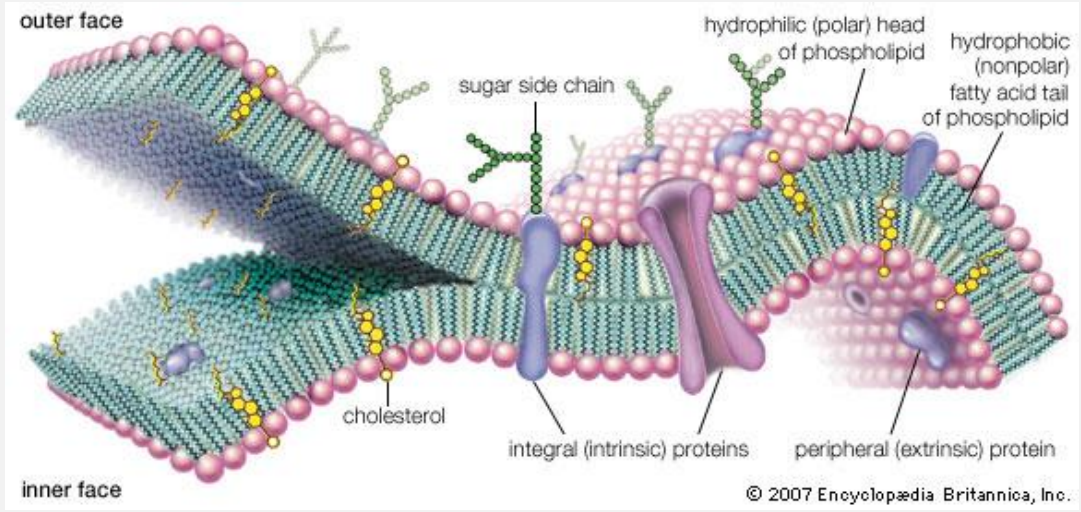
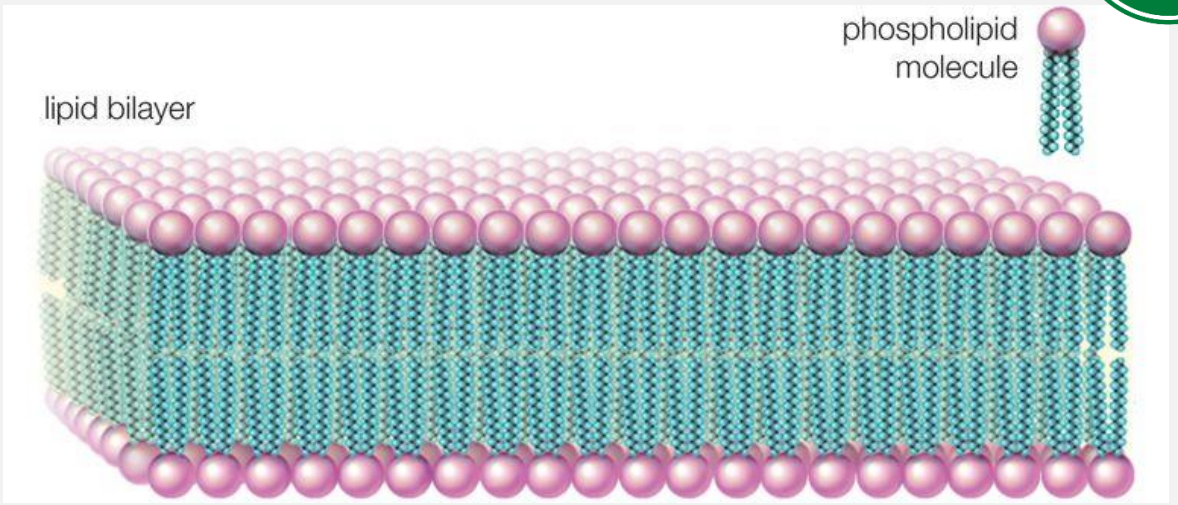
# Amber MD Simulation Experience

**Steven Pei**
**Updated 12/27/2022**

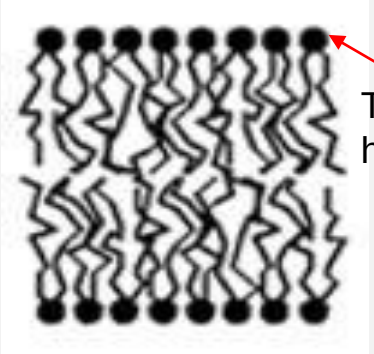
# Phospholipid phases



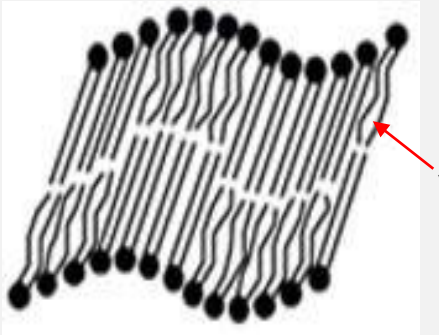

Britannica, *Encyclopedia Britannica* (2019)

**Schematical figures of the different phospholipid bilayer phases.**



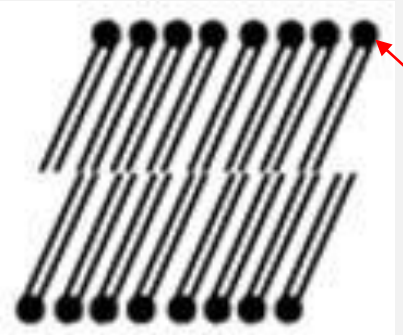
The hydrophilic head

Liquid ($L_\alpha$)



Wave behavior

Ripple($P_\beta$')

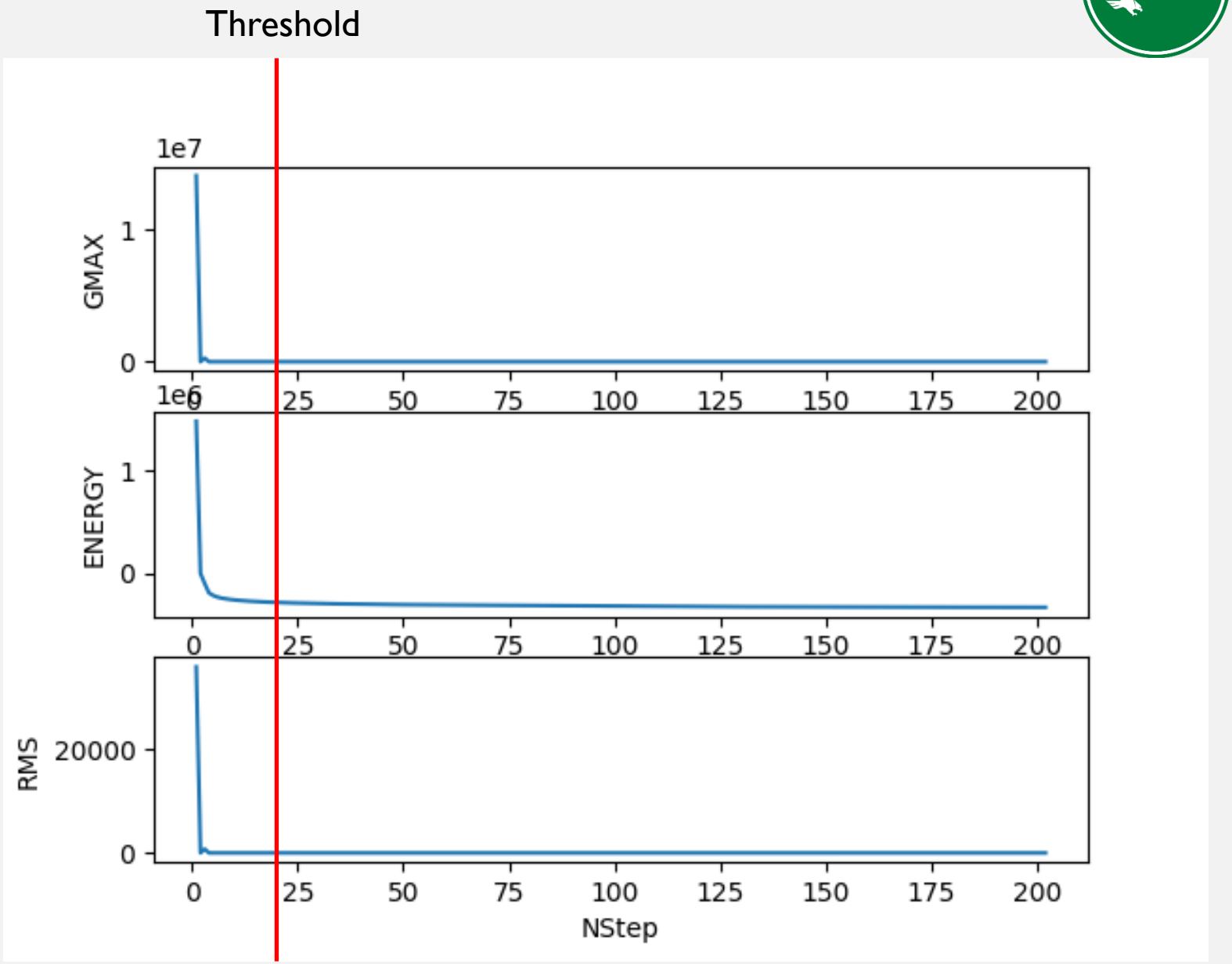


The hydrophobic tails

Gel Phase($L_\beta$')

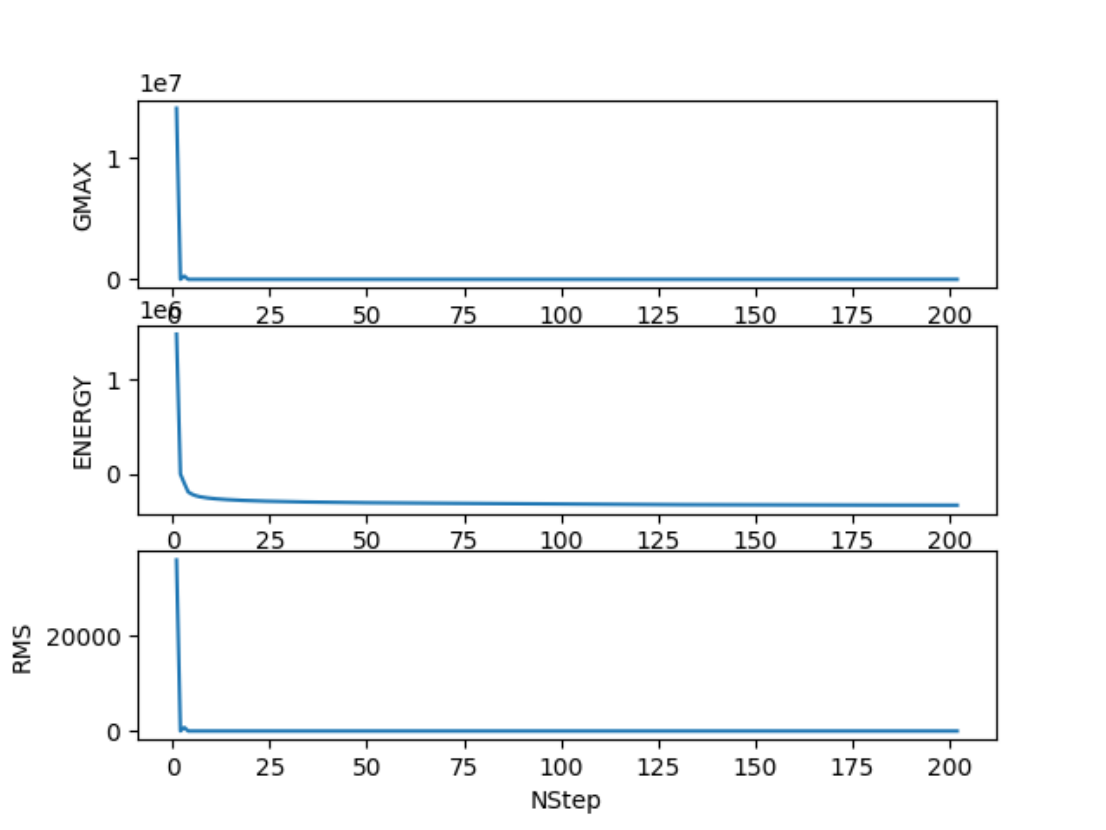
# Minimization

- NSTEP is the total number of steps of the minimization. Amber prints every NTPR steps as set in the input file.
- Energy is the total energy of the system, as determined from the force field equation, in Kcal/mol.
- RMS is the mean of the square root of the dot product of the force vectors.
- GMAX is the magnitude of the largest component of the force vectors, I.e the largest force and NAME and NUMBER are the atom that has that largest force. I.e the one that will move the most during the minimization step.
- These three parameter should decrease as the system approaches the minima.
- Because the values outlined in the graph to the right show that as the number of steps increases, the valves approach equilibrium, we should stop the calculations at 1000 steps.

