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A Physics-Aware Deep Learning Model for Shear Band Formation in Weak-to-Modest Shock Regime

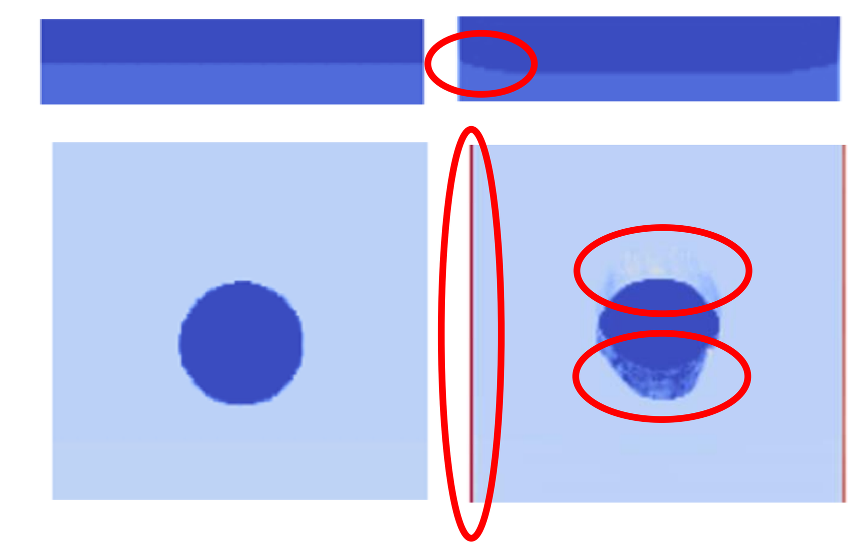
Project Objective

- Energetic material (EM) under weak to modest shocks
  - Not well understood but crucial
  - Safe storage and handling of EMs
  - Understanding of deflagration-to-detonation transition (DDT)
  - Initiation of insensitive munitions or structural reactive material
- Traditional numerical simulations are time and resource intensive
- An accurate, efficient and fast deep learning model for energetic material shear band formation

Challenges

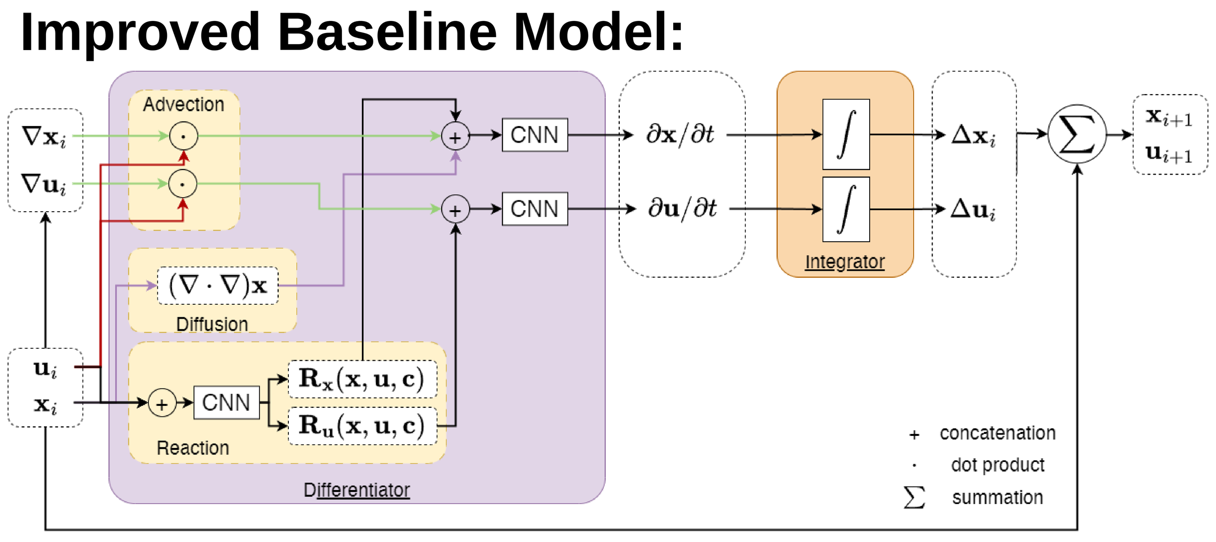
Existing model

- Accurate modeling of strong shock regime
- Artifacts appear in weak-to-moderate regime
  - Warping of material interface
  - Boundary artefacts
  - Dragging and shape irregularity
  - Long roll-out instability

