Physics-Aware Recurrent Convolutional (PARC) Neural Networks
to Assimilate Meso-scale Reactive Mechanics of Energetic Materials

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Abstract

The thermomechanical properties of energetic materials (EM) are known to be a function of their microscopic structures, i.e., morphological configurations of crystals and pores. This microstructural dependency has motivated vigorous research in the EM community, seeking to engineer material microstructures with targeted properties and performance under the materials-by-design paradigm. However, establishing the complex structure-property-performance (SPP) relationships of EMs demands extensive experimental and simulation efforts, and assimilating and encapsulating these relationships in usable models is a challenge. Here, we present a novel deep learning method, Physics-Aware Recurrent Convolutional (PARC) Neural Network, that can “learn” the meso-scale thermo-mechanics of EM microstructures during shock-to-detonation transition (SDT). We show that this new approach can produce accurate high-fidelity predictions of time-evolving temperature and pressure fields of the same quality as the state-of-the-art direct numerical simulations (DNS), despite the dramatic reduction of computing time—from hours and days on a high-performance computing cluster (HPC) to a little more than a second on a commodity laptop. We also demonstrate that PARC can provide physical insights, i.e., the artificial neurons can illuminate the underlying physics by identifying which microstructural features led to critical hotspots and what are the characteristics of “critical” versus “non-critical” microstructures. This new knowledge generated alongside the capacity to conduct high-throughput experiments will broaden our theoretical understanding of the initiation mechanisms of EM detonation, as a step towards engineering EMs with specific properties.

Introduction

Energetic materials (EMs) such as propellants, explosives, and pyrotechnics are key components in many military and civilian applications. EMs are composites of organic crystals, plasticizers, metals, and other inclusions, forming complex microstructural morphologies, which are determining factors for the properties and performance characteristics of these materials.\textsuperscript{1} For instance, the sensitivity, one of the key performance parameters for the design of EMs, is strongly influenced by their microstructures.\textsuperscript{2–4} Pores, cracks, and interfaces in EM microstructures are potential sites for energy localization, i.e., the formation of high temperature regions or “hotspots”. Hotspots that are large enough and reach sufficiently high temperatures can initiate chemical reactions to release energy, strengthening the traveling shock and triggering a self-sustaining detonation.\textsuperscript{5} Due to the strong correlation between the microstructural morphologies and initiation sensitivity, in principle, one can engineer the sensitivity of EMs by manipulating their microstructures.\textsuperscript{6} This insight has inspired an active area of research to discover quantitative relationships between EM microstructures and their thermomechanical properties and performance, and to engineer the performance characteristics in a “materials-by-design” paradigm.\textsuperscript{7–9} However, the application such a framework is still confined by the lack of method that can efficiently provide accurate quantitative estimations of EM properties and performance with given microstructures. In this work, we propose a...
deep learning approach to overcome aforementioned issues called physics-aware recurrent convolution neural networks (PARC) to assimilate reactive mechanics of shock-initiated EM microstructures.

Establishing SPP linkages\textsuperscript{10} is, in fact, a central task in materials-by-design for EMs. In current practice, properties and performance of microstructures are determined experimentally\textsuperscript{11–13} or calculated using multiscale numerical experiments.\textsuperscript{14} In the latter approach, a large number of meso-scale simulations are conducted to develop a surrogate model, which is then used to produce macro-scale predictions of sensitivity by bridging the micro- and macro- length scales.\textsuperscript{14} In previous works, surrogate models for meso-scale energy localization were constructed using Gaussian Random Process techniques; training data were obtained from ensembles of simulations performed with canonical void shapes (circular/elliptical) and other simplifying assumptions were made to reduce the model complexity and computational effort in generating the training data. Nassar et al.\textsuperscript{15} developed a machine learning (ML) based surrogate model whereby hot spot ignition is formulated as a function of pore size and applied shock loading. Roy et al.\textsuperscript{16} developed a more sophisticated surrogate model spanning a larger parameter space, including not only the pore sizes, but also the aspect ratios of pores, their orientations, and volume fractions. Other approaches to quantifying hotspot dynamics have also relied on idealized synthetic microstructures with voids represented by circles,\textsuperscript{4,14,17} ellipses,\textsuperscript{18} and rectangles.\textsuperscript{19} Surrogate models assimilated in this manner\textsuperscript{20,21} were then used to close the macro-scale system of equations to model shock-to-detonation transition and determine critical energy for initiation\textsuperscript{22} and run-to-detonation distances. Using this multi-scale framework, the relationships between microstructural parameters, meso-scale dynamics (e.g., evolution of the hot spot temperature or hot spot area) and macro-scale quantities of interest (QoI), were determined.

