Multi-scale Modelling using Recurrent Neural Network for Mesoscale Surrogation to Achieve Acceleration in Simulation of Rate-Dependent Dissipative Lattice Based and Cellular Meta-Materials

M. Mustafa, L. Wu, L. Noels
University of Liege
Computational & Multiscale Mechanics of Materials
http://www.ltas-cm3.ulg.ac.be

J. Segurado
IMDEA Materials Institute
Multiscale Materials Modelling
https://materials.imdea.org/people/javier-segurado/

19th European Mechanics of Materials Conference
30-31 May 2024

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 862015

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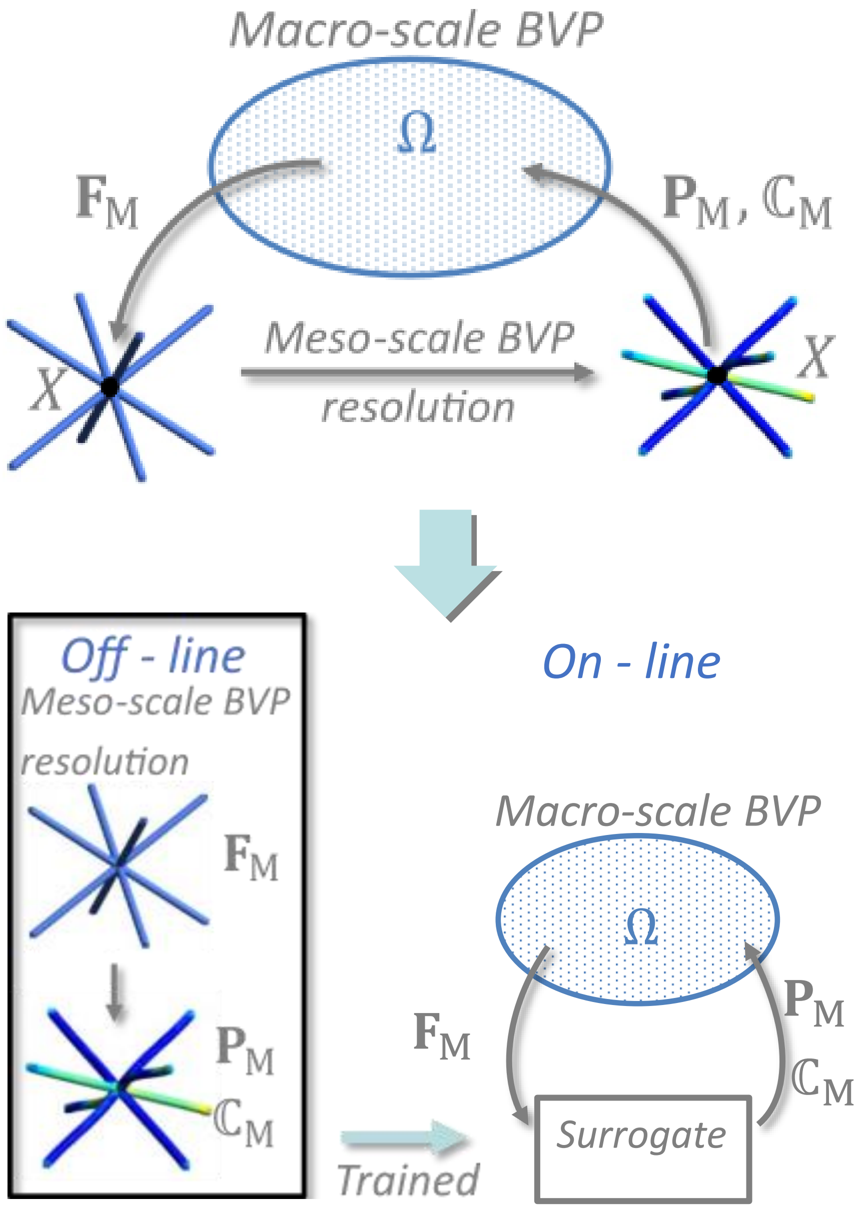
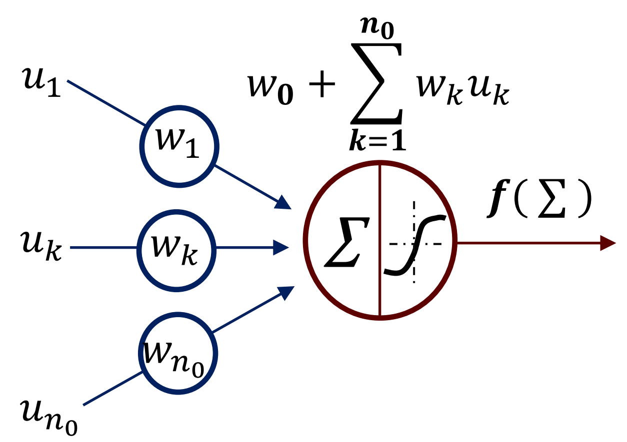
Motivation

- **Multi-scale simulations**
  - Concurrent solution at two different scales
    - Macro-scale resolution
    - Meso-scale resolution
    - Finite element simulations have FE^2 complexity
  - Impractical for lattice based meta materials
    - Material is dissipative & rate dependent
    - Fine discretization for geometrical resolution
  - Reduction of the FE^2 complexity is sought

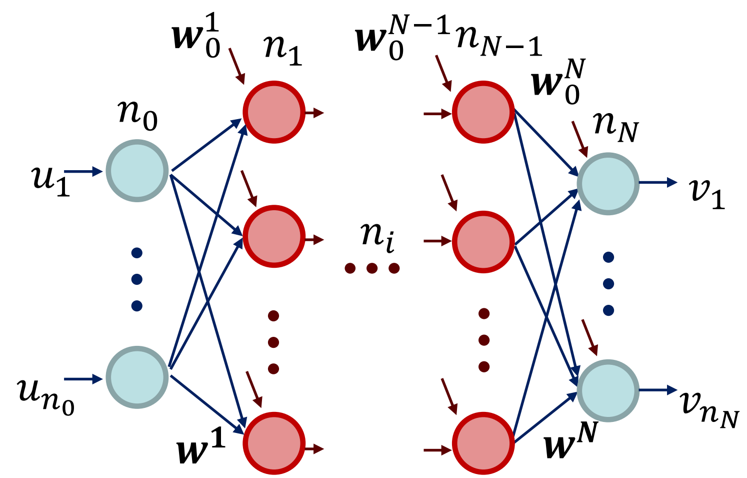
- **Accelerated Multi-scale simulations**
  - Substitute a surrogate in-place of meso-scale
    - Surrogate is trained offline
    - Substitutes expensive meso-scale FE resolution
    - Speeds up the (online) simulation



