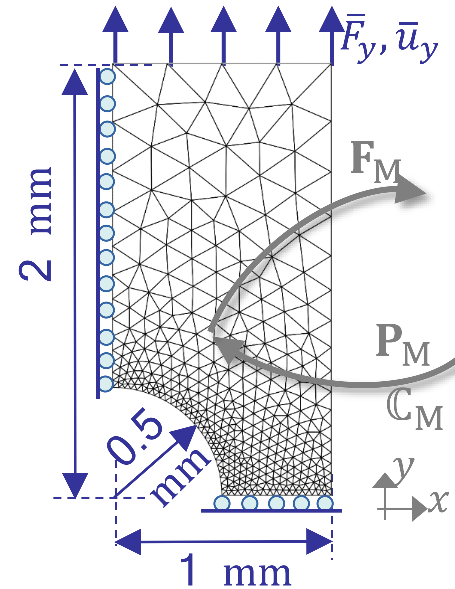
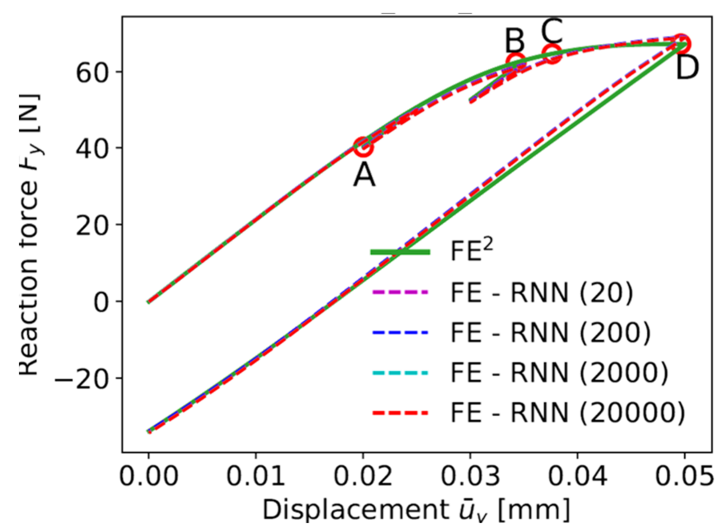




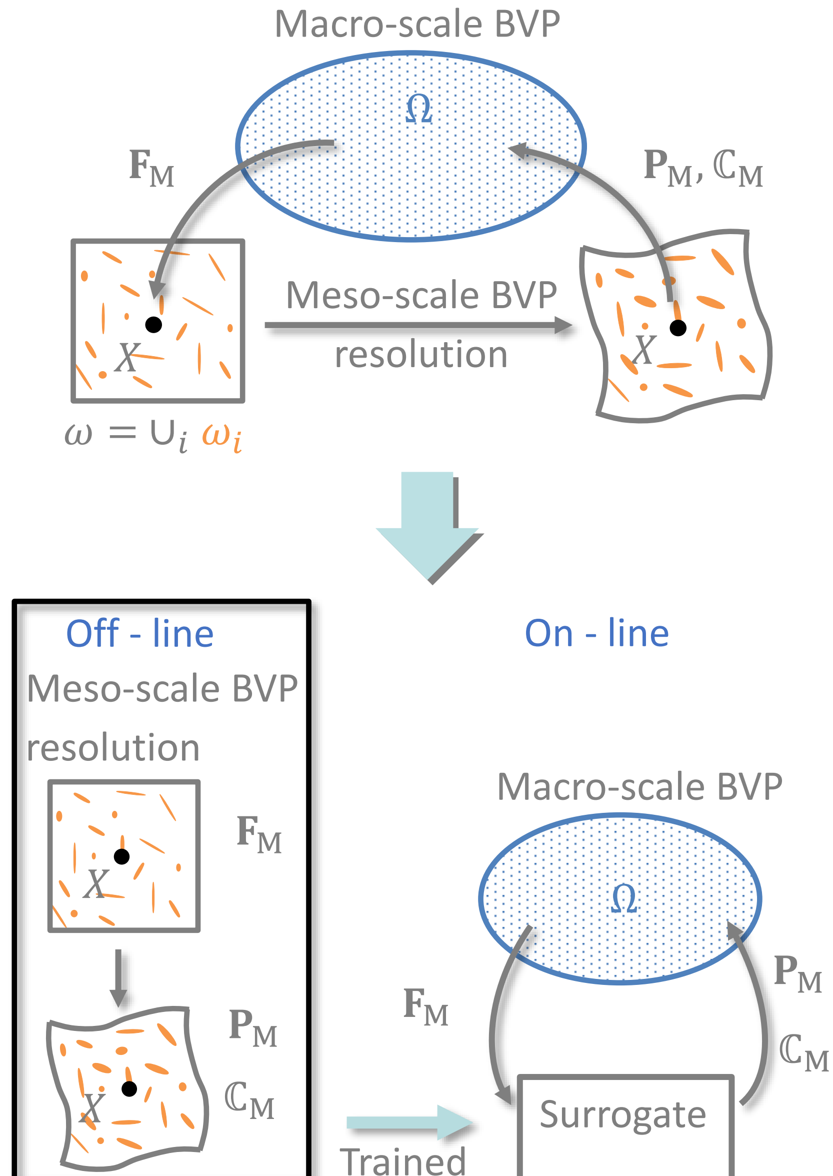
Self-Consistency Reinforced Recurrent Neural Network acting as surrogate of highly-nonlinear composite responses in multi-scale simulations

Wu Ling, Mohib Mustafa, Noels Ludovic

This project has received funding from the European Union's Horizon Europe Framework Programme under grant agreement No. 101056682 for the project ''DIgital DEsign strategies to certify and mAnufacture Robust cOmposite sTructures (DIDEAROT)''. The contents of this publication are the sole responsibility of ULiege and do not necessarily reflect the opinion of the European Union. Neither the European Union nor the granting authority can be held responsible for them

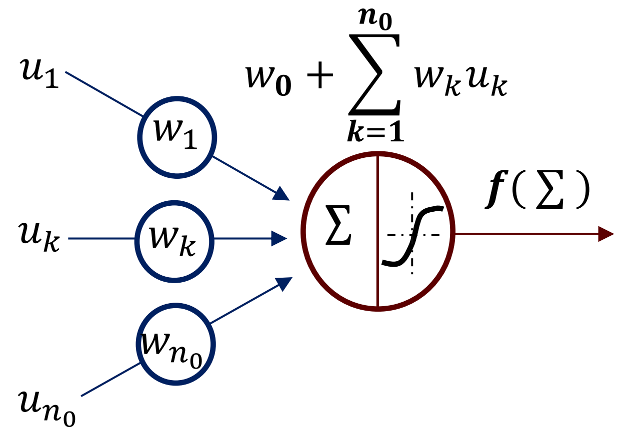
Self-Consistent Recurrent Neural Network for multi-scale simulations

- Introduction to non-linear multi-scale simulations
  - FE multi-scale simulations
    - Problems to be solved at two scales
    - Requires Newton-Raphson iterations at both scales
  - Use of surrogate models
    - Train a meso-scale surrogate model (off-line)
      - Requires extensive data
      - Obtained from RVE simulations
    - Use the trained surrogate model during analyses (on-line)
      - Surrogate acts as a homogenised constitutive law
      - Expected speed-up of several orders

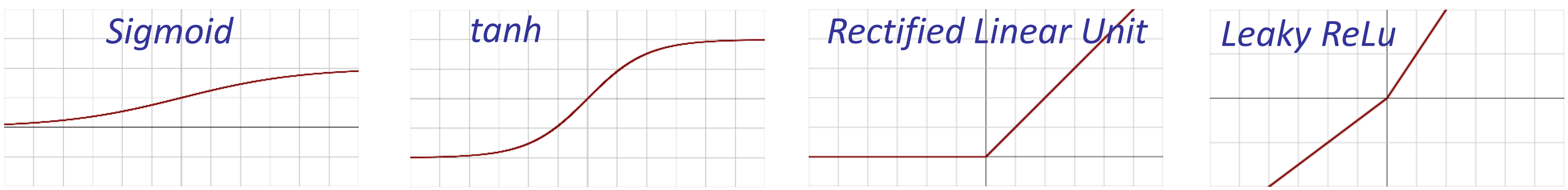


Self-Consistent Recurrent Neural Network for multi-scale simulations

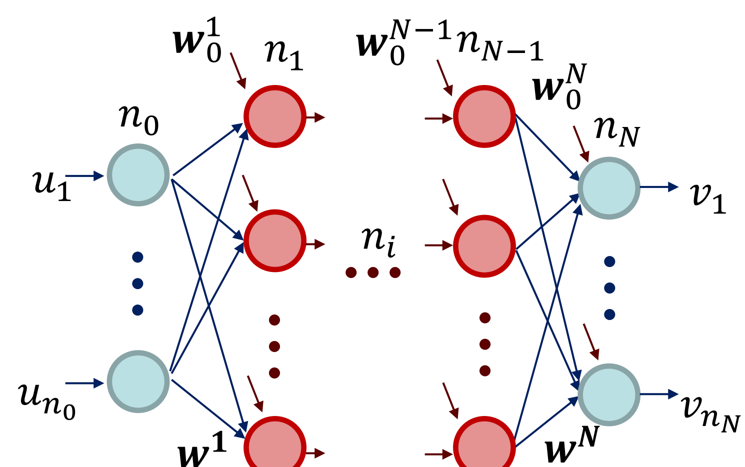
- Definition of the surrogate model
  - Artificial neuron
    - Non-linear function on n_0 inputs u_k
    - Requires evaluation of weights w_k
    - Requires definition of activation function f