The use of idealized microstructures\textsuperscript{18} or training data obtained from single void collapse calculations for surrogate modeling\textsuperscript{15} can simplify the material design space and facilitate the investigation of the SPP linkages of EMs, with tractable computational effort. However, such idealized representations may oversimplify the thermodynamics, and are unable to capture the full complexity of morphological structures (e.g., large, elongated cracks, tortuous voids) which may influence the energy localization phenomena at the meso-scale. Furthermore, simplified surrogates do not adequately model the interaction among microstructural features such as void-void interactions, contorted voids, and cracks. In addition, most surrogate models estimate the mesoscale QoI through an effective scalar value obtained by averaging techniques; therefore, such approaches cannot represent high-fidelity details and spatio-temporal variations of the hotspot dynamics. Hence, detailed local phenomena such as the origin of hotspots or the combination of multiple hotspots cannot be properly modeled. An alternative to constructing surrogate models using inputs from meso-scale calculations performed on single voids or idealized microstructures is to estimate SPP linkages of EMs directly on non-idealized, high resolution direct numerical simulations (DNS) performed on real, imaged microstructures (Figure 1b).\textsuperscript{19} However, due to the highly transient thermo-mechanics of shocked heterogeneous EMs, DNS with non-idealized microstructures are computationally intensive as numerical simulations require extremely fine grid resolutions For instance, a single, well-resolved meso-scale simulation of the reactive response of microstructures can take hours to days on high performance computing facilities. Moreover, since there is a large parameter space of stochastic micromorphy that needs to be examined during the design process, a vast number of experiments and simulations is required, leading to formidable costs for analyzing, modeling and designing new material microstructures.

The new deep learning-based approach presented in this paper, PARC, is proposed to overcome the aforementioned limitations of current approaches to establish SPP linkages of EMs. PARC is trained with DNS of image-derived or synthetic microstructures\textsuperscript{6} to assimilate the behavior of the spatio-temporal fields directly (Figure 1b). In contrast to typical input-output mapping of current deep learning methods in materials science,\textsuperscript{23–26} PARC is designed to predict the time evolution of temperature and pressure fields by modeling the governing differential equations using convolutional neural networks (CNN) in a recurrent formulation and solving them via data-driven integration. This CNN architecture design of PARC makes it “physics-aware” and interpretable, as its mathematical
formulation is reminiscent to that of typical DNS solvers. PARC is capable of predicting the evolution of temperature and pressure fields, providing a relationship between microstructures and hotspot field evolution, which cannot be attained with previous surrogate-based approaches. In addition, PARC can take complex microstructural morphologies fully into account and assimilate the hotspot dynamics with an accuracy comparable to DNS. Furthermore, once trained, PARC is computationally efficient with a steep reduction of computation time, nearly three orders of magnitude faster compared to DNS. Moreover, we also show that PARC can illuminate the mechanisms of hotspot formation and growth via neural network visualization techniques intrinsic to PARC, leading to the production of new knowledge on how and why hotspots are formed, which morphological features do or do not result in the formation of hotspots, etc. The resulting PARC-enabled capacity to run extremely high-throughput, high-fidelity simulations presented in this work, when combined with synthetic microstructure generation methods, can accelerate the EM characterization processes. These new capabilities will also allow exploration of the vast configuration space of EM microstructures and, thus, discovery of new functional structures. Furthermore, the new knowledge generated by visualizing PARC will broaden our theoretical understanding of EM meso-scale thermo-mechanics as demonstrated in the sections below.

**Physics-Aware Recurrent Convolutional Neural Network (PARC)**

PARC is trained to solve the governing differential equations that capture the ignition and growth of hotspots generated by shock passage through a real EM microstructure. In a domain tessellated into a regular Cartesian grid in a Eulerian framework, the state vector containing the temperature and pressure values at a given position \( r \) and specific time \( t \) is denoted as \( X(r; t) = [T(r; t), P(r; t)]^T \), where \( T(r; t) \) and \( P(r; t) \) are temperature and pressure fields at time \( t \) and position \( r \). The evolution of temperature and pressure fields over time is formulated as the following differential equation with initial boundary conditions.

\[
\frac{dX}{dt} = f(X, \mu) \\
T(r; t = 0) = T_0(r) \\
P(r; t = 0) = P_0(r)
\]

In Eq. (1), the microstructural shape descriptor, \( \mu \), is introduced into the computation model to account for the effect of microstructural morphologies on the evolution of the temperature and pressure. In addition, \( t = 0 \) refers to the instant when a transient shock enters the material at which the temperature field \( T(r; t = 0) \) is assumed to be constant with the value of 300K across all positions \( r(x, y) \). Solving Eq. (1), at a given time \( t = \tau \), the temperature and pressure values \( X(r; \tau) \) is computed as:

\[
X(r; \tau) = X_0(r) + \int_0^\tau f(X, \mu) \, dt
\]

