APS Topical Group on Compression of Condensed Matter GCCM

24th Biennial Conference of the APS Topical Group on Compression of Condensed Matter, Washington DC, June 22-27, 2025.

Physics-Aware Convolutional Neural Networks for Modeling Energetic Material in the *Weak Shock Regime*

Xinlun Cheng[1] (Presenter)

Yen Nguyen,[2] Joseph Choi,[1] Pradeep Kumar Seshadri,[2] Mayank Verma,[2] H.S. Udaykumar,[2] Stephen Baek[1,3]

[1] School of Data Science, University of Virginia
[2] Department of Mechanical Engineering, University of Iowa
[3] Department of Mechanical and Aerospace Engineering, University of Virginia

Visual Intelligence Laboratory

UVA DATA SCIENCE

UVA ENGINEERING

IOWA ENGINEERING

DEVCOM ARMY RESEARCH LABORATORY

NSF

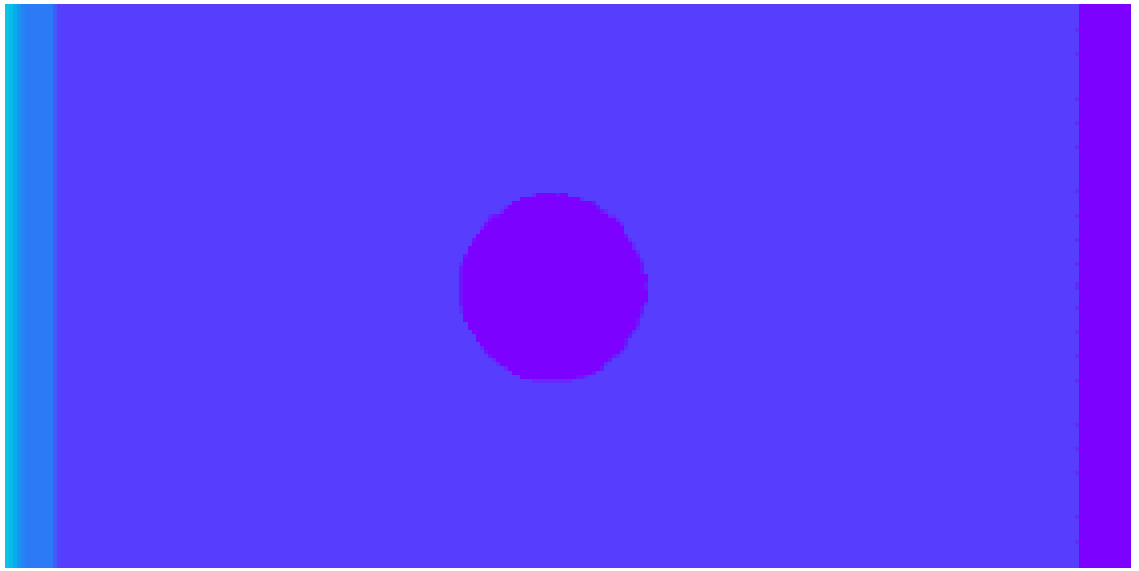
DMREF MATERIALS FOR OUR FUTURE

EM Reactive Dynamics in Different Shock Regimes

- **Strong Shock**

- Localized region of high temperature: hotspot
- Nano-second scale
- Continuum simulation: a few CPU hours
- Frequently simulated & modeled

- **Weak-to-Modest Shock**



- Multitude of physical processes
- Pico-second scale
- MD simulation: millions of CPU hours
- Continuum simulation: a few CPU hours[1,2]
- **Understudied**

[1] Herrin et al. 2024 "Pore collapse, shear bands, and hotspots using atomistics-consistent continuum models for RDX (1, 3, 5-trinitro-1, 3, 5-triazinane): Comparison with molecular dynamics calculations." *Journal of applied physics* 136, no. 13 (2024).

[2] Nguyen et al. 2024 "Continuum models for meso-scale simulations of HMX (1, 3, 5, 7-tetranitro-1, 3, 5, 7-tetrazocane) guided by molecular dynamics: Pore collapse, shear bands, and hotspot temperature." *Journal of applied physics* 136, no. 11 (2024).

EM Reactive Dynamics in Different Shock Regimes

- **Strong Shock**
  - Localized region of high temperature: hotspot
  - Nano-second scale
  - Continuum simulation: a few CPU hours
  - Frequently simulated & modeled
- **Weak-to-Modest Shock**
  - Multitude of physical processes
  - Pico-second scale
  - MD simulation: millions of CPU hours
  - Continuum simulation: a few CPU hours
  - **Understudied**

Can we go faster?

Entire simulation in seconds,
without requiring millions of training samples

Yes, with the help of physics-informed machine learning!