  - Activation functions f

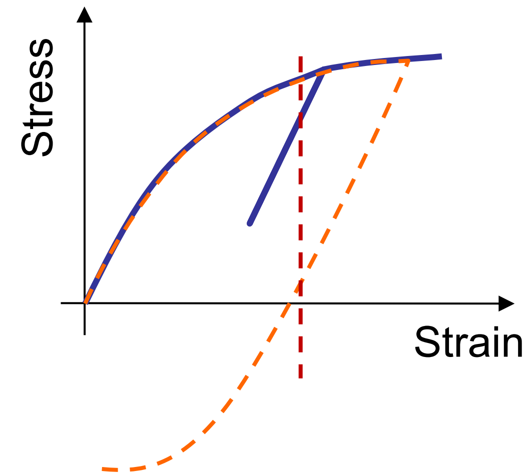


  - Feed-Forward Neuron Network
    - Simplest architecture
    - Layers of neurons
      - Input layer
      - $N-1$ hidden layers
      - Output layers
    - Mapping $\Re^{n_0} \rightarrow \Re^{n_N}: \boldsymbol{v} = \boldsymbol{g}(\boldsymbol{u})$



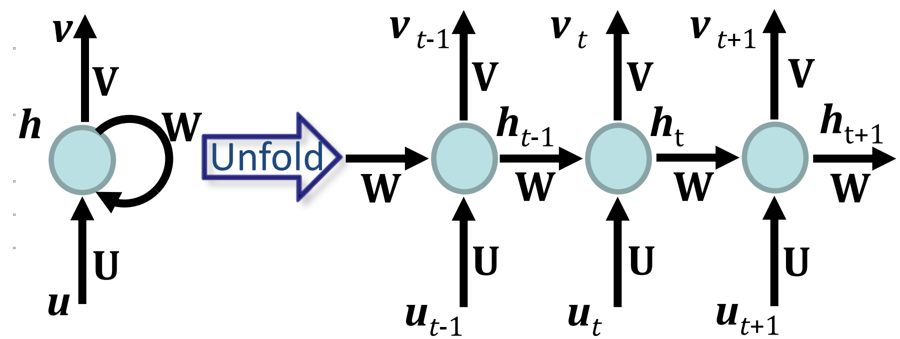
Self-Consistent Recurrent Neural Network for multi-scale simulations

- Input / output definition
  - Input: Strain (history): $\mathbf{F}_{\mathrm{M}}$
  - Output: Stress (history): $\mathbf{P}_{\mathrm{M}}$



- Elasto-plastic material behaviour
  - No bijective strain-stress relation
    - Feed-forward NNW cannot be used
    - History should be accounted for

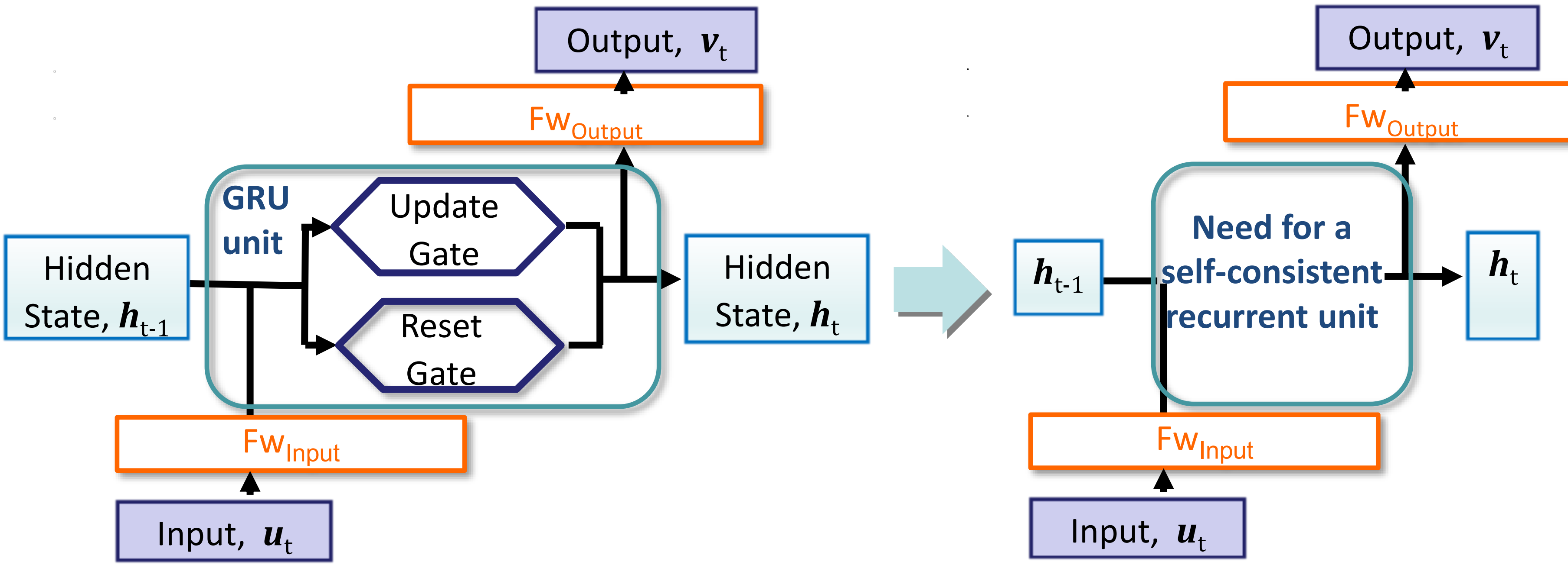
- Recurrent neural network
  - Allows a history dependent relation
    - Input: sequence $\boldsymbol{u}_t$
    - Output: sequence $\boldsymbol{v}_t = \boldsymbol{g}(\boldsymbol{u}_t, \boldsymbol{h}_{t-1})$
    - Internal variable $\boldsymbol{h}_t = \boldsymbol{g}(\boldsymbol{u}_t, \boldsymbol{h}_{t-1})$
  - Existing recurrent units
    - Oscillations / loss of accuracy can appear with GRU, LSTM* (both developed for Nature Language Processing)
    - One needs to enforce self-consistency*
    - Need to replace the GRU/LSTM unit



*Colin Bonatti, Dirk Mohr, On the importance of self-consistency in recurrent neural network models representing elasto-plastic solids, Journal of the Mechanics and Physics of Solids, 158, 2022, 104697, https://doi.org/10.1016/j.jmps.2021.104697.

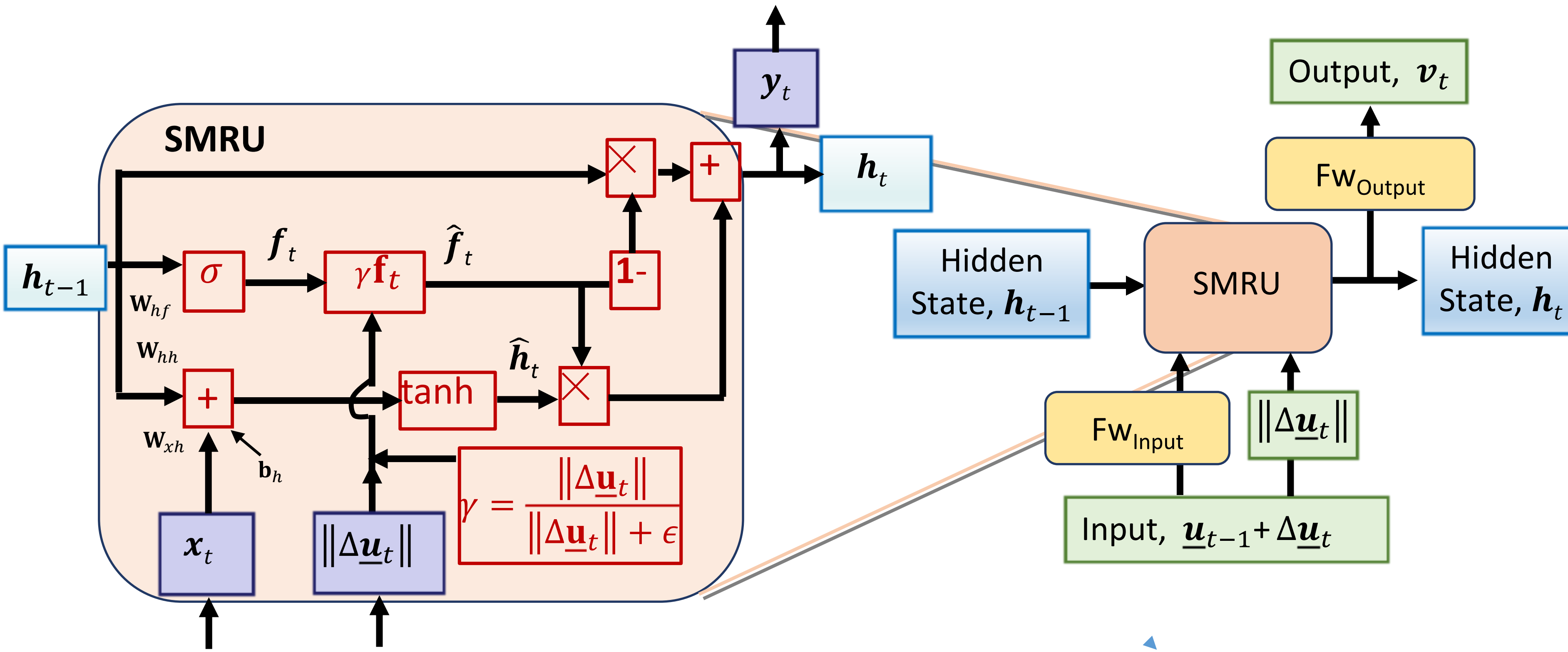
Self-Consistent Recurrent Neural Network for multi-scale simulations

- Self-Consistency reinforcement through ad hoc recurrent unit/cell
  - SC-cell originally to surrogate a constitutive model
  - Can we develop easy and fast to train surrogate for RVE responses?



