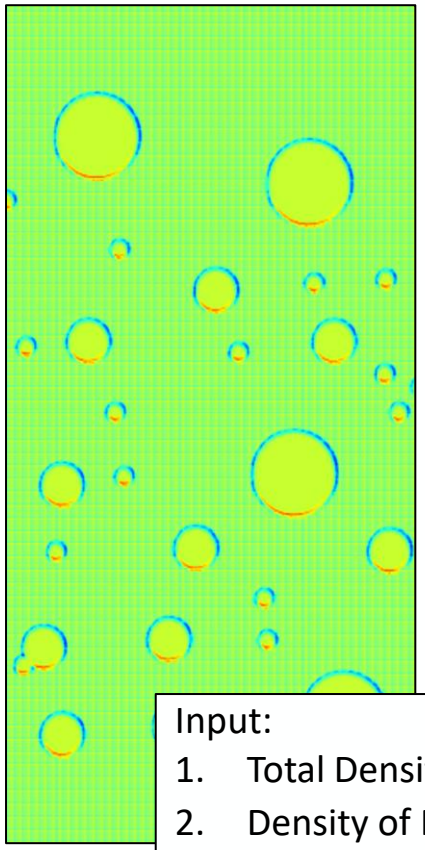
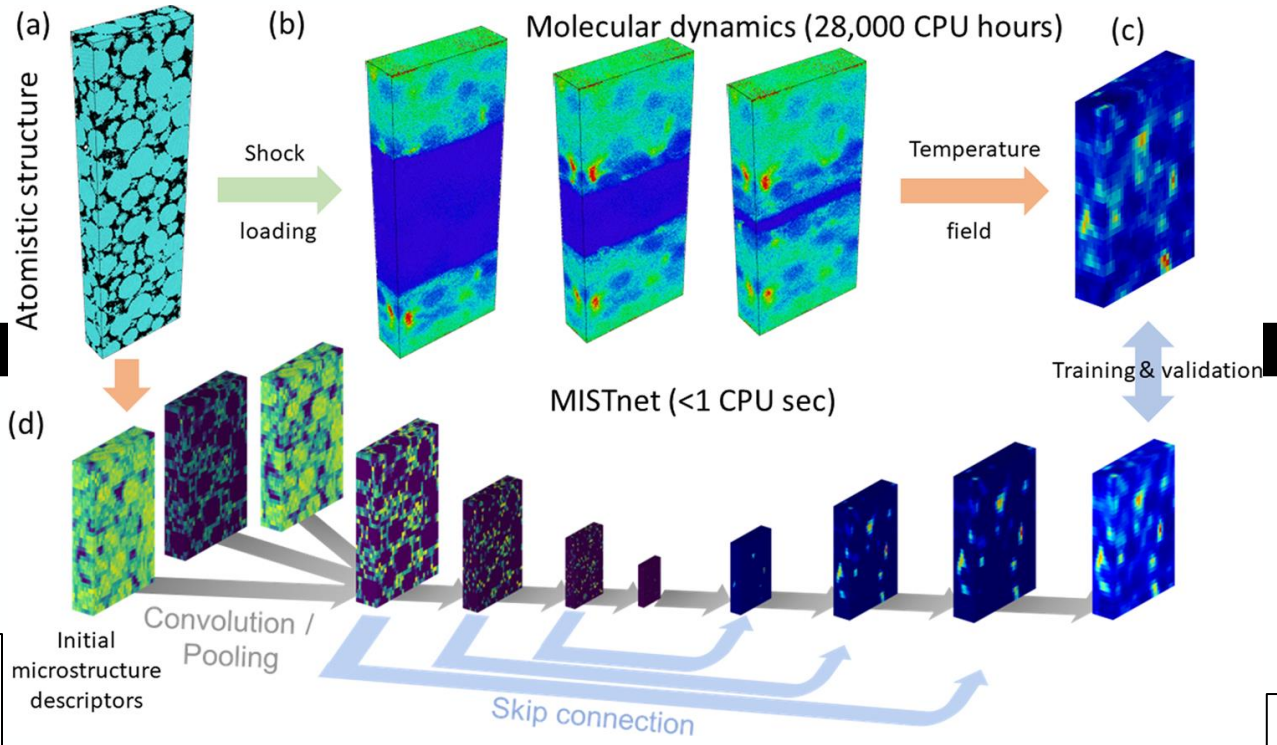
MISTnet – Mapping Microstructure to Shock-Induced Temperature Fields

Microstructure



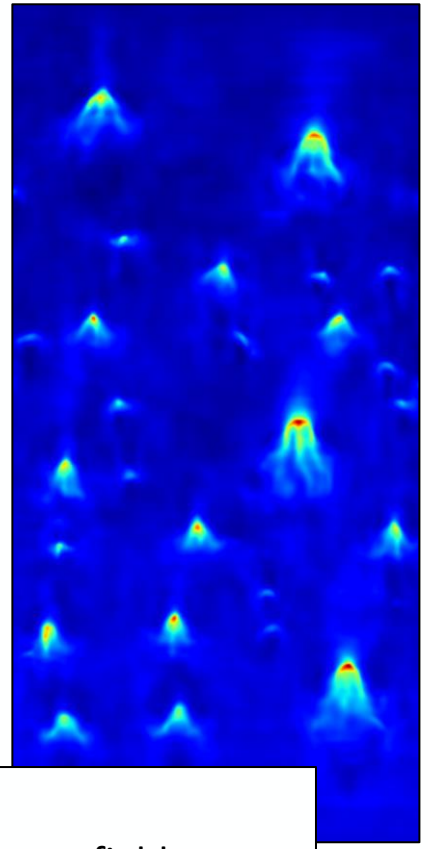
Input:

1. Total Density
2. Density of RDX
3. RDX × PS Density
4. Shock Speed



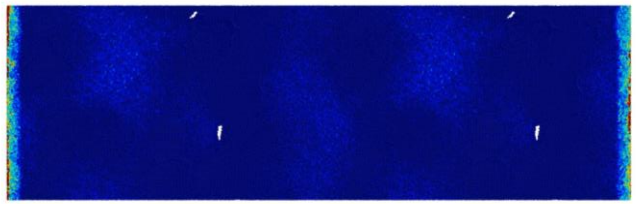
[1] Li, C., Verduzco, J.C., Lee, B.H. et al. *Mapping microstructure to shock-induced temperature fields using deep learning*. **npj Comput Mater** (2023).

Temperature Field



Output:

Temperature field, following shock loading



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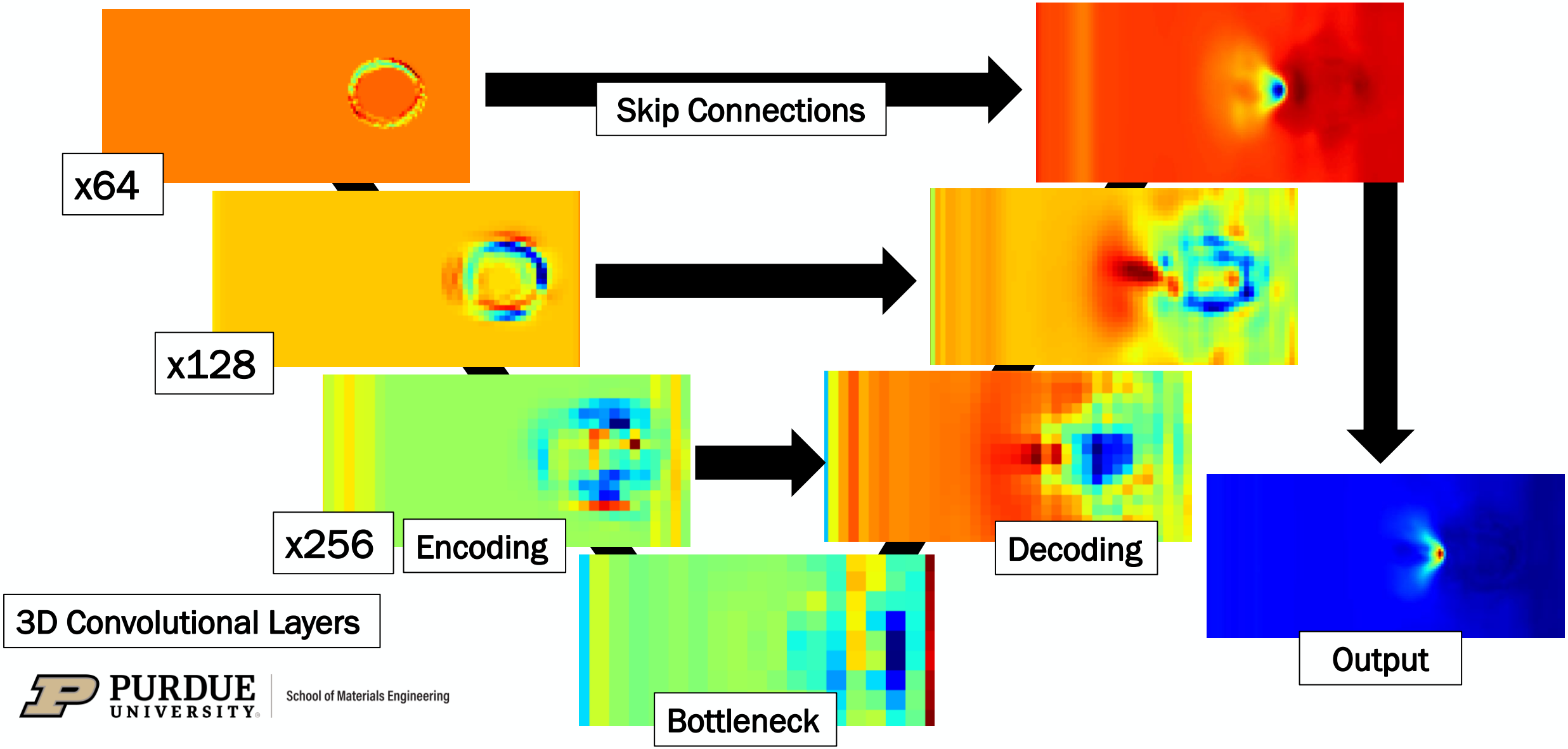
MISTnet Original Layers



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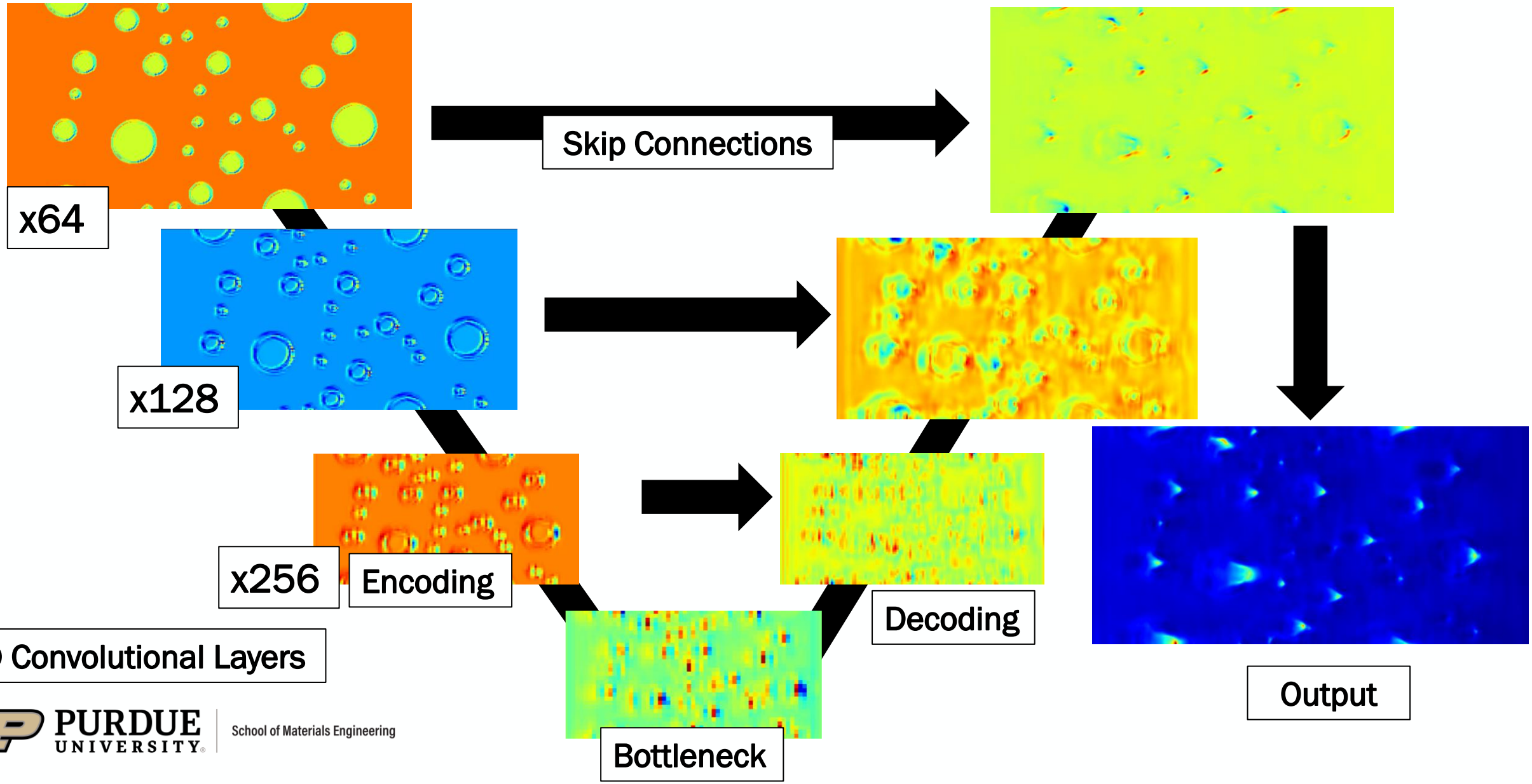
MISTnet Original Layers



