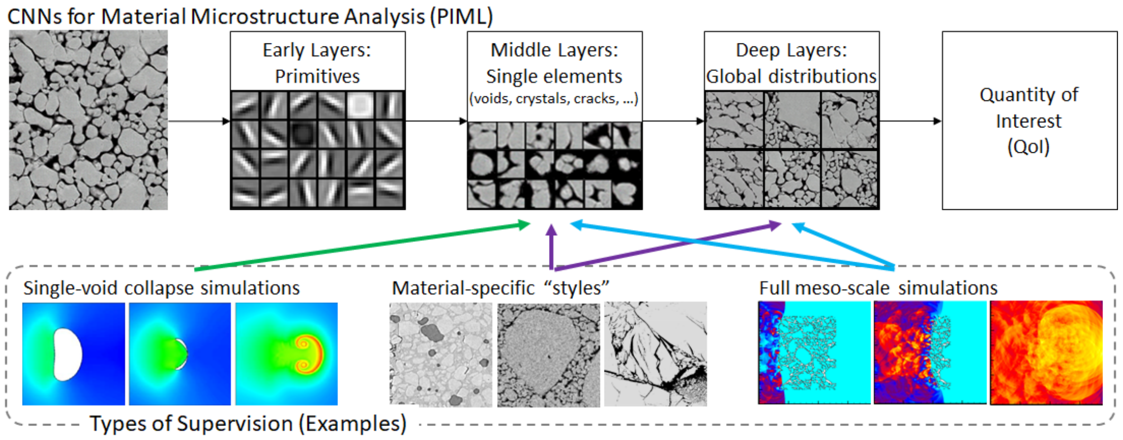
DMR-2203580

Physics-Informed Meta-Learning for Design of Complex Materials

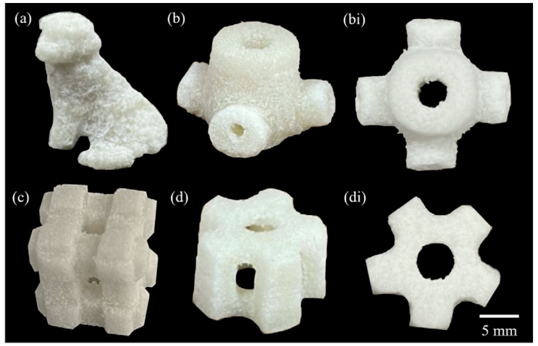
Stephen Baek, University of Virginia Main Campus

This project aims to develop new meta learning techniques to extend our previous machine-learning-based physical model of one particular energetic material (EM) species, HMX, to all known species of CHNO based EMs, such as PETN, TNT, RDX, TATB, and CL-20. Such a leap from a single material (HMX) to the comprehensive space of CHNO EM species is expensive because of the cost of running experiments. To address this challenge, meta learning methods will be used to leverage HMX-trained AI models as a springboard to accelerate development of burn models for new species.

In this reporting year (Year 2), we established a framework for describing meso-scale energy localization behaviors of **a range of CHNO materials**, ranging from the most sensitive molecule, PETN, to the least sensitive molecule, TATB. We also developed a meta-learning framework to generalize physics-aware recurrent convolutional neural networks (PARC) to other **unseen loading conditions**, as well as to bridge **different length-scales**. Furthermore, we developed a 3D printing capacity, called pressure-assisted binder jet (PBJ) process, to facilitate the **fabrication of meta-learned microstructures** and perform experimental validation.



Inexpensive training of a deep learning model via multi-scale simulation data. Small-scale, single void simulations are relatively inexpensive than full, meso-scale simulations. We hypothesize that a model can be pre-trained with a large number of single void simulations before it is scaled up to full, meso-scale simulations.