PARCv2

- Integrating ADR equations into neural network architecture
  - Inductive design philosophy
  - Numerically calculated advection & diffusion
  - Merged with learnt reaction terms
  - Predicts temporal derivatives
  - Numerical integrated to get the next step
- Proven track record in modeling extreme dynamics
  - Dynamics of localized region of high temperature[1]
  - Supersonic cylinder flow[2]
  - Achieved state-of-the-art accuracy with <100 training simulations
  - Inference in seconds on a GPU workstation

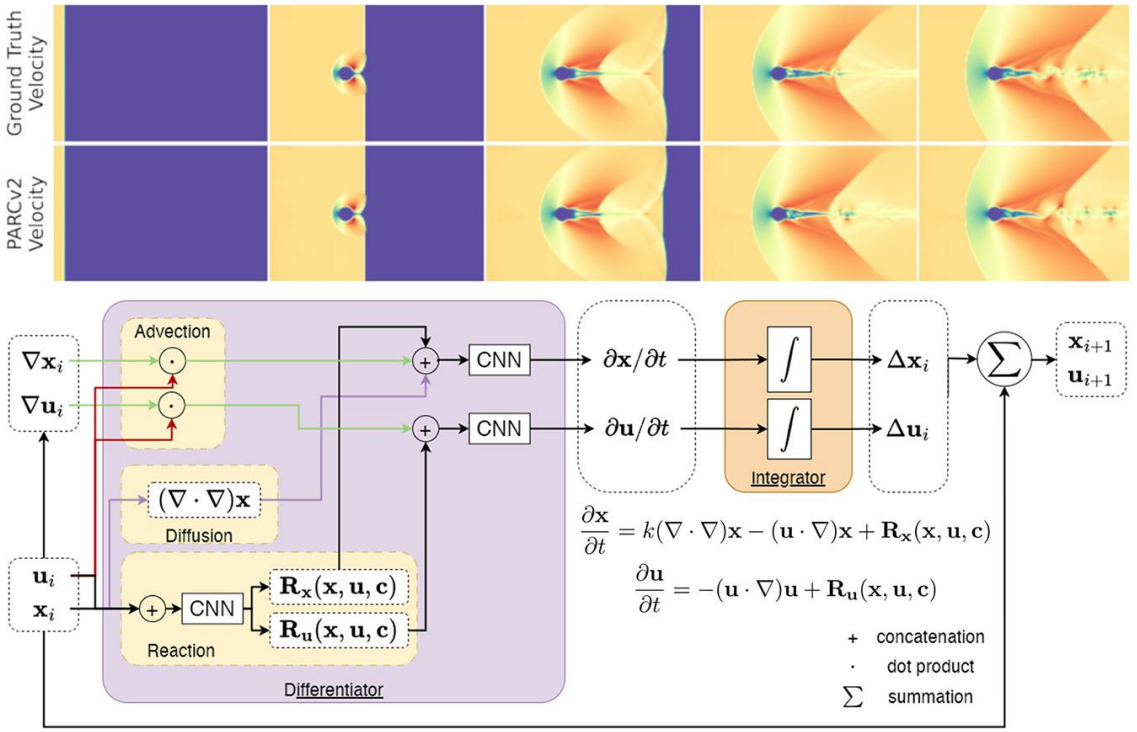


Image credit: Cheng et al. 2024[2]

PARCv2 Paper

GitHub Repo

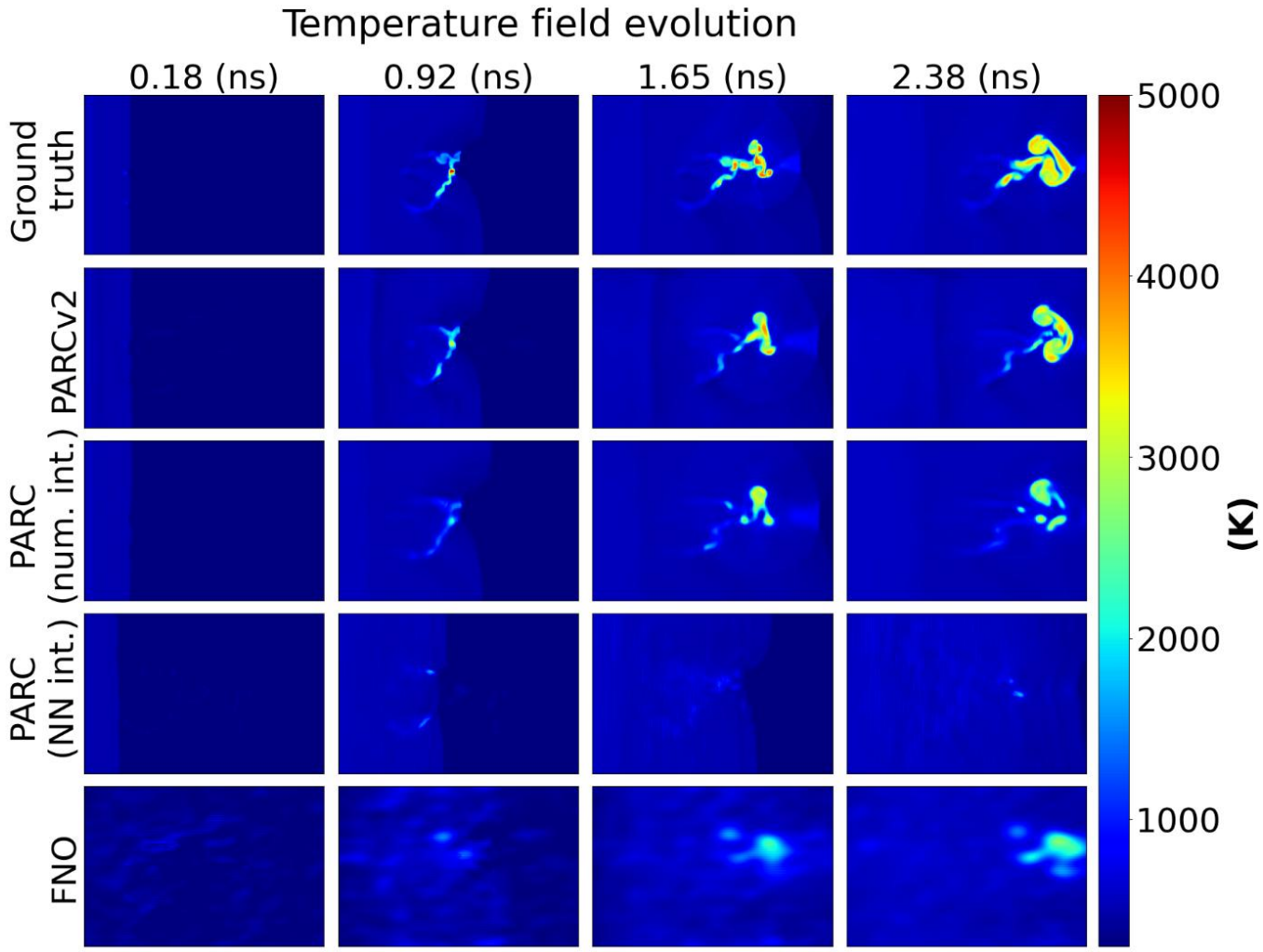
[1] Nguyen et al. 2024 "PARCv2: Physics-aware recurrent convolutional neural networks for spatiotemporal dynamics modeling." In *Proceedings of the 41st International Conference on Machine Learning*, pp. 37649-37666.

