A Convolutional Neural Network for Enhancement of Multi-Scale Localization in Granular Metallic Representative Unit Cells

(+- *my other interests*)

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Mostly from AIAA SciTech 2022

Me:

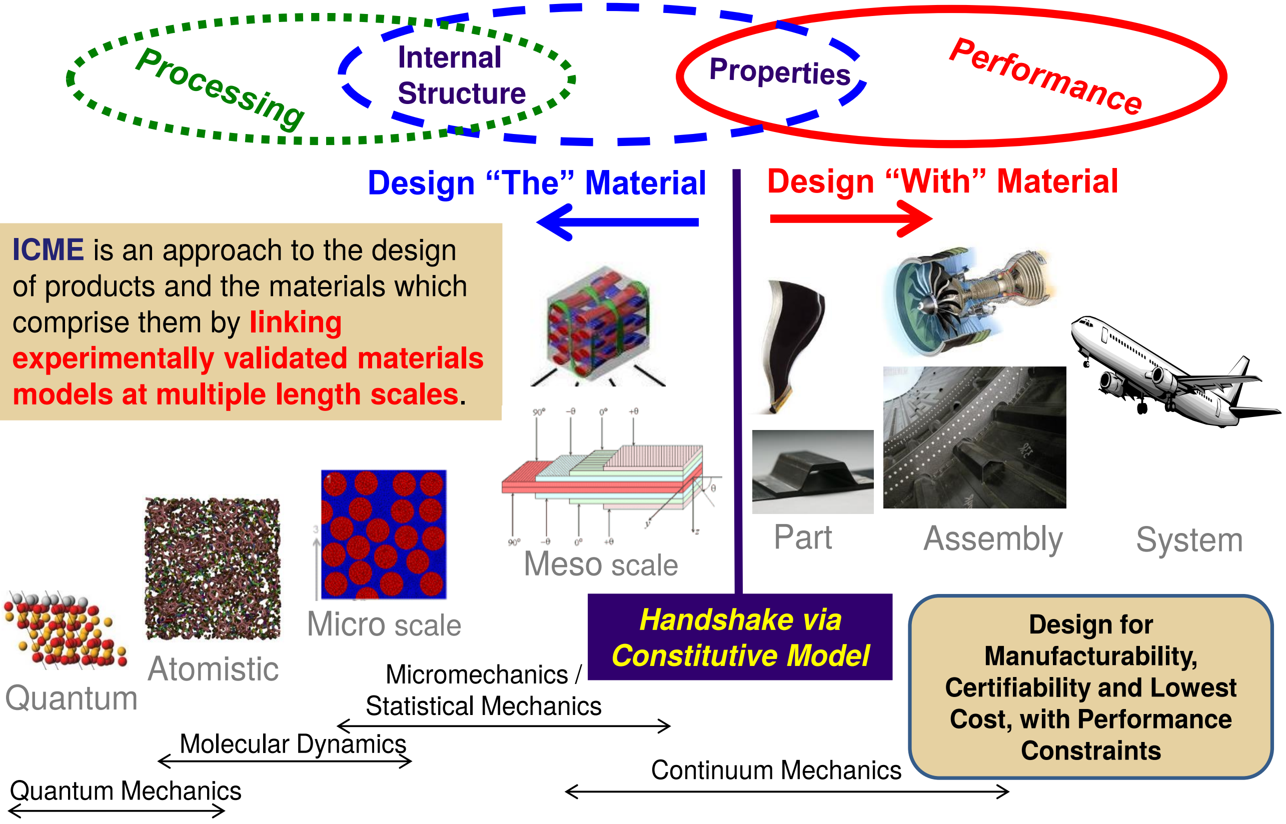
- Professor of Mechanical and Aerospace Engineering
  - On sabbatical from Western Michigan University
  - Working with Josh Stuckner, Evan Pineda
  - and others from Materials Branch (Multi-scale modeling)

- Research Interests
  - Computational Structural Mechanics (primarily FEA)
  - Aerospace Structures
  - Composite Materials
  - Biomedical Engineering (tissue modeling, devices)