Self-Consistent Recurrent Neural Network for multi-scale simulations

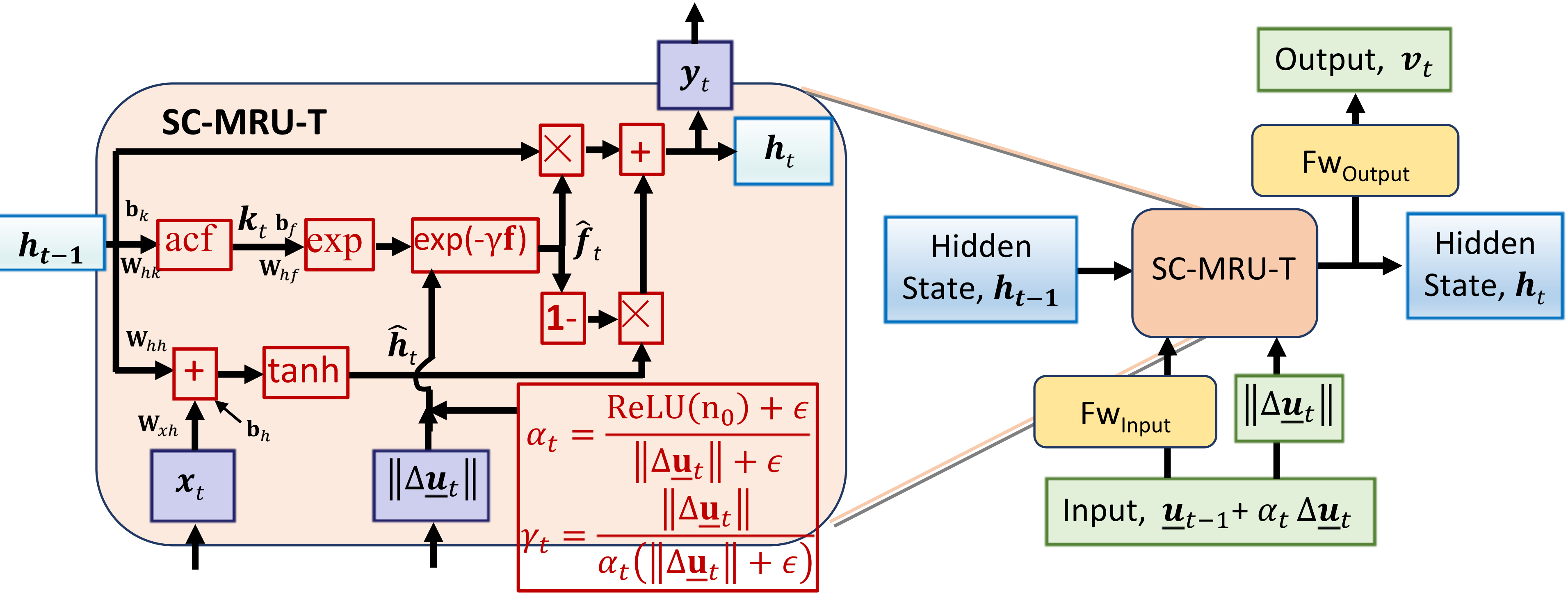
- New cell 1: New simplified recurrent unit: Simplified Minimal Recurrent Unit



- The **total form of input variable** as well as **increment norm** $\|\Delta\boldsymbol{u}_t\|$ (like SC-LMSC)
- **Self-consistency weakly enforced**
  - Using norm of $\|\Delta\boldsymbol{u}_t\|$ and
  - Data augmentation during training (i.e. subdividing randomly increments in training data)

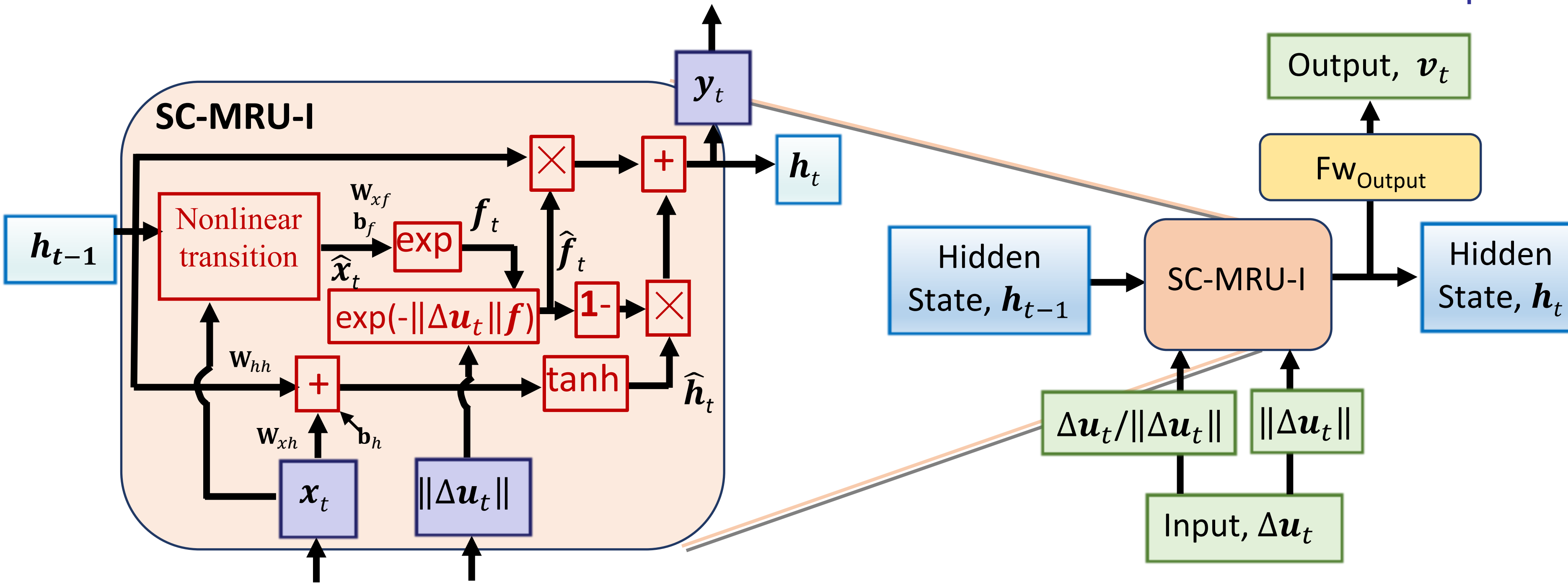
Self-Consistent Recurrent Neural Network for multi-scale simulations

- New cell 2: Self-Consistent Minimal Recurrent Unit with Total form of inputs

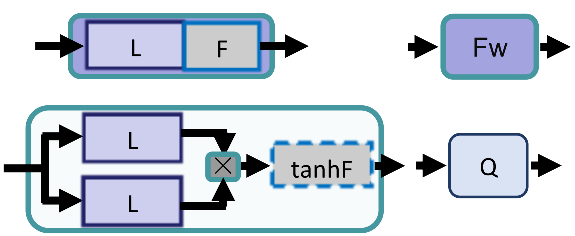


- The **total form of input variable** as well as **increment norm** $\|\Delta\boldsymbol{u}_t\|$ (like SC-LMSC)
  - Use as input $\underline{\boldsymbol{u}}_{t-1}+\alpha_t\,\Delta\underline{\boldsymbol{u}}_t$ (n_0 is a learnable parameter)
  - acf is the same activation function as in Fw$_{\text{input}}$
- **Self-consistency enforced**
  - Double exponential function $\boldsymbol{f_t} = \exp[\boldsymbol{W_f k_t} + \boldsymbol{b_f}] > \boldsymbol{0}$ & ratio $\hat{\boldsymbol{f}}_{\boldsymbol{t}} = \exp[-\gamma(\|\Delta\boldsymbol{u}_t\|)\,\boldsymbol{f_t}] \in [\boldsymbol{0}, \boldsymbol{1}]$
  - Hidden variables $\boldsymbol{h_t}$ is an element-wise interpolation (ratio $\hat{\boldsymbol{f}}_{\boldsymbol{t}}$ dependent on the norm of $\|\Delta\boldsymbol{u}_t\|$) between previous value $\boldsymbol{h_{t-1}}$ and $\hat{\boldsymbol{h}}_{\boldsymbol{t}}$

- New cell 3: Self-Consistent Minimal Recurrent Unit with Incremental form of inputs