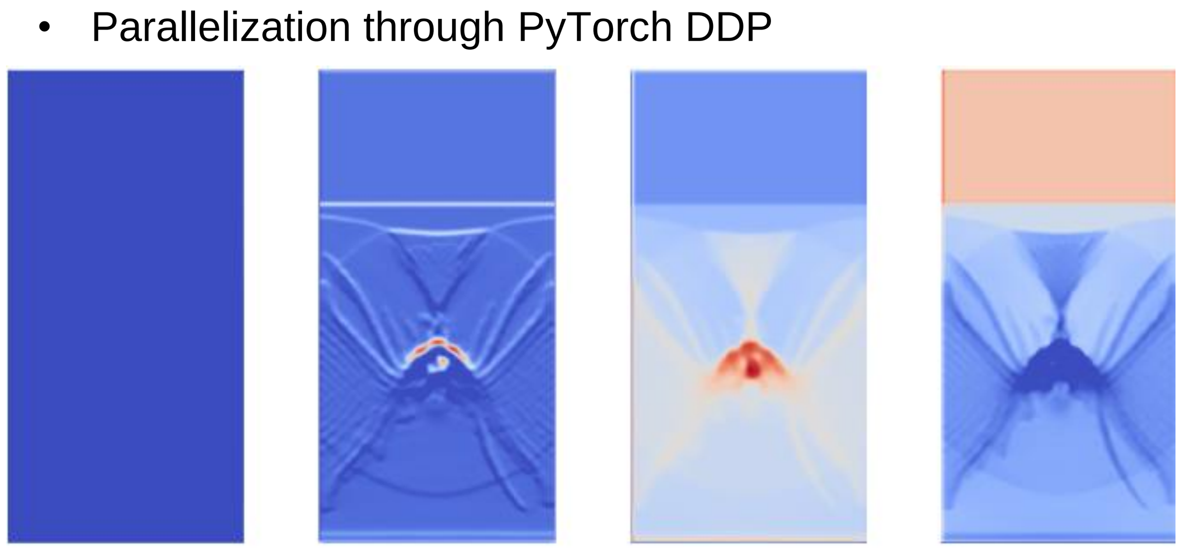


Approach/Methodology

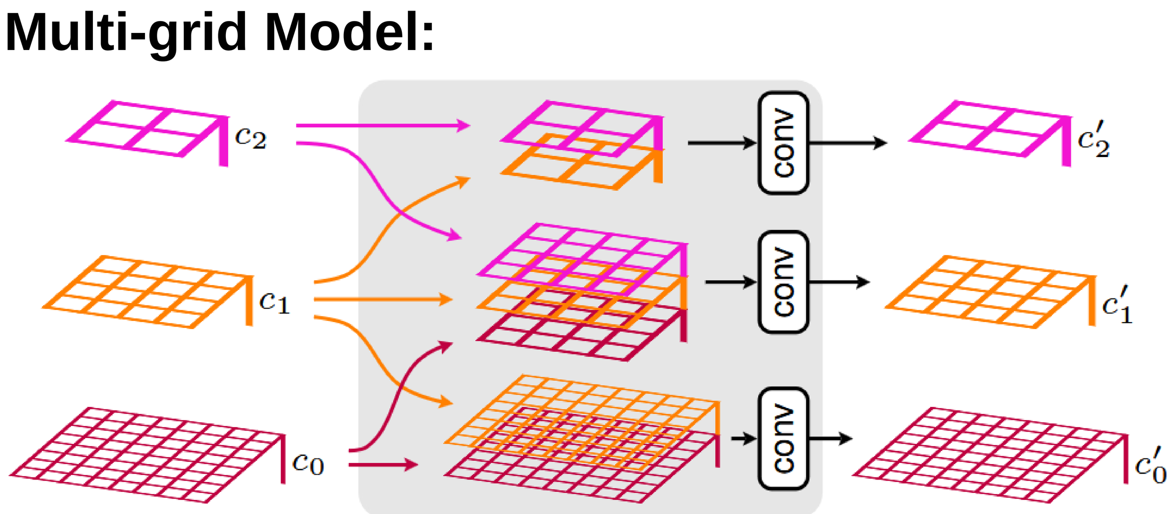
Improved Baseline Model:



- PARCv2 (Nguyen et al. 2024a, Cheng et al. 2024)
  - Physics equations built into network architecture
  - Differentiator – Integrator design
- Various improvements in this work:
  - Strict enforcement of boundary condition through custom padding
  - Curriculum training to mitigate error accumulation
  - Perception loss to encourage learning of weak shear bands
  - Parallelization through PyTorch DDP



Multi-grid Model:

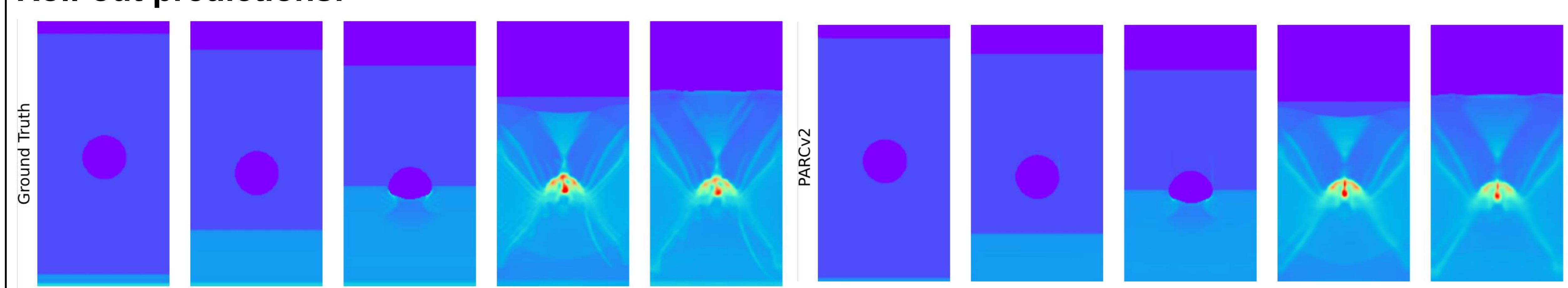


- Multi-grid PARCv2
  - Exchanging information among grid of different scales
  - Capturing large & small scale dynamics at the same time
  - Faster training convergence