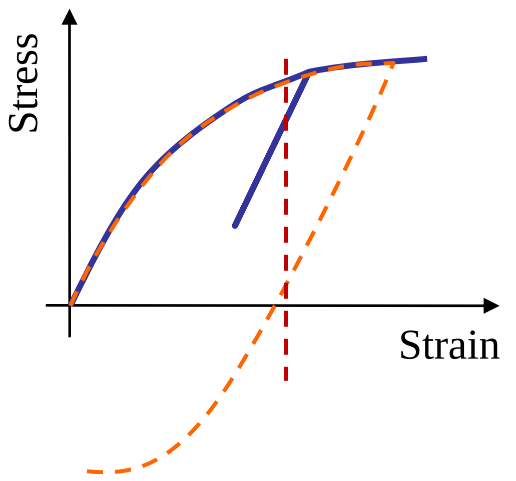
- Neural networks
  - Theoretically generic
    - Material parameters
    - Rate dependency
    - Geometrical parameters
- Basic unit of a Neural Network
  - Neuron
    - Non-linear function on n_0 inputs u_k
    - Requires evaluation of weights w_k
    - Requires definition of activation function

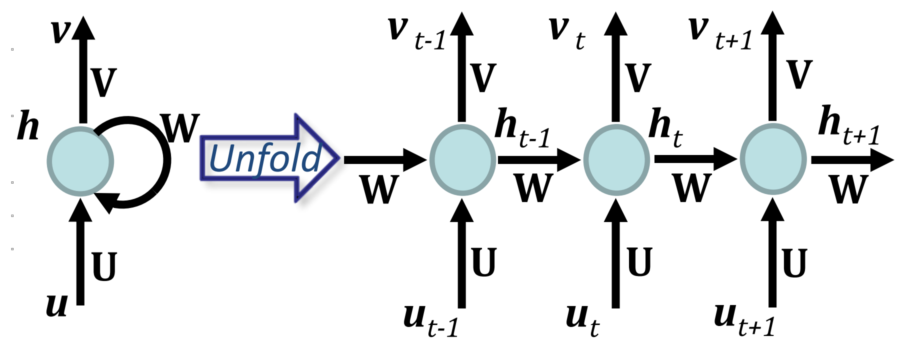


- Feed-Forward Neuron Network
  - Simplest architecture
  - Layers of neurons
    - Input layer
    - $N-1$ hidden layers
    - Output layers
  - Mapping $\Re^{n_0} \rightarrow \Re^{n_N}$: $\boldsymbol{v} = \boldsymbol{g}(\boldsymbol{u})$
  - Doesn't allow for history dependence

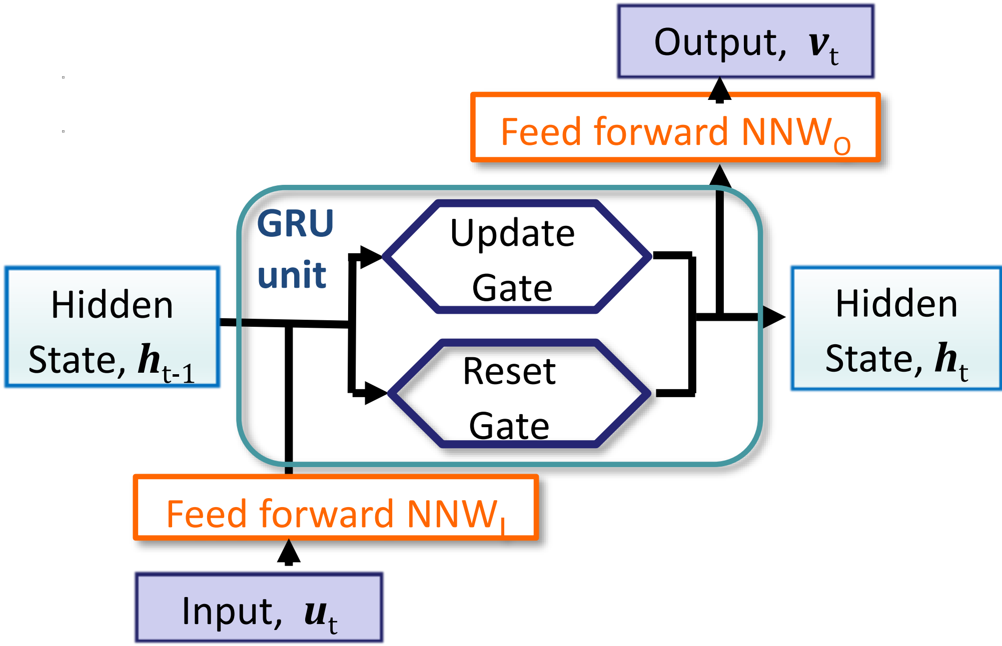


- Recurrent neural network
  - Allows a history dependent relation
    - Input $\boldsymbol{u}_t$
    - Output $\boldsymbol{v}_t = \boldsymbol{g}(\boldsymbol{u}_t, \boldsymbol{h}_{t-1})$
    - Internal variable $\boldsymbol{h}_t = \boldsymbol{g}(\boldsymbol{u}_t, \boldsymbol{h}_{t-1})$
  - Weights matrices $\mathbf{U}, \mathbf{W}, \mathbf{V}$
    - Trained using sequences
      - Inputs $\boldsymbol{u}_{t-n}^{(p)}, \ldots, \boldsymbol{u}_{t}^{(p)}$
      - Output $\boldsymbol{v}_{t-n}^{(p)}, \ldots, \boldsymbol{v}_{t}^{(p)}$