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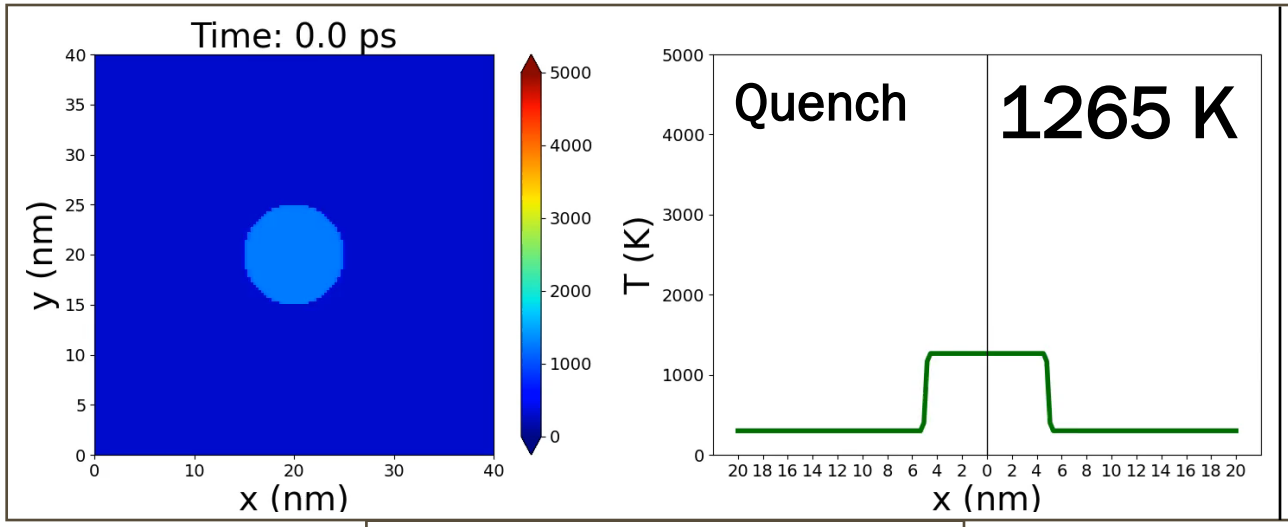
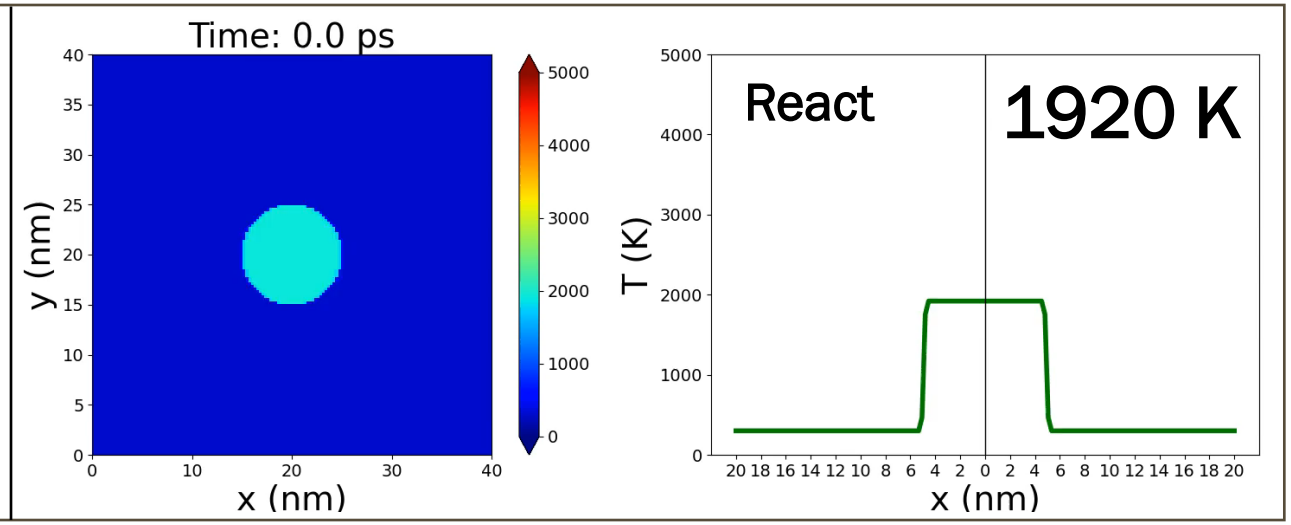
1,3,5-Trinitro-1,3,5-triazinane (RDX) Hotspots

Thermal Diffusion & Reaction w/ Arrhenius Kinetics



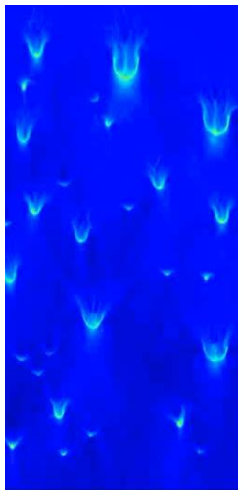


Diameter = 10 (nm)

Grid = 40 x 40 (nm)

Seeded T= 1265, 1620, 1920 (K)

Surrounding T = 300 (K)



Continuum Model: $\boldsymbol{\rho C_v \dot{T} = k\nabla^2 T - Q_1 \dot{C}_1 + Q_2 \dot{C}_3}$

Heat Diffusion: $k\nabla^2 T$

Reaction: $-Q_1 \dot{C}_1 + Q_2 \dot{C}_3$

[2] Sakano, M. et al. (2020). *Unsupervised learning-based multiscale model of thermochemistry in 1,3,5-trinitro-1,3,5-triazinane (RDX)*. The Journal of Physical Chemistry A

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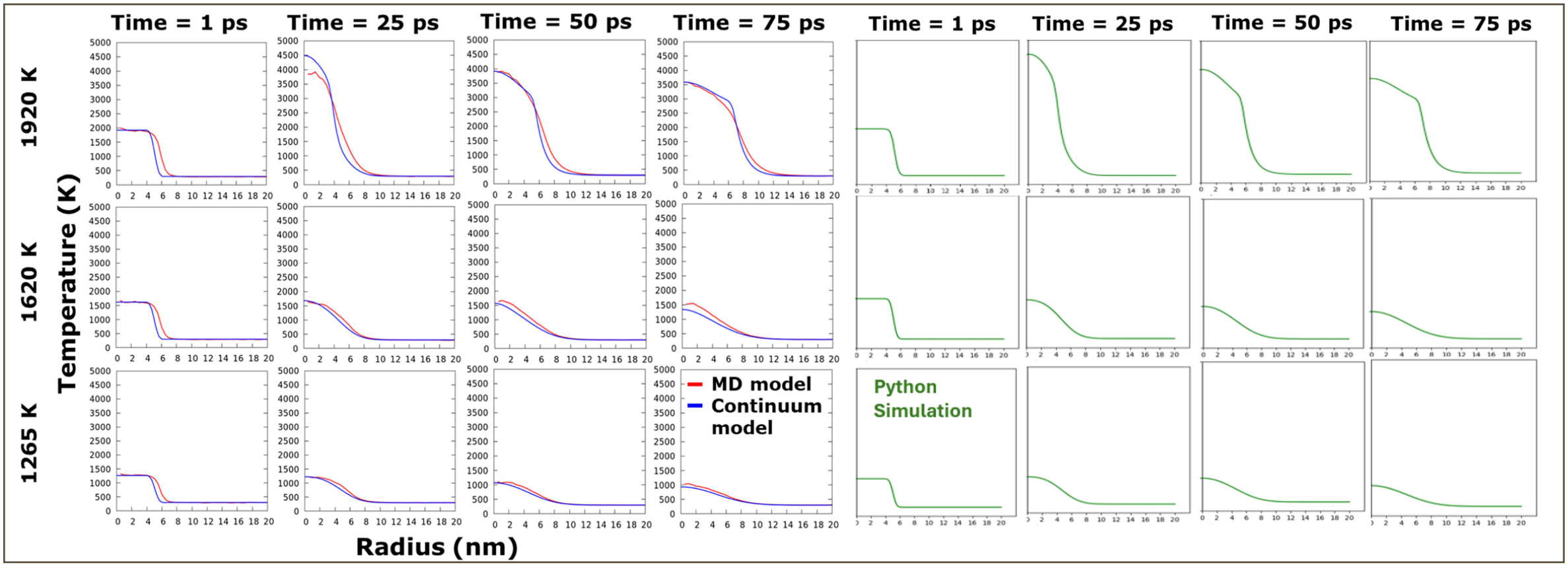
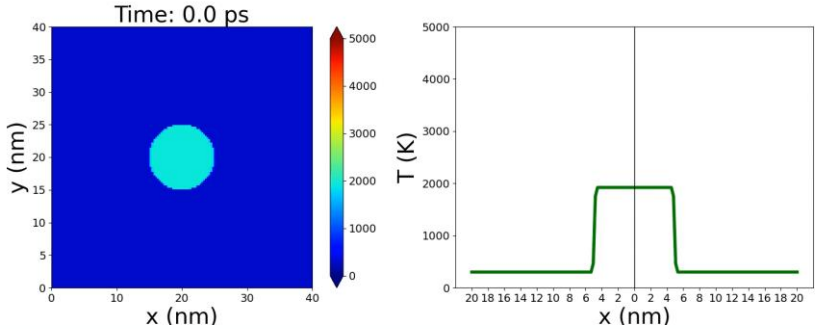
1D Temperature Profile Validation



[2] Sakano, M. et al. *Unsupervised learning-based multiscale model of thermochemistry in 1,3,5-trinitro-1,3,5-triazinane (RDX)*. The Journal of Physical Chemistry A (2020)



