Computational & Multiscale
Mechanics of Materials

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A Self-consistent Reinforced minimal Gated Recurrent Unit for surrogate modelling of elasto-plastic multi-scale problems

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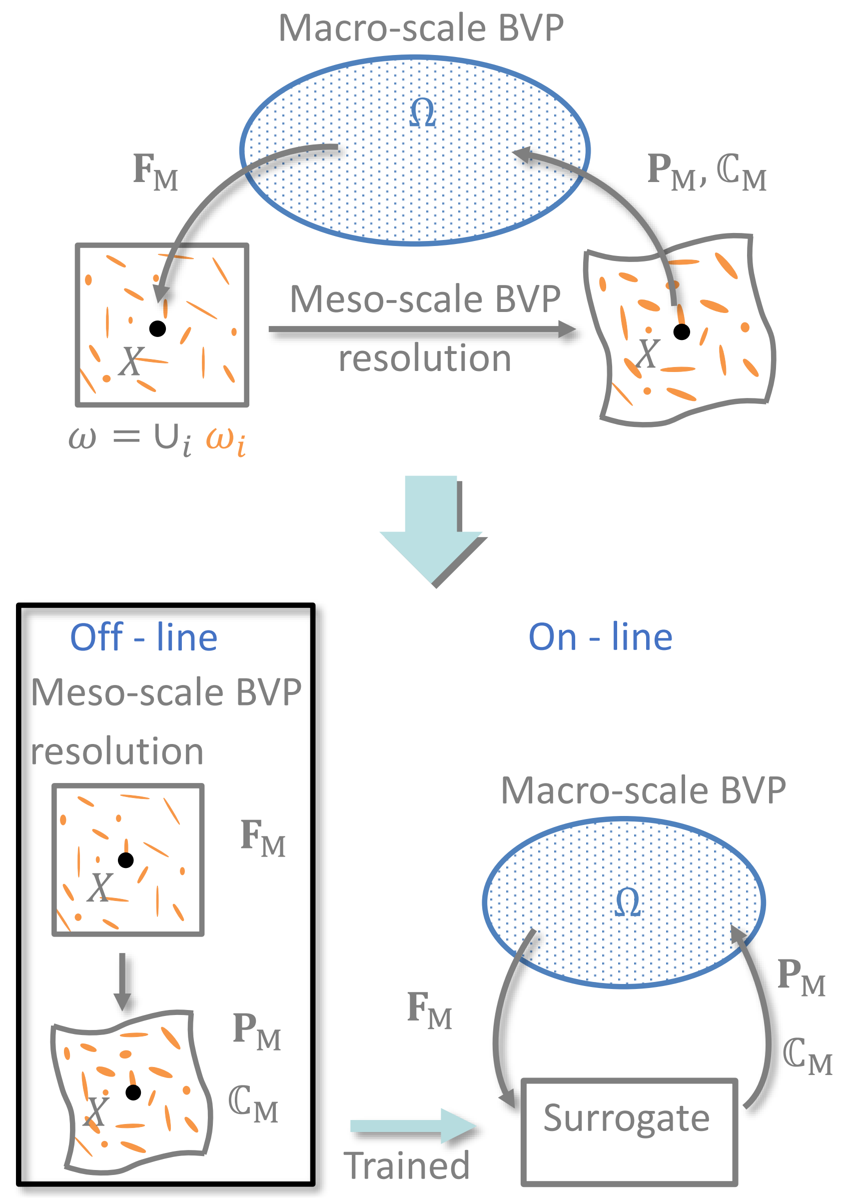
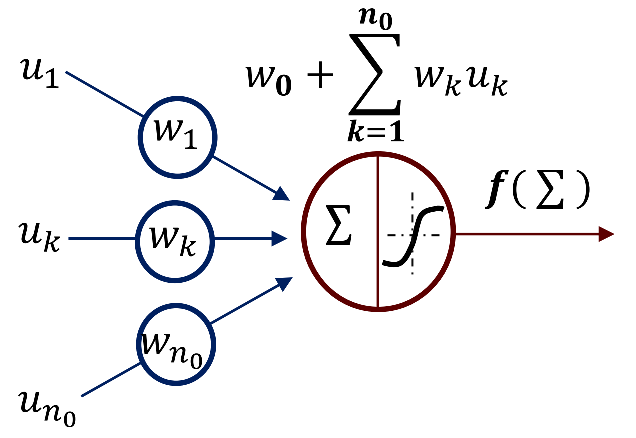
AI-accelerated multi-scale simulations

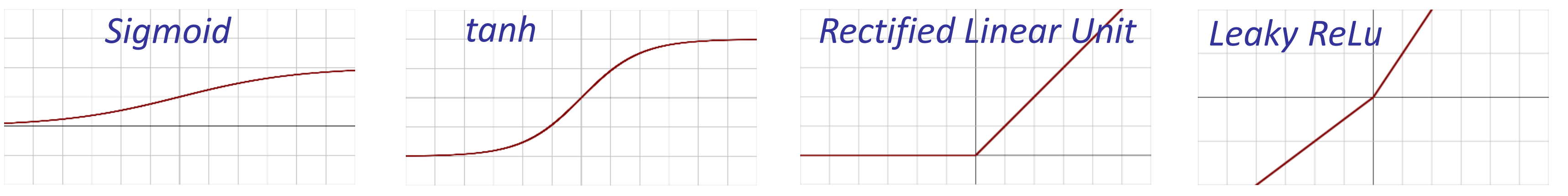
- Introduction to non-linear multi-scale simulations
  - FE multi-scale simulations
    - Problems to be solved at two scales
    - Require Newton-Raphson iterations at both scales
  - Use of surrogate models
    - Train a meso-scale surrogate model (off-line)
      - Requires extensive data
      - 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



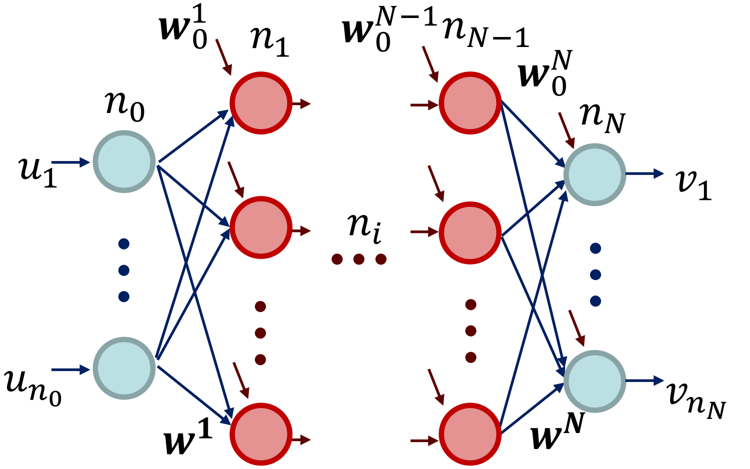
- Definition of the surrogate model
  - Artificial neuron
    - Non-linear function on n_0 inputs u_k
    - Requires evaluation of weights w_k
    - Requires definition of activation function f



  - Activation functions f

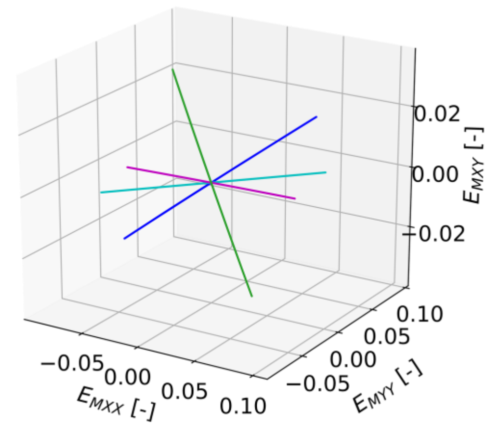


  - Feed-Forward Neuron Network
    - Simplest architecture
    - Layers of neurons
      - Input layer
      - $N-1$ hidden layers
      - Output layers
    - Mapping $\Re^{n_0} \rightarrow \Re^{n_N}: \boldsymbol{v} = \boldsymbol{g}(\boldsymbol{u})$

