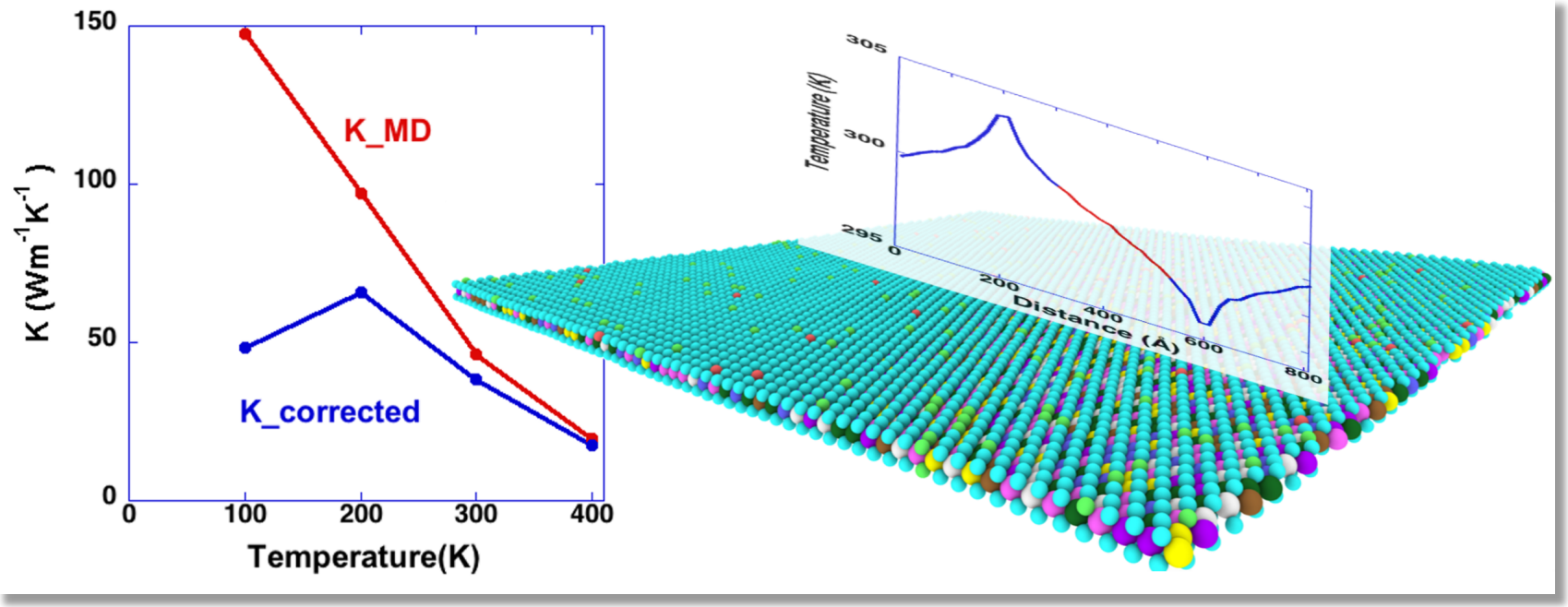
MAGICS Workshop
Thermal Conductivity Hands-On Session



Thermal Conductivity Plugins for LAMMPS used in this research was produced by USC MAGICS Center that is a part of the Computational Materials Sciences Program funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Award Number DE-SC00014607.

The goal of this session is to calculate DOS, C_v and thermal conductivity of 2-D materials with quantum correction

Configuring the Jupyter Notebook

- For our hands on session we will be using Jupyter Notebook.
- The advantage of doing this is that it lets us run jobs on the USC HPC cluster directly from our web browsers.
- Let us take a look at how we configure the Jupyter notebook.
- People with MacBooks can directly run it from the Terminal, however for people using windows we will be running it through PUTTY

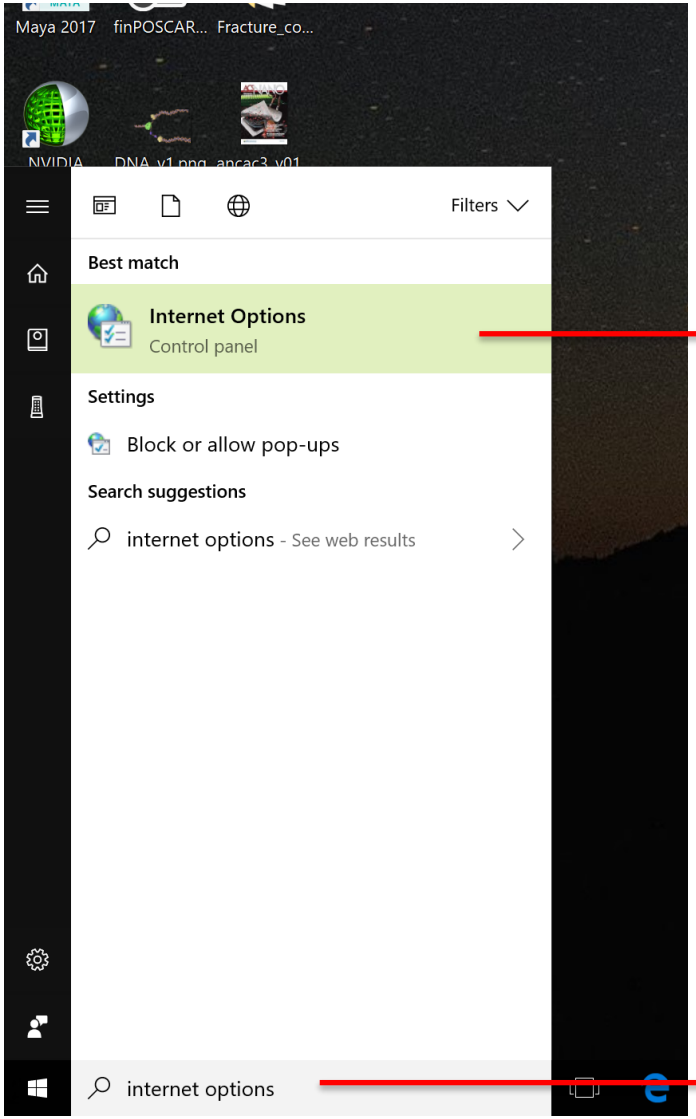
People with MacBooks, open terminal and type:

```
ssh -L localhost:89XX:localhost:89XX magicsXX@hpc-login3.usc.edu
```

Replace XX with last two
digits of your MAGICS Account

Enter your Password and you should be able to log into HPC.

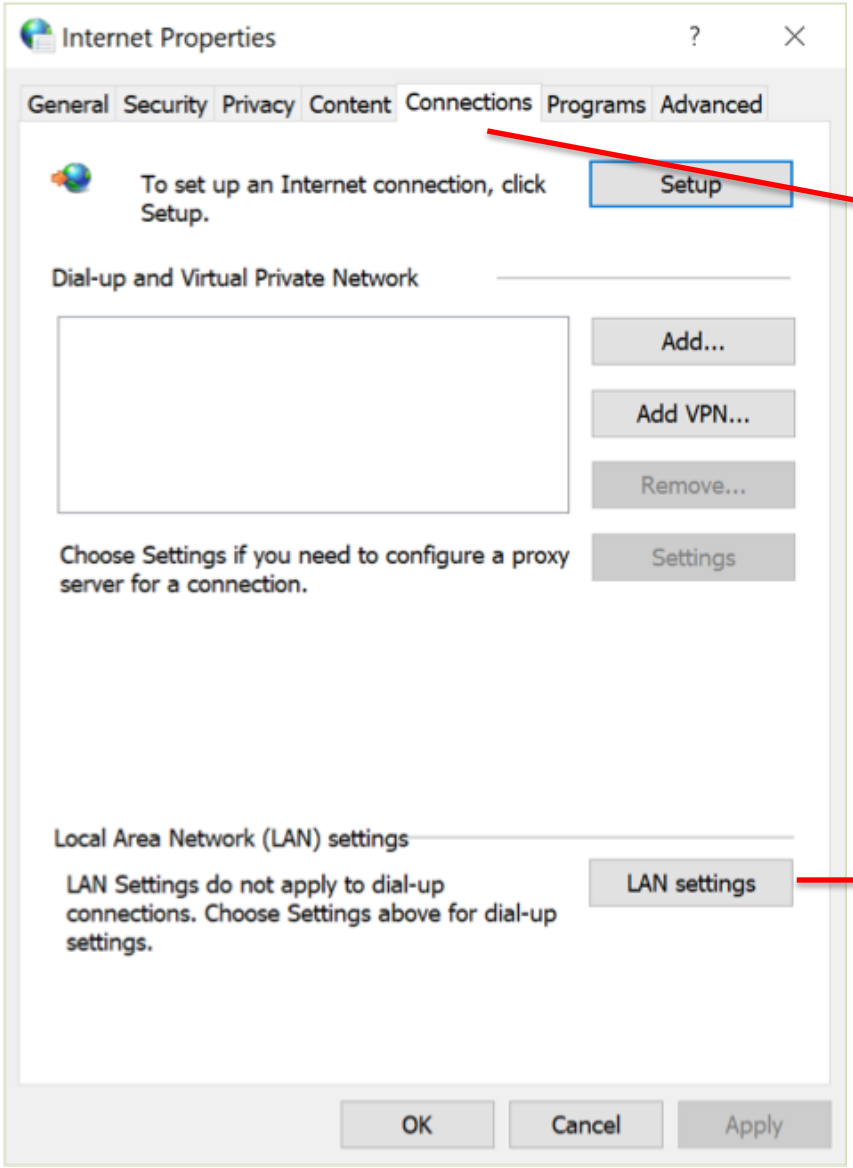
Setting up the Jupyter Notebook (Windows)