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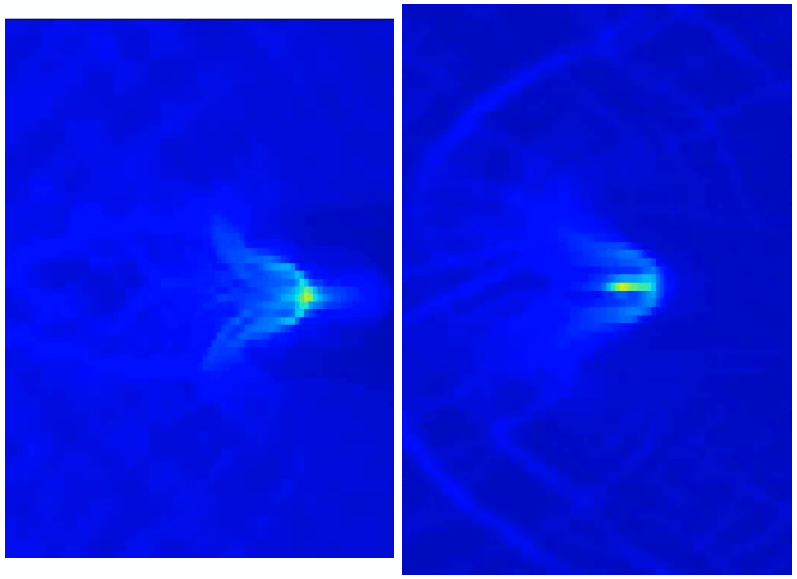
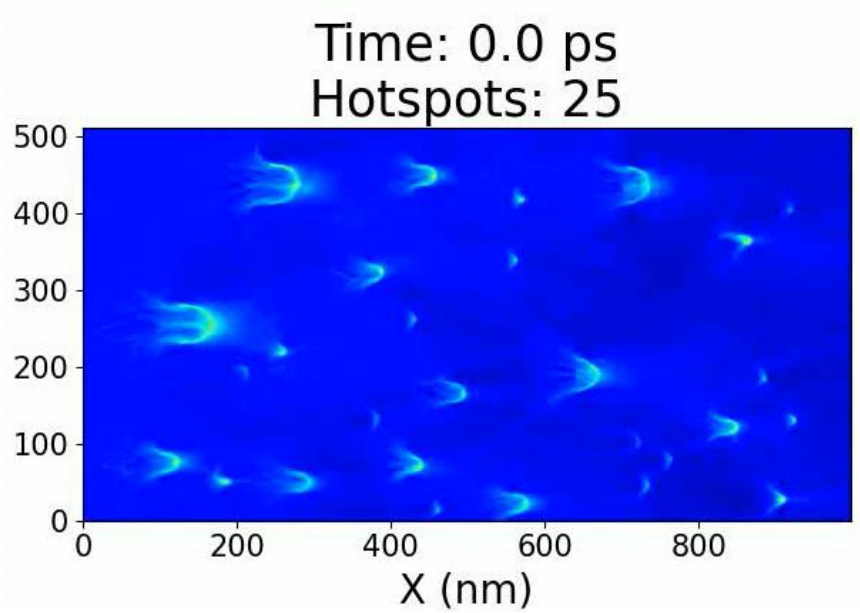
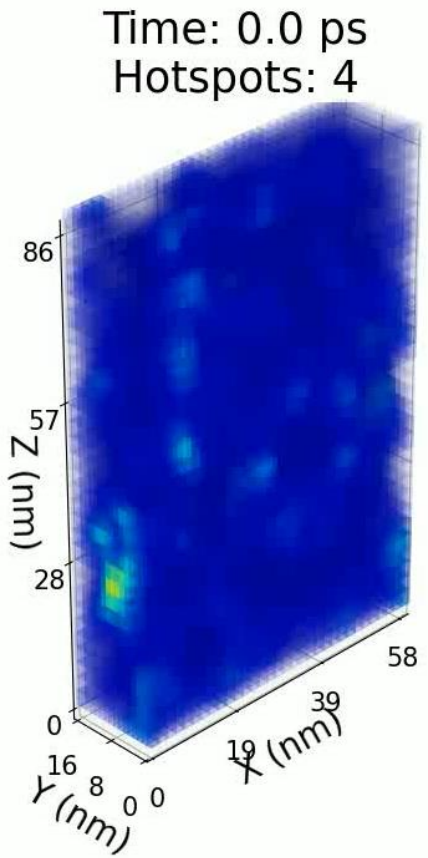
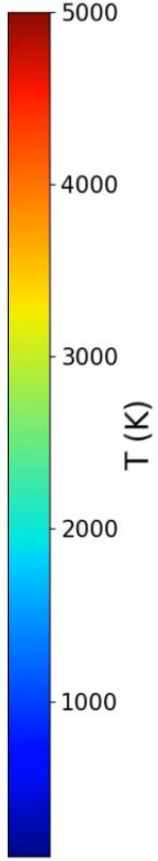
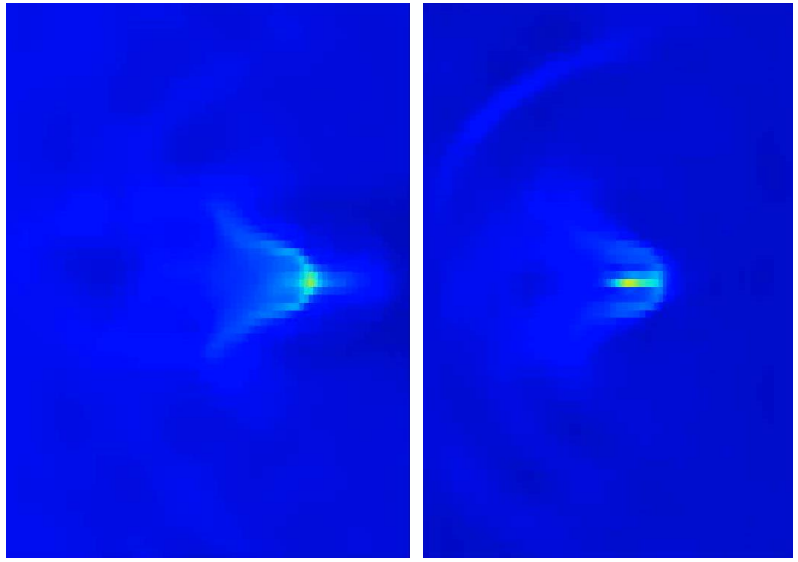
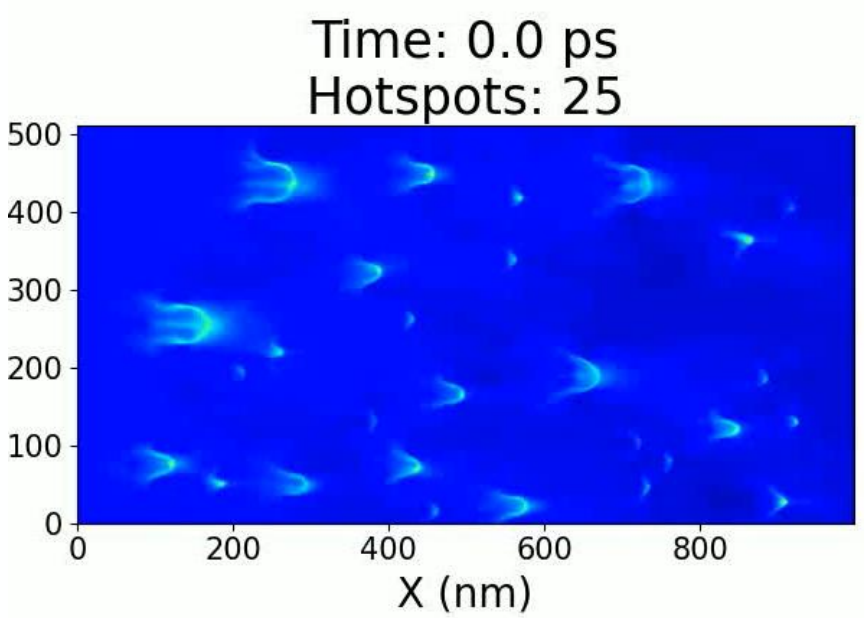
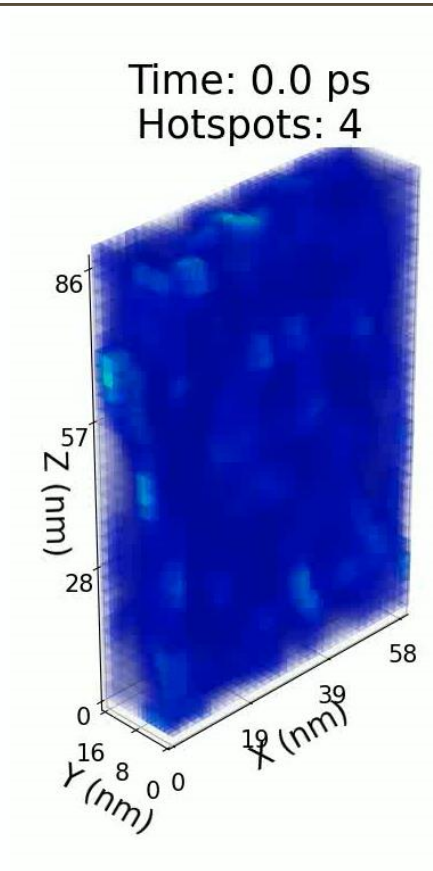
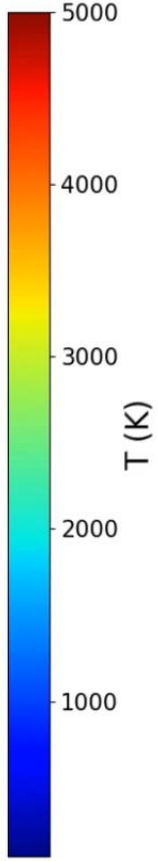
MISTnet True Data

