UCI Samueli School of Engineering | Department of Mechanical and Aerospace Engineering

Multiscale Damage Via Physics-Informed Recurrent Neural Networks

Ramin Bostanabad, Ph.D.
Assistant Professor, Mechanical and Aerospace Engineering
UC Irvine, Raminb@uci.edu

Shiguang Deng (UCI-Northwestern), **Shirin Hosseinmardi** (UCI), and **Diran Apelian** (UCI)

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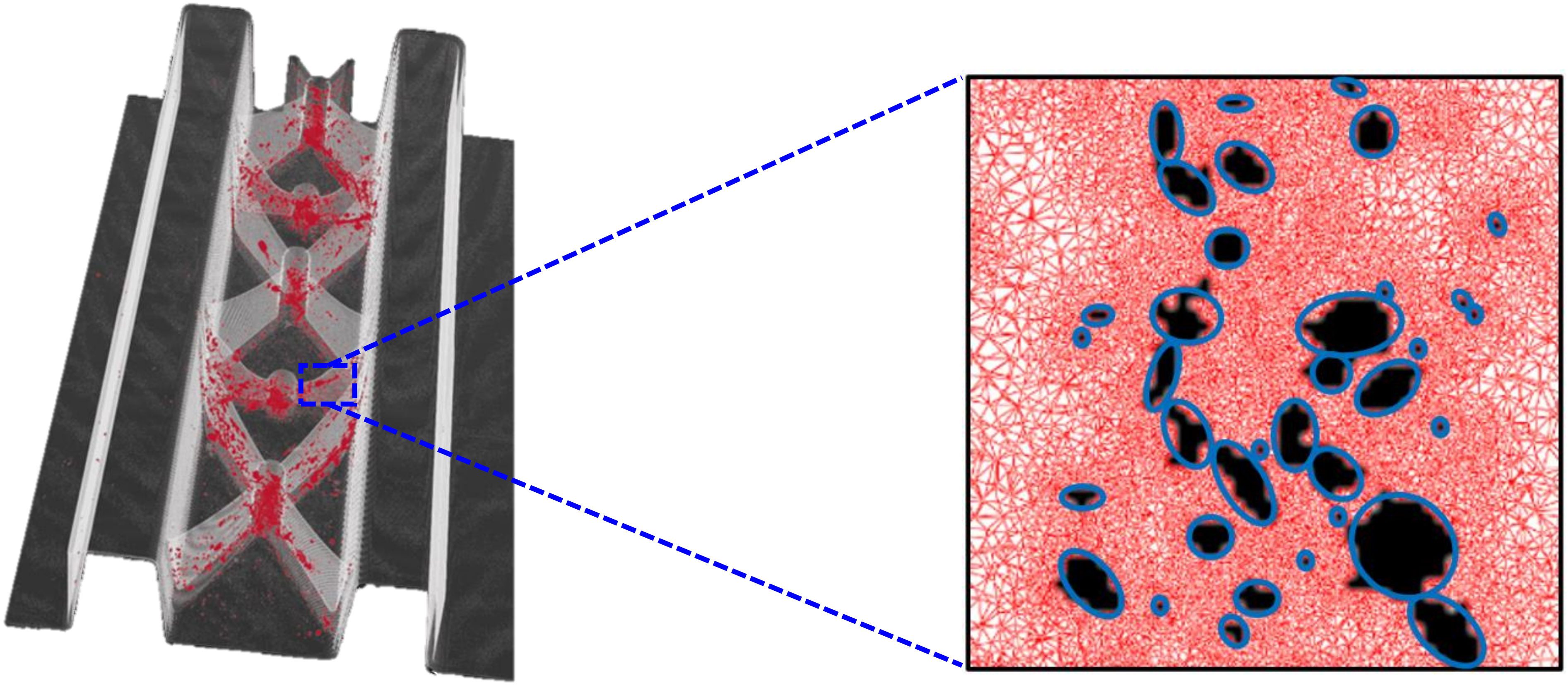
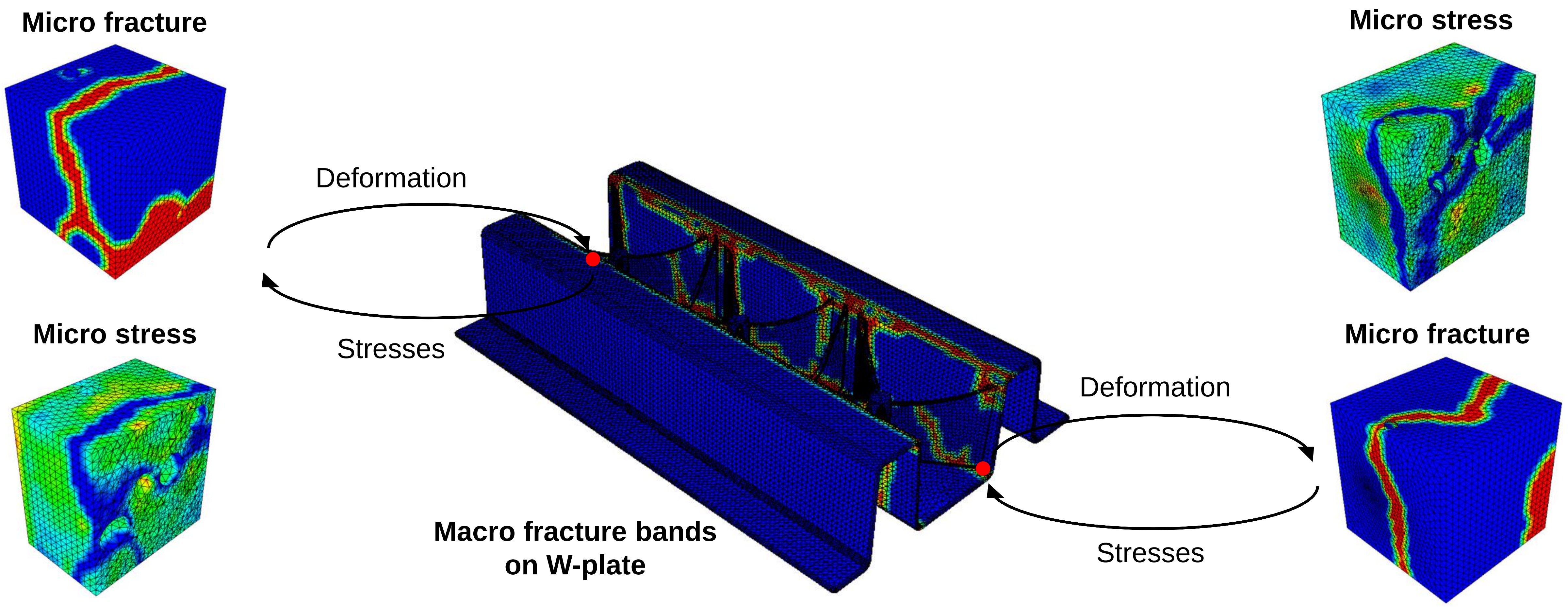
MOTIVATING APPLICATION

Understanding the effects of **micro pores** on the **damage** behavior of cast aluminum components.