Click in Internet options

Type Internet options in your start menu

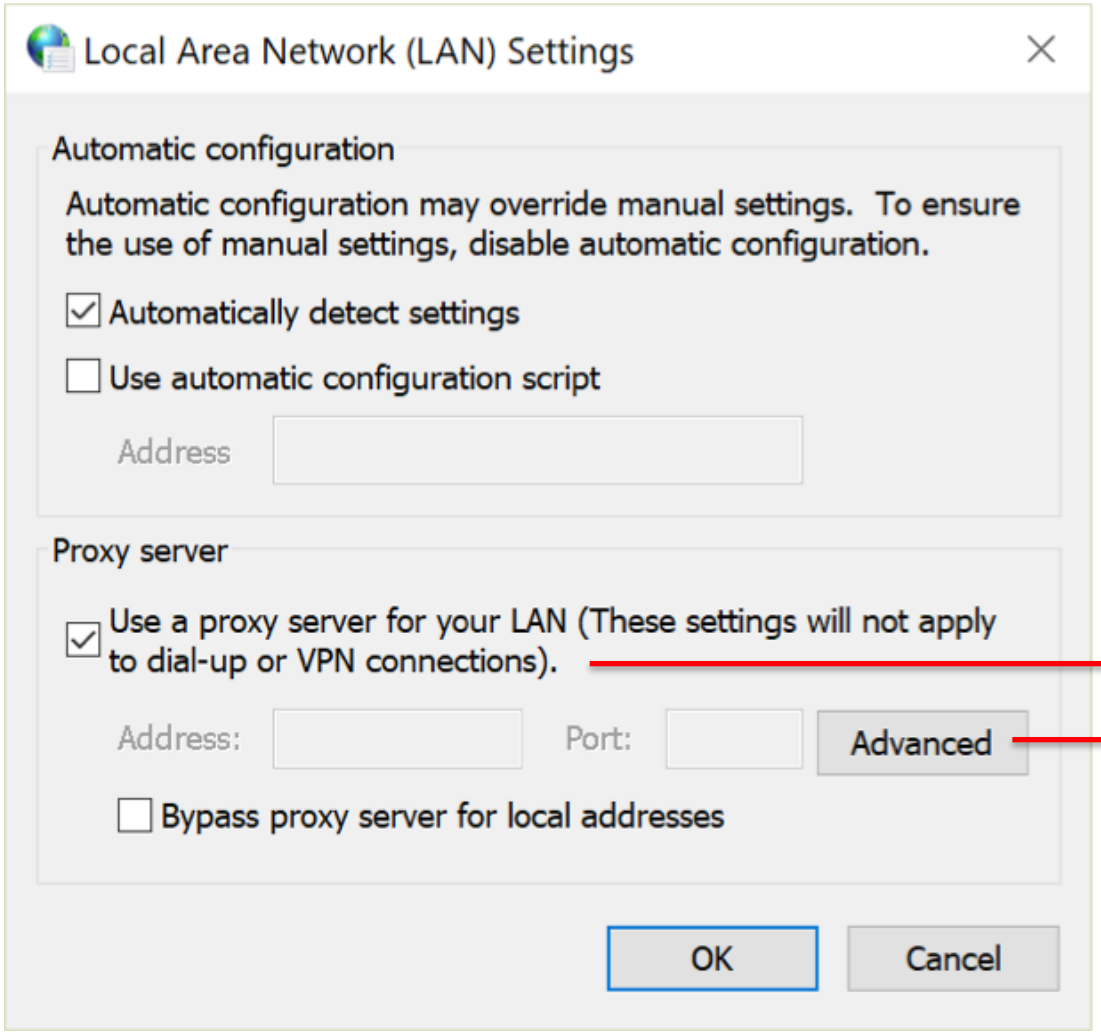
Setting up the Jupyter Notebook (Windows)



Click on Connections tab

Click on LAN Settings

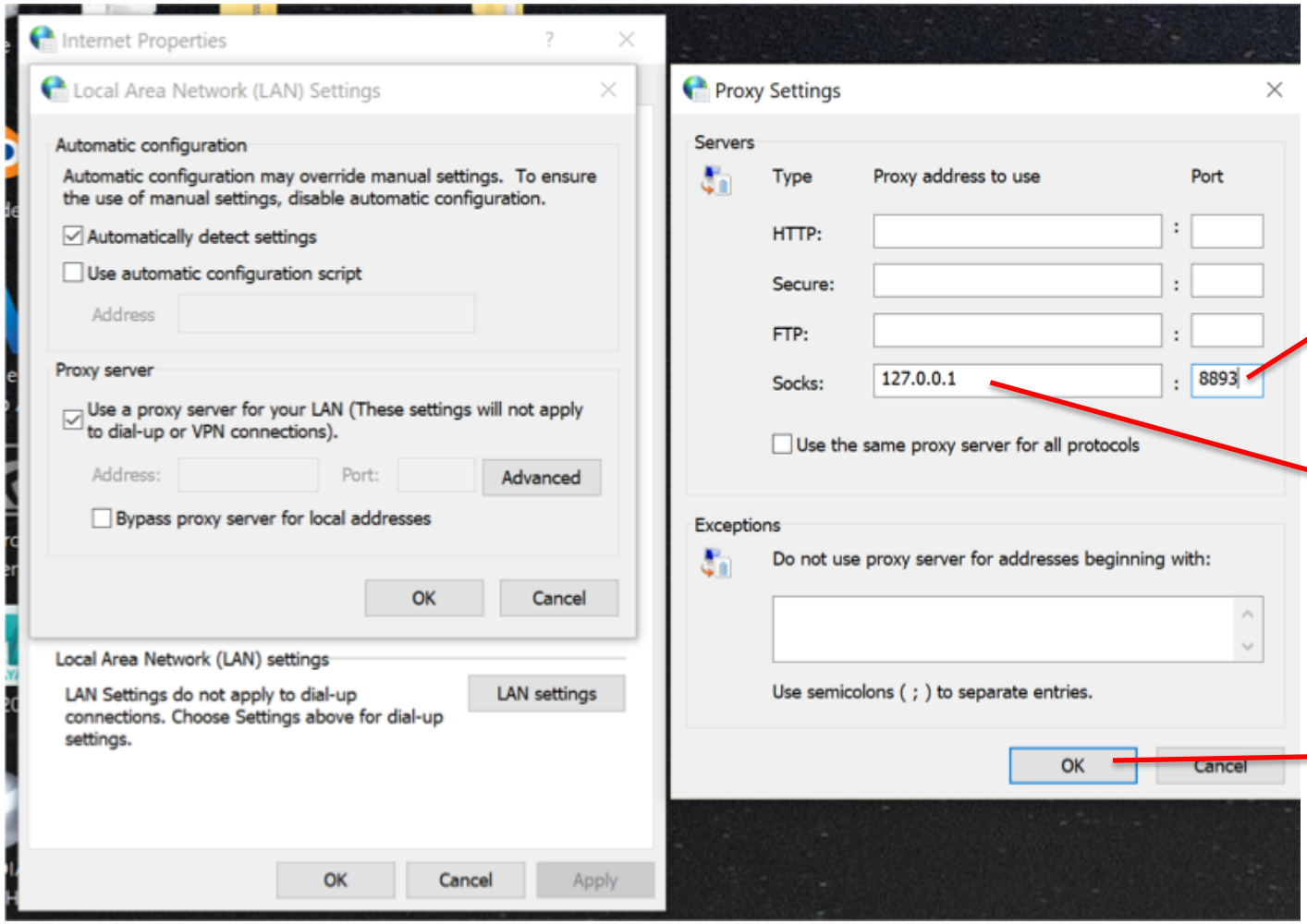
Setting up the Jupyter Notebook (Windows)



Check this box

Click on Advanced

Setting up the Jupyter Notebook (Windows)