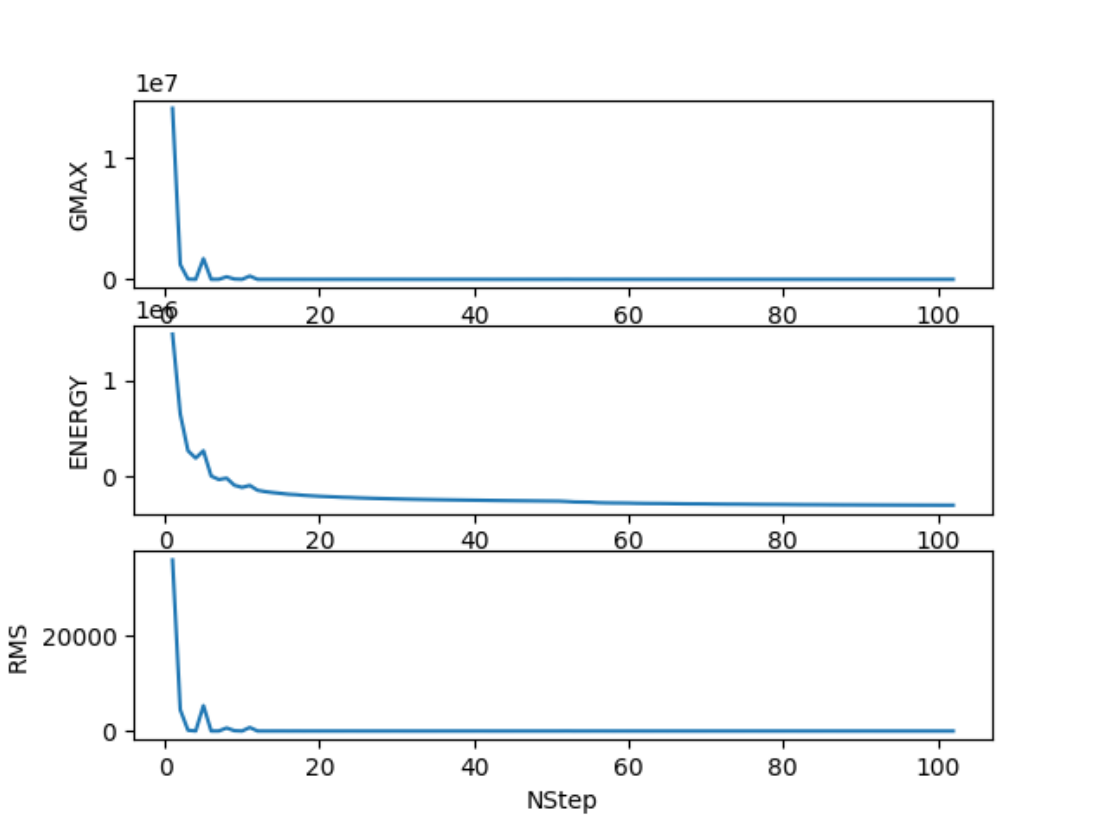


# Minimization Test

10000 Step Test - 2.36 Hours

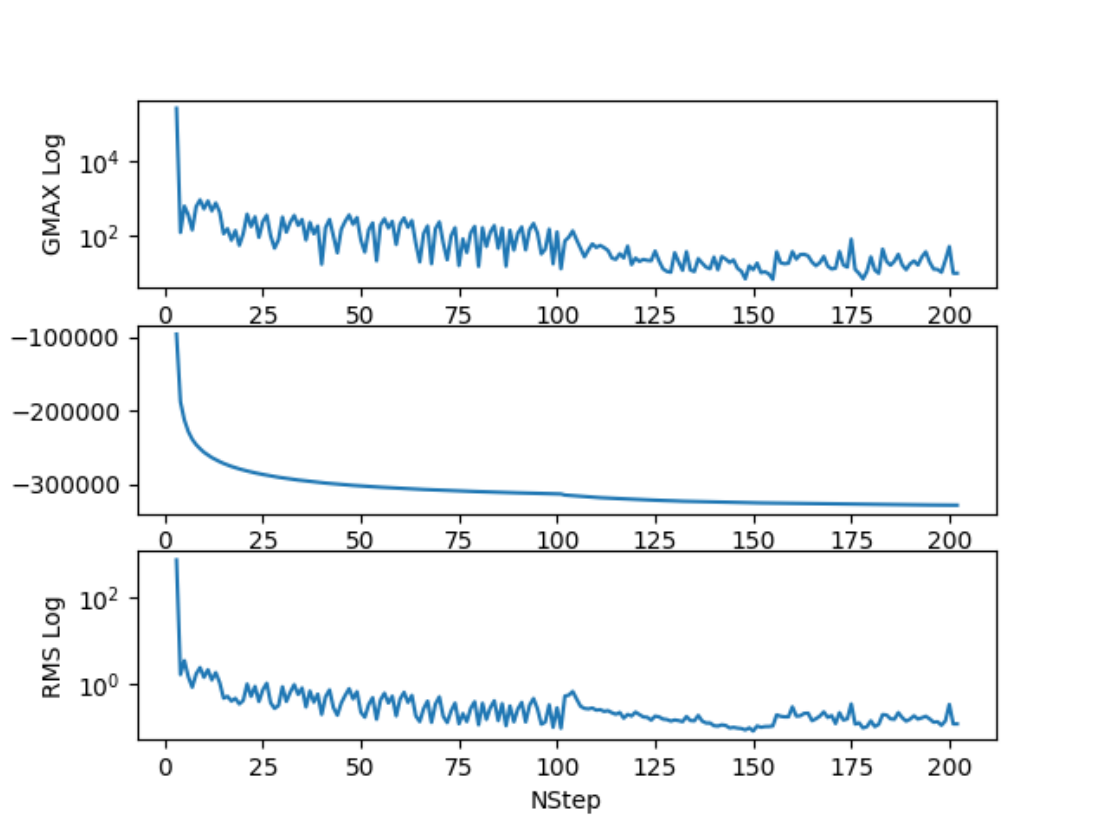



1000 Step Test – 0.25 Hours

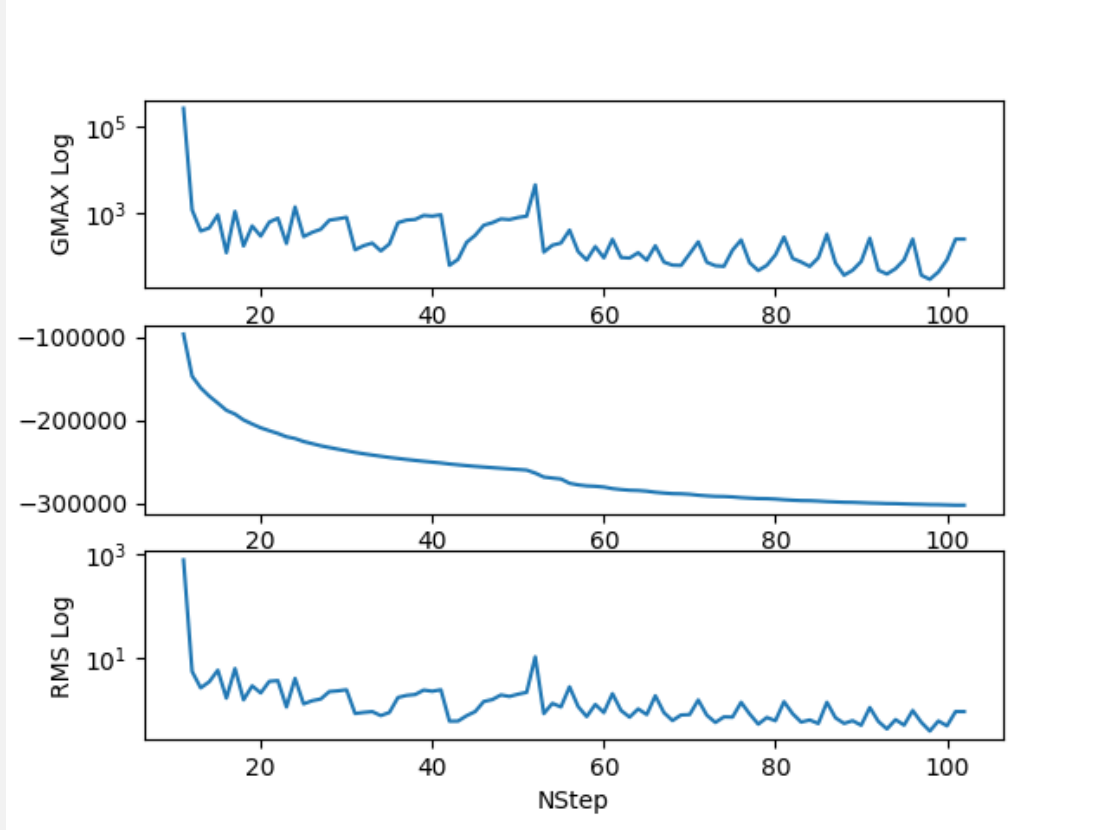


# Minimization Test Log

10000 Step Test - 2.36 Hours

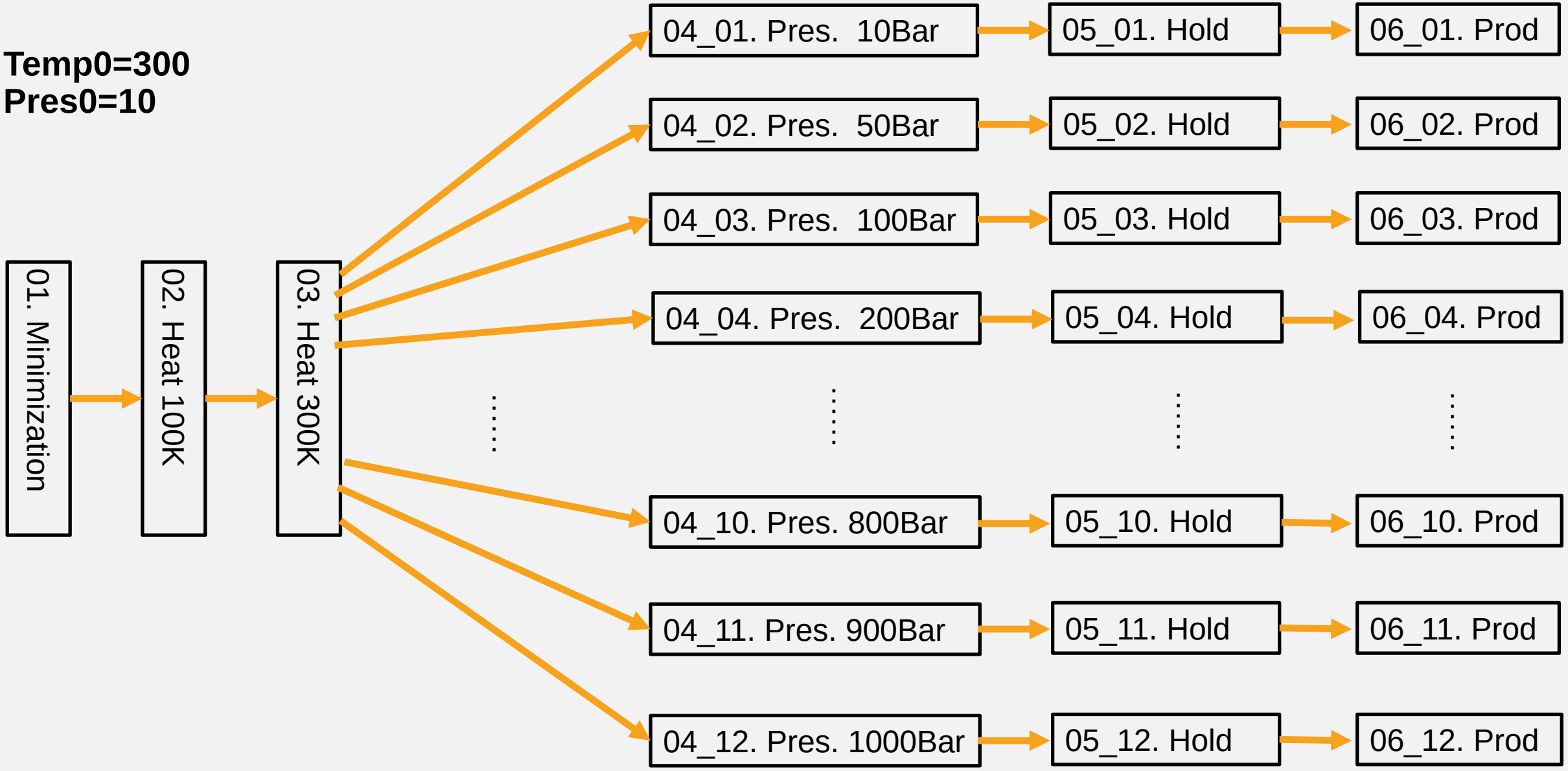



1000 Step Test – 0.25 Hours



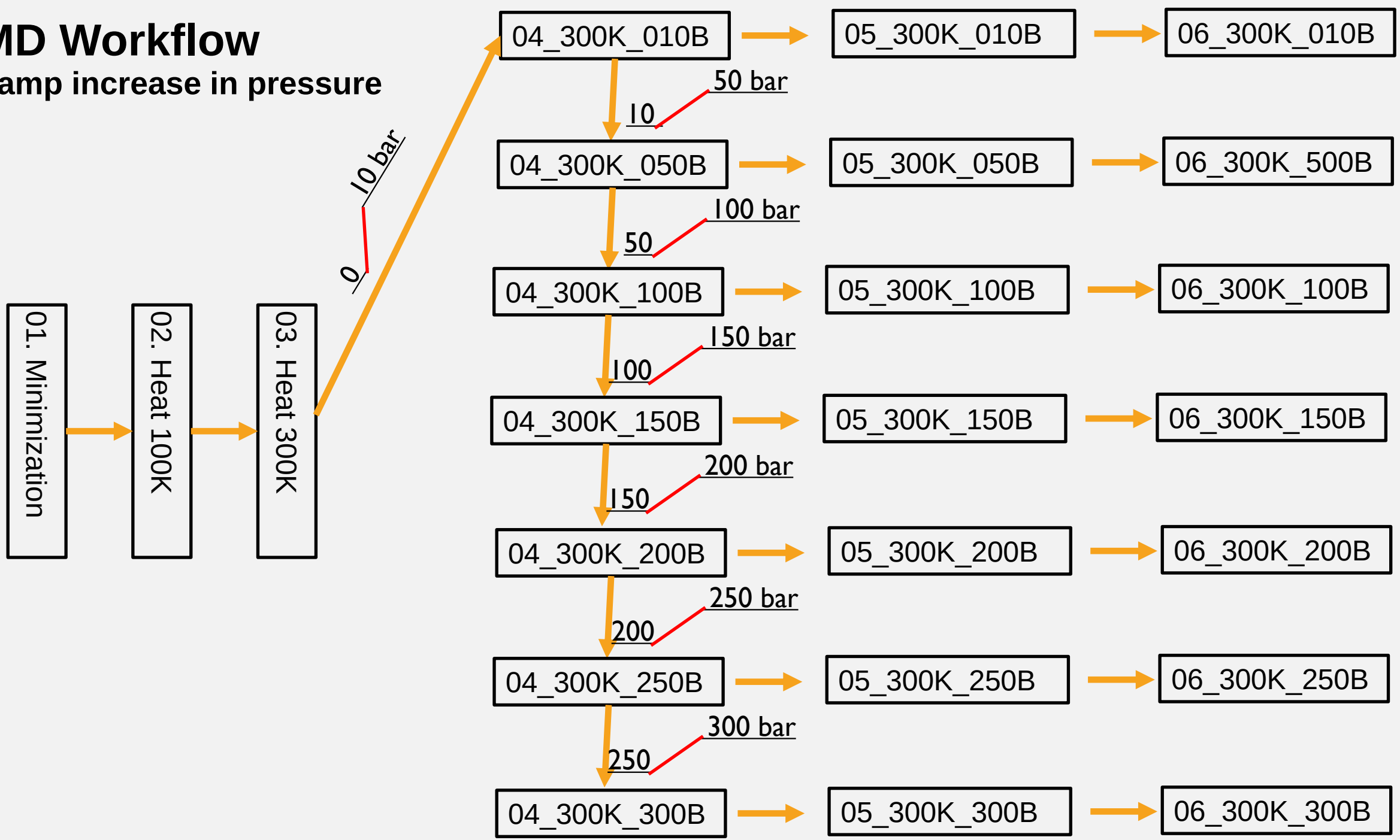
# MD Workflow

**Temp0=300**
**Pres0=10**



# MD Workflow

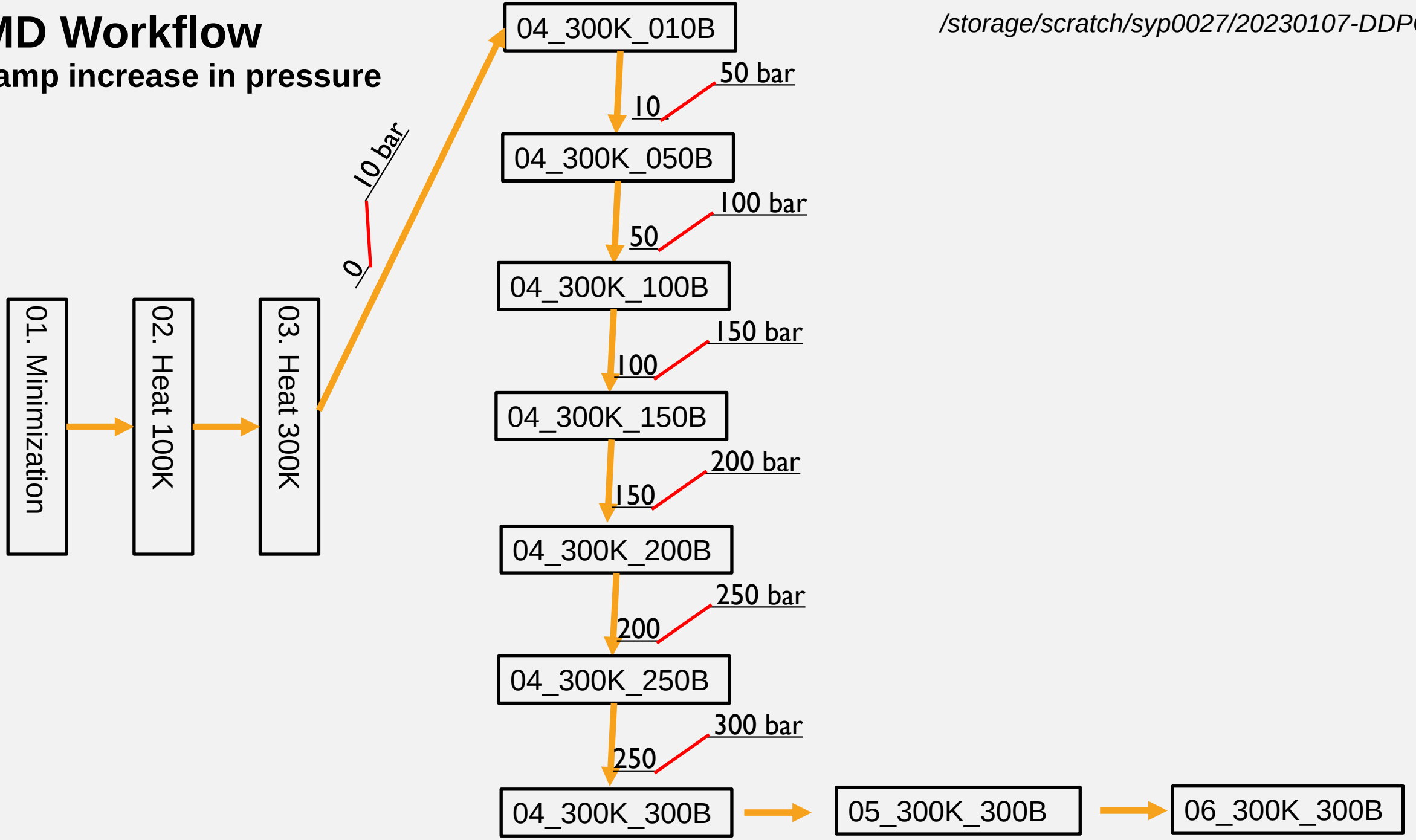
**ramp increase in pressure**



# MD Workflow

## ramp increase in pressure

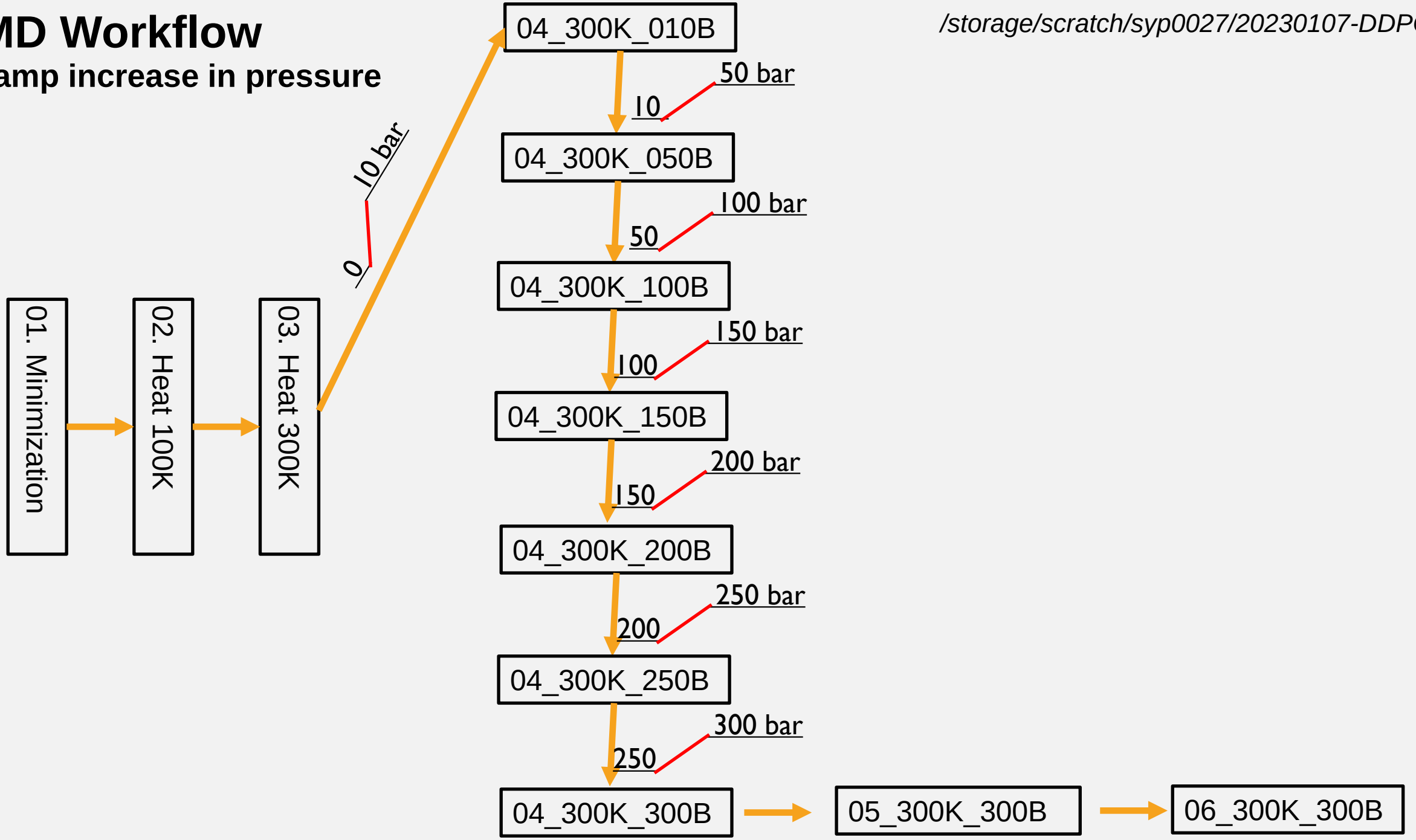
/storage/scratch/syp0027/20230107-DDPC512



# MD Workflow

## ramp increase in pressure

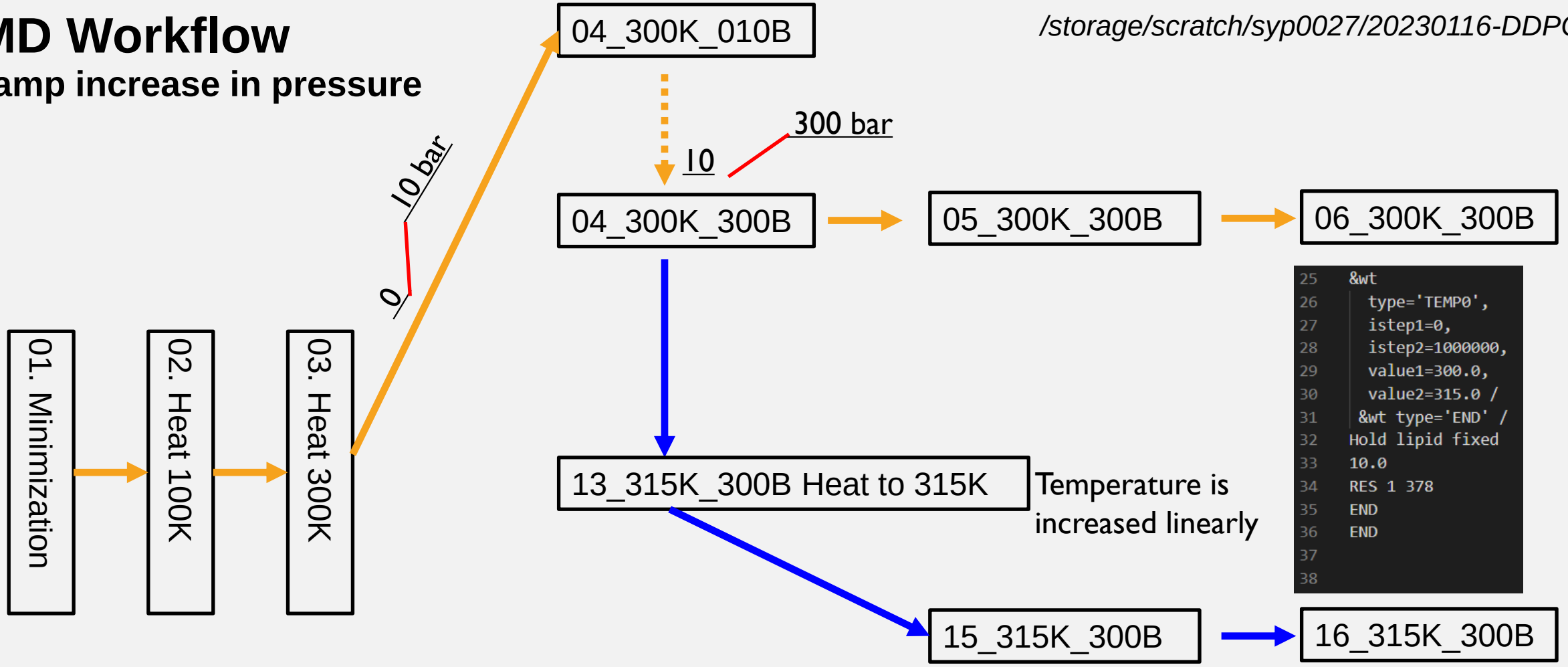
/storage/scratch/syp0027/20230107-DDPC512



# MD Workflow

## ramp increase in pressure

/storage/scratch/syp0027/20230116-DDPC512



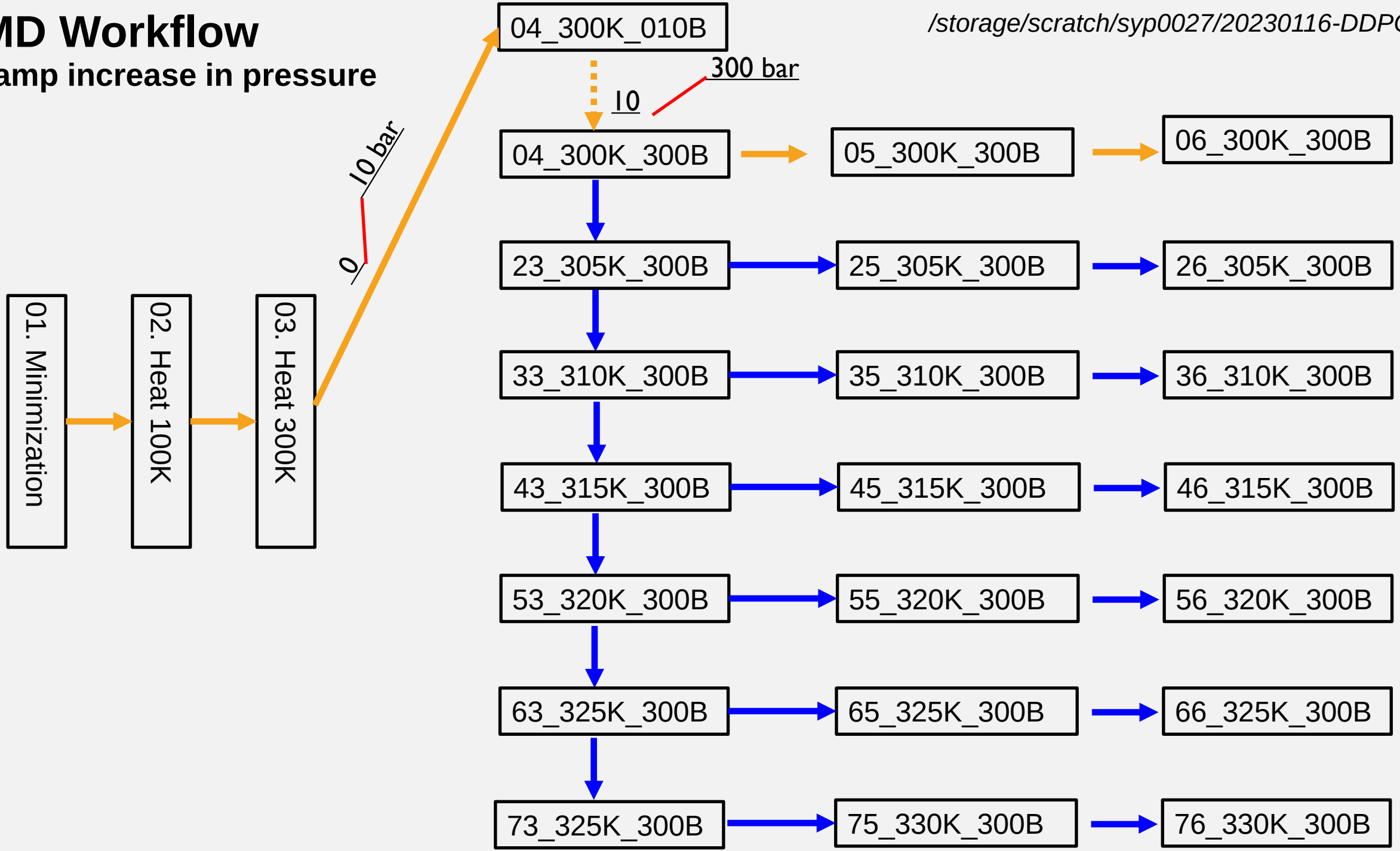

```
&wt
  type='TEMP0',
  istep1=0,
  istep2=1000000,
  value1=300.0,
  value2=315.0 /
 &wt type='END' /
Hold lipid fixed
10.0
RES 1 378
END
END
```

13 is equivalent to 03 which is a heating processing. Temp is linearly increased inside .in file. 15 is equivalent to 05 which is an equilibrium processing. 16 is equivalent to 06 which is a production processing.