[2] Cheng et al. 2024 "Physics-aware recurrent convolutional neural networks for modeling multiphase compressible flows." *International Journal of Multiphase Flow* 177 (2024): 104877.

Nguyen et al. 2024

On a Strong Shock Regime…

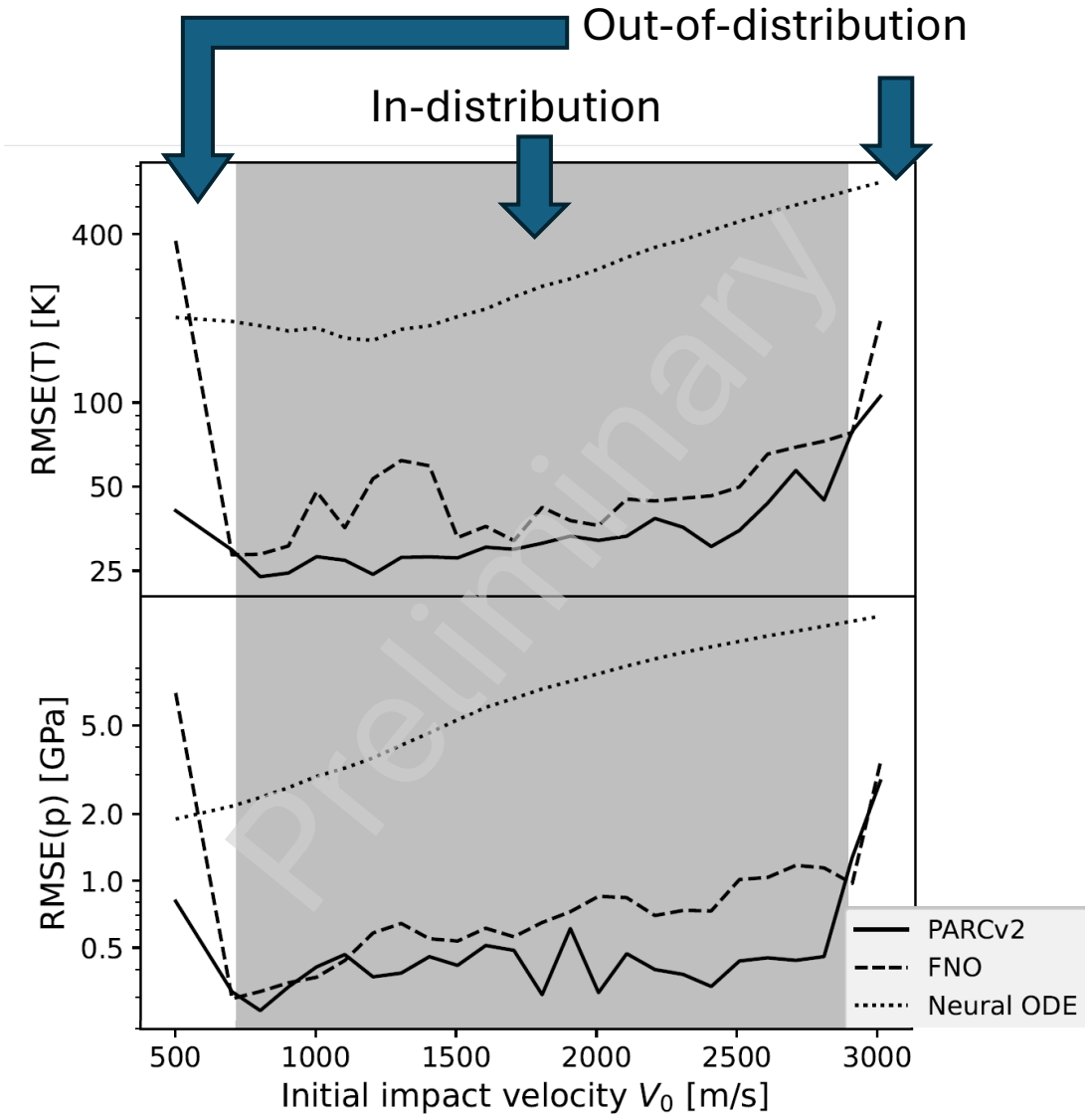
- State-of-the-art accuracy
- Inference in seconds