In Eq. (2), it is required to compute the integral term \( \int_0^\tau f(X, t) \, dt \) to determine the current temperature and pressure values at a given Eulerian grid point. However, the integral is difficult to compute due to the highly transient, extreme dynamics, presence of discontinuities and large deformations inherent in the thermo-mechanics of shocked EMs. During the shock-induced reaction of EMs, both temperature and pressure fields exhibit high spatiotemporal gradients, resulting in both temporal and spatial nonlinearities in the evolution equation (2), particularly for the long time of evolution, i.e., when the value of \( \tau \) is high. For large values of \( \tau \), predictions from Eq. (2) may diverge from the ground truth, resulting in high sensitivity to noise and high prediction errors. To
avoid such issues, the integral should be decomposed into discrete time steps with reasonable time intervals, in the form:

\[
\int_{0}^{t_i} f(X, \mu) \, dt = \int_{t_0}^{t_1} f(X, \mu) \, dt + \int_{t_1}^{t_2} f(X, \mu) \, dt + \cdots + \int_{t_{i-1}}^{t_i} f(X, \mu) \, dt
\]

\[
= \int_{t_0}^{t_{i-1}} f(X, \mu) \, dt + \int_{t_{i-1}}^{t_i} f(X, \mu) \, dt,
\]

where \( t_i = \tau \) is the total time of the simulation. Substituting Eq. (3) into Eq. (2), we obtain:

\[
X(r; t_i) = X_0(r) + \int_{t_0}^{t_{i-1}} f(X, \mu) \, dt + \int_{t_{i-1}}^{t_i} f(X, \mu) \, dt
\]

\[
= X(r; t_{i-1}) + \int_{t_{i-1}}^{t_i} f(X, \mu) \, dt,
\]

Representing the integral over the interval \([t_{i-1}, t_i]\) by a function \(S\), we have:

\[
S(f) := \int_{t_{i-1}}^{t_i} f(X, \mu) \, dt,
\]

Both \(S(f)\) and \(f(X, \mu)\) represent complex spatiotemporal behavior of the material system and can be modeled by neural networks with parameter \(\varphi\) and parameter \(\theta\), respectively. Therefore, Eq. (4) can be written as:

\[
X(r; t_i) = X(r; t_{i-1}) + S(f(X, \mu | \theta) | \varphi)
\]

The goal of PARC is to accurately model the spatiotemporal evolution of both temperature and pressure fields calculated from shock-initiated reaction simulations. To this end, training of neural networks \(S(f)\) and \(f(X, \mu)\) is cast as an optimization problem in which the following loss function is minimized with respect to \(\theta\) and \(\varphi\):

\[
L(\theta, \varphi | \hat{X}) = \lambda_1 \int_{0}^{\infty} \left\| \hat{X}(r; \tau) - X_{i-1} - S(f(X, \mu | \theta) | \varphi) \right\|_2^2 \, d\tau
\]

\[
+ \lambda_2 \int_{0}^{\infty} \left\| \hat{\chi}(r; t) - f(X, \mu | \theta) \right\|_2^2 \, dt.
\]

Here, the quantities with the upper hat represents the ground truth data derived from DNS. The continuous training objective in Eq. (7) can be processed in the discretized form with a suitable time interval value \(\Delta t\). As a result, the loss function of Eq. (7) in the discretized from is:

\[
L(\theta, \varphi | \hat{X}) = \lambda_1 \sum_{t_i} \left\| \hat{X}(r; t) - X_{i-1} - S(f(X, \mu | \theta) | \varphi) \right\|_2^2 + \lambda_2 \sum_{t_i} \left\| \hat{\chi}(r; t) - f(X, \mu | \theta) \right\|_2^2
\]
Figure 2 illustrates how we modeled Eq. (6) as well as the loss function in Eq. (8) in the PARC neural network architecture. First, the morphology parameter $\mu$ is learned directly from the microstructure image $I(x, y)$ and the position map $U(x, y)$. Here the position map is a mapping $U: (x, y) \mapsto x$ introduced to represent how far each structural element is from the shock front. This is a necessary step because CNNs are translationally equivariant[i.e., CNNs are inherently incapable of distinguishing the relative position of structural elements from the shock front. We drop the vertical coordinate $y$ in the position map because the shock travels horizontally in our setting. We employ the U-Net architecture,[28] informed by the previous success of employing the U-Net as a morphology descriptor.[30] The U-Net architecture takes the microstructure image $I(x, y)$ and the position map $U(x, y)$ as inputs and returns a X-dimensional feature vector $\mu$ (morphology descriptor) as an output.

In the next step, the derivative solver takes the U-Net-encoded morphology descriptor $\mu$ and the initial temperature and pressure fields $X_0 = [T_0, P_0]^T$ as input and computes the time derivatives of temperature and pressure fields. The derivative solver essentially is a CNN whose architecture is illustrated in Figure 3(b), which models the governing differential equation $f$ in Eq. (1). The outputs of the derivative solver are comprised of the time derivatives of temperature and pressure fields, namely, $\frac{dX}{dt} = \left[\frac{dT}{dt}, \frac{dP}{dt}\right]$, which are then sent to the integral solver to compute the temperature and pressure fields after the time step $\Delta t$, namely $X_1 = [T_1, P_1]^T$. The integration solver is also a CNN as illustrated in Figure 3(c), which models the integral term $S(f)$ in Eqs. (6-8). We hypothesize that such a data-driven integration approach should compensate the numerical integration error arising from the discretization of extreme dynamics. This hypothesis will be tested in the following section.