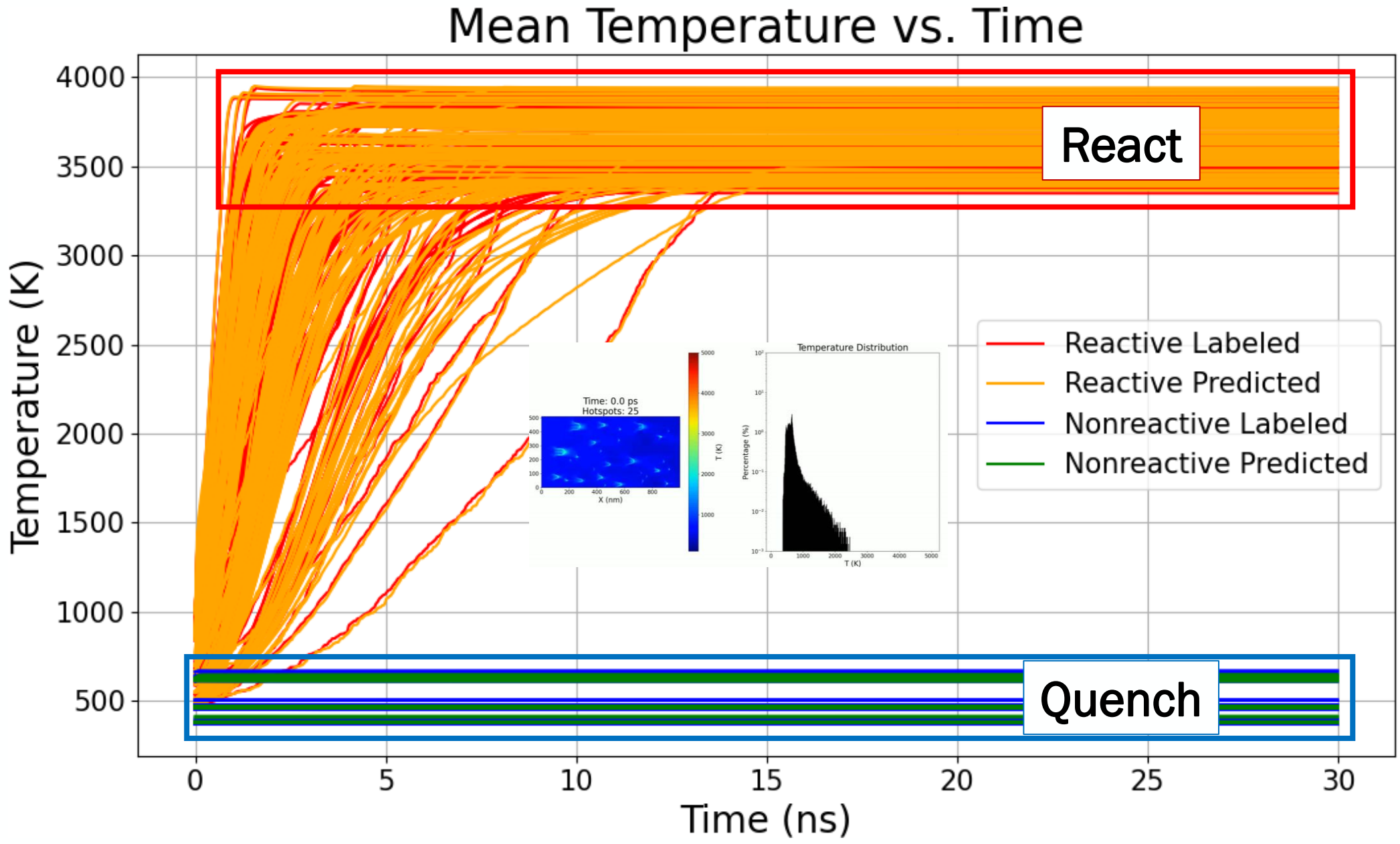
Single Pore	Multi Pore	Original
		

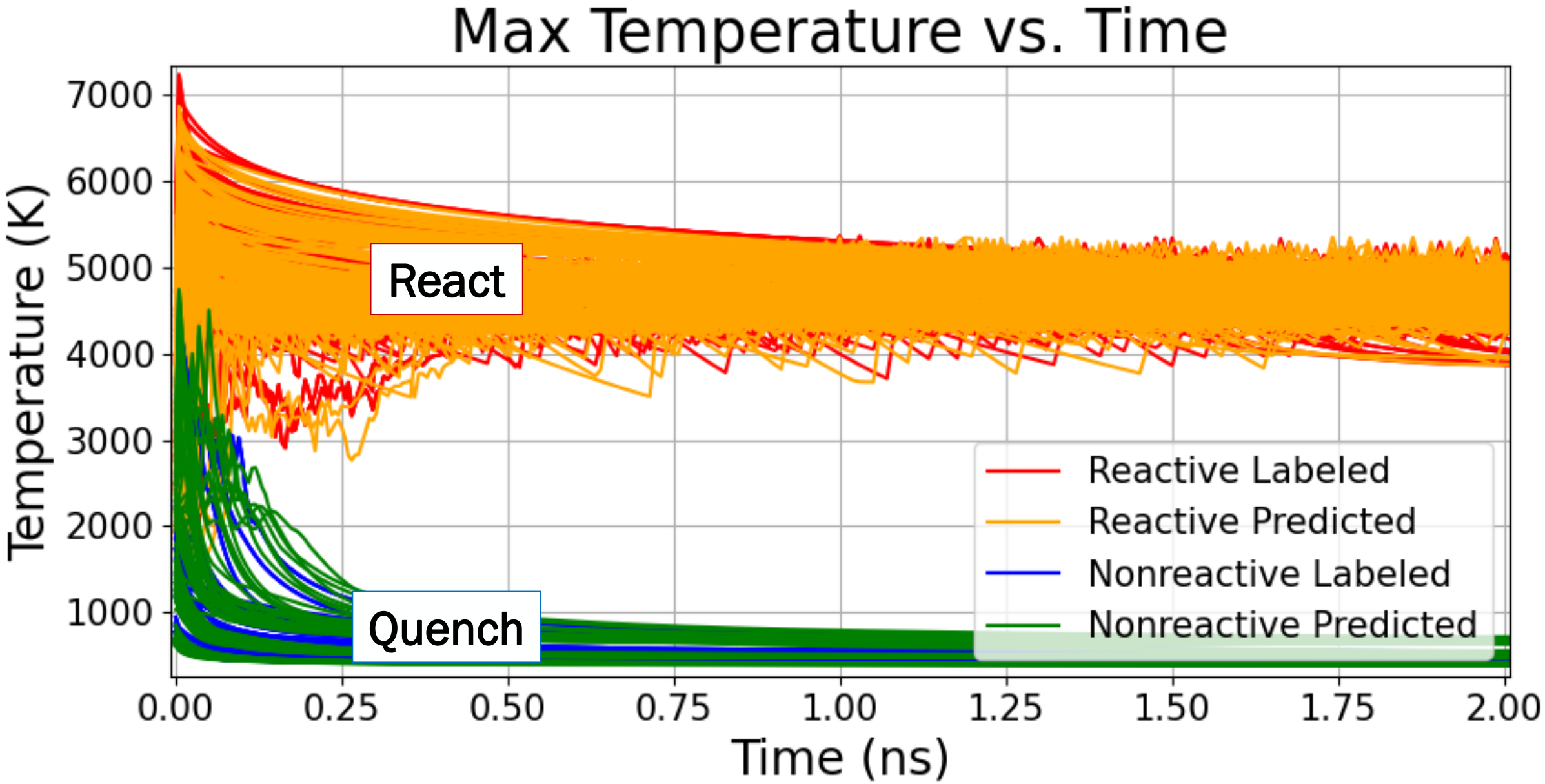


MISTnet Predicted Outputs

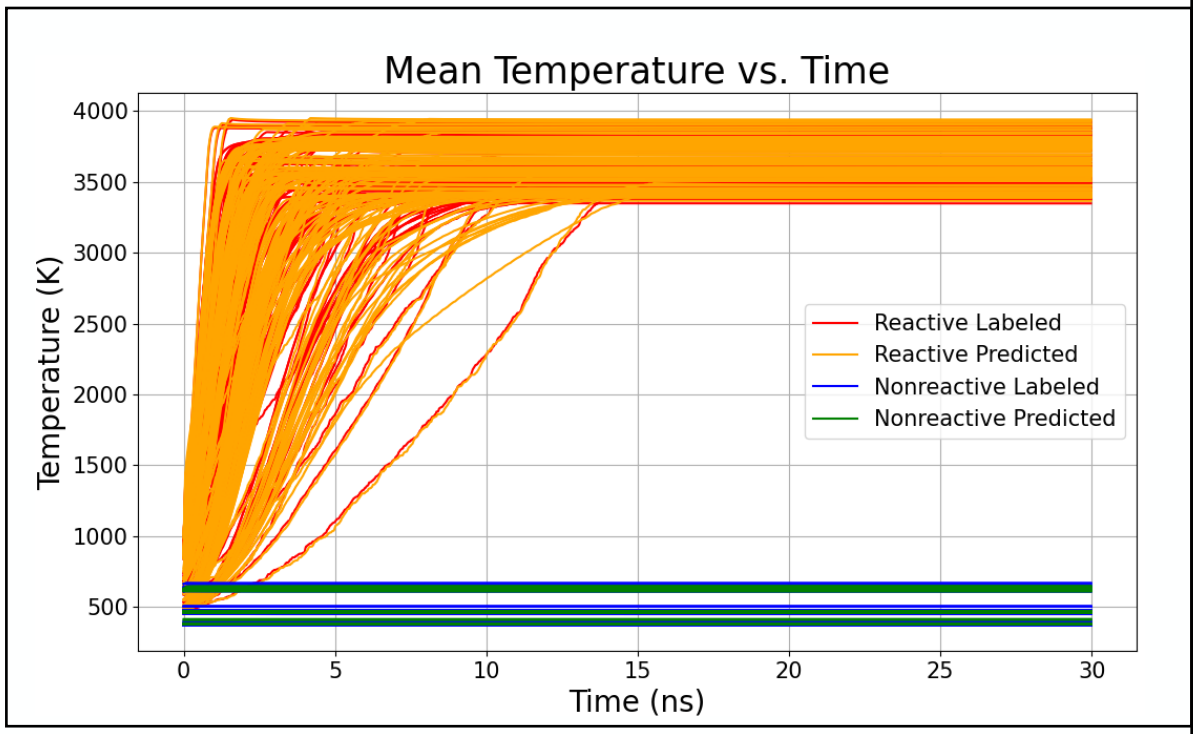
Single Pore	Multi Pore	Original
		

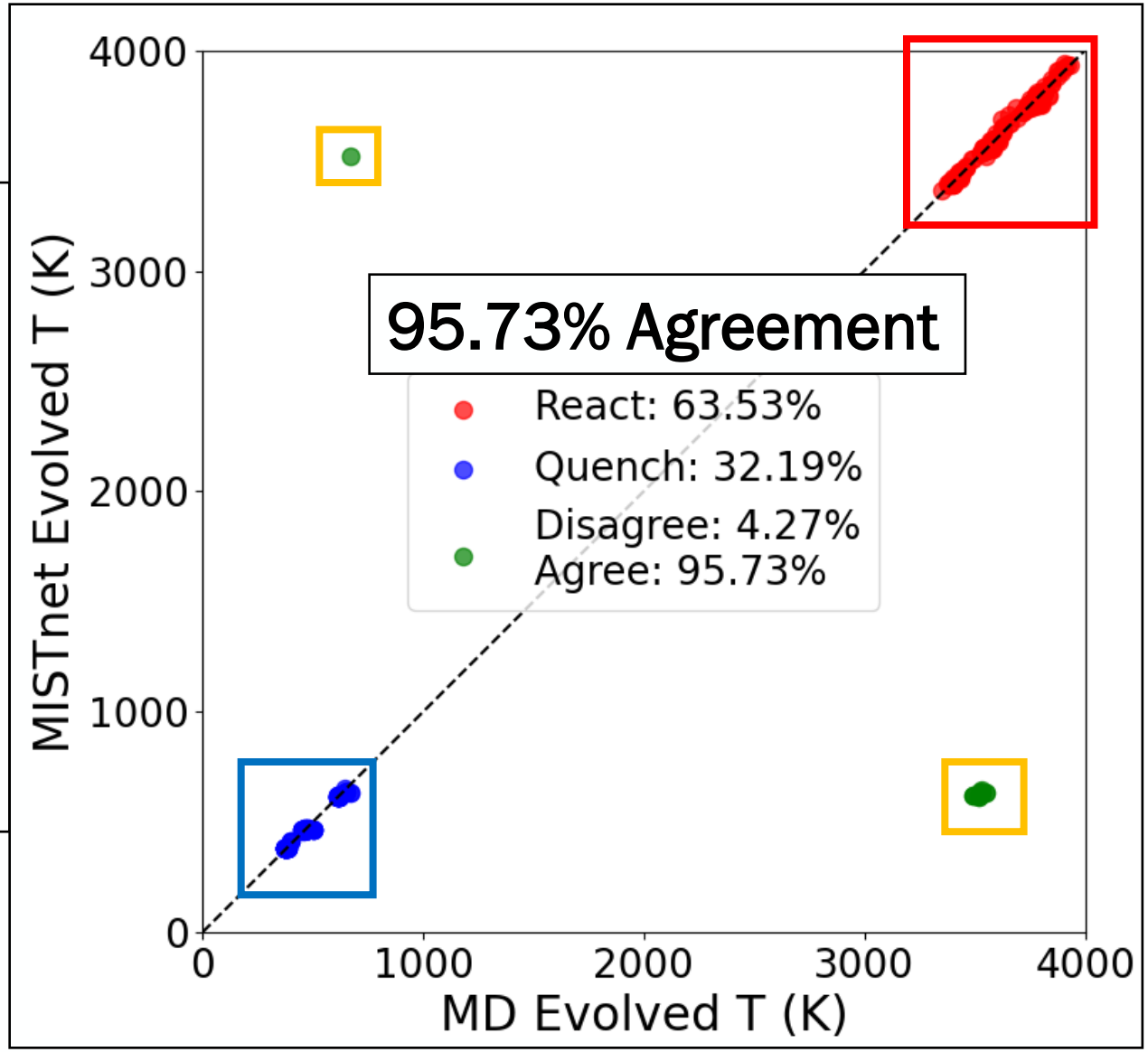



Mean Temperature vs. Time
Temperature (K)
Time (ns)
React
Quench
Reactive Labeled
Reactive Predicted
Nonreactive Labeled
Nonreactive Predicted
Time: 0.0 ps
Hotspots: 25
X (nm)
T (K)
Temperature Distribution
Percentage (%)


Max Temperature vs. Time
Temperature (K)
7000
6000
5000
4000
3000
2000
1000
0.00
0.25
0.50
0.75
1.00
1.25
1.50
1.75
2.00
Time (ns)
React
Quench
Reactive Labeled
Reactive Predicted
Nonreactive Labeled
Nonreactive Predicted

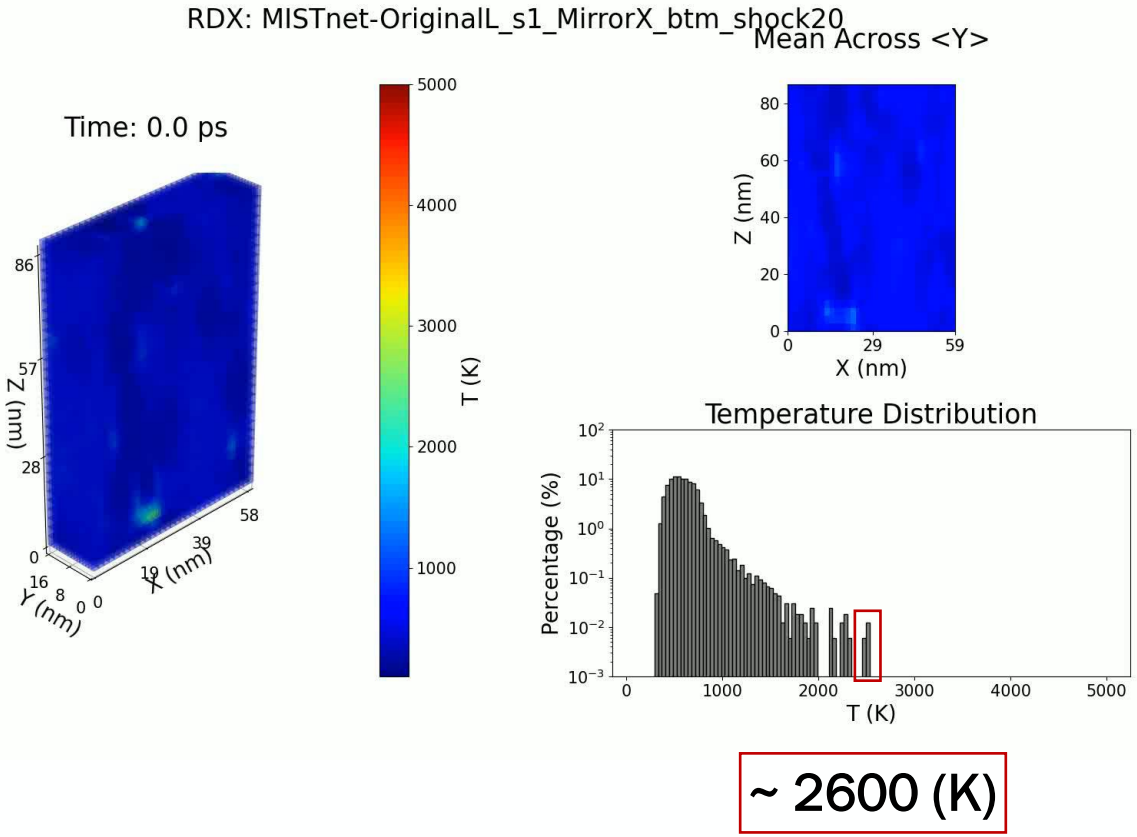
MISTnet vs MD Evolved Equilibrium T





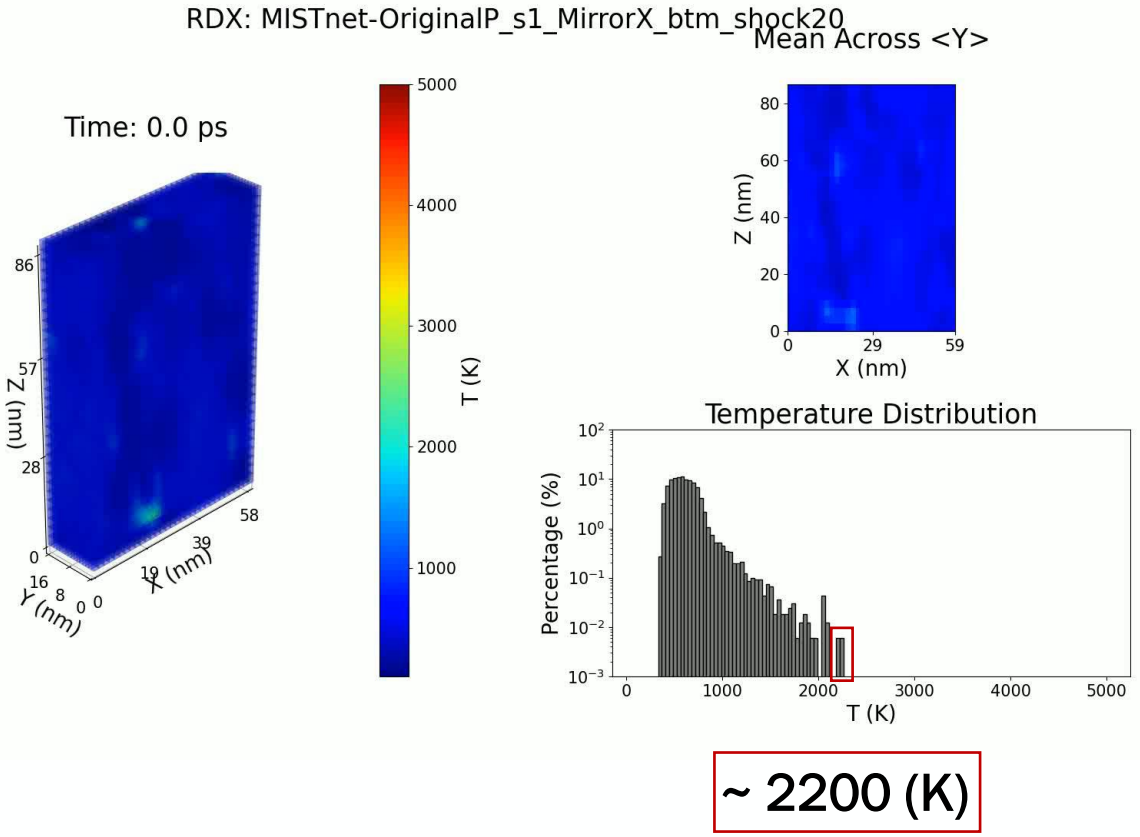
Disagreement Example:

MD Simulation



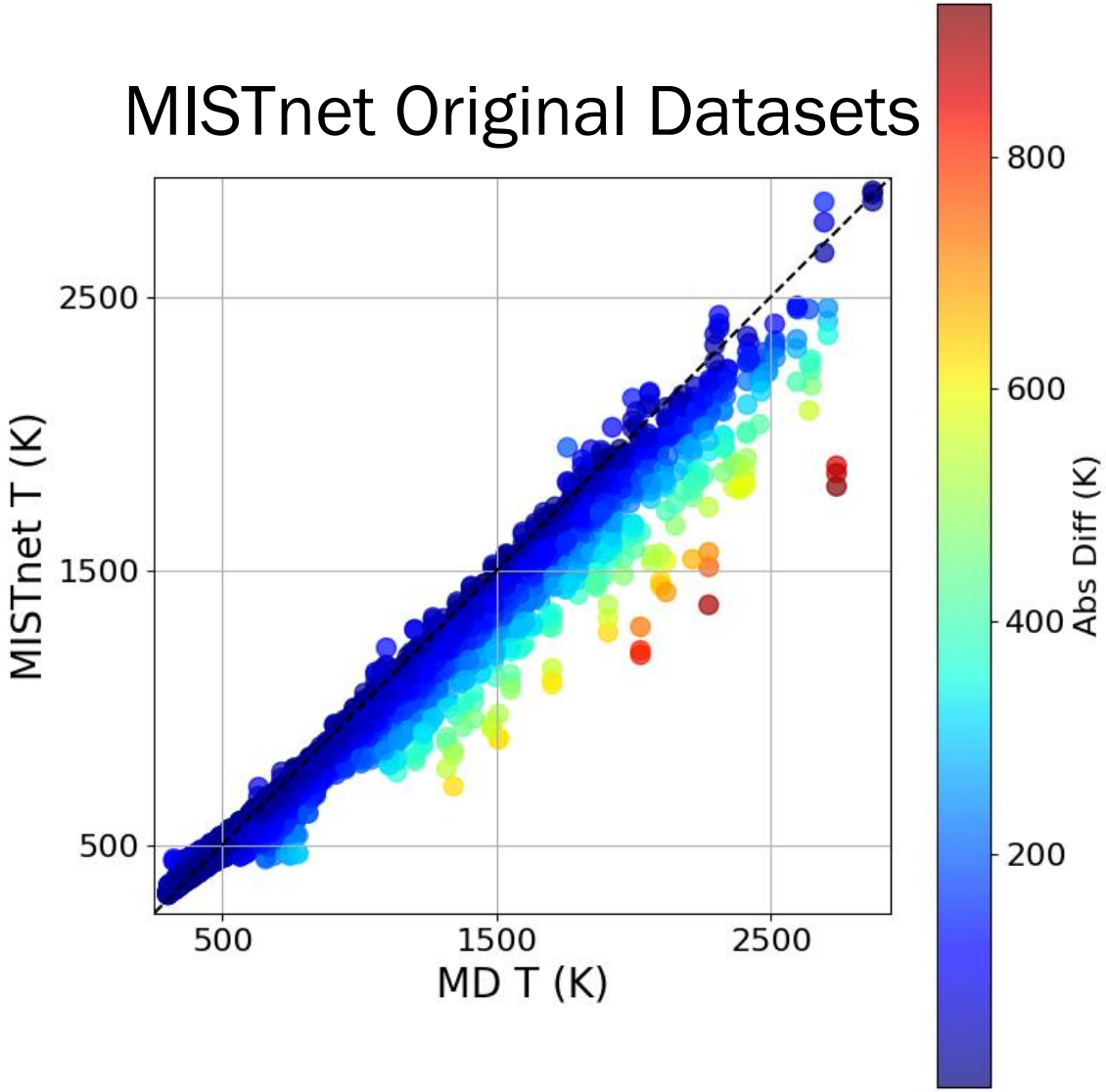
~ 2600 (K)

MISTnet Prediction

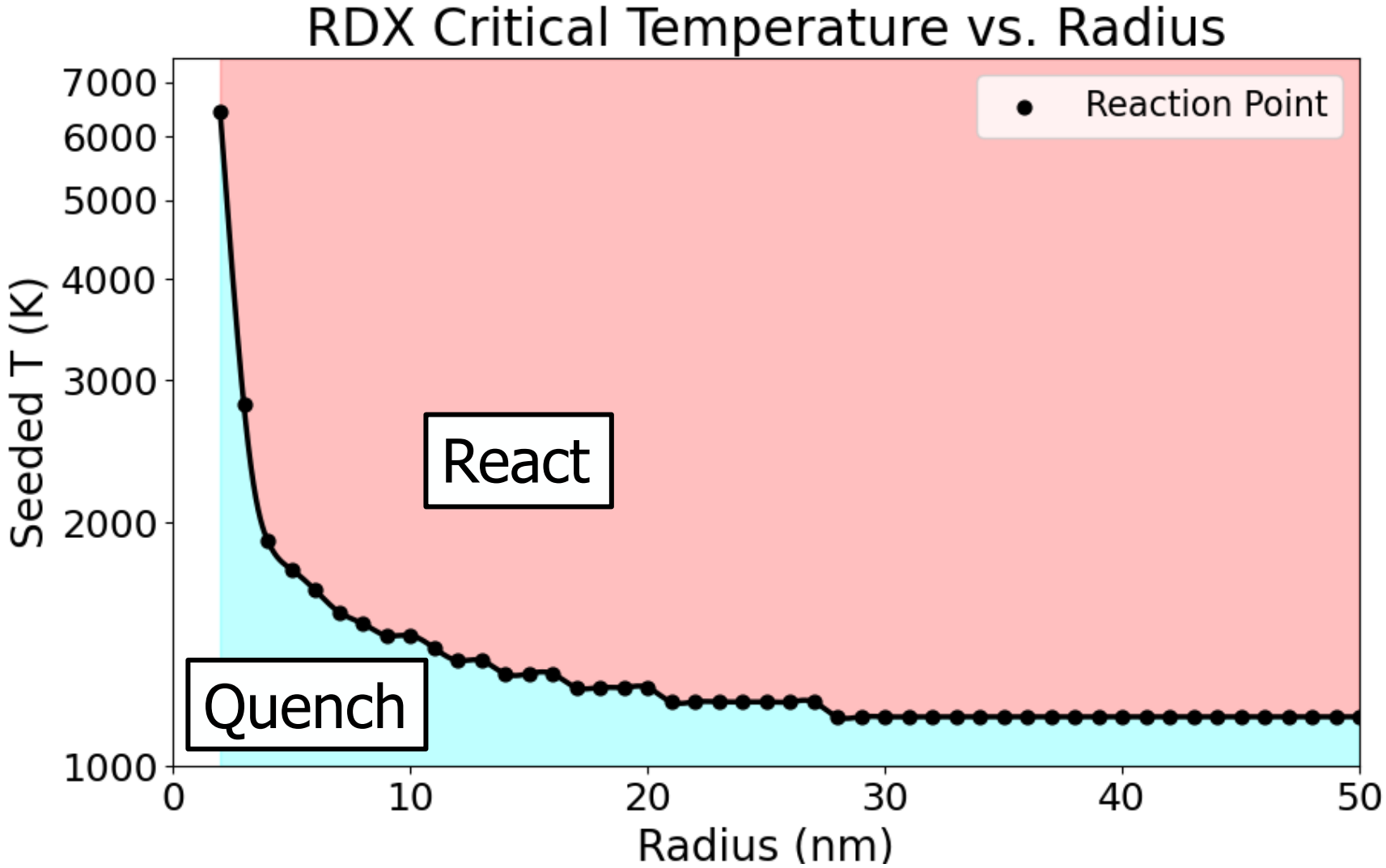


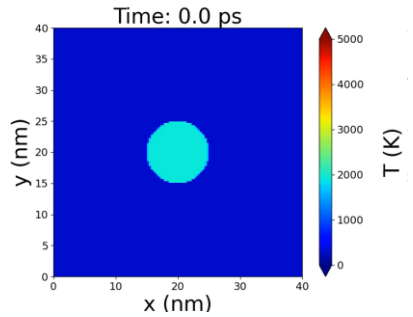
~ 2200 (K)