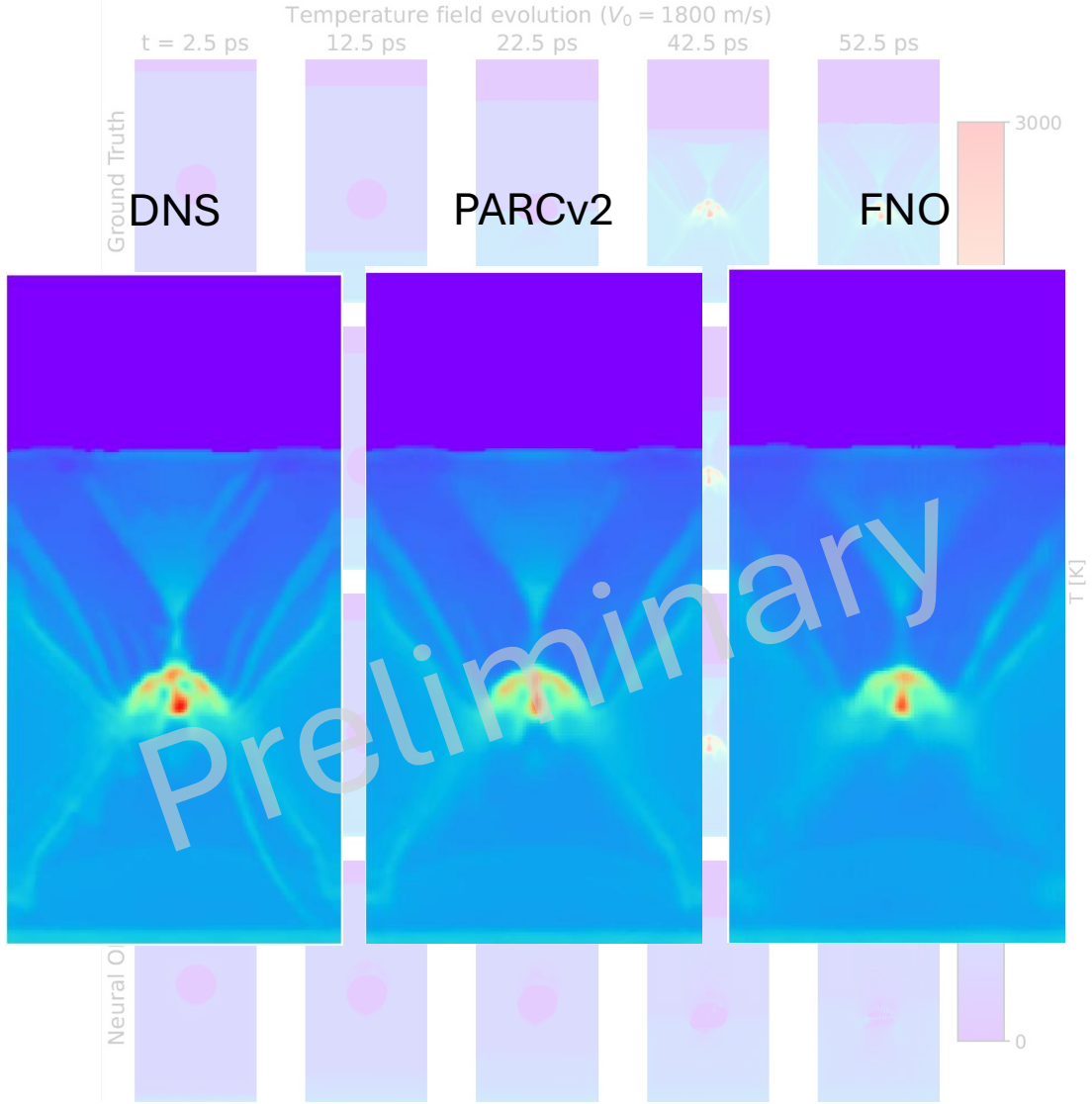
*For more details, please visit **Poster 105** this evening.

