Experiment Report: Training Losses at 300K vs 1000K

This report presents the training losses observed when machine learning models are trained at different temperatures (300K and 1000K) for the molecules Pb, I, N, C, H. The key metrics of interest include energy and force errors, as well as root mean square errors (RMSE). The results are detailed for both the training and validation stages. The losses at 1000K were observed to be higher than those at 300K, as discussed below.

1. Training Losses at 300K

Learning Rate	0.002
Training Loss (total)	0.021203
Training Loss (energy)	0.000415
Training Loss (forces)	0.020787
Validation Loss (total)	0.021380
Validation Loss (energy)	0.000002
Validation Loss (forces)	0.021378

2. Training Losses at 1000K

Learning Rate	0.002
Training Loss (total)	0.083535
Training Loss (energy)	0.002305
Training Loss (forces)	0.081229
Validation Loss (total)	0.105628
Validation Loss (energy)	0.000880

Validation Loss (forces)	0.104748

Conclusion

From the experiment, we observe that training and validation losses are significantly higher at 1000K compared to 300K. The increase in both energy and force errors suggests that the models struggle to maintain the same level of prediction accuracy at higher temperatures. This indicates a temperature-dependent variation in the training performance for these molecules.

The training losses and validation errors increase with temperature, pointing toward potential model adjustments required for high-temperature simulations.

For further details, refer to the GitHub repository: https://github.com/chirag1701/nequip_project_ttu