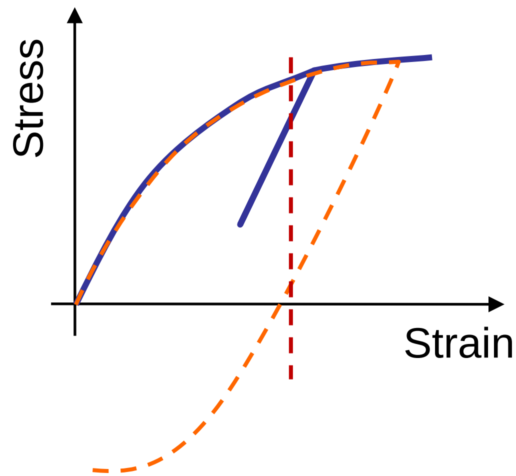


Recurrent Neural Network-accelerated multi-scale simulations

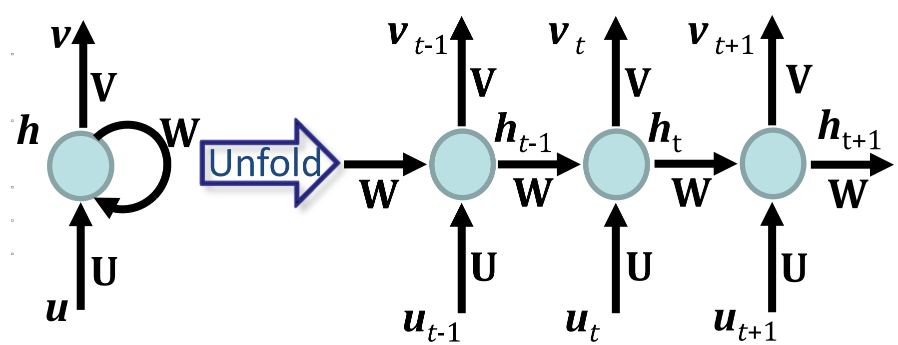
- Input / output definition
  - Input: Strain (history): $\mathbf{F}_{\mathrm{M}}$
  - Output: Stress (history): $\mathbf{P}_{\mathrm{M}}$



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

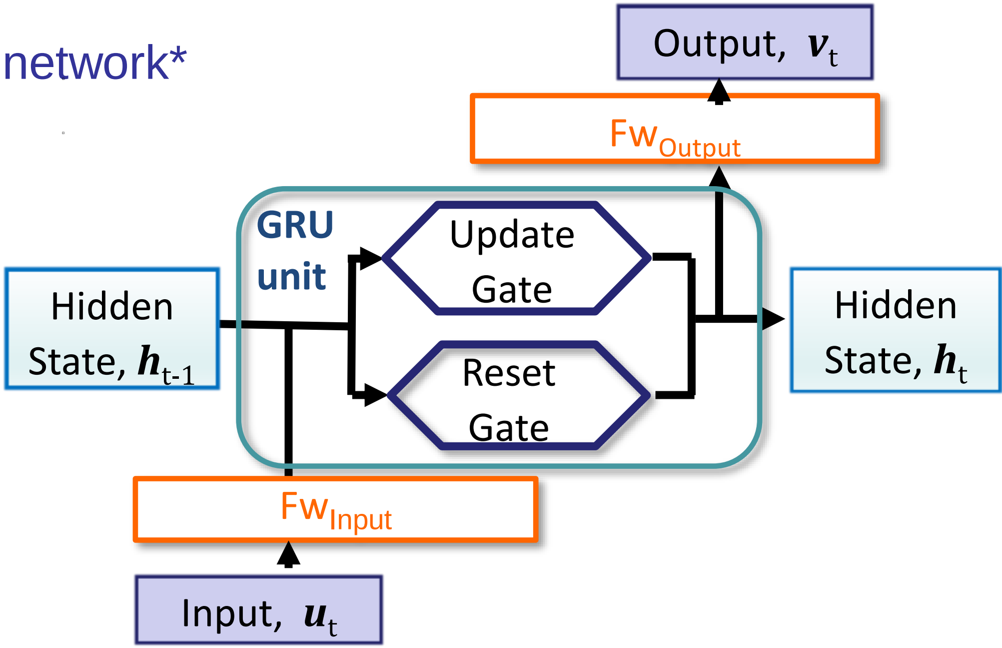


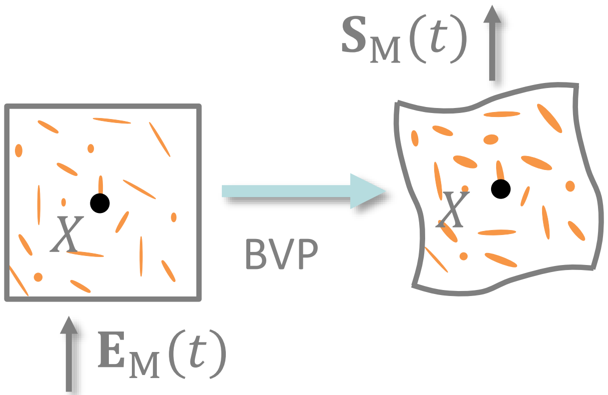
- Recurrent neural network
  - Allows a history dependent relation
    - Input $\boldsymbol{u}_t$
    - Output $\boldsymbol{v}_t = \boldsymbol{g}(\boldsymbol{u}_t, \boldsymbol{h}_{t-1})$
    - Internal variable $\boldsymbol{h}_t = \boldsymbol{g}(\boldsymbol{u}_t, \boldsymbol{h}_{t-1})$
  - Weights matrices $\mathbf{U}, \mathbf{W}, \mathbf{V}$
    - 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-accelerated multi-scale simulations

- Previous Work with recurrent neural network*
  - 1 Gated Recurrent Unit (GRU)
    - Reset gate: select past information to be forgotten
    - Update gate: select past information to be passed along
  - 2 feed-forward NNWs
    - $\mathrm{FW_{Input}}$ to treat inputs $\boldsymbol{u_t}$
    - $\mathrm{FW_{Output}}$ to produce outputs $\boldsymbol{v_t}$
  - Details
    - $\boldsymbol{u_t}$: homogenised GL strain $\mathbf{E}_\mathrm{M}$ (symmetric)
    - $\boldsymbol{v_t}$: homogenised 2nd PK stress $\mathbf{S}_\mathrm{M}$ (symmetric)
    - 100 hidden variables $\boldsymbol{h_t}$
    - $\mathrm{FW_{Input}}$ one hidden layer of 60 neurons
    - $\mathrm{FW_{Output}}$ two hidden layers of 100 neurons

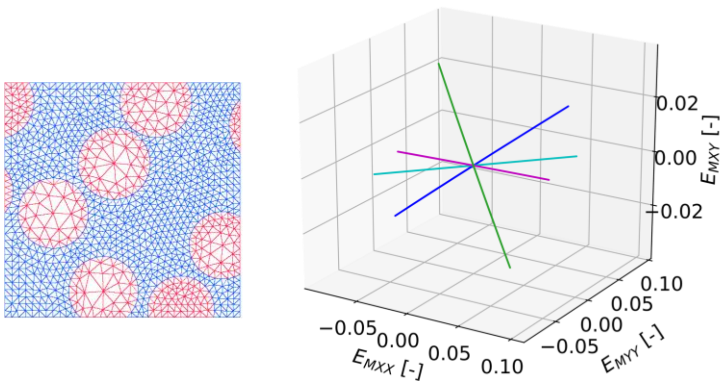


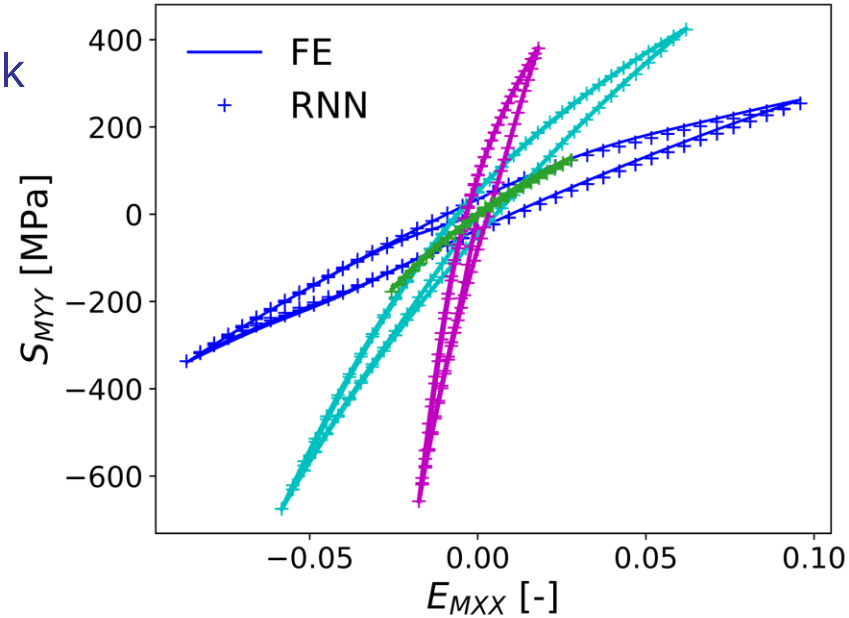


*L. Wu, V. D. Nguyen, N. G. Kilingar, and L. Noels. "A recurrent neural network-accelerated multi-scale model for elasto-plastic heterogeneous materials subjected to random cyclic and non-proportional loading paths." Computer Methods in Applied Mechanics and Engineering, 369 (01 September 2020): 113234. doi:10.1016/j.cma.2020.113234

