Physics-Aware Convolutional Neural Networks for Modelling Energetic Material in the Strong Shock Regime

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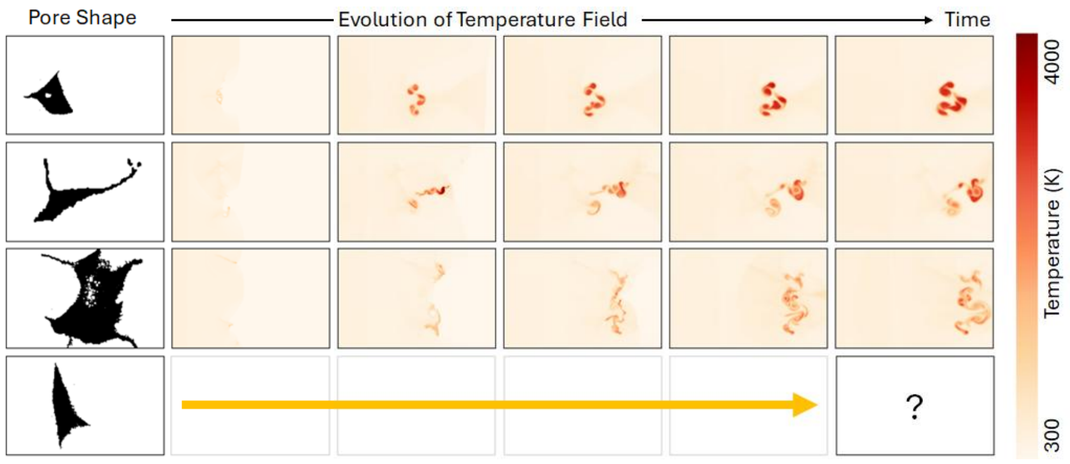
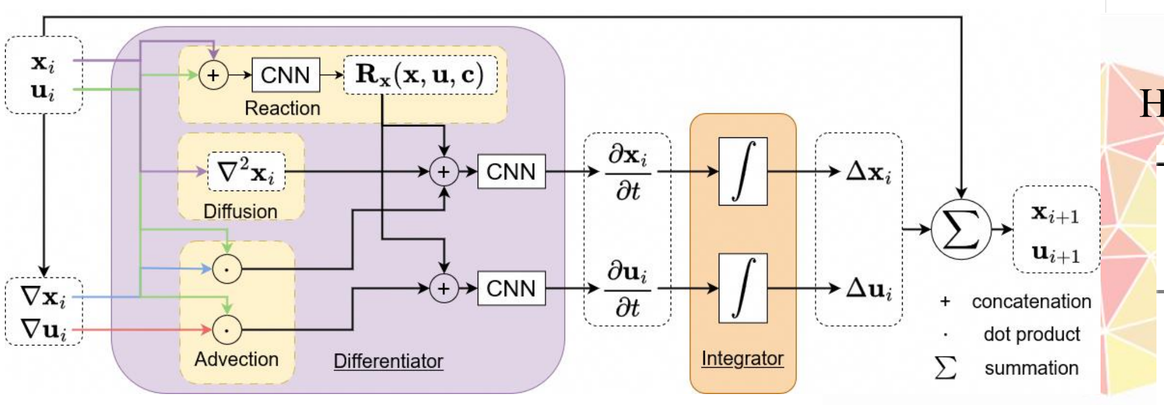
Introduction



- Sensitivity-performance balance
- Governed by molecular structure and **microstructure**
- Structure-Property-Performance (S-P-P) linkages in EM
- Traditional DNS takes days on HPC
- Can we do it in seconds on a workstation?
- Without requiring millions of training samples

PARCv2

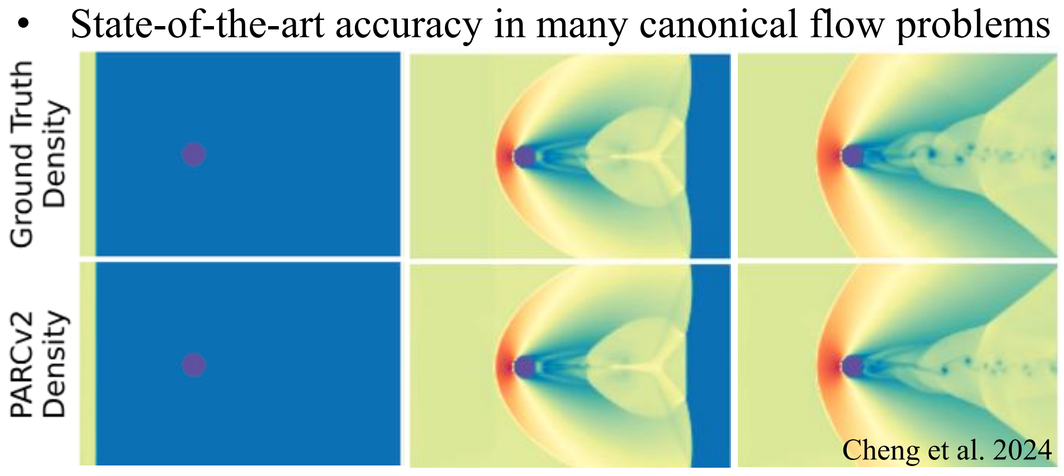


- Physics-aware Recurrent Convolutional Neural Network (PARCv2)
- Building the structure of ADR equations into the architecture
  - Numerically calculated advection & diffusion
  - Merged with learnt reaction terms
  - Predicts temporal derivatives
  - Numerical integrated to get the next step