Such a process of derivation and integration is repeated recursively through the final time step $t_N$ and PARC returns the predictions of temperature and pressure fields $X_1, \ldots, X_N$ for discrete time steps $t_1, \ldots, t_N$, respectively. Here, the neural network parameters (weights and biases) of the derivative and integration solvers are applied recursively, making these convolutions recurrent in the PARC architecture. Such a recurrent convolutional architecture is what makes PARC physically-aware, resembling the way of how dynamic systems are simulated in typical DNS solvers. As we will see in the later sections, this unique architecture makes PARC more interpretable compared to other black-box machine learning methods in which the input-output relationships are regressed in a simplistic manner. For more details of the PARC architecture design and implementation, please see Appendix.

**Prediction Performance of PARC**

PARC was trained on a data set from 42 instances of shock-initiated reaction simulations on two different classes of pressed EMs: fluid-energy-milled (FEM) and Class V (Figure 4(a) and (b)). The microstructures of these two materials were obtained from SEM images with spatial dimensions of $25 \mu m \times 25 \mu m$ resolved into $240 \times 240$ pixels (104.17 nanometers per pixel). Sequences of temperature and pressure fields evolving over time were computed from a DNS, performed using the multi-material reactive dynamics code, SCIMITAR3D. The calculations were performed using methods and models described in several publications. For this experiment, the microstructural samples were loaded with a shock of 9.5 (GPa) pressure applied at the left boundary of the domain, which then traverses through the microstructure from the left to right (Figure 4(c)). The total time scale of the simulation was 15.01 nanoseconds (ns), which was sufficient for the shock to traverse the entire sample shown in Figure 4(c) and for the collapse of all voids in the material. Hotspot ignition and growth ensued in the time period of 15 ns, creating an evolving field of hotspots that evolve in the post-shock region. The temperature and pressure field data were recorded at equal time intervals leading to 19 snapshots spaced at $\Delta t = 0.79$ ns time interval. In addition, during these simulations, the initial microstructures were deformed and advected with the post-shock flow velocity. To relate the initial void field in the microstructure to the final hotspot field in the current Eulerian framework, temperature and pressure fields were backtracked using the algorithm described in the Appendix. This pre-processing step resulted in 38 images of temperature and pressure fields having dimensions of $240 \times 240$ pixels. The supplementary information shows videos of the evolving microstructure and the resulting hotspot fields.
for some sample cases. In addition, the data set was normalized to have pixel values ranging from $-1$ to $1$. Finally, the data set was split into training, validation, and testing sets, with 30, 3, and 9 instances, respectively. The neural network parameters were initialized using normalized He initialization method\textsuperscript{31} and the ADAM optimizer\textsuperscript{32} with the learning rate of $10^{-4}$ was used to train PARC.

In this setting, the ability of PARC to accurately predict the evolution of the temperature and pressure fields was evaluated with the DNS predictions as the ground truth. First, PARC prediction results for both temperature and pressure fields were in a good agreement with those from the DNS predictions qualitatively, as shown in Figure 5 as an example. Notably, PARC was also capable of identifying the formation of hotspots and the locations and patterns of hotspot areas derived by PARC were in a good agreement with those derived from the DNS (Figure 5). Similarly, the propagation of shock waves in the microstructure during the simulation was well captured as indicated in both temperature and pressure field evolutions.

Quantitatively speaking, the average root-mean-square-error (RMSE) was 853.46 K for the temperature field predictions and 1.72 GPa for the pressure field predictions across nine independent test samples set aside from the training. More importantly, we also validate the prediction accuracy of PARC via several sensitivity QoIs that are known to be crucial for the design of EMs. Particularly, the sensitivity of EMs is measured via (1) the intensity of void collapse and ignition likelihood of critical hotspots, represented by the average hot spot temperature, where hotspots are identified as the locations in the domain having temperature value larger than 875K; (2) the growth rate and contribution of hotspots to energy localization, represented by the average area of hot spots; and (3) the rate of energy deposition at the meso-scale represented by the rates of change in average hot spot temperature and area.\textsuperscript{33} These sensitivity QoIs, the average hotspot temperature, the average hotspot area, and their rates of change, are computed as follows. In a given temperature field, being discretized into a $M \times N$ Euclidean grid, the average hotspot temperature, $T_{hs}$, and the average hot spot area, $A_{hs}$, at a given time, $t_k$, is compute as:

$$T^{hs}(t_k) = \frac{\sum_{i=1}^{M} \sum_{j=1}^{N} \left( T_{ij}(t_k) A_{ij}^{hs}(t_k) \right)}{A^{hs}(t_k)},$$

$$A^{hs}(t_k) = \sum_{i=1}^{M} \sum_{j=1}^{N} A_{ij}^{hs}(t_k),$$ \hspace{1cm} (9) \hspace{1cm} (10)

with:

$$T_{ij}^{hs}(t_k) = \begin{cases} T_{ij}(t_k) & \text{if } T_{ij}(t_k) \geq 875K \\ 0 & \text{if } T_{ij}(t_k) < 875K \end{cases}.$$ \hspace{1cm} (11)