Recurrent Neural Network-accelerated multi-scale simulations

- Previous Work with recurrent neural network
  - Good accuracy on testing data



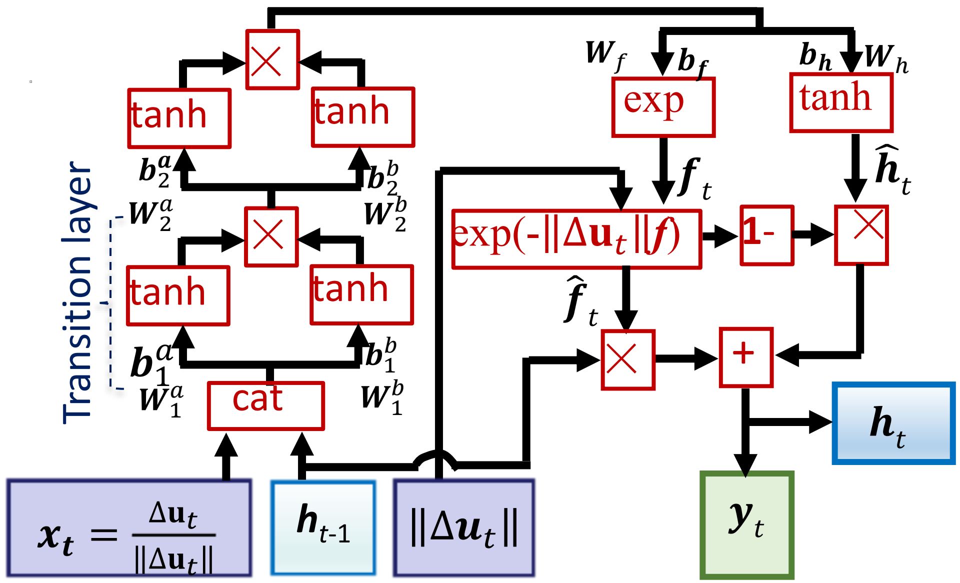


  - Sequence increment $\boldsymbol{\Delta u_t} = \Delta \mathbf{E}_{\mathrm{M}}$ of comparable order of magnitude between training and testing data

- What if online simulations use smaller increments?
  - 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.

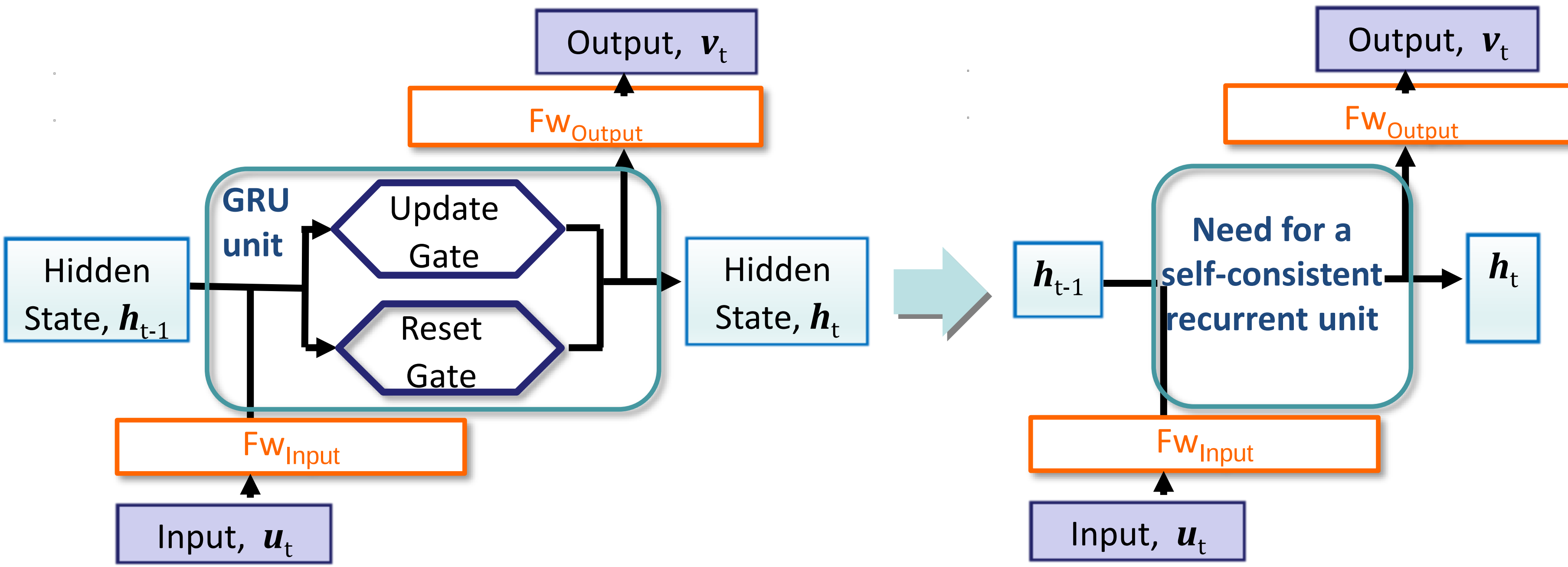
- Self-Consistent Linearized Minimal State Cell (SC-LMSC)*



