Physics-based machine learning in materials modeling and multiscale simulation

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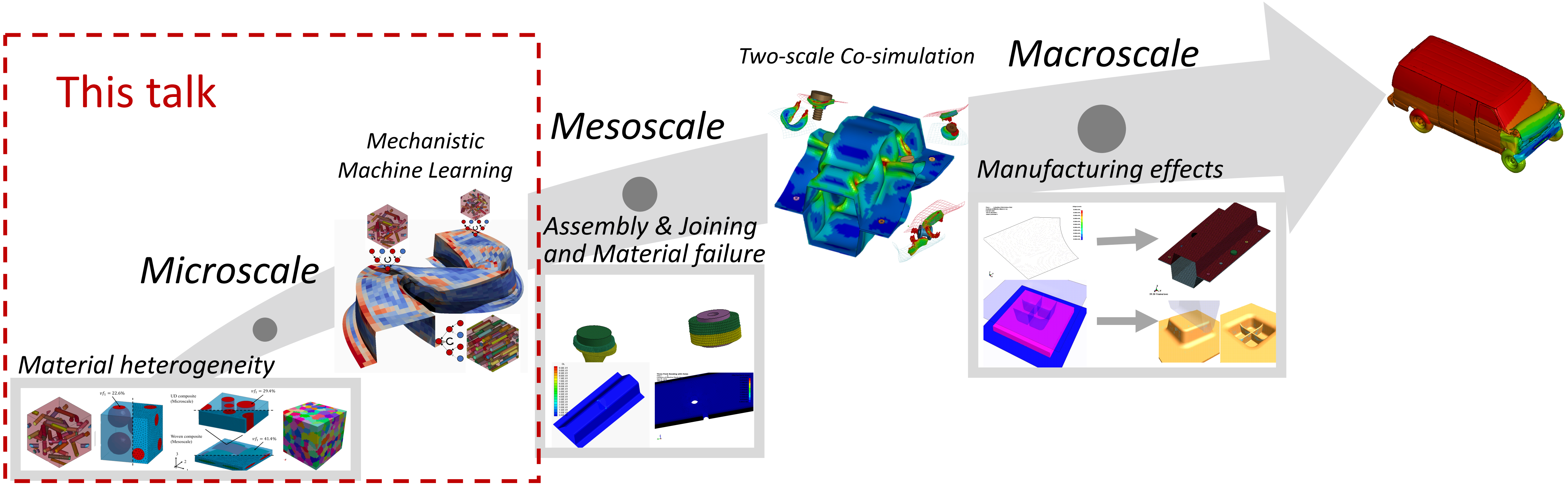
Background

- Multiscale problems inevitably arise in many fields, including crashworthiness.
- In cars, fine-scale solutions impact the accuracy of crash prediction.
- It is impractical to resolve all details at a single scale in CAE software.
- Effective space-time multiscale methods need to be introduced.



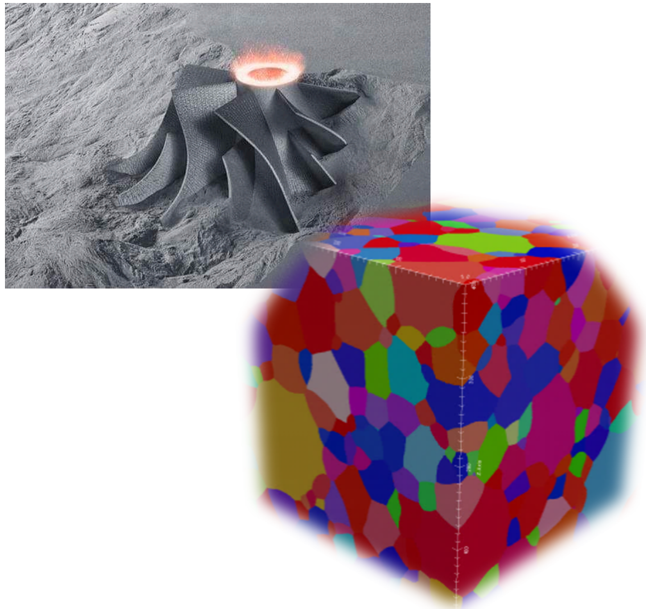
Content of this talk

- **Multiscale materials modeling and simulation**
  - Challenges and opportunities
  - Machine learning
- **Deep material network:** embedding physics into machine learning model
- **A data-driven multiscale framework:** from process to structural analysis
  - Data-generation and training
  - Transfer learning
  - Concurrent multiscale simulation
- **Q&A**

What is multiscale materials modeling

Structural analysis

Manufacturing



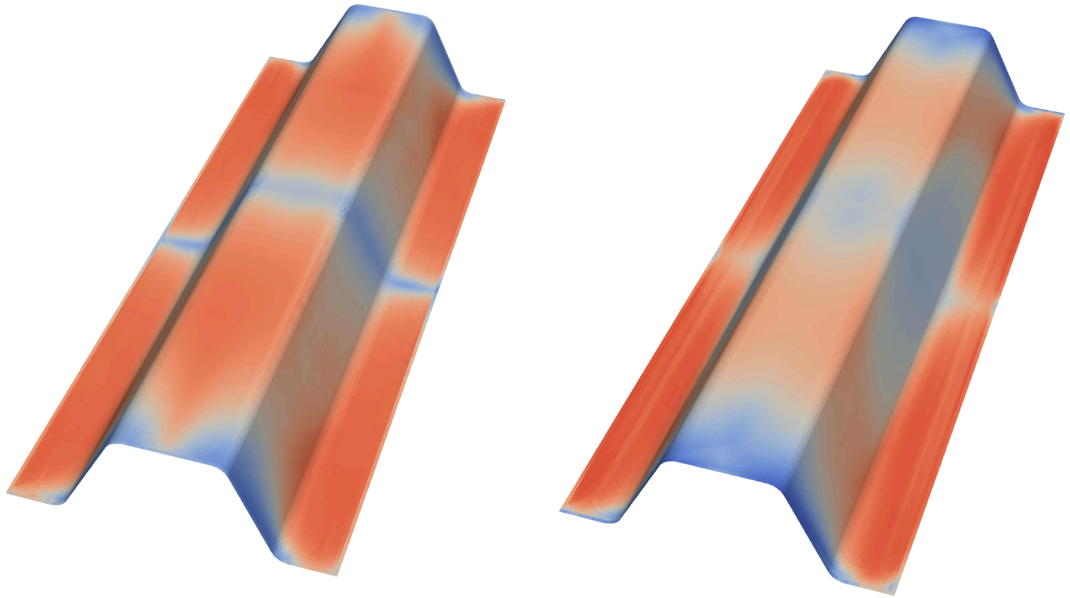
Materials design

- Phenomenological materials model ? - Complexity, Calibration, Design …
- Representative Volume Element (RVE) and Homogenization

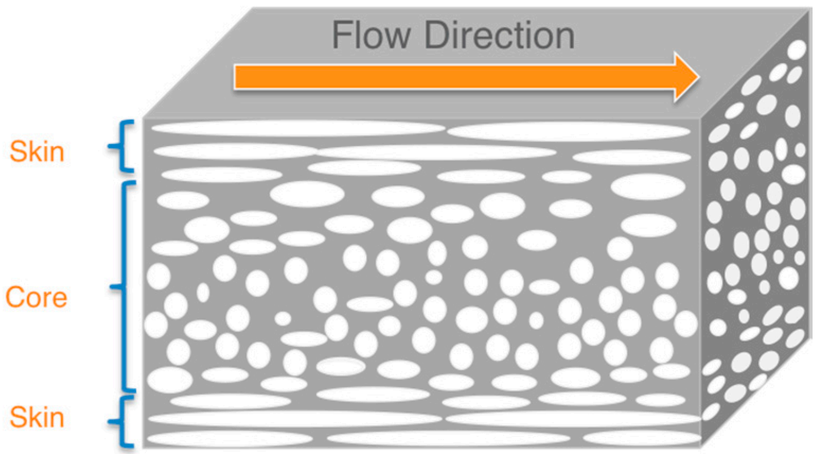
Spatially varying microstructures from manufacturing processes

- Injection molded short fiber reinforced composite

Shear layer (surface) Mid layer



"skin-core-skin" structure

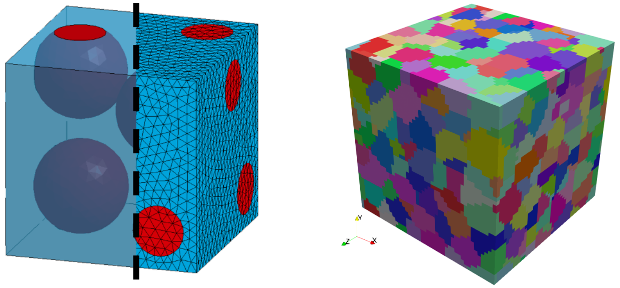


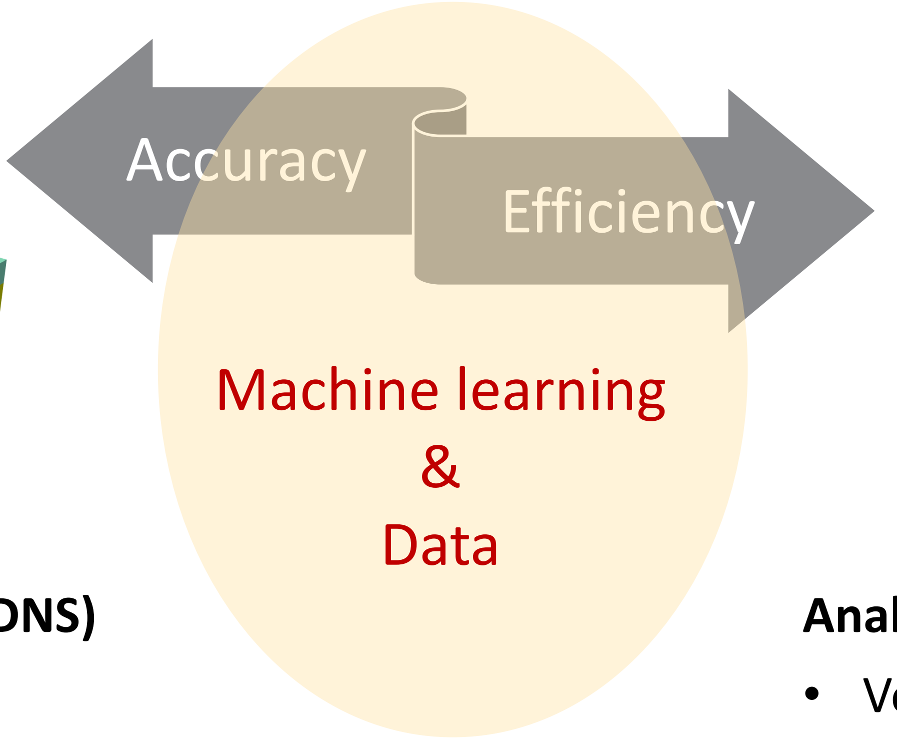
Bärwinkel et al. Materials (2016)

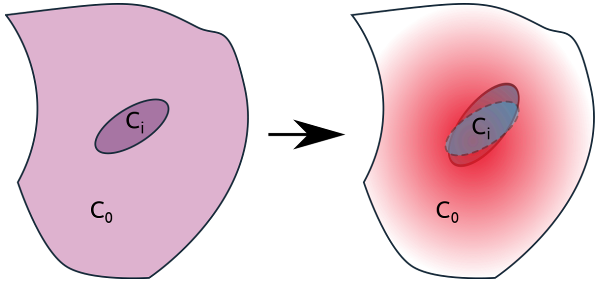
- Compressive molding, additive manufacturing, metal forming …

Existing methods for microstructure modeling

- **Objectives:** Arbitrary morphology, material nonlinearity (ex. plasticity), geometric nonlinearity.
- **Applications:** Concurrent multiscale simulation, materials design …







Direct numerical simulation (DNS)

- Finite element
- Meshfree and particle methods
- FFT-based method…

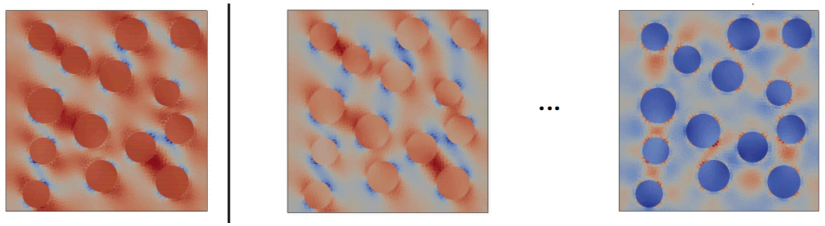
Analytical micromechanics methods

- Voigt and Reuss bounds
- Mori-Tanaka method (most popular)
- Self-consistent method…

Machine learning in materials modeling

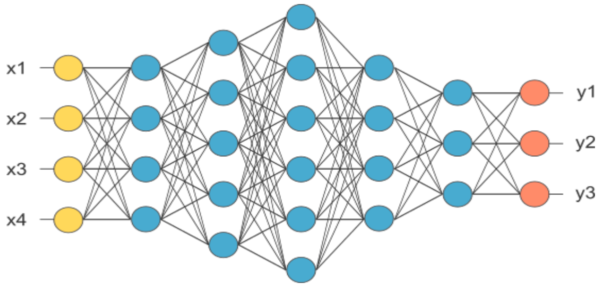
- **Eigen-decomposition:** Singular value decomposition (SVD), PCA, POD ….