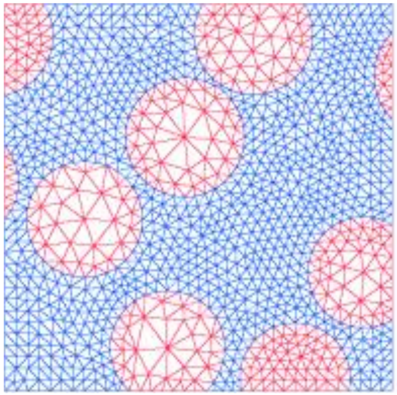
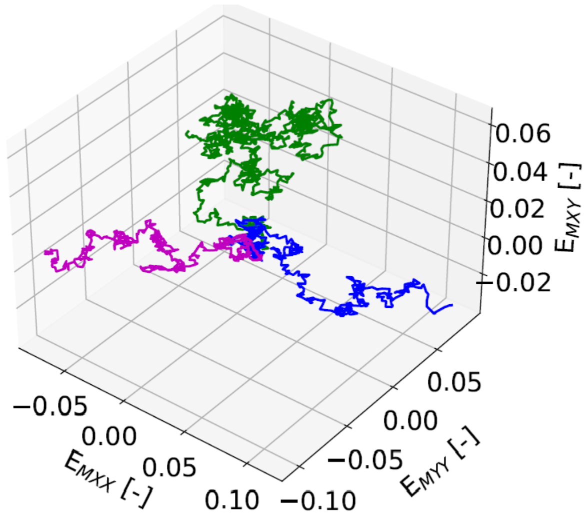


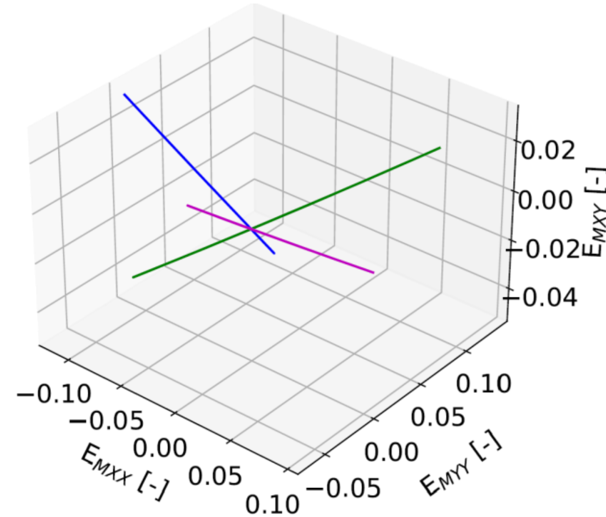
- The **incremental form of input variable** as well as **increment norm** $\|\Delta u_t\|$ (like LMSC)
  - Use as input $\Delta u_t/\|\Delta u_t\|$ and $\|\Delta u_t\|$
  - Non-linear transition blocks:



- **Self-consistency enforced**
  - Double exponential function $f_t = \exp[W_{xf}\hat{x}_t + b_f] > 0$ & ratio $\hat{f}_t = \exp[-(\|\Delta u_t\|)\, f_t] \in [0, 1]$
  - Hidden variables h_t is an element-wise interpolation (ratio $\hat{f}_t$) between previous value h_{t-1} and $\hat{h}_t$

- Training strategy
  - Elasto-plastic composite RVE

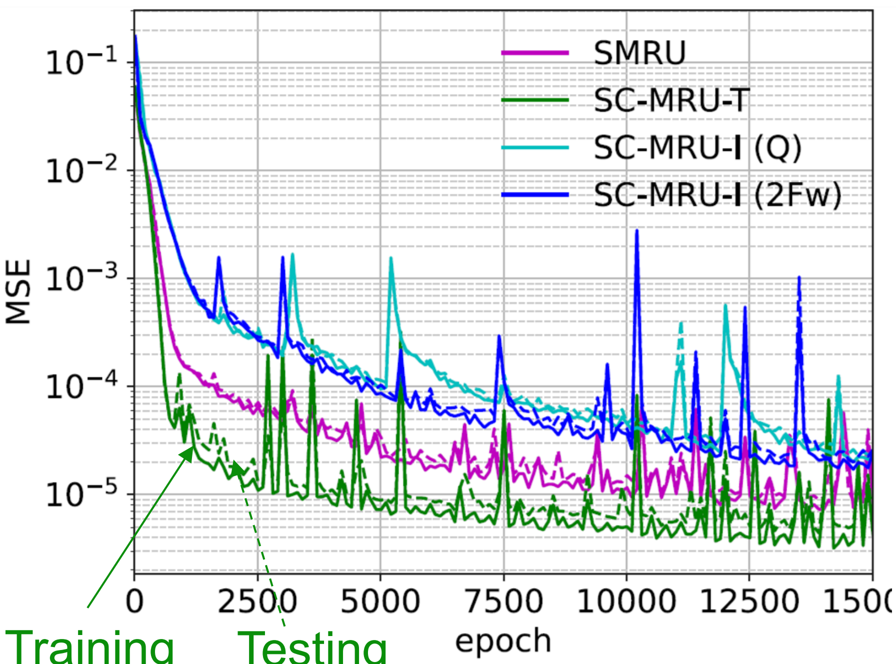


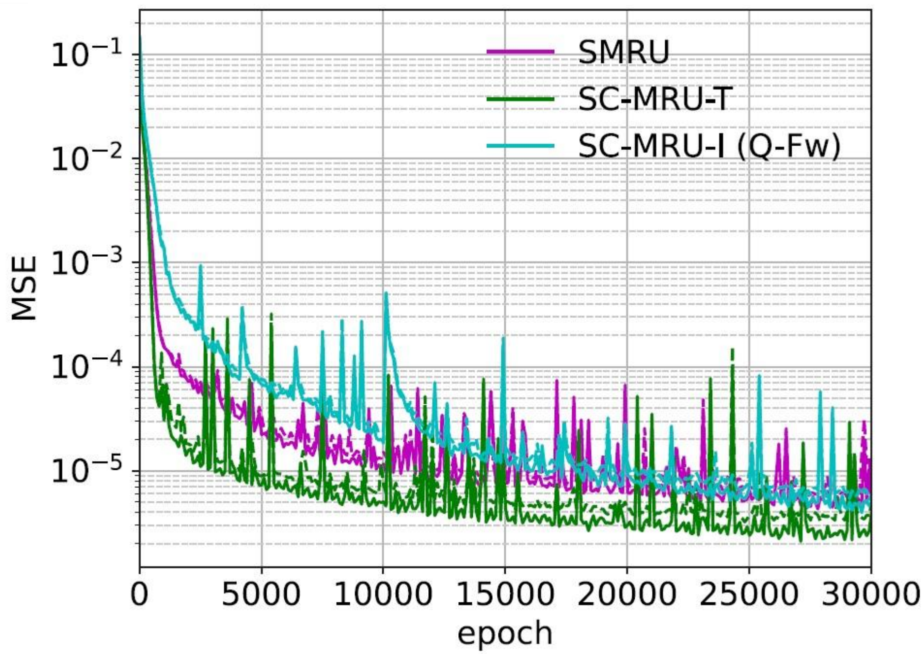
  - Training data
    - Should cover full range of possible loading histories
    - Use random walking strategy
    - Completed with random cyclic loading
    - Bounded by a hypercube of 12% deformation

Self-Consistent Recurrent Neural Network for multi-scale simulations

- Training stage
  - Learnable parameters for 120 hidden variables

Recurrent unit	SMRU	SC-MRU-T	SC-MRU-I		
Transition block	-	-	Q	Fw-Fw	Q-Fw
Learnable parameters	44 284	58 925	59 644	59 284	74 164

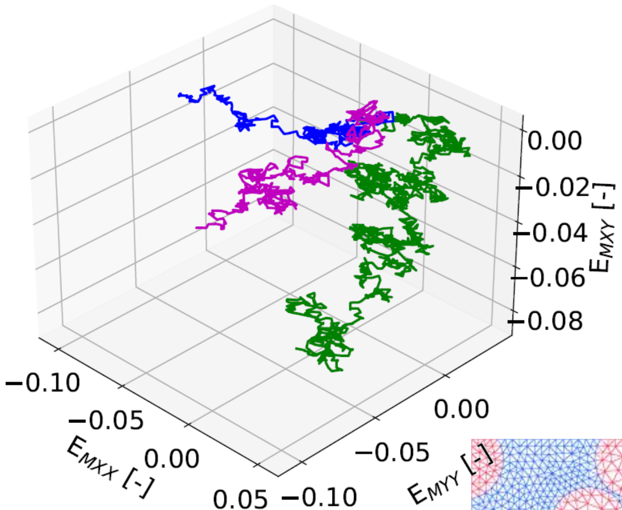


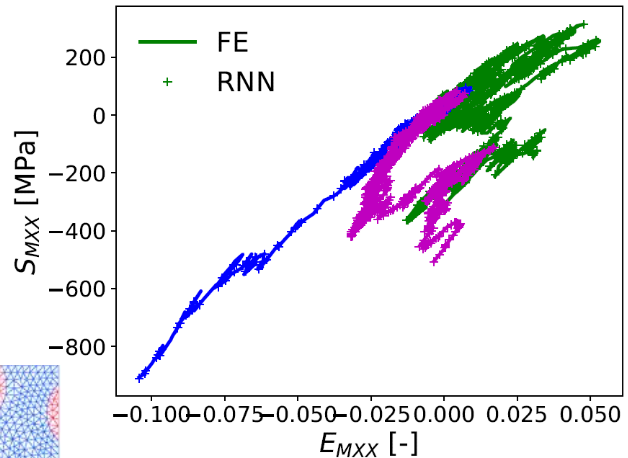


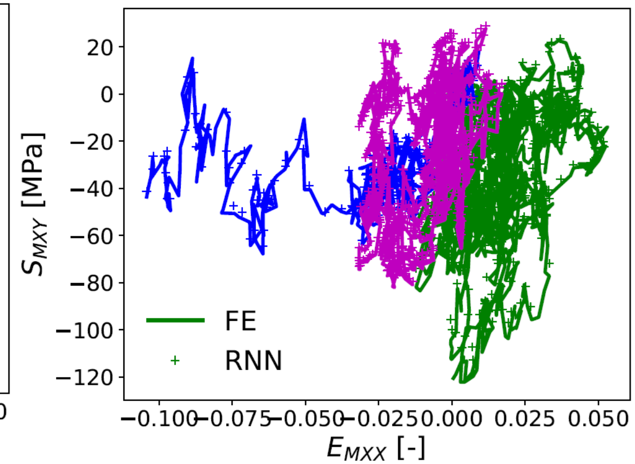
Self-Consistent Recurrent Neural Network for multi-scale simulations