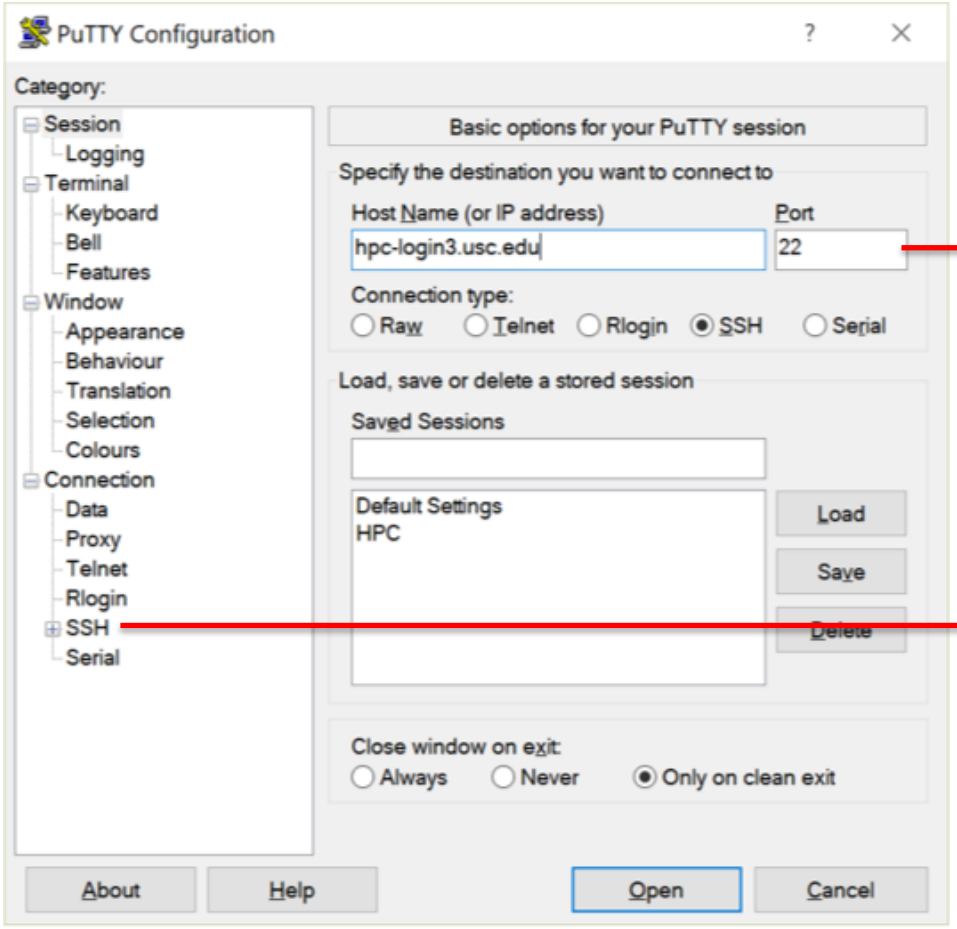


Replace 88XX with the last two digits of your MAGICS account

Enter 127.0.0.1 In the socks tab

Hit OK

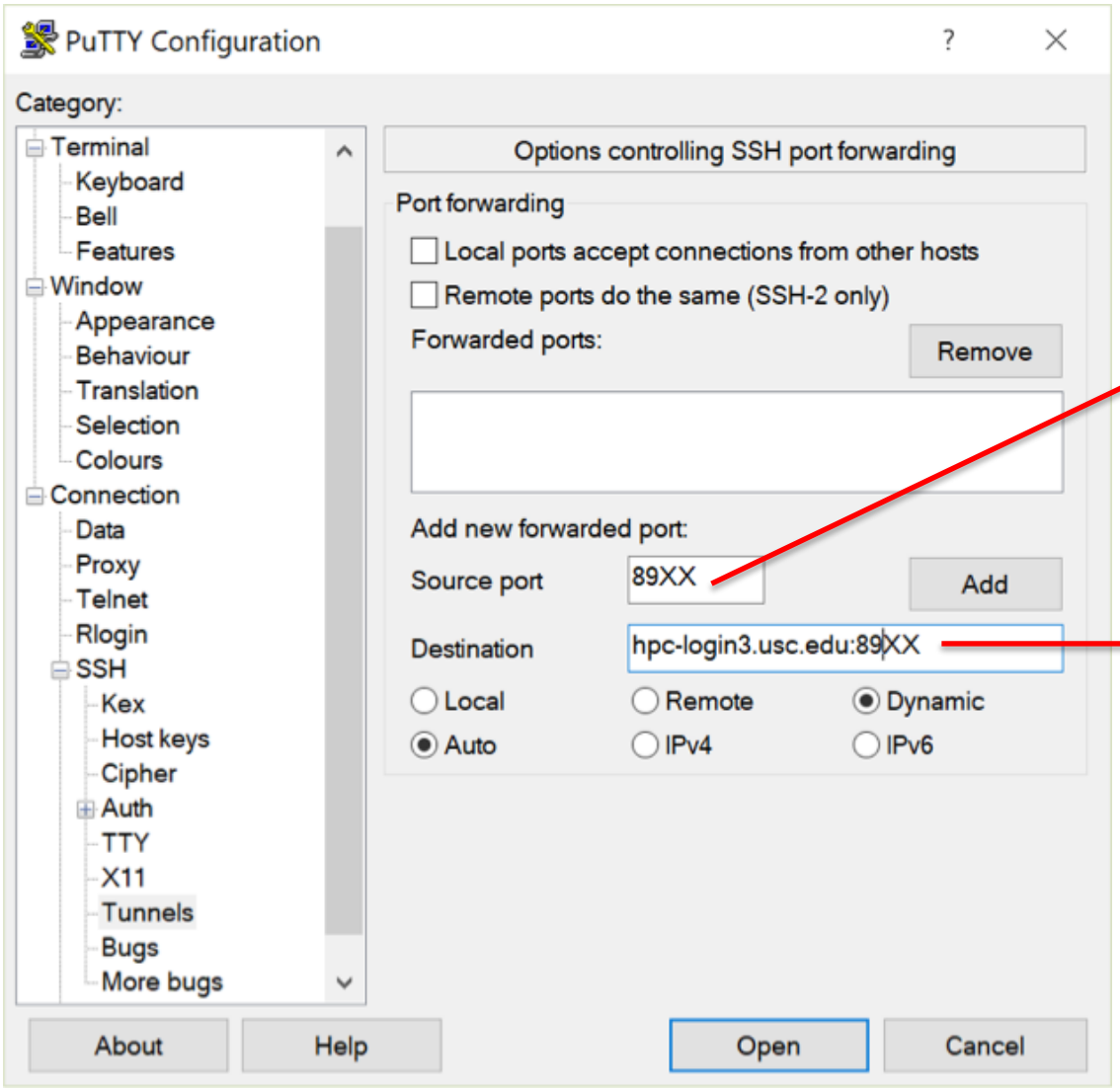
Setting up the Jupyter Notebook (Windows)



Make sure to enter the hostname as shown with the correct Port value

Click on the plus sign next to SSH

Setting up the Jupyter Notebook (Windows)

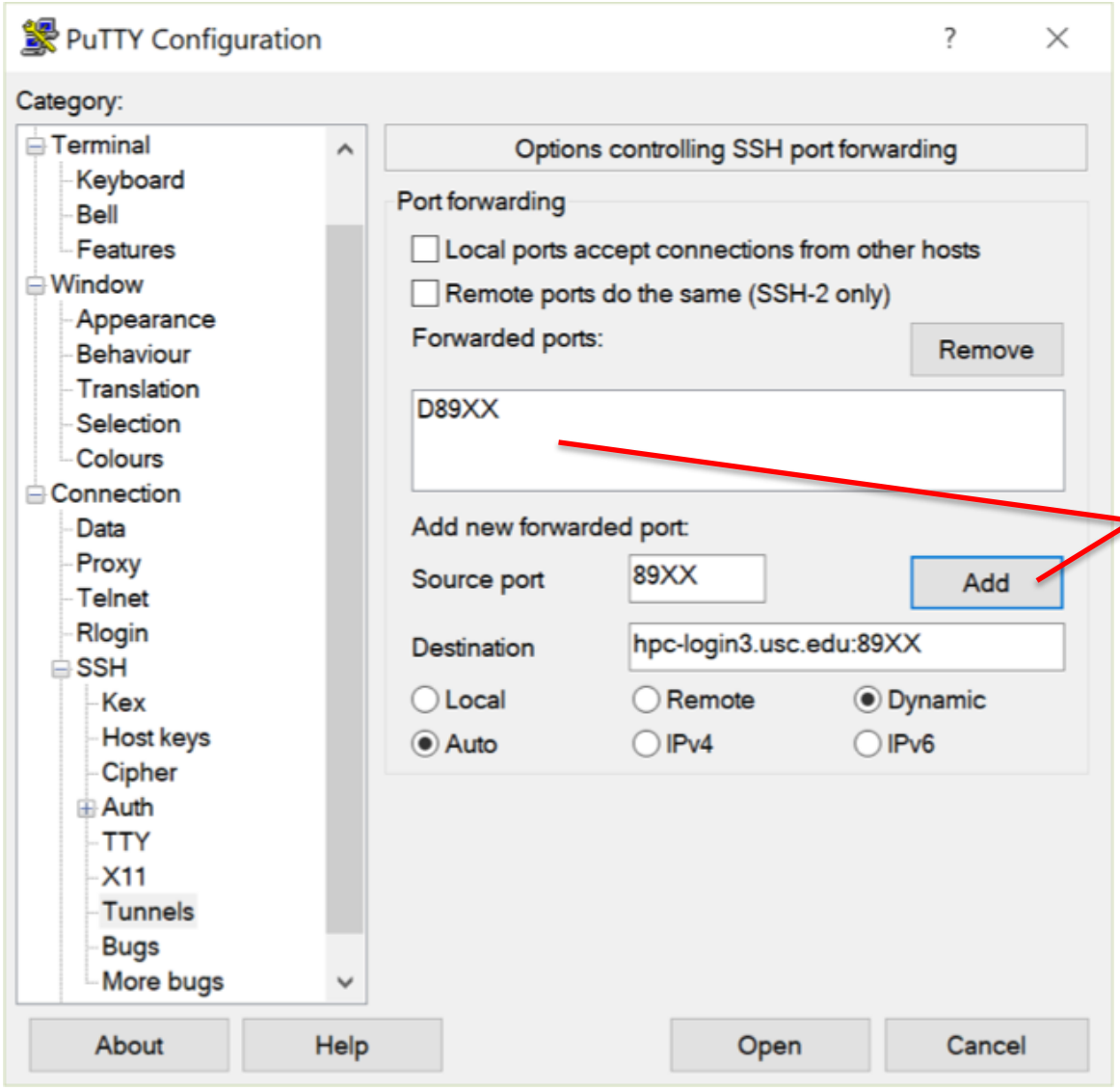


Make sure to replace XX with the last two digits of your MAGICS Account.

Example : if you're magics32 enter 8932

Do the same here. Replace XX with last two digits of you MAGICS account

Setting up the Jupyter Notebook (Windows)



Once you've replaced the XX with the last two digits of your MAGICS account Click ADD

Once you click Add you should be able to see your port appear here

Setting up the Jupyter Notebook

Once you log on to HPC navigate to the staging directory like so

```
cd /staging/magics18/magicsXX/Day1_Handson
```

Make sure to change XX to your MAGICS account number

Start a Python jupyter Notebook with the following command

```
jupyter notebook --no-browser --port=89XX
```

Make sure to replace XX with your MAGICS account number

Copy and Paste the link that the terminal throws up on to your browser.

Outline

- Thermal conductivity calculation in MoS_2
  - Length scaling
  - Temperature scaling
- PDOS, DOS and C_v calculation
- Quantum correction for thermal conductivity

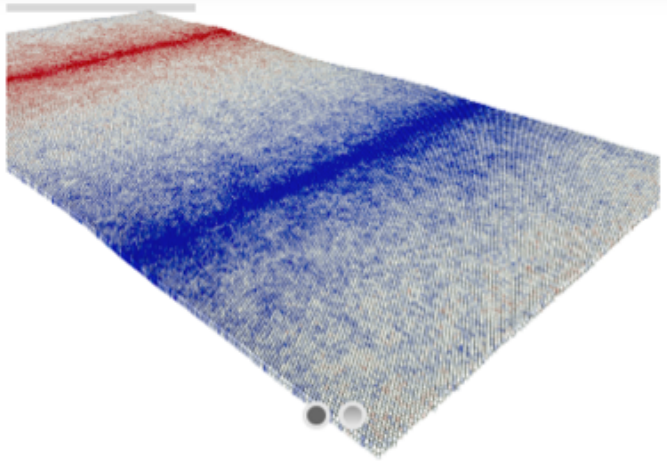
Software Download

LAMMPS Plugins for Thermal Conductivity Calculation

https://magics.usc.edu/thermal-conductivity-plugin/

Thermal Conductivity Plugins for LAMMPS

- Thermal conductivity with isotopes and quantum correction
- Velocity autocorrelation and Phonon Density of States using multiple initial conditions
- Specific heat from Phonon DOS as a function of temperature



Thermal conductivity tools is a series of plugins for thermal properties — velocity autocorrelation functions, phonon density of states, specific heat and thermal conductivity from MD using LAMMPS.