In Eqs. (9-11), $T_{ij}^{hs}$ and $T_{ij}$ are the hot spot temperature and the temperature values at the examined grid location. Meanwhile, $A_{ij}^{hs}$ is the area of the examined grid and is a constant value as a Euclidean grid is applied. The hot spot temperature and area rate of change at a given time $t_k$ with $k > 0$, denoted as $\Delta T_{k}^{hs}$ and $\Delta A_{k}^{hs}$, are computed as described in Eq. (12) and (13).

$$\Delta T^{hs}(t_k) = \frac{T^{hs}(t_k) - T^{hs}(t_{k-1})}{t_k - t_{k-1}},$$ \hspace{1cm} (12)
\[ \Delta A^{hs}(t_k) = \frac{A^{hs}(t_j) - A^{hs}(t_{j-1})}{t_k - t_{k-1}} \]  

Figure 6 illustrates the time evolution of the average hot spot temperature, average hot spot area values and their rate of change that are derived from the PARC analysis result of nine independent test samples. In particular, for each examined time step, the QoI of all test samples are derived from PARC analysis result and their mean and 95% prediction interval are computed. Those computed values are stored and plotted with respect to the time variation. As depicted in Figure 6, across nine test instances, mean values of all four QoIs derived from PARC estimation are in agreement with those derived from DNS at all observed time steps. Specifically, as observed from Figure 6, the PARC predicted average hot spot area and its rate of change are nearly identical with those derived from DNS. In addition, Table 1 reports the validation for PARC-predicted QoI via several metrics, including normalized root mean squared error (Norm. RMSE), Pearson’s correlation coefficient (PCC), and Kullback-Leibler Divergence (KLD). From Table 1, quantitatively, PARC-predicted values strongly agree with DNS results as the normalized RMSE are low across all QOIs. In addition, PARC has an extraordinary capability in predicting hot spot area and hot spot area rate of change as beside normalized RMSE, the PARC-predicted results have extremely low KLD and relatively high PCC compared to DNS result. For hot spot average temperature and temperature rate of change, the prediction results also show agreement with ground truth data as given that the normalized RMSE are low (Table 1) and the predicted values follow the trend of ground truth data (Figure 6(a) and (b)).

|                  | Hot spot ave.          | Hot spot ave.          | Hot spot ave.          | Hot spot ave.          |
|------------------|------------------------|------------------------|------------------------|------------------------|
|                  | temp. temperature      | temp. rate of change   | area                    | area rate of change    |
| Norm. RMSE       | 0.0924                 | 0.0231                 | 0.0327                 | 8.49 × 10^{-7}         |
| KLD              | 8.03                   | 3.72                   | 0.026                  | 0.092                  |
| PCC              | 0.511                  | 0.19                   | 0.8703                 | 0.7795                 |

**Reduction of Computational Time**

Despite the high accuracy and high fidelity of the results, PARC showed a dramatic improvement in computational time. Table 2 reports the average computational times for a prediction instance for PARC and DNS, alongside the hardware resources used for the computations. As reported, the computational time with PARC is significantly reduced, averagely 0.5(s) with GPU and 9.2(s) without GPU, compared to about 24 hours with that of DNS using SCIMITAR3D solver. The superior computational efficiency is a huge advantage of PARC over DNS, making it more suitable for being utilized in design optimization.
Table 2. Computation efficiency comparison between PARC and DNS. PARC drastically reduce the computation time (more than 9000 times) while requires less computational resources.

|                  | PARC (on CPU)                             | PARC (on GPU)                             | DNS               |
|------------------|-------------------------------------------|-------------------------------------------|-------------------|
| Computation time (Average) | ~ 9.2 seconds                             | ~ 0.5 seconds                             | ~ 24 hours        |
| Hardware capacity | • Intel® Core™ i9-11900 CPU @ 2.50GHz (16 processors) | • Intel® Core™ i9-11900 CPU @ 2.50GHz (16 processors) | • Intel® Xeon E5-2699v4 CPU @ 2.80 GHz (1320 processors) |
|                  | • RAM: 64GB DDR4                           | • RAM: 64GB DDR4                           | • RAM: 128GB DDR4 |
|                  | • GPU: N/A                                 | • GPU: Nvidia RTX A5000                   | • GPU: Nvidia P100 |

Physics-Awareness and Interpretability of PARC

In addition to such high accuracy, fidelity, and efficiency, the physics-awareness of PARC is another benefit that separates it from the most of other “black-box” ML models used in the materials science community. Currently, in the literature, there are three common ways to achieve the physics-awareness of an ML model—namely observational bias, learning bias, and inductive bias approaches. An observational bias approach aims to embed physics into an ML model by training it with observational data reflecting the underlying physical principles. While being straightforward to implement, observational bias approaches, however, require a huge amount of data to reinforce the physics bias and to produce predictions that follow certain physical laws. Such a large data dependency makes it almost prohibitive to apply an observational bias approach to many materials science applications, given that generating data via either numerical or physical experiments is generally expensive. On the other hand, a learning bias approach injects physics knowledge into an ML model via custom physics-based loss functions (training objectives). These approaches tend to be model-agnostic, as they rely only on the definition of loss functions, and therefore more scalable and generalizable. However, as physics is embedded via soft constraints or penalties, these approaches can approximate physics laws only roughly and, therefore, are not capable of producing accurate and high-fidelity results. Finally, an inductive bias approach embeds physics into an ML model by tailoring the mathematical formulation and the architecture of the ML model to reflect the underlying laws of physics. Similar to how PARC models the governing differential equation of the EM thermodynamics and the process of solving these equations, the inductive bias approaches attempt to express the underlying physics laws in the form of ML model parameters or architecture design. Compared to the other two approaches, inductive bias approaches pose a few advantages. First, ML models designed in such a manner do not generally require a large quantity of data and can be trained with a small number of training samples (e.g., only 30 simulation instances in case of PARC), as the physics embedded in the model architecture and formulation serves as a strong prior for the learning process. Furthermore, as already demonstrated with PARC, inductive bias approaches can generate high-fidelity predictions, in contrast to learning bias models.