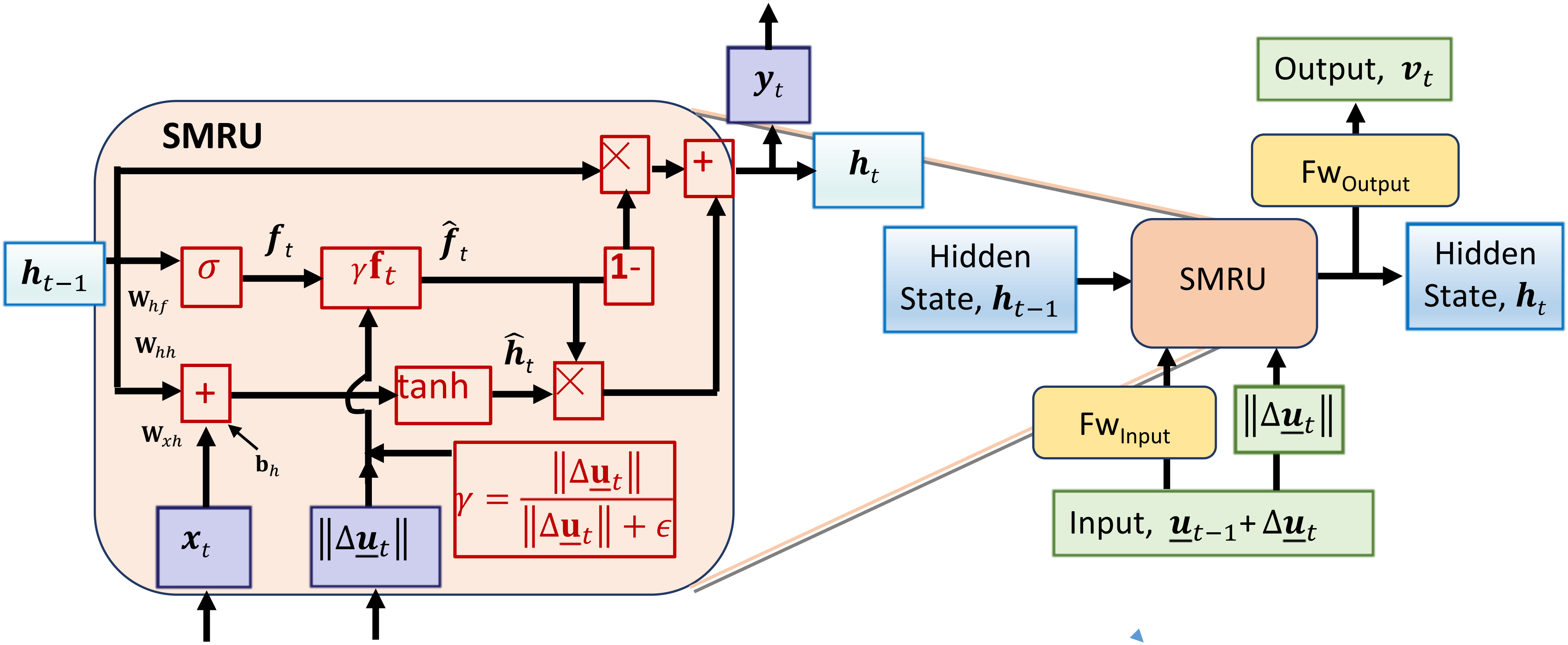
– Ingredients:
  - Incremental form of input variables converted to its direction $\frac{\Delta \boldsymbol{u}_t}{\|\Delta \boldsymbol{u}_t\|}$ and norm $\|\Delta \boldsymbol{u}_t\|$ *
  - Activations layers fed by direction $\frac{\Delta \boldsymbol{u}_t}{\|\Delta \boldsymbol{u}_t\|}$ and previous hidden variable direction $\boldsymbol{h}_t$
  - Double exponential activation function on output $\boldsymbol{O}_t$ of activation layers:
    – $\boldsymbol{f}_t = \exp\left[\boldsymbol{W}_f \boldsymbol{O}_t + \boldsymbol{b}_f\right] > 0$ and ratio $\hat{\boldsymbol{f}}_t = \exp[-\|\Delta \boldsymbol{u}_t\|\ \boldsymbol{f}_t] \in [0, 1]$
    – Hidden variables $\boldsymbol{h}_t$ are an element-wise interpolation (ratio $\hat{\boldsymbol{f}}_t$ dependent on the norm of $\|\Delta \boldsymbol{u}_t\|$) between previous value $\boldsymbol{h}_{t-1}$ and $\hat{\boldsymbol{h}}_t$

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



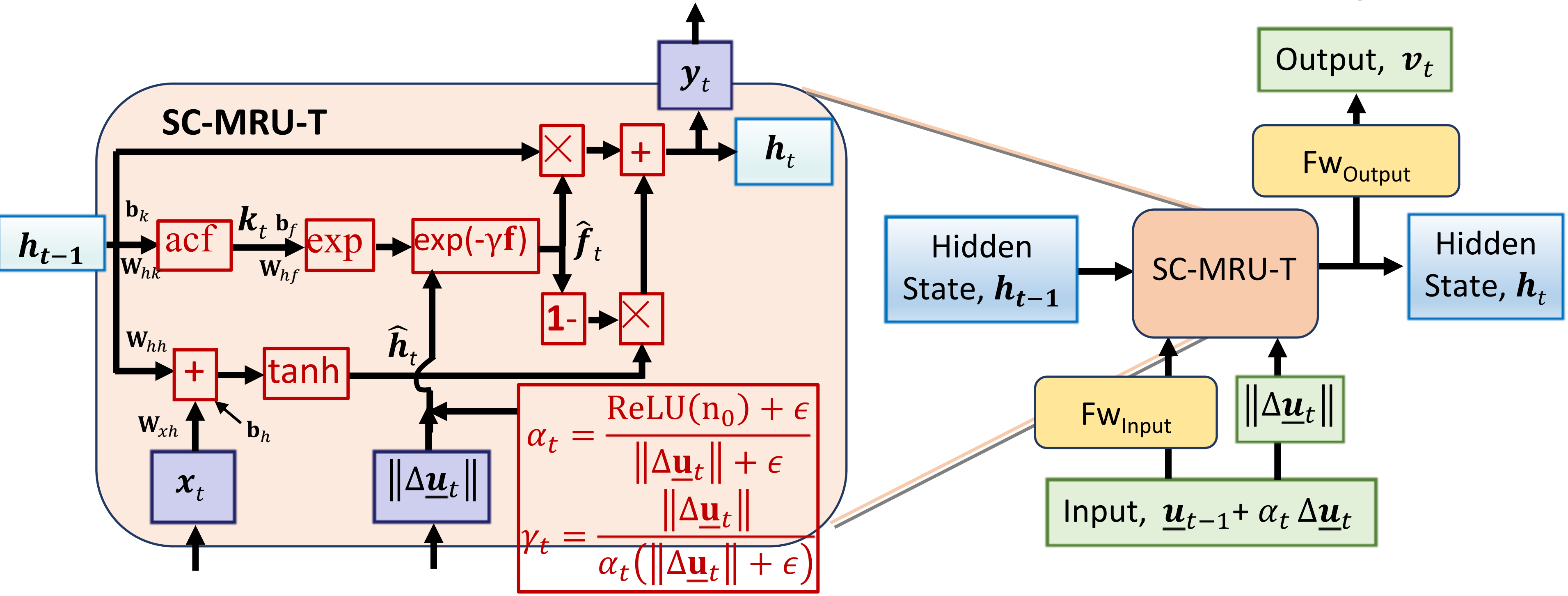
- New cell 1: New simplified recurrent unit: Simplified Minimal Recurrent Unit



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

Self-Consistent Recurrent Neural Network

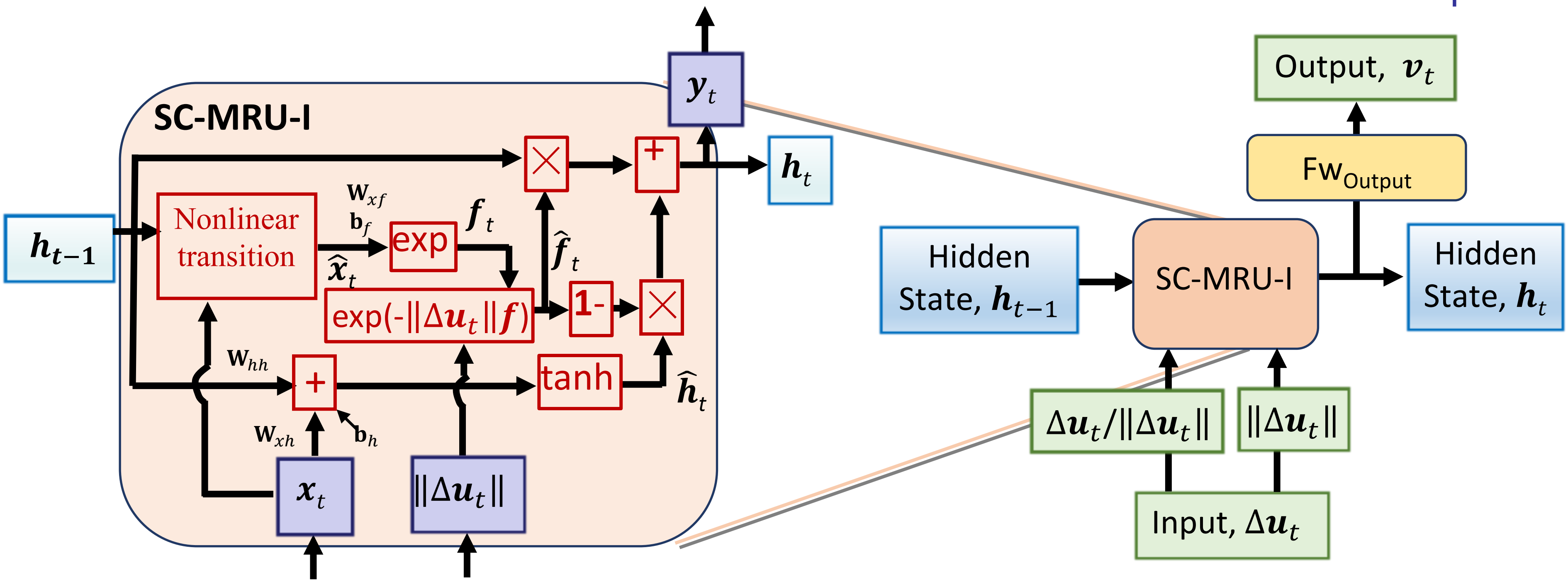
- New cell 2: Self-Consistent Minimal Recurrent Unit with Total form of inputs