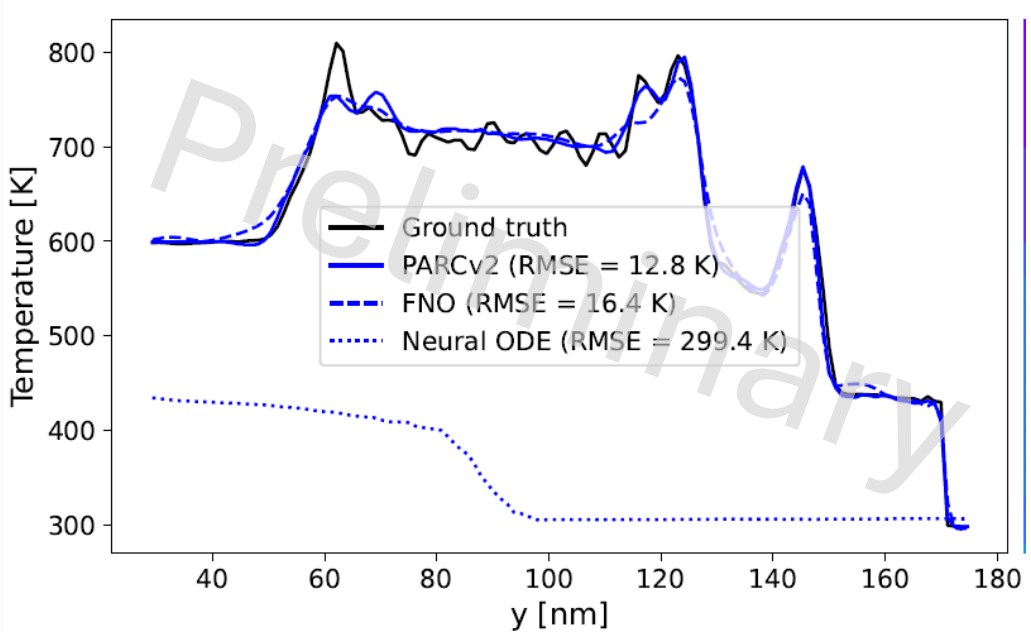
On Weak-to-Modest Shock Regimes

- PARCv2 consistently achieves smallest prediction error
  - Across wide range of impact velocities
  - On average a 3x decrease compared to FNO
  - More than 10x decrease compared to neural ODE
- PARCv2 has superior accuracy and ability to generalize