MISTnet vs MD - Binned Pixel Parity

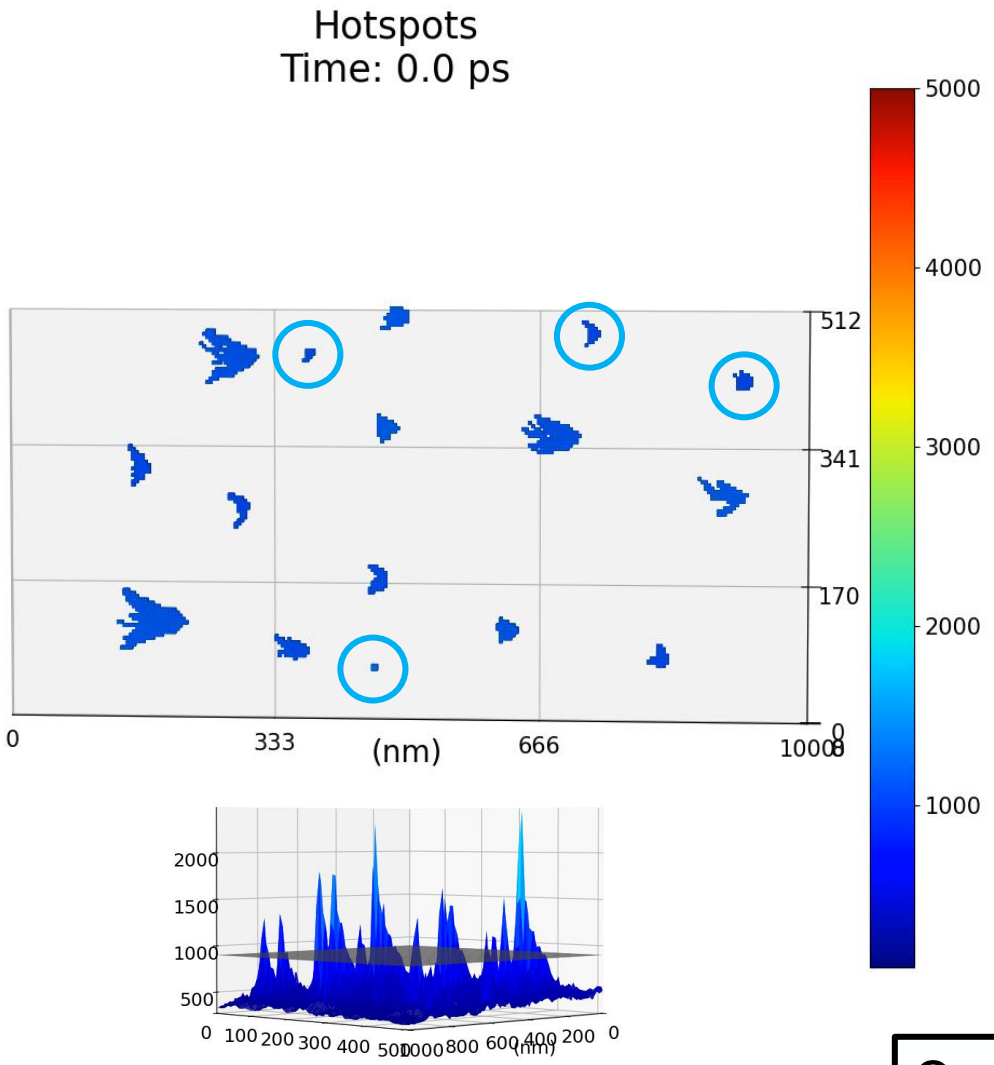


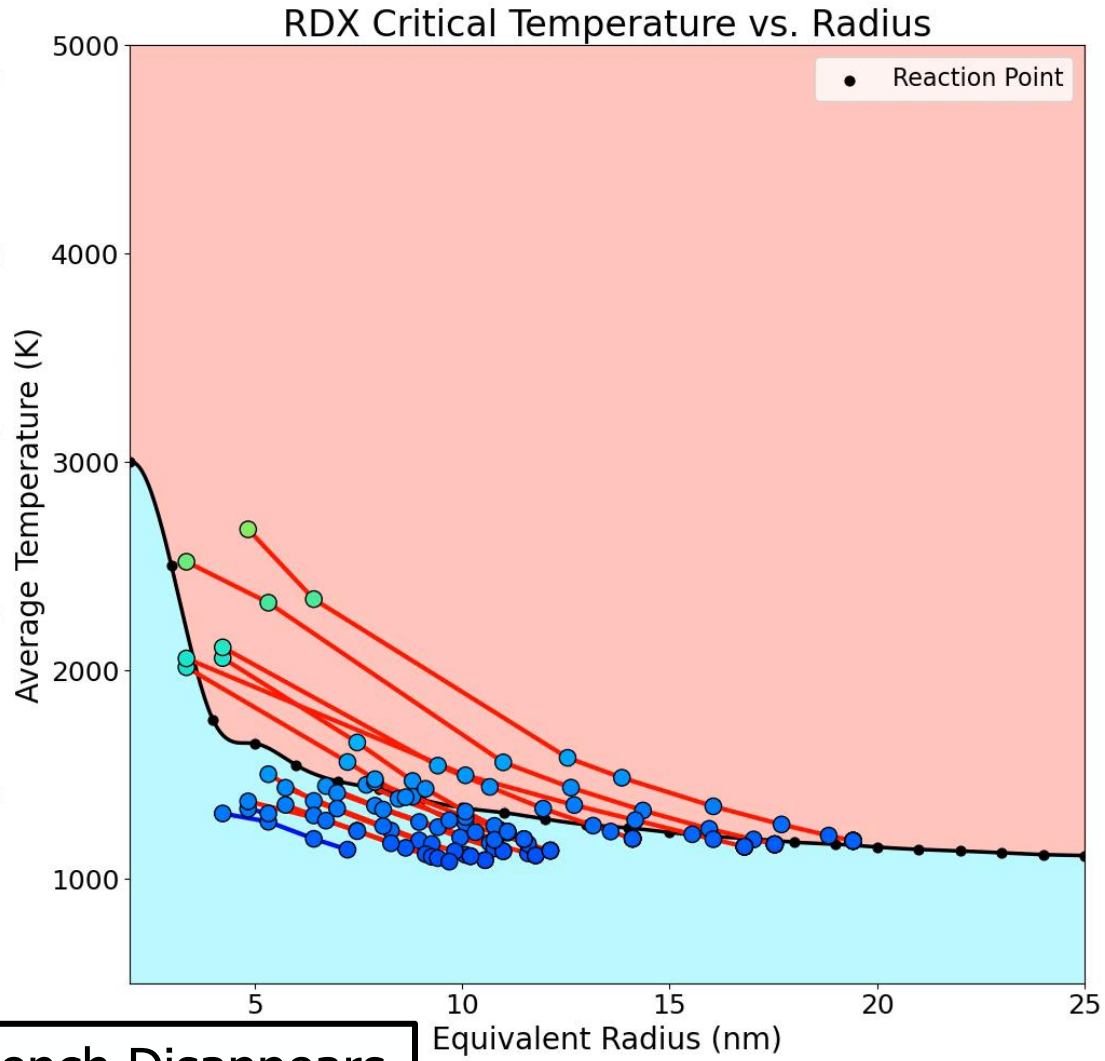
Critical Size-T Curve





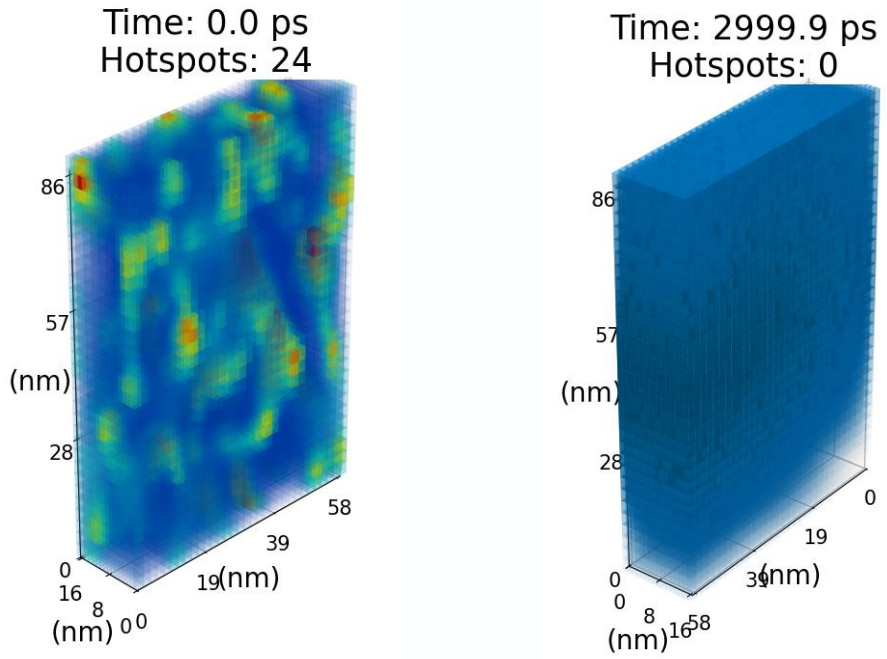
Hotspot (Size & Temperature) Function

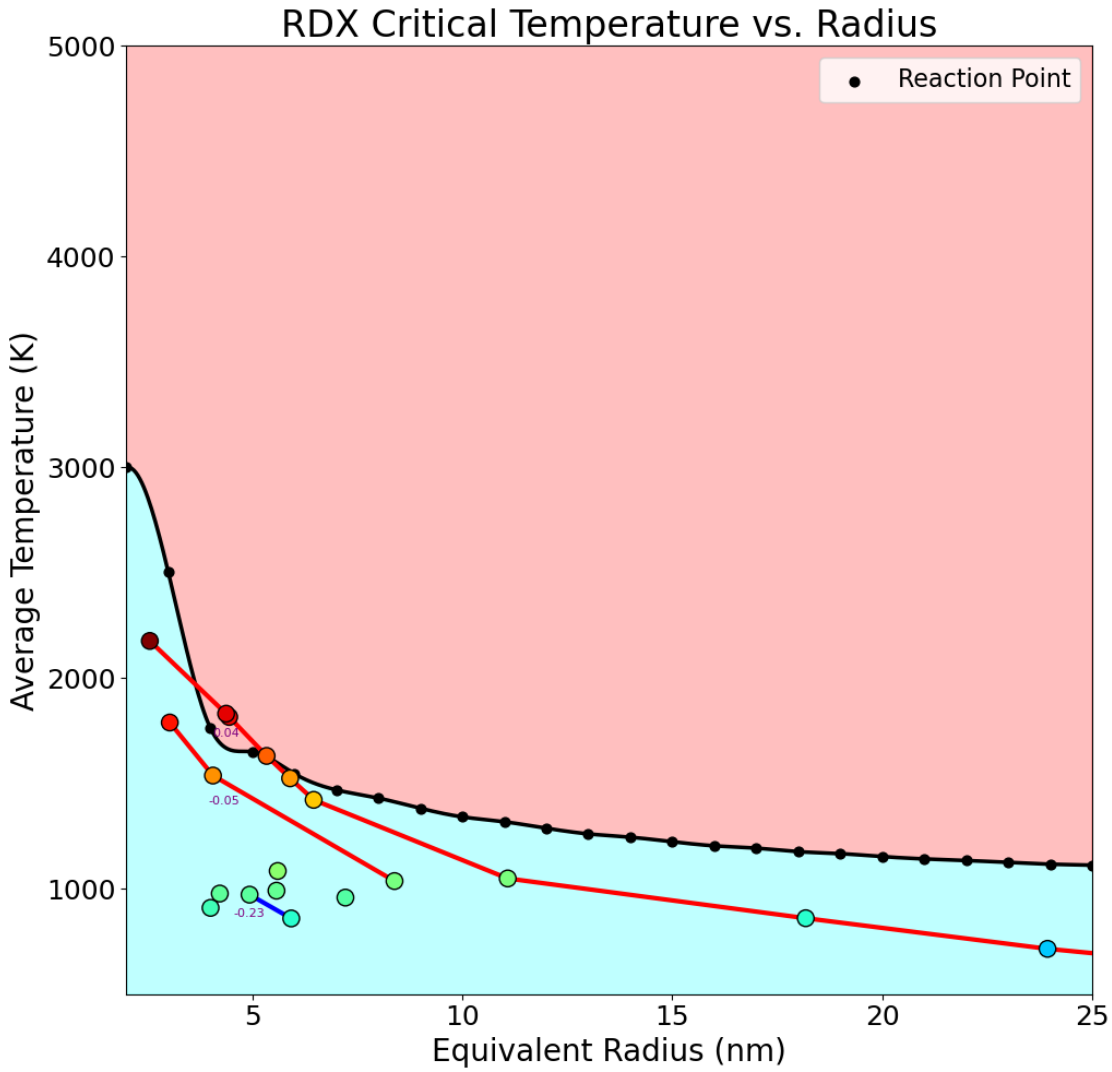




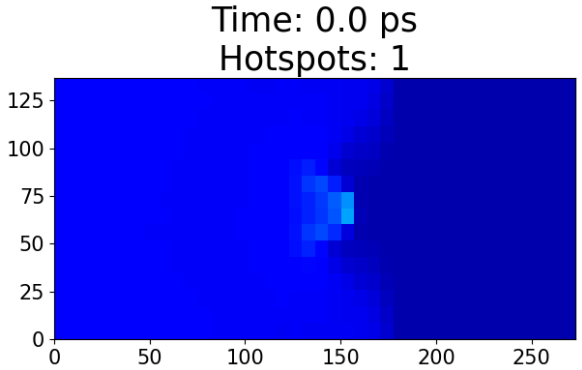
Quench Disappears

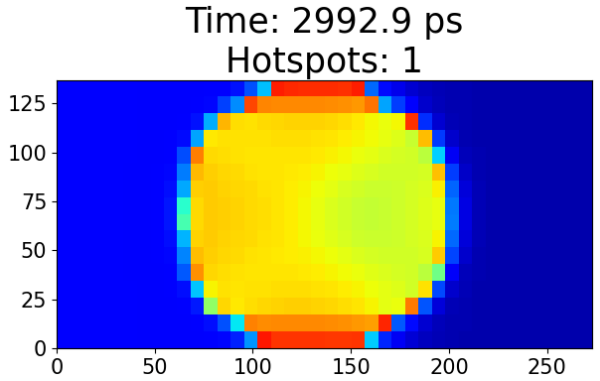
Hotspot (Size & Temperature) Function

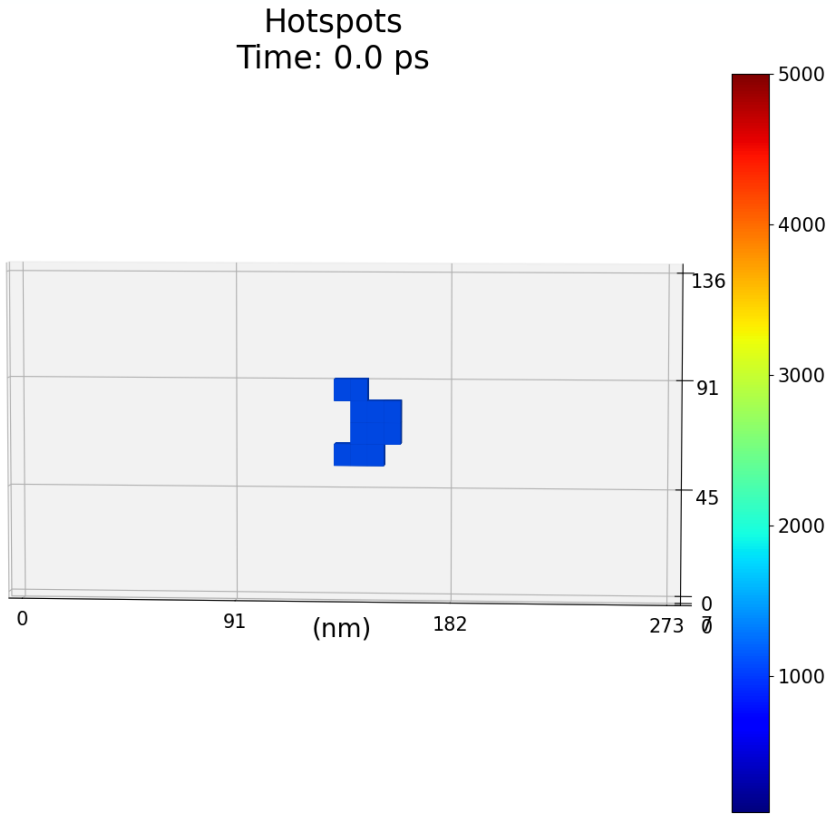


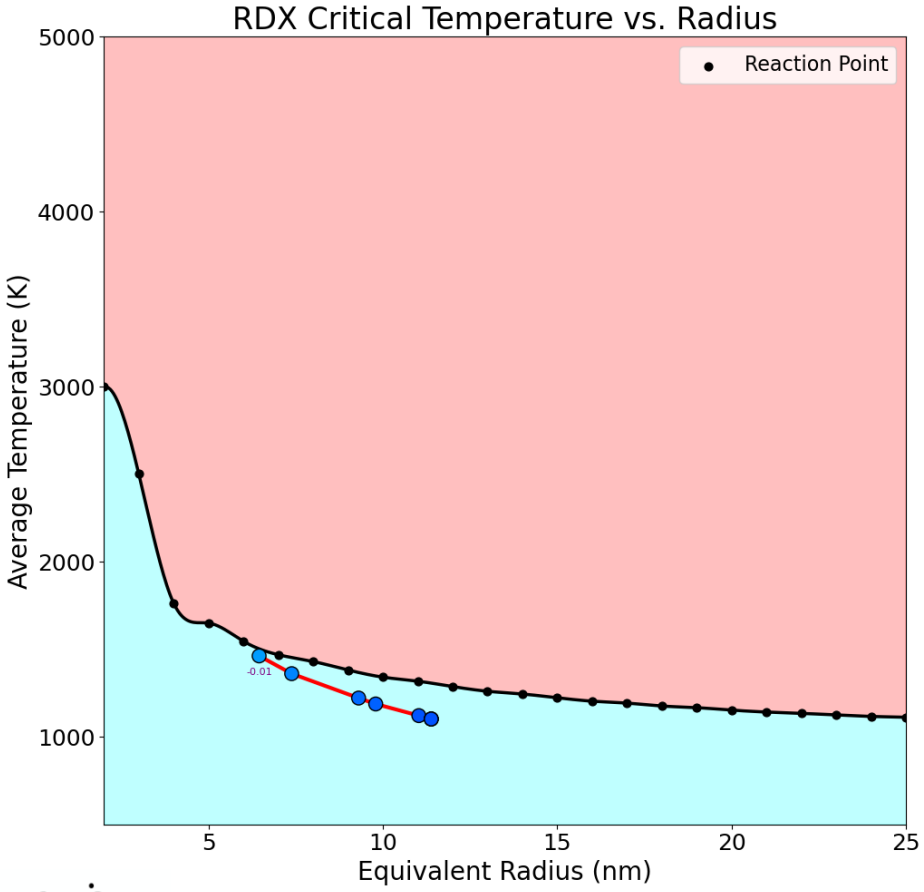


Hotspot (Size & Temperature) Function









Governing Process: $\rho C_v \dot{T} = k\nabla^2 T - Q_1 \dot{C}_1 + Q_2 \dot{C}_3$