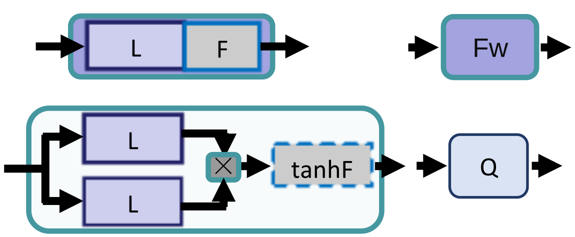
- The **total form of input variable** as well as **increment norm** $\|\Delta\boldsymbol{u}_t\|$ (like SC-LMCS)
  - Use as input $\underline{\boldsymbol{u}}_{t-1} + \alpha_t\,\Delta\underline{\boldsymbol{u}}_t$ (n_0 is a learnable parameter)
  - acf is the same activation function as in $\mathrm{Fw}_{\mathrm{input}}$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

Self-Consistent Recurrent Neural Network

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



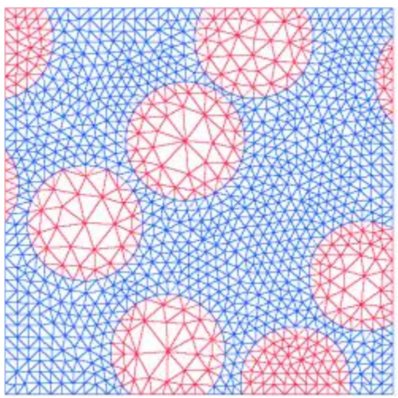
- The **incremental form of input variable** as well as **increment norm** $\|\Delta\boldsymbol{u}_t\|$ (like LMCS)
  - Use as input $\Delta\boldsymbol{u}_t/\|\Delta\boldsymbol{u}_t\|$ and $\|\Delta\boldsymbol{u}_t\|$
  - Non-linear transition blocks:

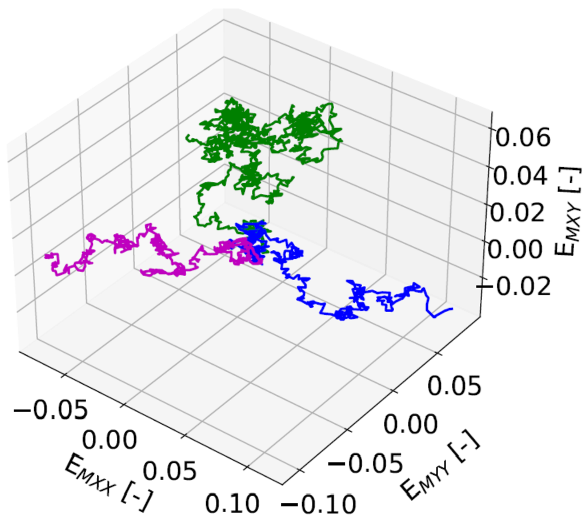


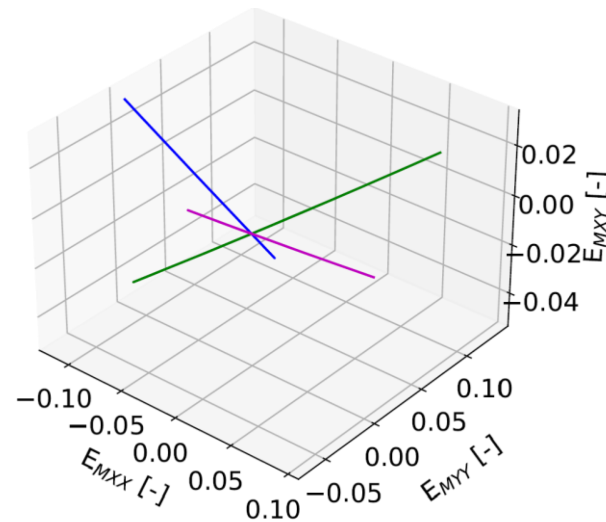
- **Self-consistency enforced**
  - Double exponential function $\boldsymbol{f}_t = \exp[\boldsymbol{W}_{xf}\widehat{\boldsymbol{x}}_t + \boldsymbol{b}_f] > \mathbf{0}$ & ratio $\widehat{\boldsymbol{f}}_t = \exp[-(\|\Delta\boldsymbol{u}_t\|)\,\boldsymbol{f}_t] \in [\mathbf{0}, \mathbf{1}]$
  - Hidden variables $\boldsymbol{h}_t$ is an element-wise interpolation (ratio $\widehat{\boldsymbol{f}}_t$) between previous value $\boldsymbol{h}_{t-1}$ and $\widehat{\boldsymbol{h}}_t$

Training of Recurrent Neural Network

- Training strategy
  - Elasto-plastic composite RVE





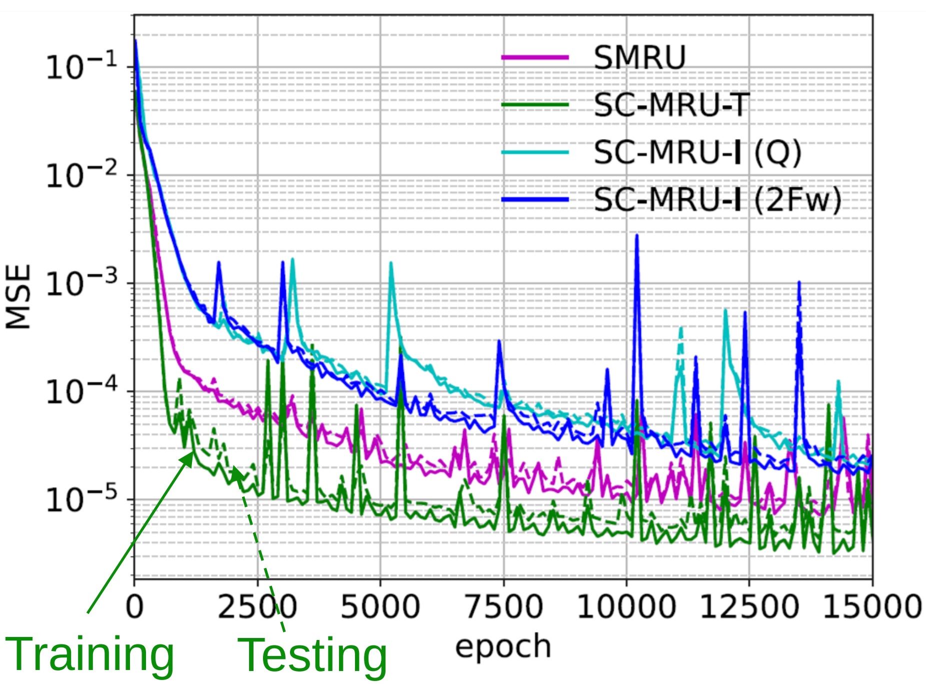


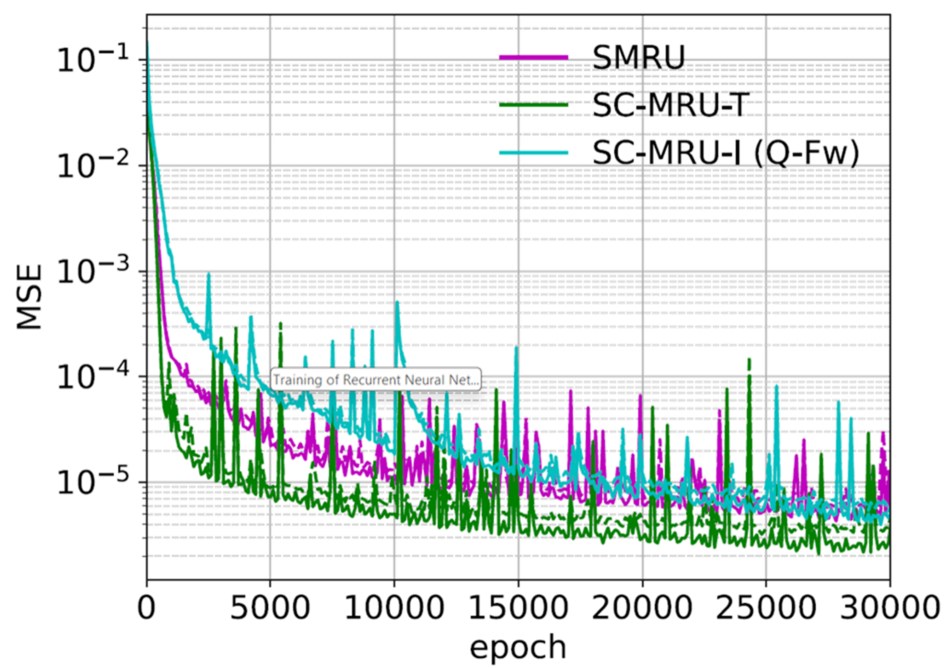
  - Training data
    - Should cover full range of possible loading histories
    - Use random walking strategy
    - Completed with random cyclic loading
    - Bounded by a hypercube of 12% deformation