MULTISCALE SIMULATIONS



Challenges:

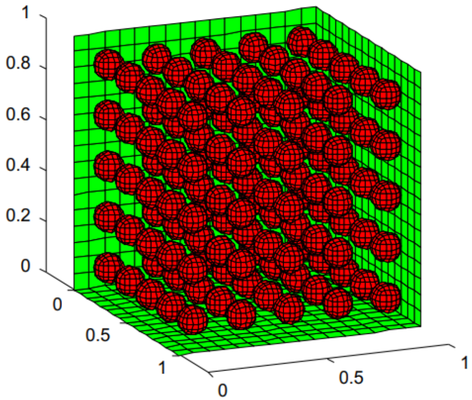
- Extremely fine mesh
- Very small explicit integration steps
- Large storage requirements
- Long simulation time

MICROSCALE ANALYSES

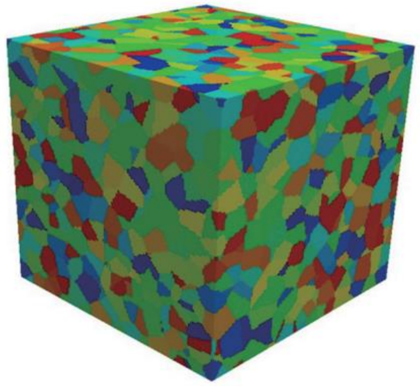
Direct numerical simulation (DNS):

- Finite element method
- Boundary element method
- Meshfree method
- Fast Fourier Transformation

B. Drach et al., IJSS, 96 (2016) 48–63



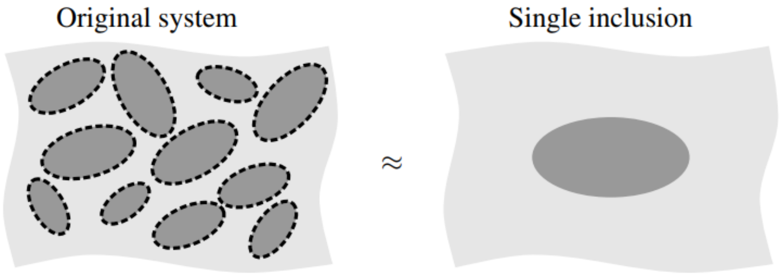
Jacek Ptaszny, CM (2015) 56:477–490



Takayuki Otsuka, et al., Nippon Steel (2018), 18-25

Analytical micromechanics:

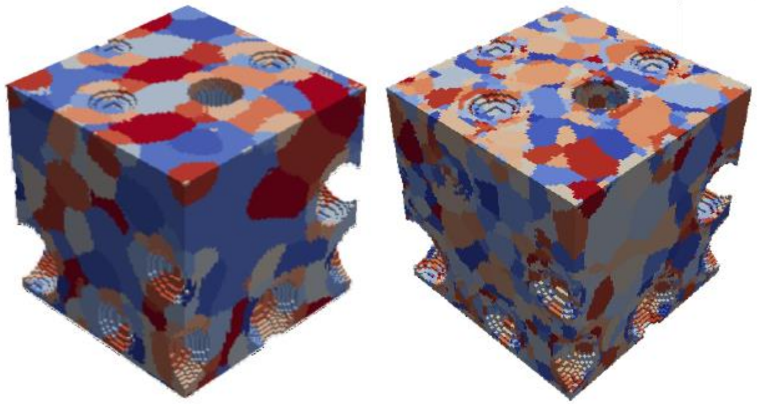
- Mori-Tanaka method
- Voigt and Reuss bounds
- Self-consistent theory



Jan Stransky, et al., Micromachines (2011): 129-149.

Mechanistic reduced-order model (ROM):

- Transform field analysis
- Singular value decomposition: PCA, POD
- Clustering-based analysis

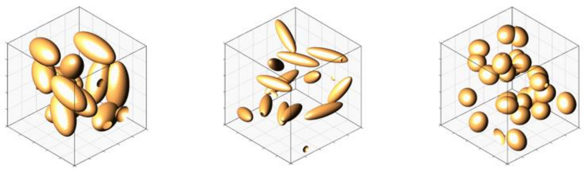


Z. Liu et al., CMAME. 330 (2018) 547–577

EVEN MORE SPEEDUPS: DATA DRIVEN MICRO MODEL

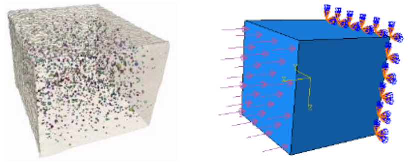
Representation

(3) Reconstruction:
- Generate microstructure designs according to design variables at each DoE point



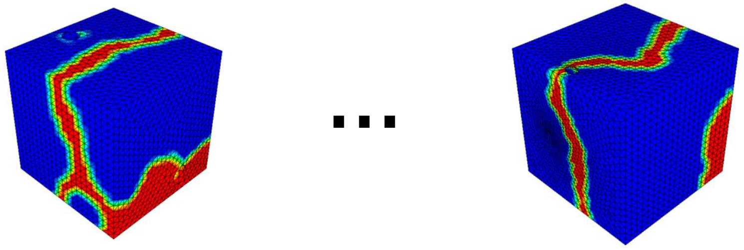
(2) Domain exploration:
- Explore input space with design of experiment (DoE)
- Check feasibility of each DoE point

(1) Characterization:
- Pore morphology
- Constitutive property
- Boundary conditions