# MD Workflow

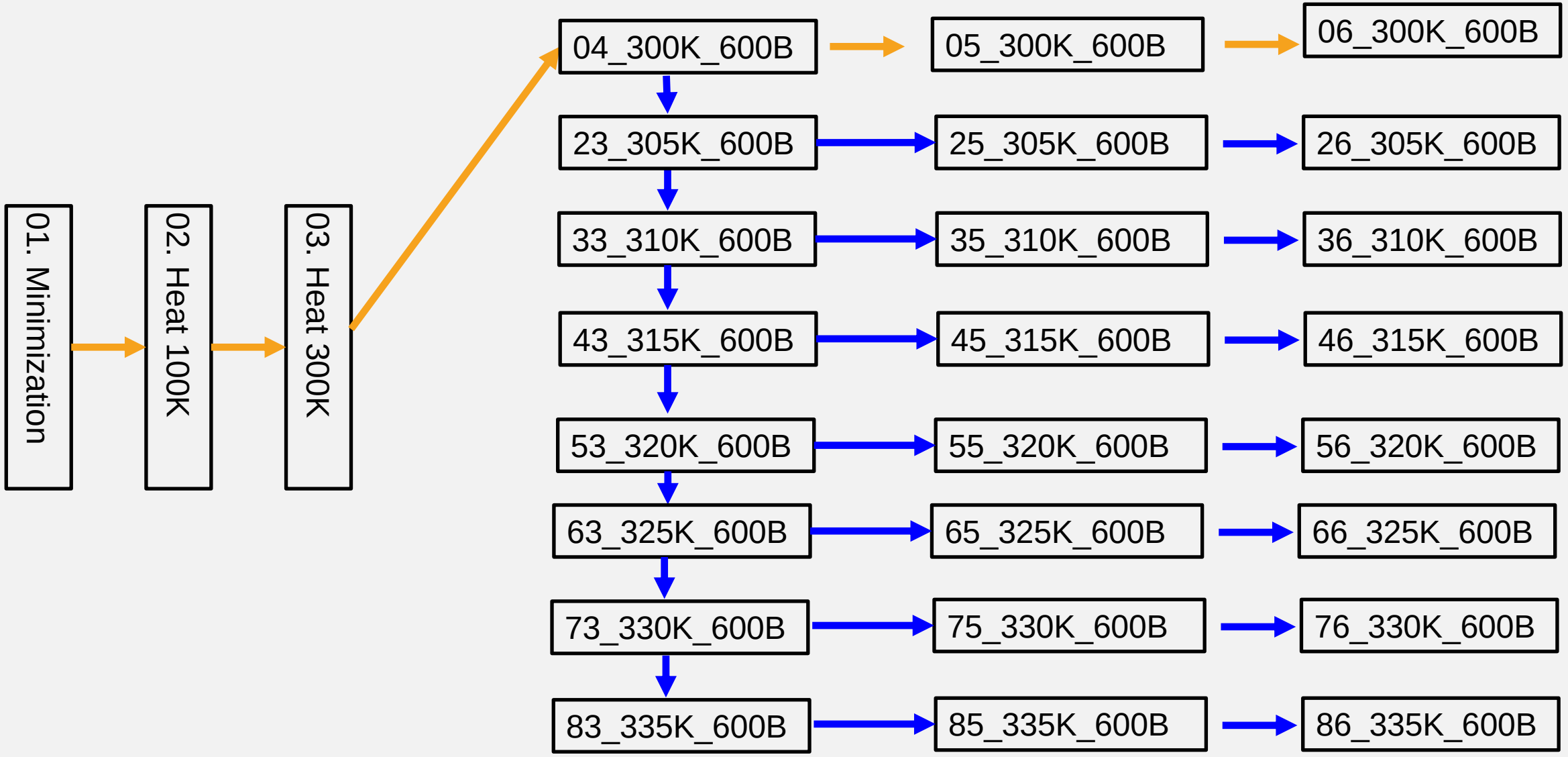
## ramp increase in pressure

*/storage/scratch/syp0027/20230116-DDPC512*



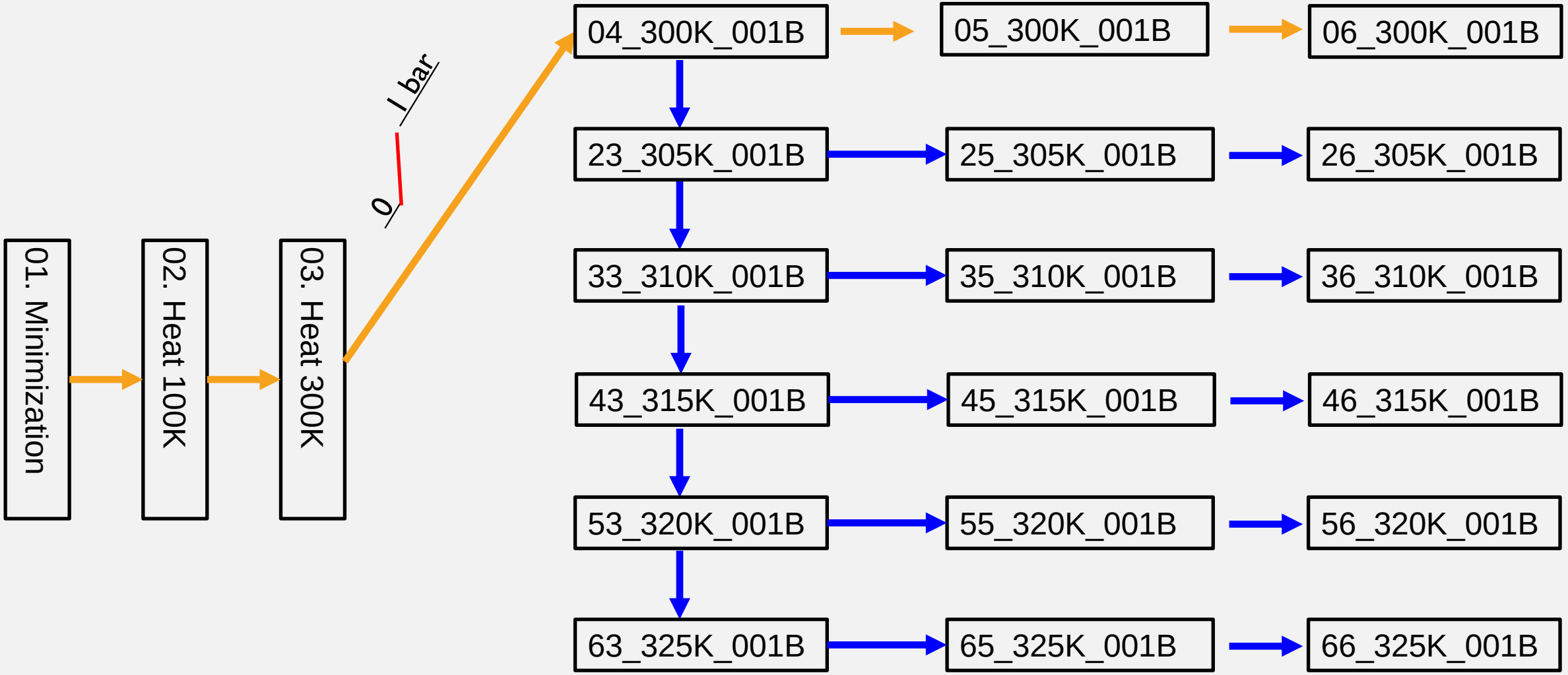
# MD Workflow 600 Bar

*/storage/scratch/syp0027/20230116-DDPC512*



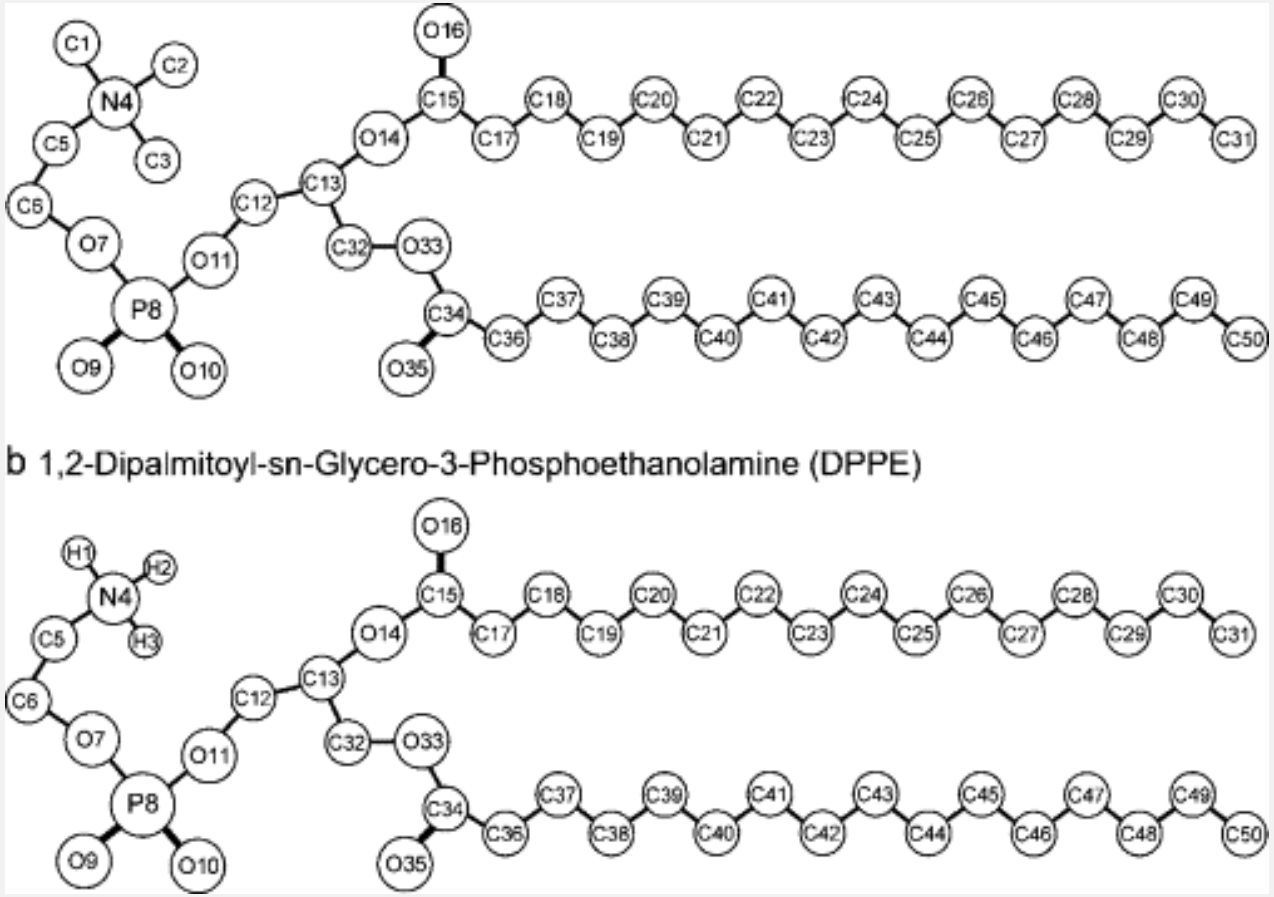
# MD Workflow 1 Bar

*/storage/scratch/syp0027/20230116-DDPC512*

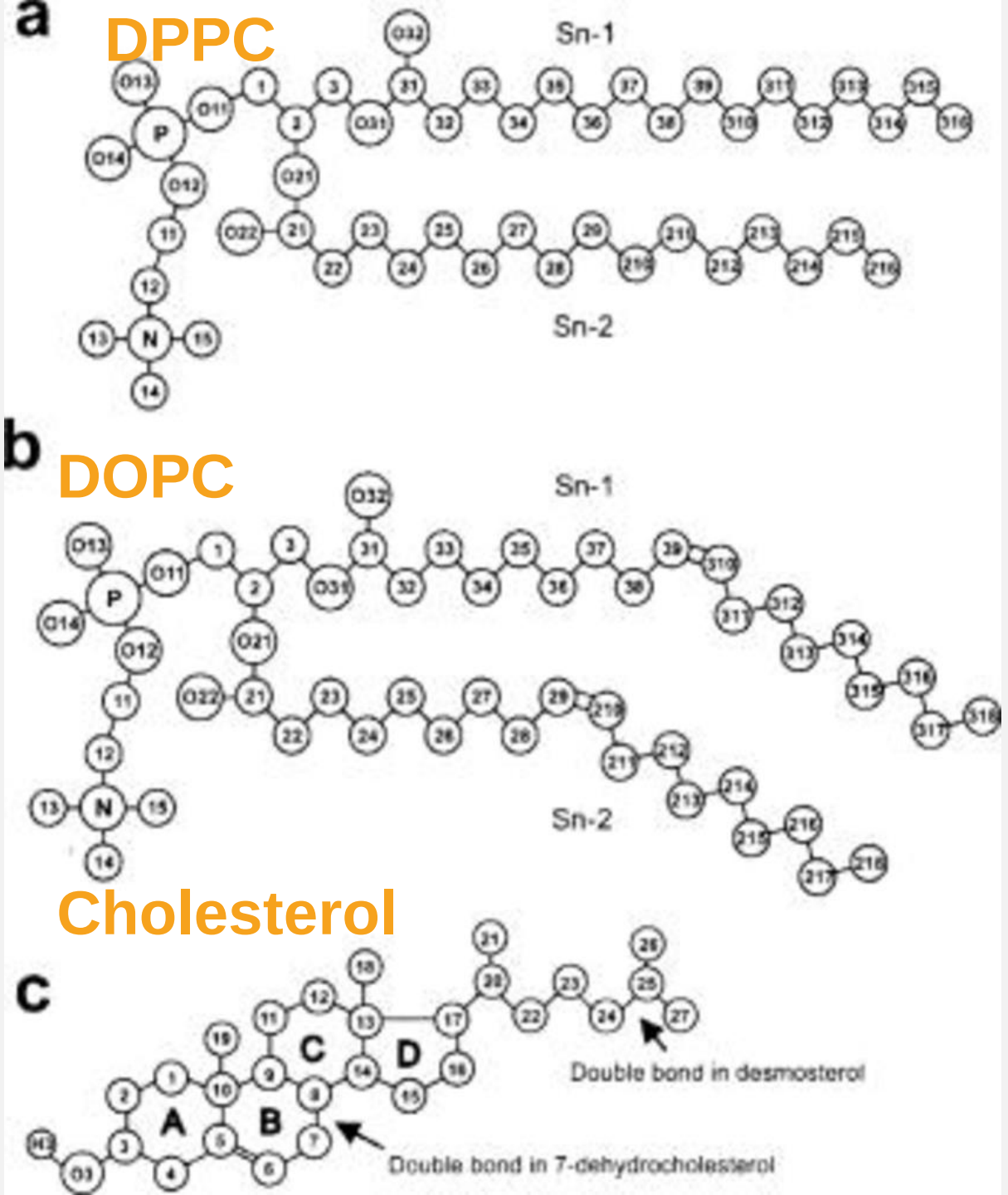


# Molecule Structure

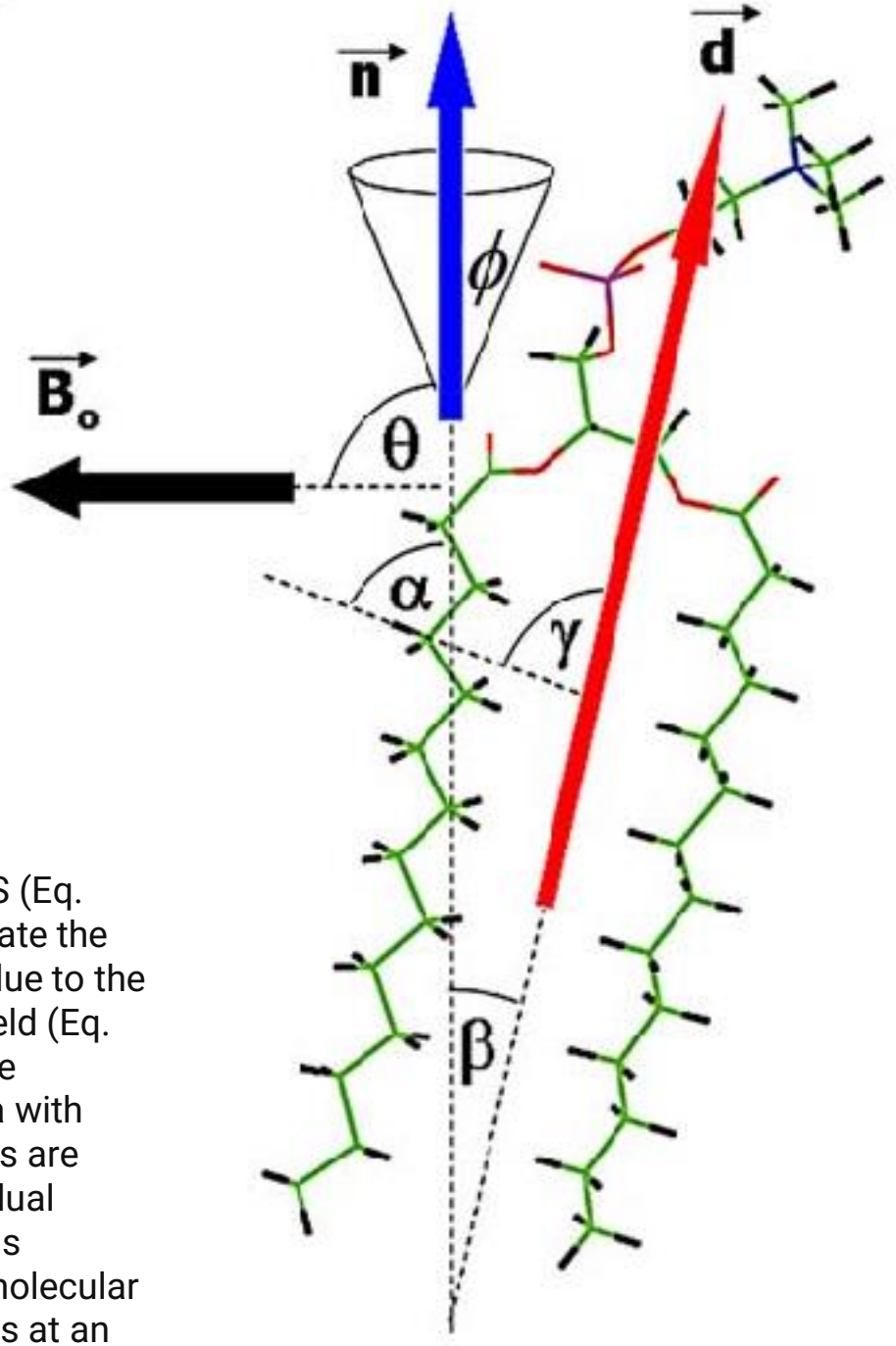
Figure 1. Molecular structures and assigned numbering of atoms for (*a*) DPPC and (*b*) DPPE. Chemical symbols are carbon (C), hydrogen (H), nitrogen (N), oxygen (O), and phosphorus (P).