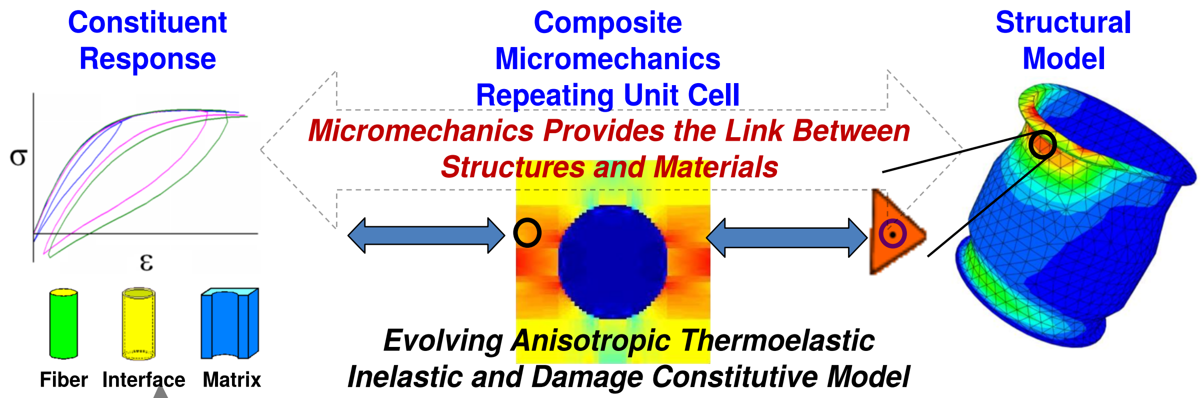
- Learning goals for the sabbatical
  - Multi-scale modeling
  - Machine learning

Relevance and Background

Integrated Computational Materials Engineering (ICME) Is The Future



Multiscale Modeling



Continuum Deformation and damage models

Macro-level Constitutive Equations

$$\bar{\sigma} = B^*\left(\bar{\varepsilon} - \bar{\varepsilon}^I - \bar{\varepsilon}^T\right)$$

$$B^* = \frac{1}{dhl}\sum_{\alpha=1}^{N_\alpha}\sum_{\beta=1}^{N_\beta}\sum_{\gamma=1}^{N_\gamma} d_\alpha h_\beta l_\gamma C^{(\alpha\beta\gamma)} A^{(\alpha\beta\gamma)}$$

$$\bar{\varepsilon}^I = \frac{-\left[B^*\right]^{-1}}{dhl}\sum_{\alpha=1}^{N_\alpha}\sum_{\beta=1}^{N_\beta}\sum_{\gamma=1}^{N_\gamma} d_\alpha h_\beta l_\gamma C^{(\alpha\beta\gamma)}\left(D^{(\alpha\beta\gamma)}\varepsilon_s^I - \varepsilon^{I(\alpha\beta\gamma)}\right)$$

$$\bar{\varepsilon}^T = \frac{-\left[B^*\right]^{-1}}{dhl}\sum_{\alpha=1}^{N_\alpha}\sum_{\beta=1}^{N_\beta}\sum_{\gamma=1}^{N_\gamma} d_\alpha h_\beta l_\gamma C^{(\alpha\beta\gamma)}\left(D^{(\alpha\beta\gamma)}\varepsilon_s^T - \varepsilon^{T(\alpha\beta\gamma)}\right)$$

Micro-level Field Equations (subcell)

$$\varepsilon^{(\alpha\beta\gamma)} = A^{(\alpha\beta\gamma)}\bar{\varepsilon} + D^{(\alpha\beta\gamma)}\left(\varepsilon_s^I + \varepsilon_s^T\right)$$

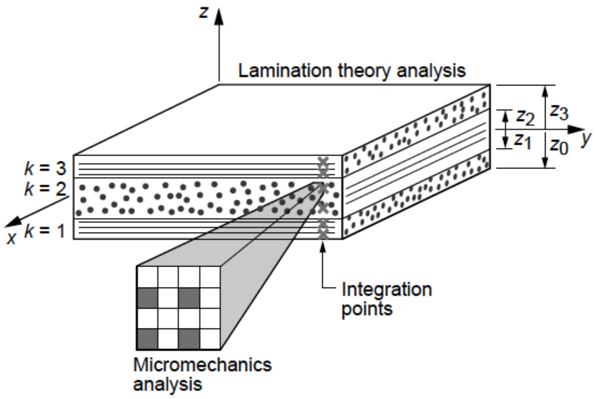
$$\sigma^{(\alpha\beta\gamma)} = C^{(\alpha\beta\gamma)}\left[A^{(\alpha\beta\gamma)}\bar{\varepsilon} + D^{(\alpha\beta\gamma)}\left(\varepsilon_s^I + \varepsilon_s^T\right) - \left(\varepsilon^{I(\alpha\beta\gamma)} + \varepsilon^{T(\alpha\beta\gamma)}\right)\right]$$

Aboudi, J., Arnold, S.M., and Bednarcyk, B.A. (2013) *Micromechanics of Composite Materials: A Generalized Multiscale Analysis Approach*, Elsevier, Oxford, UK., pp 1-984.