Eigenvectors

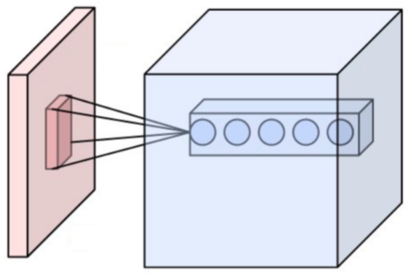


  - *Extensive offline sampling*
  - *Limitations of linear basis*

- **(Deep) neural network:** Convolutional, Recurrent, Generative nets, Reinforcement learning …

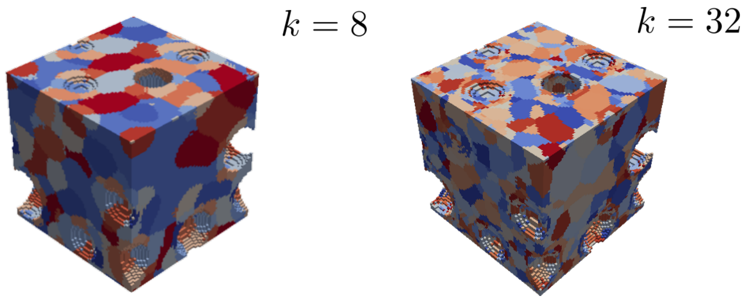


Feedforward Neural Network



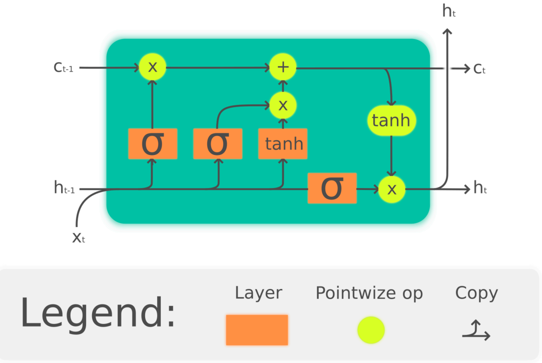
CNN

- **Clustering analysis:** Self-consistent clustering analysis ….



K-means clustering

  - *Micromechanical assumption*
  - *Computational complexity*

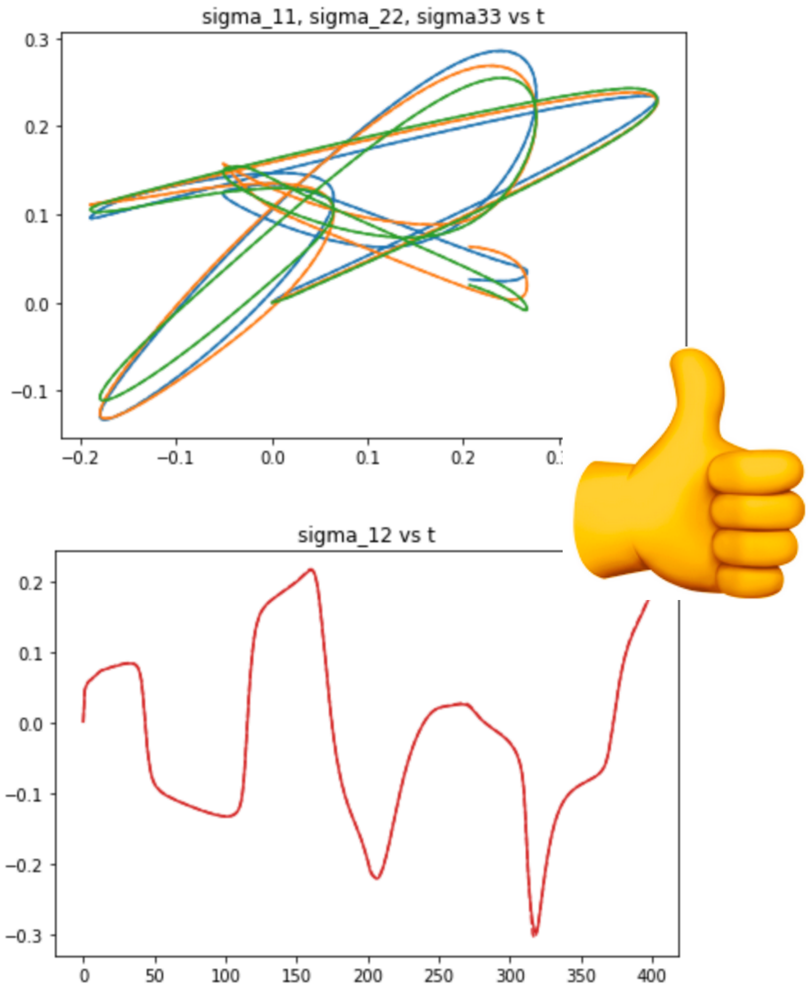


RNN: Long Short-Term Memory (LSTM)

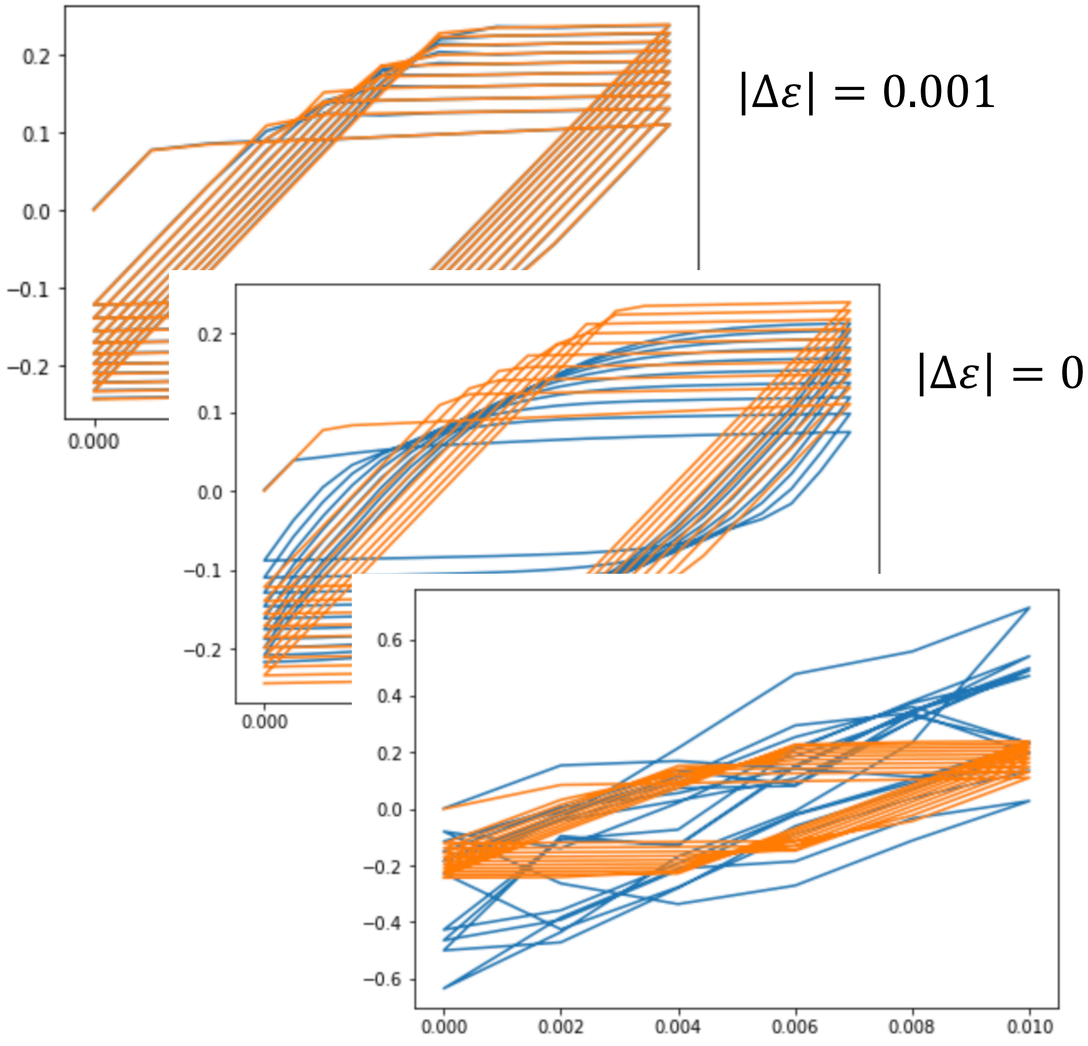
A recurrent net for von-Mises (J2) plasticity?

Training with 2000 random paths

$|\Delta\varepsilon| = 0.001$



Generalization/prediction for cyclic loading

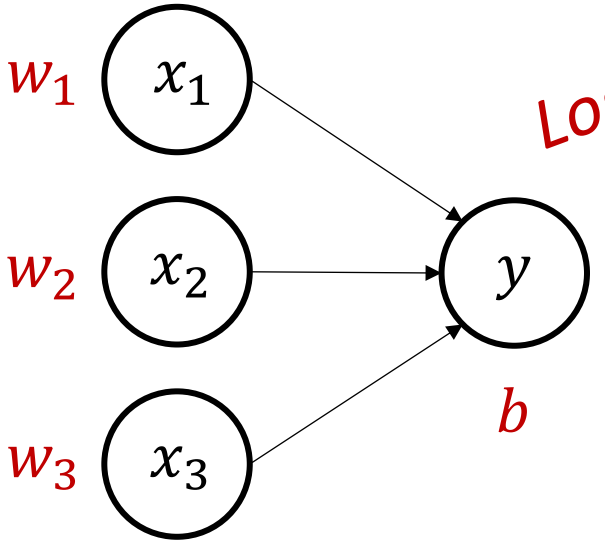


$|\Delta\varepsilon| = 0.001$

$|\Delta\varepsilon| = 0.0005$

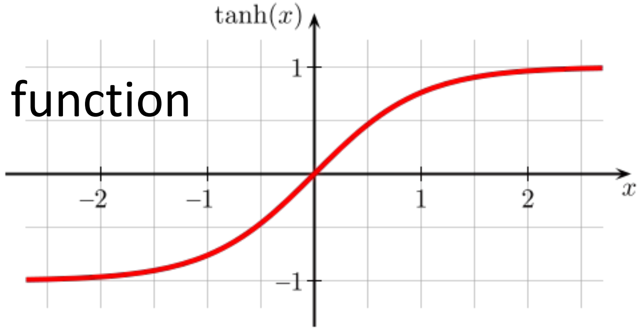
$|\Delta\varepsilon| = 0.002$

The building block of a generic neural network



$$y = a\left(\sum_{i=1}^{n} w_i x_i + b\right)$$

a: activation function

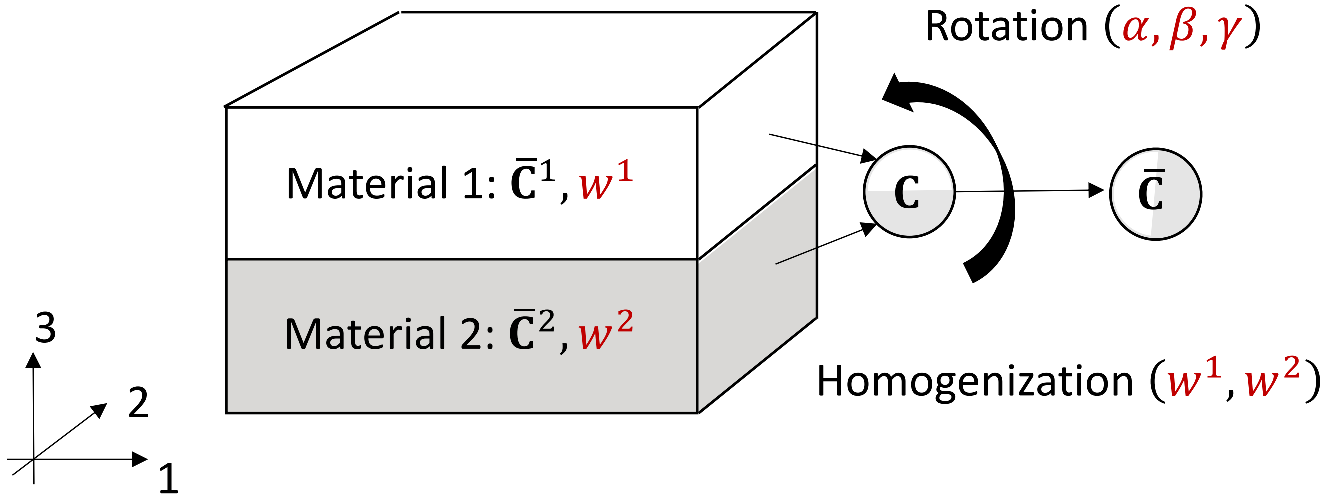


How to embed mechanics/physics into the building block of a network structure?