Heat Diffusion: $k\nabla^2 T$

Reaction: $-Q_1 \dot{C}_1 + Q_2 \dot{C}_3$

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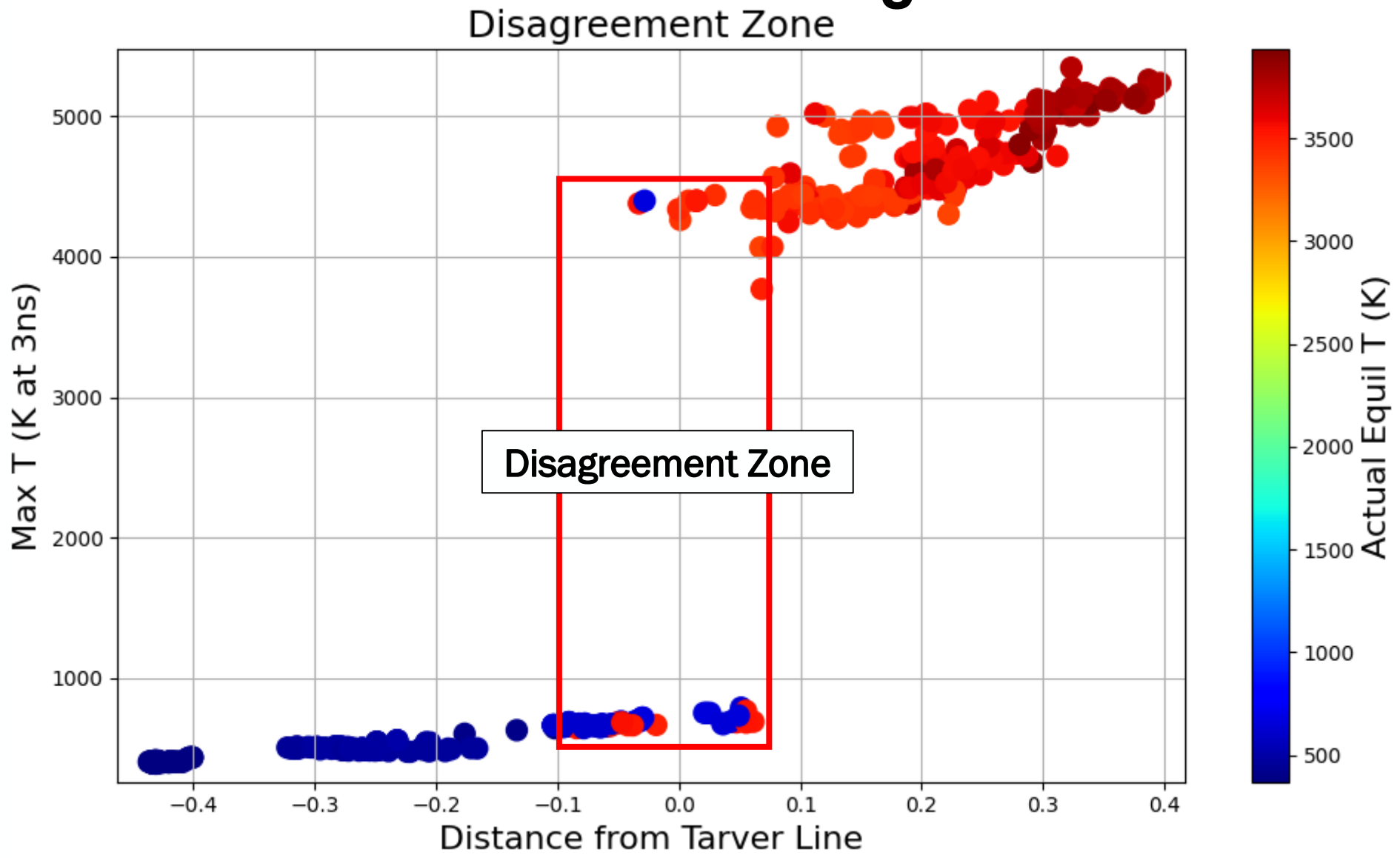
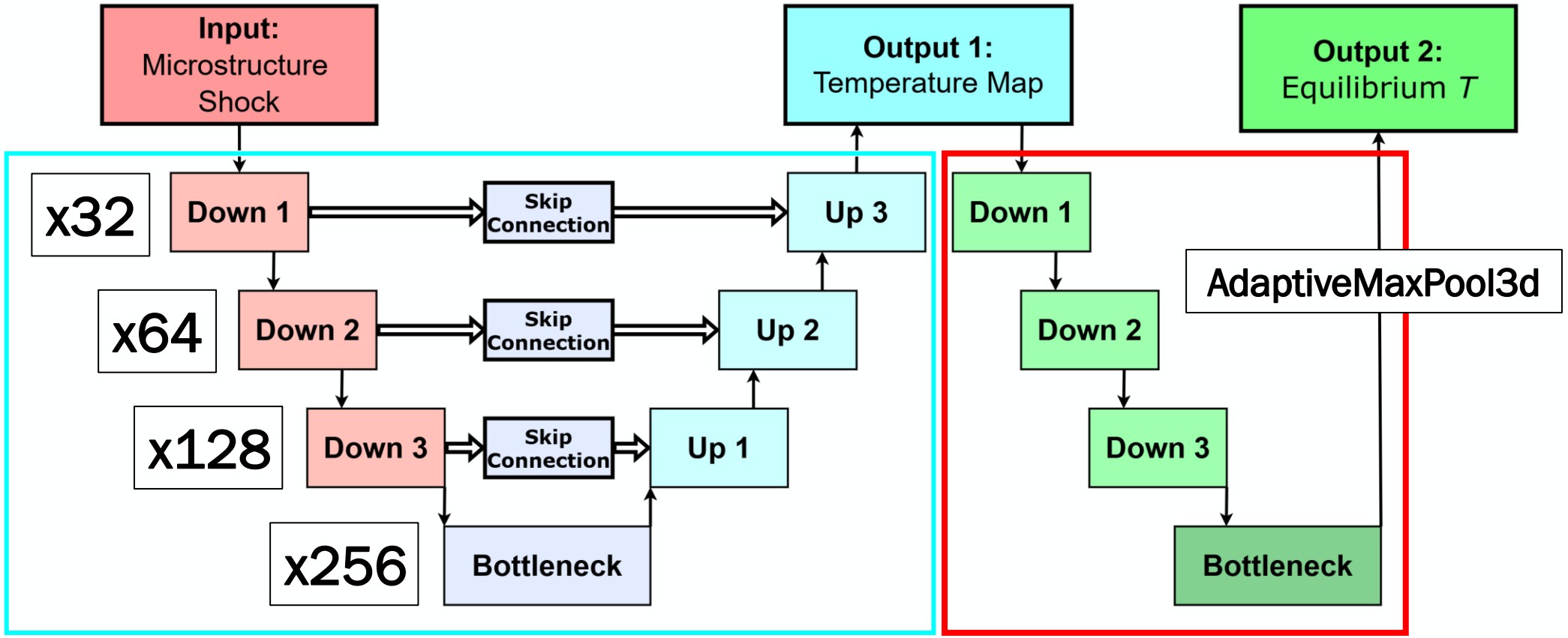
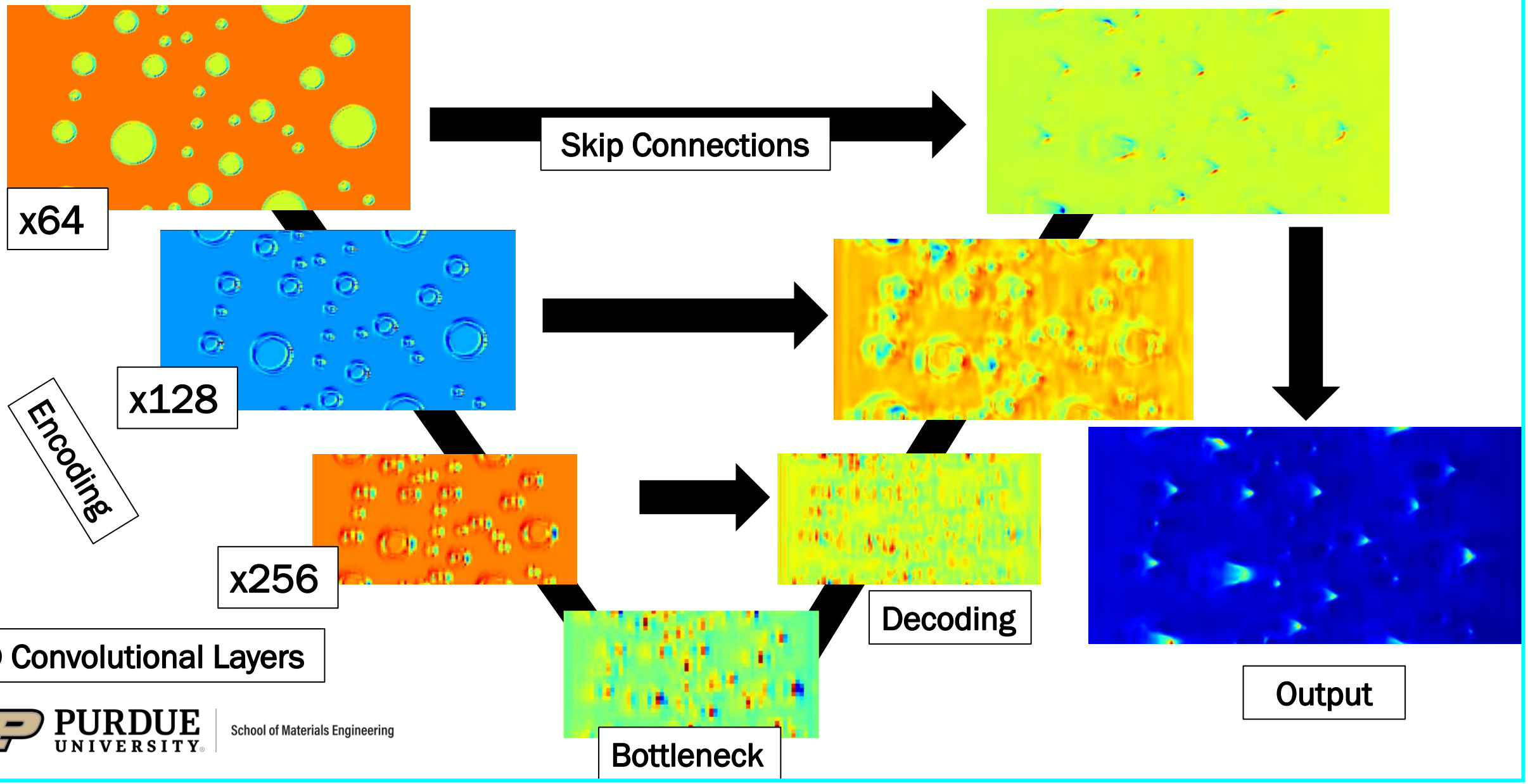
MISTnet Evolved Disagreement



MISTnet Multi-Model



MISTnet Original Layers



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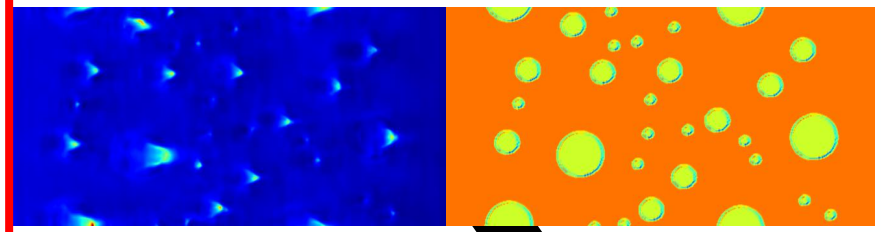
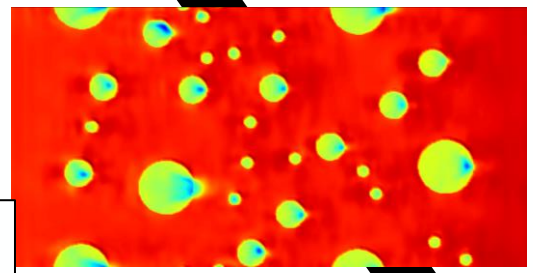
MISTnet Equil Layers

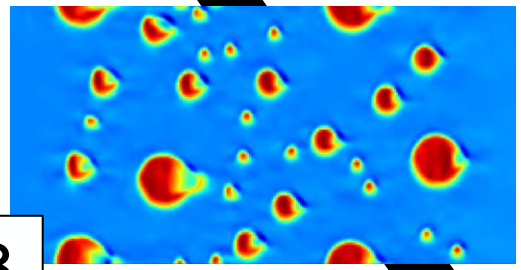


1 channel (T) + 3 channel (Density 1,2,3)