Molecular structures of (a) DPPC, (b) DOPC, and (c) cholesterol molecules with numbering of atoms. The cholesterol rings are labeled A, B, C, and D. The chemical symbol for carbon atoms C is omitted. In desmosterol the bond C24–C25 is a double bond

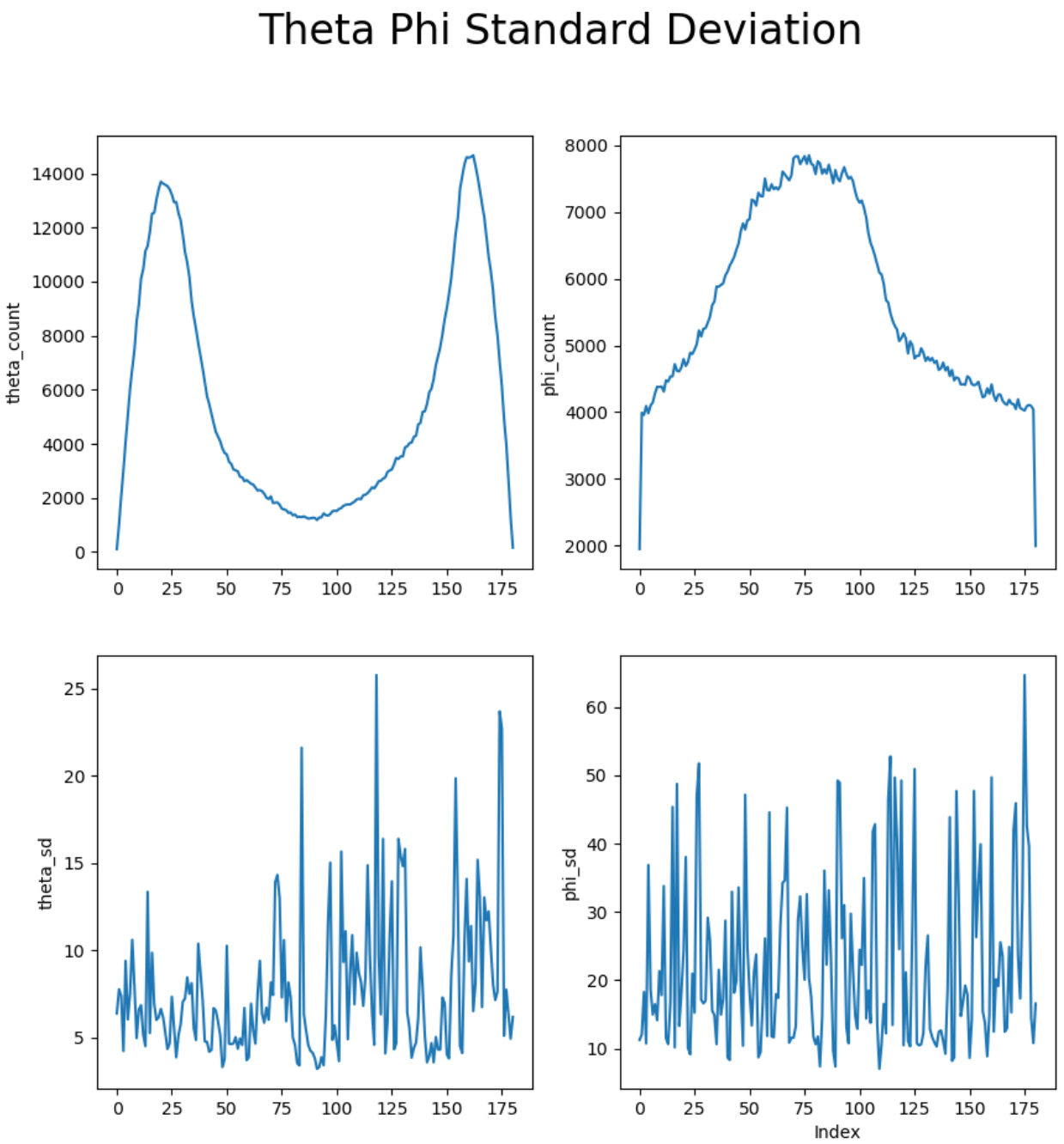


# Movie

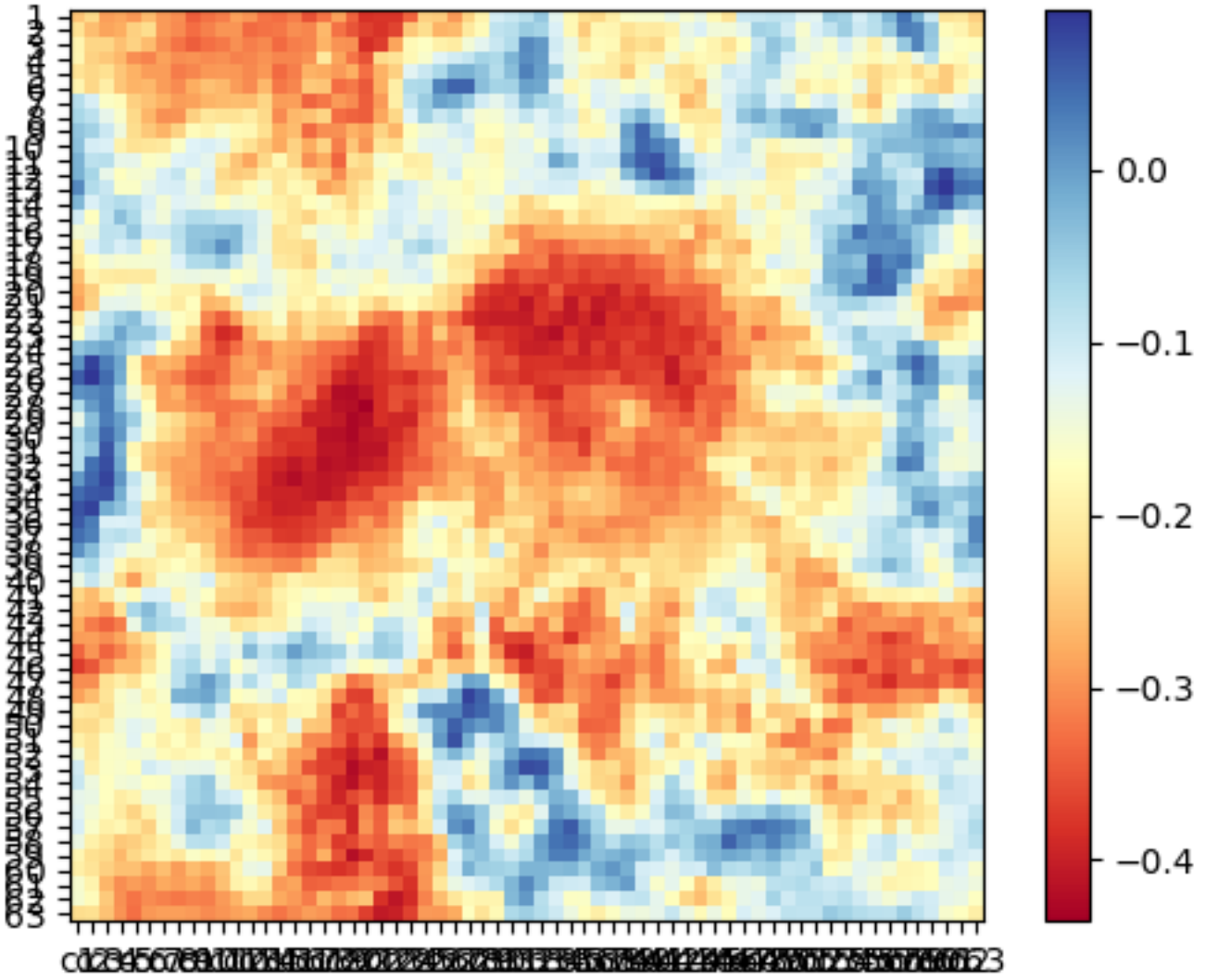



Visual representation of different contributions to the observed order parameter S (Eq. 2a). Fast rotations of lipids about the vector normal to the bilayer permit to separate the contribution to the order parameter due to this movement from the contribution due to the overall positioning of the oriented bilayer with respect to the external magnetic field (Eq. 2b). The bilayer normal, symbolized by the vector n, is oriented at an angle h to the external magnetic field B 0 (Eq. 2c). The observed CD vector is tilted at an angle a with respect to the bilayer normal (Eq. 2d). If the rotations of lipids about different axes are independent, the order parameter may be represented as the product of all individual contributions (Eq. 2e). The bilayer normal is subject to fluctuations, shown here as wobbling of the vector n within a cone, characterized by an angle / (Eq. 2f). The molecular director d is at an angle b to the bilayer normal (Eq. 2g). The observed CD vector is at an angle c with respect to the molecular director (Eq. 2h)

# Heatmap


Theta Phi Standard Deviation
theta_count
phi_count
theta_sd
phi_sd
Index

# Heatmap

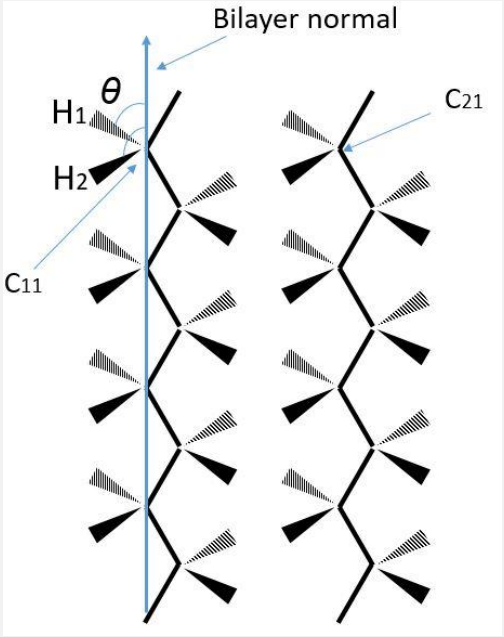


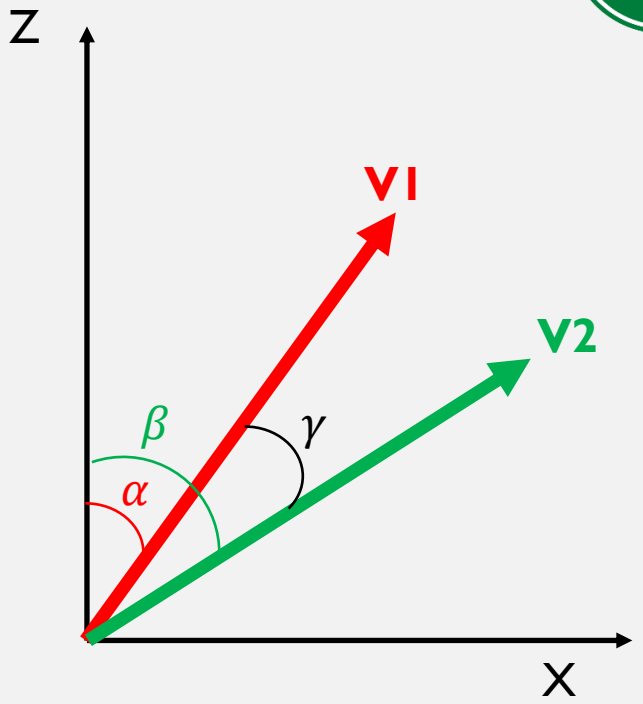
# Dot product

$$\mathbf{a} \cdot \mathbf{b} = |\mathbf{a}| \times |\mathbf{b}| \times \cos(\theta)$$

$$\mathbf{a} \cdot \mathbf{b} = a_x \times b_x + a_y \times b_y + a_z \times b_z$$

$$Scd = \frac{3\cos^2\theta - 1}{2}$$

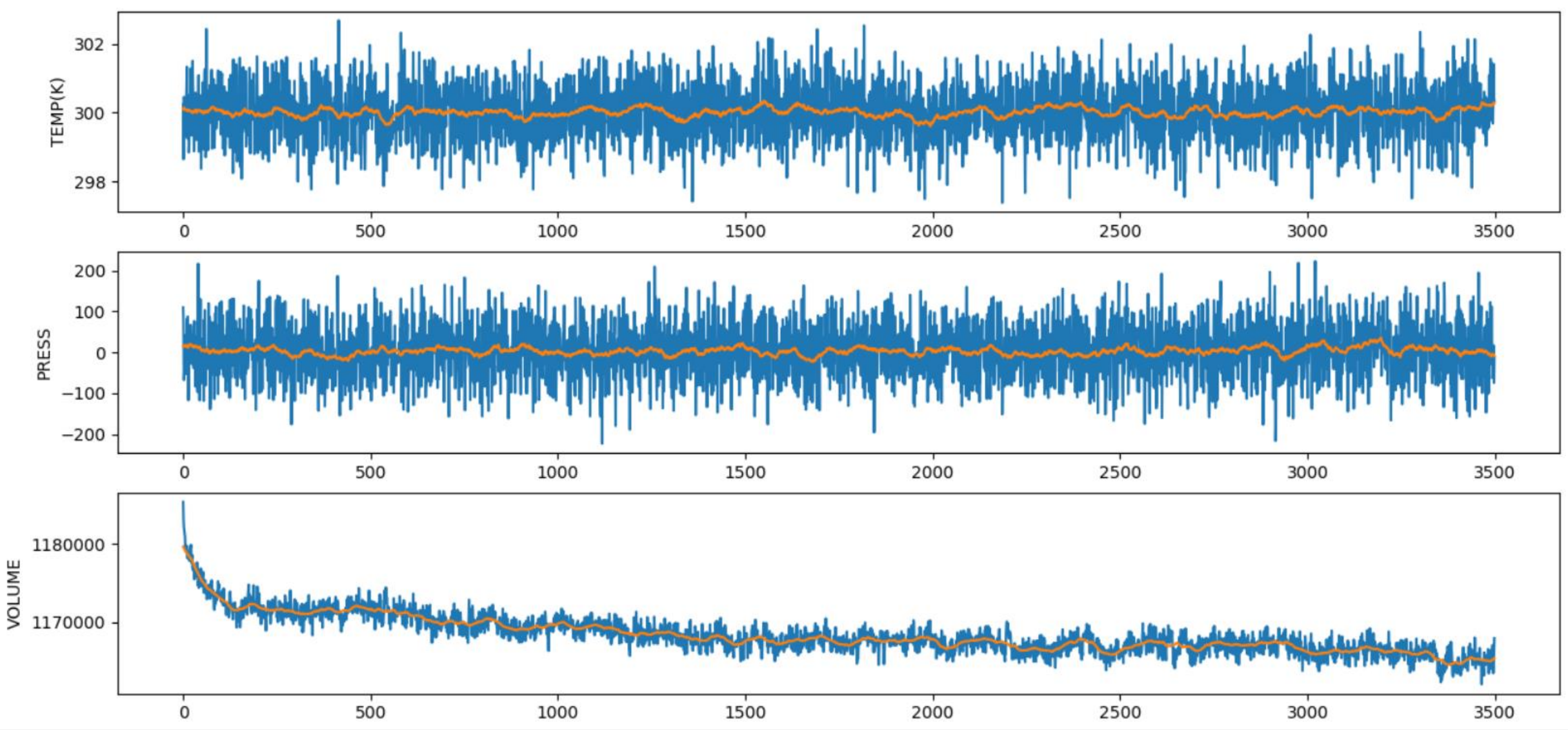



But line 118 in SCD.py file

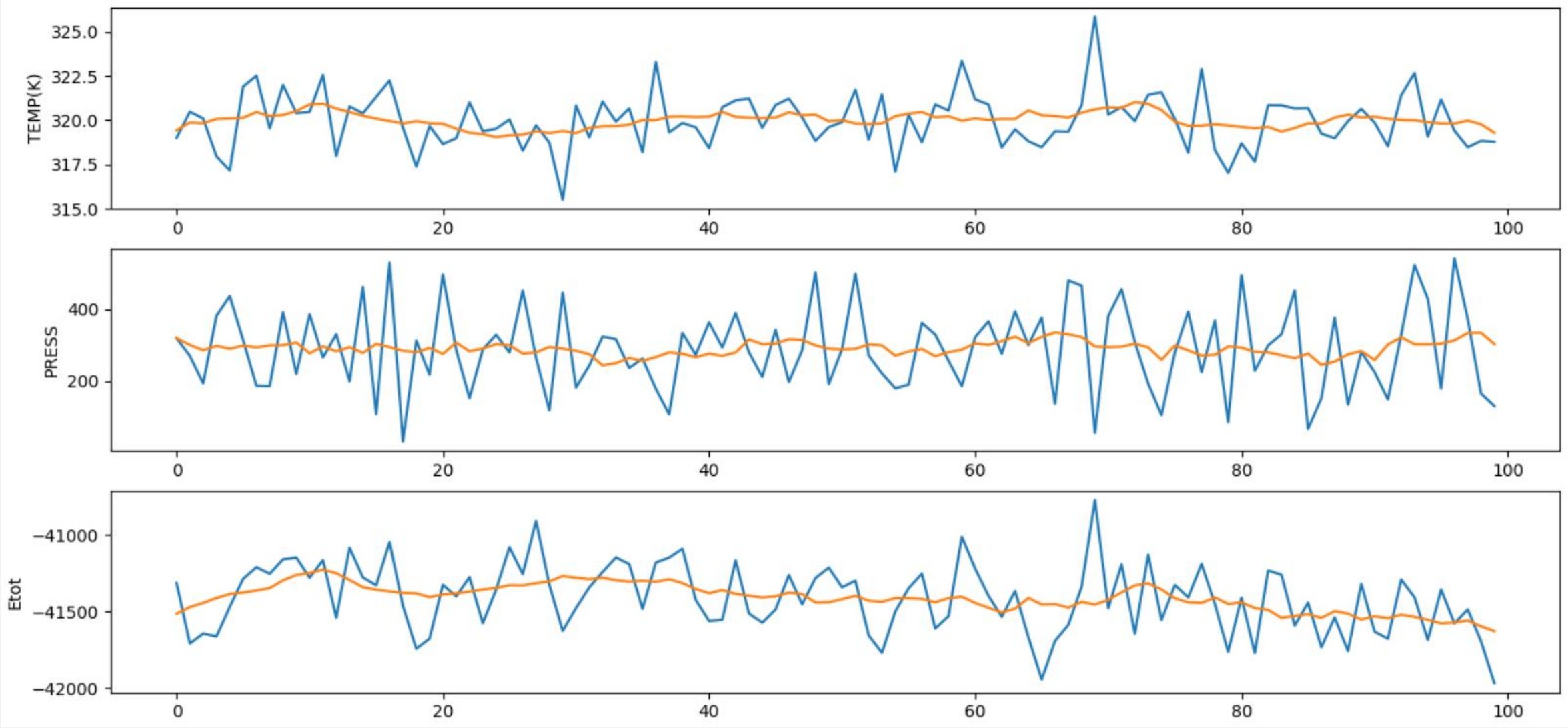
$$Scd = \frac{\frac{3\cos^2\theta}{2} - 1}{2}$$

# 04 Pressure Plot



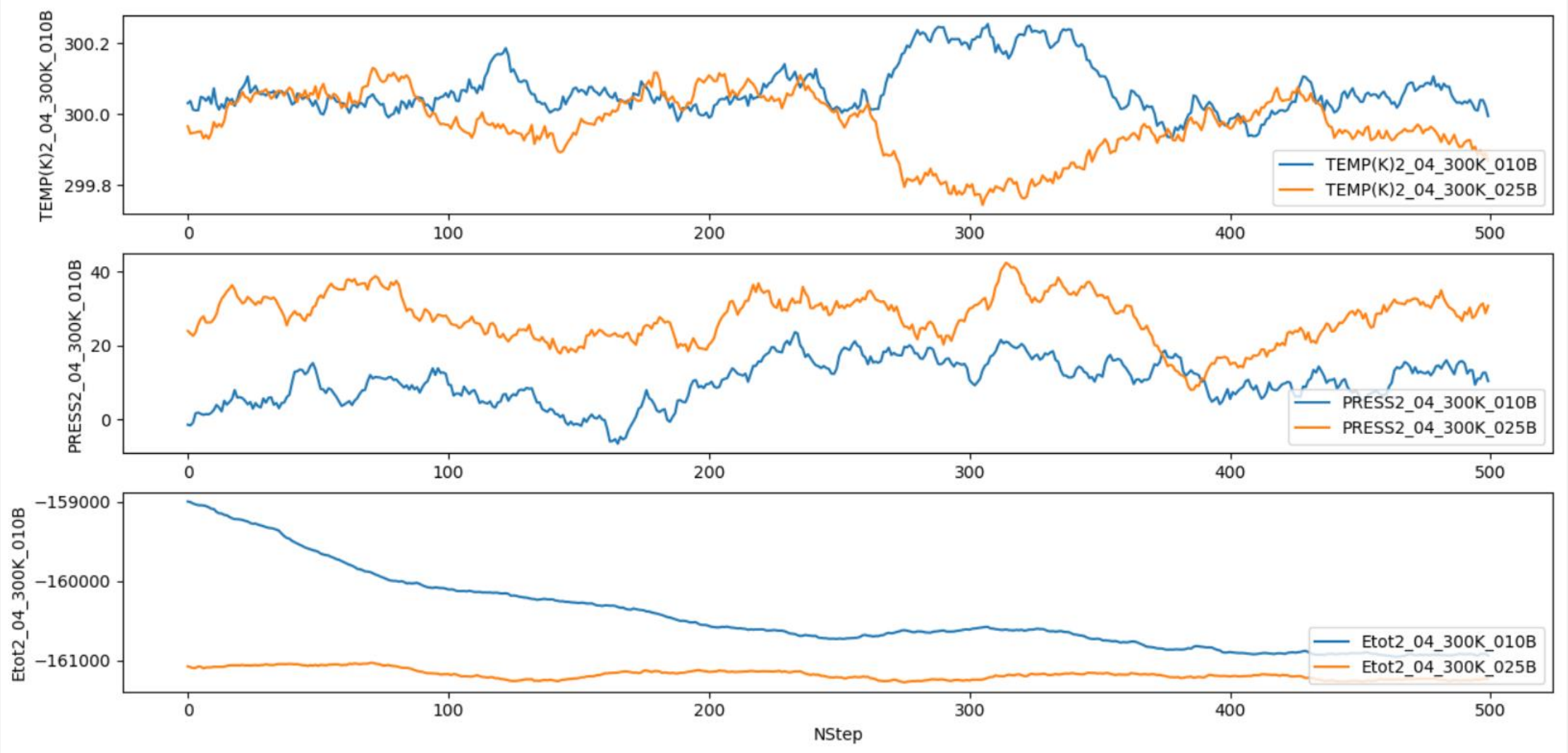

Every 500 steps is a single file. For instance, 0-500 is 04_300K_010B.out and 501-1000 is 04_300K_050B.out. The graph has plotted the energy, temperature, and PRESS. The orange line represents a 51 moving average curve, while the blue line represents the original data points.

# Alireza 04 Pressure Graph



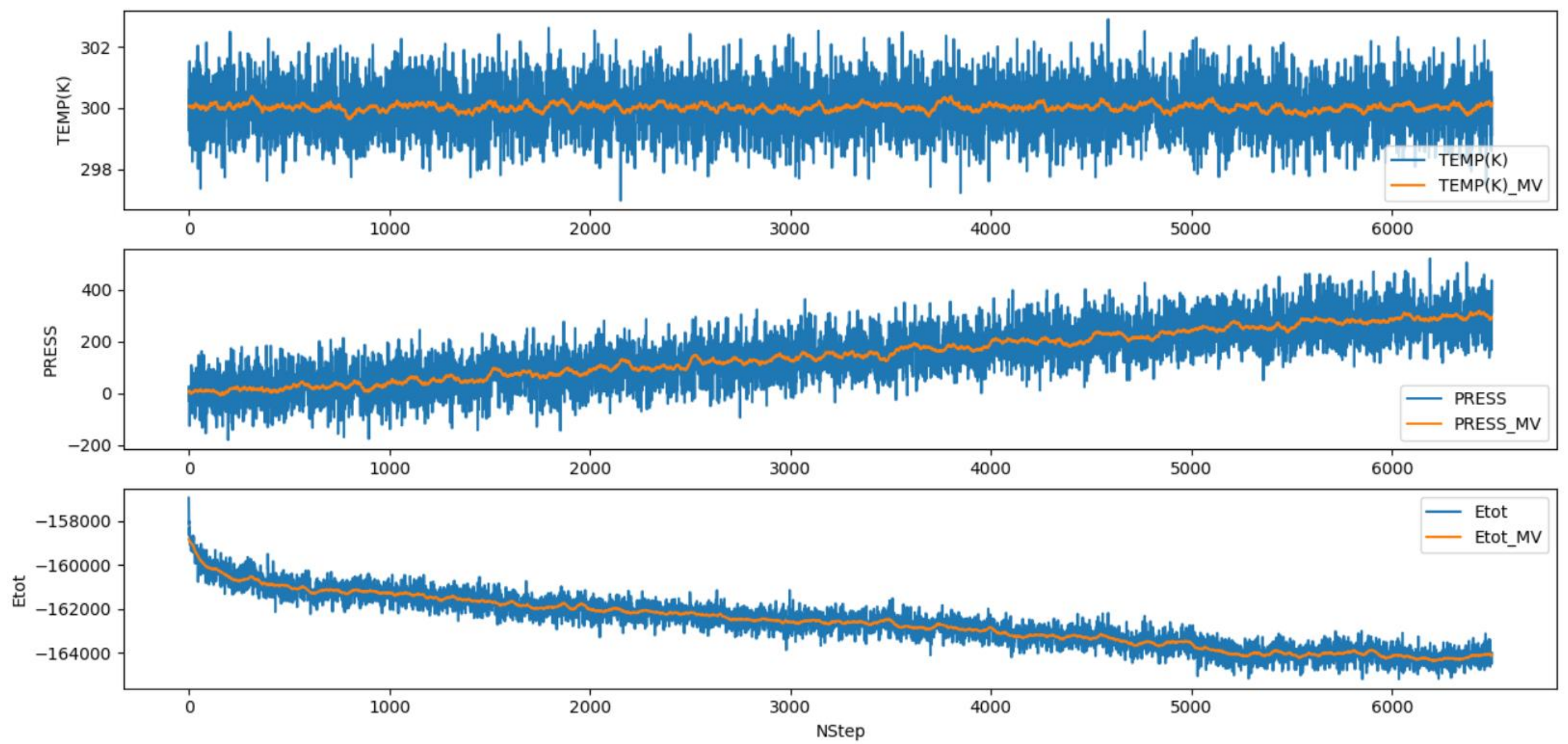

Graph for energy, temperature, and PRESS of 04_Pressure_275_8.out located at /storage/group/yan/backup/Alireza_Javadi/Computational/DPPC. One thing to note is that PRESS fluctuates often, with a range between 400 and 0. The orange line represents a 11 moving average curve, while the blue line represents the original data points.