Deep Material Network (DMN)

1. *Zeliang Liu, C.T. Wu, M. Koishi. CMAME 345 (2019): 1138-1168.*
2. *Zeliang Liu, C.T. Wu. JMPS 127 (2019): 20-46.*
3. *Zeliang Liu, C.T. Wu, M. Koishi. Computational Mechanics (2019)*
4. *Zeliang Liu, CMAME 363 (2020): 1132913*

Deep material network: Physics-based building block



Existence of analytical solutions

↓

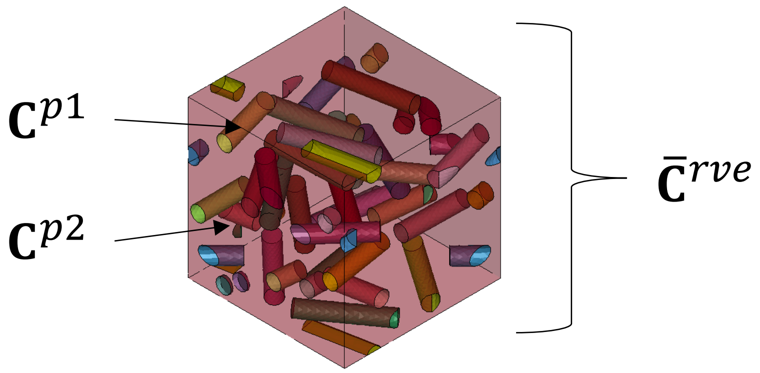
- Automatic differentiation
- Backpropagation

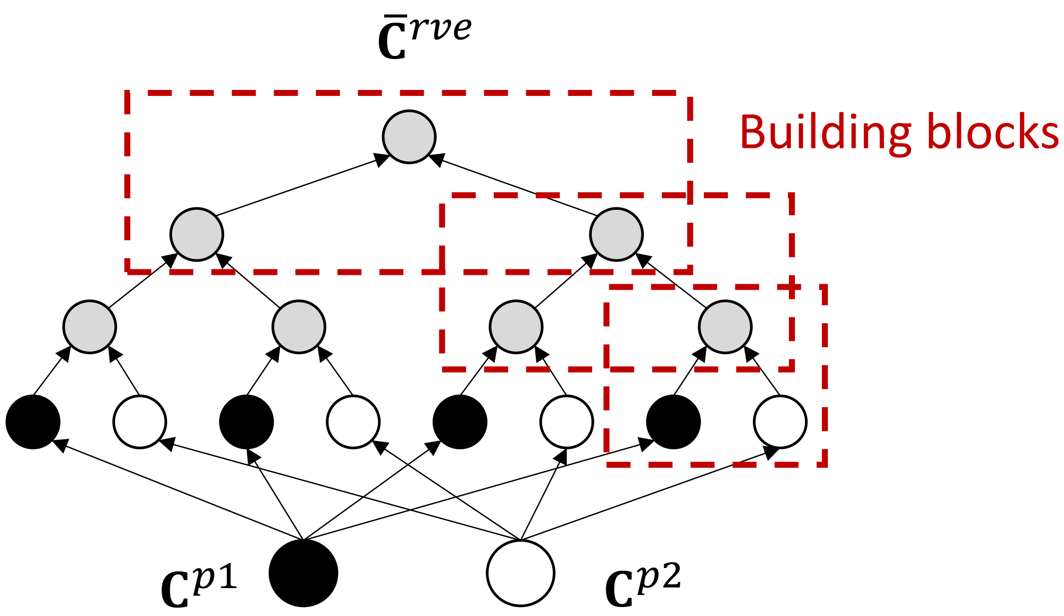
- ❑ Interfacial equilibrium conditions: $\sigma_3^1 = \sigma_3^2, \quad \sigma_4^1 = \sigma_4^2, \quad \sigma_5^1 = \sigma_5^2$
- ❑ Interfacial kinematic constraints: $\varepsilon_1^1 = \varepsilon_1^2, \quad \varepsilon_2^1 = \varepsilon_2^2, \quad \varepsilon_6^1 = \varepsilon_6^2$
- ❑ Weights (w^1, w^2) are determined by the activations z in the bottom layer

Deep material network: Architecture, input, output

Input: Microscale stiffness tensor $\mathbf{C}^{p1}$, $\mathbf{C}^{p2}$

Output: Overall stiffness tensor $\bar{\mathbf{C}}^{rve}$





$$\underbrace{\bar{\mathbf{C}}^{rve}}_{\text{Output}} = \mathbf{f}_2(\underbrace{\mathbf{C}^{p1}, \mathbf{C}^{p2}}_{\text{Inputs}}, \overbrace{z^{j=1,2,\ldots,2^{N-1}}, \alpha_{i=1,\ldots,N}^{k=1,2,\ldots,2^{i-1}}, \beta_{i=1,2,\ldots,N}^{k=1,2,\ldots,2^{i-1}}, \gamma_{i=1,2,\ldots,N}^{k=1,2,\ldots,2^{i-1}}}^{\text{Fitting parameters}}).$$

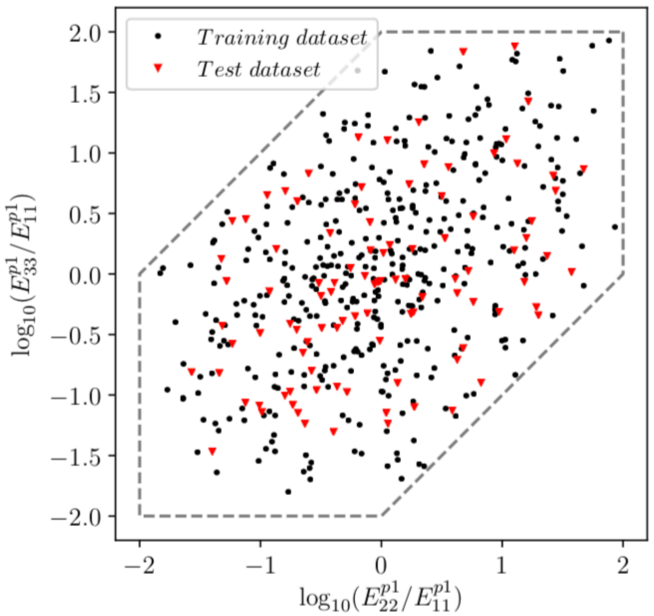
Data Generation → Training → Prediction & Extrapolation

Data generation: Sampling of phase properties

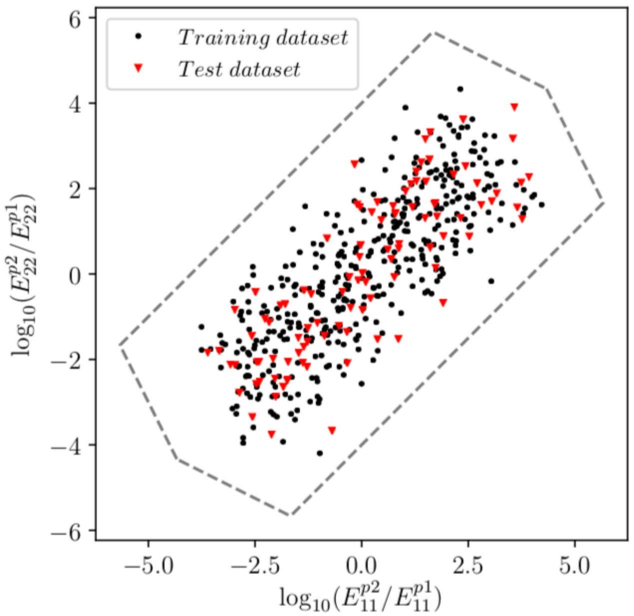
Design of Experiments (DoE)

- Only linear elastic materials
- Strong material anisotropy and phase contrast
- Analyzed using LS-DYNA RVE package

$$
\mathbf{D}^{pi} = \begin{Bmatrix}
1/E_{11}^{pi} & -\nu_{12}^{pi}/E_{22}^{pi} & -\nu_{31}^{pi}/E_{11}^{pi} & & & \\
 & 1/E_{22}^{pi} & -\nu_{23}^{pi}/E_{33}^{pi} & & & \\
 & & 1/E_{33}^{pi} & & & \\
 & & & 1/(2G_{23}^{pi}) & & \\
 & & & & 1/(2G_{31}^{pi}) & \\
 & & & & & 1/(2G_{12}^{pi})
\end{Bmatrix}
$$



(a) Anisotropy of phase 1.



(b) Contrasts of moduli between phase 1 and 2.

Data Generation | Training | Prediction & Extrapolation

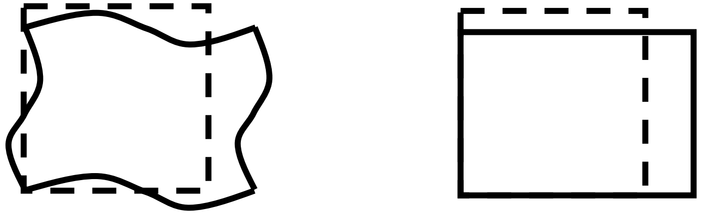
Data generation: LS-DYNA RVE package

- ❑ RVE homogenization module in small-strain and finite-strain formulations.
- ❑ Homogenized stress-strain results are saved to database file.