Paper
Nguyen et al. 2024

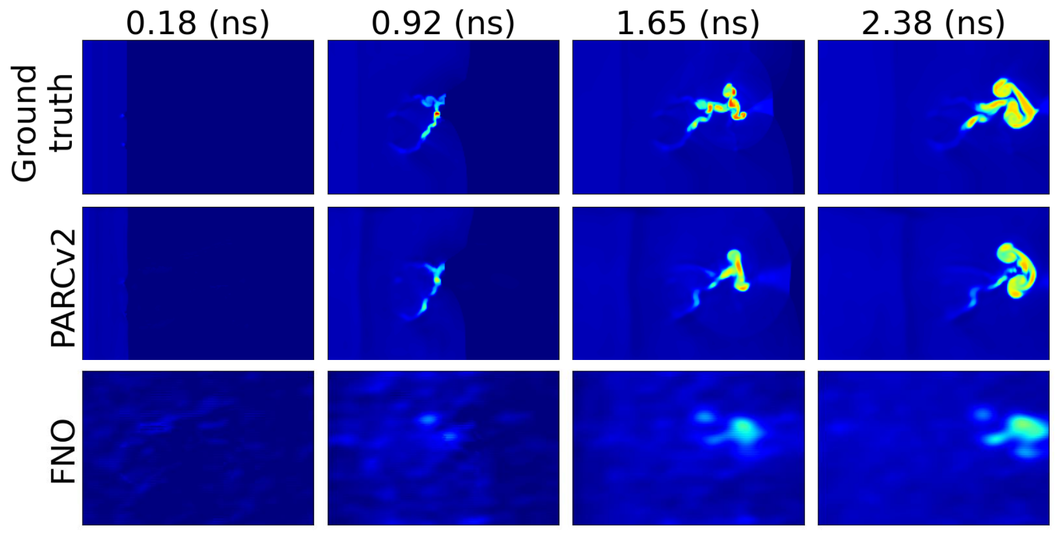
Github repo

- State-of-the-art accuracy in many canonical flow problems



- Comparison model -- Fourier neural operator (FNO)
  - Learning the operators mapping between Fourier space
- Comparison model -- PARC
  - No ADR structure, black box NN approximation of governing equations

Results



Prediction error:

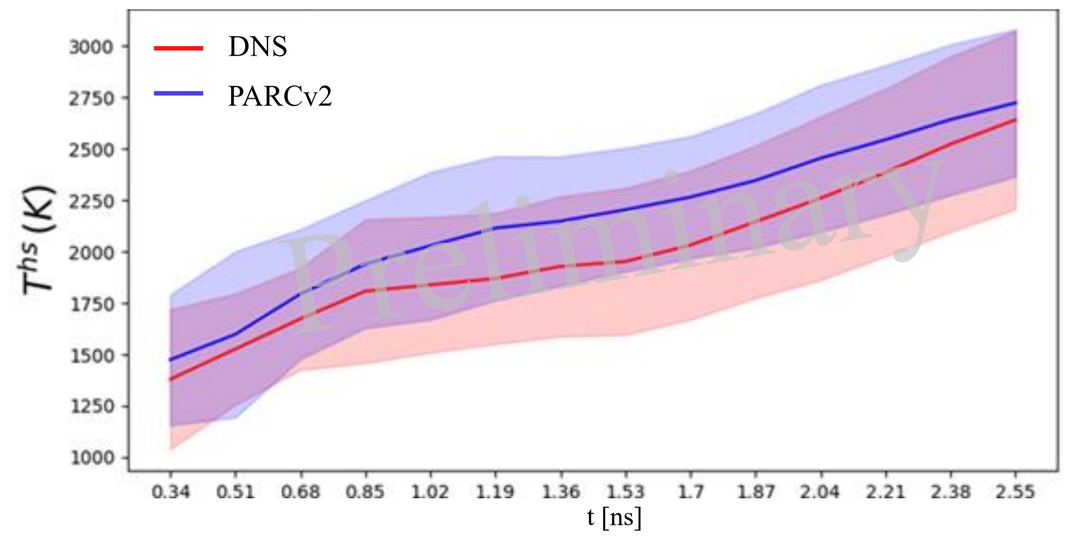
Model	Energetic Materials $RMSE_T(K)$	Energetic Materials $RMSE_P(GPa)$
PARC (numerical int.)	249.99	1.491
PARC (data-driven int.)	306.99	4.111
FNO	248.39	2.685
PARCv2 (This Study)	229.52	1.634

Hotspot characteristics:

Model	Energetic Materials $\varepsilon_{T^{hs}}$ (K)	$\varepsilon_{A^{hs}}$ (μm^2)	$\varepsilon_{\dot{T}^{hs}}$ (K/ns)	$\varepsilon_{\dot{A}^{hs}}$ $(\mu m^2/ns)$
DNS	-	-	-	-
PARC (numerical int.)	409.58	0.0253	269.09	0.0248
PARC (data-driven int.)	972.38	0.0728	839.64	0.0681
FNO	622.60	0.0431	425.91	0.0527
PARCv2 (This Study)	149.27	0.0060	228.98	0.0094

PARCv2 achieves best accuracy over the entire domain and in regions of scientific interest

Future Works



- Consistent overprediction of hotspot temperature
- Modeling more complex problems
  - Multi-pore microstructure
  - Single model multiple material
  - Different shock strength

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