Software Download Links

SOURCE CODE

Thermal Conductivity Calculation

Phonon DOS and Specific heat

Documentation download

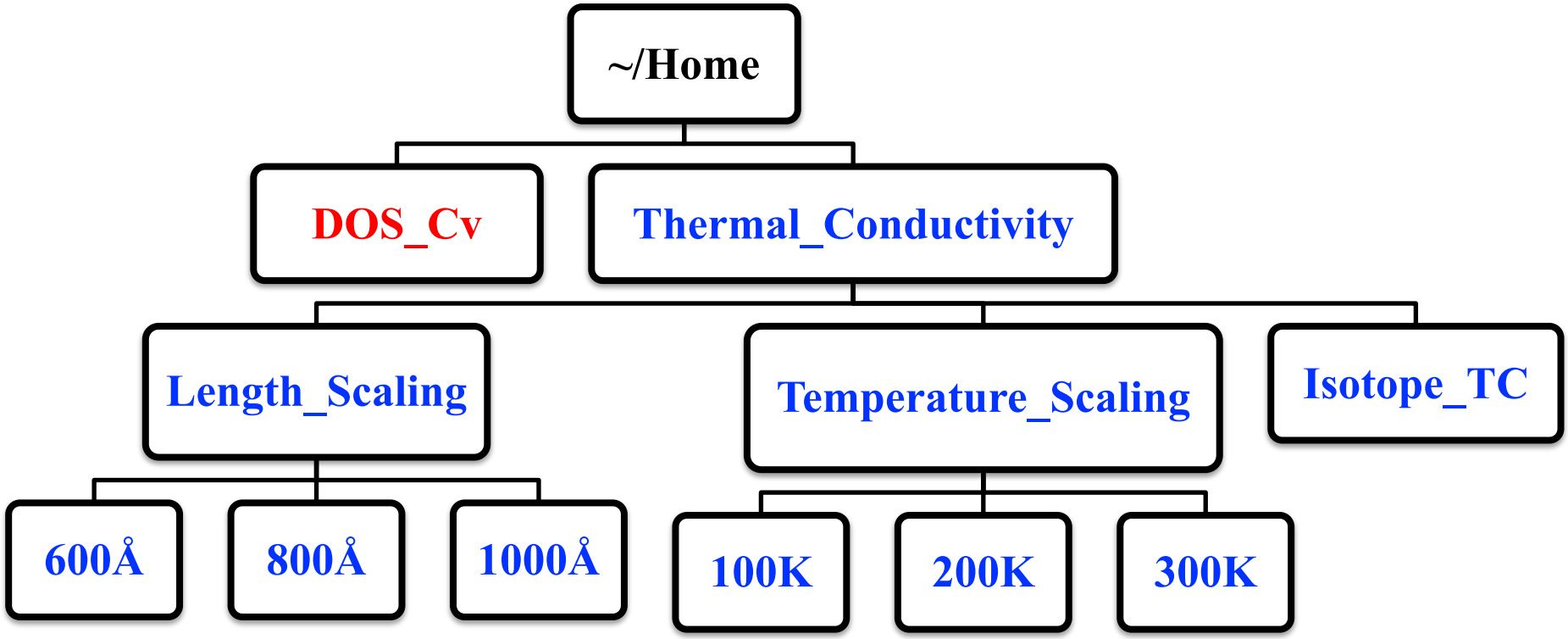
PDF of quick start guide can be downloaded here

Frequently Asked Questions

For frequently asked questions, please click here ?

LAMMPS Plugins for Thermal Conductivity

Contents of your Home Directory



LAMMPS Plugins for Thermal Conductivity

Each sub directory of Length_Scaling and Temperature_Scaling following files

1. **in.relax:** ***LAMMPS script to create a relaxed system at a given Temperature***
2. **in.heatflux:** ***LAMMPS script to for thermal conductivity calculation***
3. **in.variables:** ***Variable definitions that are used in the LAMMPS Script***
4. **MoS_2.data:** ***Input unit cell coordinate of MOS_2 monolayer***
5. **MoS_2.sw:** ***SW Interaction potential for MOS_2***
6. **MoS_2.restart:** ***Restart file to be used by LAMMPS.***
7. **job.pbs:** ***PBS file used to submit jobs to the HPC***
8. **calthermal_conductivity.py:** ***Python code to post-process LAMMPS data to compute thermal conductivity value***
9. **input.txt:** ***Input parameters for calthermal_conductivity.py***

First Set of Job Submissions

STEP 1: Go to Thermal_Conductivity folder in your home directory

```
cd ~/Thermal_Conductivity
```

STEP 2: Navigate to Length_Scaling folder

```
cd ./Length_Scaling
```

STEP 3: Navigate to 1000A folder

```
cd ./1000A
```

STEP 4: Submit your first Job

```
qsub job.pbs (qstat -u username to check status)
```

First Set of Job Submissions (Contd.)

STEP 1: Get back to Length_Scaling folder

```
cd ~/Thermal_Conductivity/Length_Scaling
```

STEP 2: Navigate to 800A folder

```
cd ./800A
```

STEP 3: Submit your second Job

```
qsub job.pbs (qstat -u username to check status)
```

Steps for Thermal Conductivity Calculation

Step 1: Create a relaxed system at Temperature = TK

use LAMMPS script: in.relax

Step2: Add/remove heat to/from the system for 10-12ns

use LAMMPS script: in.heatflux

Step3: Compute thermal conductivity

post process LAMMPS output file using calthermal_conductivity.py

LAMMPS Walkthrough: Simulation Units

Units used in LAMMPS here for Molecular dynamics Simulation – Metal.

Example : 1 Femtosecond as timestep = 0.001 (in LAMMPS Metal unit)

Parameter	Units
Distance	Angstroms (Å)
Time	Picoseconds (ps)
Energy	Electron Volts (eV)
Temperature	Kelvin (K)

Step 1: Create a relaxed system

Input script: *in.relax*

1. *Create a system*
2. *Do energy minimization*

```
units           metal
atom_style      atomic
boundary        p p p
processors      ${px} ${py} ${pz}
read_data       MoS2.data
replicate       ${xnum} ${ynum} ${znum}
group           watom type 1
group           seatom type 2
neighbor        2.0 bin
neigh_modify    delay 0 every 1 check yes
pair_style      sw
pair_coeff      *  *  MoS2.sw Mo S
thermo_style    custom step temp pe ke etotal press vol
thermo          50
dump            1 all atom 100 dump.min
min_style       cg
minimize        1.0e-8 1.0e-8 5000 10000
```

Input Crystal structure

Interaction potential

Energy minimization

Step 1: Create a relaxed system

Input script: ***in.relax***

3. *Heat to temperature T*
4. *Relax to temperature T*

```
velocity        all create ${SysTemp100} 156467 mom yes rot yes dist gaussian
fix             2a all  nve
run             ${Steps40ps}

fix             5 all nve
dump            4 all atom 50000 dump300.nve
run             ${Steps600ps}
unfix           5
write_restart   MoS2.restart
```

Heat to T

Relax at T

Input file for in.heatflux for thermal conductivity

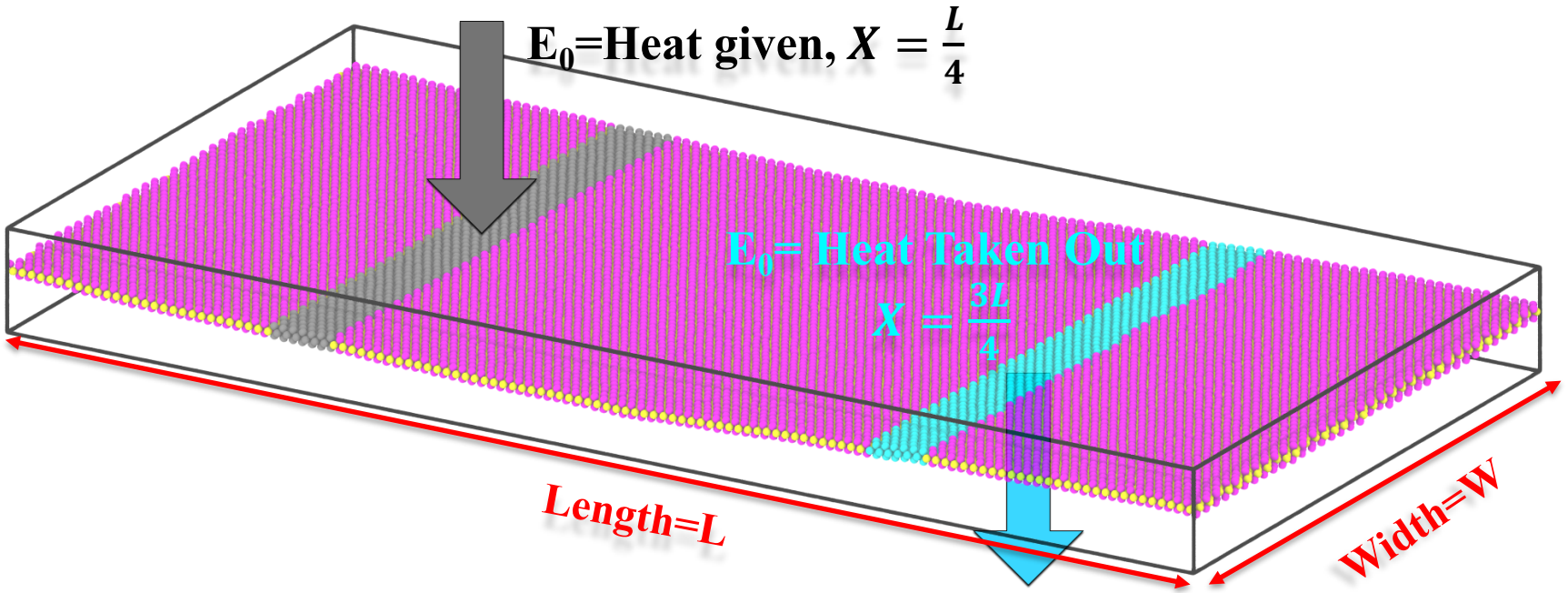
LAMMPS Walkthrough: Variables

File: ***in.variables***

- ***Contains variable definitions***
- ***Here are some of the important ones***

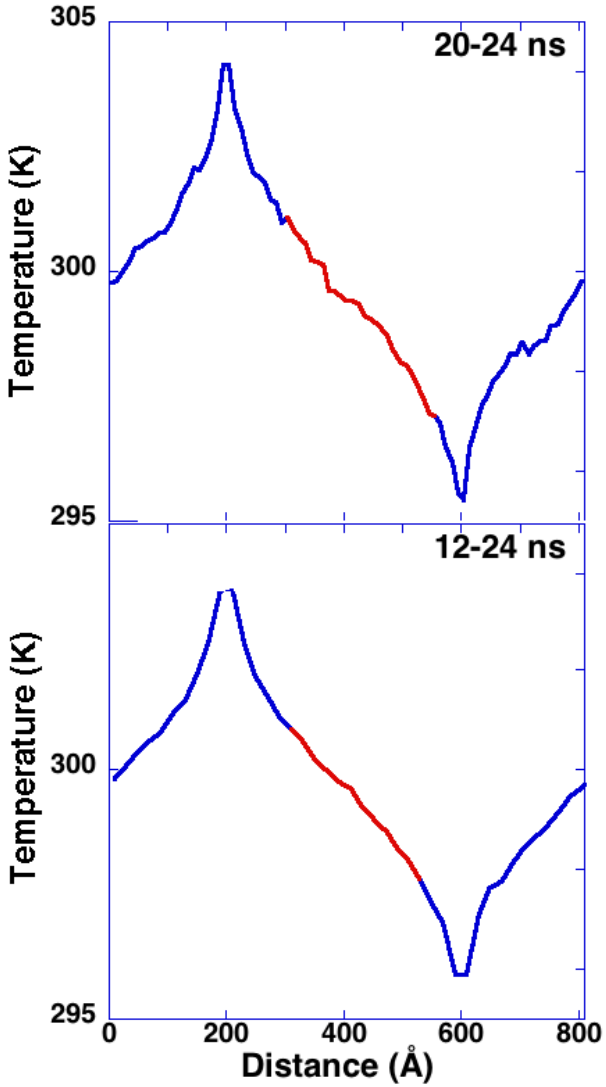
```
variable  px equal 20 # Number of processors in the x direction
variable  py equal 4  # Number of processors in the y direction
variable  pz equal 1  # Number of processors in the z direction
variable  SimTimestep equal 0.001 # Timestep used. Here 1 femtosecond
variable  Steps300K equal 300000 # Number of steps to run. Here 300000
variable  HeatAdded equal 0.00431*100 # Amount of heat added. 0.431eV
variable  HeatRemoved equal -0.00431*100 # Amount of heat removed
                                         0.431eV
```

Schematic of Thermal Conductivity Simulation Setup



- Define Hot and Cold region in the system at X=L/4 and X=3L/4 respectively
- E_0 heat is given to the hot region and E_0 heat is taken away from cold region.