Woven composite *Particle-reinforced composite*

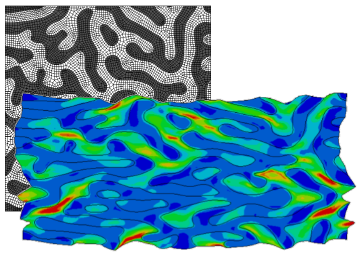
a) Arbitrary RVE morphologies in both 2D and 3D

Periodic BC *Displacement BC*

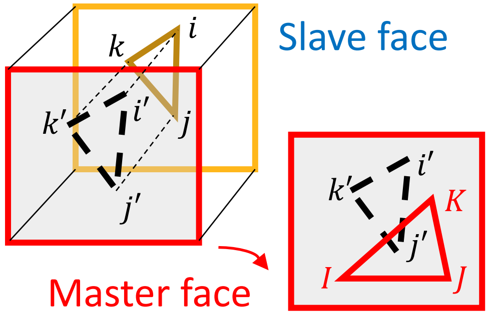


b) Various types of boundary conditions

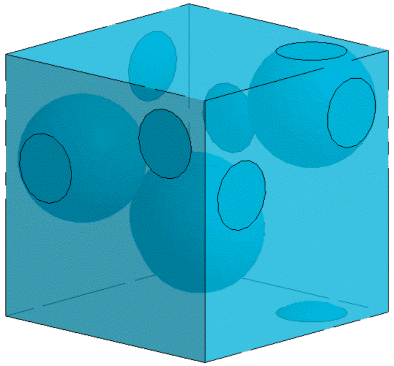
Example in 2D



Example in 3D



c) Treatment of non-matching 2D & 3D meshes



d) Arbitrary material and loading conditions

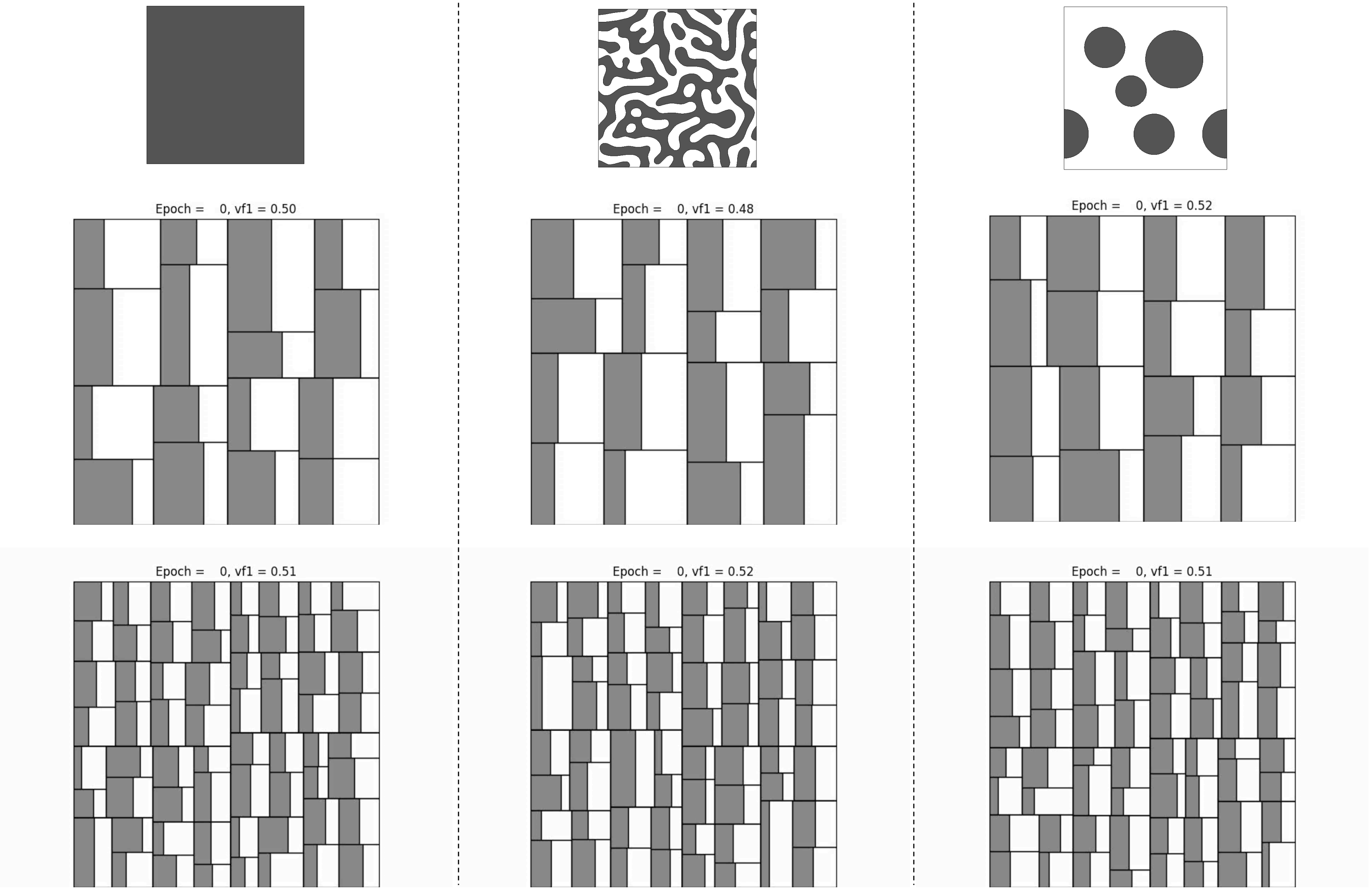
Data Generation → Training → Prediction & Extrapolation

Evolutions of weights during the training process (2D RVEs)

Depth

$N = 5$

$N = 7$



$vf_{dns} = 29\%$

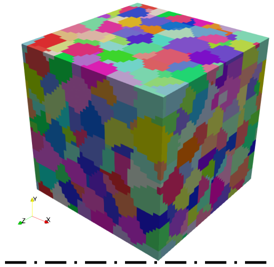
$vf_{n=5} = 30\%$

$vf_{n=5} = 28\%$

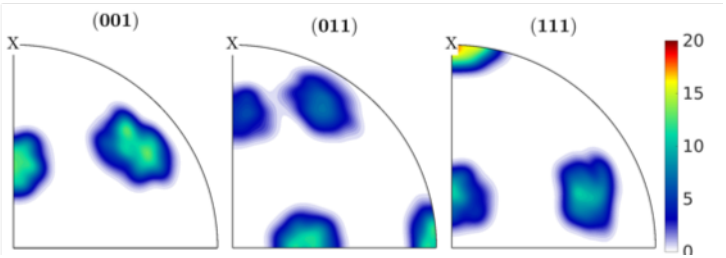
Hidden Geo Info

Data Generation | **Training** | Prediction & Extrapolation

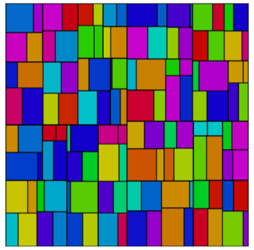
Hidden geometric information encoded in fitting parameters



Grain orientation map
of DNS (hidden in data)

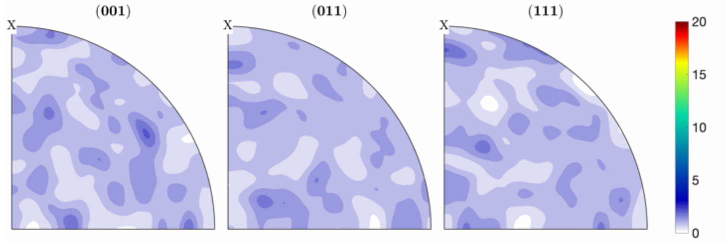


DMN with 8 layers

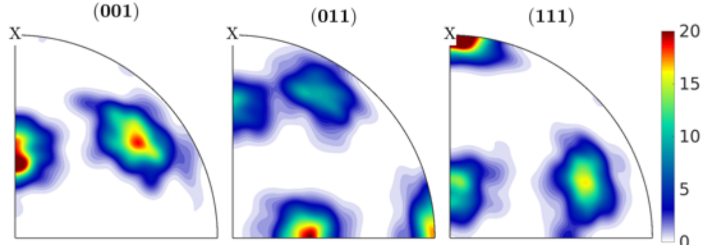


(c) $N = 8, N_a = 128$

In training
(first 2000 epochs),



After 20000 epochs,



$$\underbrace{\bar{\mathbf{C}}^{rve}}_{\text{Output}} = \mathbf{f}_2(\underbrace{\mathbf{C}^{p1}, \mathbf{C}^{p2}}_{\text{Inputs}}, \overbrace{z^{j=1,2,\ldots,2^{N-1}}, \alpha_{i=1,\ldots,N}^{k=1,2,\ldots,2^{i-1}}, \beta_{i=1,2,\ldots,N}^{k=1,2,\ldots,2^{i-1}}, \gamma_{i=1,2,\ldots,N}^{k=1,2,\ldots,2^{i-1}}}^{\text{Fitting parameters}}).$$

Data Generation | **Training** | Prediction & Extrapolation

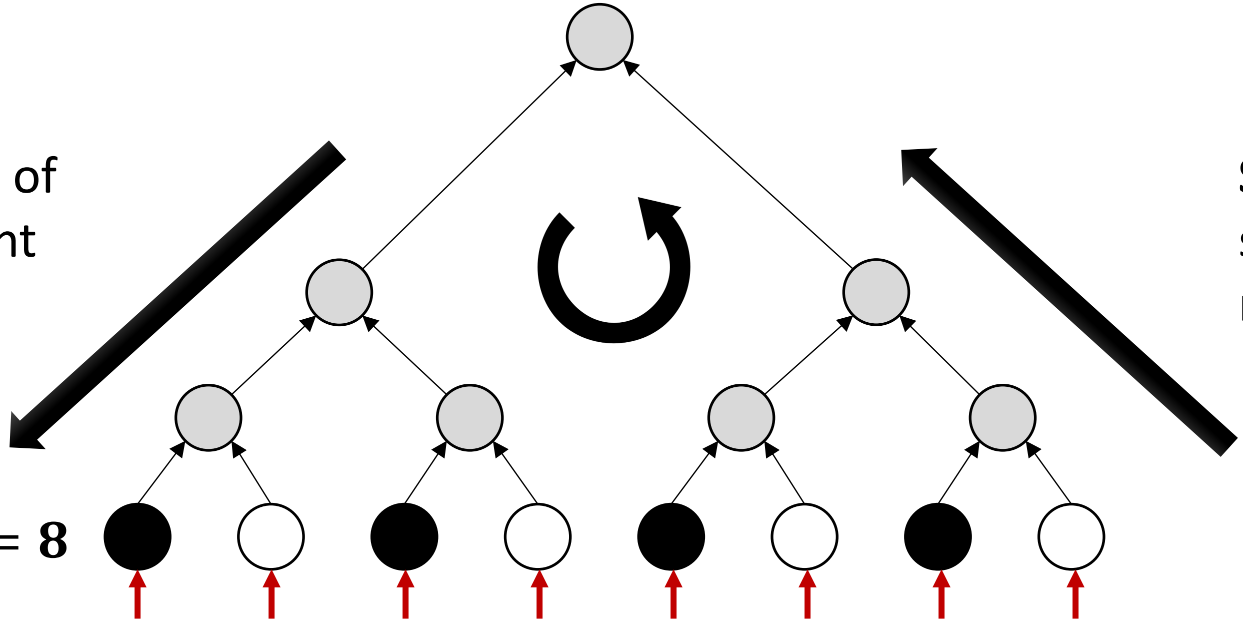
Online prediction: Material nonlinearities, large deformation

Step 3: Macroscale boundary condition evaluation

Step 4: Propagation of deformation gradient $\Delta\mathbf{P}$ and stress $\Delta\mathbf{F}$

Step 2: Propagation of stiffness matrix $\mathbf{A}$ and residual stress $\delta\mathbf{P}$

$\boldsymbol{N_{dof}} = \mathbf{8}$



Step 1: Microscale material law evaluations

"Computational cost of one iteration" = $O(N_{dof})$

Data Generation | Training | **Prediction & Extrapolation**

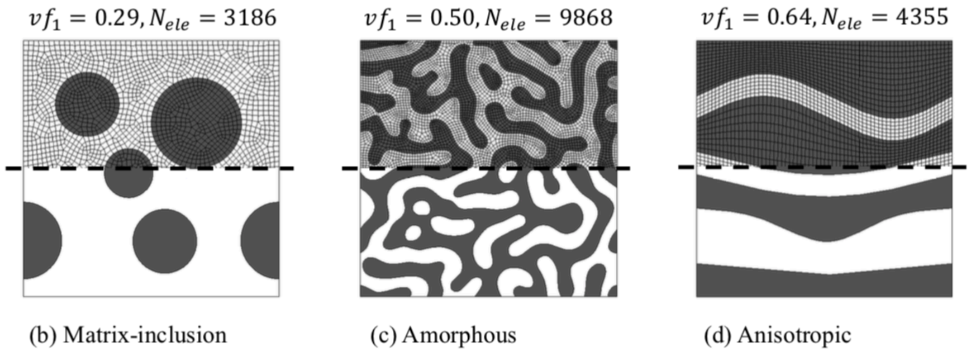
Applications to 2D and 3D RVEs

2D materials:

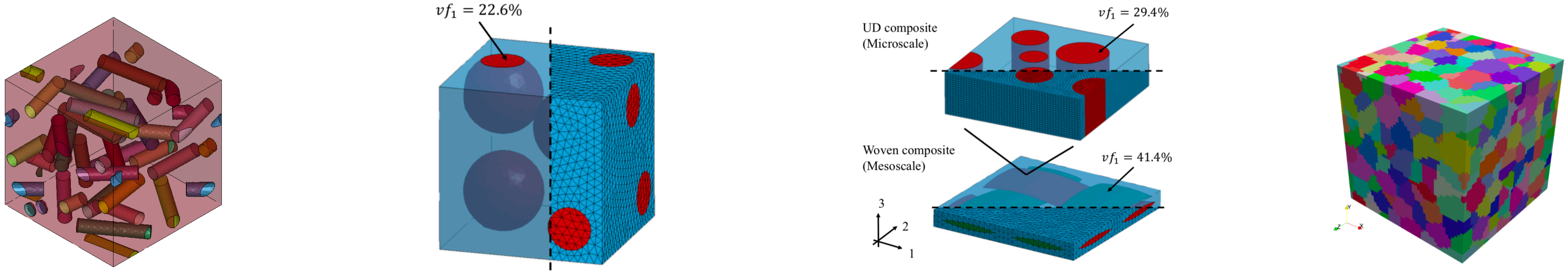
- Mooney-Rivlin hyperelasticity
- Von Mises plasticity

3D materials:

- Mooney-Rivlin hyperelasticity with Mullins effect
- Von Mises plasticity
- Rate-dependent crystal plasticity

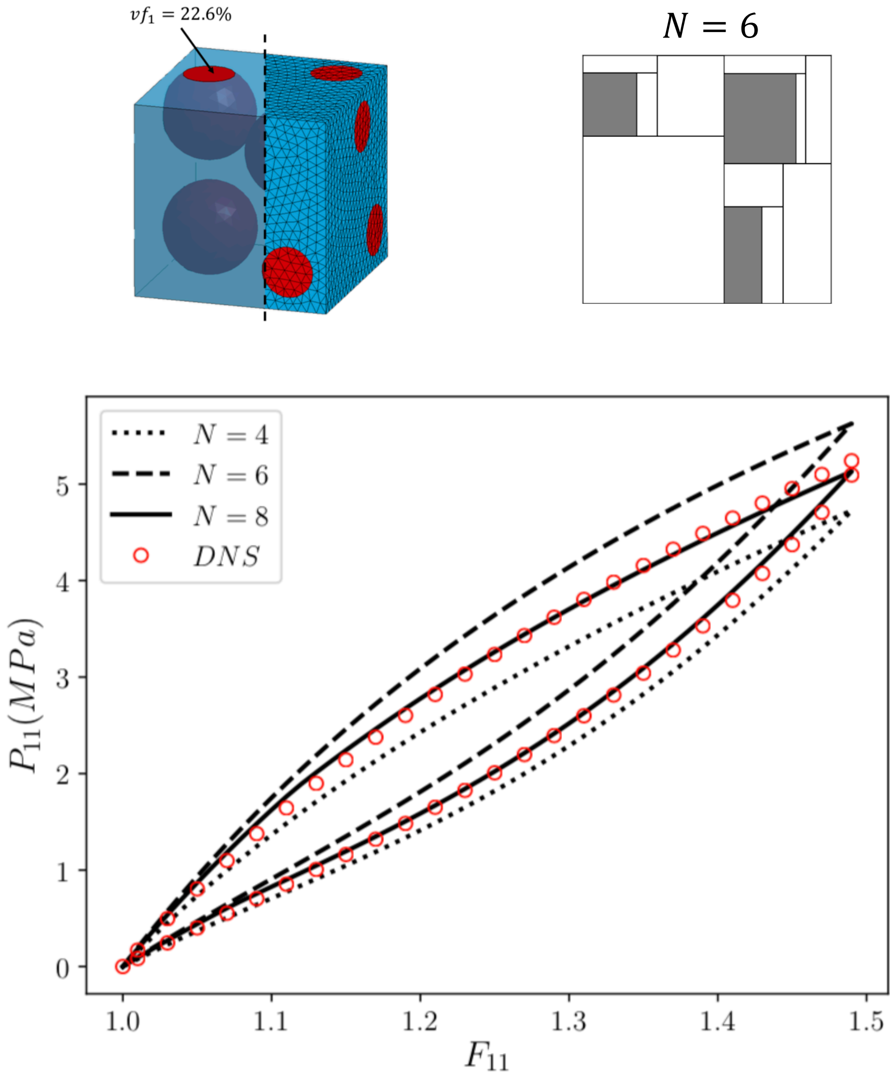


1. *Zeliang Liu, C.T. Wu, M. Koishi. CMAME 345 (2019): 1138-1168.*
2. *Zeliang Liu, C.T. Wu. JMPS 127 (2019): 20-46.*

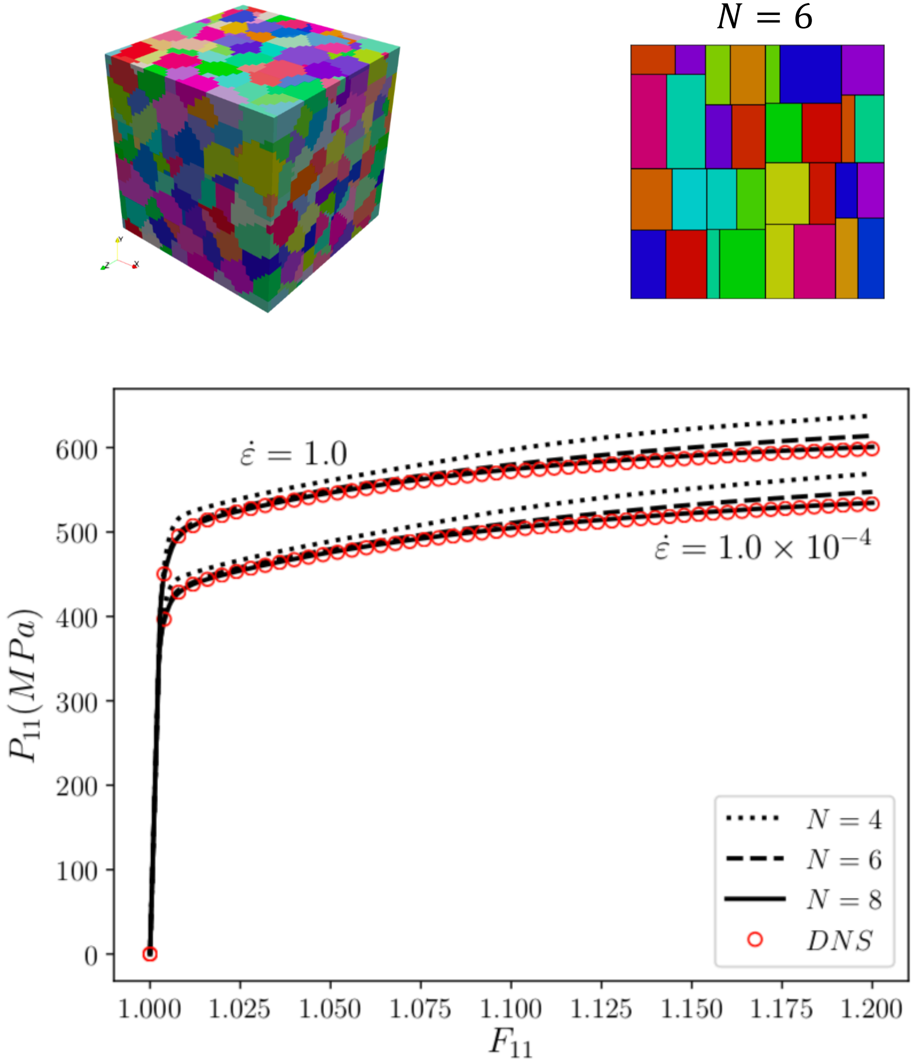


Short-fiber Composites | Particle-reinforced Rubber | UD & Woven Fiber Composites | Polycrystals

Online predictions: Hyperelasticity, crystal plasticity…



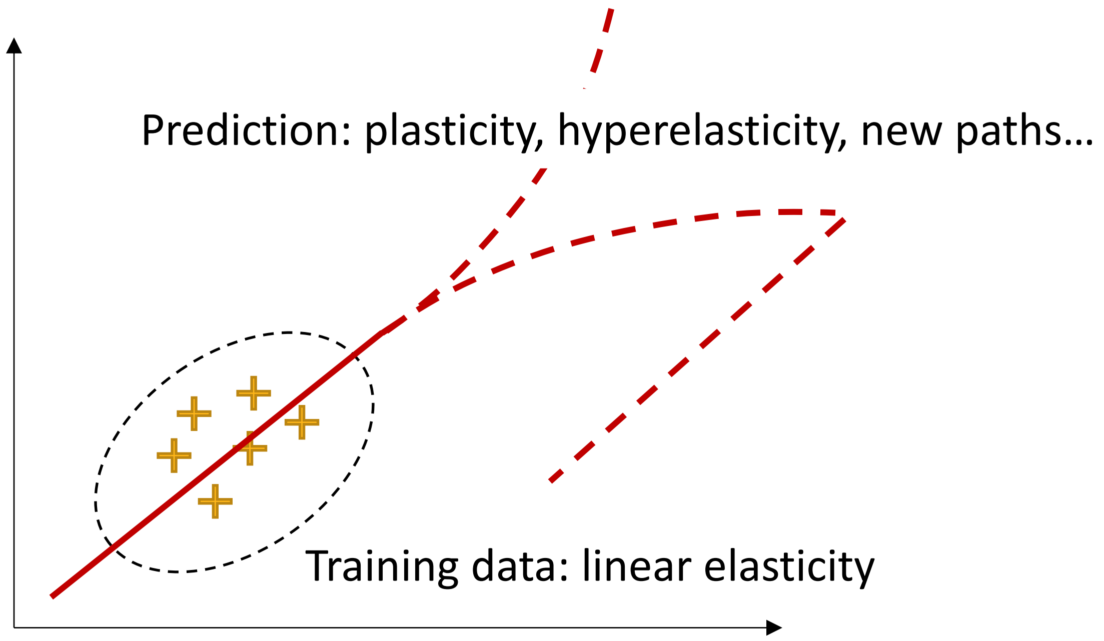
(a) Uniaxial tension.

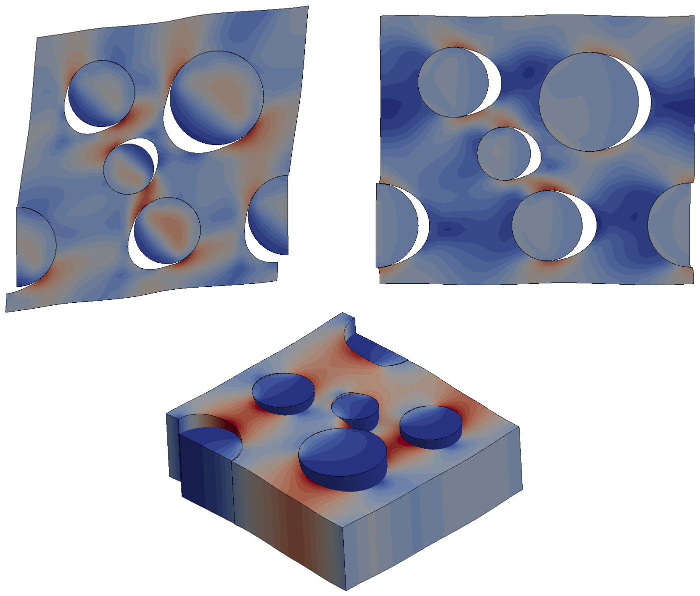


(a) Random ODF.

Key features of deep material network

- Physics-based building block with interpretable fitting parameters
- Extrapolation capability for material and geometric nonlinearities with only linear elastic training data
- Efficient online inference: "Computational cost" = $O(N_{dof})$
- Extension to debonding and failure analysis.