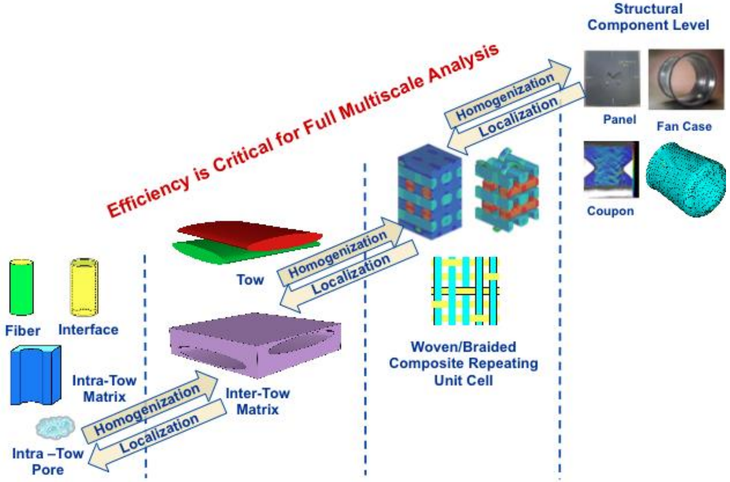
NASA tools heavily dependent on the **Generalized Method of Cells**

Robust Multiscale Modeling Framework Enables Efficient Analysis of Composite Materials and Structures

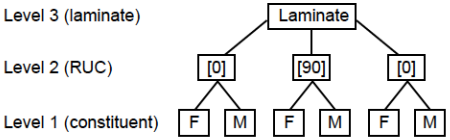
Classical Lamination Theory (CLT)



Woven/Braided Composite Systems

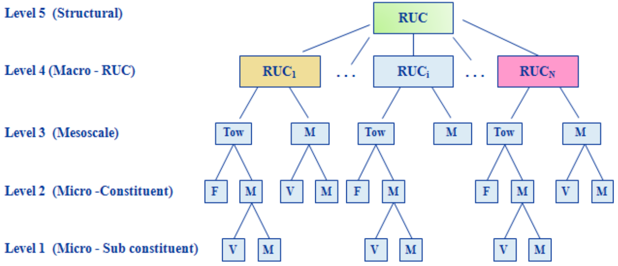


Multiscale Analysis Diagrams (MsGMC):



3 Scales with 2 Homogenizations/Localizations

5 Scales with 4 Homogenizations/Localizations



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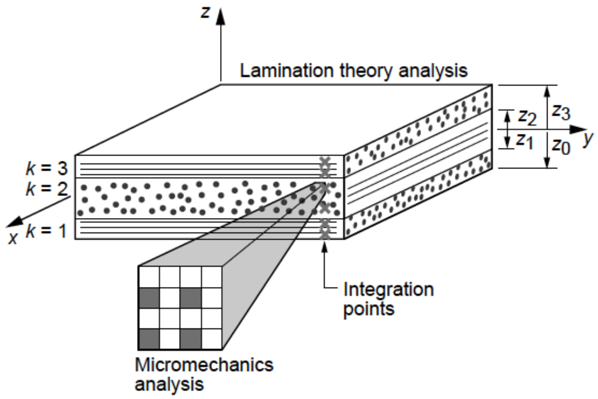
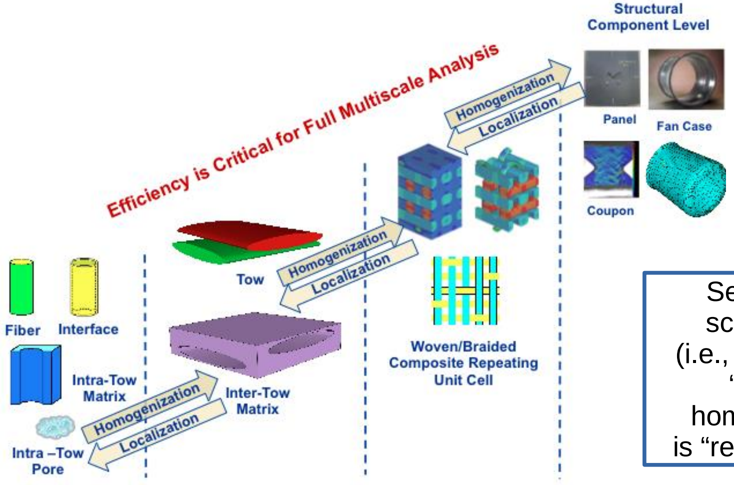
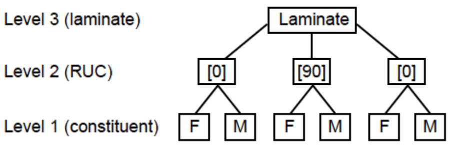


Woven/Braided Composite Systems



Separation of scales critical (i.e., localization is “uniform”, homogenization is “representative”)