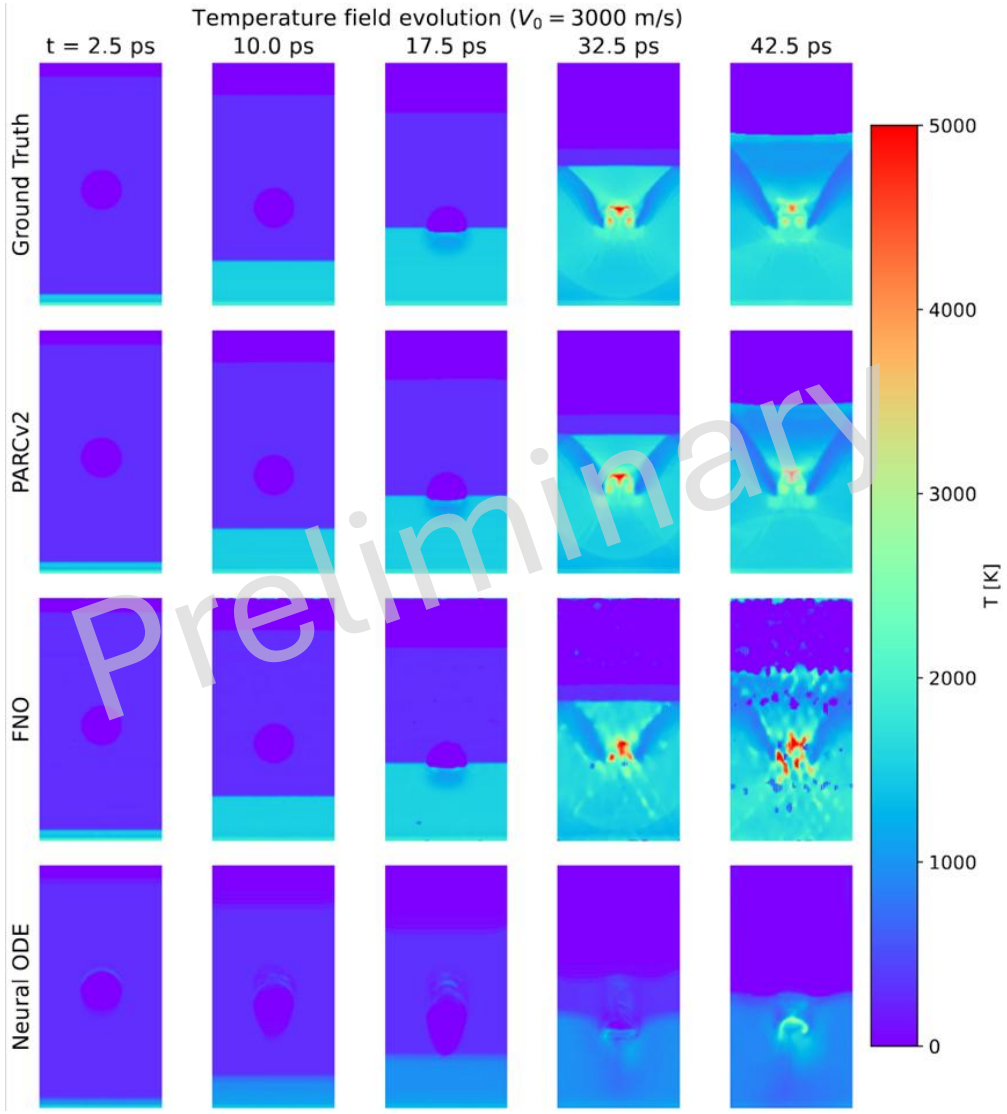
In-distribution Rollout Sequences

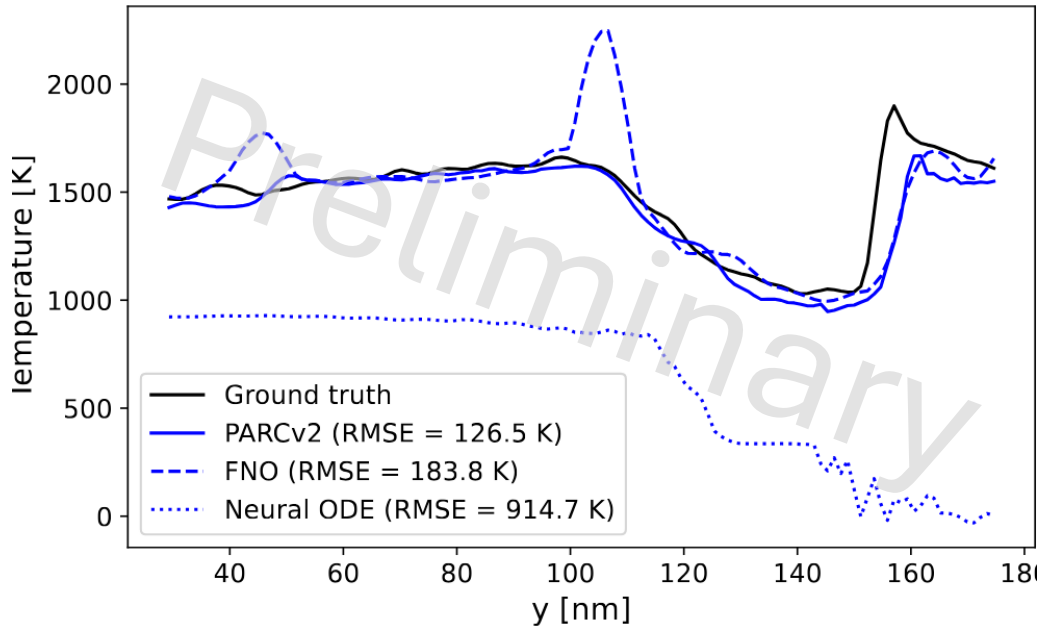




- Comparison with FNO
  - Sharper prediction
  - Much more accurate reaction dynamics
  - More detailed shear bands
- Comparison with Resnet Neural ODE
  - Explicit calculated advection/diffusion gives large performance boost