3D printed meso architectures via pressure-assisted binder jet

Broader Impacts

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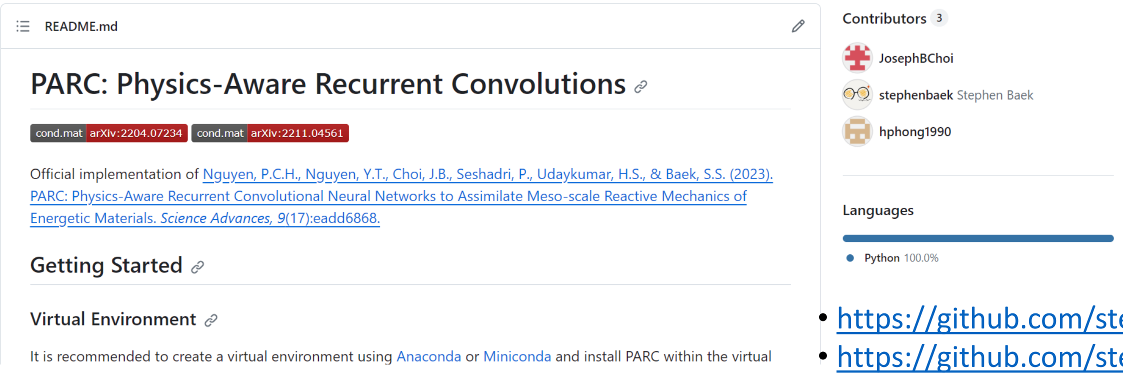
We have also made a meaningful progress towards constructing an open-source PyTorch library for the meta-learning source codes. There is already a TensorFlow version of research code made available to public at a GitHub repository (https://github.com/stephenbaek/parc) and a University of Virginia (UVA) undergraduate student is working on migrating the TensorFlow code to PyTorch for better extension to different use case scenarios and compatibility with other scientific machine learning (SciML) codes such as physics-informed neural networks (PINN).

There is another undergraduate student project in progress that aims to develop graphical user interface for the MaterIQ design framework. The students currently are working on developing React.js JavaScript front-end user interface. The goal is to have an interface that curates synthetic microstructure designs, pipelines different physics-aware machine learning models, and other design optimization tools in intuitive graphical user interface.


README.md

PARC: Physics-Aware Recurrent Convolutions

cond.mat arXiv:2204.07234 cond.mat arXiv:2211.04561

Official implementation of Nguyen, P.C.H., Nguyen, Y.T., Choi, J.B., Seshadri, P., Udaykumar, H.S., & Baek, S.S. (2023). PARC: Physics-Aware Recurrent Convolutional Neural Networks to Assimilate Meso-scale Reactive Mechanics of Energetic Materials. *Science Advances*, 9(17):eadd6868.

Getting Started

Virtual Environment

It is recommended to create a virtual environment using Anaconda or Miniconda and install PARC within the virtual

Contributors 3

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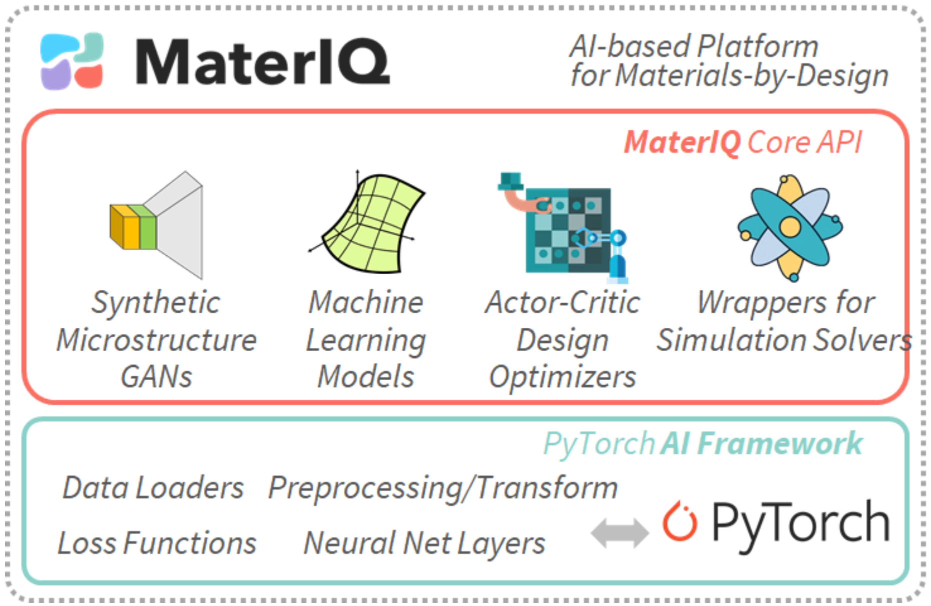
Languages