Multiscale Analysis Diagrams (MsGMC):



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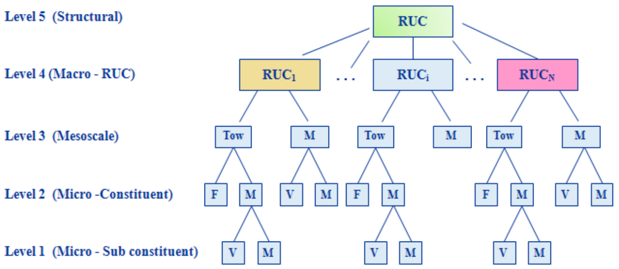
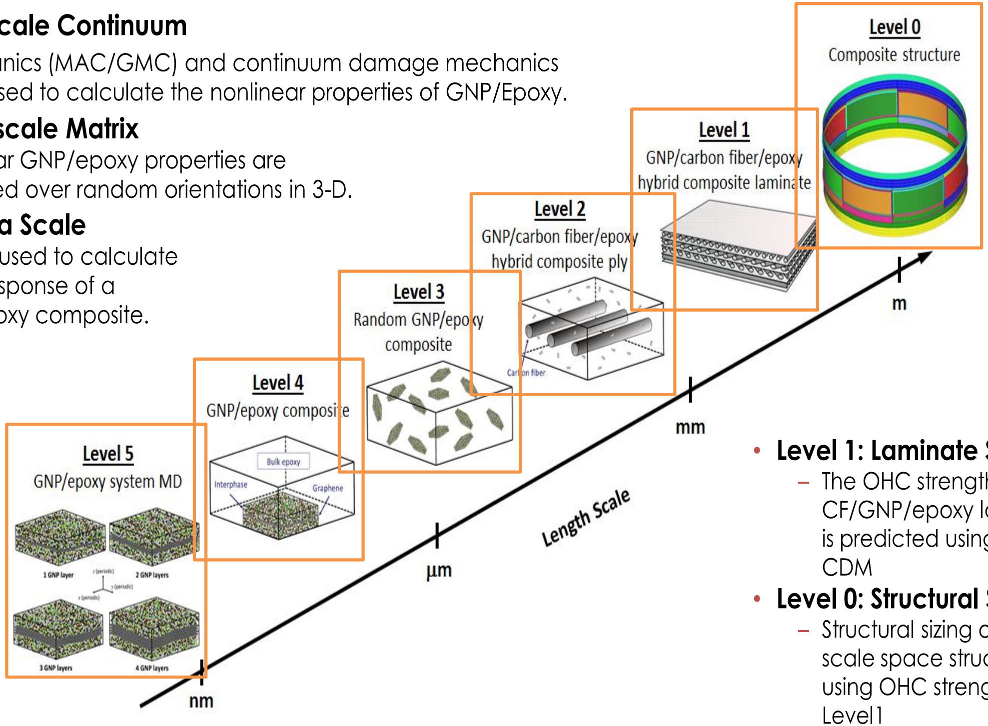


Thermomech. Multiscale Modeling of Large Space Structure Including GNP

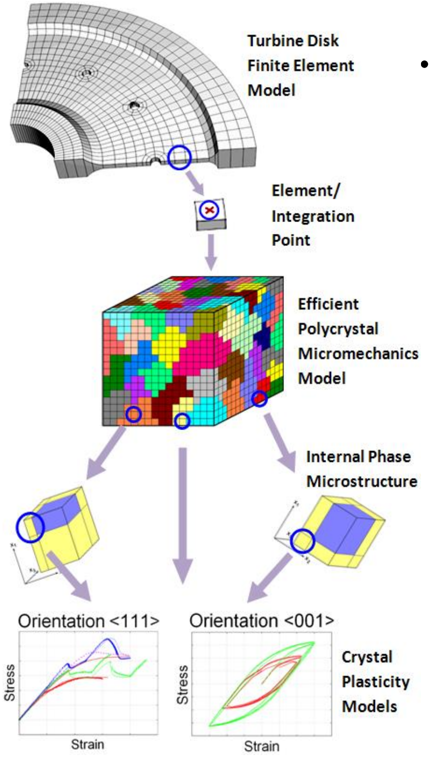
- **Level 5: Nanoscale**
  - LAMMPS Molecular Dynamics (MD) code used to predict thermoelastic properties of GNP/epoxy
- **Level 4: Nanoscale Continuum**
  - Micromechanics (MAC/GMC) and continuum damage mechanics (CDM) are used to calculate the nonlinear properties of GNP/Epoxy.
- **Level 3: Microscale Matrix**
  - The nonlinear GNP/epoxy properties are homogenized over random orientations in 3-D.
- **Level 2: Lamina Scale**
  - MAC/GMC used to calculate nonlinear response of a CF/GNP/Epoxy composite.