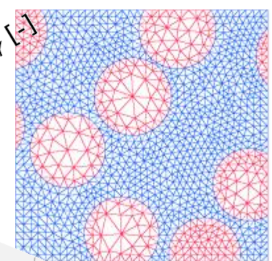
- SC-MRU-T: Testing data with inserted extra-points

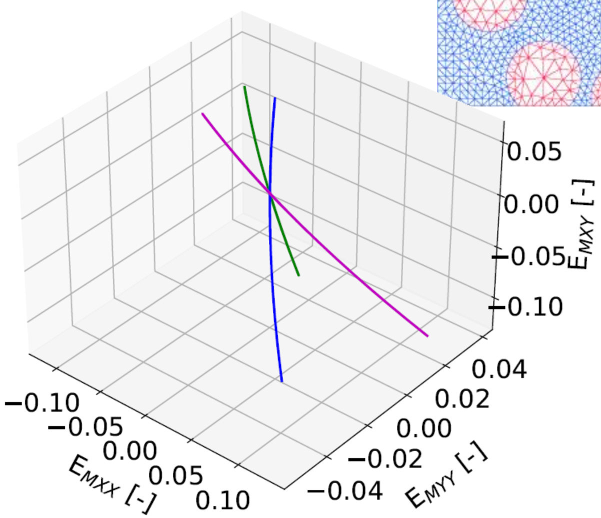
Maximum inserted data points is **5**, **20**, **60** in each loading step

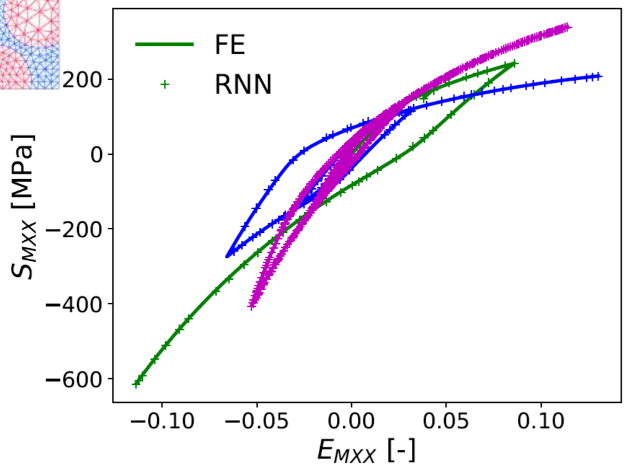


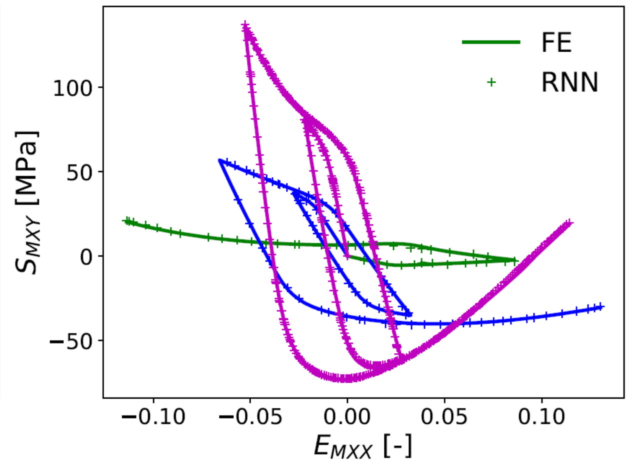






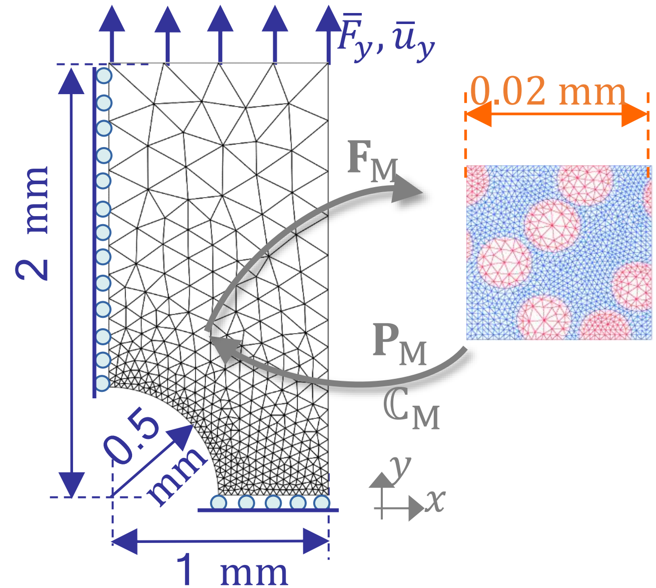


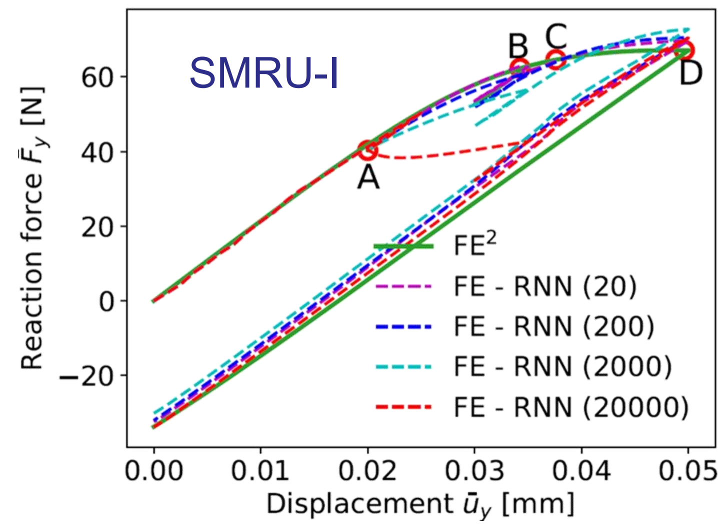


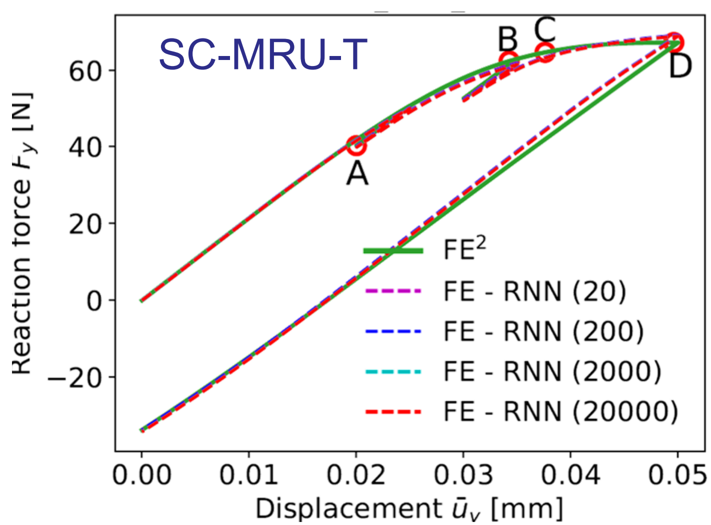


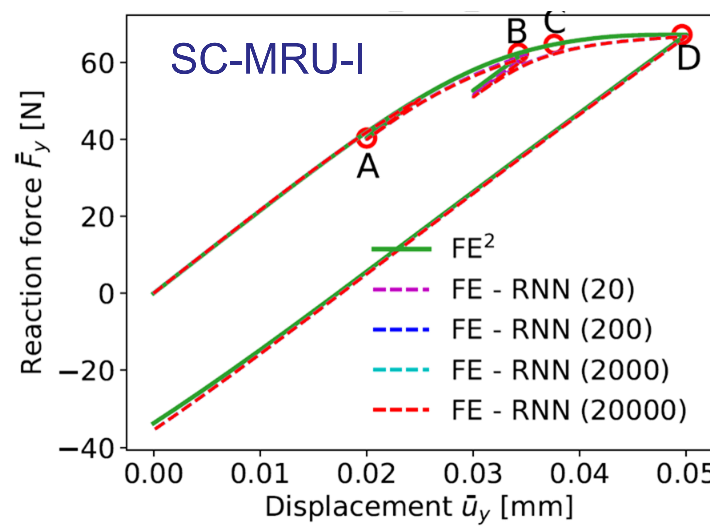
Self-Consistent Recurrent Neural Network for multi-scale simulations

- FE2 vs. FE-RNN: Change in the increment size (between points A&B)