# Pressure Verification



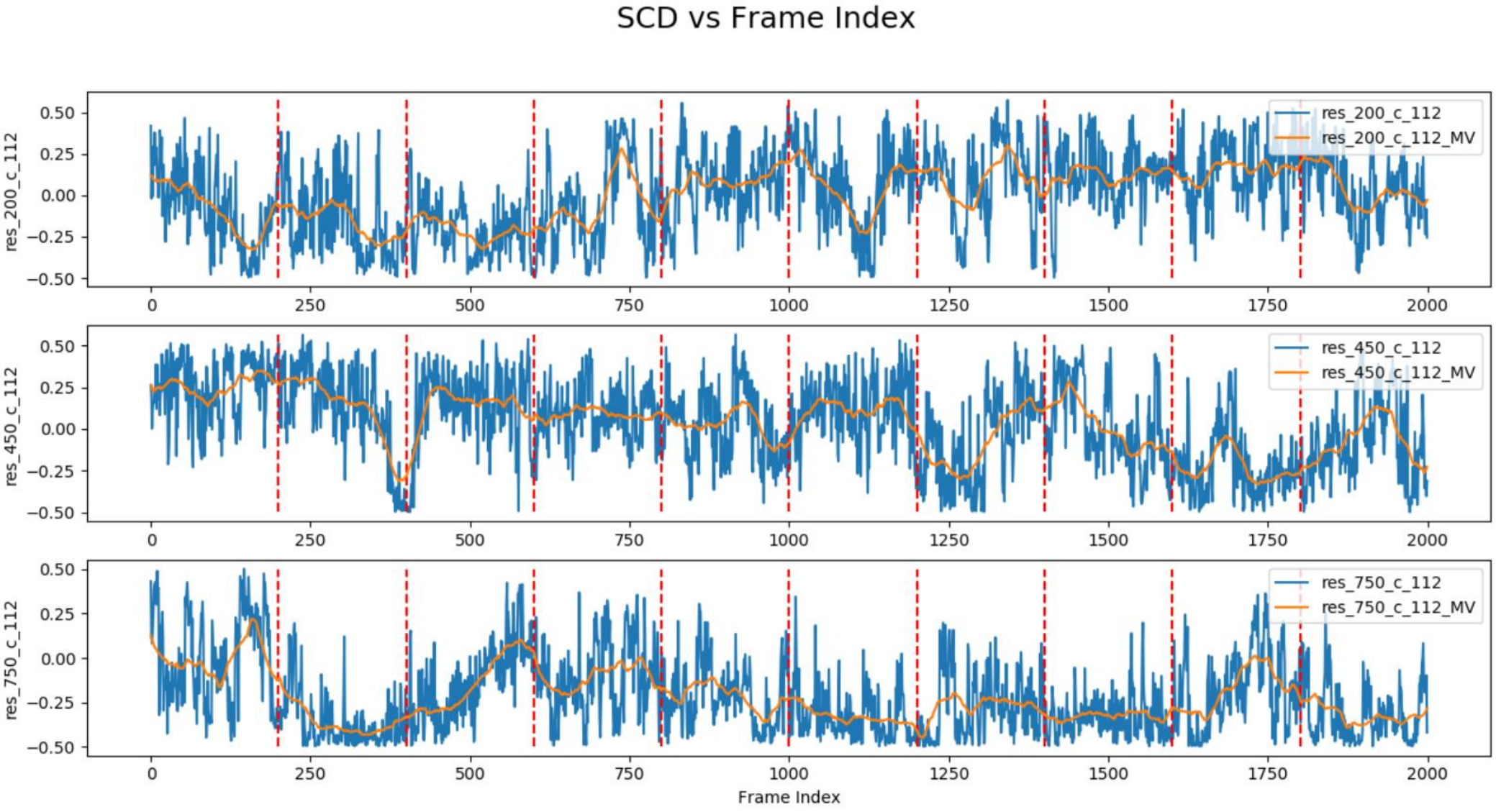

The graph above compares the 71-point moving average for the newly run 04_300K_010B.out and 04_300K_025B.out. It shows that the average pressures is 25 bars for the 04_300K_025B.out file and 10 bars for the 04_300K_010B.out file, which is consistent with the design. Thus, our implementation is correct.

# 04 Pressure Plot Verification



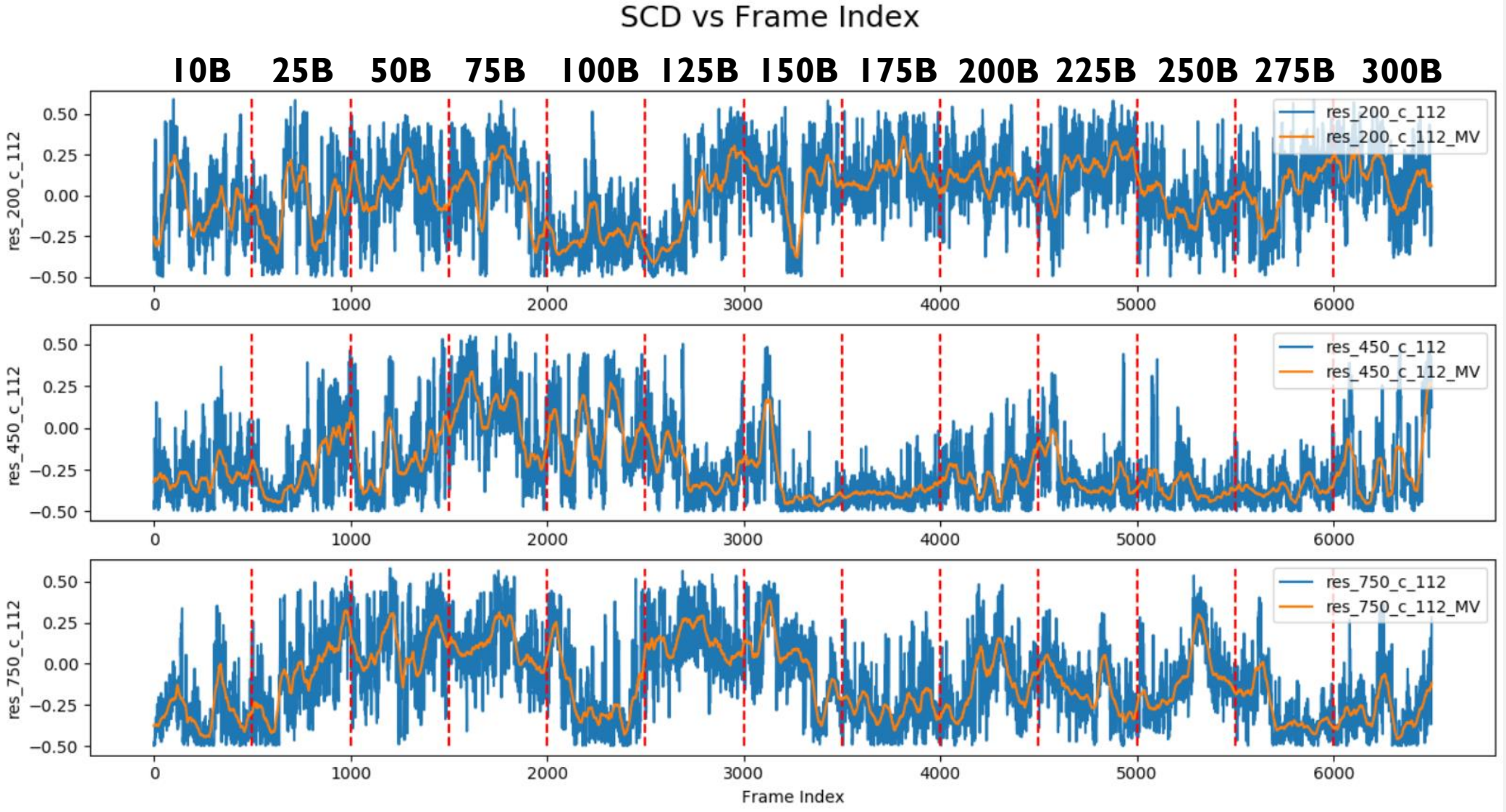

After running the 04 input files again with the modified changes and graphing the results, we can see that the output files have generated the desired pressure, temperature, and energy amounts. The orange line represents the 51-point moving average of the output files and the blue lines represent the original data.

# SCD vs Frame Index Graph from 06



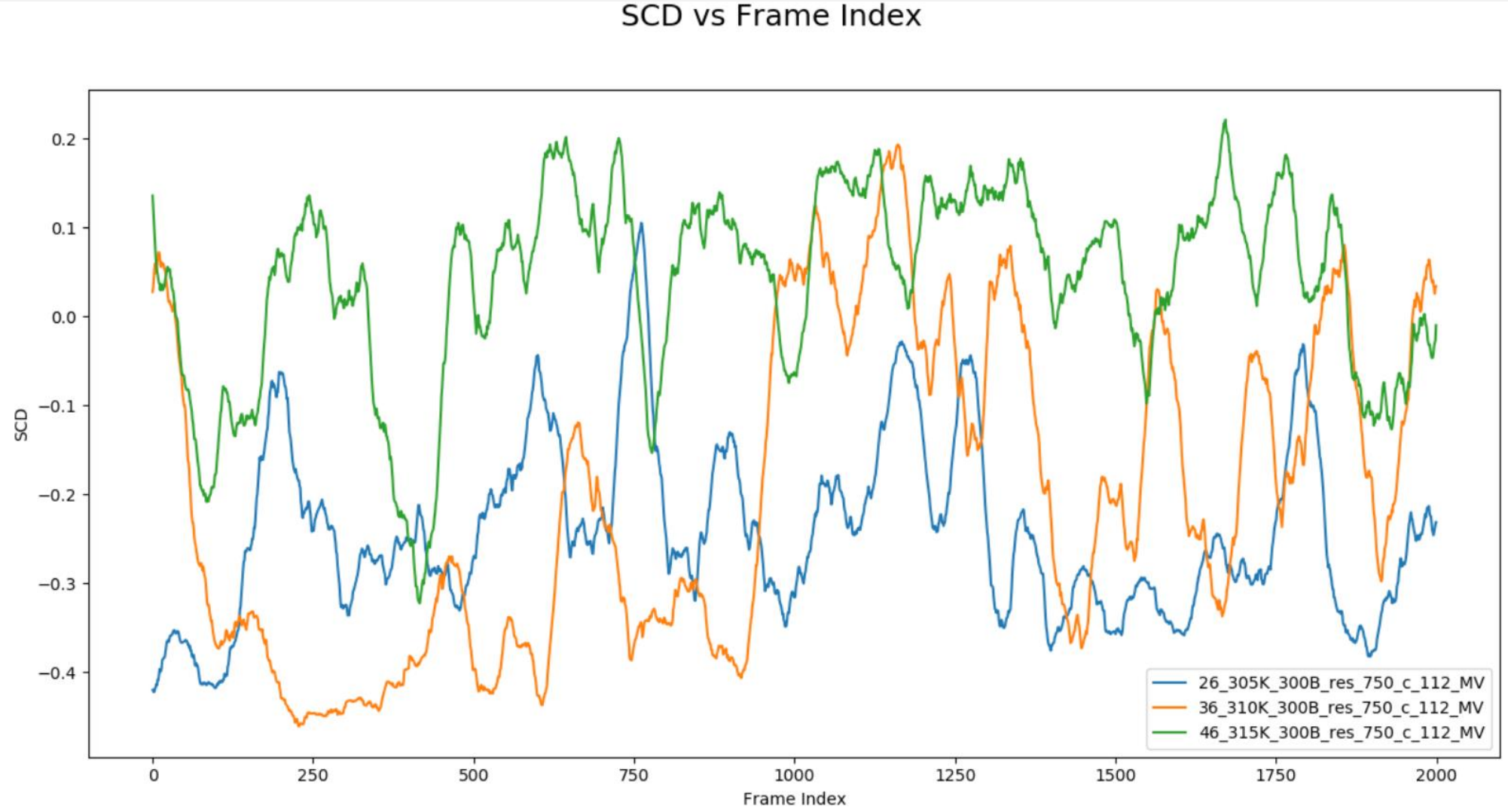

The graph represents the SCD plot for carbon 112 in three residues from the 06 stage. The blue line represents the original data points while the orange line represents the 51-point moving average. The data within the red lines are from different files. The data points are confusing, however, in that they are, in general, negative when we expect them to be positive.

# SCD vs Frame Index Graph from 04



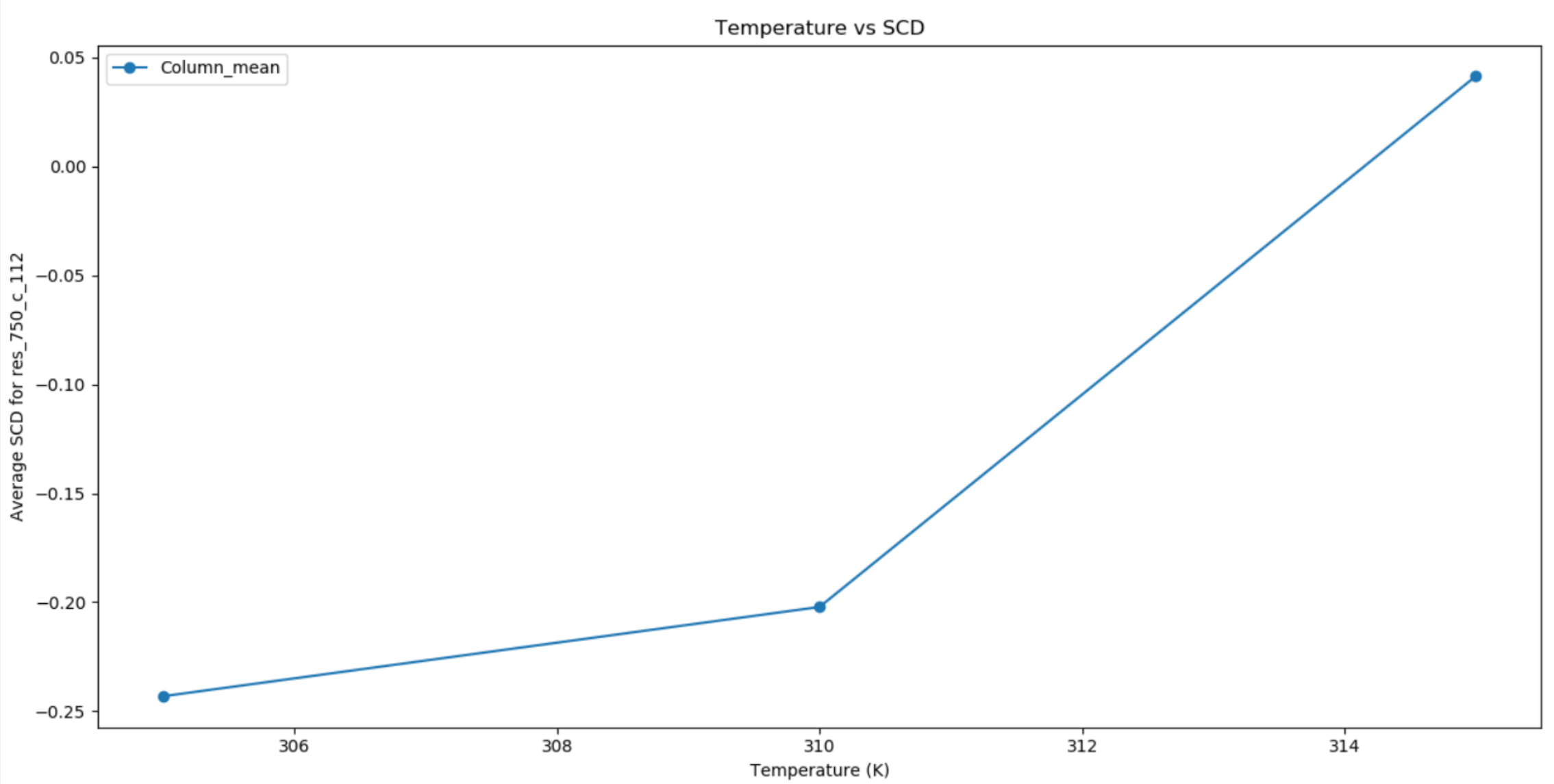

The graph represents the SCD plot for carbon 112 in three residues from the 04 stage. The blue line represents the original data points while the orange line represents the 51-point moving average. The data within the red lines are from different files. The data points are confusing, however, in that although the pressure is ramped for every file, the SCD does not increase with pressure.

# SCD vs Temperature Graph



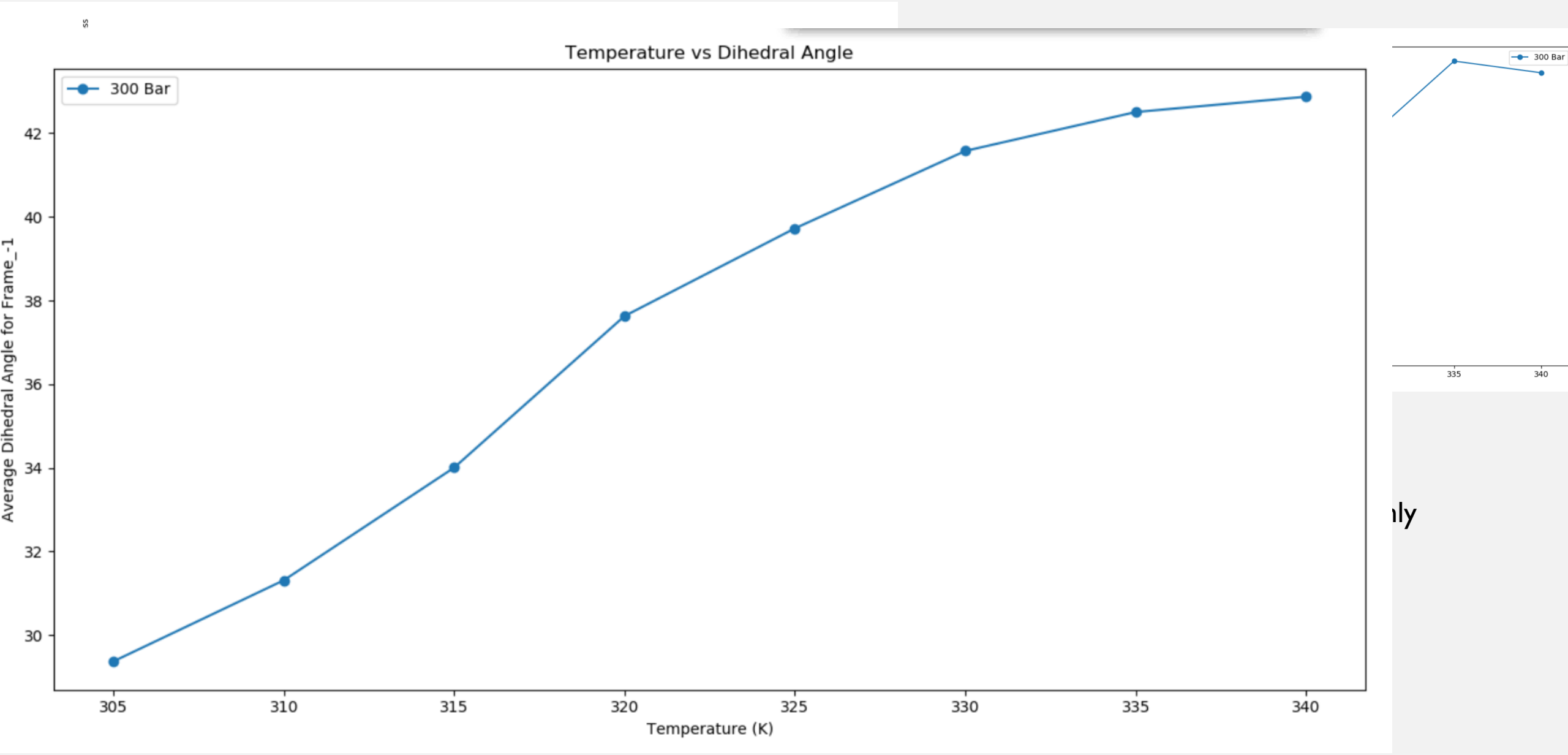

In this graph, we can see that the overall SCD for 46_315K_300B was greater than 26_305K_300B and 36_310K_300B. Note that 46_315K_300B_res_750_c_112_MV means that the SCD value is the moving average from carbon 112 in PA residue 750 from file 46_315k_300B. This is the same for 26 and 36.