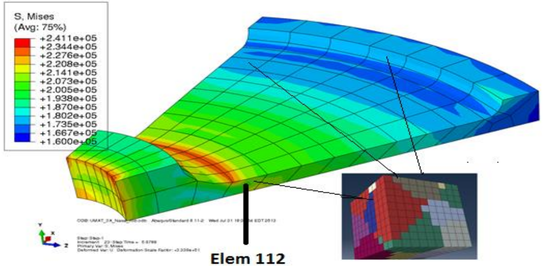
- **Level 1: Laminate Scale.**
  - The OHC strength of CF/GNP/epoxy laminates is predicted using FEA and CDM
- **Level 0: Structural Scale.**
  - Structural sizing of full-scale space structure using OHC strengths from Level1

Multiscale Model for Polycrystalline Structures
Microstructure/Property Relationship

Challenge Problem

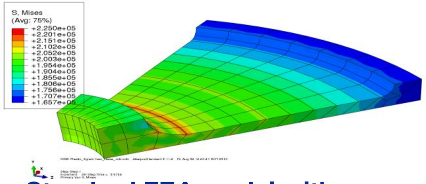


- Utilizes NASA's ultra-efficient micromechanics methods to link grain and sub-grain behavior to the performance of the structure.
- For polycrystals consisting of 10s to 100s of grains – GMC exhibited 2 to 3 orders of magnitude speed up compared to conventional FEA with minimal loss of accuracy.



FEAMAC used to link macro-scale to micro-scale (each grain crystal plasticity)

Von Misses stress distribution

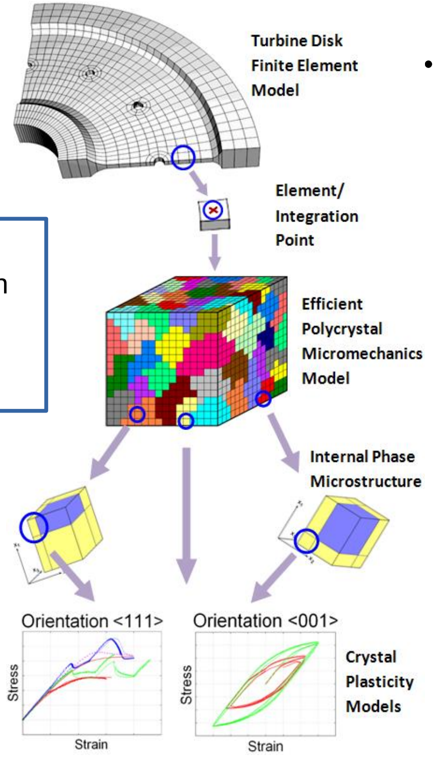


Standard FEA model with macroscale constitutive relationship

Multiscale Model for Polycrystalline Structures

Microstructure/Property Relationship

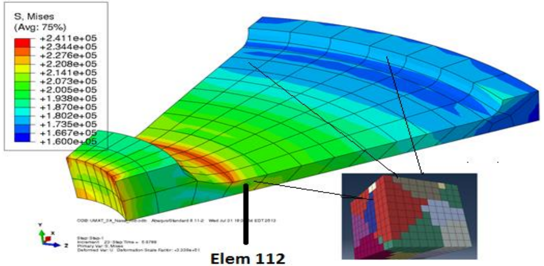
Challenge Problem



This presentation focused on this problem!!!

- Utilizes NASA's ultra-efficient micromechanics methods to link grain and sub-grain behavior to the performance of the structure.
- For polycrystals consisting of 10s to 100s of grains – GMC exhibited 2 to 3 orders of magnitude speed up compared to conventional FEA with minimal loss of accuracy.

For homogenization (when comparable assumptions included)



FEAMAC used to link macro-scale to micro-scale (each grain crystal plasticity)

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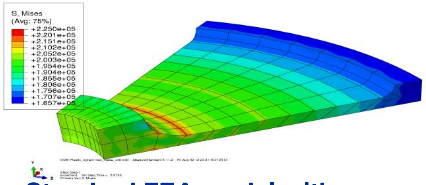