- Recurrent neural network design
  - 1 Gated Recurrent Unit (GRU)
    - Rest gate: select past information to be forgotten
    - Update gate: select past information to be passed along
    - Hidden variables account for history dependence
  - 2 feed-forward NNWs
    - NNW_I to treat inputs $\boldsymbol{u_t}$
    - NNW_O to produce outputs $\boldsymbol{v_t}$

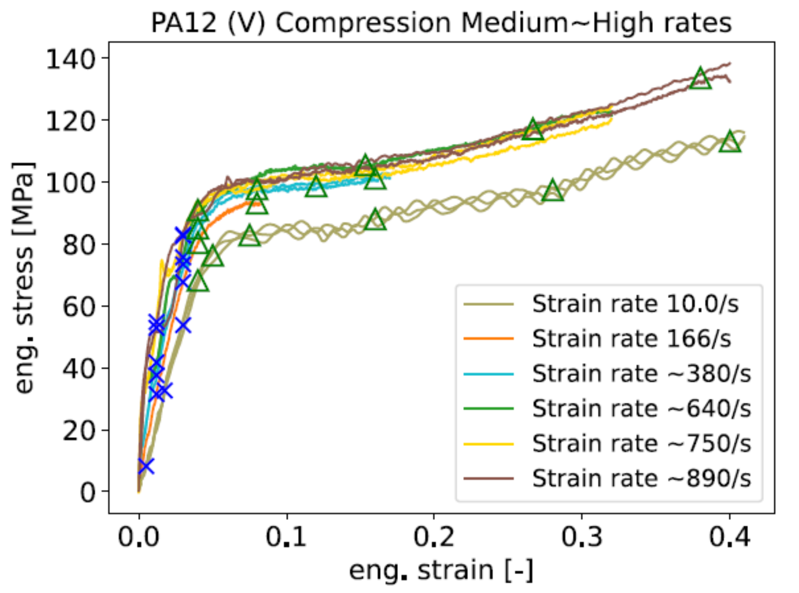


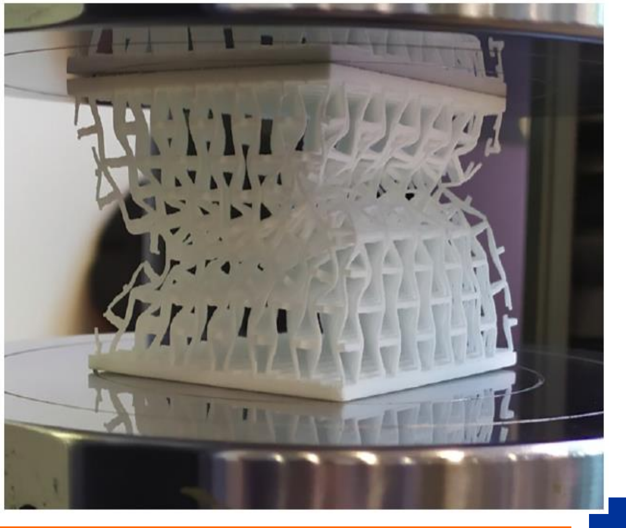
Recurrent Neural Network accelerated multi-scale simulations

- Identification of inputs & outputs of the training dataset
- Generation of training & testing datasets
- Training of the meso-scale surrogate
- Validation of the meso-scale surrogate
  - Against testing data
  - Against FE2 simulations
  - Against experimental tests

Identification of inputs & outputs of the training dataset

- Focus is on lattice based meta materials:
  - Polymeric base material – Polyamide 12 (PA12):
    - Visco elastic – visco plastic constitutive behavior
    - Stress - Strain relation is not a one-to-one mapping which must be accounted for
    - Stress – Stress relation is rate-dependent which must be tracked
  - Topology of the lattices
    - Different lattices display different mechanical response e.g., auxetic behavior
    - Different volume fractions of the unit lattices result in different mechanical response





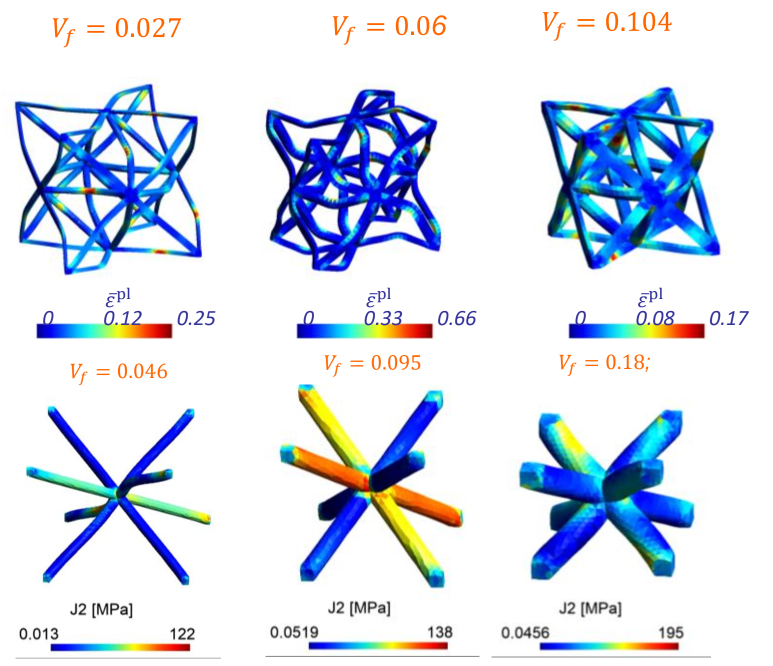
Identification of inputs & outputs of the training dataset

- Hence the input parameters of the dataset must be rich in:
  - Rate dependent strain (history): $\mathbf{E}_{\mathrm{M}}, \dot{\mathbf{E}}_{\mathrm{M}}$
  - Geometrical parameters: $\boldsymbol{\varphi}_{\mathrm{m}}$

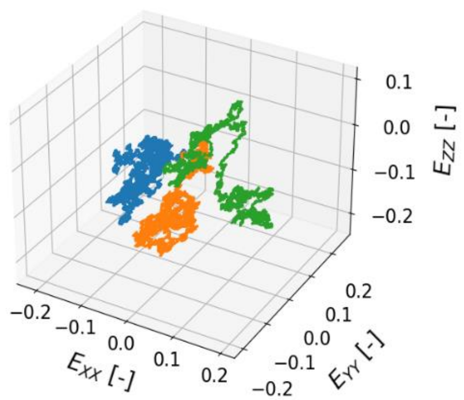
- Such that the output parameters of the dataset span the prediction space
  - Homogenized stress (history): $\boldsymbol{S}_{\mathrm{M}}$