In addition to the advantages of small data learning and high-fidelity prediction, the unique physics-aware architecture presents several additional benefits. For example, as described in Figure 2, PARC incorporates the U-net-encoded microstructure shape descriptor, $\mu$, for the prediction of the time derivatives of temperature and pressure fields. The physics-aware architecture of PARC then allows us to unveil the effect of microstructure morphology on the formation of hot spots. Figure 7 highlights microstructures with high influence on the hot spot formation as visualized by the saliency map technique. As explained in ‘Methods’ section, the saliency map visualizes regions in the microstructure image that predicted large temperature changes in the derivative solver. Here, it is interesting to observe that the regions highlighted by the saliency map were all within voids and cracks.
in the microstructure images. This observation is, in fact, in accordance with the prior knowledge of the EM research community that hot spots are formed as a result of the release of chemical energy during the collapse of cracks and voids in EM microstructures.

Based on the saliency map visualization, we further analyzed the microstructural influence on the hot spot formation by classifying those voids and cracks into ‘critical’ and ‘non-critical’ ones. Figure 8(a) and (b) show some samples of critical and non-critical voids, respectively, randomly selected from the saliency map visualization results. Interestingly, we found that most of the critical voids were thin and elongated, as well as oriented in parallel to the direction of shock propagation (from left to right), as one may also be able to find from the samples in Figure 8(a). This, in fact, aligns with the observations of the prior work of Nassar et al.,43 Rai and Udaykumar,44 and Nguyen et al.45 which have demonstrated the strong influence of void aspect ratios and void orientations on the formation of hot spot. To further validate this trend, we fitted an ellipsoid to these voids and cracks to compute the void size, aspect ratio, and orientation (Figure 8 (c)). The morphometry analysis result shows that voids with average diameter of 0.835 ± 0.175 (μm), aspect ratio of 2.97 ± 0.73 and the angle of 17.724 ± 10.16(°) w.r.t the shock direction are the most responsible for the formation of hot spot. Meanwhile, non-critical microstructures have void average diameter of 1.061 ± 0.344 (μm), aspect ratio of 4.23 ± 1.81, and create angle of 49.65 ± 25.88(°) w.r.t to shock direction. In addition, our two-sample t-test46 also confirmed a clear difference in the morphometry distribution of critical and non-critical microstructures with P-value of 0.003, 0.001, and 0.001 for void average diameter, aspect ratio and orientation, respectively.

All of the above creates remarkable new research opportunities for the EM research community. As a matter of fact, there has been no work that studied the linkage between the real microstructure morphology and hot spot ignition mechanism, to the best of our knowledge. All previous works, including the one by Rai and Udaykumar44 relied on some idealized shapes such as elliptical voids to understand the structure-property relationships thus far. We anticipate the new lenses enabled by the physics-aware PARC architecture will significantly accelerate the research of microstructure influence on a various QoIs in the EM community. In particular, more detailed statistical morphometry analysis conducted on critical and non-critical voids may lead to more in-depth, foundational understanding of the hot spot ignition, and ultimately, to the capability to design and fabricate performance-optimized EM microstructures with engineered material properties. While more in-depth, quantitative investigation of the microstructure influence on the hot spot formation is deferred to the future research, we can at least conclude here that the unique physics-aware architecture of PARC creates new research opportunities that were impossible before.

**Conclusion**

In this work, we proposed a new deep learning model for prediction of shock-initiated reactions in EM. The validation results with FEM and class V materials showed that PARC is capable of predicting high-fidelity and accurate predictions of temperature and pressure field evolutions. PARC could predict EM sensitivity QoIs including hotspot temperature, hotspot area, and their rate of change over time with the accuracy comparable to DNS. Despite the strong agreement with the DNS, the computation cost was multiple orders of magnitude lower (from a day to less than a second). In addition, we demonstrated that the physics-aware architecture of PARC could create new kinds of observations that were previously impossible. For instance, with the saliency map visualization, voids and cracks that have the most influence on hotspot formation could be determined, enabling comparative analyses between critical and non-critical voids.