Equations to Compute K



- Temperature gradient($\frac{dT}{dx}$) is calculated from the temperature vs distance plot.
- Thermal conductivity (K) is calculated using these formula

Heat Flux: $J_y = -\frac{1}{2}\frac{E_0}{A \times \Delta t}$

$$J_y = -K\frac{dT}{dx}$$

A= Cross-sectional area of MoS_2

E_0= Input Heat/ Heat taken out from the system

Δt=time interval between consecutive E_0

Step 2: Add/Remove heat to/from system

Read relaxed structure coordinate

```
boundary        p p p
processors      ${px} ${py} ${pz}
read_restart    MoS2.restart
neighbor        2.0 bin
```

Input script: ***in.heatflux***

1. *Read relaxed structure coordinate*
2. *Define two strips L/2Å apart*
3. *Add/remove heat from these strip*
4. *Run system for 4ns*
5. *Take temperature average over 4ns*
6. *Continue this process at least thrice*

Define strips and add/remove heat from these regions

```
region          hot  block  240 260  INF INF INF INF units box
region          cold block  740 760 INF INF INF INF units box
group           hot region  hot
group           cold region cold
fix             1 hot  heat 100 ${HeatAdded} region hot
fix             2 cold heat 100 ${HeatRemoved} region cold
```

Step 2: Add/Remove heat to/from system

Input script: ***in.heatflux***

1. *Read relaxed structure coordinate*
2. *Define two strips L/2Å apart*
3. *Add/remove heat from these strip*
4. ***Run system for 4ns***
5. ***Take temperature average over 4ns***
6. ***Continue this process for at least 3 time***

Take Temperature average for 4ns

```
compute          myKE all ke/atom
variable         atemp atom c_myKE/(1.5*8.621738*0.00001)
timestep         ${SimTimestep}
fix              6b all ave/spatial 1 ${T_avg4ns} ${T_avg4ns} x lower
                 20.0 v_atemp file Temperature.txt units box
run              ${T_avg4ns}
```

Hands on Calculations

Length Scaling:

1. Pre-relaxed system at 300K for 12ns is inside L_scaling folder:
   a) 600Å×100Å : MOS2_600L.restart
   b) 800Å×100Å: MOS2_800L.restart
   c) 1000Å×100Å: MOS2_1000L.restart

   } Already Submitted Earlier

2. Run in.heatflux for 300000 steps
4. Compute thermal conductivity using calthermal_conductivity.py

Check Status of your jobs

Job Submission: Job 3 (Length Scaling)

STEP 1: Navigate to Thermal_Conductivity folder in your home directory

```
cd ~/Thermal_Conductivity
```

STEP 2: Navigate to Length_Scaling folder

```
cd ./Length_Scaling
```

STEP 3: Navigate to 600A folder

```
cd ./600A
```

STEP 4: Submit your Third Job

```
qsub job.pbs
```

Job Submission: JOB1 (Temperature Scaling)

STEP 1: Get to Temperature_Scaling folder

```
cd ~/Thermal_Conductivity/Temperature_Scaling
```

STEP 2: Navigate to 100K folder

```
cd ./100K
```

STEP 3: Submit your fourth Job

```
qsub job.pbs
```

Hands on Calculations

Temperature Scaling:

1. Pre-relaxed system at 100K, 200K, 300K for 12ns is inside T-scaling folder:
   a) 800Å×100Å , 200K : MOS2_200T.restart
   b) 800Å×100Å , 100K : MOS2_100T.restart
   c) 800Å×100Å , 300K : MOS2_200T.restart

   } Already Submitted Earlier

2. Run in.heatflux for 300,000
3. Compute thermal conductivity using calthermal_conductivity.py

Step 3: Compute Thermal Conductivity

Compute thermal conductivity using *calthermal_conductivity.py*

- **Input parameters for calthermal_conductivity.py is defined in input.txt**

```
height      3.5       # height of your system.
                      # This value can be seen from lammps dump file
width       197.45    # width of your system.
                      # This value can be seen from lammps dump file
energy      0.2586    # energy input into the system in ev/ps.
                      # Should be equal to eheat/rheat of in.heatflux file
frequency   1000      # how frequently heat is supplied/extracted from system.
                      #Should be equal to value of fix hot/cold  in.heatflux file
dtstep      0.001     # time step used in your md simulation in ps
```

Note: you can find these parameters in in.heatflux and lammps dump file

Sourcing Python

Before we start plotting anything we must source python. Follow these steps

STEP 1: Go to your home directory

```
cd ~/
```

STEP 2: Source Python

```
source /usr/usc/python/default/setup.sh
```

Step 3: Compute Thermal Conductivity

Compute thermal conductivity using *calthermal_conductivity.py*

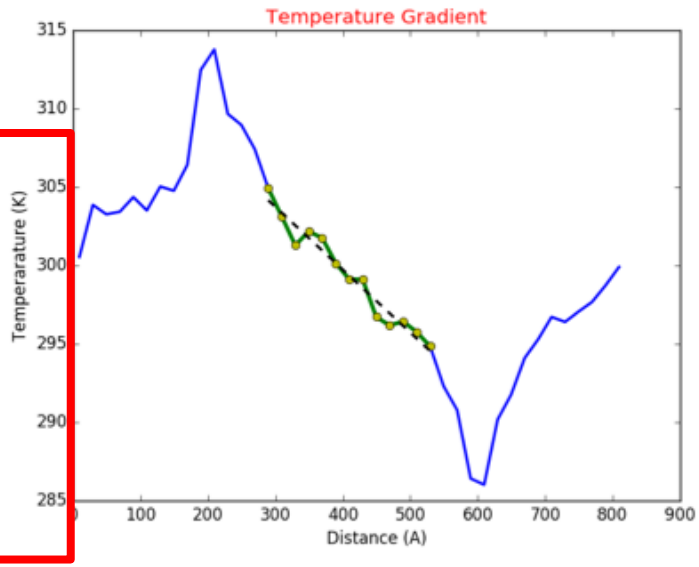
```
python3.5 calthermal_conductivity.py Temperature.txt
```

File: Temperature.txt

1. *Contains Temperature profile averaged over 300K Steps (0.3 ns)*
2. *Noisy*

Output :
Length: 39.99 1/Length 0.025
Mean Thermal Conductivity value and standard deviation 249.71 0.00
1/(Thermal_Conductivty) value and standard deviation 0.004 0.00

Also Outputs : 300K_steps.png



Step 3: Compute Thermal Conductivity (4ns data)

Compute thermal conductivity using *calthermal_conductivity.py*

```
python3.5 calthermal_conductivity_4ns.py 20Temperature4.txt
```

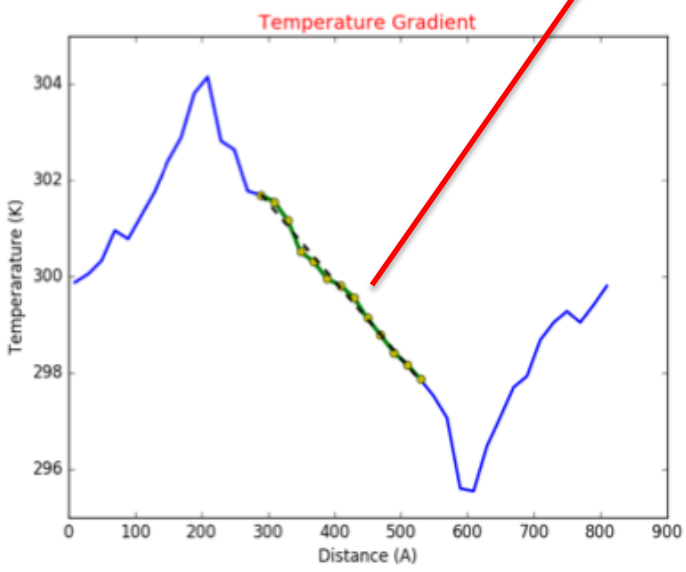
File: 20Temperature4.txt

1. *Contains Temperature profile averaged over 4ns*
2. *Much Less Noise*

Output : Length: 39.99 1/Length 0.025
Mean Thermal Conductivity value and standard deviation 18.61 0.00
1/(Thermal_Conductivty) value and standard deviation 0.054 0.00

Also Outputs :4ns.png

Much Better Fit compared to 300Ksteps



Job Submission: JOB 2 Temperature Scaling

STEP 1: Navigate to Thermal_Conductivity folder in your home directory

```
cd ~/Thermal_Conductivity
```

STEP 2: Navigate to Temperature_Scaling folder

```
cd ./Temperature_Scaling
```

STEP 3: Navigate to 200K folder

```
cd ./200K
```

STEP 4: Submit your Fifth Job

```
qsub job.pbs
```

Job Submissions : Isotope (JOB 1)

STEP 1: Get to Isotope_TC directory

```
cd ~/Thermal_Conductivity/Isotope_TC
```