# Temperature vs SCD graph




In this graph, there are 3 points that represent the means of carbon 112 in residue 750 in 3 files: 26_305K_300B, 36_310K_300B, and 46_315K_300B. Note that while the pressure was kept constant at 300B, the temperature increased from 300 to 315 in intervals of 3, which the means of such outputs are displayed on the graph.

# Minimization







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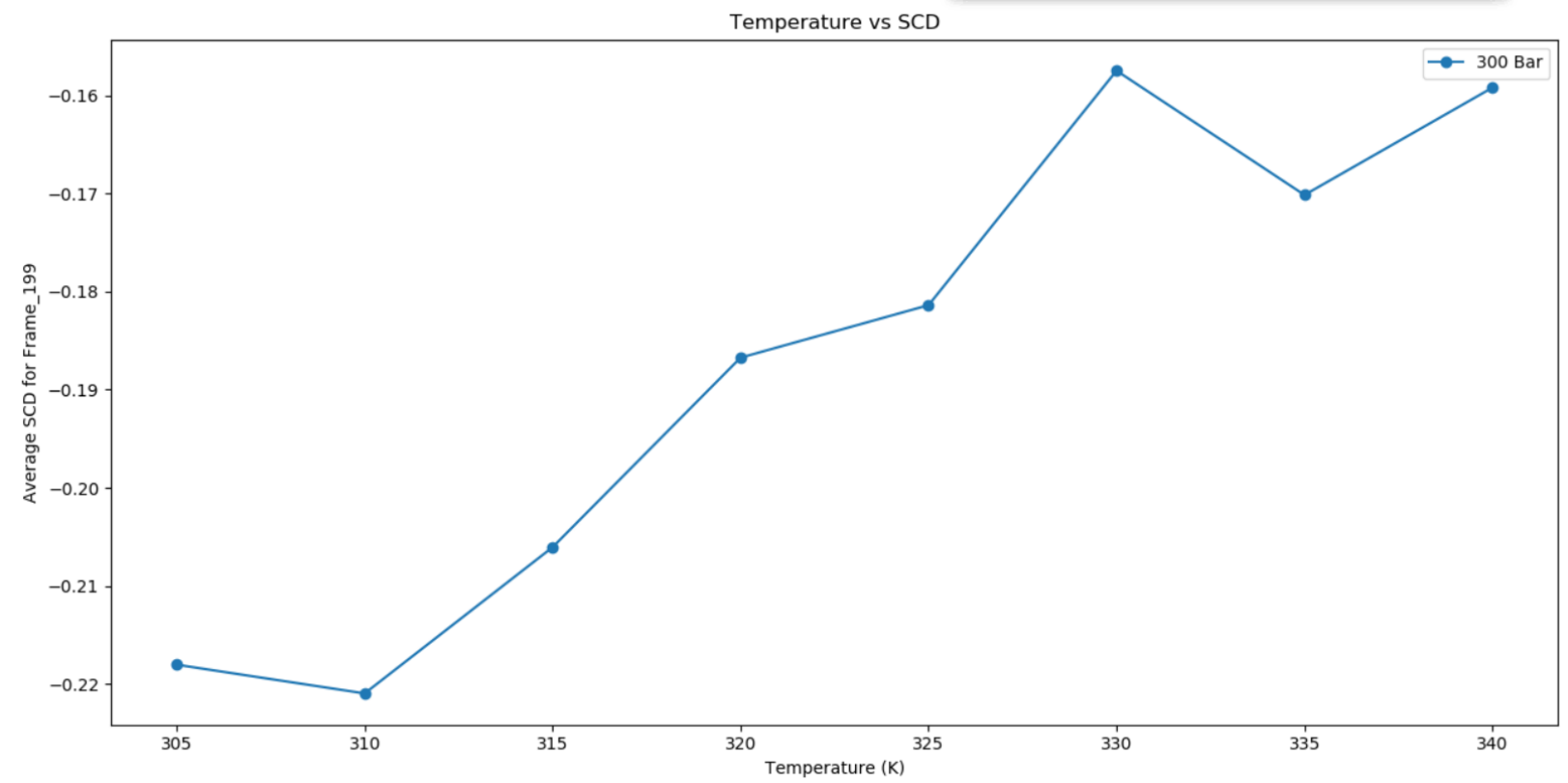
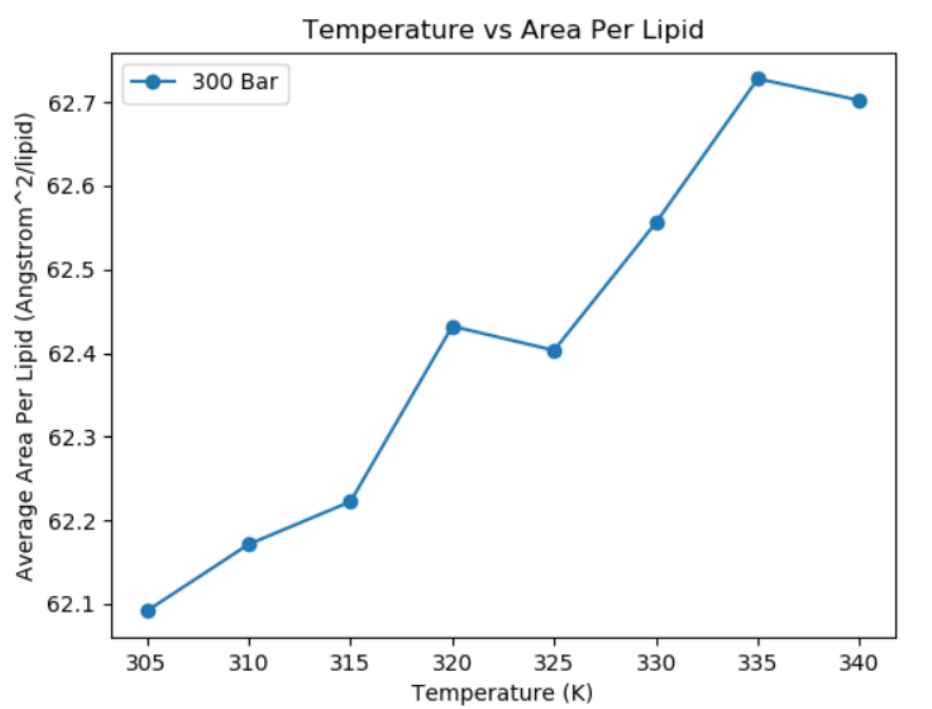
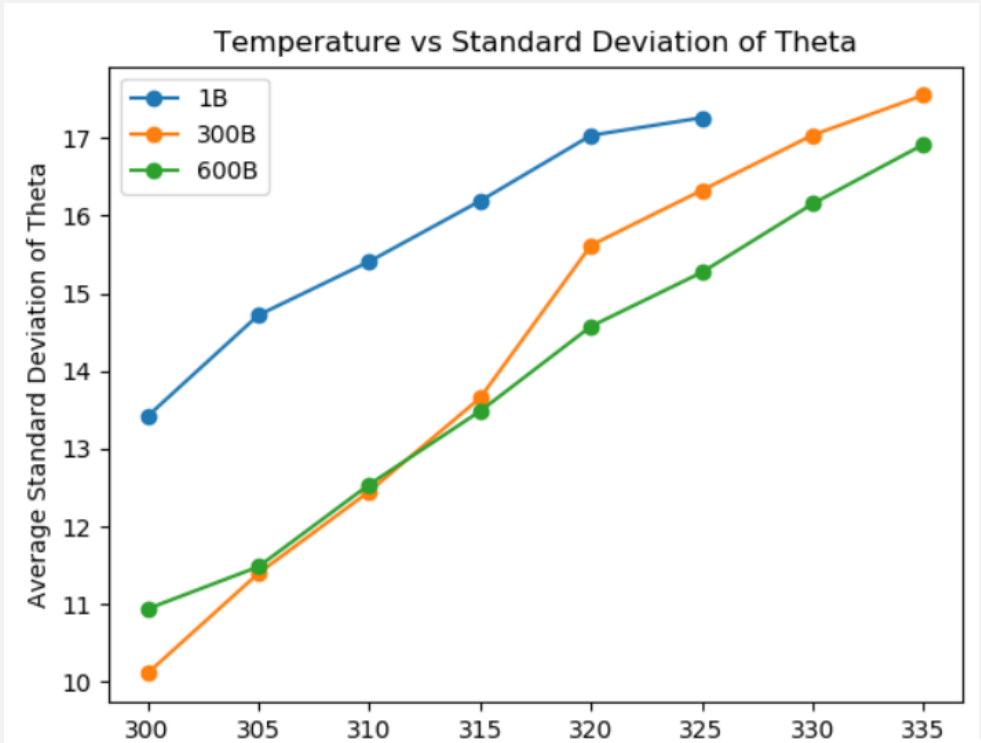
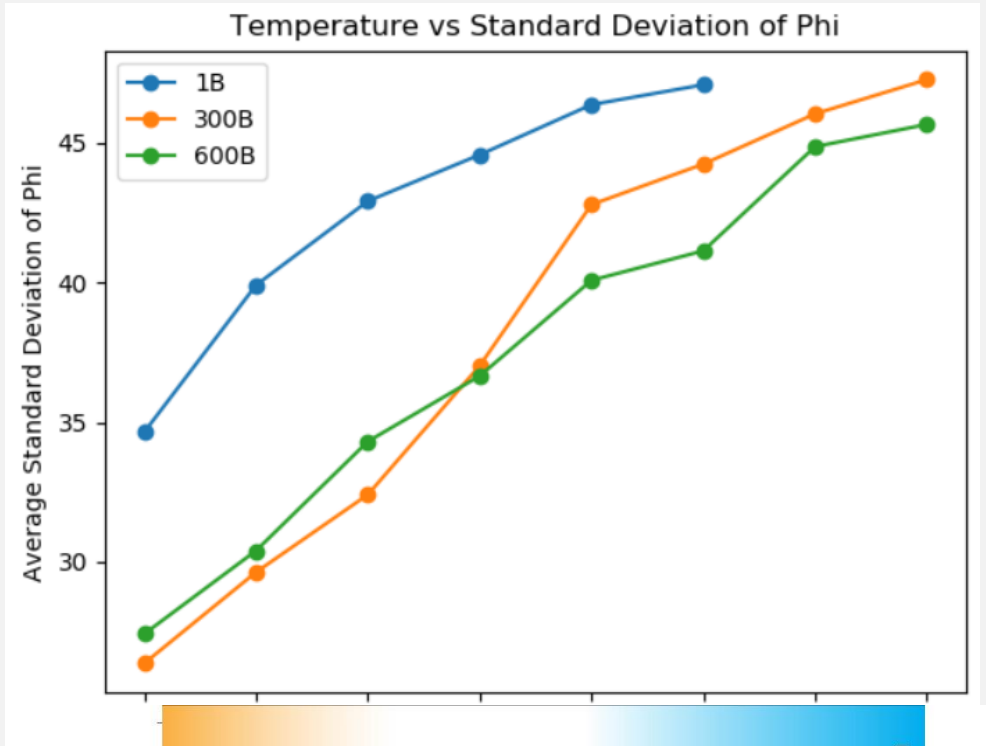
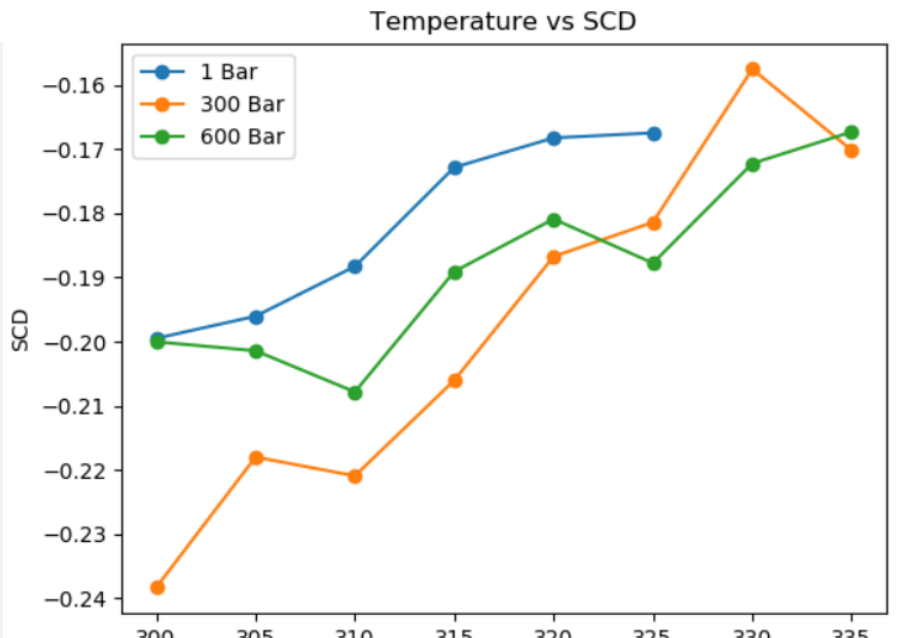
# Minimization

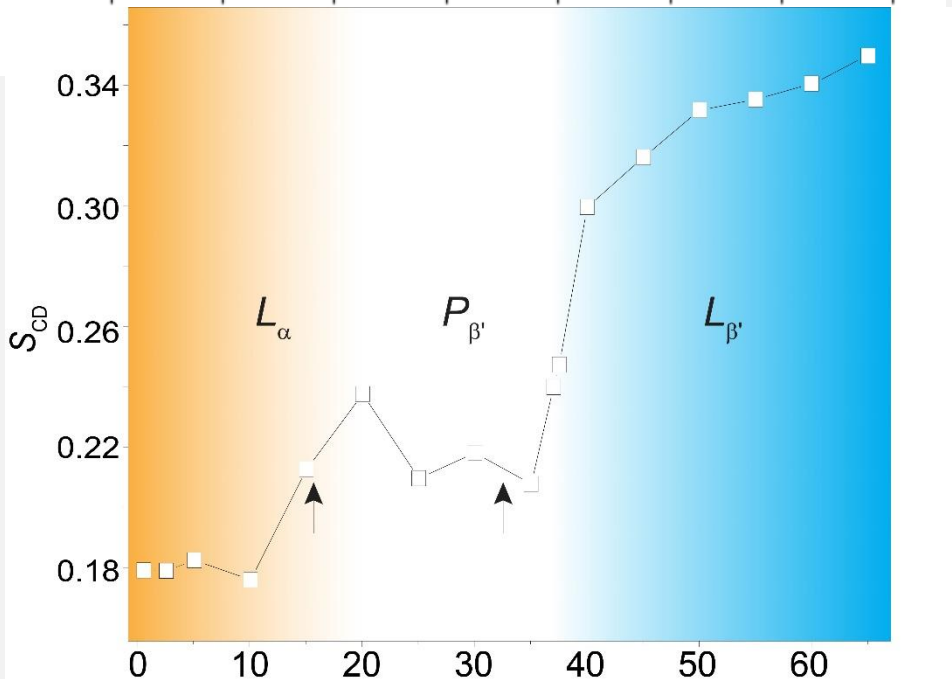


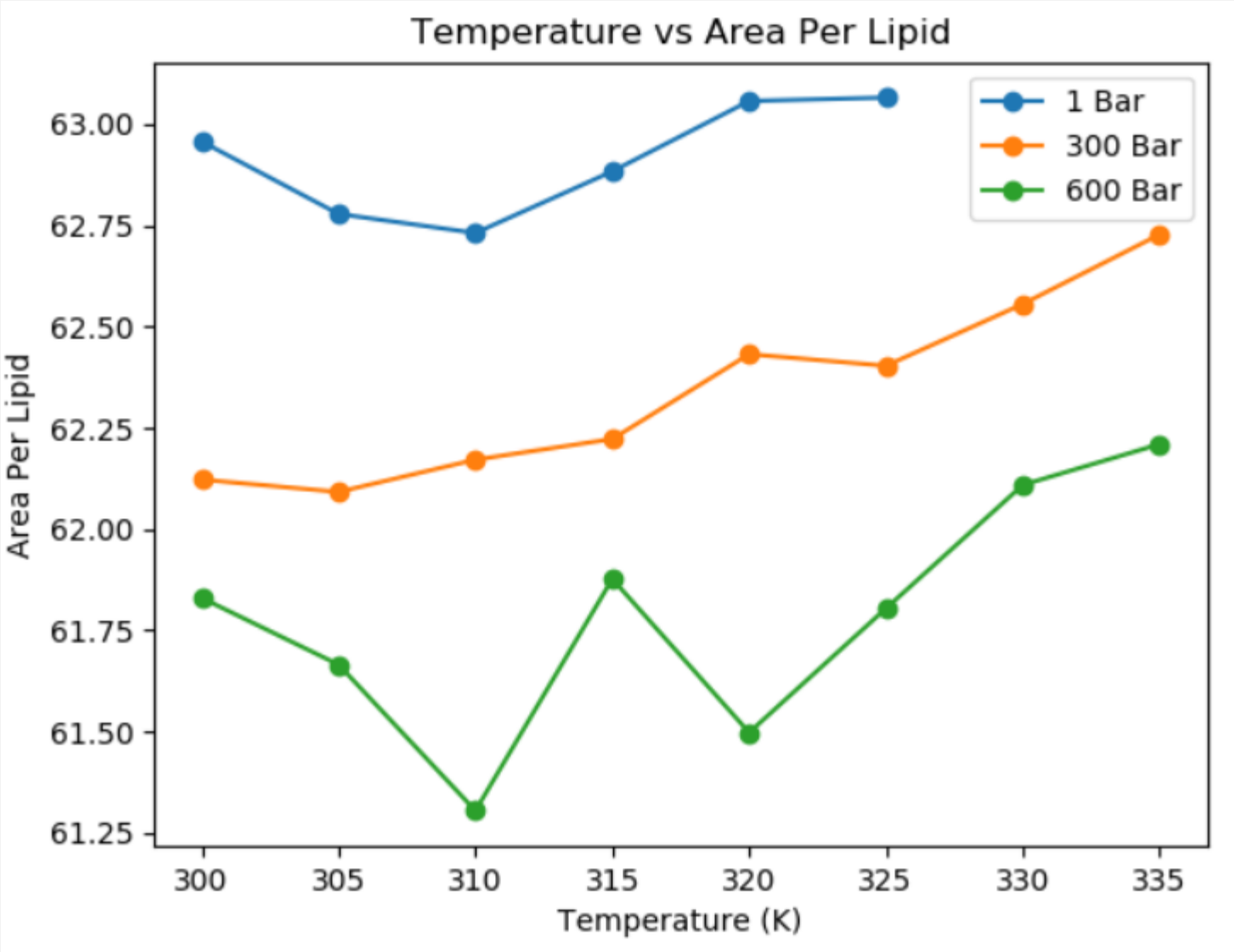

Temperature vs Standard Deviation of Theta
Average Standard Deviation of Theta
1B
300B
600B
10
11
12
13
14
15
16
17
300
305
310
315
320
325
330
335


Temperature vs Standard Deviation of Phi
Average Standard Deviation of Phi
1B
300B
600B
30
35
40
45

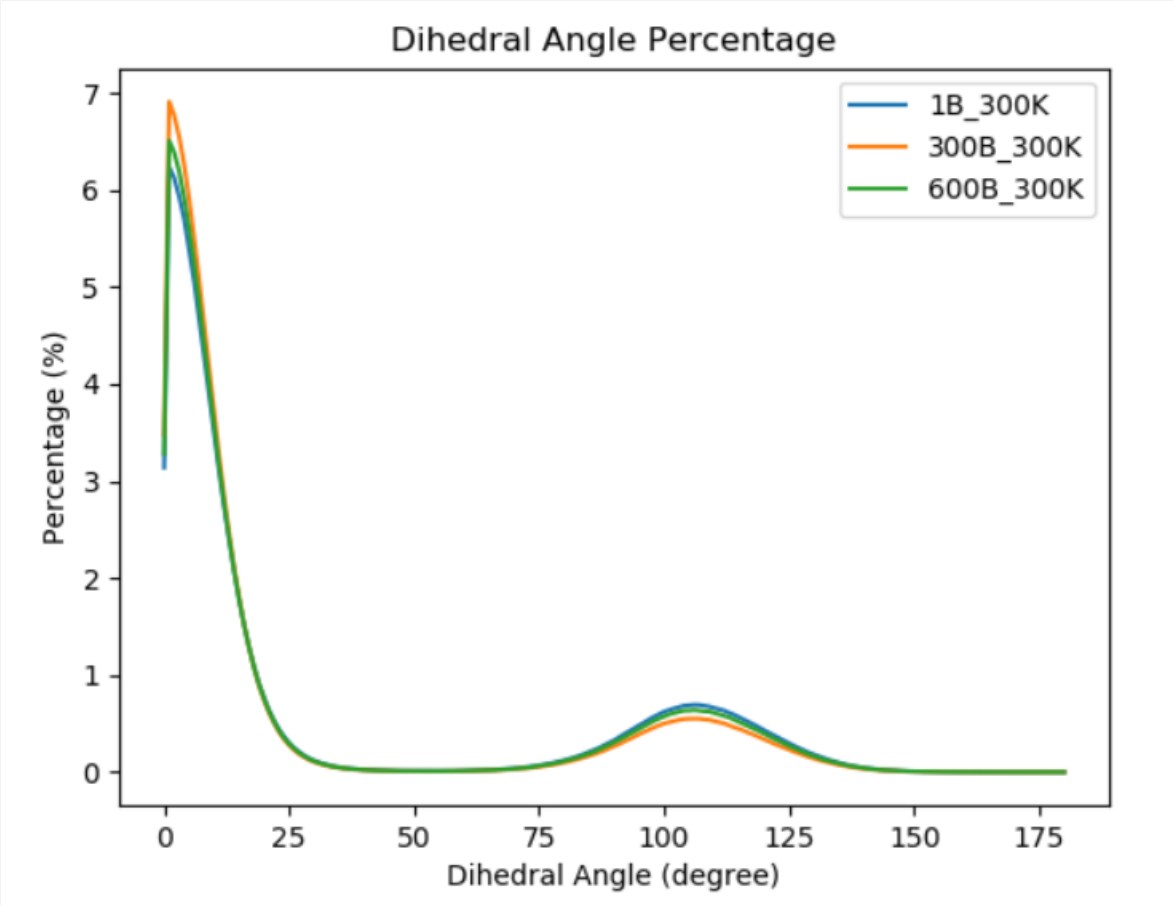

Temperature vs SCD
SCD
1 Bar
300 Bar
600 Bar
−0.16
−0.17
−0.18
−0.19
−0.20
−0.21
−0.22
−0.23
−0.24

