High Pressure Material Phase Identification with Gaussian Kernel Neural Networks

CAMERON RYAN

SUPERVISED BY SHUAI ZHANG

University of Rochester, Laboratory for Laser Energetics

Background

- Phase identification is a process of classifying a certain spatial configuration of atoms as a certain type of ‘phase’, which is often a periodic crystal lattice
- Common methods for phase identification are based around comparing an observed structure to an ideal structure.
- A shortcoming of these methods is that they are extremely specialized to a few specific simple structures, and they are unable to classify non-periodic structures, such as amorphous, or melt
- Erhard et al. presented a method for crystal identification which involves classifying crystal structures using Dynamic Graph Convolutional Neural Networks (DGCNN)
- Erhard’s method is an extremely accurate, however slow to compute. We present a novel method for phase identification using machine learning which possesses similar accuracy with an extreme computational speedup.

Gaussian Kernel Model Derivation

- Work by Tancik et al. shows that in low dimensional, high frequency input domains, neural networks learn best on Fourier features because the Neural Tangent Kernel can represent the spatial proximity of points
- According to Rahimi et al. for points in Euclidean space, their representations as Fourier features with frequencies drawn from a kernel distribution will have dot products that approximate the kernel:

$$\mathbf{z}(r_k)^T\mathbf{z}(r) \approx k(r_k - r)$$

- Therefore, taking the sum Fourier features for each point in a local environment, and then applying the first weight matrix of a neural network approximates the Gaussian Kernel sum between each point and a set of ‘latent’ sample points

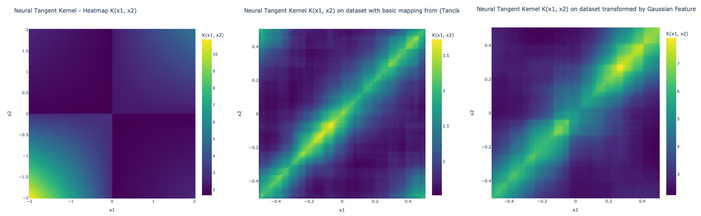
$$\sum_{i=1}^{n}(\mathbf{z}(\vec{r}_1)^T\mathbf{z}(r_i),...,\mathbf{z}(\vec{r}_m)^T\mathbf{z}(r_i))^T \approx \sum_{i=1}^{n}\left(e^{-\frac{|\vec{r}_1-r_i|^2}{2\sigma^2}},...,e^{-\frac{|\vec{r}_m-r_i|^2}{2\sigma^2}}\right)^T$$

Neural Tangent Kernel

- According to Jacot et al. a neural network will converge to the Neural Tangent Kernel as the number of hidden units goes to infinity

$$k_{\mathrm{NTK}}(\mathbf{x}_i,\mathbf{x}_j) = \mathbb{E}_{\theta\sim\mathcal{N}}\frac{\partial f(\mathbf{x}_i;\theta)}{\partial\theta}\cdot\frac{\partial f(\mathbf{x}_j;\theta)}{\partial\theta}$$

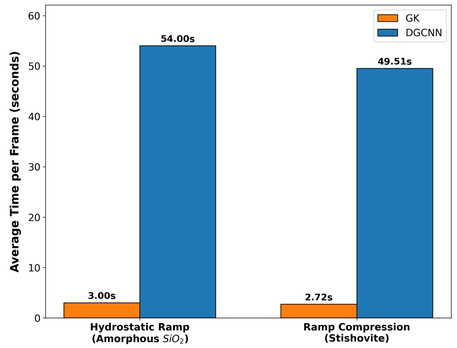
- To validate the theoretical efficiency of our method, we view the Neural Tangent Kernel of a neural network with a one dimensional input for (a) No transformation of the input, (b) Fourier features of input (like Tancik et al.) (c) Gaussian Kernel Features for a set of evenly distributed detectors
- Gaussian Kernel features give a highly diagonal/stationary NTK