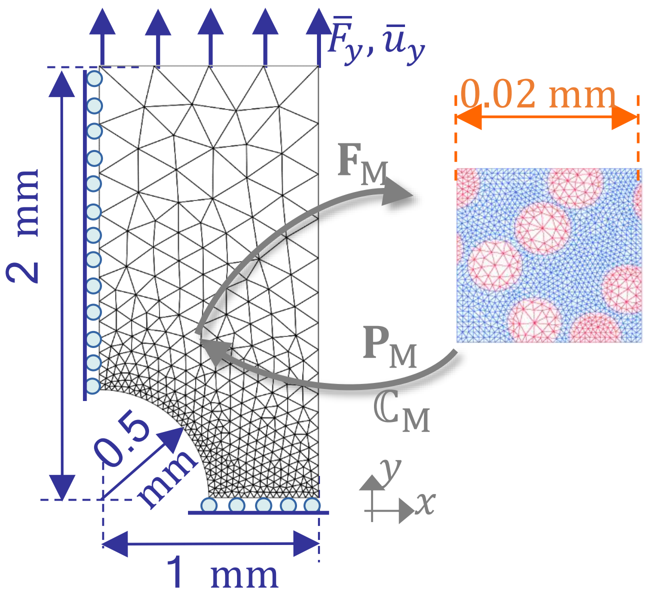






Self-Consistent Recurrent Neural Network for multi-scale simulations

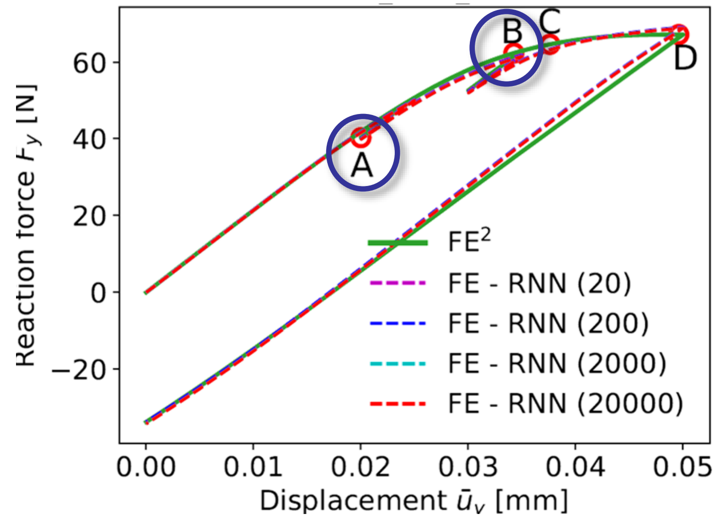
- FE2 vs. FE-RNN: Cost comparison



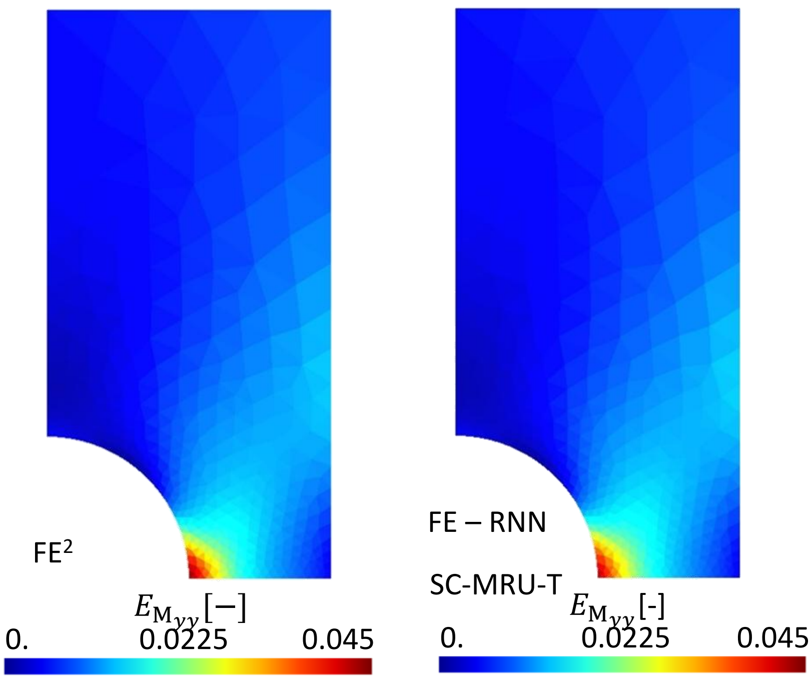
Off-line	FE^2	SMRU	SC-MRU-T	SC-MRU-I
Data generation	-	23500 h-cpu		
Training	-	< 10 h-cpu		
On-line	**FE^2**	**SMRU**	**SC-MRU-T**	**SC-MRU-I**
Simulation	18000 h-cpu	0.27 h-cpu	0.38 h-cpu	0.28 h-cpu