Identification of inputs & outputs of the training dataset

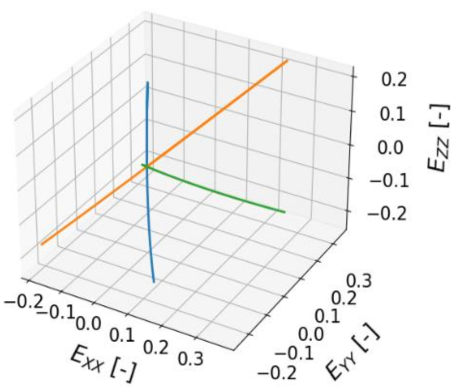
- Dataset Composition:
  - Input:
    - Random rate dependent strain (history): $\mathbf{E}_{\mathrm{M}}, \dot{\mathbf{E}}_{\mathrm{M}}$
      - Random Walk Strain Paths
      - Cyclic Strain Paths
    - Random geometrical parameters: $\boldsymbol{\varphi}_{\mathrm{m}}$
      - Type of unit lattice cell
      - Volume fraction specified as the radius of unit lattice strut



Unit lattices in increasing order of volume fraction subjected to random walk & cyclic strain paths



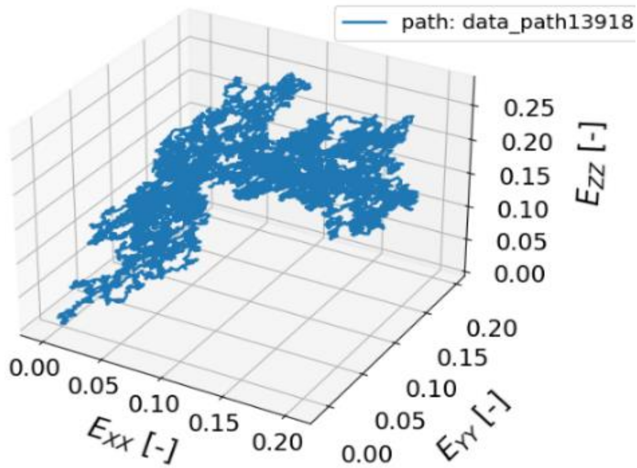
Random walk strain paths



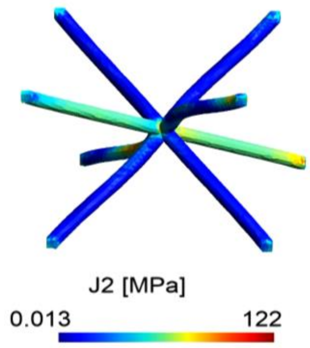
Cyclic strain paths

Identification of inputs & outputs of the training dataset

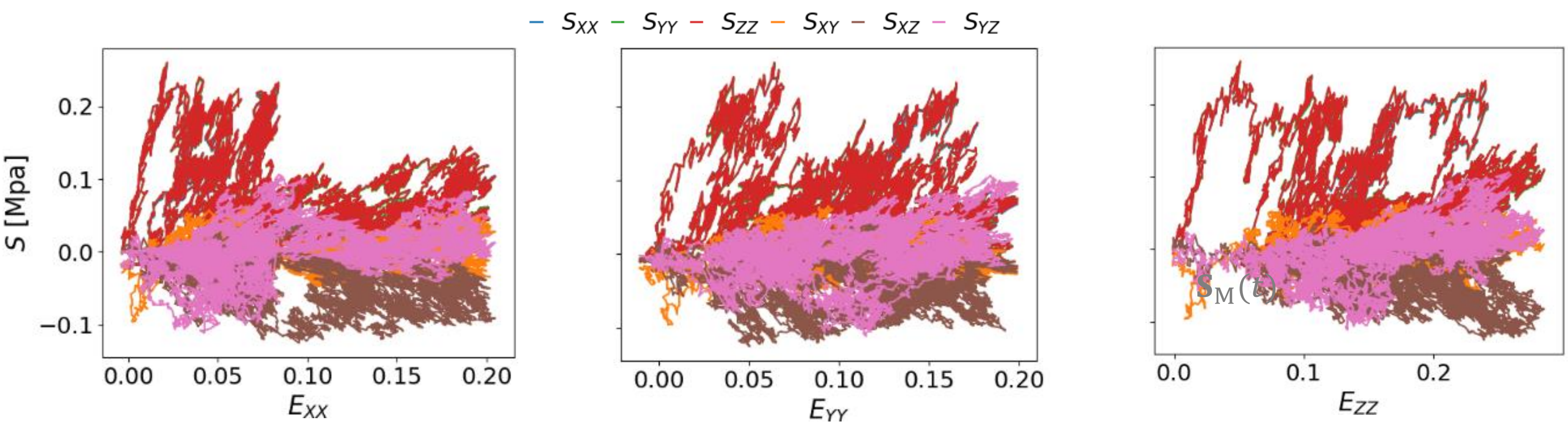
- Dataset Composition:
  - Input:
    - Random rate dependent strain (history): $\mathbf{E}_{\mathrm{M}}, \dot{\mathbf{E}}_{\mathrm{M}}$
    - Random geometrical parameters: $\boldsymbol{\varphi}_{\mathrm{m}}$
  - Output:
    - Homogenized stress (history): $\mathbf{S}_{\mathrm{M}}$