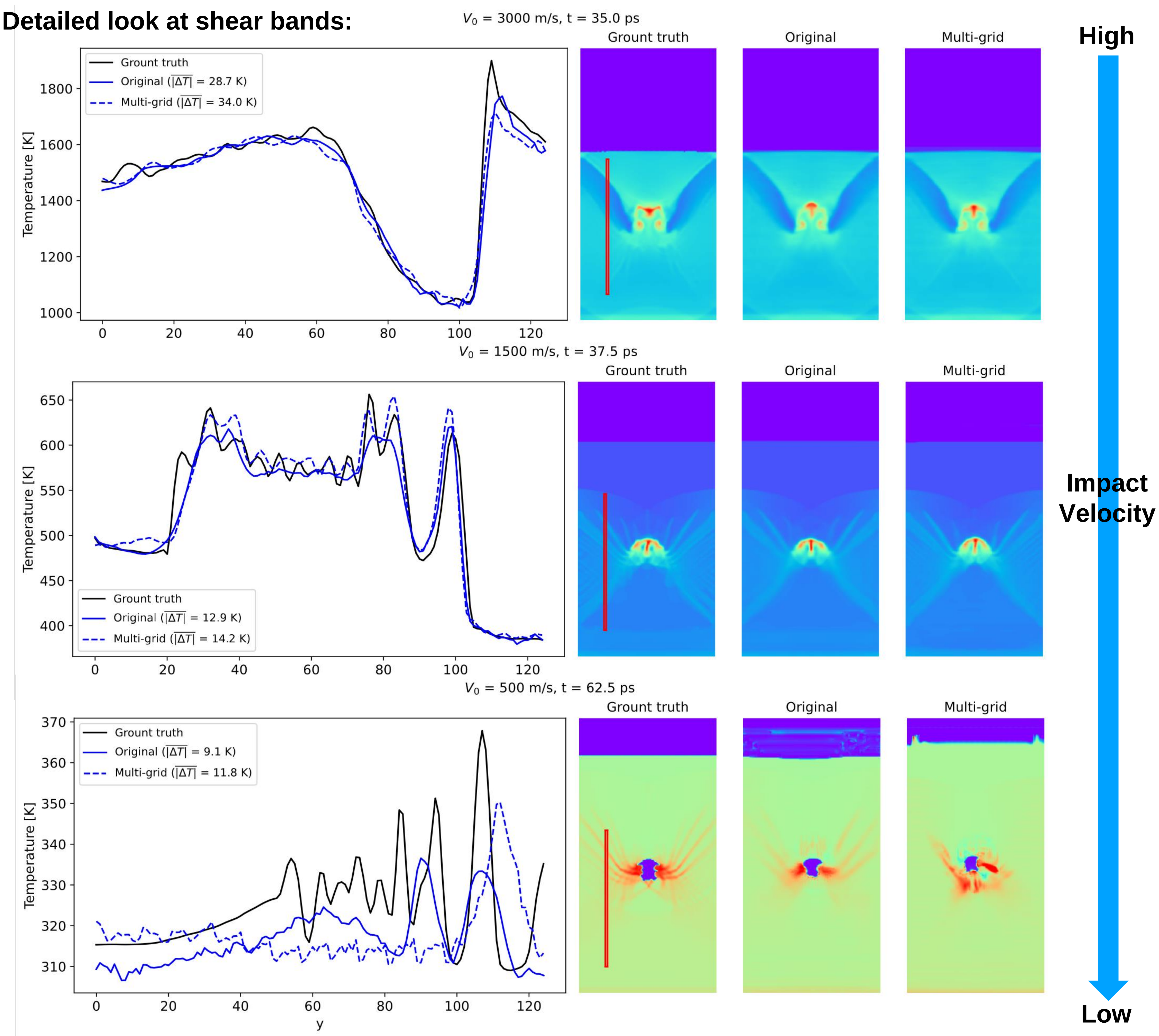
- Training data from SCIMITAR3D DNS (Nguyen et al. 2024b)
  - Includes low/high velocity extrapolation test set
  - Shock travel -> void collapse -> reverse ballistics

Results

Roll-out predictions:



Detailed look at shear bands:



Future Plans

- Improving low impact velocity cases prediction accuracy
- Improving extrapolation test set prediction accuracy
- Experimental validation

Enabling Impact

- Highlighting existing challenges in physics-informed machine learning
- Guiding future development of PIML models
- Blueprint for developing AI accelerated simulations of extreme physics
- Enables rapid new material development
- Better understanding of extreme dynamics

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