Python 100.0%

- https://github.com/stephenbaek/parc
- https://github.com/stephenbaek/PARCtorch



Overview of the MaterIQ software framework (backend) being developed in this project.

DMREF-specific

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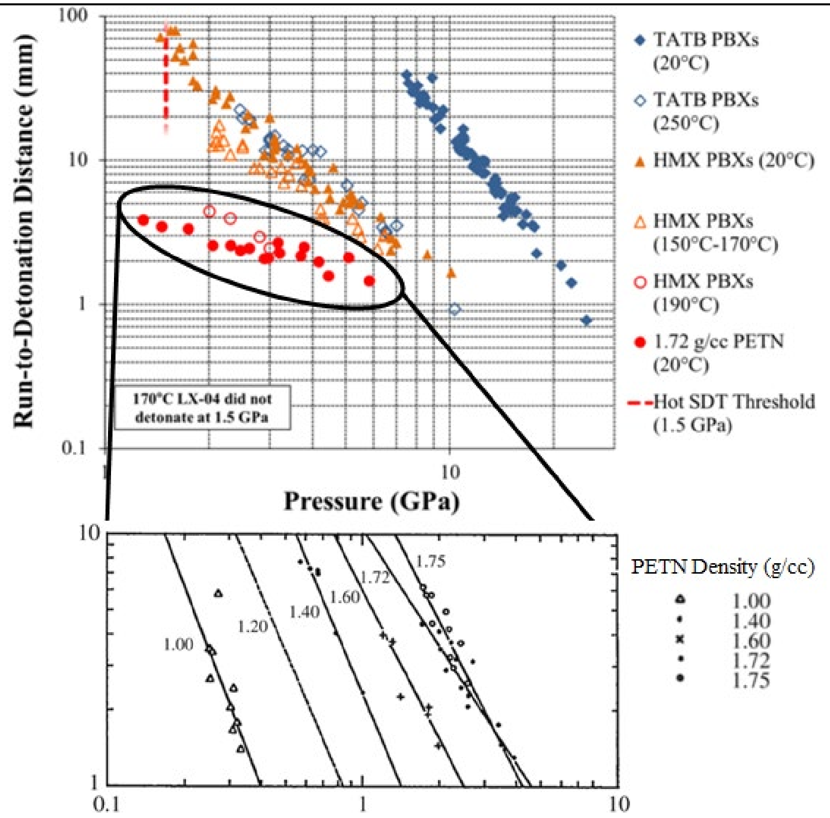
The progress we made in Year 2 contributes towards accelerating materials discovery and understanding of the fundamental knowledge of thermodynamics of energetic materials (EM) that are critical to various civilian and military (Air Force in particular) applications. For example, through PARC and the scale bridging, we were able to obtain a pop-plot numerically, based on rapid machine learning predictions, that aligns well with experimentally-obtained pop-plot. This is multiple-orders in magnitude of reduction of time and effort required to produce a pop-plot, which is critical for, e.g., engineering the sensitivity of EMs.

This project also supported 4 PhD students and 2 postdoctoral researchers both financially and by providing intellectually stimulating research problems. We also added an Air Force NRO student to the team in Year 2 to develop a momentum for the collaboration with AFRL. These next generation of scientists and engineers were trained and mentored in a multi-university and trans-disciplinary setting.



Pop-plots for various EMs showing the wide variation in sensitivity across different species (top) and across different microstructures (density) within the same species, PETN (bottom). Establishment of such data for different quantities of interests and for varying operating condition greatly facilitates the discovery of EMs.