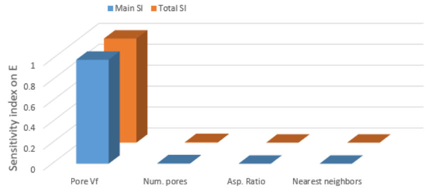
Analysis

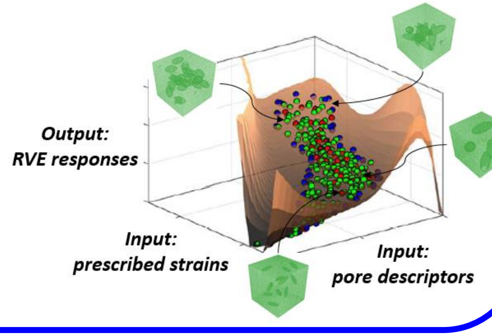
(4) Reduced-order model



Machine learning

(5) Metamodeling development:
- Model training
- Sensitivity analysis





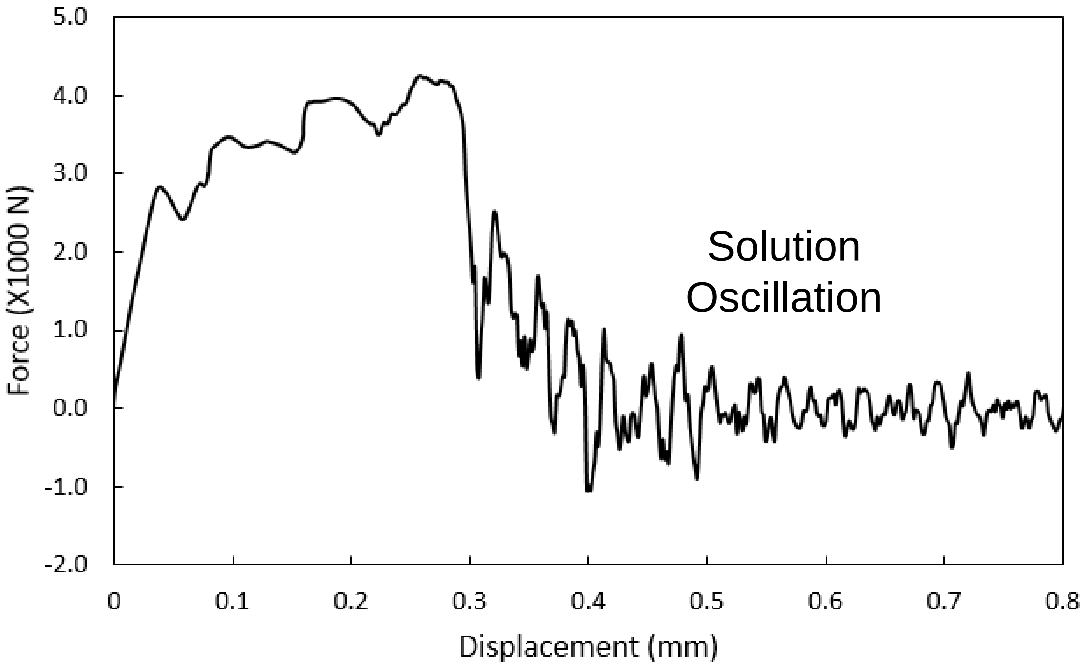
CHALLENGES WITH THE ANALYSIS STEP

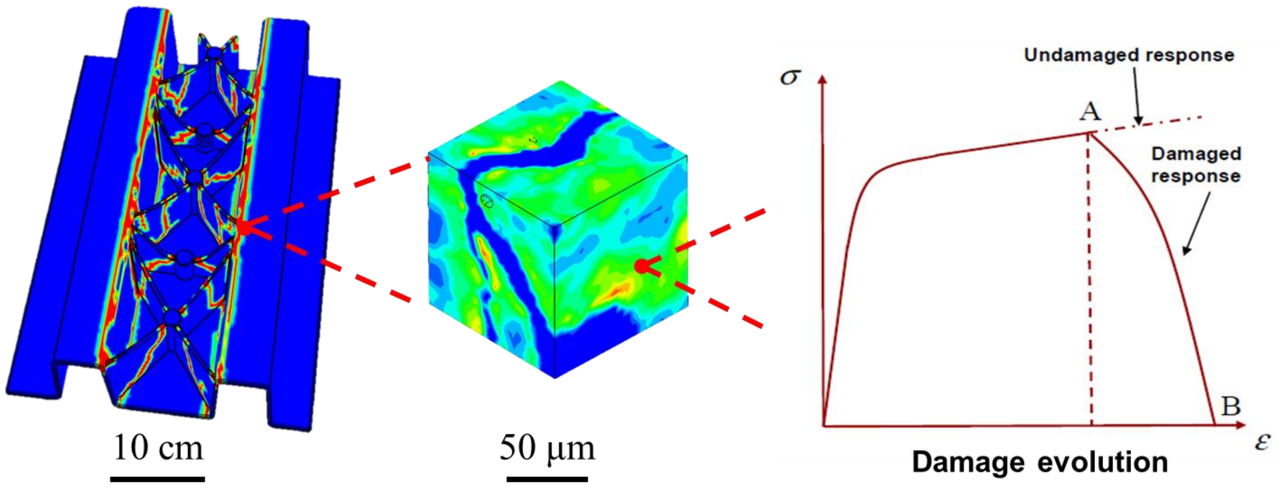
Explicit solvers:

- Solves displacements via **MU”=F**
- Always positive definite mass matrix (**M**)
- Conditionally stable but smaller step sizes
- No convergence check on displacements
- Excessive scaling/damping/smoothing leads to unrealistic solutions

Implicit solvers:

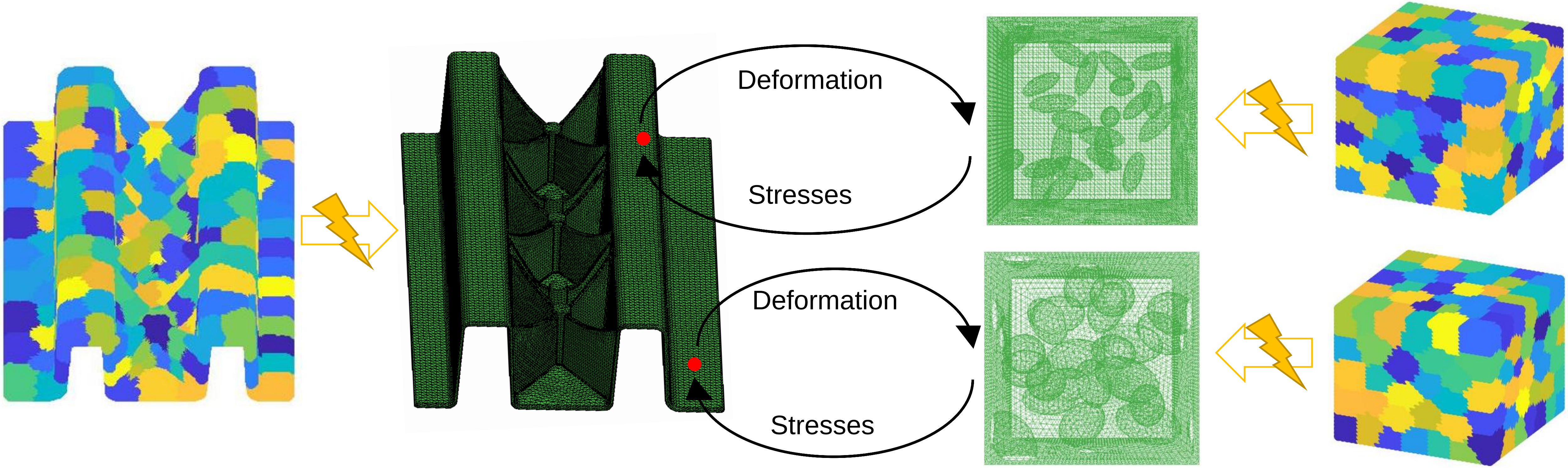
- Solving displacement via **KU=F**
- Stiffness matrix (**K**) must be invertible
- Solutions convergence is checked
- Unconditionally stable
- Large step sizes: high efficiency
- Job abortion due to damaged elements (singular **K**)





PHYSICS-BASED REDUCED ORDER MODELS (ROMs)

Adaptive **spatiotemporal** reduction of degrees of freedom



Reduced-order macro model | Macroscale FEA | Microscale FEA | Reduced-order micro model