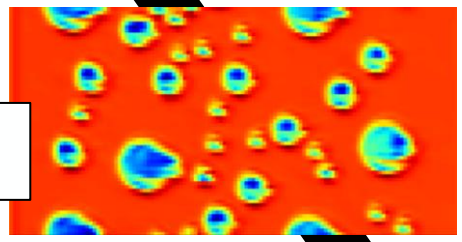


x64

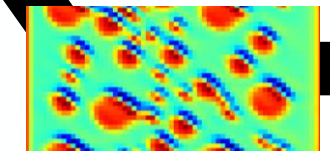
Encoding



x128

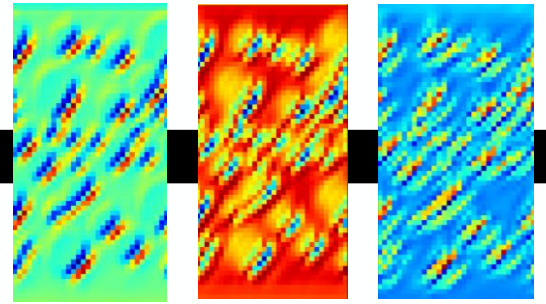


x256



x256

3D Convolutional Layers



Bottleneck

3568 (K)

Output

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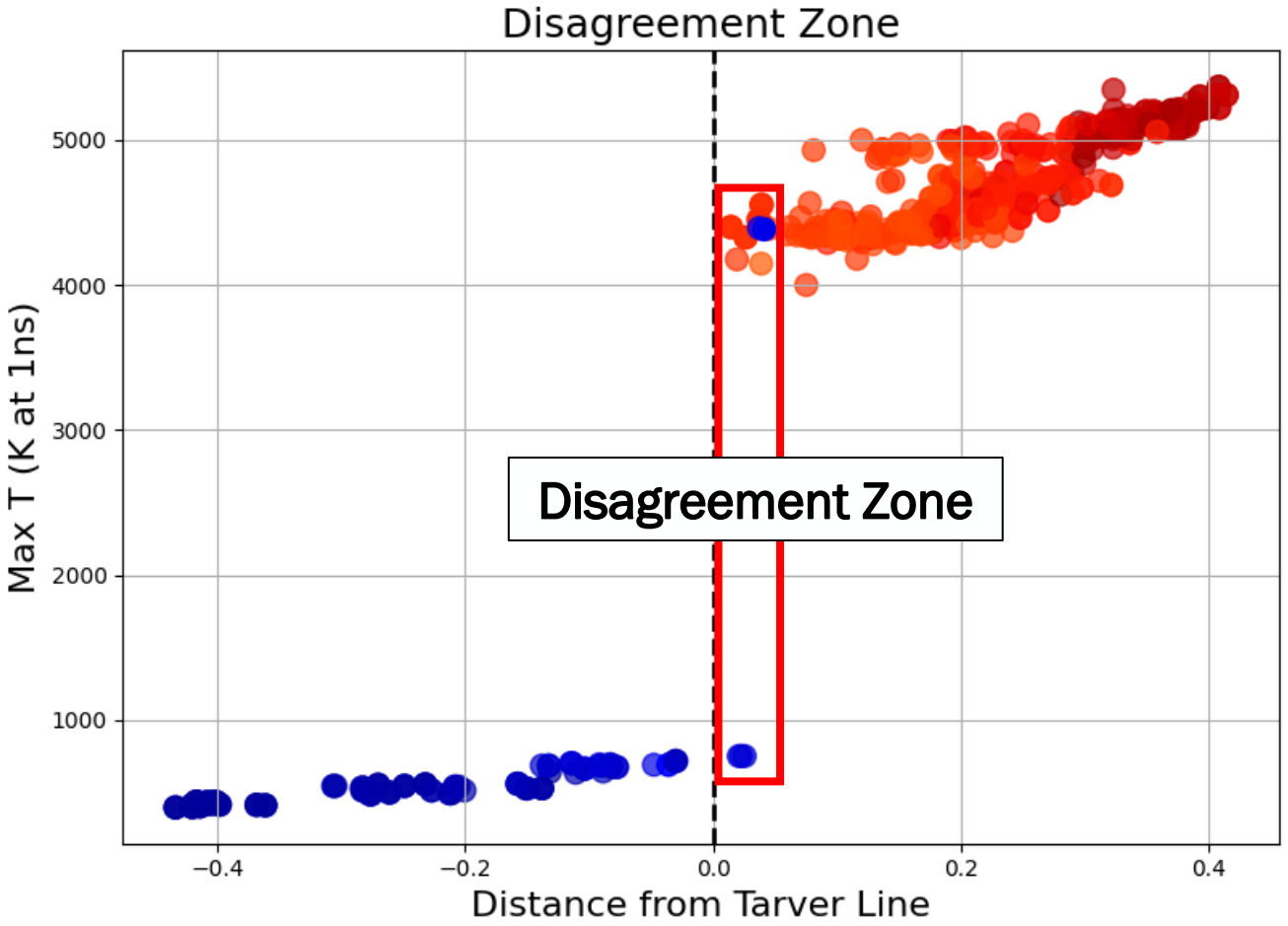
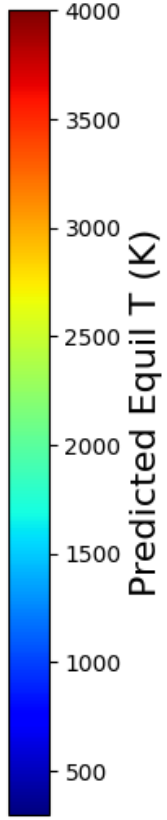
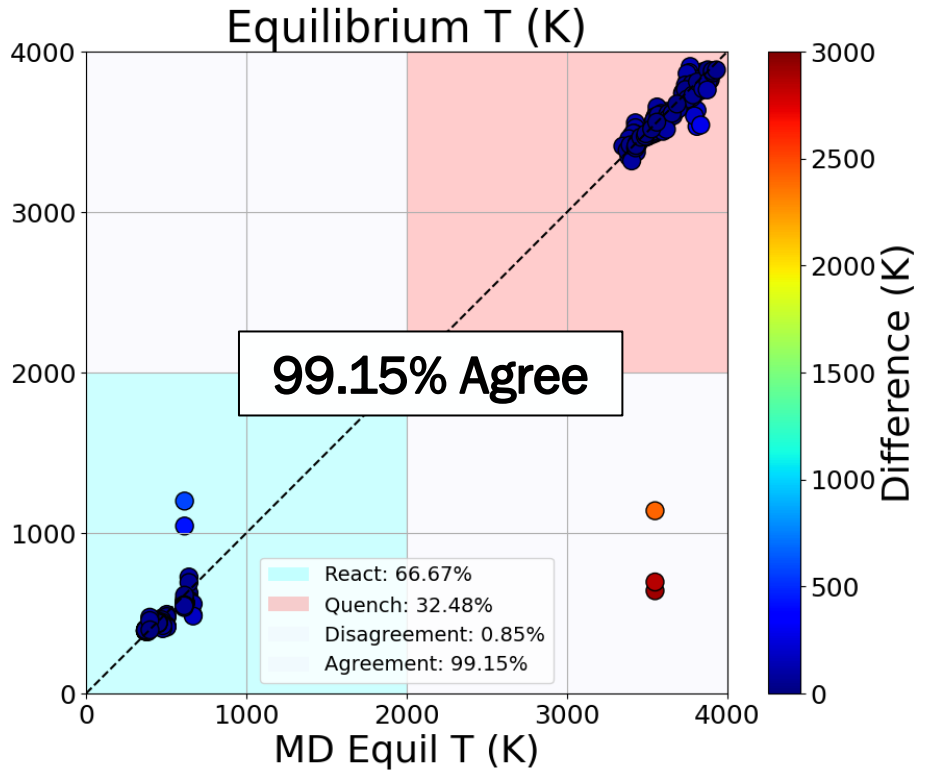
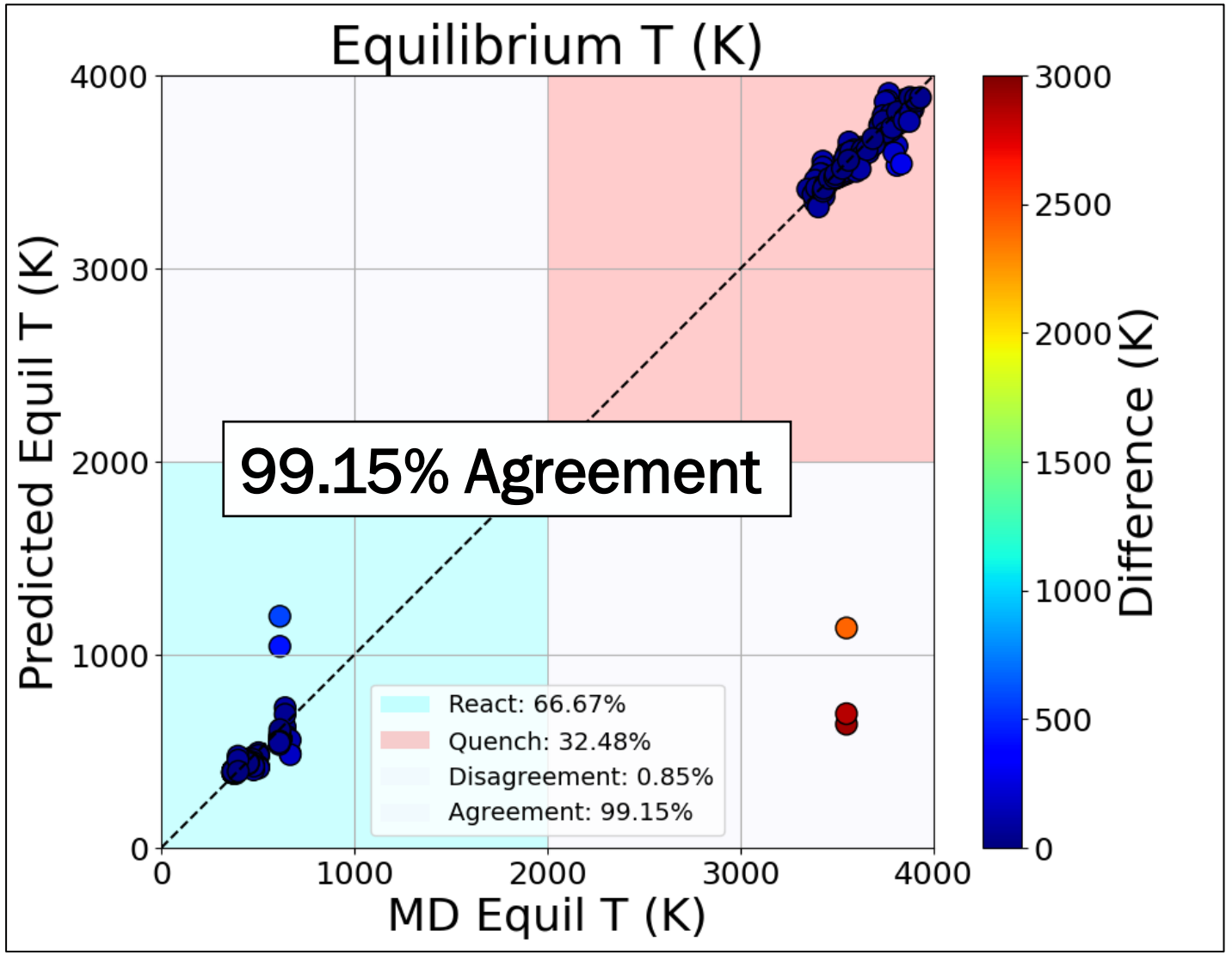
Best Equil T Prediction



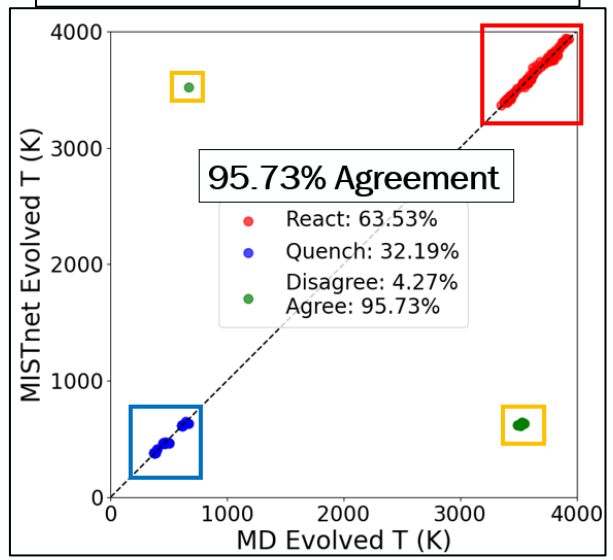




MD Evolved T vs MISTnet Evolved T vs Predicted Equil T



MD Evolved T
vs
MISTnet Evolved T



References

1. Li, C., Verduzco, J.C., Lee, B.H. *et al. Mapping microstructure to shock-induced temperature fields using deep learning.* **npj Comput Mater 9**, **178** (2023). https://doi.org/10.1038/s41524-023-01134-0
2. Sakano, M. N., Hamed, A., Kober, E. M., Grilli, N., Hamilton, B. W., Islam, M. M., Koslowski, M., & Strachan, A. (2020). *Unsupervised learning-based multiscale model of thermochemistry in 1,3,5-trinitro-1,3,5-triazinane (RDX)*. **The Journal of Physical Chemistry**, 124(44), 9141–9155. https://doi.org/10.1021/acs.jpca.0c07320