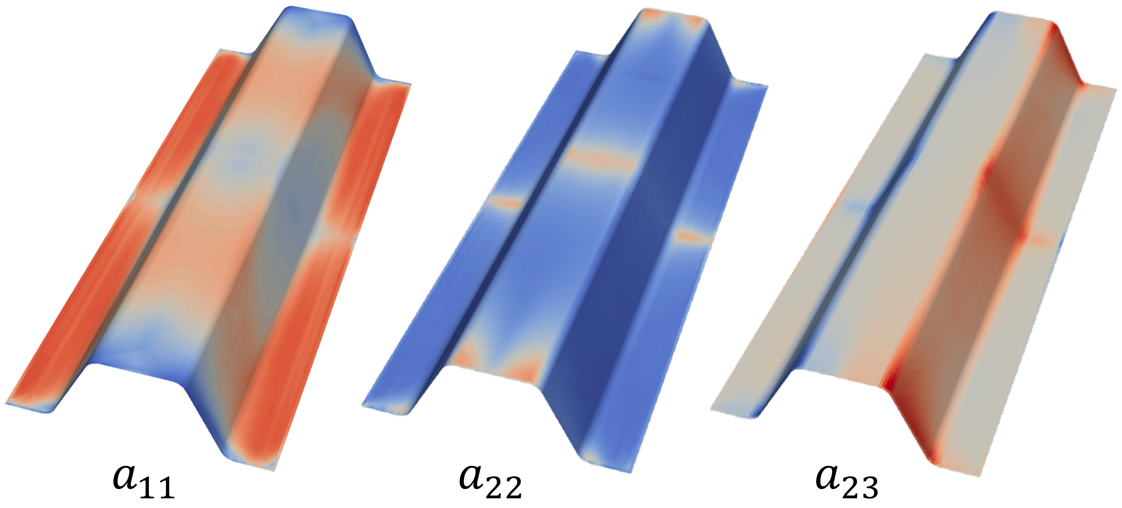


Zeliang Liu, CMAME 363 (2020): 1132913

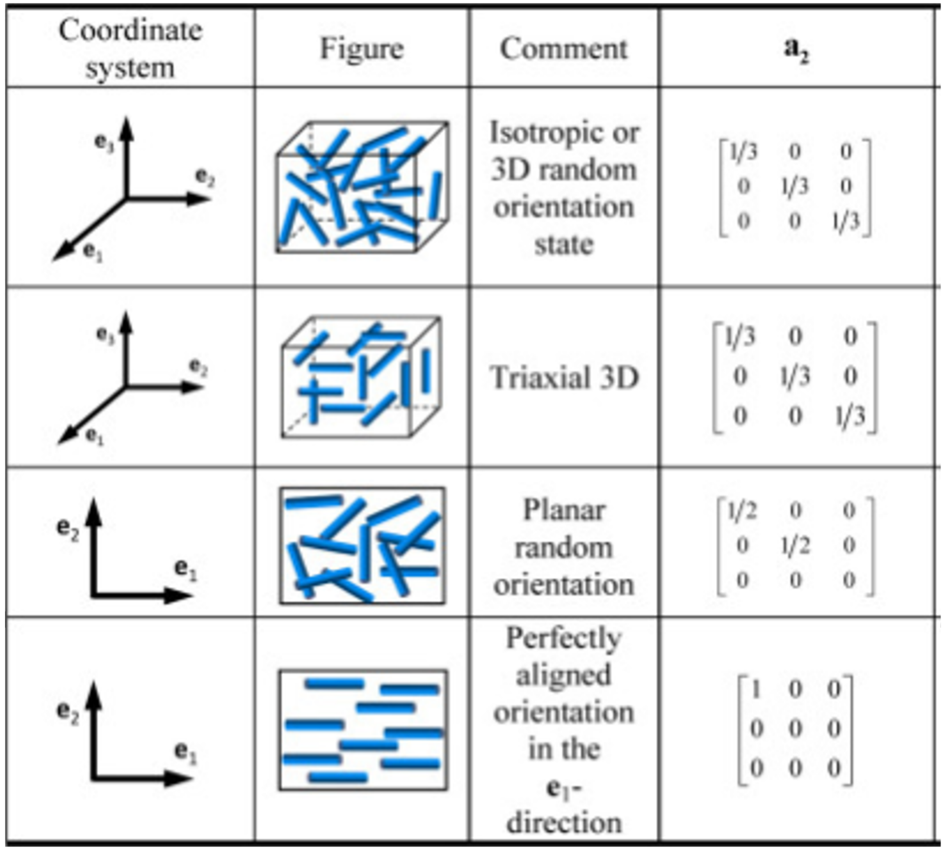
An exemplar on short fiber reinforced composites

<u>Orientation tensor A</u>

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$



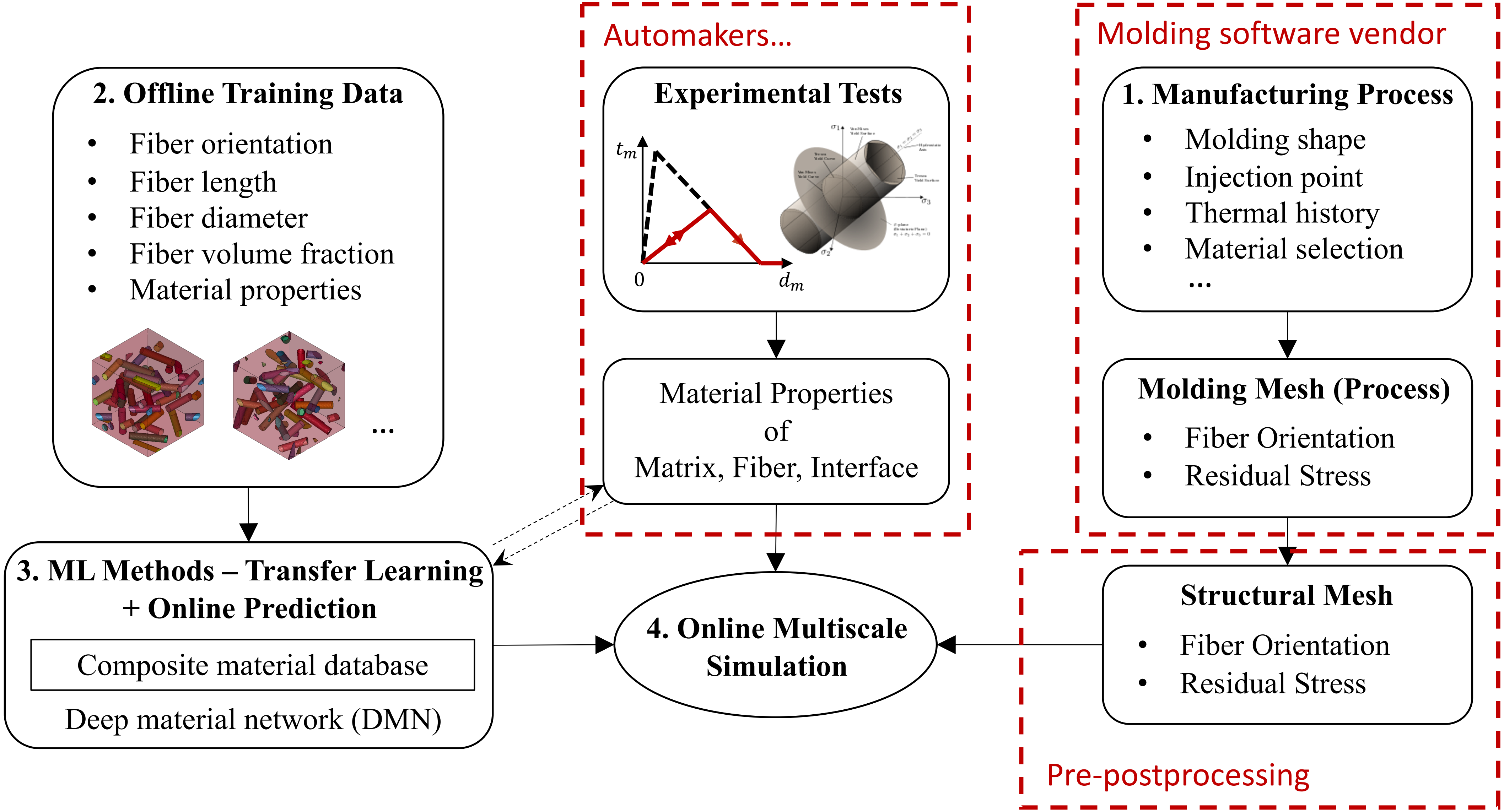
- Higher order tensors exists, but typically not available



Coordinate system	Figure	Comment	$\mathbf{a}_2$
$\mathbf{e}_3$, $\mathbf{e}_2$, $\mathbf{e}_1$		Isotropic or 3D random orientation state	$\begin{bmatrix} 1/3 & 0 & 0 \\ 0 & 1/3 & 0 \\ 0 & 0 & 1/3 \end{bmatrix}$
$\mathbf{e}_3$, $\mathbf{e}_2$, $\mathbf{e}_1$		Triaxial 3D	$\begin{bmatrix} 1/3 & 0 & 0 \\ 0 & 1/3 & 0 \\ 0 & 0 & 1/3 \end{bmatrix}$
$\mathbf{e}_2$, $\mathbf{e}_1$		Planar random orientation	$\begin{bmatrix} 1/2 & 0 & 0 \\ 0 & 1/2 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
$\mathbf{e}_2$, $\mathbf{e}_1$		Perfectly aligned orientation in the $\mathbf{e}_1$-direction	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$

https://www.sciencedirect.com/topics/engineering/fibre-orientation-distribution

Data-driven framework for short fiber reinforced composites



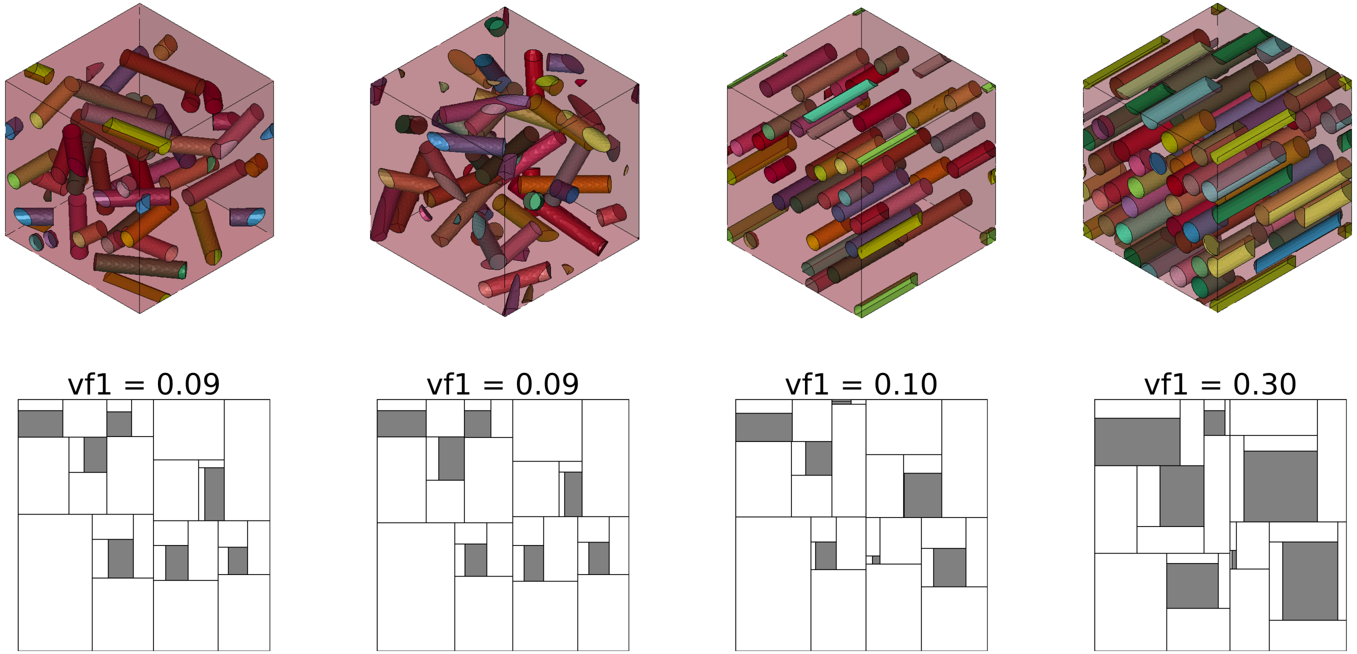
Zeliang Liu, Haoyan Wei, Tianyu Huang, C.T. Wu. 16-th LS-DYNA user conference

Training results with transfer learning

3D random (10%) | 2D random (10%) | Aligned (10%) | Aligned (30%)