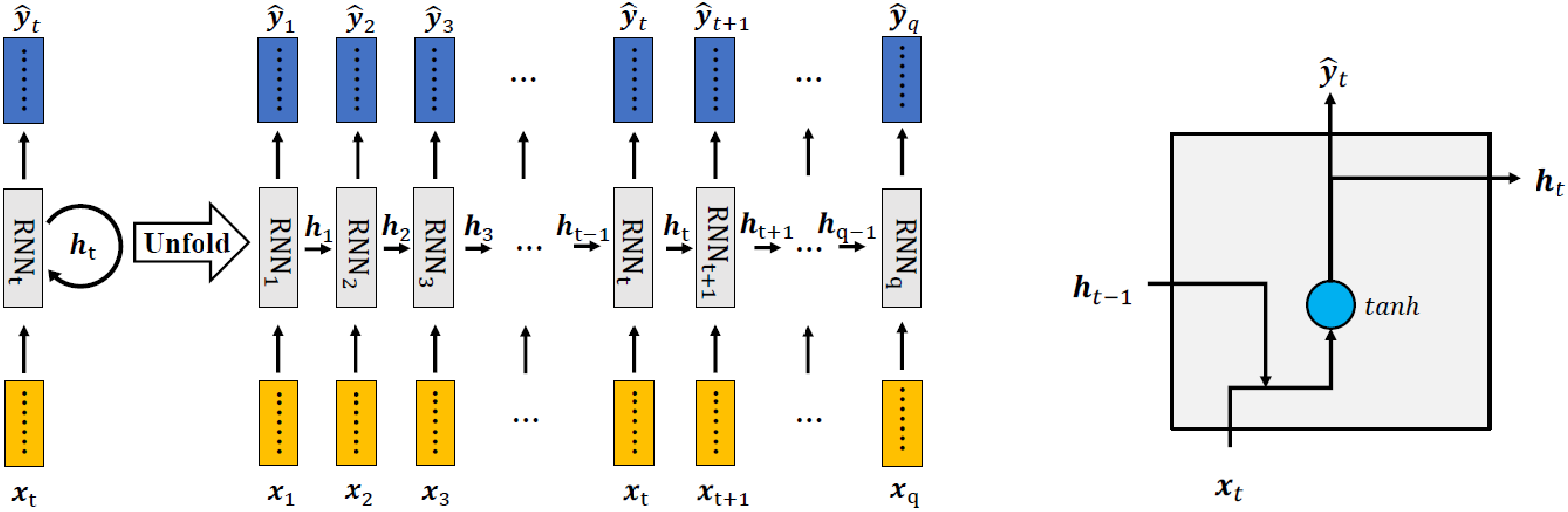
Deng, S., Soderhjelm, C., Apelian, D., & Bostanabad, R. (2022). Reduced-order multiscale modeling of plastic deformations in 3D alloys with spatially varying porosity by deflated clustering analysis. Computational Mechanics, 70(3), 517-548.

Deng, Shiguang, Diran Apelian, and Ramin Bostanabad. "Adaptive spatiotemporal dimension reduction in concurrent multiscale damage analysis." Computational Mechanics 72.1 (2023): 3-35.

PHYSICS-INFORMED NEURAL NETWORK

History dependent microstructure response → Sequence learning

History + $\boldsymbol{E}_n$ → **Data-driven Material Model** → $\boldsymbol{S}_n$ and D_n