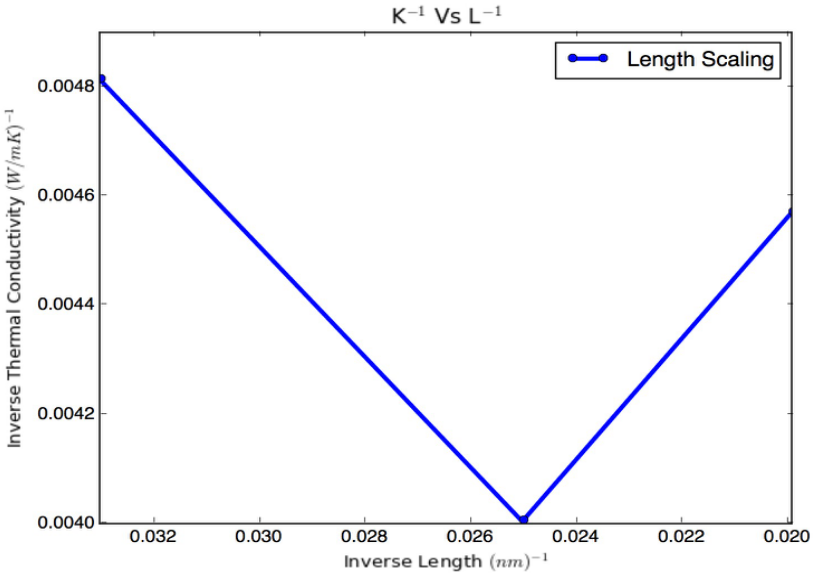
STEP 2: Submit job

```
qsub job.pbs
```

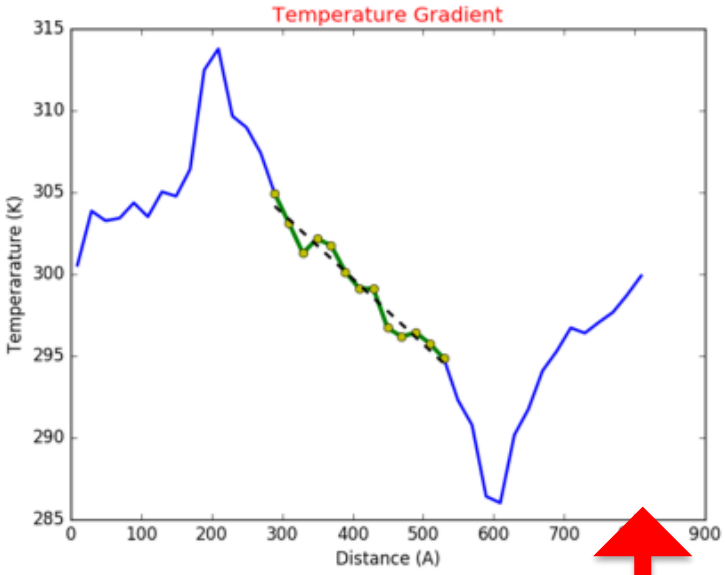
Step 4: Plot Length scaling

For 600Å×100Å, 800Å×100Å, 1000Å×100Å
compute K value and plot K^{-1} vs L^{-1}

plot K^{-1} vs L^{-1}



Temperature profile



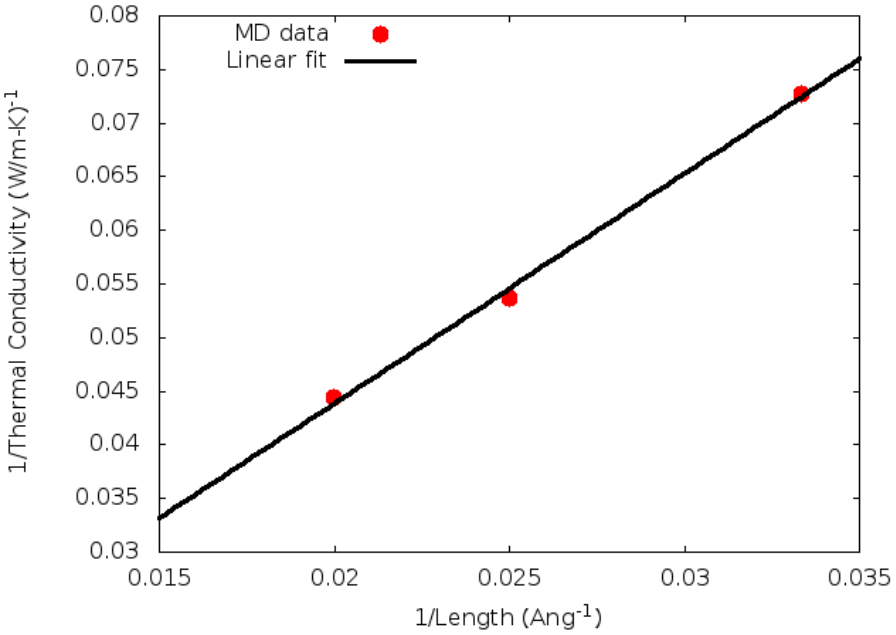
1. **Poor Length Scaling because of insufficient time averaging**
2. **Extremely noisy temperature gradient**

Step 4: Plot Length scaling (4ns System)

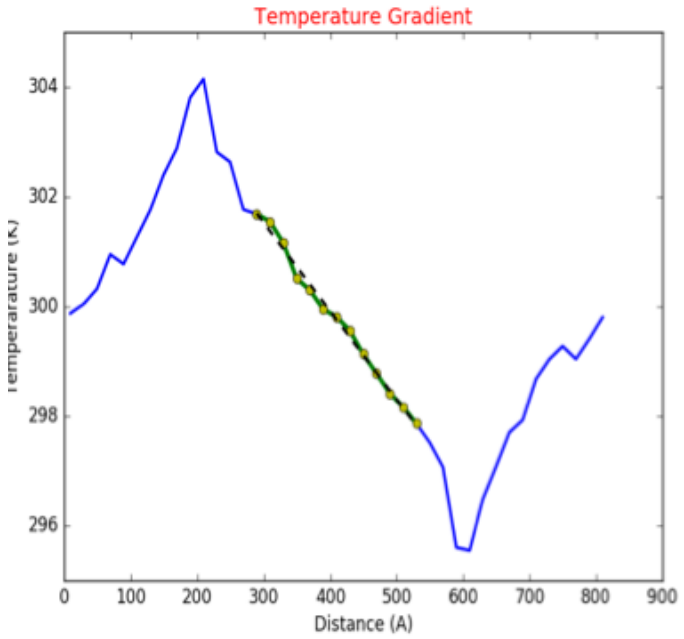
For 600Å×100Å, 800Å×100Å, 1000Å×100Å *compute K value and plot K^{-1} vs L^{-1} using 20Temperature4.txt*

Note: Temperature profiles have been averaged over 4 ns instead of 0.3ns (300Ksteps)

plot K^{-1} vs L^{-1}



Temperature profile



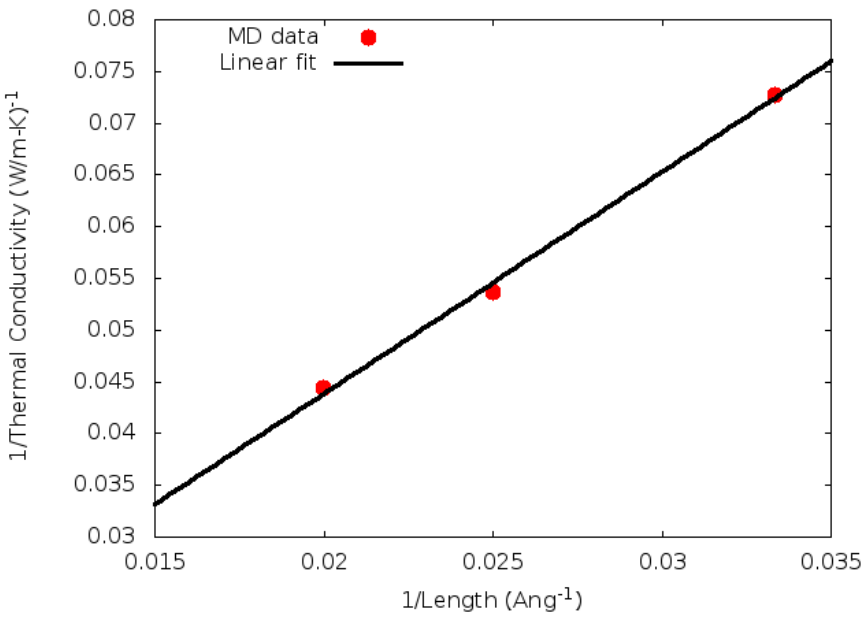
Step 4: Plot Length scaling (4ns System)

To Plot Length Scaling we have provided you with a GNUPLOT script inside the Length_Scaling folder

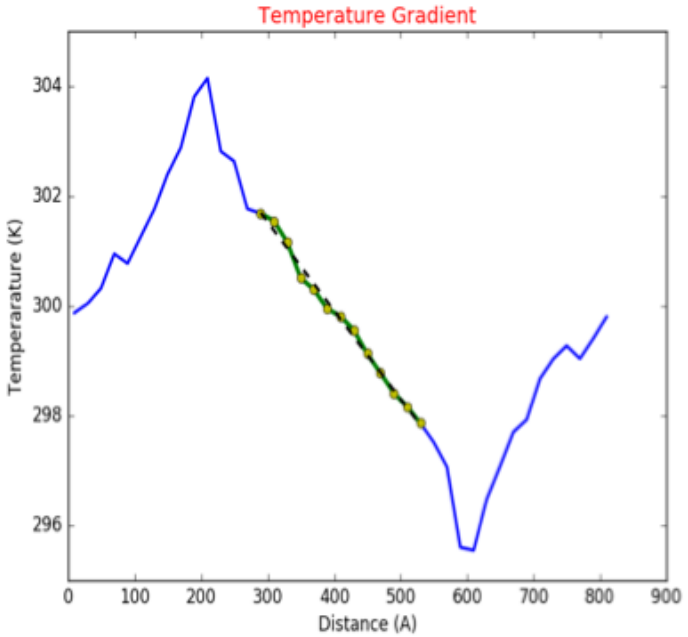
```
$ gnuplot sket.ch
```

This outputs length_scaling.png Transfer it to your machine and view the plot

plot K^{-1} vs L^{-1}



Temperature profile

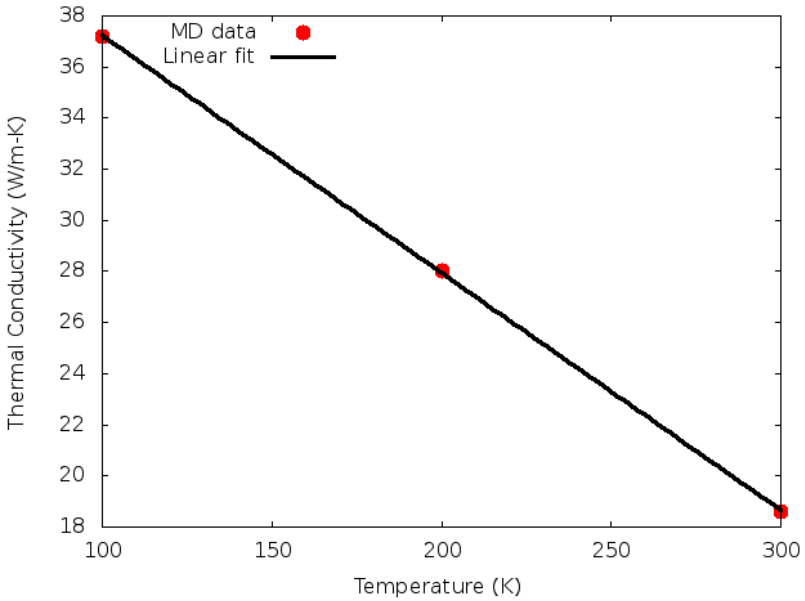


Step 5: Plot Temperature scaling

For 800Å×100Å at temperature 100K, 200K and 300K
compute K value and plot K vs T

Note: **For 800Å×100Å at 300K use the Thermal conductivity value from the Length Scaling System**