Out-of-distribution Rollout Sequences

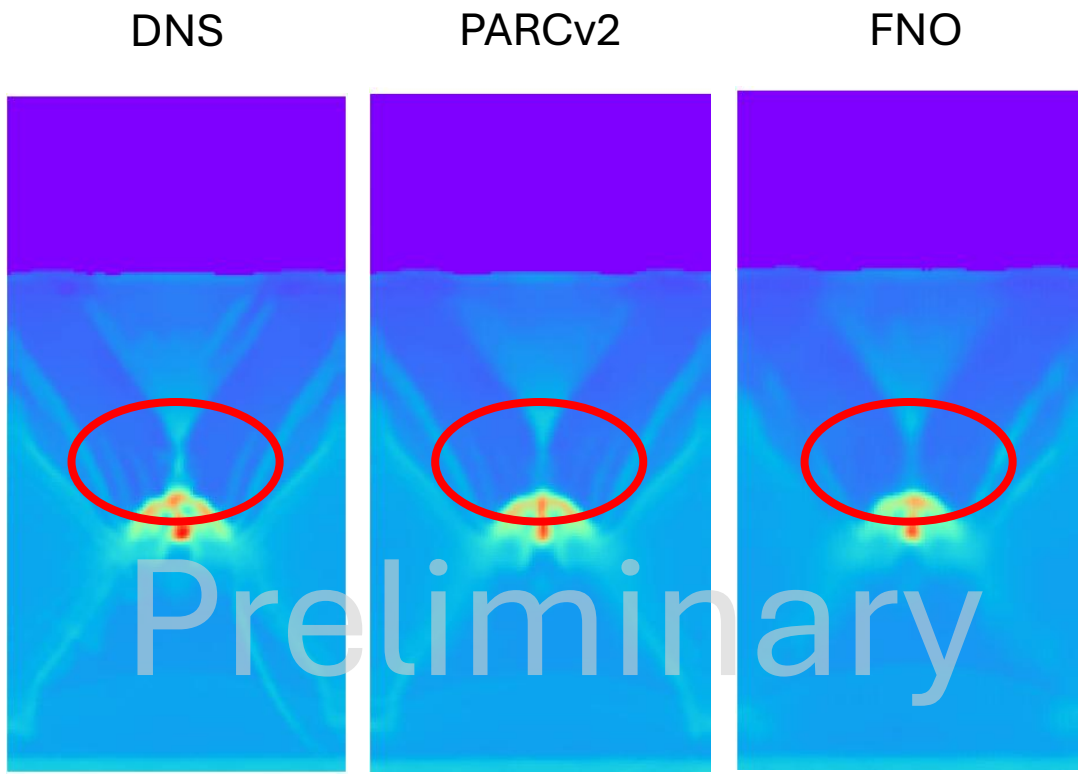




- Extrapolation
  - PARCv2 can still achieve satisfactory accuracy
  - FNO shows significant artifacts