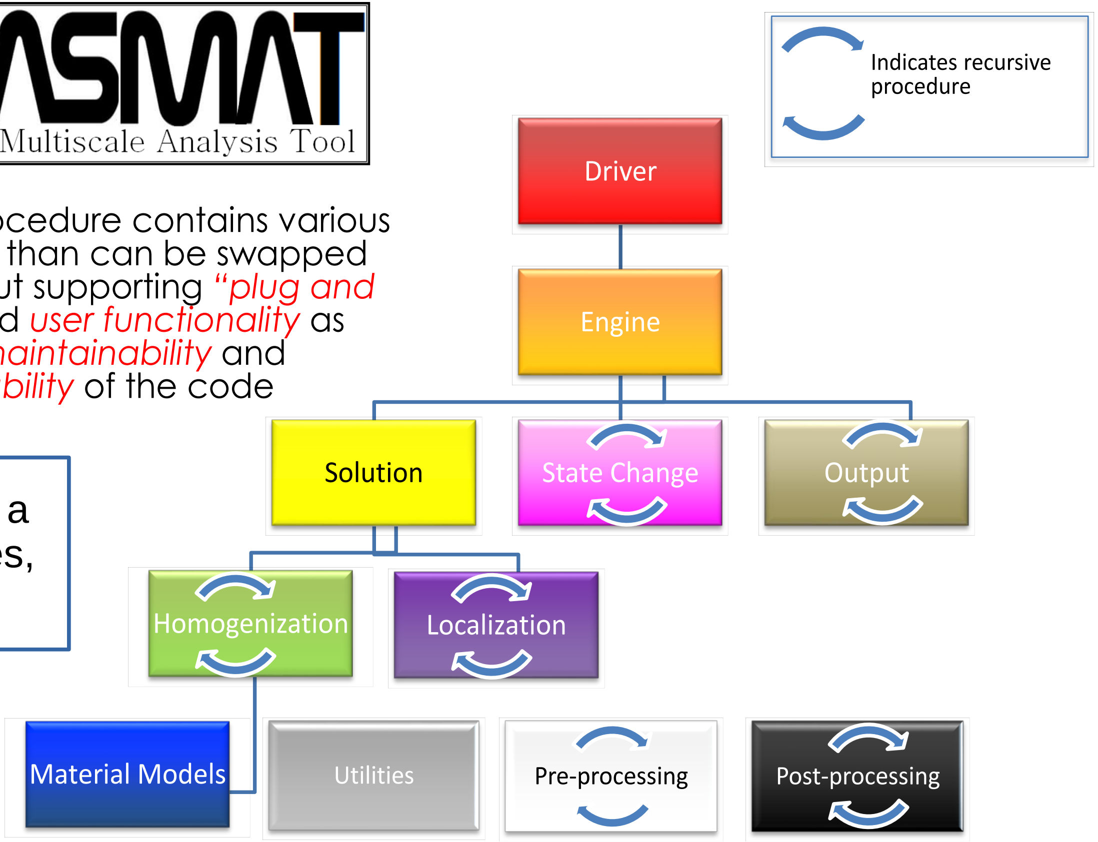
Standard FEA model with macroscale constitutive relationship

"Damage" (i.e., yield, fracture, etc) typically dependent on invariants

NASA Multiscale Analysis Tool

NASMAT
NASA Multiscale Analysis Tool

- Each procedure contains various modules than can be swapped in and out supporting *"plug and play"* and *user functionality* as well as *maintainability* and *upgradability* of the code

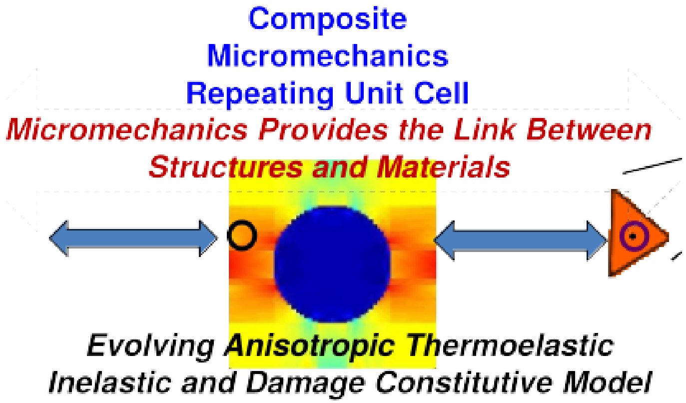


Note: parallelization is a challenge across scales, (current push)

Method of cells limitations (GMC)
(especially with respect to localization of damage mechanics)

- Normal stresses are assumed constant, consequently shear stresses are also assumed constant

$$\sigma_{xx,x} + \sigma_{yx,y} + \sigma_{zx,z} + b_x = \rho\, a_x$$
$$\sigma_{xy,x} + \sigma_{yy,y} + \sigma_{zy,z} + b_y = \rho\, a_y$$
$$\sigma_{xz,x} + \sigma_{yz,y} + \sigma_{zz,z} + b_z = \rho\, a_z$$



- There is no normal-shear stress coupling in equilibrium (i.e., no shear lag)
    - Lack of coupling draws into question localized damage
    - Especially when not invariant based
- The spatial distribution of invariants within GMC are impacted