To Plot Temperature Scaling we have provided you with a GNUPLOT script inside the Temperature_Scaling folder




```
$ gnuplot sket.ch
```

This outputs temperature_scaling.png
Transfer it to your machine and view the plot

PDOS, DOS and C_v Calculation

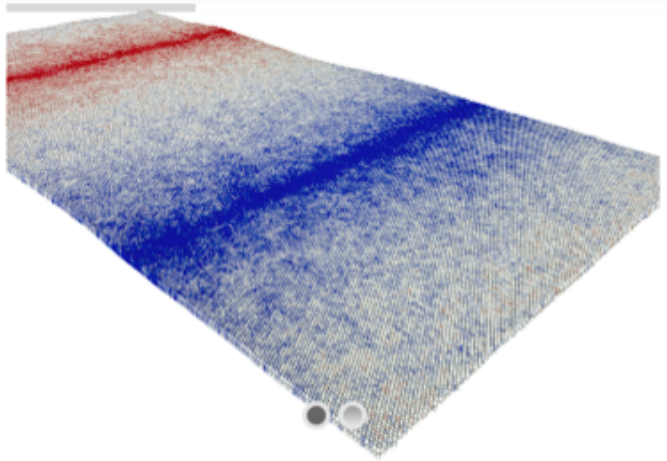
Software Download

LAMMPS Plugins for Thermal Conductivity Calculation

https://magics.usc.edu/thermal-conductivity-plugin/

Thermal Conductivity Plugins for LAMMPS

- Thermal conductivity with isotopes and quantum correction
- Velocity autocorrelation and Phonon Density of States using multiple initial conditions
- Specific heat from Phonon DOS as a function of temperature



Thermal conductivity tools is a series of plugins for thermal properties — velocity autocorrelation functions, phonon density of states, specific heat and thermal conductivity from MD using LAMMPS.

Software Download Links

SOURCE CODE

Thermal Conductivity Calculation

Phonon DOS and Specific heat

Documentation download links

quick start guide can be downloaded here

Frequently Asked Questions

For frequently asked questions, please click here ?

LAMMPS Plugins for Thermal Conductivity

DOS_Cv: Contains following files

1. **in.dos:** *LAMMPS script to create a relaxed system at Temperature=T K*
2. **MOS_2.data:** *Input unit cell coordinate of MOS_2 monolayer*
3. **MoS_2.sw:** *SW Interaction potential for MOS_2*
4. **caldos.py:** *Python script to run dos.c and save images of of velocity autocorrelation, PDOS, FDOS, C_v in the folder image.*
5. **dos.c:** *C program to compute velocity autocorrelation, PDOS, TDOS, C_v from LAMMPS dump file*
6. **dos.h:** *header file for dos.c*
7. **input.txt:** *contains input parameters for DOS calculation , used by dos.c*

Major steps involved in calculating DOS

Step 1: Create a relaxed system at a given Temperature

use LAMMPS script in.dos

Step2: Compute DOS from LAMMPS Dump file

use caldos.py

Step 1: Create a relaxed system

Input script: *in.dos*

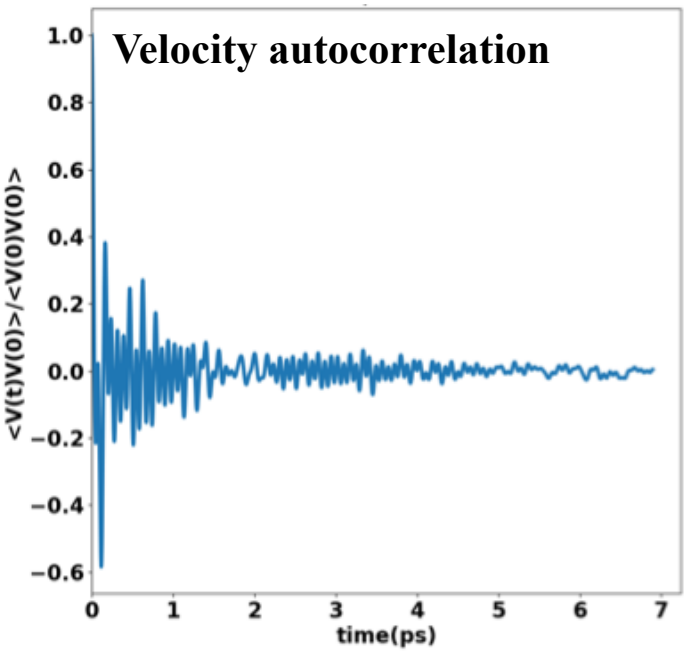
1. ***Create a system***
2. ***Do energy minimization***
3. ***Heat and relax to temperature T***
4. ***Save coordinates for analysis***

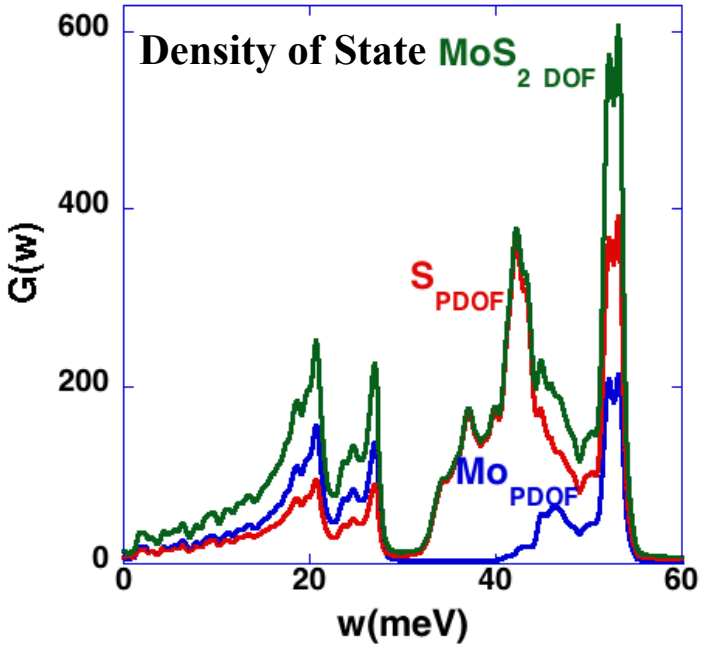
```
reset_timestep  0
fix             5 all nve
fix             6a all momentum 1000 linear 1 1 1
dump            3 all custom 1000 dump100relax.nve id type x y z vx vy vz
variable        tt0 equal step
run             200000
undump          3
unfix           6a
#save coordinates of thermalized system for analysis
dump            4 all custom 10 dumpdos.nve id type x y z vx vy vz
dump_modify     4 sort id
run             10500
unfix           5
write restart   mos2.restart
```

Used to calculate Velocity autocorrelation, PDOS, DOS and Cv by caldos.py

Hands on Calculations

Compute Velocity autocorrelation, Density of states using LAMMPS dump file





- Compute Velocity autocorrection (Z_α) for Mo & using 50 initial condition
- Partial Density of State:

$$G_\alpha(\omega) = \frac{6N_\alpha}{\pi}\int_0^\infty Z_\alpha(t)cos(\omega t)dt$$

- Total Density of State :

$$G(\omega) = \sum_\alpha G_\alpha(\omega)$$

Hands on Calculations

Velocity autocorrelation, Density of states, C_v calculation:

1. **Dump file for a relaxed system is inside DOS_cv_plugins folder:**
   - **dumpdos.nve**
2. **Compute velocity autocorrelation, density of states and C_v**

```
python3.5 caldos.py dumpdos.nve
```

Note: caldos.dy run a C program called dos.c which does this calculations. dos.h is header file for dos.c(no need to edit this file).Various parameters required for the calculation is defined inside input.txt file(you will need to change parameters here).

Output : images and values of DOS, Velocity autocorrelations of each element and Specific Heat.

Input parameters for dos.c

Input parameter file: input.txt

```
Ninitial        10      #Total number of initial condition
Corlength       7000    #Correlation length for each initial condition
Ngap    100     #Gap between two initial condition
TFREQ   10      #Timestep between two consecutive saved frame
dT      0.001   #timestep in ps
massW   95.940  #mass of atom type 1
massSe  32.065  #mass of atom type 2
```

from in.dos file:

```
#save coordinates of thermalized system for analysis
dump            4 all custom 10 dumpdos.nve id type x y z vx vy vz
dump_modify     4 sort id
run             10500
unfix           5
write restart   mos2.restart
```