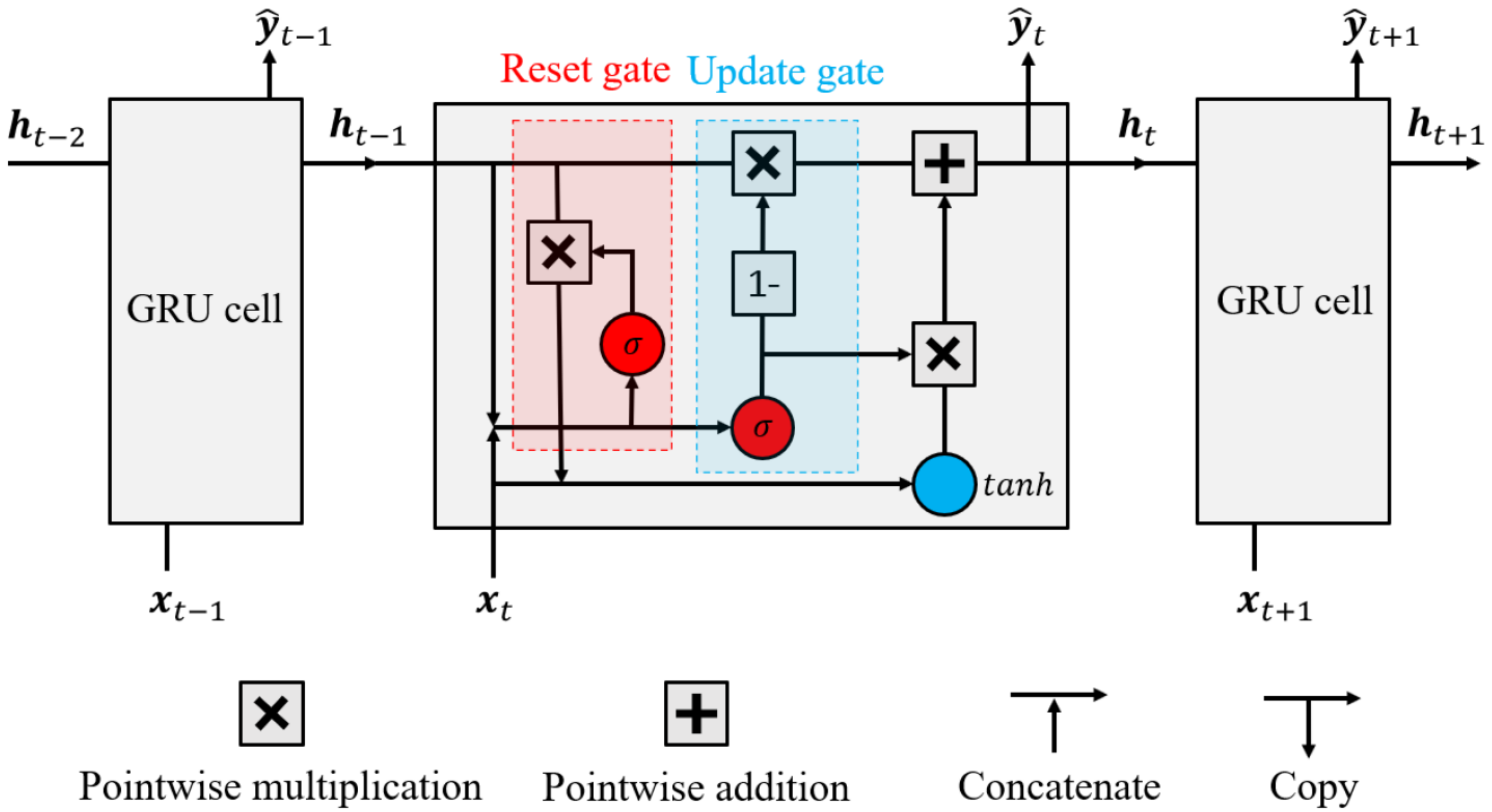


(a) Folded and unfolded RNN

(b) Vanilla RNN cell

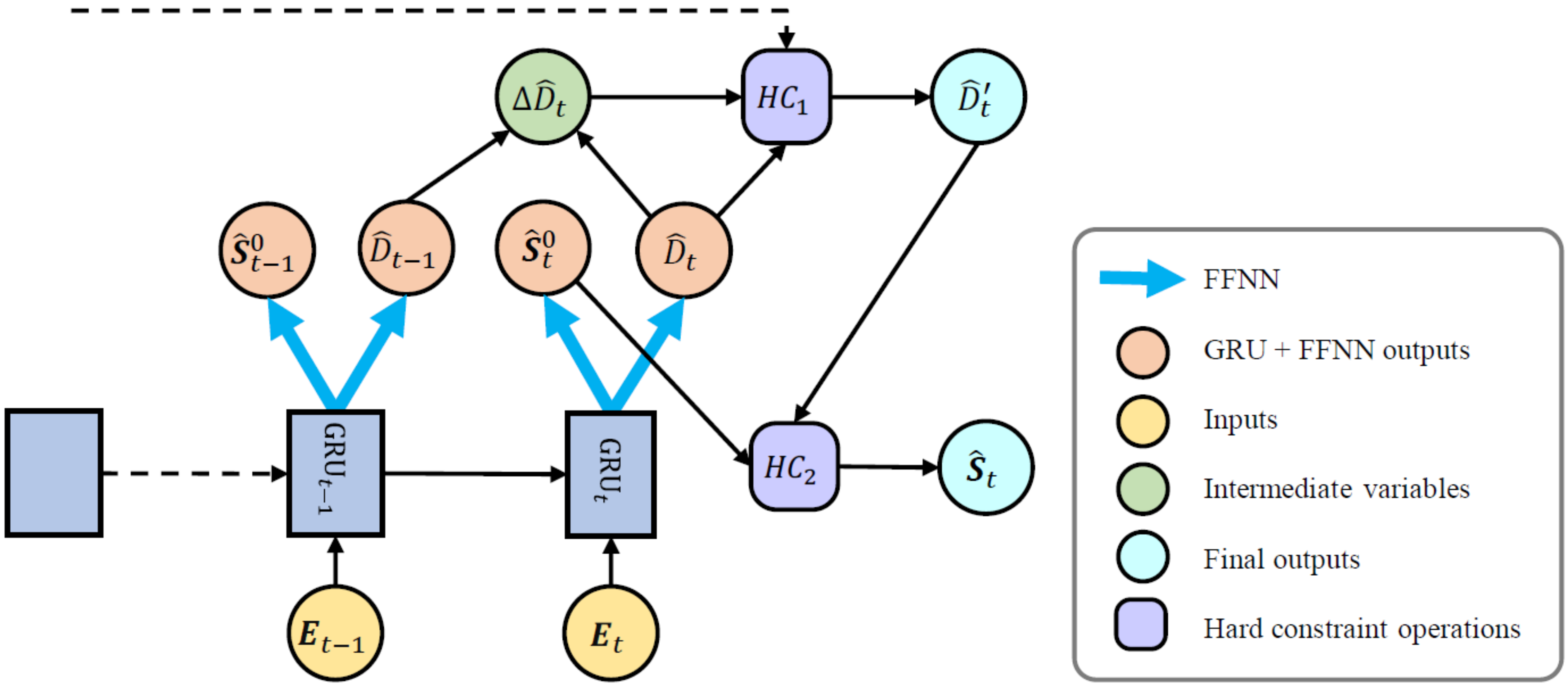
PHYSICS-INFORMED NEURAL NETWORK

History dependent microstructure response → Sequence learning



MODEL ARCHITECTURE

We design the architecture based on the mechanics of the problem:



$$\dot{D}_t = \frac{\partial D_t}{\partial t} \geq 0 \Rightarrow \hat{D}'_t = \hat{D}_t + \sum_{\tau=1}^{t} \left(\Delta\hat{D}_\tau \times \left(0.5 \times \text{sign}(\Delta\hat{D}_\tau) - 0.5 \right) \right) \quad \forall t \in \{1, 2, \ldots, n_{load} - 1\}$$

$$\hat{\boldsymbol{S}}_t = (1 - \hat{D}'_t)\hat{\boldsymbol{S}}^0_t$$

LOSS FUNCTION

We design a composite loss function that is minimized via mini-batch stochastic gradient descent.

- 1st component is the reconstruction error at any arbitrary time instance:

$$l_t^0 = \frac{1}{d_{out}} \frac{1}{n_b} \sum_{b=1}^{n_b} \| \boldsymbol{y}_t^b - \hat{\boldsymbol{y}}_t^b \|_2$$

- 2nd part requires the total internal work at an arbitrary macro integration point to be non-negative at any time instance:

$$l_t^1 = \frac{1}{n_b} \sum_{b=1}^{n_b} ReLU(-\sum_t (\hat{\boldsymbol{S}}_t^b : \Delta \boldsymbol{E}_t^b))$$

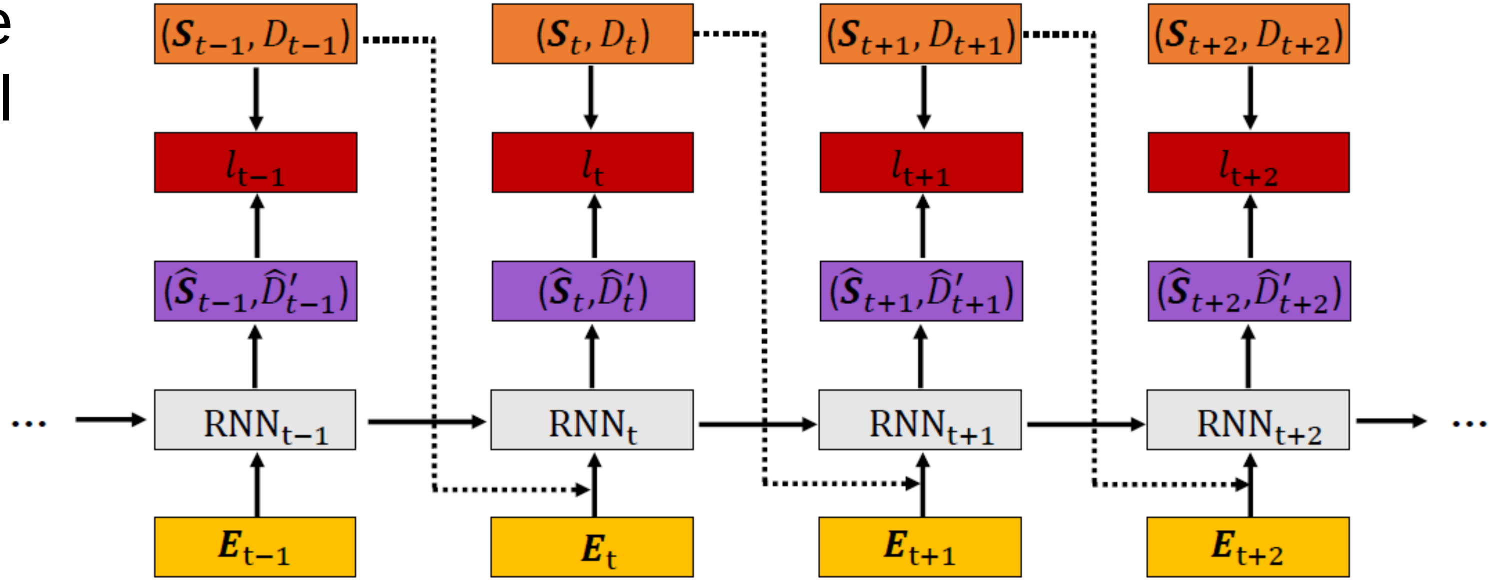
Total loss:

$$\mathcal{L} = \sum_{t=1}^{n_{load}} l_t; \qquad l_t = l_t^0 + \lambda l_t^1$$

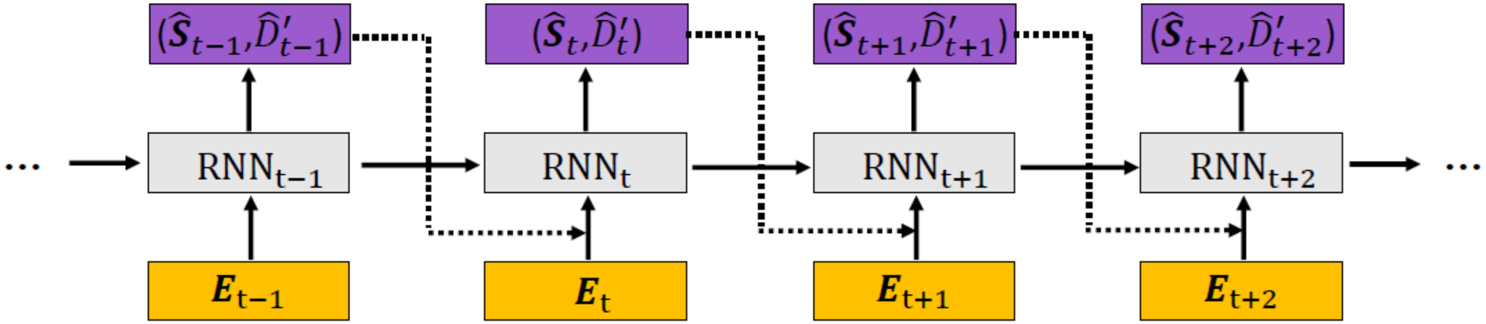
TEACHER FORCING

- It refers to networks whose outputs are fed back into model via recurrent connections.

- Training and testing are done differently: in training stage, we provide the ground truth at the previous time step as inputs at the next time step. In testing, we use the predictions at the previous time step since the ground truth is unavailable.



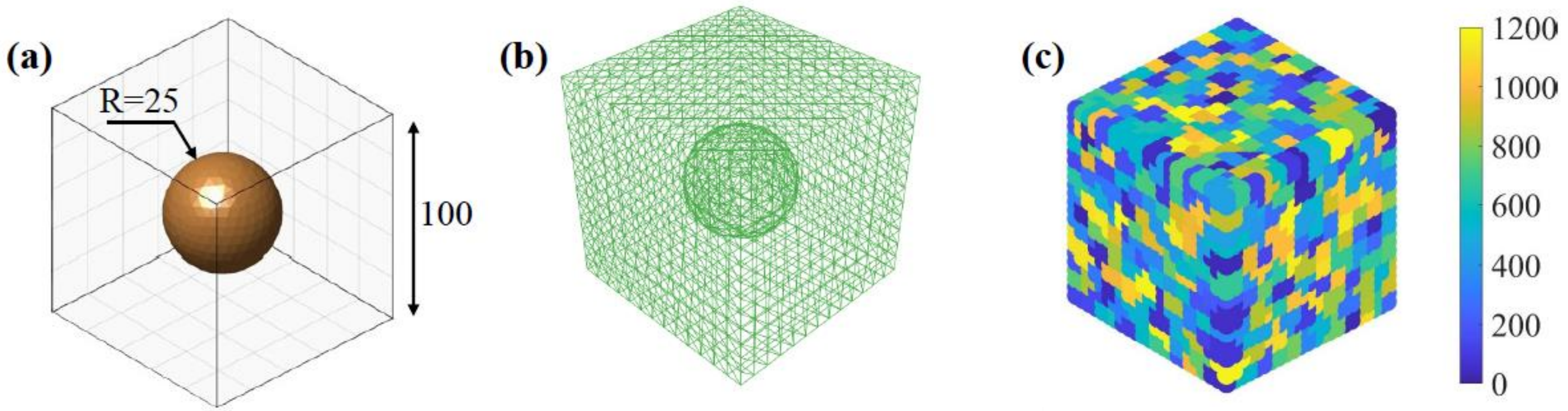
(a) Teacher forcing during training



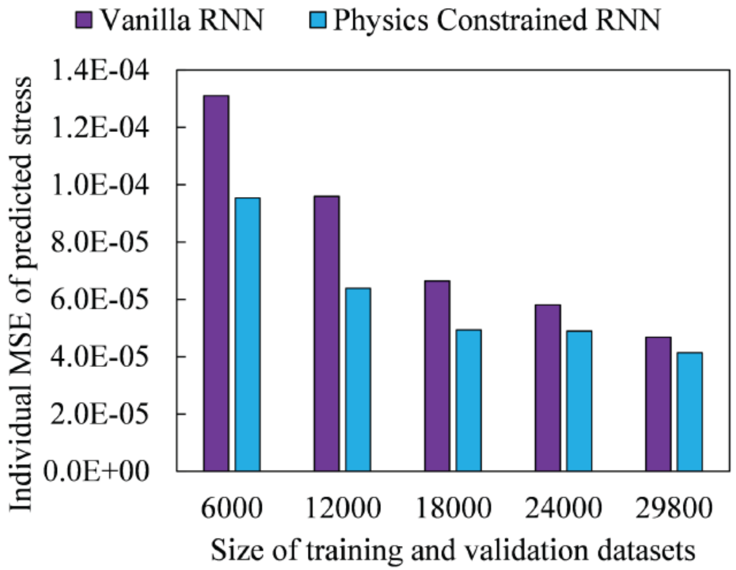
(b) Teacher forcing during testing

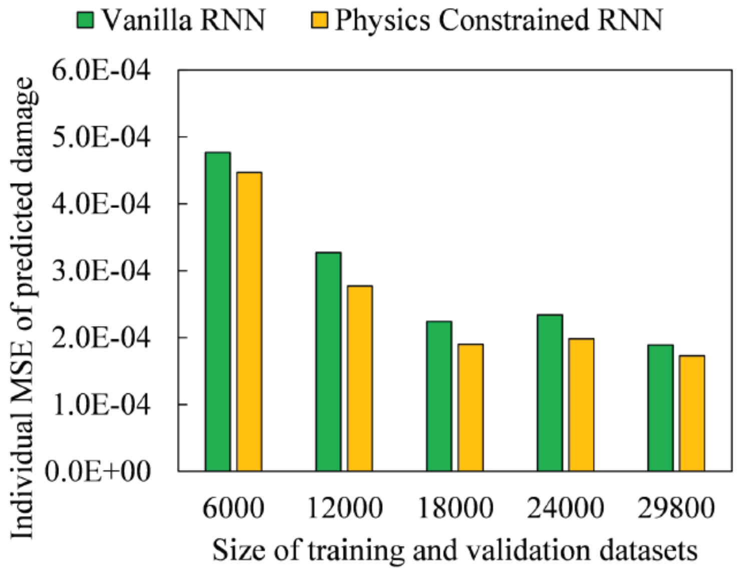
IMPACTS OF PHYSICS CONSTRAINTS (SINGLE SCALE)