Training of Recurrent Neural Network

- Training stage
  - Learnable parameters for 120 hidden variables

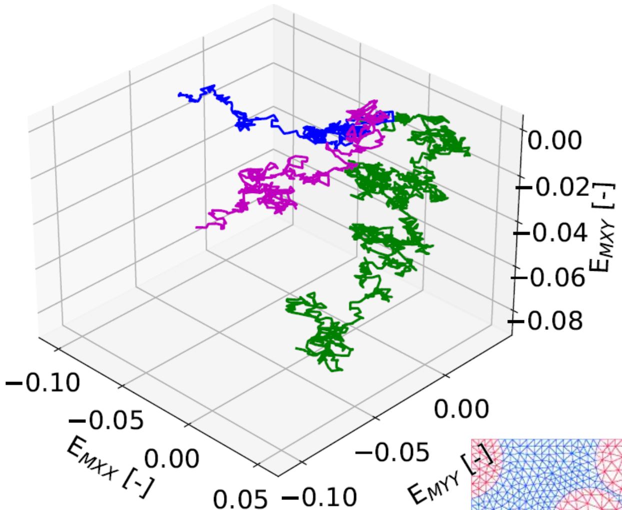
Recurrent unit	SMRU	SC-MRU-T	SC-MRU-I		
Transition block	-	-	Q	Fw-Fw	Q-Fw
Learnable parameters	44 284	58 925	59 644	59 284	74 164



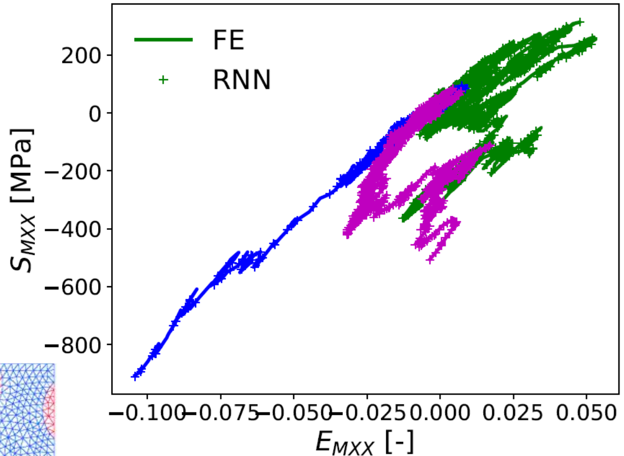


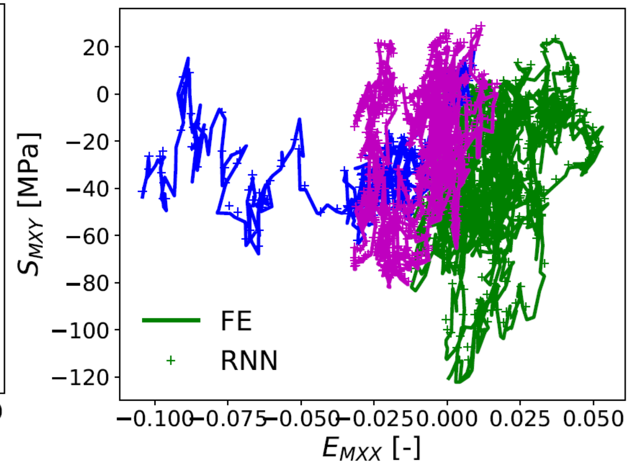
Testing of Recurrent Neural Network

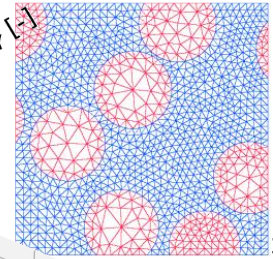
- SC-MRU-T: Testing data with inserted extra-points

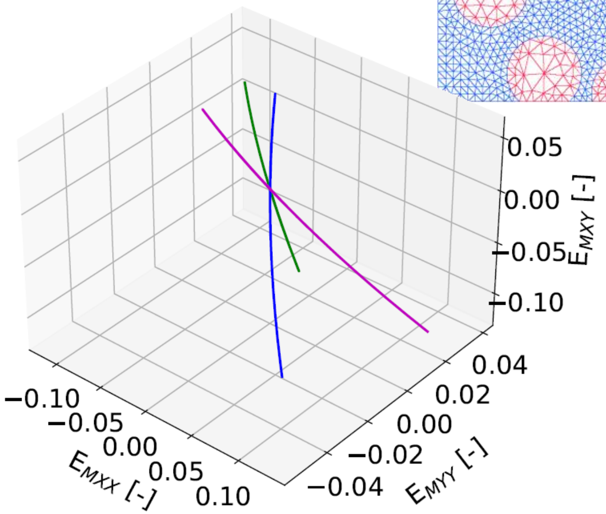


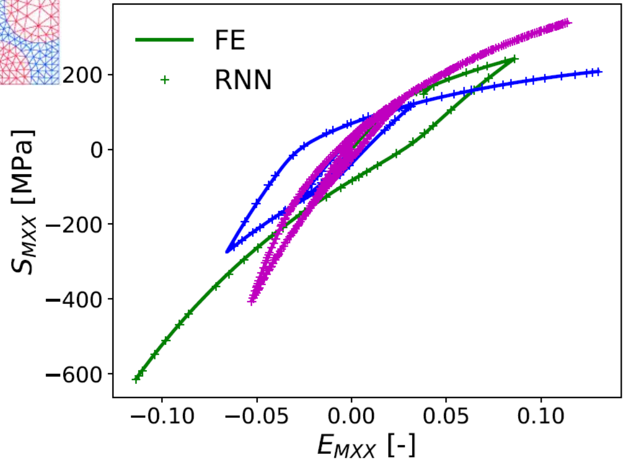
Maximum inserted data points is 5, 20, 60 in each loading step