TFREQ in input.txt

NFRAME

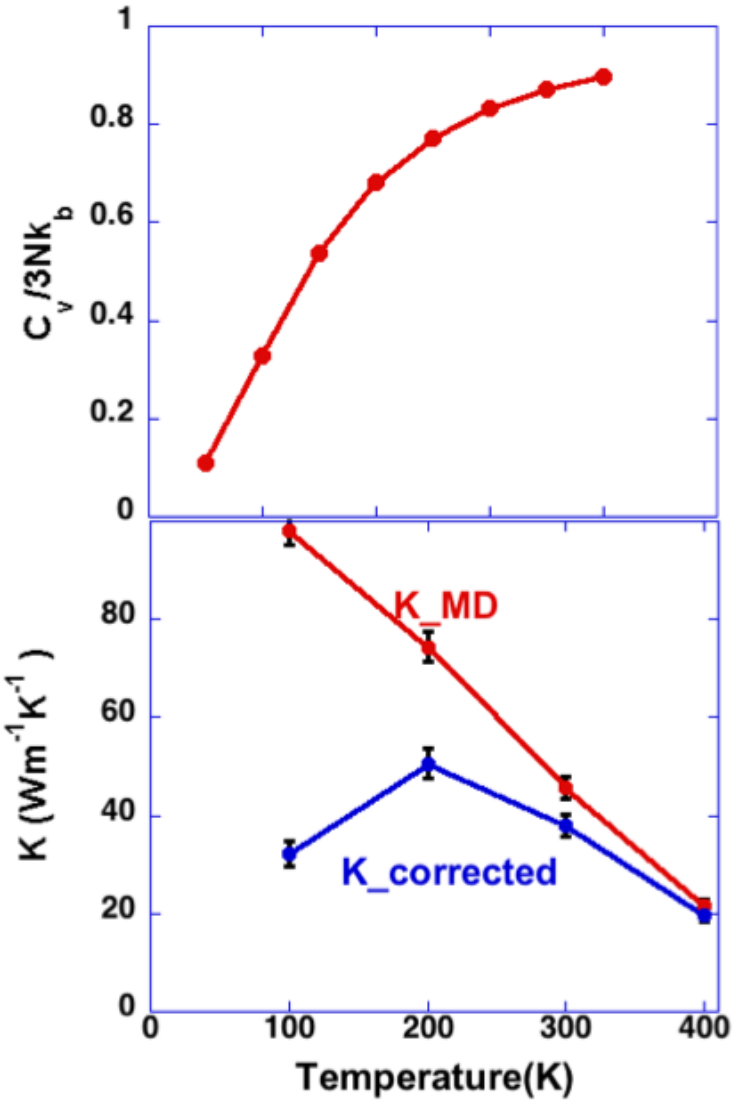
Note: $Ninitial \times Ngap + \text{Corlength} \leq NFRAME$

If this condition is not satisfied you will get error message

Hands on Calculations

1. Calculate Velocity autocorrelations, PDOS,DOS and C_v with one initial condition (Ninitial =1) and with 10 initial condition (Ninitial =10)
2. Compare the results

Quantum Corrected Thermal Conductivity



$$\frac{C_v}{3Nk_b} = \frac{\int_0^\infty \frac{u^2 e^u}{(e^u-1)^2} G(\omega) d\omega}{\int_0^\infty G(\omega) d\omega}, \mathrm{u} = \frac{\hbar\omega}{k_B t}$$

$$\mathrm{K_{corrected}} = \left(\frac{C_v}{3Nk_b}\right) \times \mathrm{K_{MD}}$$

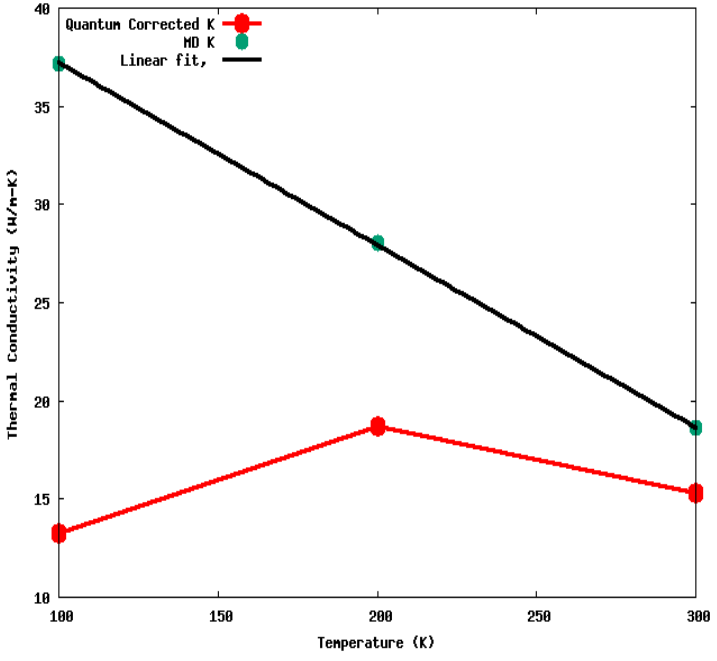
Hands-on Calculation:

1. Take the value of C_v at 100K,200K and 300K from *Specific_heat.txt* file
2. Take the value of K computed at 100K, 200K and 300K for 800Å×100Å system
3. Multiply these two number to get quantum corrected K value

Quantum Corrected Thermal Conductivity

Hands-on Calculation:

1. Take the value of C_v at 100K,200K and 300K from *Specific_heat.txt* file
2. Take the value of K computed at 100K, 200K and 300K for 800Å×100Å system
3. Multiply these two number to get quantum corrected K value
4. To plot Thermal Conductivity with Quantum Corrections we have provided you with a folder named Quantum_corrected_TC.
5. Inside this folder you will find a gnuplot script file that will plot out the values.
6. To run type : `gnuplot sket.ch`
7. This outputs a file Quantum_correction_TC.png Transfer to view it in your machine



Hands on Calculations : Isotope Effect

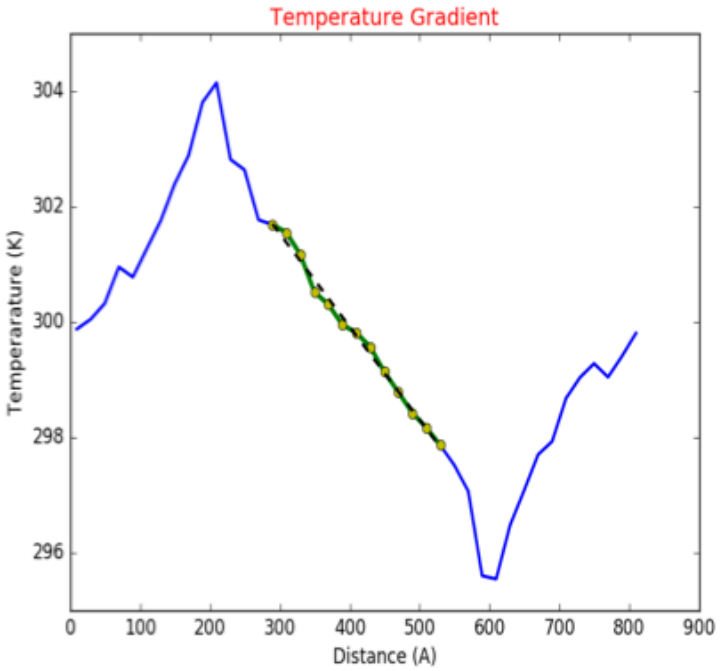
- **Compute thermal conductivity value of 800Å×100Å at 100K with isotopes**

```
python2.7 calthermal_conductivity.py Temperature.txt
```

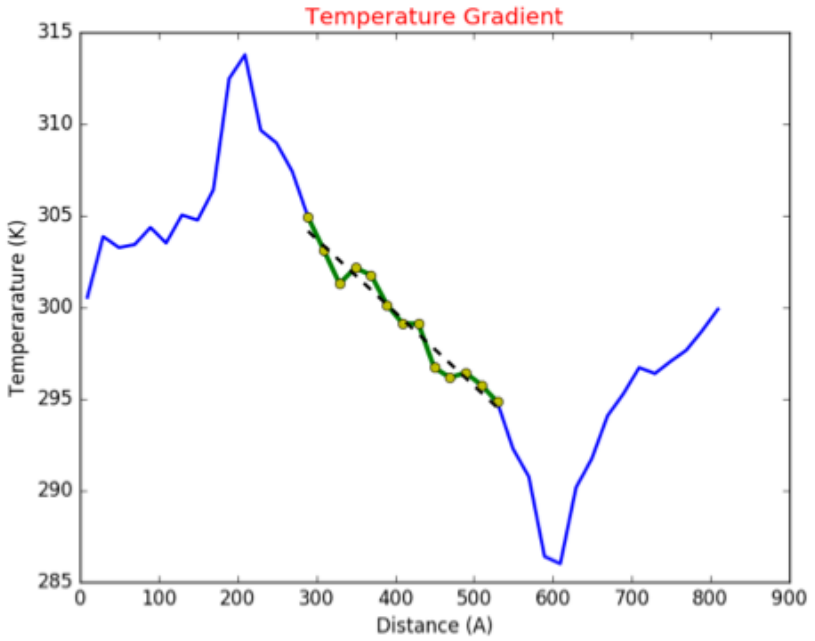
- **Compare the thermal conductivity value of 800Å×100Å at 100K with and without isotopes**

Stuff to keep in mind - 1

Average temperature over longer time



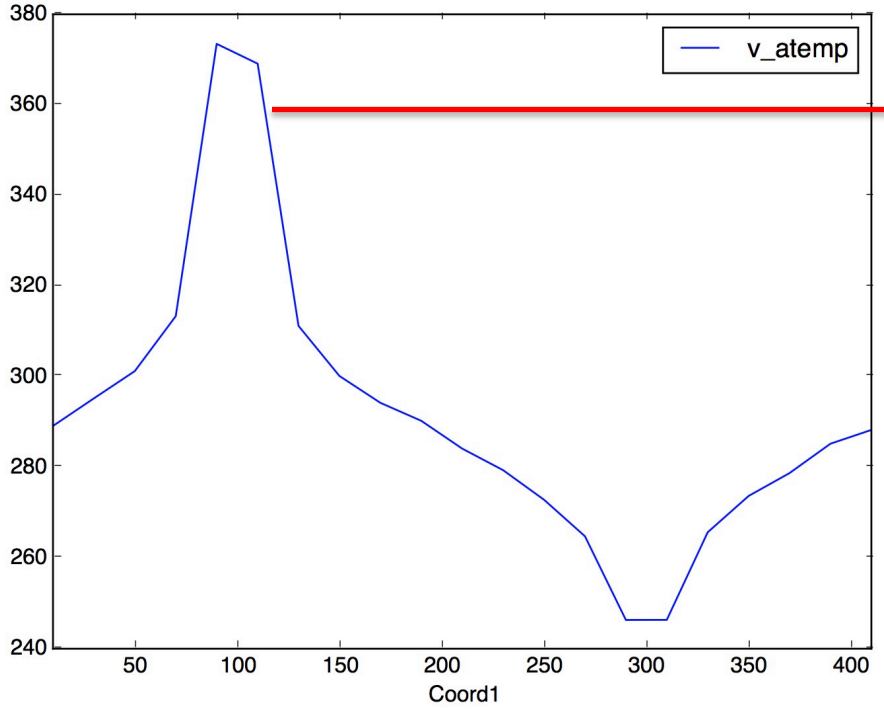
Averaging for longer gives a very clean gradient and almost a linear gradient



Extremely Noisy Temperature gradient. Gives erroneous slope values

Stuffs to keep in mind - 2

Heating rate is important : Very high heating rate can give anomalous result



Note the weird bump at heat source. This can be avoided using a reasonable heating rate.
Also Note the rather flat heat sink.