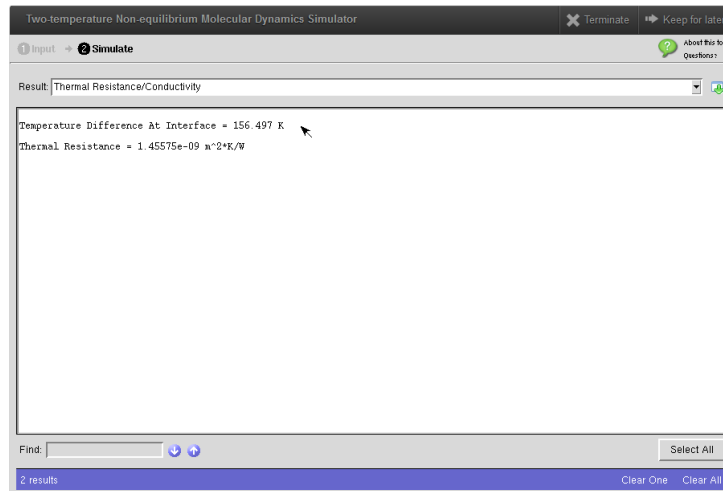
In the Si-Cu(LJ) case, we can change the simulation mode between conventional phononic MD and two-temperature electron-phonon coupled MD, through the “Enable TTM?” selection. Here let us do a simple comparison between these two modes.

- **Conventional Phononic MD: Unchecking “Enable TTM?”**

The temperature profile is given below, showing the phonon temperatures.

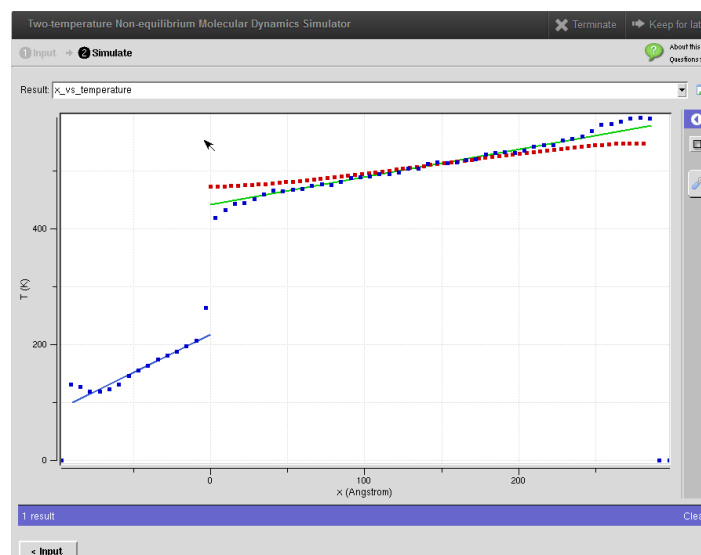


The tool can also export the interfacial thermal resistance directly, as shown below. The thermal resistance is  $\sim R_{INT} = 1.46 \times 10^{-9} \text{ m}^2 \text{ K/W}$ .



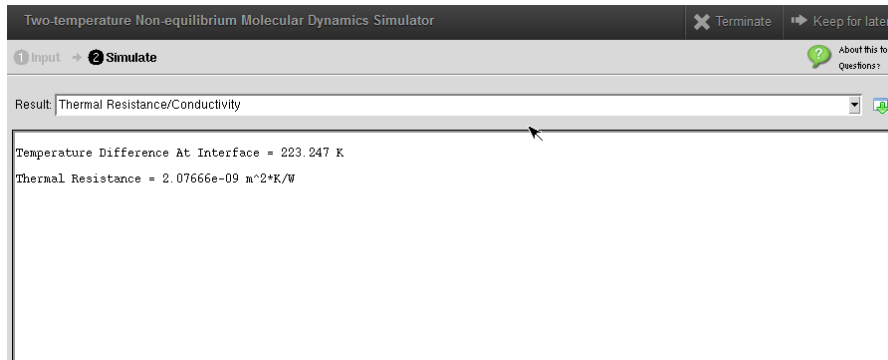
■ TTM-MD: Checking “Enable TTM?”

The temperature profile is shown below, where both electron (red symbols) and phonon (blue symbols) temperatures are shown. The slope of the electron temperature is zero near the interface, which means that electron energy cannot transport across the interface. On the other hand, the slope of the phonon temperature is large at the interface than away from it, which is because electrons at the interface must transfer their energy to phonons, and, hence, phonons are transporting more energy (higher slope) compare to other parts.





As can be seen from the output shown below, the interfacial thermal resistance from TTM-MD is  $R_{INT} = 2.08 \times 10^{-9} \text{ m}^2 \text{ K/W}$ .



Therefore, we find that  $R_{INT}$  from TTM-MD is higher than that from conventional MD, which is consistent with literature (Yan Wang, Xiulin Ruan, and Ajit K. Roy, *Phys. Rev. B* 85, 205311 (2012)).

## Limitations and Future Work

The current version only supports the simulation of very limited types of materials, e.g., Cu as the metal, and Si or C as the nonmetal. It is good to use the current version for systems like CNT/Cu, Si/Cu, Graphene/Cu, pure Cu, diamond/Cu, etc. More types of materials will be supported in future versions.

## References

- [1] nanoHUB – Web page from nanoHUB.org and nanoHUB Wiki  
<https://nanohub.org/infrastructure/rappture/>
- [2] LAMMPS Molecular Dynamics Simulator – Web page from LAMMPS homepage  
<http://lammps.sandia.gov>
- [3] RAPPTURE (**R**apid **a**pplication **i**nfrastructure) – Web page from NanoHUB.org  
<https://nanohub.org/infrastructure/rappture/>
- [4] Yan Wang, Xiulin Ruan, and Ajit K. Roy, *Phys. Rev. B* 85, 205311 (2012)