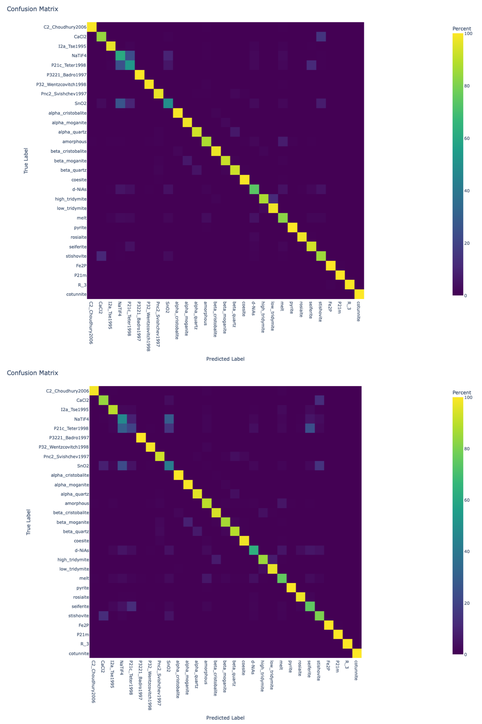
Hyperparameter Experimentation

- More hidden layers are detrimental to model accuracy
- More hidden units improve model accuracy
- Lower learning rates improve model accuracy

Computation Time Comparison to Leading Method



Confusion Matrix

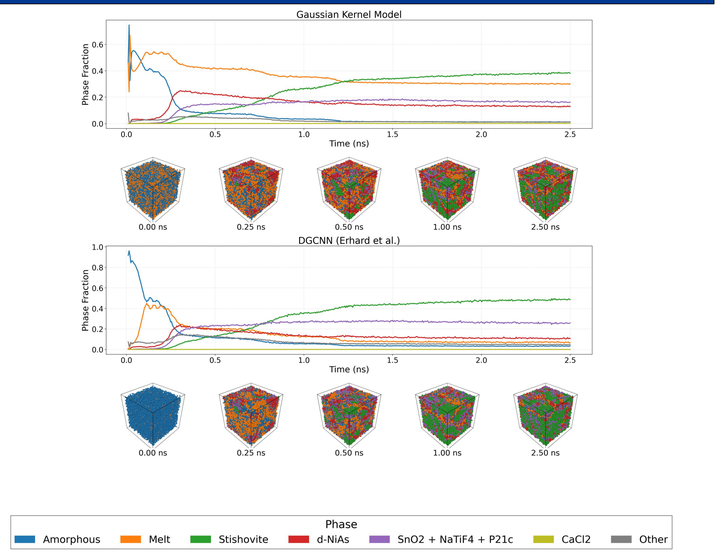


Test Accuracy Comparison to Leading Method

- Even with the extreme computational speedup, this method maintains better or comparable accuracies to the leading method

Environment Size	DGCNN (Erhard et al.)	Gaussian Kernel Model (This Work)
16	75%	78%
32	85%	86%
64	92%	90%

SiO2 Shock Simulation



Conclusion and Future Work

- We present a novel method for material phase identification using neural networks that presents comparable accuracies with a large computational speedup compared to the leading method
- Future work will involve increasing the hidden units and decreasing learning rate to develop more accurate models, and incorporate new structure types

References

- **[1]** L. C. Erhard, D. Utt, A. J. Klomp, K. Albe, "Crystal structure identification with 3D convolutional neural networks with application to high-pressure phase transitions in SiO_2," *Modelling and Simulation in Materials Science and Engineering* **32**, 065029, 2024. doi:10.1088/1361-651X/ad64f3
- **[2]** L. C. Erhard, C. Otzen, J. Rohrer, C. Prescher, K. Albe, "Understanding phase transitions of α-quartz under dynamic compression conditions by machine-learning driven atomistic simulations," *npj Computational Materials* **11**, 2025. doi:10.1038/s41524-025-01542-4
- **[3]** A. Jacot, F. Gabriel, C. Hongler, "Neural Tangent Kernel: Convergence and Generalization in Neural Networks," *arXiv:1806.07572*, 2020.
- **[4]** M. Tancik, P. P. Srinivasan, B. Mildenhall, S. Fridovich-Keil, N. Raghavan, U. Singhal, R. Ramamoorthi, J. T. Barron, R. Ng, "Fourier Features Let Networks Learn High Frequency Functions in Low Dimensional Domains," *Advances in Neural Information Processing Systems* **33** (NeurIPS 2020). arXiv:2006.10739
- **[5]** A. Rahimi, B. Recht, "Random Features for Large-Scale Kernel Machines," *Advances in Neural Information Processing Systems* **20**, 2007.
- **[6]** A. P. Bartók, R. Kondor, G. Csányi, "On representing chemical environments," *Physical Review B* **87**, 184115, 2013. doi:10.1103/PhysRevB.87.184115

This material is based upon work supported by the Department of Energy [National Nuclear Security Administration] University of Rochester “National Inertial Confinement Program” under Award Number(s) DE-NA0004144.