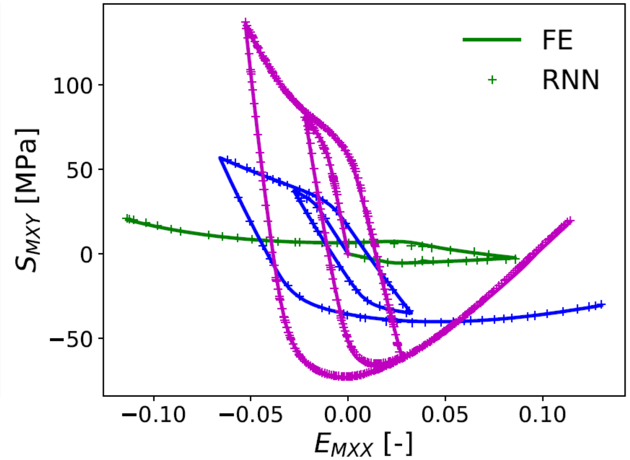




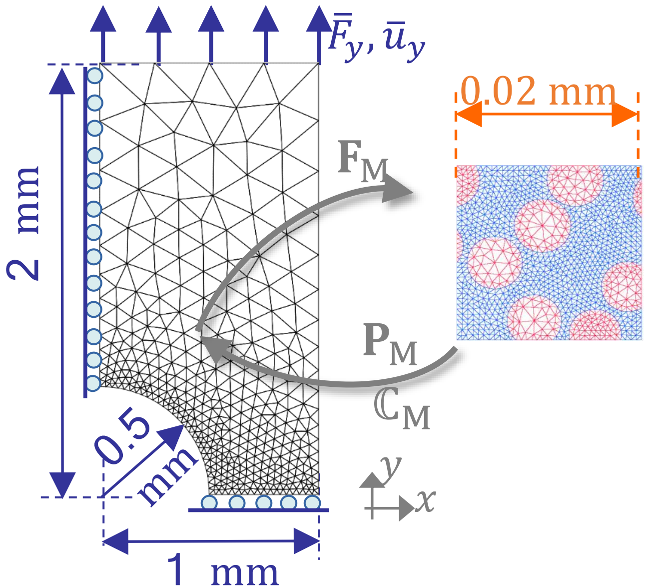


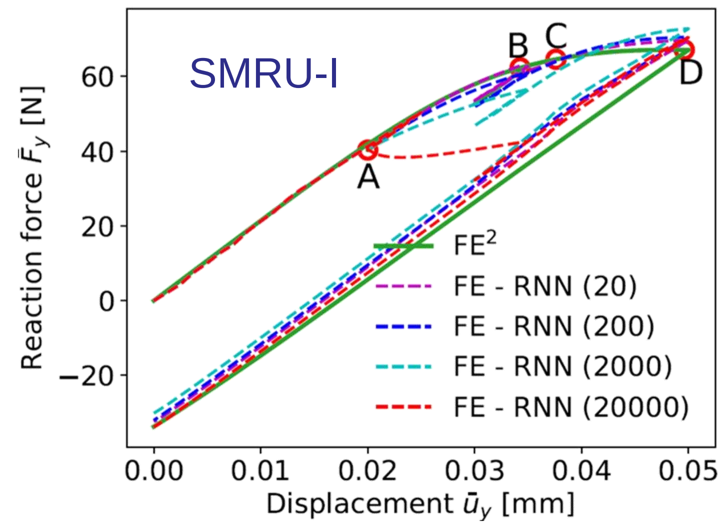


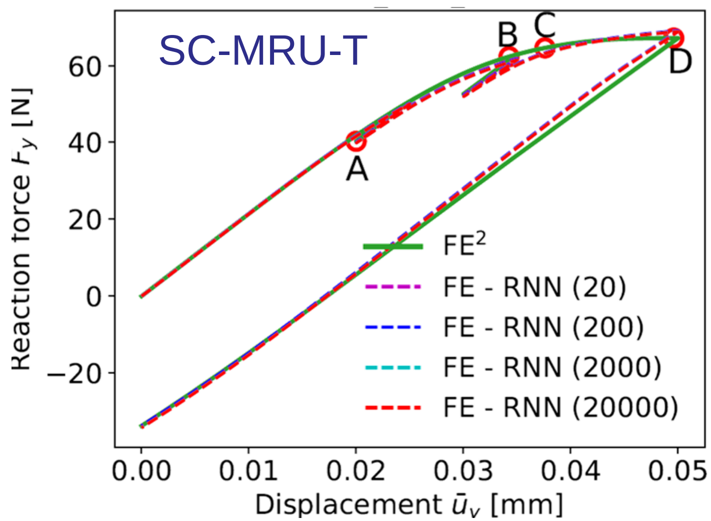


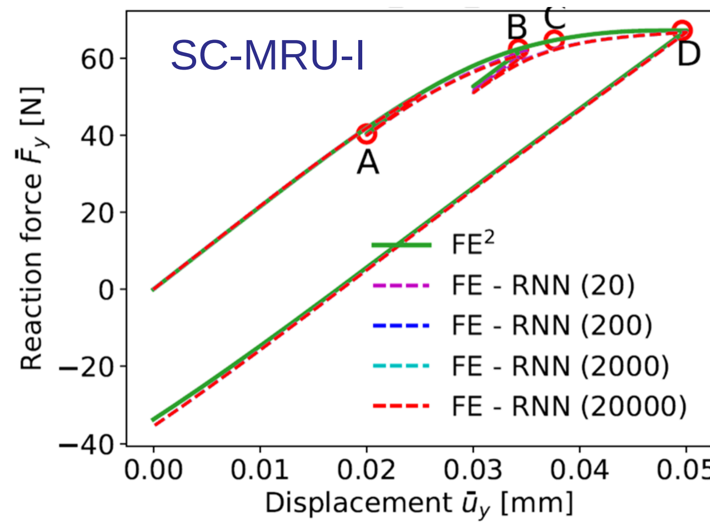


- FE2 vs. FE-RNN: Change in the increment size (between points A&B)



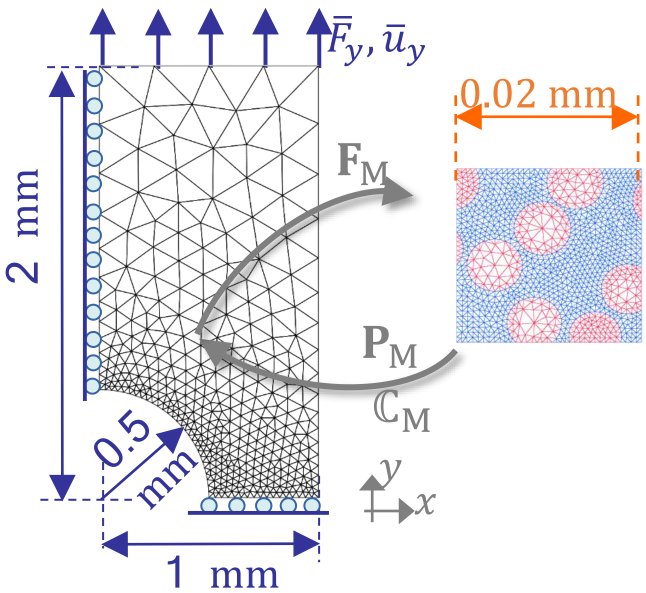






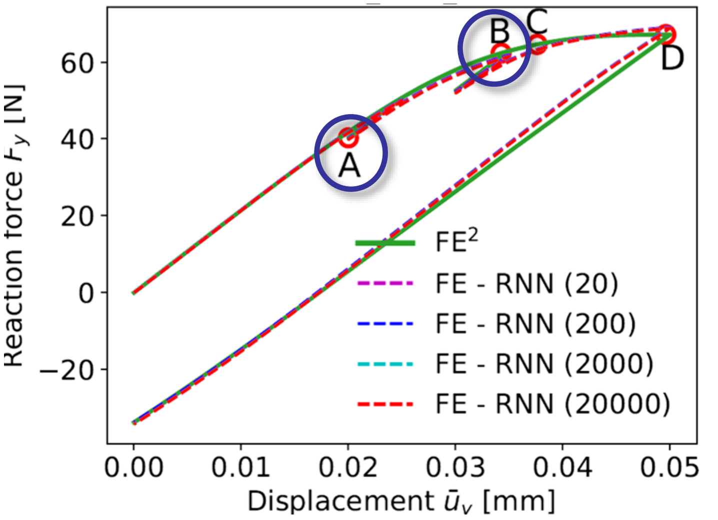
Multi-scale simulations with Recurrent Neural Network