Strain Path in volumetric Space



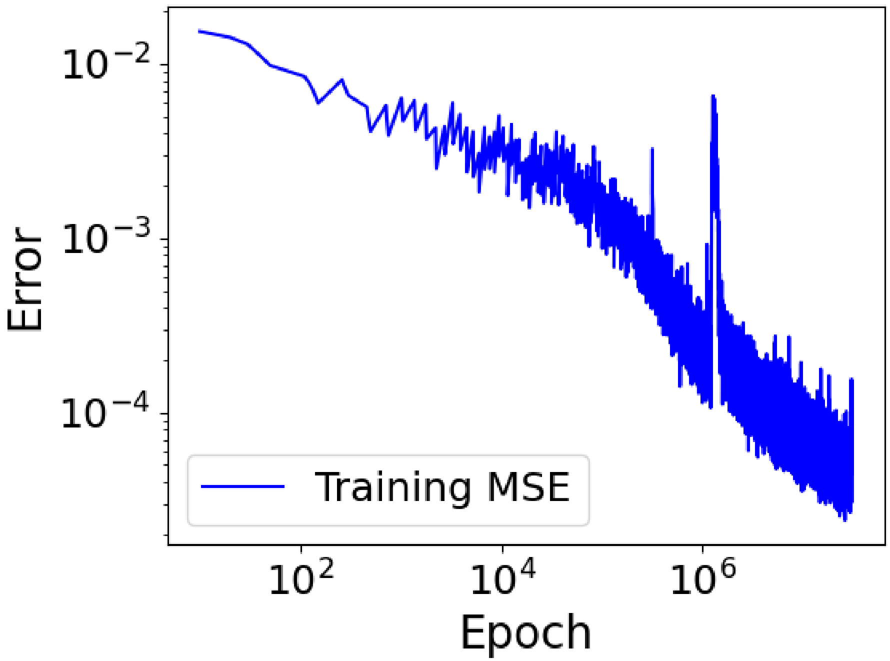
Unit lattice cell subjected to strain path for generating stresses

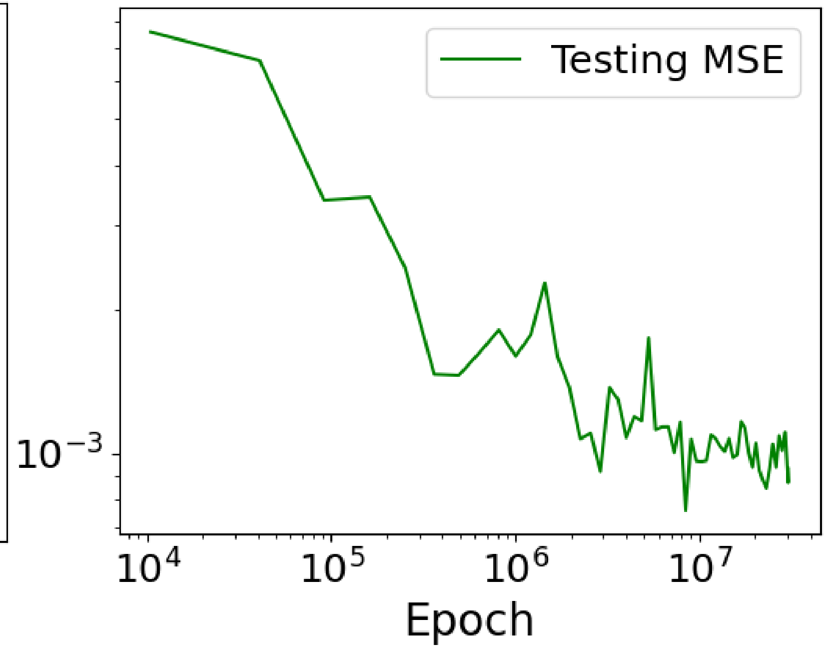


Homogenized stress plotted against (volumetric) strain path

Training of mesoscale surrogate

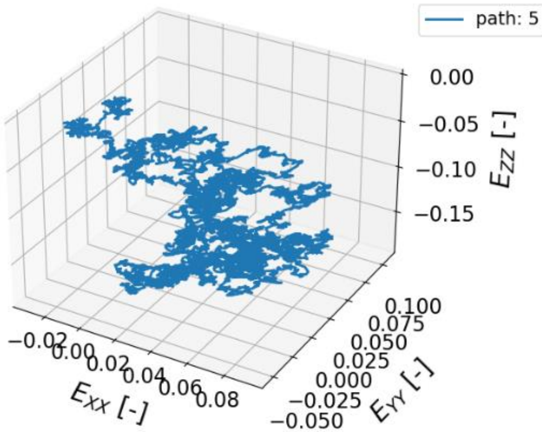
- Mean square error (MSE) evolution during training
  - Computed on training and testing data (Excluded from training data - Pristine)



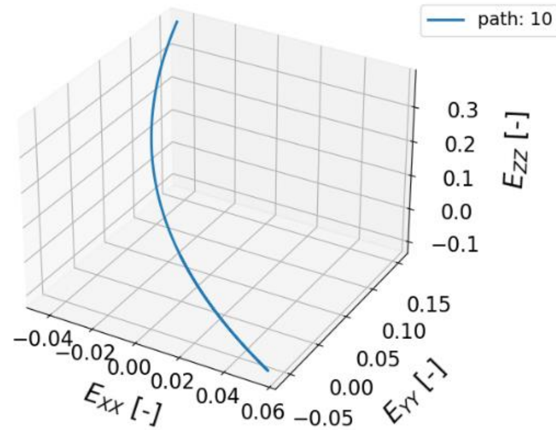


Validation of the recurrent neural network

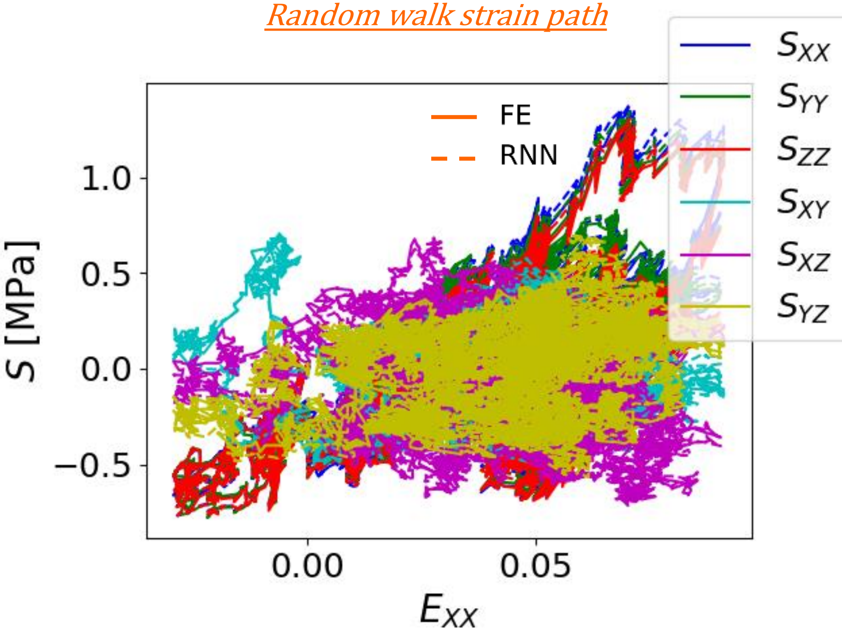
- Performance evaluation on testing data [Actual vs RNN prediction]



