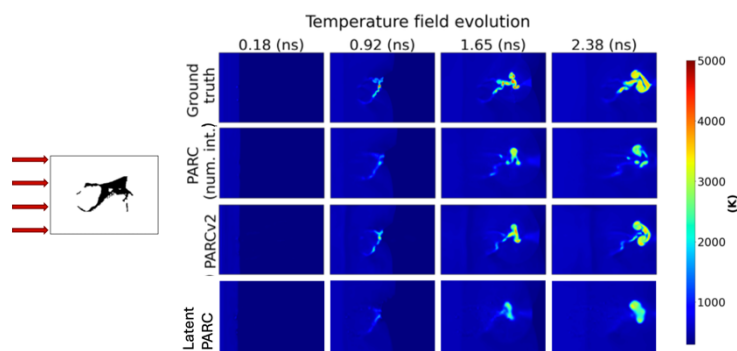


Modeling Dynamical Systems of Energetic Materials: Physics-Aware Convolutional Neural Networks in a Latent Space (LatentPARC)

Physics-informed machine learning has recently become popular for use in complex physics simulation due to its ability to extract complex features, handle nonlinearity, and perform well with fewer training data. However, when given insufficient data, machine learning models struggle to model dynamical systems that exhibit fast transient flows and sharp gradients. Here, we show that the challenge of learning complex spatio-temporal dynamics can be simplified by decoupling the problem into the tasks of learning complex geometric features of a dynamical system and of learning dynamics over these features. To do so, we build on previous work on physics-aware recurrent convolutional neural networks (PARC) [1, 2]. PARC embeds knowledge of the underlying dynamics into a neural network architecture to learn the dynamics of a given physics dataset more efficiently and make more accurate predictions. Previously, it was shown that PARC could effectively learn the thermomechanical behavior of energetic materials (EM) during shock-induced initiation using a relatively small set of high-resolution direct numerical simulations (DNS).

In this work, we further accelerate PARC and reduce its computational cost by projecting the original dynamics onto a lower-dimensional invariant manifold, or 'latent space' using a convolutional autoencoder. The projected latent representation encodes complex geometry of evolving fields (e.g., temperature and pressure) in a set of data-driven features. The reduced dimension of this latent space allows us to learn the dynamics of an EM problem with a lighter and more efficient version of PARCv1. We observe a significant decrease in training time and a 10x and 30x reduction in inference time when compared to PARCv1 and PARCv2, respectively. LatentPARC does this while maintaining predictive quality comparable to PARC, as shown in the figure below. This research also reveals information about latent dynamics specific to the EM problem. Our results further the understanding of latent dynamics of EM physical systems and



provide a base ML model which can be further expanded upon for additional investigation into the latent dynamics of highly nonlinear systems. This work can also be applied to other materials or difficult dynamical problems, with highly non-linear systems more benefited by this method than simpler systems.

[1]. Nguyen, P. C. H., Cheng, X., Azarfar, S., Seshadri, P., Nguyen, Y. T., Kim, M., Choi, S., Udaykumar, H. S., & Baek, S. (2024). PARCv2: Physics-aware Recurrent Convolutional Neural Networks for Spatiotemporal Dynamics Modeling. *arXiv (Cornell University)*. <https://doi.org/10.48550/arxiv.2402.12503>

[2]. Nguyen, P. C. H., Nguyen, Y., Seshadri, P. K., Choi, J. B., Udaykumar, H. S., & Baek, S. (2023). A Physics-Aware deep learning model for energy localization in multiscale Shock-To-Detonation simulations of heterogeneous energetic materials. *Propellants Explosives Pyrotechnics*, 48(4). <https://doi.org/10.1002/prep.202200268>