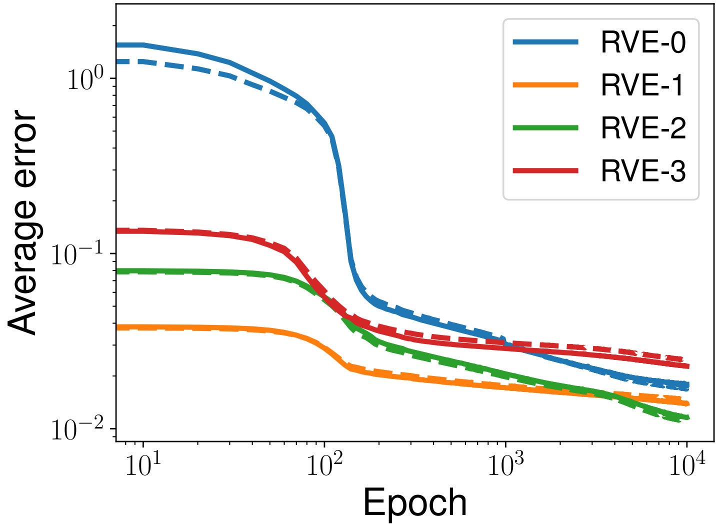
RVE Geometry

DMN Architecture

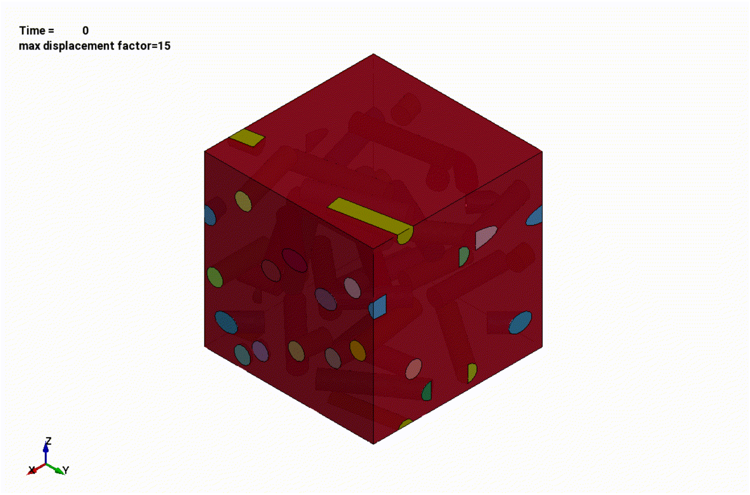


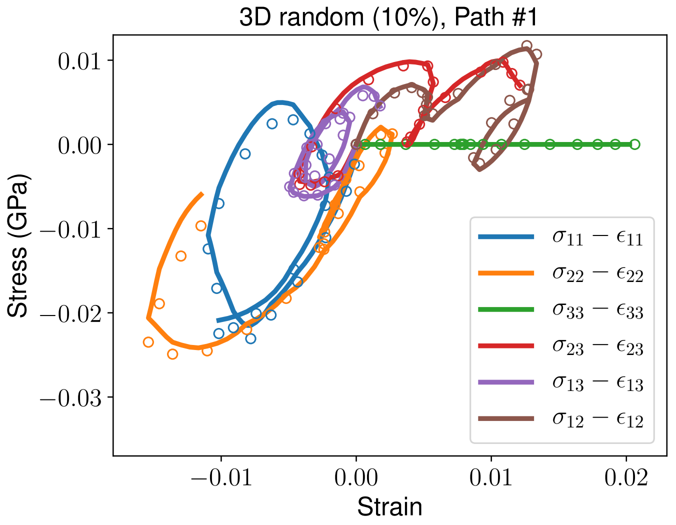
Transfer learning: DMNs with identical architectures

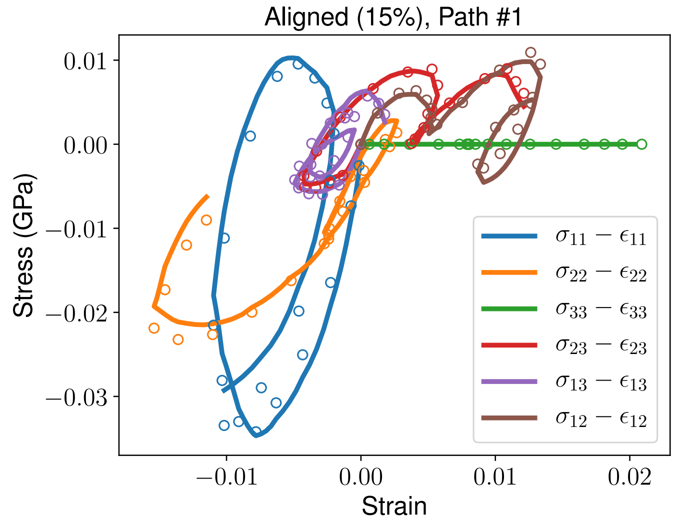
Training history

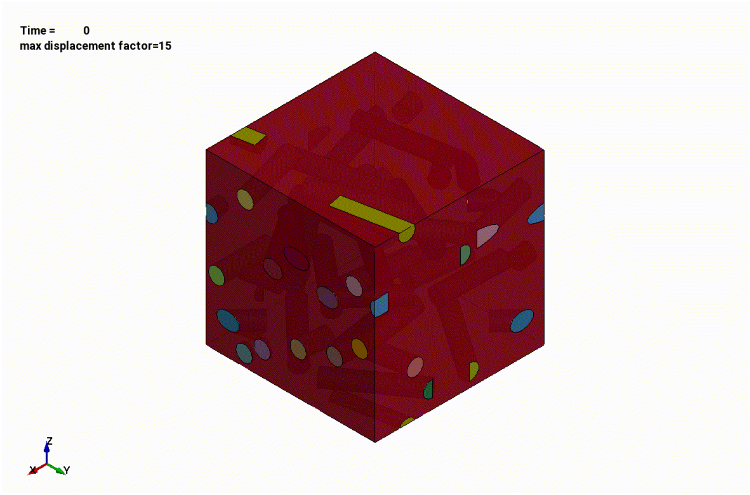


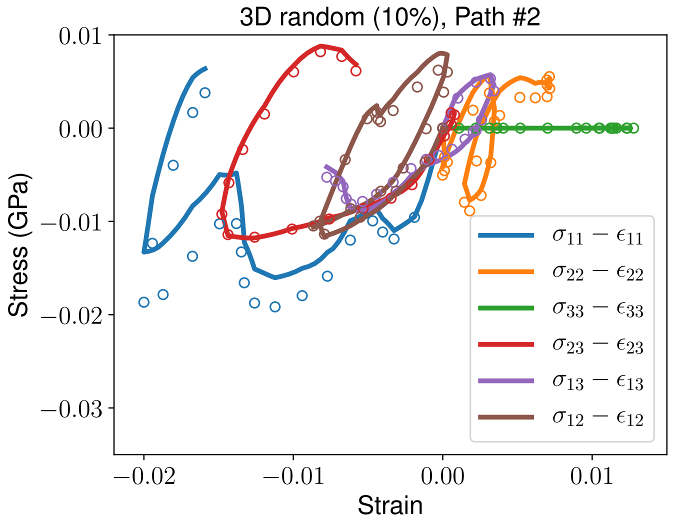
Prediction results (nonlinear): Matrix plasticity, random paths

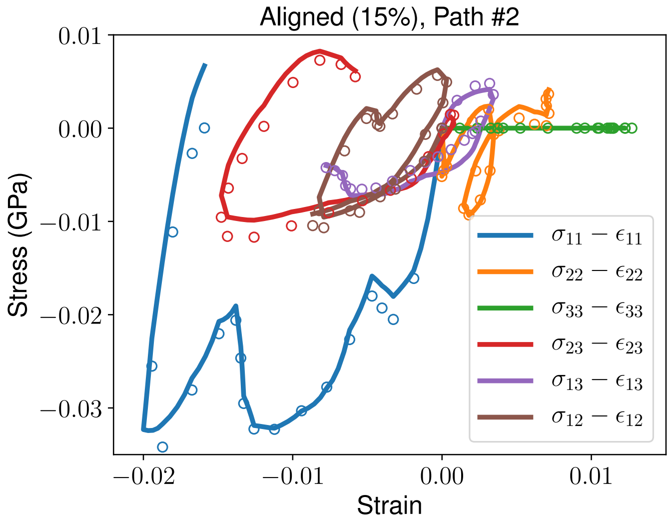




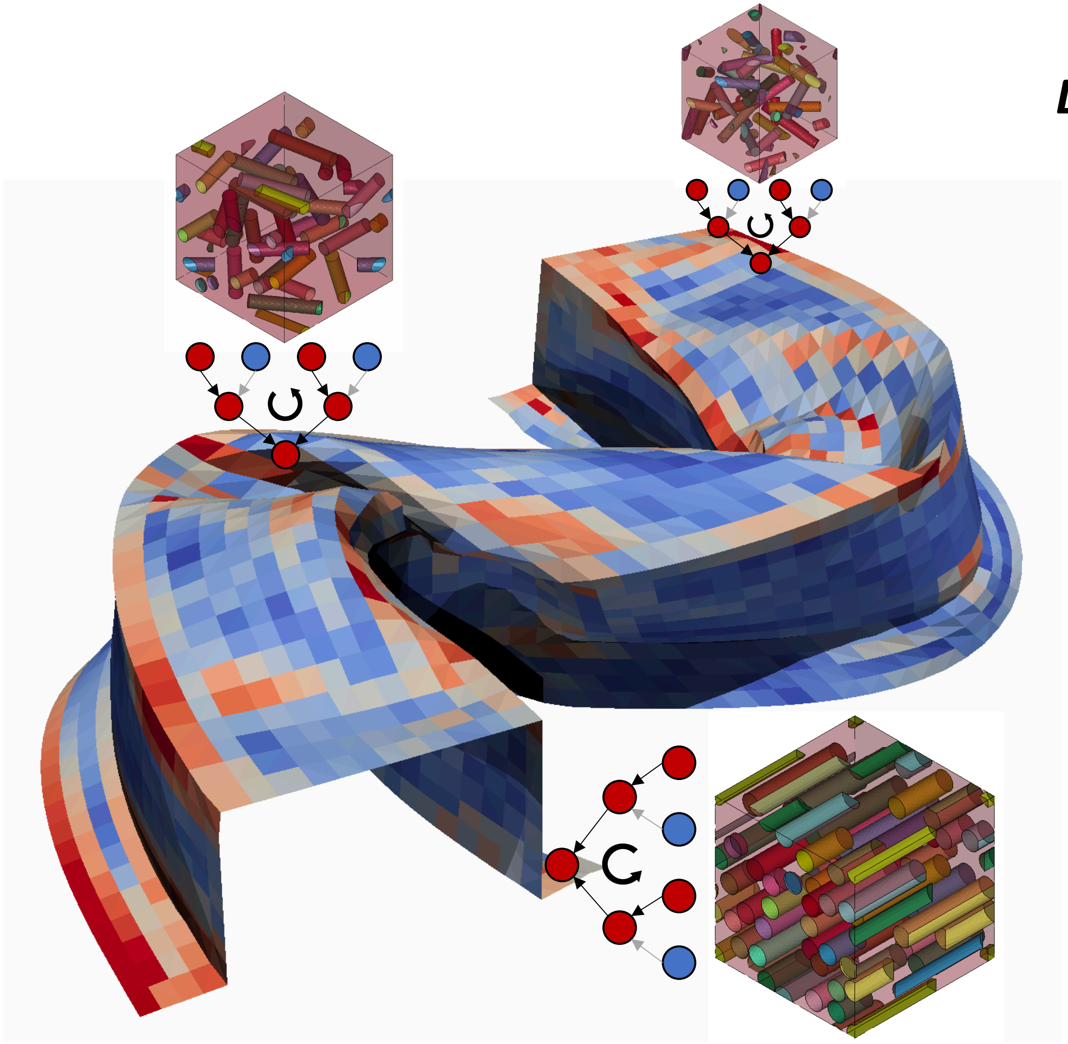








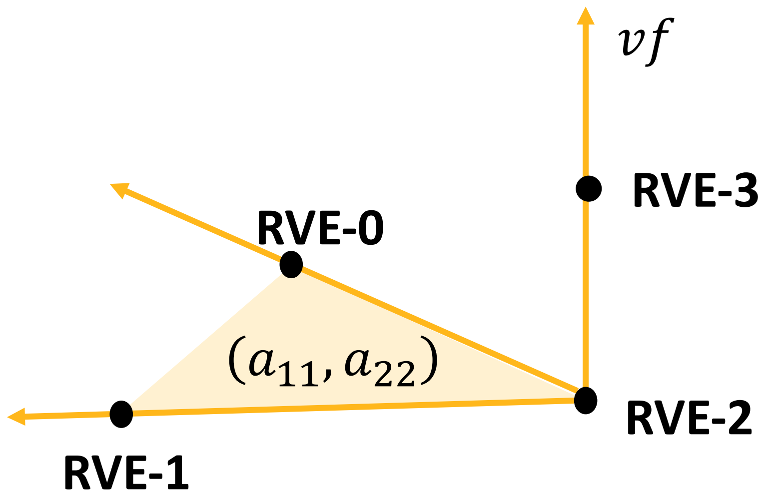
Multiscale concurrent simulations in LS-DYNA