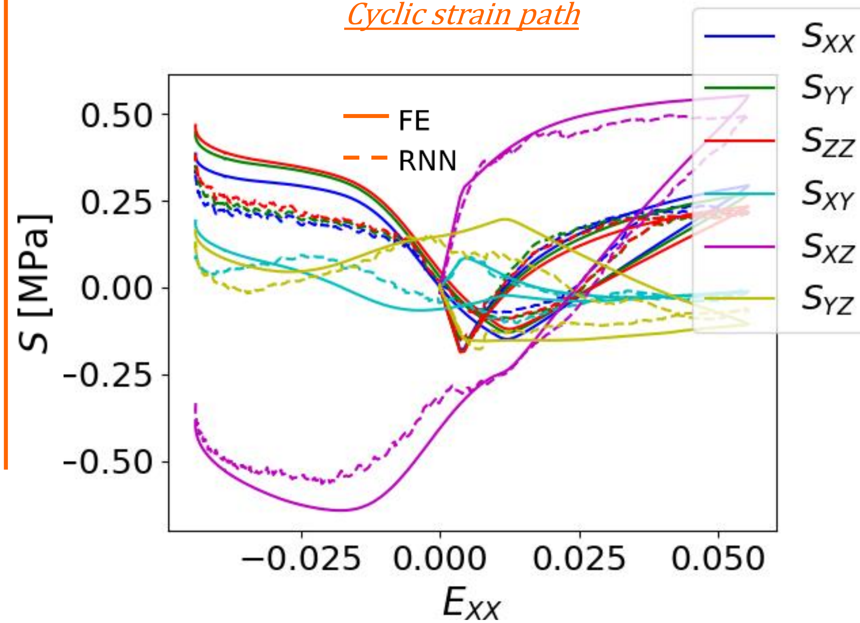
Random walk strain path



Cyclic strain path



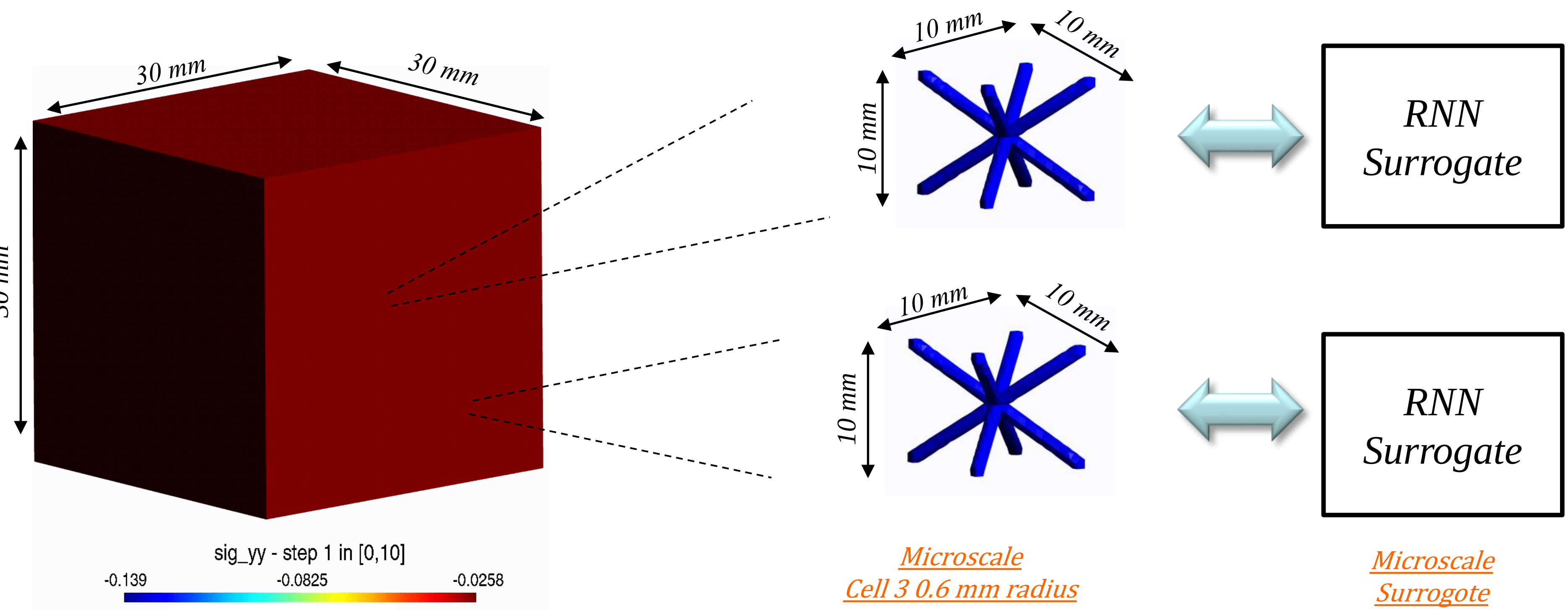
FE (actual solution) vs RNN prediction



FE (actual solution) vs RNN prediction

Testing of mesoscale surrogate

- Performance evaluation on multiscale (FE^2) simulations.
  - Establishing control for comparison using uniaxial compression test
  - Substituting microscale FE resolution by RNN surrogate in the uniaxial compression test