Self-Consistent Recurrent Neural Network for multi-scale simulations

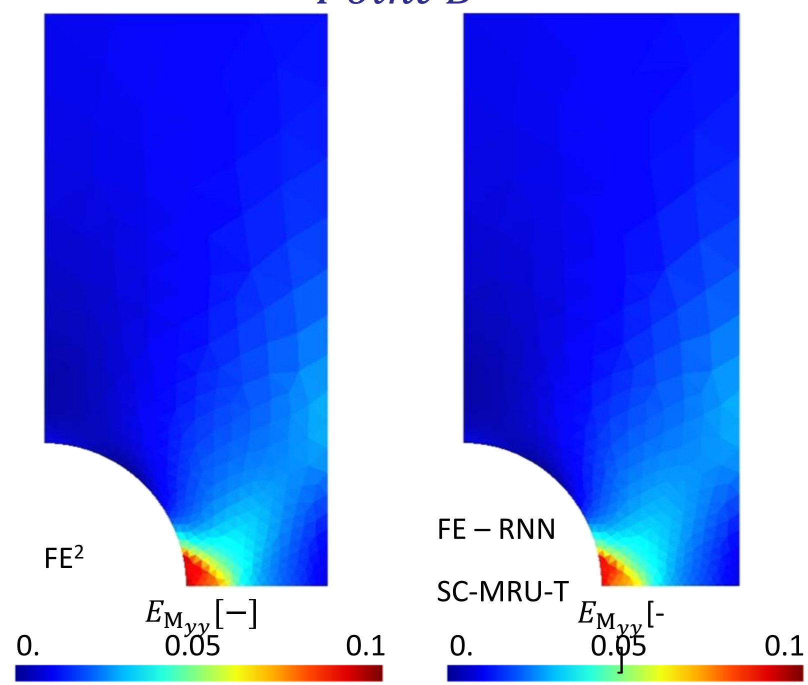
- FE2 vs. FE-RNN: Fields distribution



Point A

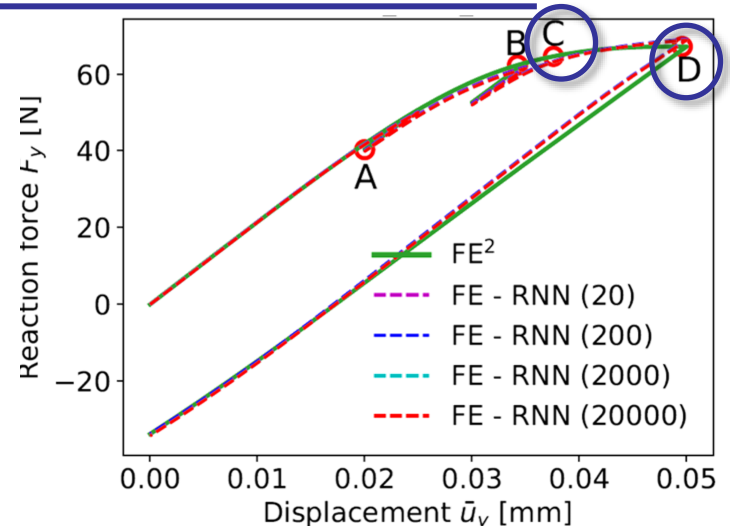


Point B

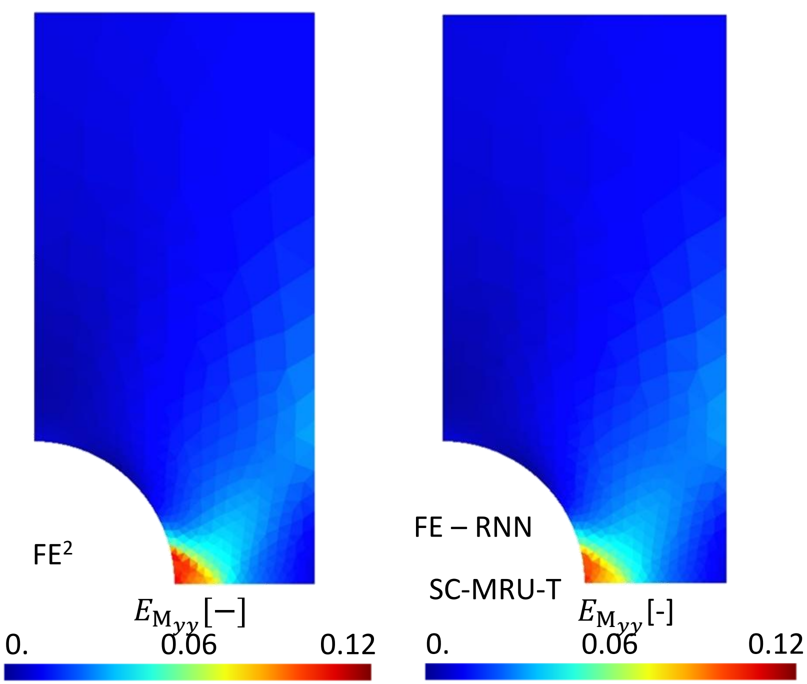


Self-Consistent Recurrent Neural Network for multi-scale simulations

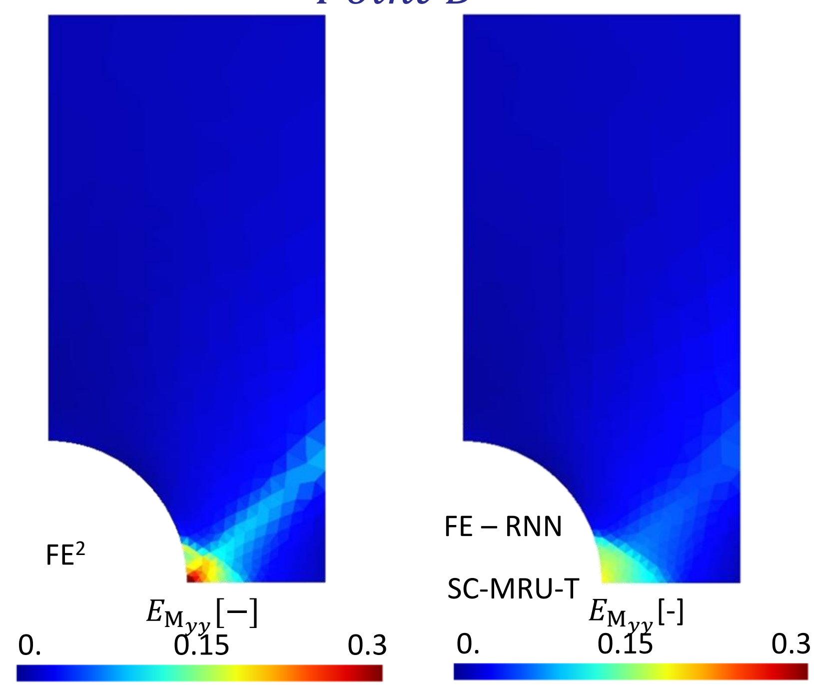
- FE2 vs. FE-RNN: Fields distribution



Point C

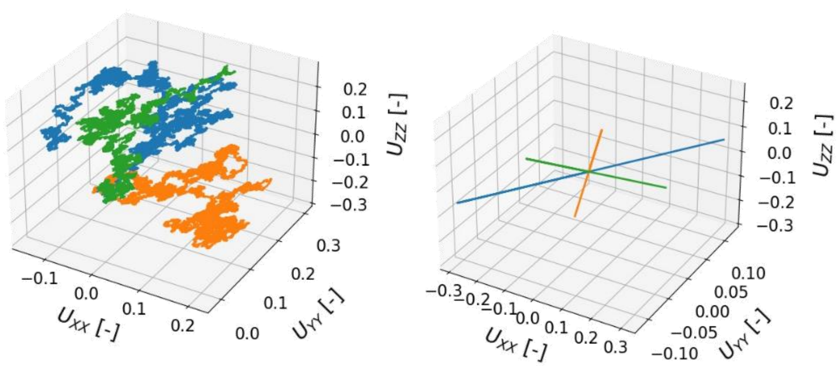


Point D

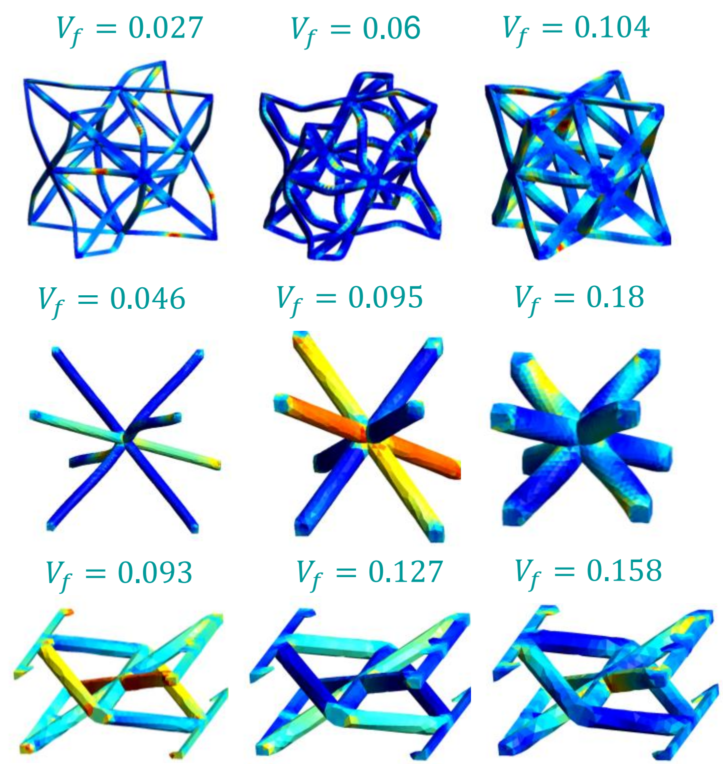


Self-Consistent Recurrent Neural Network for multi-scale simulations

- Self-Consistent model of VE-VP lattice cell response of arbitrary diameter value
  - Objective: Predict response of lattice cell
    - Complex visco-elastic-visco-plastic material response
    - Different strain-rate
    - Arbitrary geometrical parameters $\boldsymbol{\vartheta}_{\mathrm{geo}}$ (e.g. struts diametre)
  - Data
    - Inputs (depend on the surrogate)
      - $\mathbf{E}_{\mathbf{M}_t}$: strain sequence
      - Geometrical parameters $\boldsymbol{\vartheta}_{\mathrm{geo}}$
    - Outputs
    - $\mathbf{S}_{\mathbf{M}_t}$: stress sequence

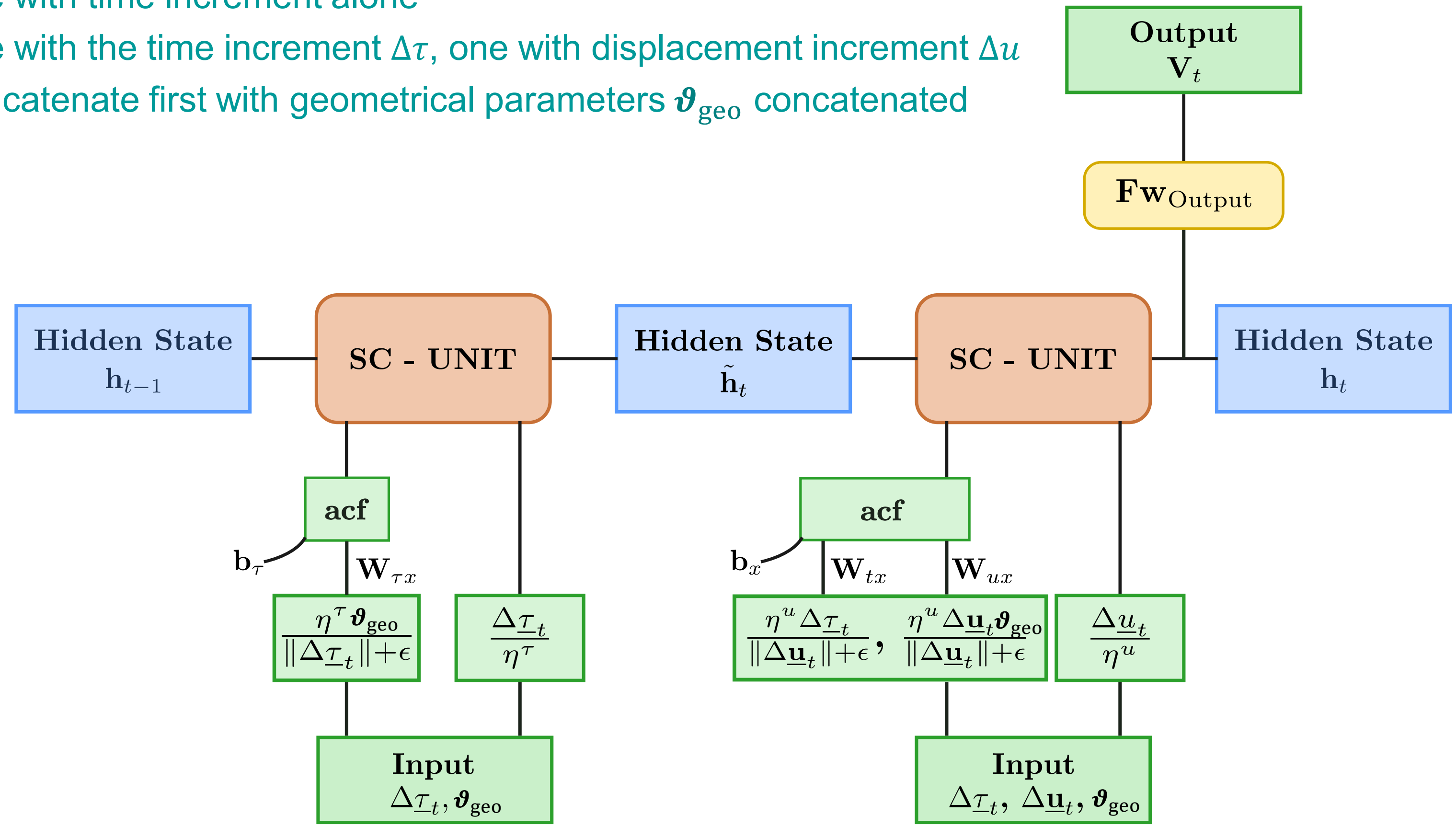


Loading histories at varying strain rate, RW & CC



Self-Consistent Recurrent Neural Network for multi-scale simulations

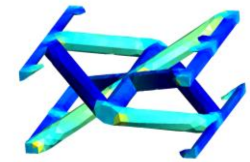
- Self-Consistent model of VE-VP lattice cell response of arbitrary diameter value
  - Key-idea: Use 2 SC units
    - One with time increment alone
    - One with the time increment $\Delta\tau$, one with displacement increment Δu
    - Concatenate first with geometrical parameters $\boldsymbol{\vartheta}_{\text{geo}}$ concatenated