Goals

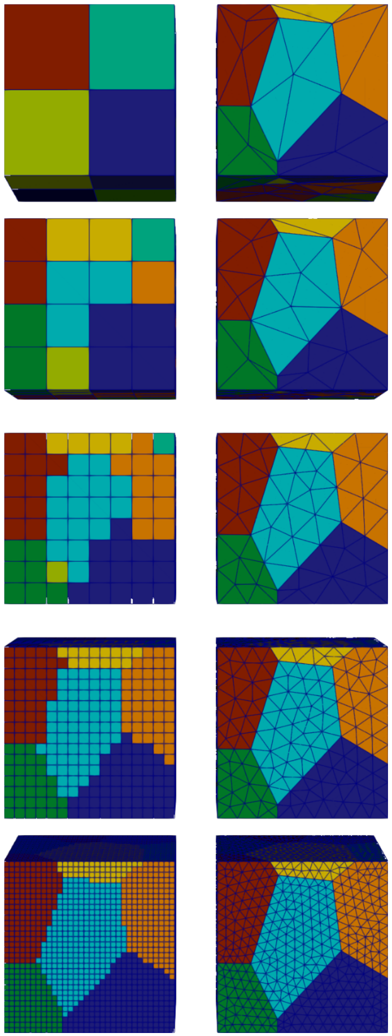
- To increase the accuracy of GMC models <u>without sacrificing speed</u>
  - Primarily focused on hierarchical multi-scale models and <u>***localization***</u>
    - (In my view, accurate damage prediction requires accurate localization whereas accurate stiffness converges quickly via homogenization)
  - Permit accurate shear-normal coupling to allow for effective failure analysis
    - (and filtering or down-selection for hierarchical models)

Side Note: My work is complementary to Josh's ML work on NASMAT

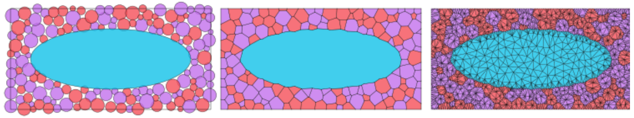
- Josh is generating ML GMC/HFGMC model predictions
  - GMC/HFGMC inputs used as ML inputs for GMC/HFGMC outputs
  - Fast, including damage mechanics
  - <u>Still subject to the limitations inherent in the generalized method of cells (or HFGMC)</u>

Method - Models

- Training data:
  - Finite element and GMC models
  - GMC RUCs with varying numbers of subcells per model.
- The left column visualizes both the GMC microstructural representation and the voxelized finite element model (C3D8)
- The right columns represent varying mesh densities of the same microstructure.
  - ML models were trained for all of these mesh densities
  - General approach less dependent of mesh density?



Process for generating ML result



- MicroStructPy
  - Create 3D grain structure
  - Based on Voronoi
- Gmsh (Initial meshing)
- CalculiX CGX (Mesh Order Change)
- Python scripts
  - Voxelized FE and NASMAT
  - BCs and Loads
- CalcuiliX CCX (FEA solver)
- NASMAT
- Hdf5 for data storage
- Paraview (postprocessing)
- Tensorflow (Machine Learning)

Gmsh

A three-dimensional finite element mesh generator with built-in pre-processing facilities

Christophe Geuzaine and Jean-François Remacle

Download | Documentation | Licensing | Screenshots | Links | References |

Gmsh is an open source 3D finite element mesh generator with a built-in CAD engine and post-processor. Its design goal is to provide a fast, l meshing tool with parametric input and advanced visualization capabilities. Gmsh is built around four modules: geometry, mesh, solver and po specification of any input to these modules is done either interactively using the graphical user interface, in ASCII text files using Gmsh's own s files), or using the C++, C, Python or Julia Application Programming Interface (API).

See this general presentation for a high-level overview of Gmsh and recent developments, the screencasts for a quick tour of Gmsh's graphic reference manual for a more thorough overview of Gmsh's capabilities, some frequently asked questions and the documentation of the C++, C

The source code repository contains many examples written using both the built-in script language and the API (see e.g. the tutorials and the