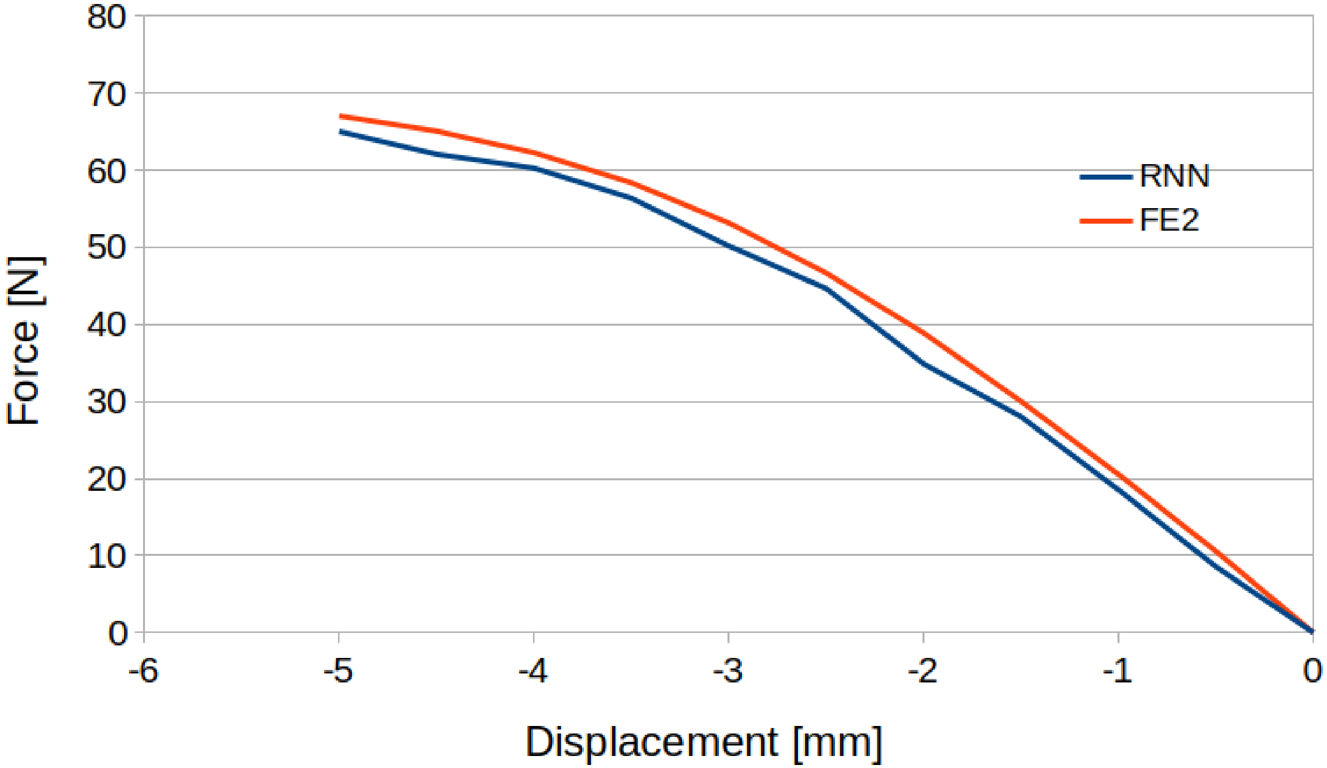
Macroscale
Single Element

Microscale
Cell 3 0.6 mm radius
Discretized SVEs

Microscale
Surrogote

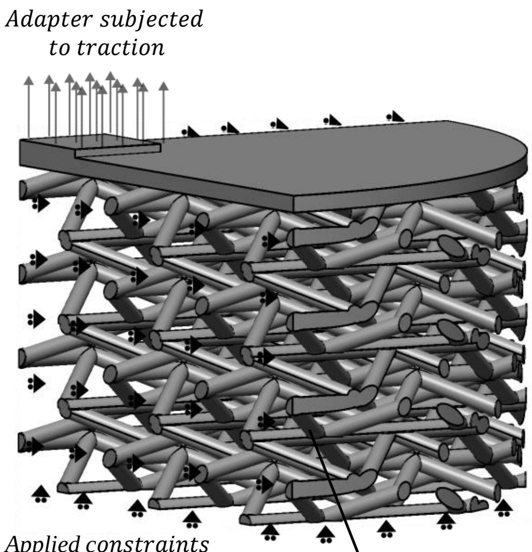
Testing of mesoscale surrogate

- Comparison between Multiscale (FE2) and RNN surrogate predictions.
  - Uni-axial compression test

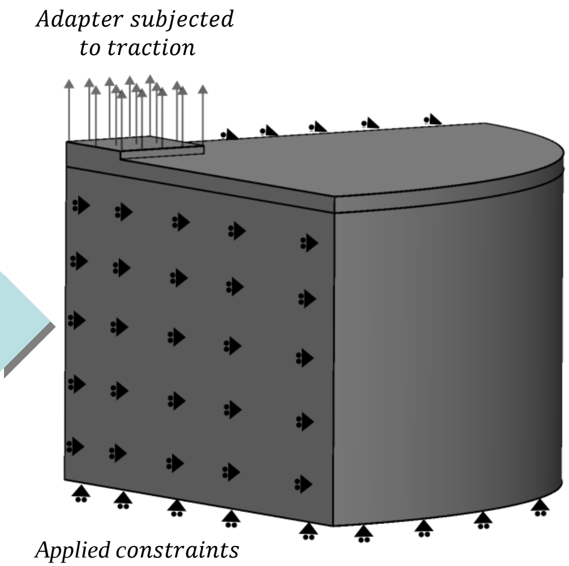


Testing of mesoscale surrogate

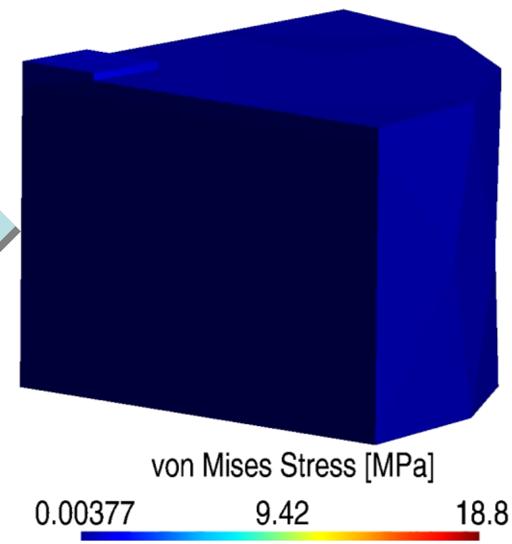
- Validation against experimental data
  - ¼ sample of a cylinder constituting of a repeated unit lattices subjected to a tensile force