Microstructure under consideration:

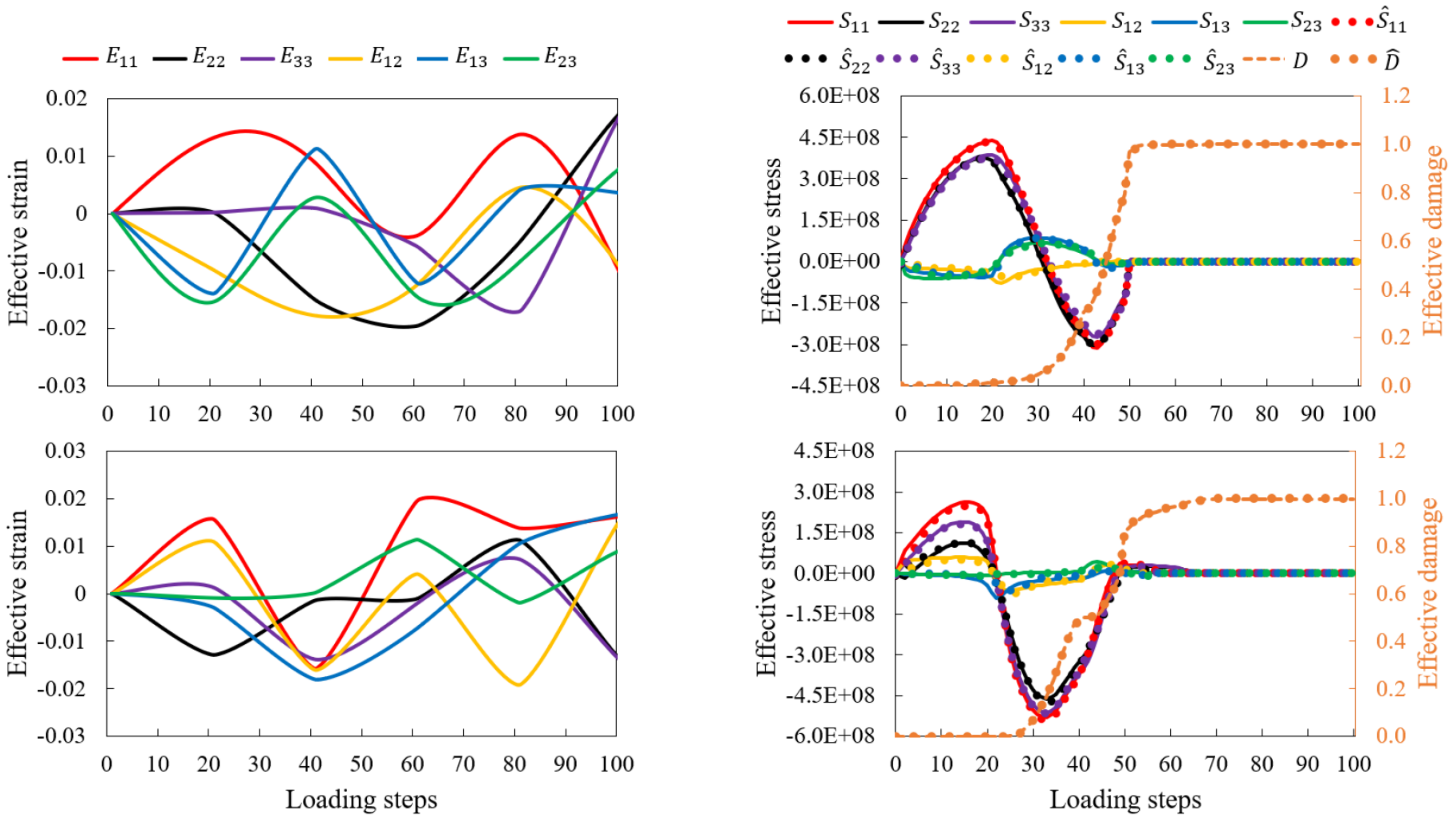


The physics-informed model consistently improves the predictions.