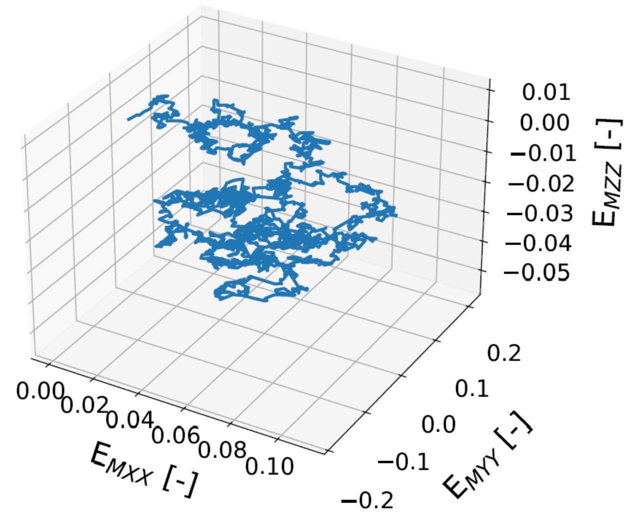


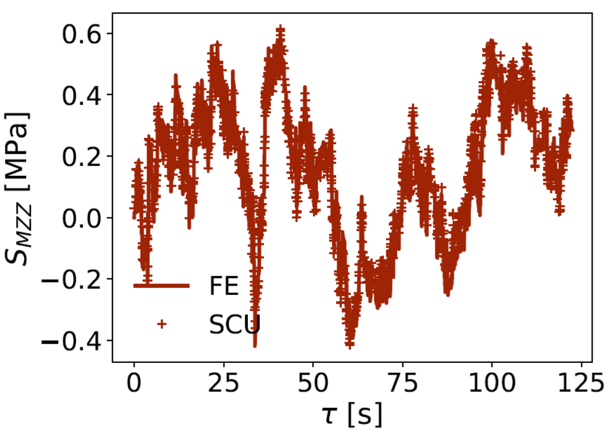
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 862015

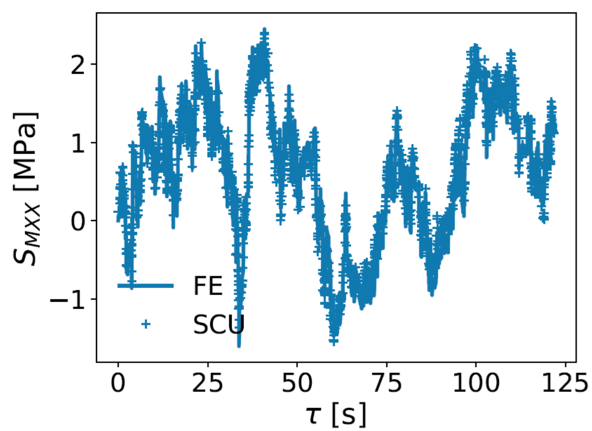
Self-Consistent Recurrent Neural Network for multi-scale simulations

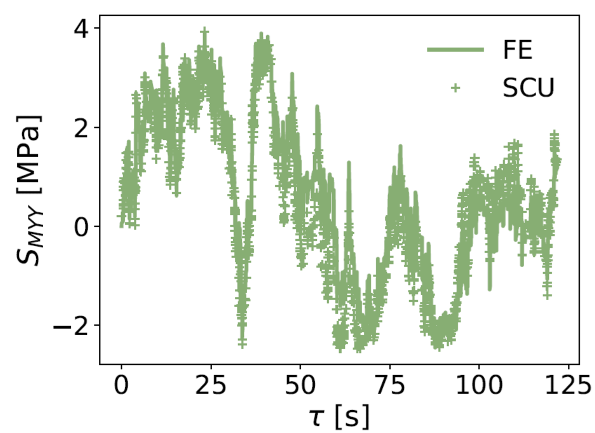
- Testing
  - Inputs (depend on the surrogate)
    - $\mathbf{E}_{\mathbf{M}_t}$: new unseen strain sequence
    - New unseen geometrical parameter realisation $\boldsymbol{\vartheta}_{\text{geo}}$
  - Outputs
    - $\mathbf{S}_{\mathbf{M}_t}$: stress sequence





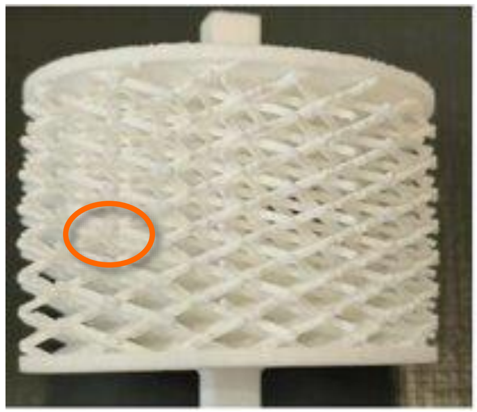


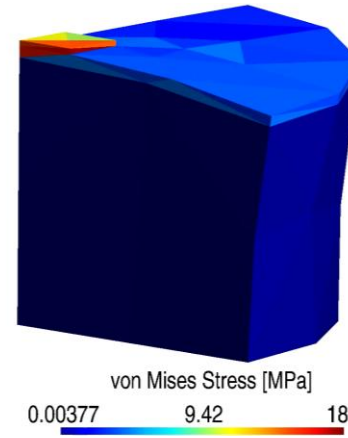




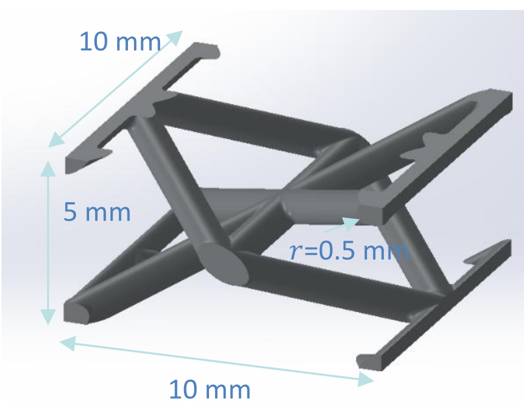
Self-Consistent Recurrent Neural Network for multi-scale simulations

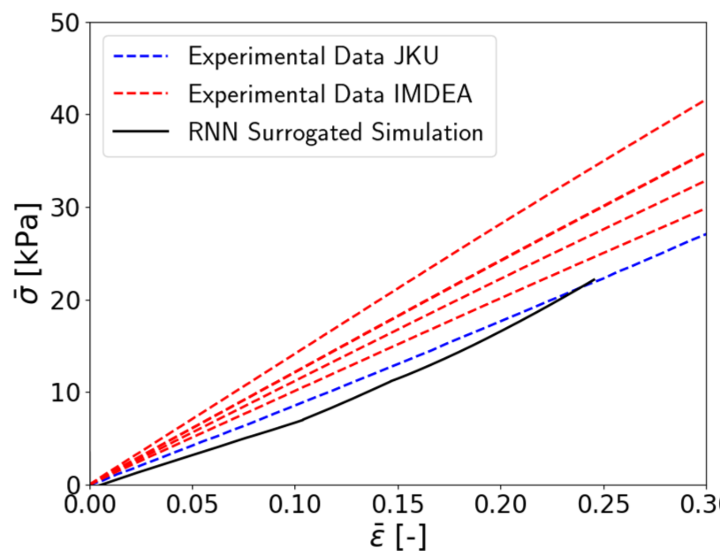
- Validation of meso-scale surrogate model for lattice meta-materials
  - Tension/compression on USF lattice





micro-structure parameter $\boldsymbol{\vartheta}_{\text{geo}}$ not seen in the training stage





References

- DIDEAROT project (https://www.didearot-project.eu/)
  - CENAERO, HEXAGON, SONACA, ULiège (Belgium)
  - Tecnalia, Aernnova, Barcelona Supercomputing Center (Spain)
  - Inegi (Portugal)

- Publication
  - L. Wu, L. Noels, Self-consistency Reinforced minimal Gated Recurrent Unit for surrogate modelling of history-dependent non-linear problems: Application to history-dependent homogenized response of heterogeneous materials, *Computer Methods in Applied Mechanics and Engineering* 424 (2024) 116881, doi: https://doi.org/10.1016/j.cma.2024.116881

- Data and code on
  - Repository: https://gitlab.uliege.be/didearot/didearotPublic/publicationsData/2024_scmru
  - Doi: http://dx.doi.org/10.5281/zenodo.10551272