Experimental Setup



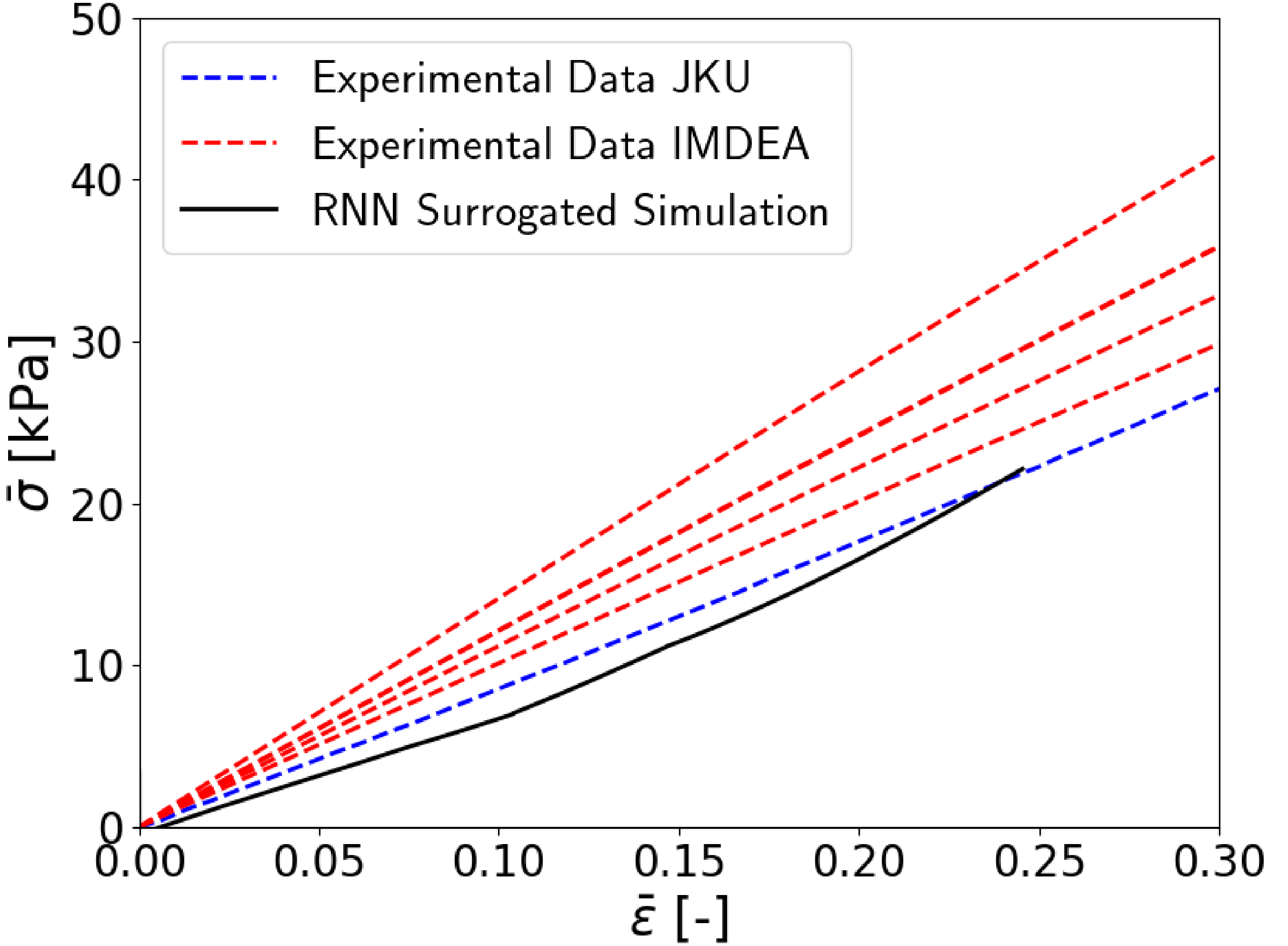
Equivalent Multiscale Setup



Simulation using RNN surrogate at the mesoscale

Testing of mesoscale surrogate

- Validation against experimental data
  - ¼ sample of a cylinder constituting of a repeated unit lattices subjected to a tensile force



- Conclusions
  - Neural Network based surrogates can be employed to accelerate multiscale simulations, this approach reduces the FE2 complexity and enables simulations within reasonable time and resources
  - Recurrent Neural Network were investigated for accelerated multi-scale simulations involving lattice based meta-materials
    - Results and validations indicate that RNN can predict scenarios that involve
      - Rate dependent dissipative mesoscale response
      - Geometrically variant mesoscale response
  - Training an effective surrogate requires careful identification of Input-Output parameters such that the surrogate is sensitive to the desired predictions
  - Time and resource gains observed in the online phase of the simulation are dependent on the training done during the offline phase.
  - Predictions sought outside the range of the training dataset will severely reduce the quality of the results, however additional training with new data can be performed to increase the range and applicability of the surrogates.

Public access repository

- Public Access Repository
  - https://gitlab.uliege.be/moammm/moammmPublic/syntheticdata/sveresponses

main sveresponses History Find file Clone

README | Creative Commons Attribution 4.0 International

Name	Last commit
Cell3	[HOT-FIX] - Duplicate folders
Cell6	[DataPath Update 041223]
Cell9	[Feature, Refractor] - Post Processing for HO DataPaths
Scripts	[DataPath Update 041223]
LICENSE	clean history
README.md	Merge branch 'dev_mm' into 'main'

sveResponses

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This repository contains:

- Data generated by simulation of synthetic volume elements (SVE) constructed using lattices under investigation in MOAMMM project.
- Code to visualize and generate further SVE data.
- Recurrent Neural Network (RNN) based surrogate models, trained on the SVE data.
- Code to train surrogate model and visualize its predictions against the testing data.