As such, PARC has a great potential to accelerate materials-by-design of EMs and to facilitate the scientific discovery of their SPP linkage, which is currently limited by the low-fidelity and oversimplified surrogate-based approaches. For instance, with the ability of incorporating non-idealized microstructures and featuring fast,
accurate, and high-fidelity analysis of EM shock-initiated reaction, PARC could accelerate the design optimization process and shorten time to discover desired EMs. Currently, we are working on developing a design optimization framework that integrates PARC as properties estimator for inverse microstructure design. Further, we plan to investigate deeper into expanding the interpretability of PARC, which as we saw, has a huge potential in providing additional lenses for the study of EM SPP linkages by shedding light on identifying the types of microstructures that lead to high energy concentration. Finally, we also plan to make additional improvements on PARC prediction accuracy and fidelity and expand its application for other groups of materials.

Methods

Simulation Method Meso-scale simulations are performed to simulate the collapse of voids in the microstructure due to the passage of a shock wave. The shock is parameterized by the pressure $P_s$. Reactive calculations are performed using methods discussed extensively in previous works.\(^\text{19}\) By performing the meso-scale simulations, temperature, pressure and species field data are utilized to quantify the response of the pressed material to the imposed shock. In the present context, the quantities of interest (QoIs) used to quantify the effect of microstructure on the sensitivity of the material are the evolution of the temperature field and the reaction product mass fraction in the sample. The temperature field $T(x, t)$ in the domain measures the intensity of a hot spot resulted from the process of void collapse. Higher temperature hot spots formed due to collapse of voids in the material lead to higher chemical decomposition rates. The reaction product mass fraction of HMX i.e., the total mass of solid HMX material converted to gaseous species at any time $t$, is used to quantify the physio-chemical response of the material and is given by the following equation:

$$F(t) = \frac{M_{\text{reacted}}(t)}{M_{\text{HMX}}}$$

$M_{\text{HMX}}$ is the mass of HMX in the total sample prior to the beginning of the chemical reaction process in the material, while $M_{\text{reacted}}$ is the mass of complete reaction products resulting from the burning of solid HMX to result in final gaseous reaction products. Complete conversion of the solid HMX to product gases is reached when $F = 1$. The reaction zone defines the hot spot in the domain, which is defined as the region where the temperature of the material exceeds the value of the temperature ($T_{\text{bulk}}$) reached after the passage of a planar shock wave. The hot spot area $A_{hs}$ is a significant QoI for determining sensitivity and is calculated as the area of the domain where the temperature $T(x, t) > T_{\text{bulk}}$. The hot spot area is recorded throughout the simulation to track the evolution of the hot spots.

Back Tracking Temperature and Pressure Field The raw temperature distribution from the simulation had a shifting effect along the shock propagation. We hence calibrated the temperature data by integrating back the velocity field. More precisely, Eulerian approach was taken to calculate the relationship between the initial microstructure and the final hot spot field. The backtracking of any QoI values from time step $t_{i+1}$ to the previous time step $t_i$ is conducted under the assumption that each material point lying at grid node moves with velocity $U$ associated with each grid node. Thus, the displacement $\Delta x$ of material associated with grid node at $t_{i+1}$ can be taken as $0.5(U_{i+1} + U_i)\Delta t$, in which $\Delta t$ is the time interval between two frames. For any non-consecutive two time steps $t_i$ and $t_j$, in which $i - j > 1$, the backtracking procedure is done by a step-wise approach. Starting from $t_j$, backtracking the field variable to $t_{j-1}$ and the process is repeated until reach time step $t_i$. As we consider the evolution history of material points starting from the first time step $t_0$, thus for any time step $t_i$, we need to fully backtrack its QoI variable to time step $t_0$.\(^\text{19}\)
**U-Net for shape descriptor extraction**

U-Net (Figure 2) is an encoder-decoder-like neural network that is widely used for semantic segmentation task. U-Net contains two network paths: encoder and decoder. The encoder takes an image as an input and gradually decrease the spatial size to compute feature maps at abstraction levels. On the other hand, the decoder gradually increases the spatial size, starting at low-resolution feature maps produced from the encoder and moves to full-resolution feature maps. In this work, both the encoder and the decoder contain three blocks that consist of repeated two convolutional layers followed by rectified linear unit layers (ReLU). For the encoder, a max-pooling operation with stride of two is applied for each block and decoder contains up-sample layers in each block. The number of channels in each blocks double as the depth goes deeper. Also, for each symmetric block, decoder concatenates the intermediate encoder feature map to yield a multilevel, multiresolution feature representation. Finally, unlike the original U-Net, the output of shape descriptor extractor has 128 feature maps, containing shape descriptors extracted from different resolution.

**Integral & Derivative Solver Networks**

The structure of convolutional layers in integral and derivative solver networks are identical except their inputs. The derivative solver network takes QoI field of the current time step $X$ (temperature and pressure field) and shape descriptor $\mu$ as input. On the other hand, only the derivative over time domain of QoI field, $\frac{\partial X}{\partial t}$, i.e., the output of the derivative solver, is taken as input for the integral solver network. As illustrated in Figure 2, both networks contain three components: two ResNet blocks and a super-resolution-like blocks. Zero padding was used for all convolutional layers thus the size of the input QoI fields is not varied during the computation.