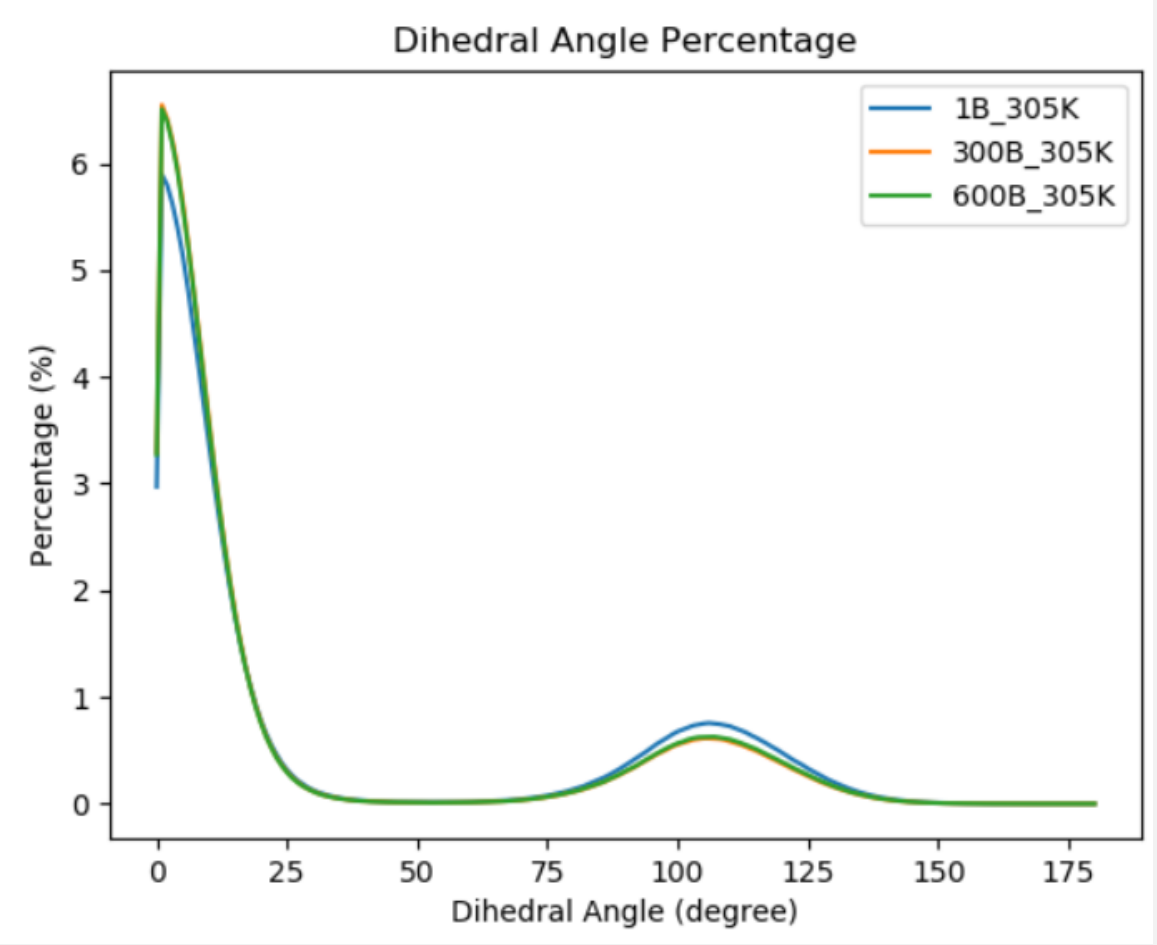

$S_{CD}$
0.18
0.22
0.26
0.30
0.34
$L_\alpha$
$P_{\beta'}$
$L_{\beta'}$
0
10
20
30
40
50
60