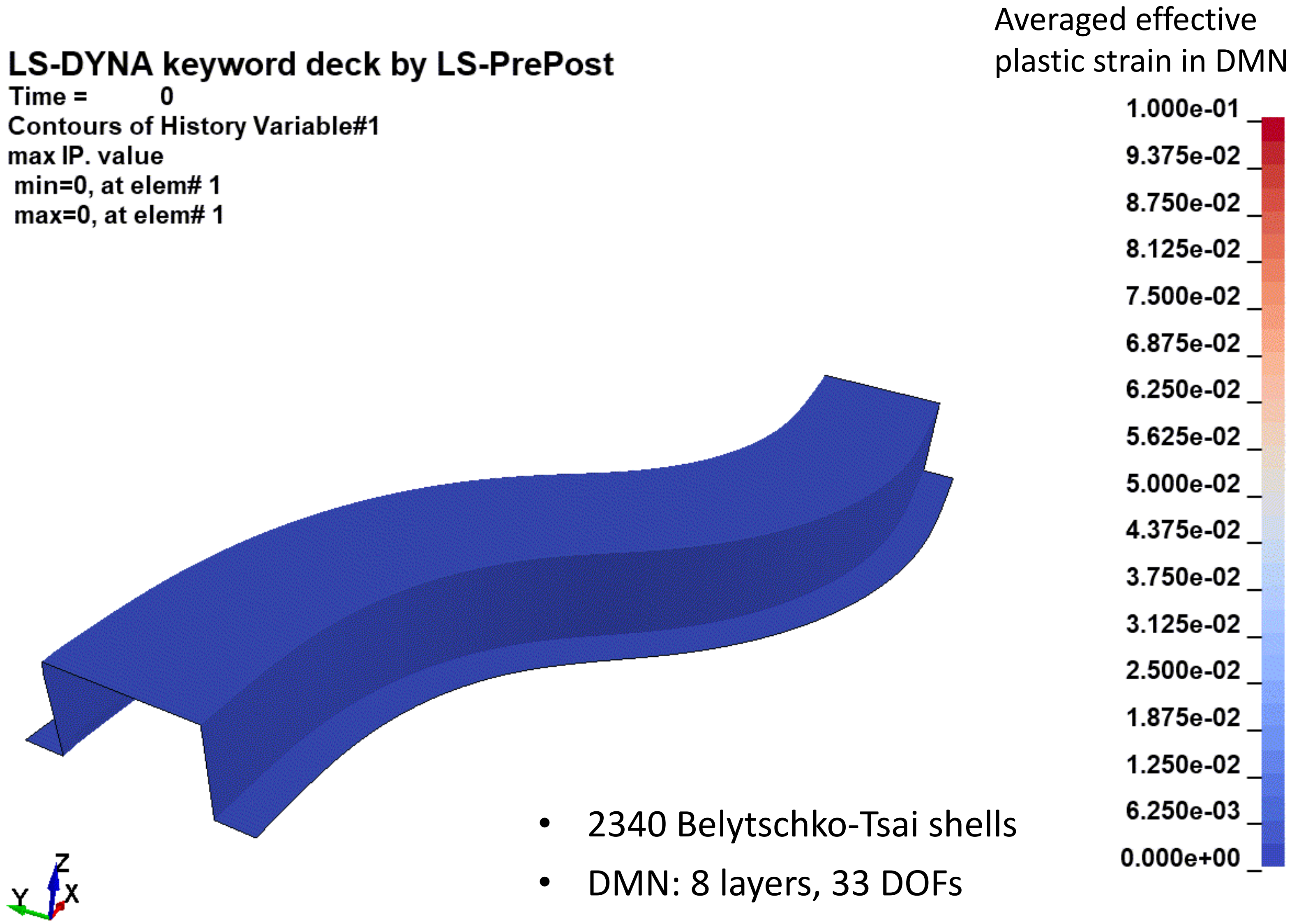
DMN + Transfer Learning + Network interpolation

(Only 4 RVEs are trained in the offline)

- Any RVE in design space.
- Arbitrary material law (e.g. plasticity).
- Any loading path.
- Efficient and accurate.

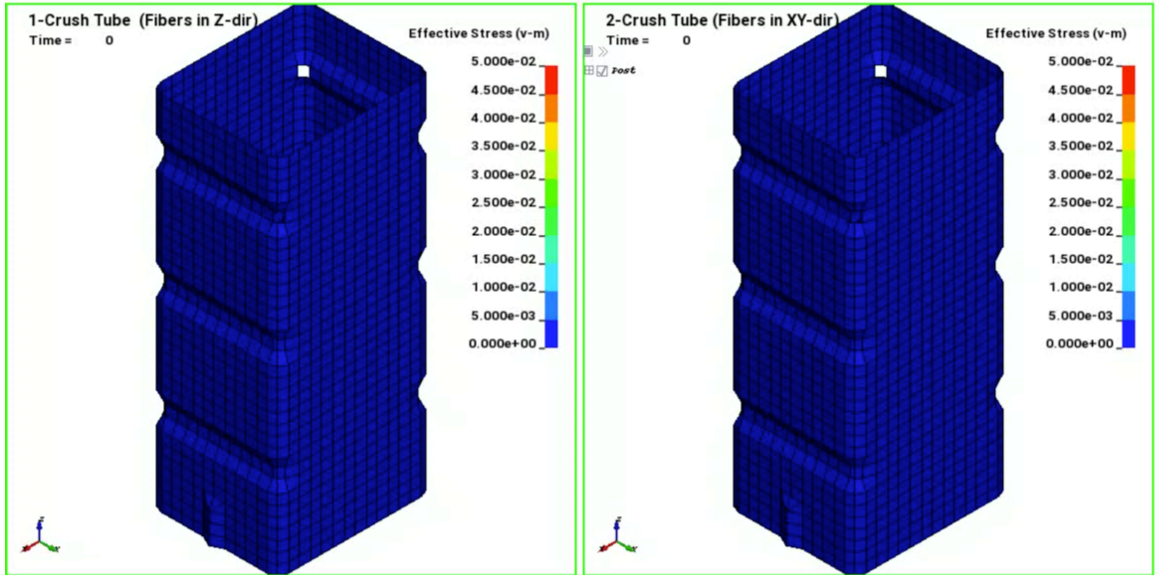


Concurrent simulation for the S-shaped rail

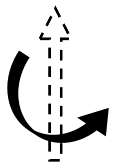


- 2340 Belytschko-Tsai shells
- DMN: 8 layers, 33 DOFs

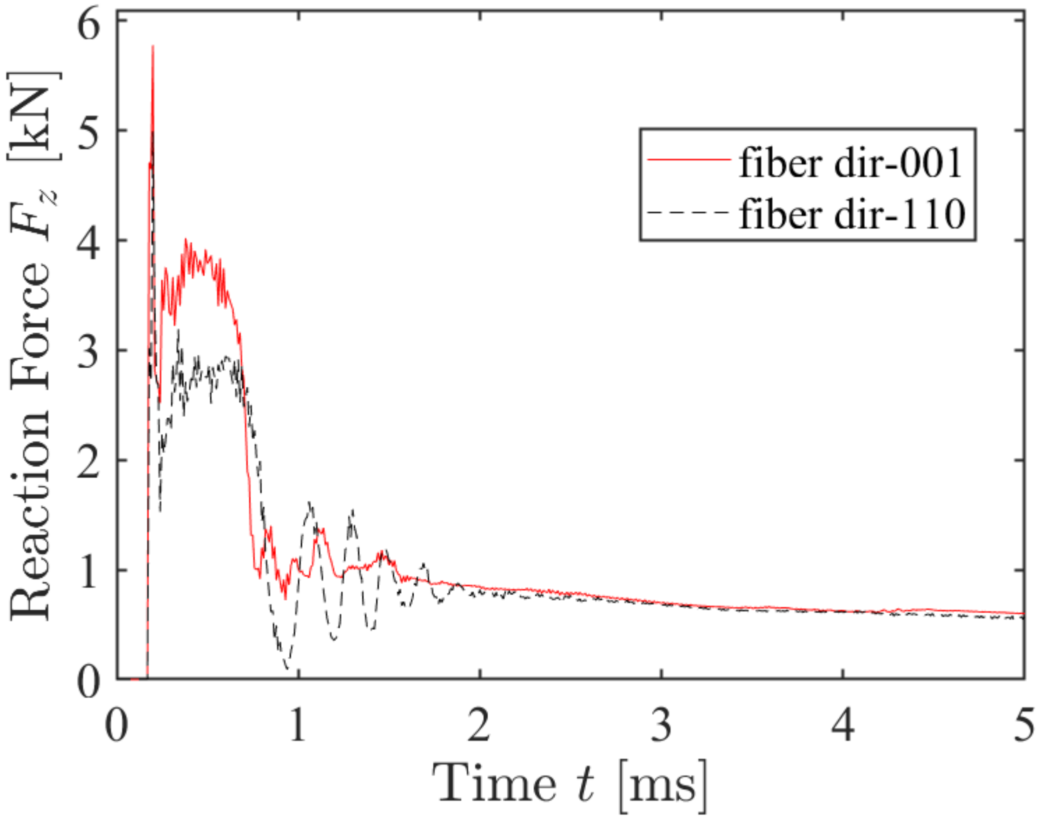
Crush tubes with different fiber directions



Fiber dir
001



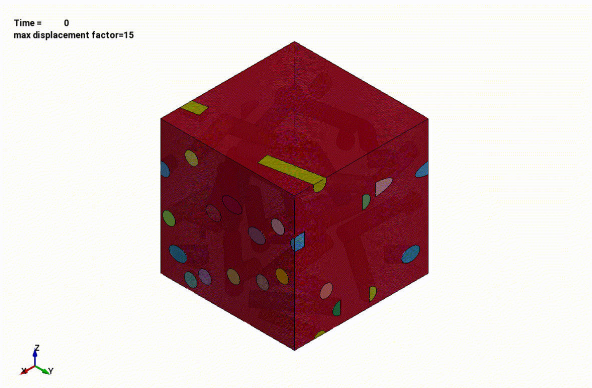
Fiber dir
110



Computational time

RVE-scale single material-point test (random path):

DNS (Finite Element, 360K DOFs)	DMN (8 layers, 33 DOFs)
1100s on 8 CPUs	3s on 1 CPU



Concurrent multiscale simulation with DMN:

Macroscale model			**Computational wall time (min)**		
Name	Num of Elements	Loading cycles	$N_{CPU} = 1$	$N_{CPU} = 4$	$N_{CPU} = 16$
S-shaped rail	2340	17372	224.0	65.5	18.1
Crush tube	641 (Sym)	17640	68.4	24.5	11.0

*All the computations are performed on a workstation with 20 Intel® Xeon® CPU E5-2640 v4 2.40 GHz processors.

Summary

- **Multiscale materials modeling using RVE analysis**
  - LS-DYNA RVE package.
  - Challenges: Efficiency and accuracy, lack of data, and danger of extrapolation.
- **Deep material network in data-driven materials modeling**
  - Physics-based building block.
  - Data generation, training, extrapolation, and transfer learning.
- **Concurrent simulation with intelligent materials models**
  - Prototyping via LS-DYNA user material interface.
  - Short fiber reinforced composite (injection molding)
- **Near-future plans**
  - Workflow integration
  - Material damage and failure analysis, experimental validations
  - Research on implicit concurrent simulations