**Saliency Map**

To calculate the saliency map, we first infer the microstructure image to our proposed model and produce the output temperature and pressure field. Consequently, a backward pass is used to calculate the derivative $G(x)$ with respect to the input image:

$$G(x) = \frac{df(x)}{dx} \quad \text{(14)}$$

Here, $f(x)$ is the predicted temperature field and $x$ is the input image. $G(x)$, representing the saliency map, is a tensor having the same dimension of the input microstructure $x$. In the case of PARC, there are multiple predicted temperature field from different time step; therefore, the final saliency map is the sum of derivative w.r.t microstructure image from all time step, such:

$$G(x) = \sum_{i=1}^{N} \frac{df_i(x)}{dx} \quad \text{(15)}$$

Finally, as the raw saliency map can be fuzzy and difficult to interpret, a threshold value $\varepsilon$ is applied to filter out the area with small gradient value, such:

$$\begin{align*}
G(x) &= G(x) \quad \text{if} \quad G(x) \geq \varepsilon \\
G(x) &= 0 \quad \text{if} \quad G(x) < \varepsilon
\end{align*} \quad \text{(16)}$$

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Figure 1: The establishment of SPP linkages is among most crucial tasks in materials-by-design for EM (a). DNS on non-idealized microstructures is the most ideal solution for SPP linkage estimation. However, such that approach is costly and time-consuming due to the requirement of extreme fine grid resolutions for complex geometry. PARC (b) is trained with DNS result of shock-initiated reaction simulations to assimilate the thermos-mechanics of EMs during their SDT. The proposal of PARC features an efficient, accurate and high-fidelity SPP model which can accelerate the materials-by-design process, thus, shorten time consumption for designing new EM.
Figure 2: Architecture of the proposed model. The inputs to the model are binarized microstructure image, position field, and initial condition of the temperature and the pressure field. Initially, the U-Net takes microstructure image and the position field as an input and produces the shape descriptor $\mu$. Consequently, $\mu$ and the initial condition $X(t_0)$ are inserted to the derivative solver (purple boxes) to produce the derivative over time, $\dot{X}$, of QoI. The predicted $\dot{X}$ value is sent to the integral solver (orange boxes) to compute the QoI rate of change $\int \dot{X} dt$. Finally, the derived value is then added to the QoI value $X(t)$ to produce the QoI of next time step, $X(t + \Delta t)$. The process is repeated recurrently until the final time step, resulting in the sharing of network hyperparameters between derivative and integral solvers at different time steps.
Figure 3: The detail architecture design of the shape descriptor extractor (a), the derivative solver (b), and the integral solver (c). The shape descriptor extractor (a) used three-level U-net architecture. All convolutional layers of the shape descriptor extractor have kernel size of 5 and the dimension of feature map is reduced/increased twice after each max-pooling/upsampling layers. Conversely, the dimension of feature maps in both derivative (b) and integral solvers (c) does not change after convolutions. Both solvers are started with two ResNet block with kernel size of 64 and 128 and finished with a super-resolution-like block. The number of feature maps for each convolutional layers in the super-resolution-like block is 128, 64, 32, 2, while the kernel size of them is 7, 1, 1, 3, respectively. The shape descriptor extractor derives a 240x240x128 feature map of shape descriptor that will be used to for the derivative solver while both derivative and integral solvers have the output dimension of 240x240x2.
Figure 4: FEM (a) and class V (b) microstructures are used to create training data for PARC. (c) The shock-initiated simulation is conducted with shock pressure of 9.5 GPa entering the EM microstructure with dimension of $25 \times 25 \text{ (\mu m)}$ from the left.

Figure 5: Predicted Temperature & Pressure Field by PARC with given input microstructure. The first and third row corresponds to ground truth temperature and pressure field respectively. The second row and fourth row are the model predicted temperature and pressure field. As can be seen, PARC is capable of deriving accurate and high-fidelity analysis with almost all hotspots being correctly predicted. In addition, the shock wave entering microstructure, the hotspot ignition and growth are also well-recognized.
Figure 6: The sensitivity metrics prediction of EMs produced by PARC: (a) average hot spots temperature, (b) average rate of change of hot spots temperature, (c) average hot spot area, (d) the average rate of change of hot spots area. As being shown, there is an agreement between the prediction and the ground truth data.
Figure 7: Hot spot identification using saliency map. The saliency map is derived by computing the derivative of the corresponding temperature field with respect to the input microstructure image. Consequently, the saliency map is registered to the corresponding microstructure image. Voids that are highlighted by the saliency map are classified as ‘critical’ microstructure.
Figure 8: From the identification result provided by the saliency map, “critical” (a) and “non-critical” (b) microstructures are cropped for morphometry analysis (c). The morphometry analysis result (c) shows clear distinction between “critical” and “non-critical” microstructures as their P-value of two samples t-test are low (0.003 for void diameter, and 0.001 for void orientation and aspect ratio). The morphometry analysis result agrees with previous findings on the size and shape of voids that can potentially lead to energy concentration which cause the ignition of hot spot.