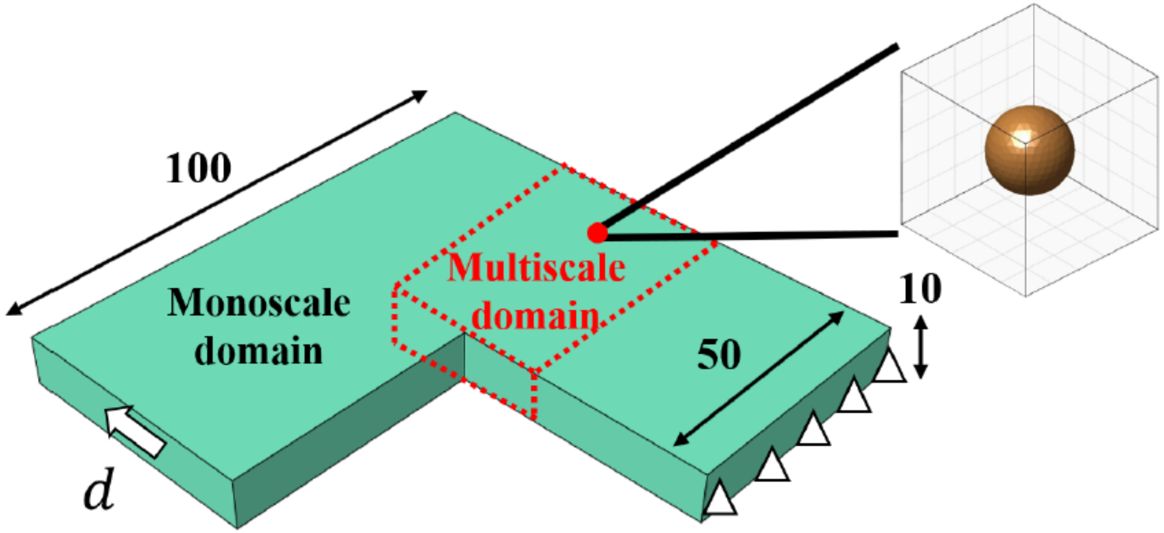


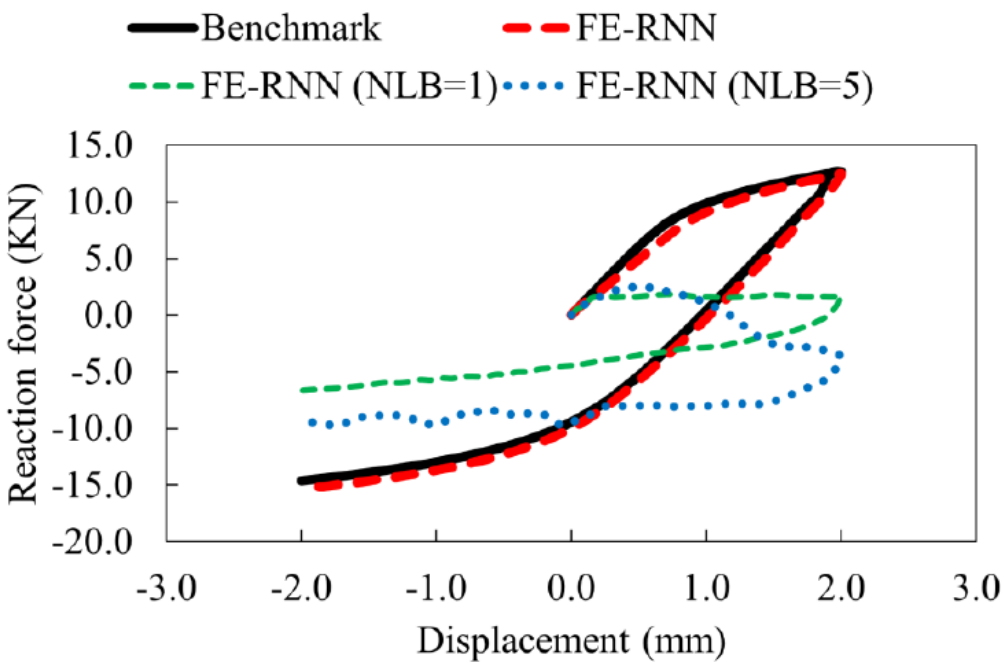


PREDICTION FOR RANDOM LOAD PATHS



We match the benchmark where ROM is used at the microscale.





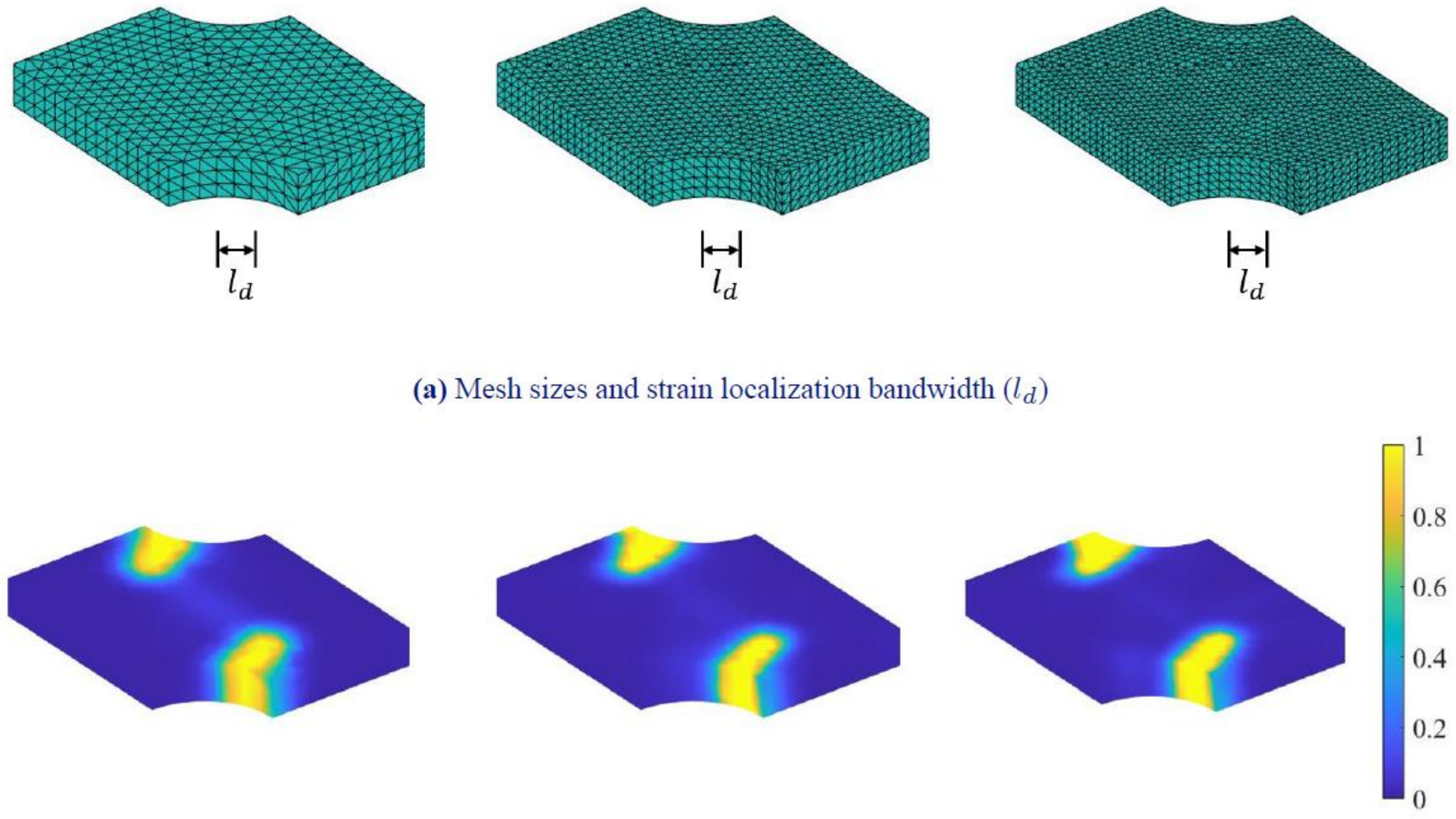
Teacher forcing for single-scale (with ground truth fed back):

	No teacher forcing	Teacher forcing (NLB=1)	Teacher forcing (NLB=5)
Total MSE	2.52	1.98	1.91
MSE_S	4.14	4.62	4.54
MSE_D	17.30	9.67	9.24

MULTISCALE DAMAGE: MESH CONVERGENCE

- A challenge in using continuum mechanics to simulate softening is preventing fracture bands from residing in single-element-wide layers.

- We use our model to a new 3D model to assess its robustness in predicting damage behavior while changing the mesh size.



(a) Mesh sizes and strain localization bandwidth (l_d)

(b) Damage patterns

CONCLUDING REMARKS

- Leveraging mechanics principles reduces the reliance on expensive data.

- Developing physics-based reduced order models is still needed for building/validating ML models.

- Advanced ML techniques such as teacher forcing do not *directly* translate to multiscale simulations.

ACKNOWLEDGMENT

Thank you!

Questions?