- FE2 vs. FE-RNN: Cost comparison

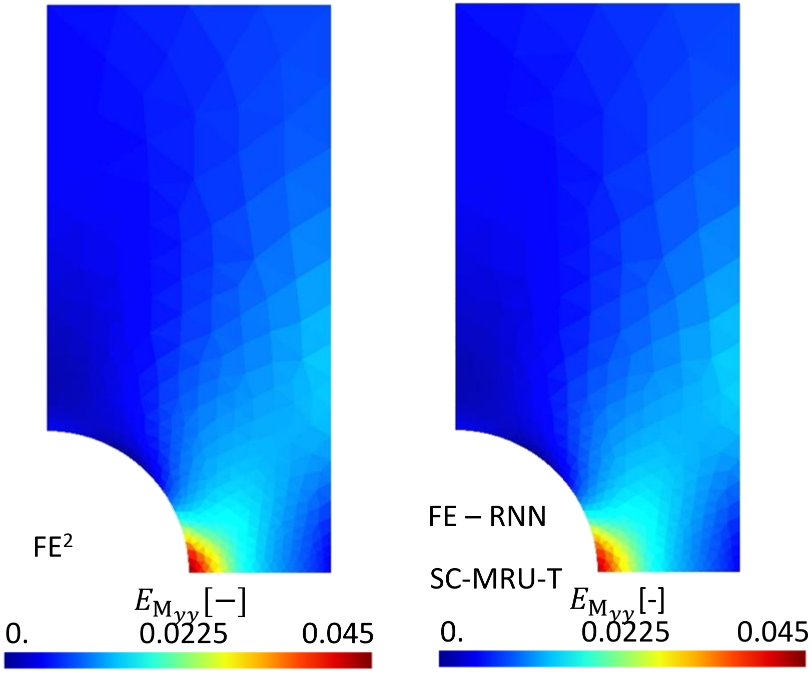


Off-line	FE^2	SMRU	SC-MRU-T	SC-MRU-I
Data generation	-	23500 h-cpu		
Training	-	< 10 h-cpu		
On-line	**FE^2**	**SMRU**	**SC-MRU-T**	**SC-MRU-I**
Simulation	18000 h-cpu	0.27 h-cpu	0.38 h-cpu	0.28 h-cpu

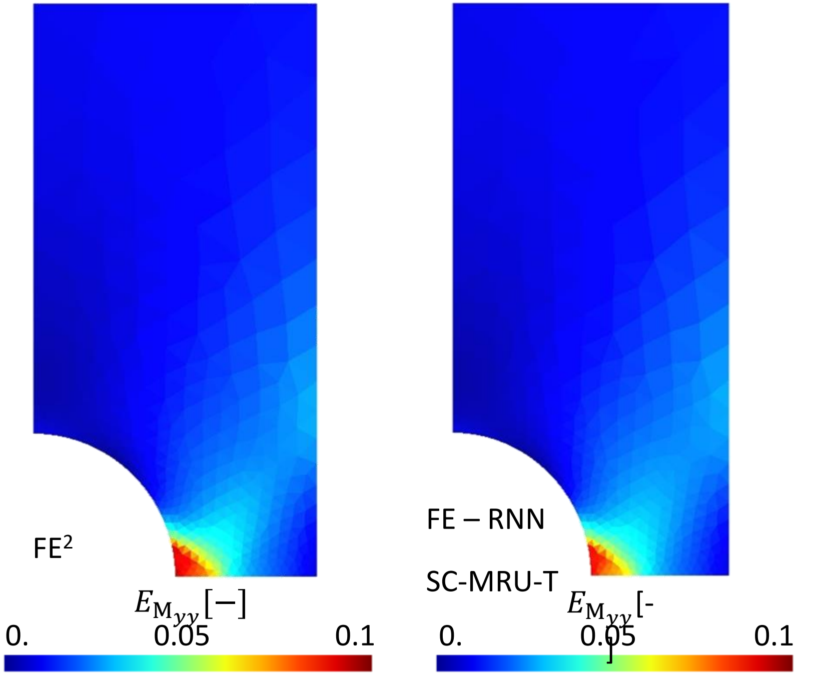
- FE2 vs. FE-RNN: Fields distribution



Point A

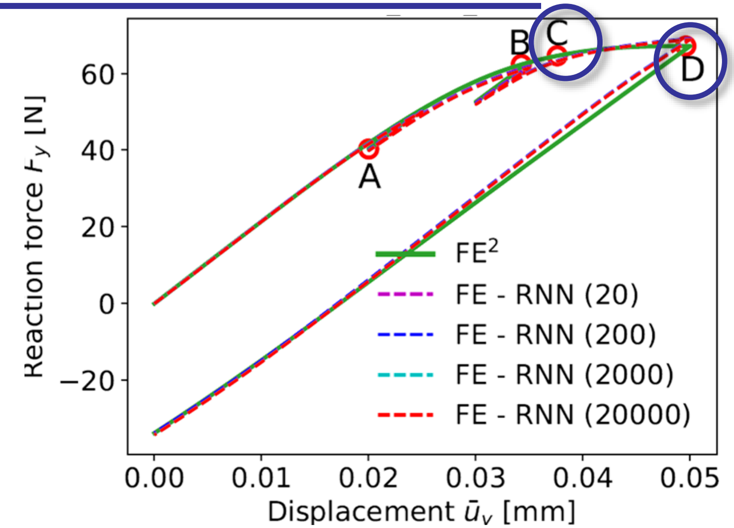


Point B

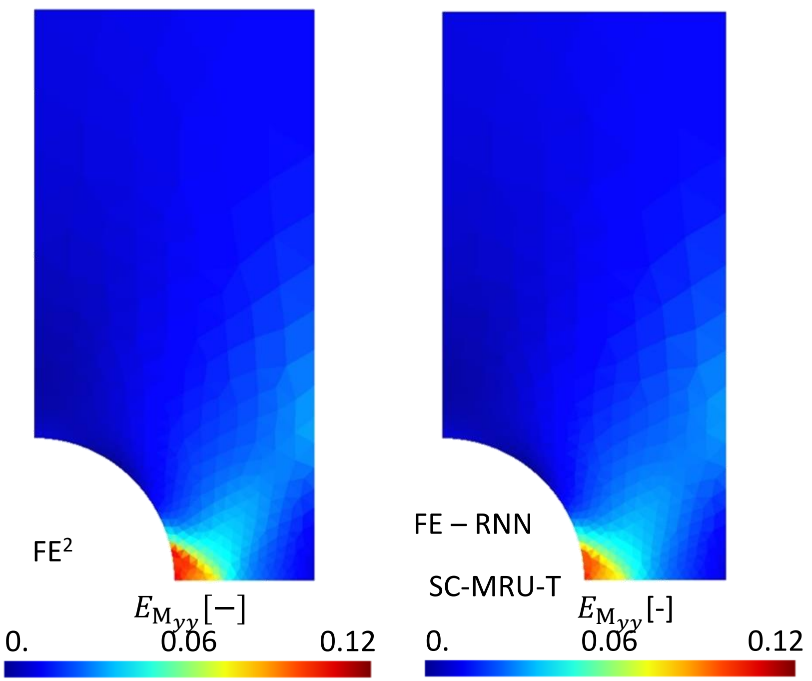


Multi-scale simulations with Recurrent Neural Network

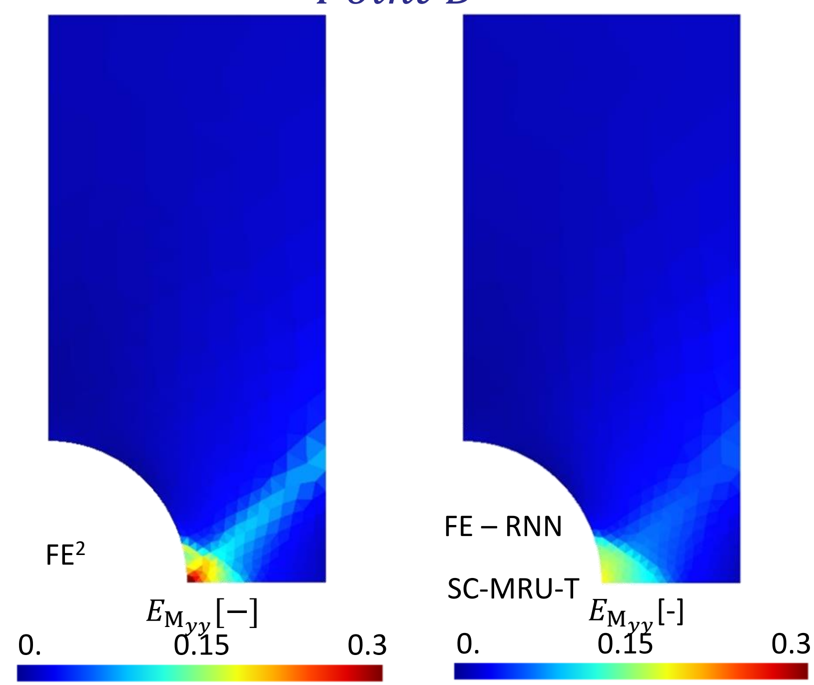
- FE2 vs. FE-RNN: Fields distribution



Point C



Point D



References

- Publication
  - L. Wu, L. Noels, Self-consistency Reinforced minimal Gated Recurrent Unit for surrogate modeling 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