# Minimization

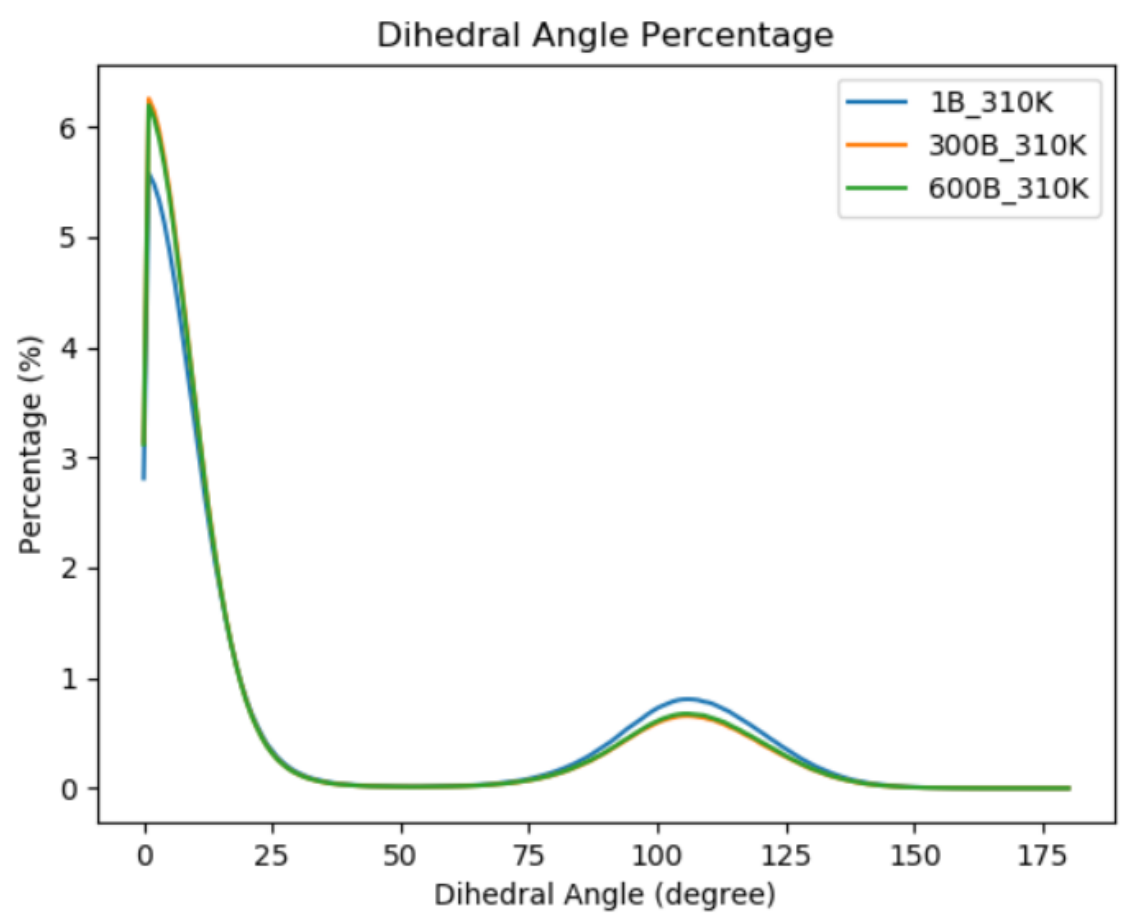


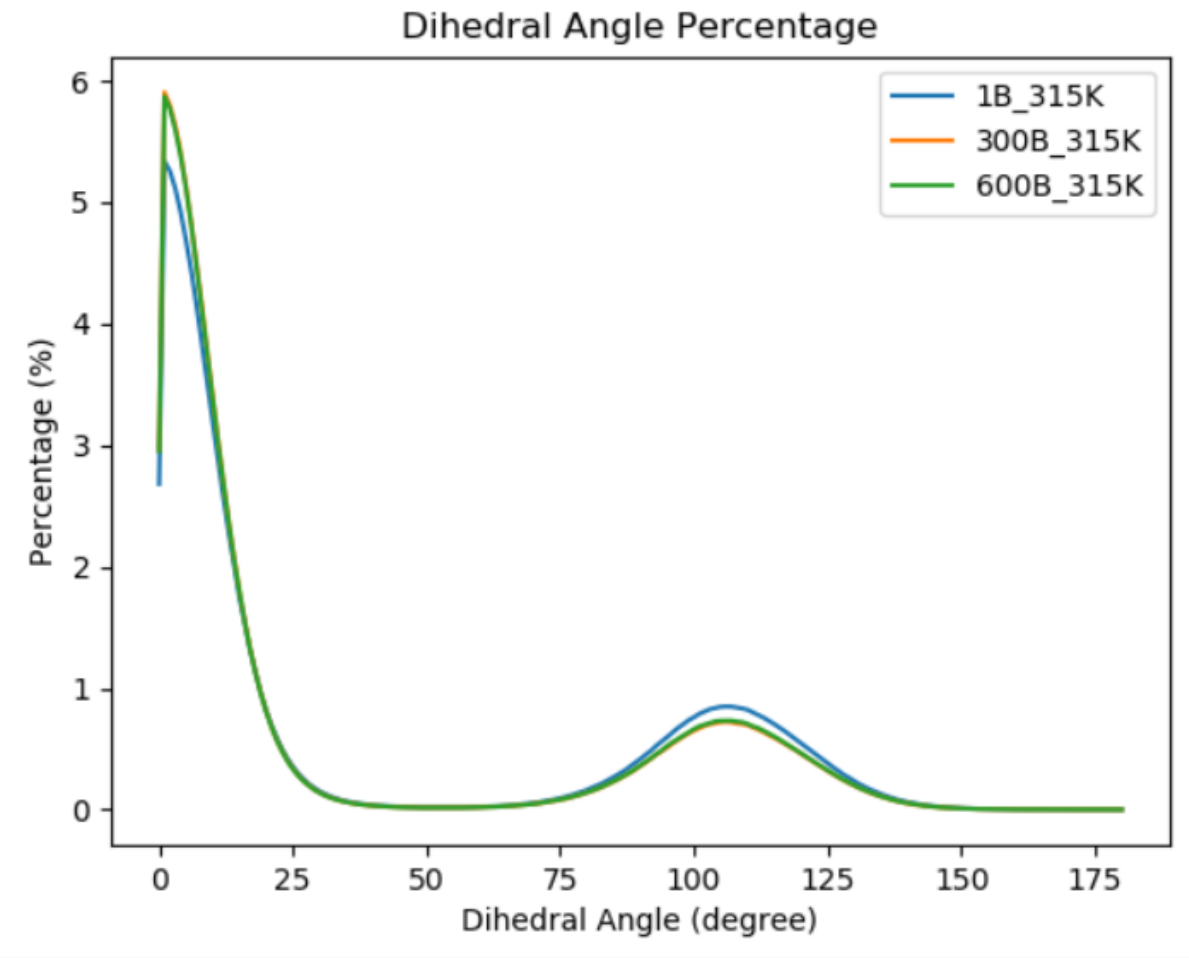
# Minimization



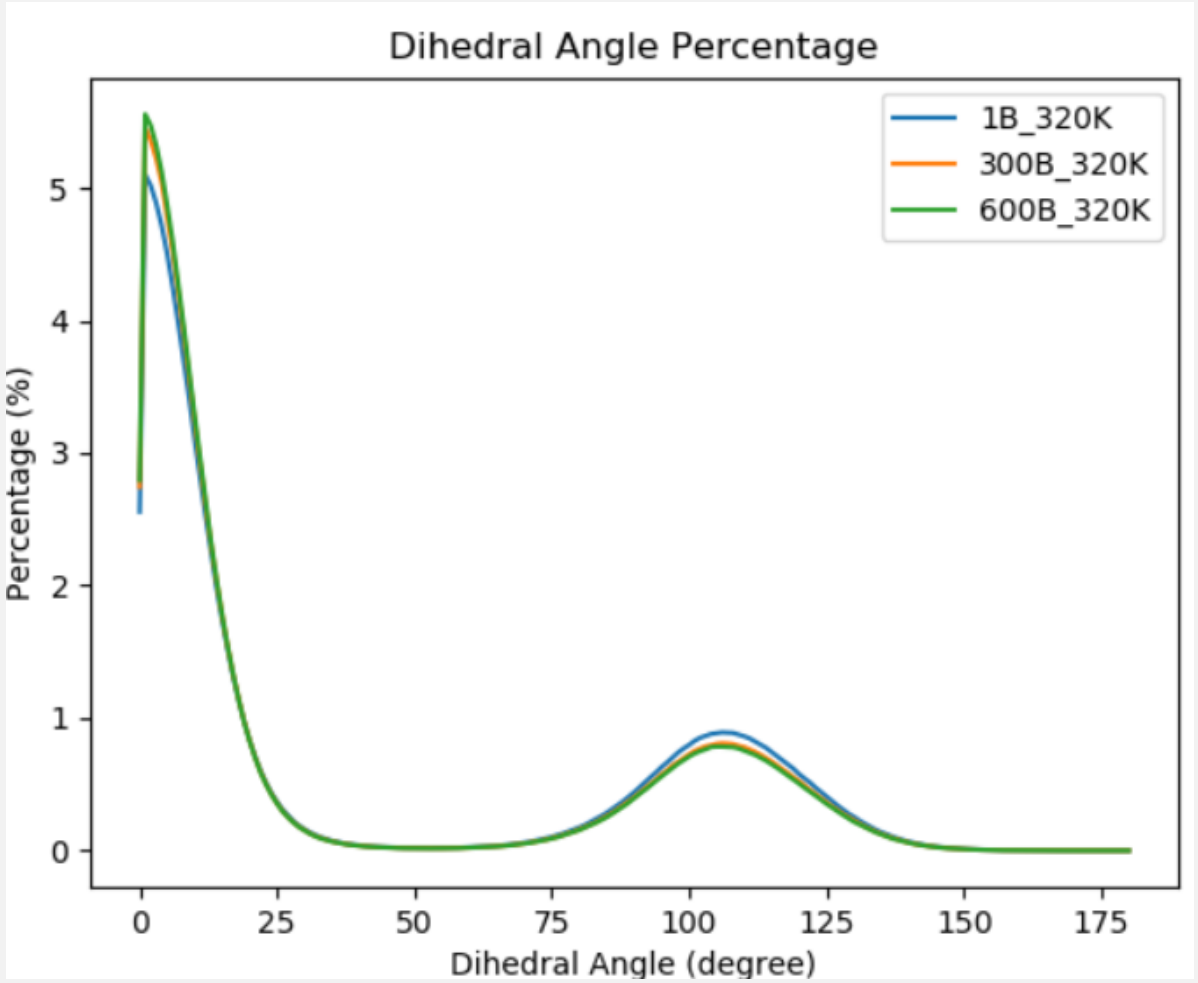



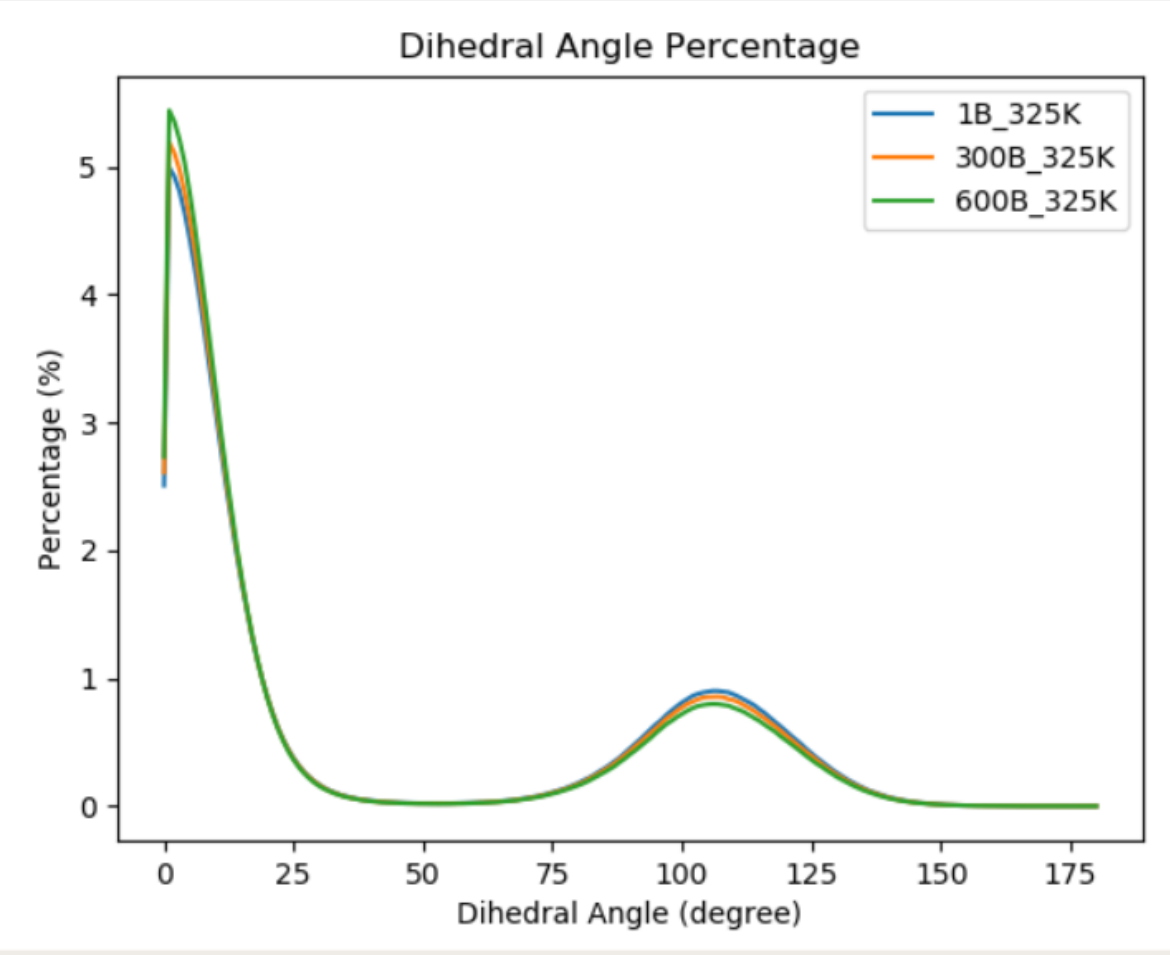
# Minimization



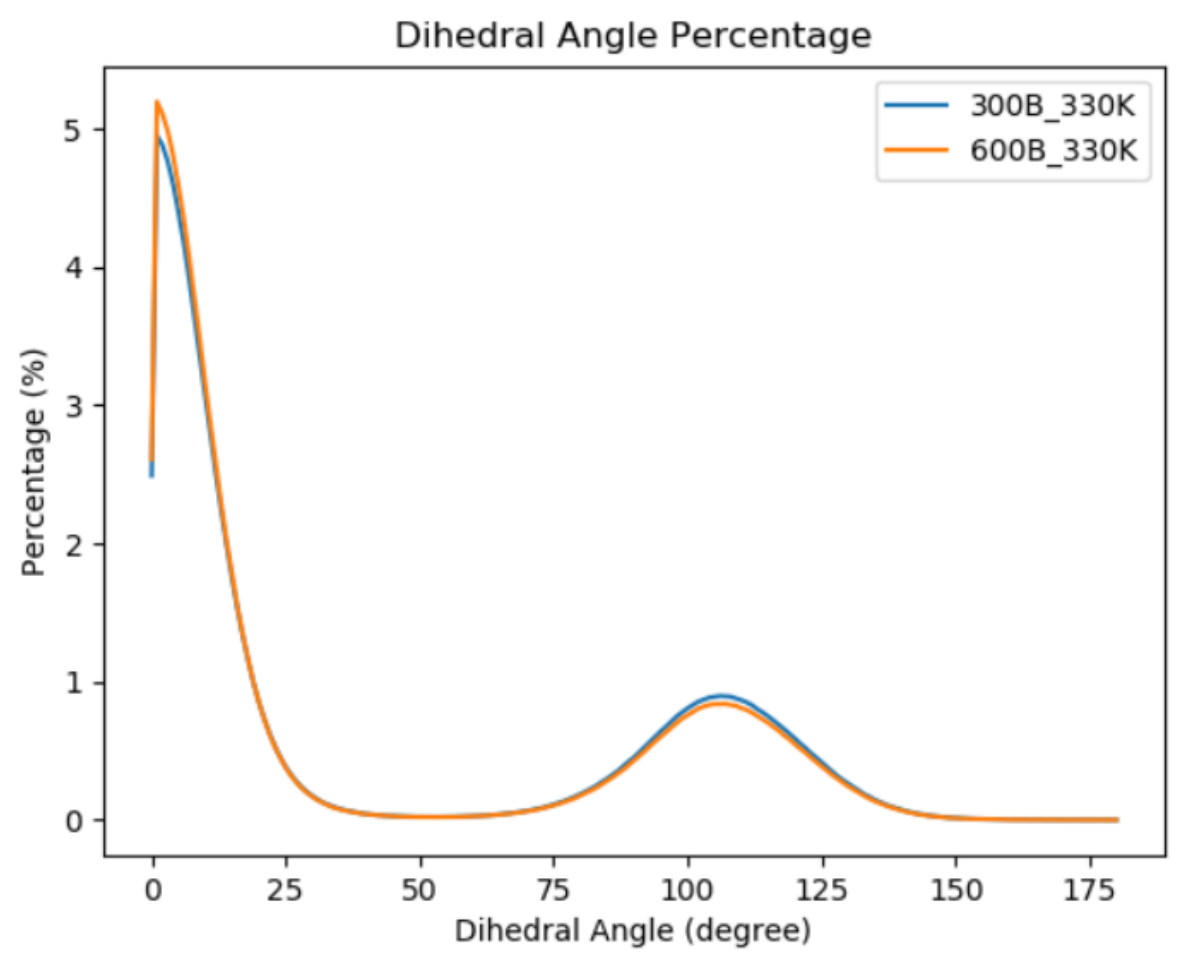



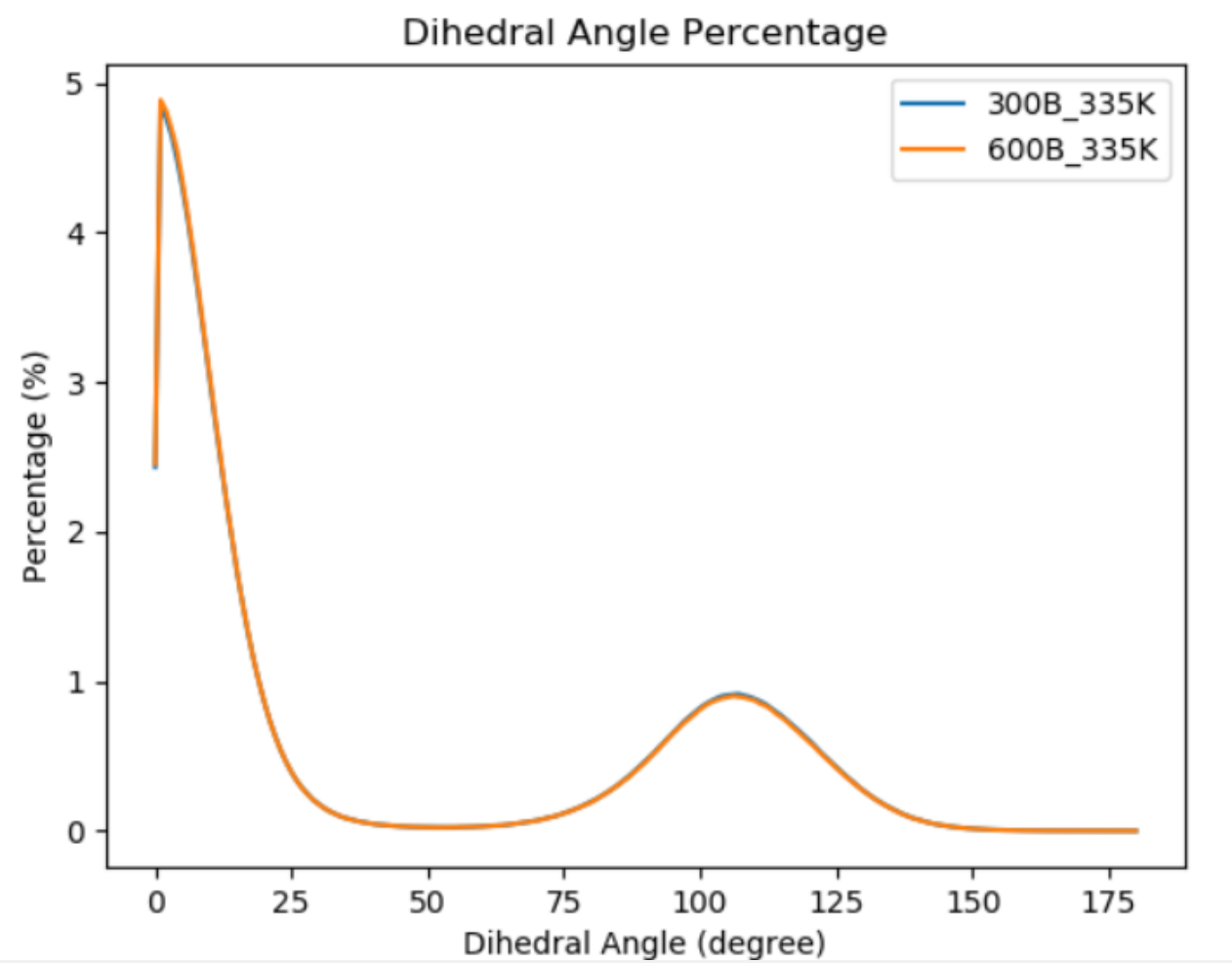
# Minimization



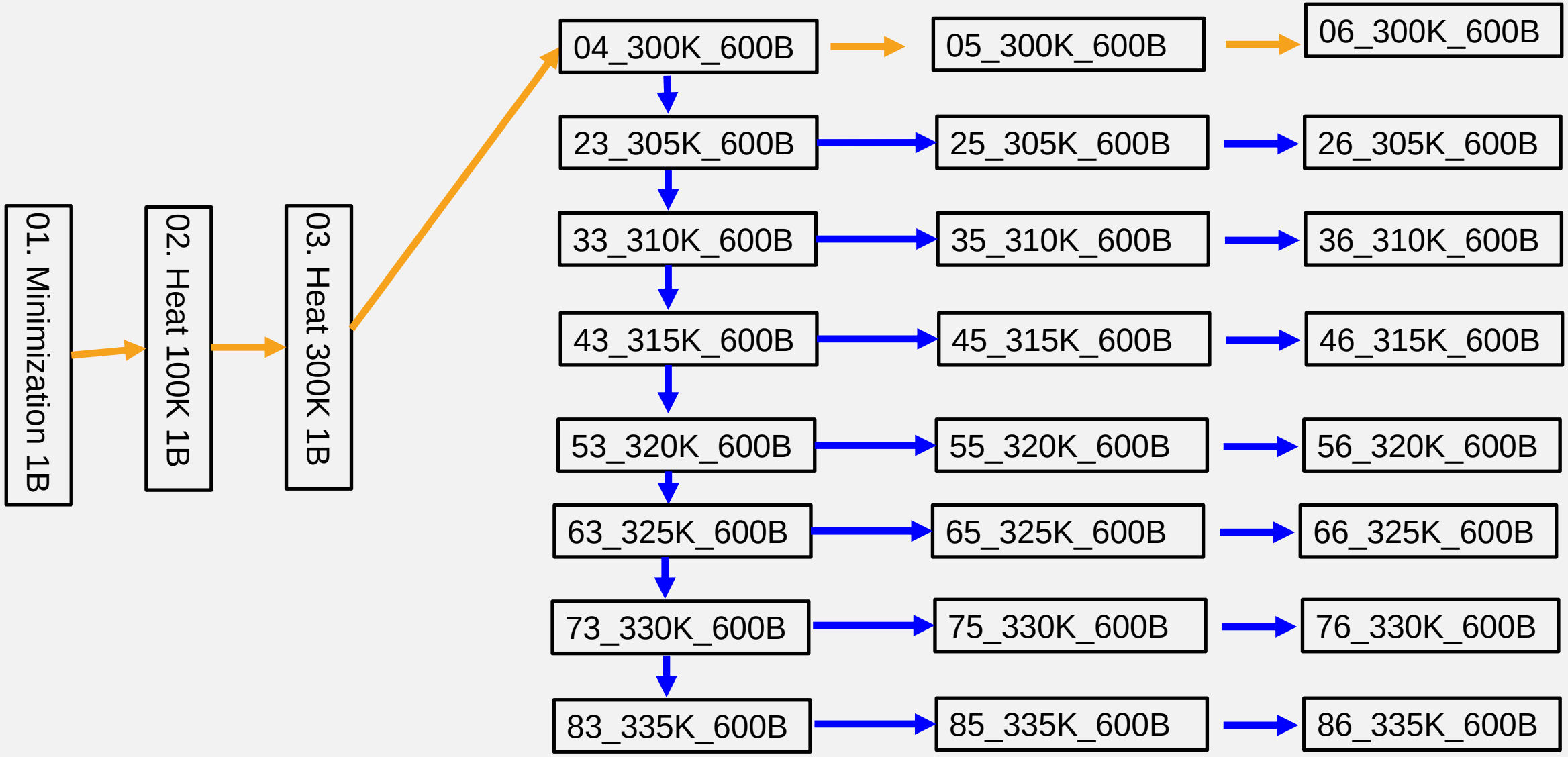
# Minimization



# MD Workflow DPPC 512 2% He 600B

*/storage/scratch/syp0027/DPPC_512_He2/600B*



# MD Workflow DPPC 512 2% He 300B

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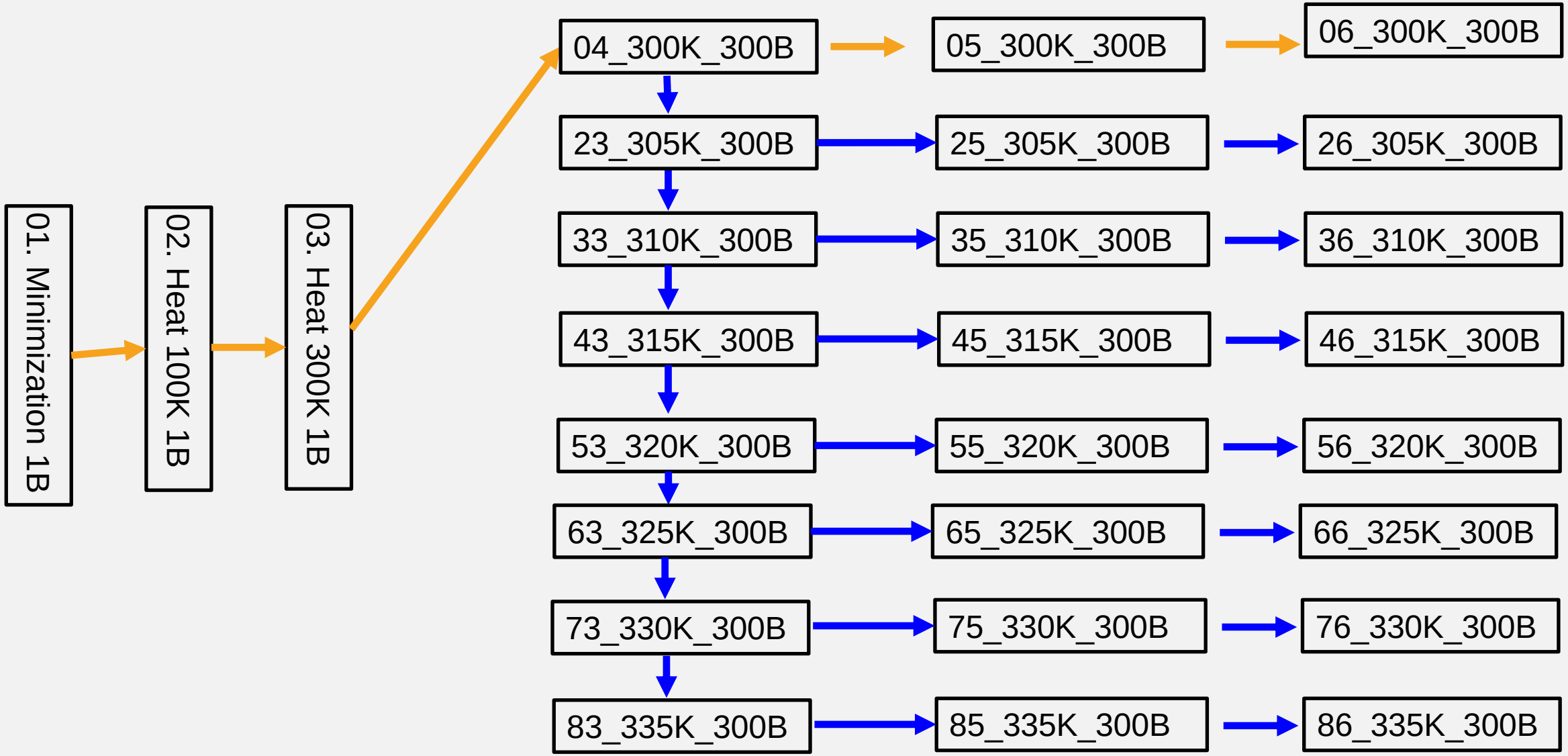
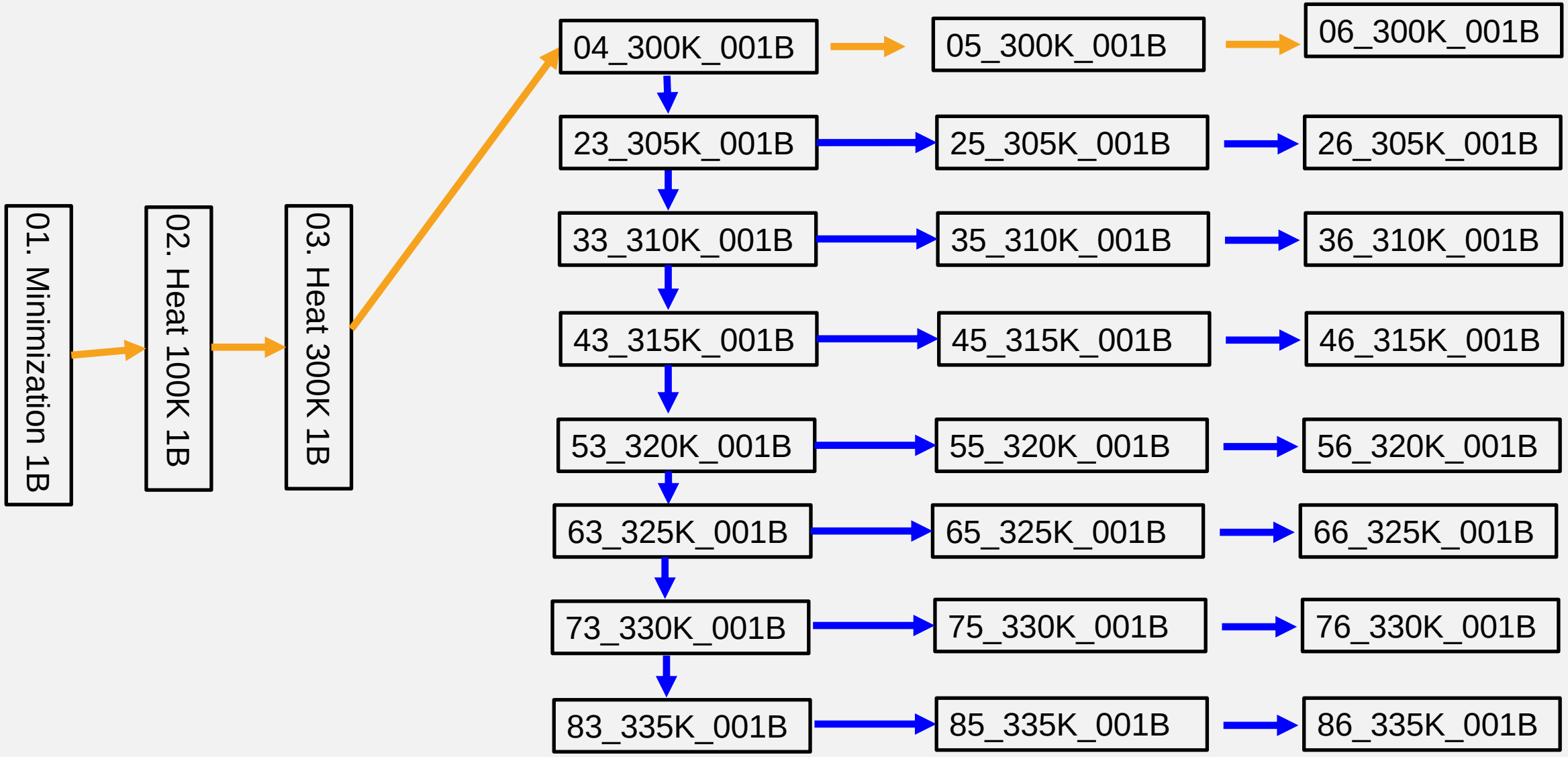
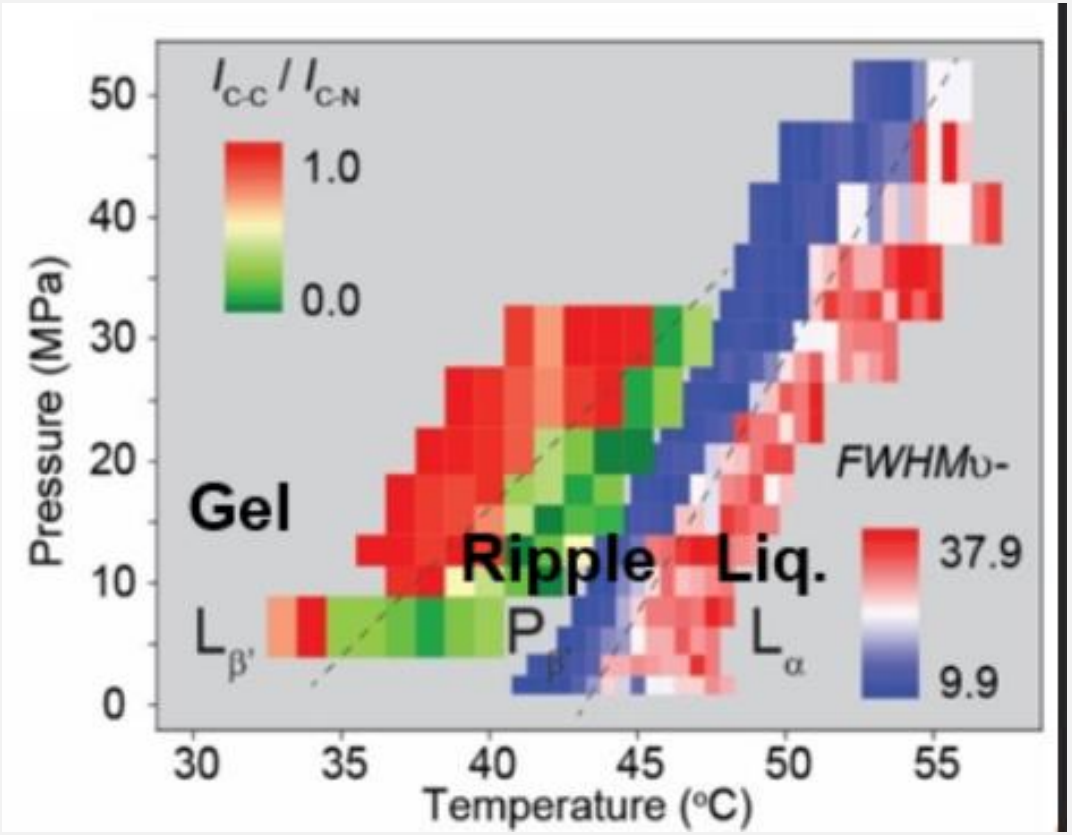


# MD Workflow DPPC 512 2% He 001B

*/storage/scratch/syp0027/DPPC_512_He2/001B*



# Phase Change Temperatures under different Pressures




| | 1B | 300B | 600B |
|---|---|---|---|
| Gel | 31C – 305K | 40C – 310K | 50C – 325K |
| Ripple | 43C – 315K | 46C – 320K | 55C – 330K |
| Liquid | 50C – 325K | 55C – 330K | 60C – 335K |


# Q&A

## Amber MD Simulation Experience

**Steven Pei 12/27/2022**

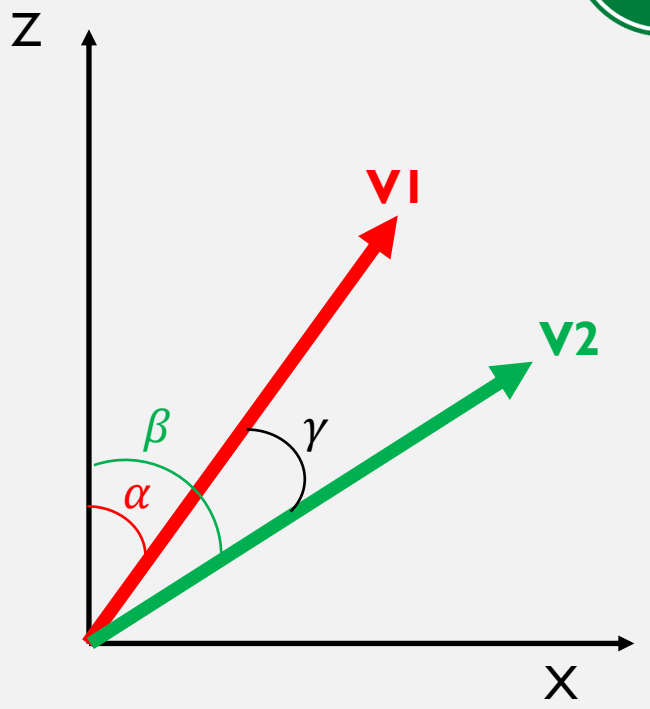
# Potential errors

$$\cos\gamma = \cos(\beta - \alpha)$$
$$= \cos\beta\cos\alpha + \sin\beta\sin\alpha$$
$$= \cos\beta\cos\alpha + \sqrt{1-\cos^2\beta}\ \sqrt{1-\cos^2\alpha}$$

where

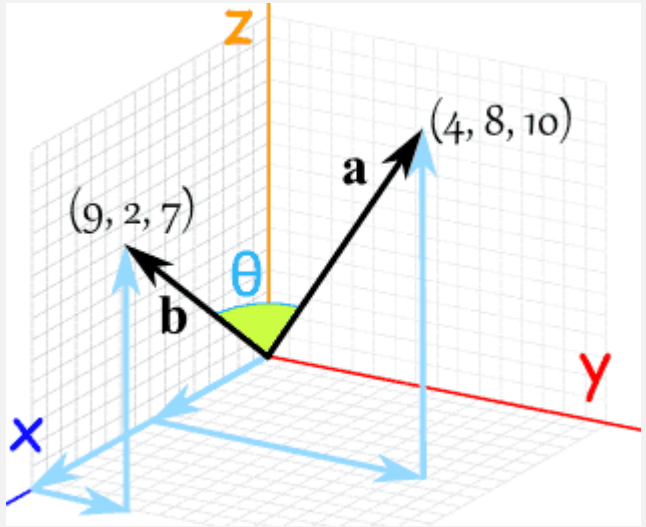
$$\cos\alpha = v1[2]$$
$$\cos\beta = v2[2]$$

$$\cos\alpha = v1[2]$$




But line 66 in SCD.py file

$$\cos^2\gamma = \cos^2\alpha + \cos^2\beta$$



# Minimization

- NSTEP is the total number of steps of the minimization. Amber prints every NTPR steps as set in the input file.
- Energy is the total energy of the system, as determined from the force field equation, in Kcal/mol.
- RMS is the mean of the square root of the dot product of the force vectors.
- GMAX is the magnitude of the largest component of the force vectors, I.e the largest force and NAME and NUMBER are the atom that has that largest force. I.e the one that will move the most during the minimization step.
- These three parameter should decrease as the system approaches the minima.