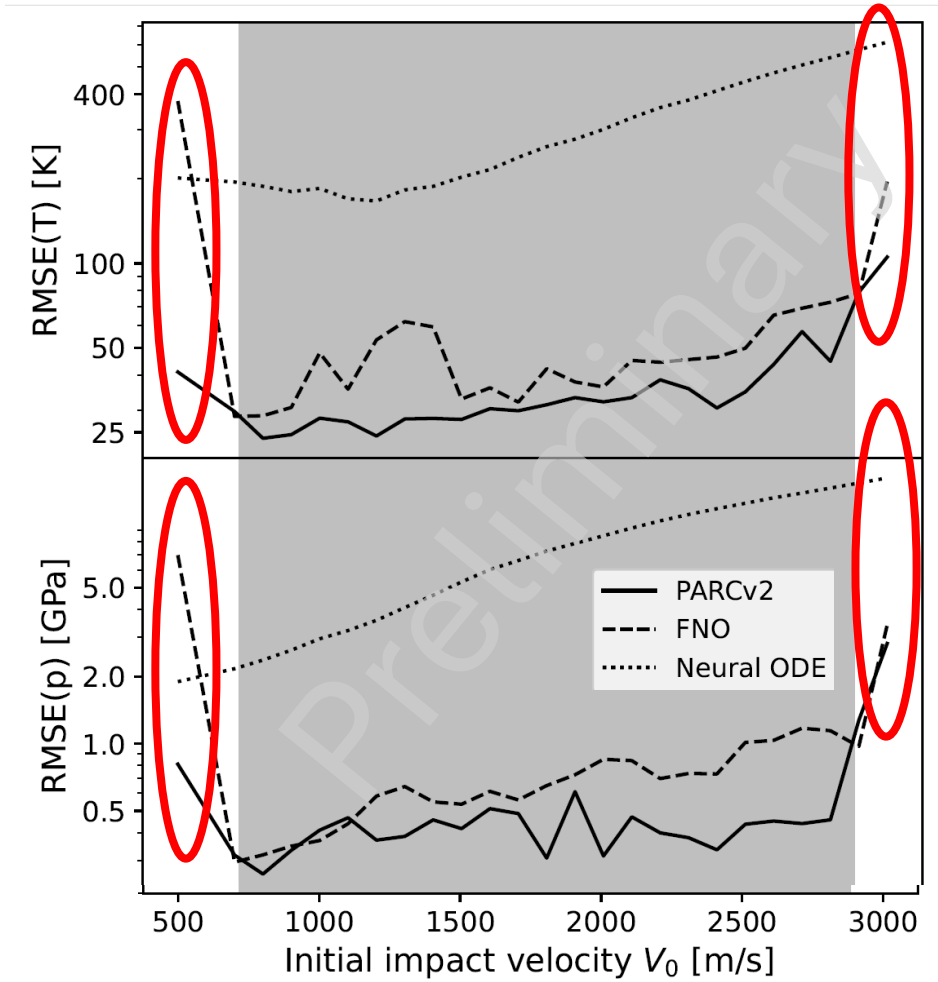
Cheng et al. in prep

Limitations



Struggles with predicting finer details

- Blurry edge of the shear bands
- Missing weaker shear bands

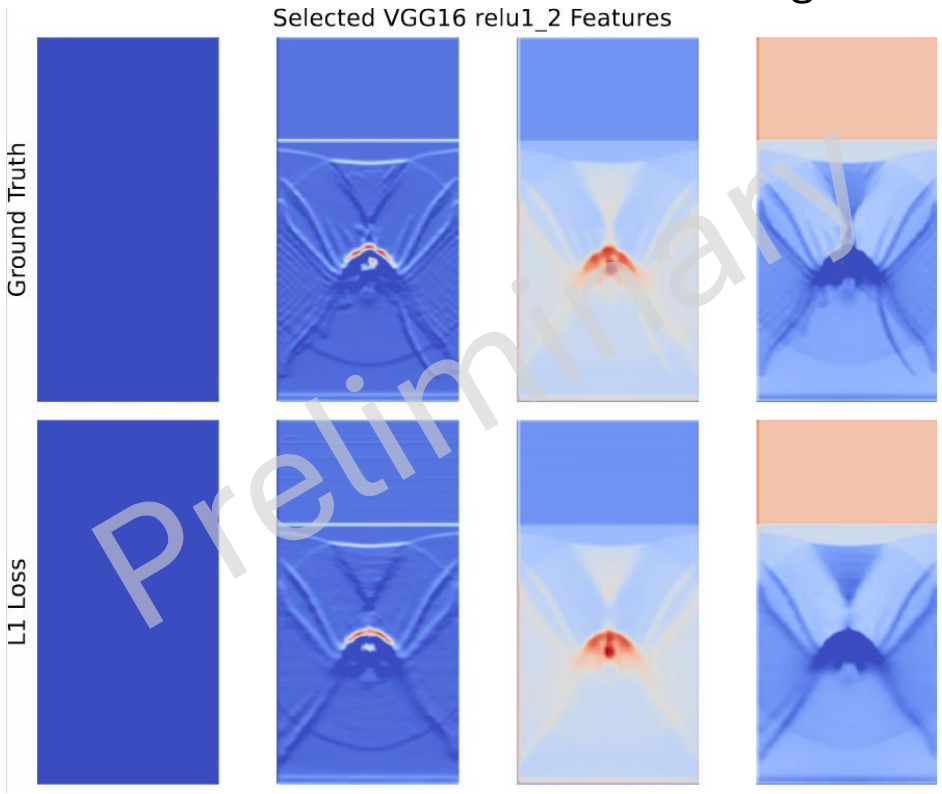


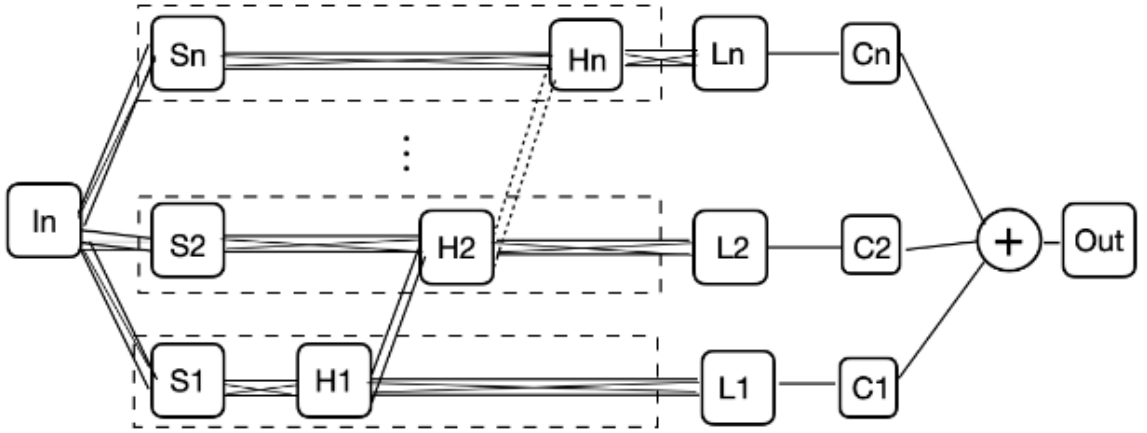
Deteriorated accuracy in extrapolation, particularly in low velocity cases

Cheng et al. in prep

Improving PARCv2

- Perceptual loss[1]
  - Loss term on high frequency features extracted with a pretrained image classifier
  - Stronger penalization on finer details
- Multi-resolution[2,3]
  - Traditional CNN: hierarchical, deeper layer larger scale
  - MR-Net: parallel, exchange information between different scales





[1] Johnson et al. 2016. “Perceptual losses for real-time style transfer and super-resolution” in *Computer Vision–ECCV 2016 Proceedings, Part II 14 pp. 694–711*. 2016

[2] Ke et al. 2017. “Multigrid neural architectures” In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, pp. 6665-6673. 2017

[3] Paz et al. 2022. "Multiresolution neural networks for imaging." In *2022 35th SIBGRAPI conference on graphics, patterns and images (SIBGRAPI)*, vol. 1, pp. 174-179. IEEE, 2022

Conclusion

- PARCv2 significantly speeds up simulations of EM reactive dynamics
  - From a few CPU hours on HPC to seconds on a workstation
- PARCv2 achieves state-of-the-art accuracy on modeling extreme dynamics
  - Across a wide range of problems and initial conditions
  - Training + validation of ~100 simulations
  - Better in-dist and extrapolation accuracy than the most popular PIML models
- Future improvements of PARCv2
  - More sophisticated loss function for capturing fine details even better
  - Multi-resolution architecture to exchange information between different scales

Thank you!

Contact: xc7ts@virginia.edu

This work was supported by the U.S. Army Research Office (ARO) Energetics Basic Research Center (EBRC) program under Grant No. W911NF-22-2-0164 and partially by the U.S. National Science Foundation (NSF) DMREF Program under Grant No. 2203580.