Download

CALCULIX

A Free Software Three-Dimensional Structural Finite Element Pro

Version 2.18 is available

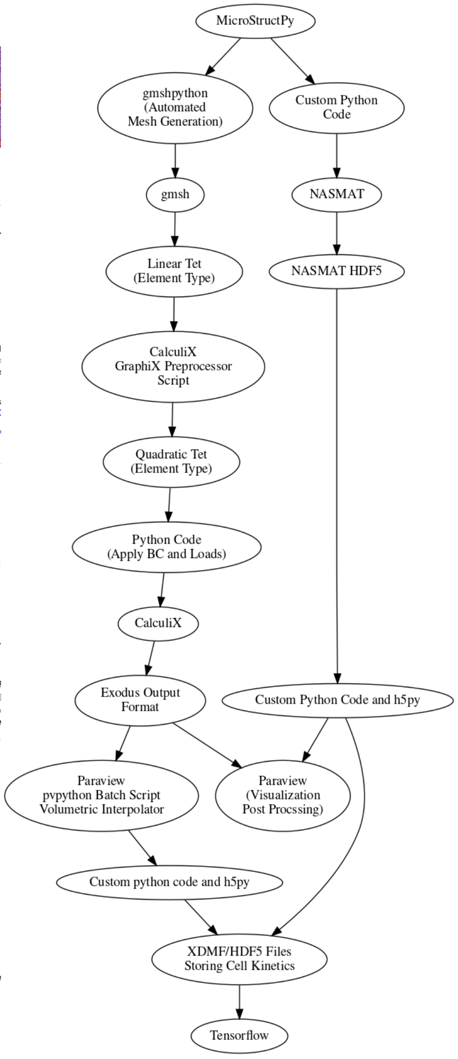
Last updated: 19. Sep 19:29:40 CEST 2021

CalculiX is a package designed to solve field problems. The method used is the finite element method.

With CalculiX Finite Element Models can be built, calculated and post-processed. The pre- and post-processor is an interactive 3 openGL API. The solver is able to do linear and non-linear calculations. Static, dynamic and thermal solutions are available. Bot used independently. Because the solver makes use of the abaqus input format it is possible to use commercial pre-processors as w pre-processor is able to write mesh related data for nastran, abaqus, ansys, code-aster and for the free-cfd codes dolfyn, duns, ISA OpenFOAM. A simple step reader is included. In addition external CAD interfaces are available. The program is designed to run platforms like Linux and Irix computers but also on MS-Windows.

ParaView

TensorFlow



Model boundary conditions

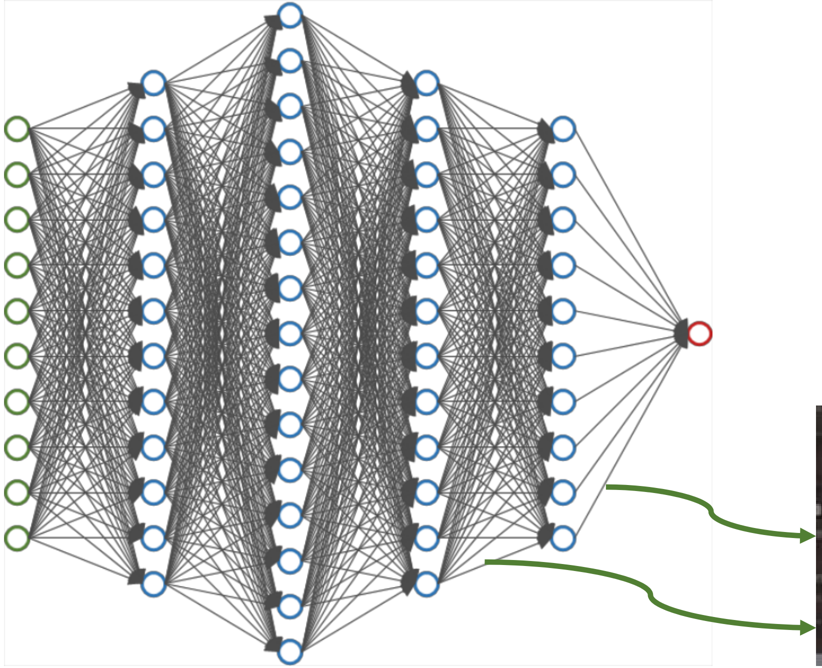
- FEA
  - Planar MPCs for face nodes, controlled by corner nodes
  - Strain control imposed on corner nodes as steps
- NASMAT
  - User strain control (one strain per model)
  - Traction periodicity on boundary subcell faces (NASMAT standard)
- Both
  - 6 isolated strain components at +- 0.001 level
  - 12 total loads (in 12 steps or 12 models)
- 1000 Randomized microstructures, 12,000 total samples

Tensorflow details

TensorFlow

- Strains were scaled by a factor of 1000
  - (thus, were approximately in the range of -1 to 1).
- Stresses were scaled by a factor of 1/1000
  - (and thus were also in the -1 to 1 order of magnitude).
- Data sets were split into training (80%), validation (15%), and testing (5%)
- The ‘relu’ activation function was used in each layer
  - **Except the final dense layer**
  - Utilized a ‘linear’ activation function to permit tensile and compressive output
- Loss function - ‘mean squared error’
- Optimizer - ‘adam’.

Training (Obligatory Representation Satisfied)

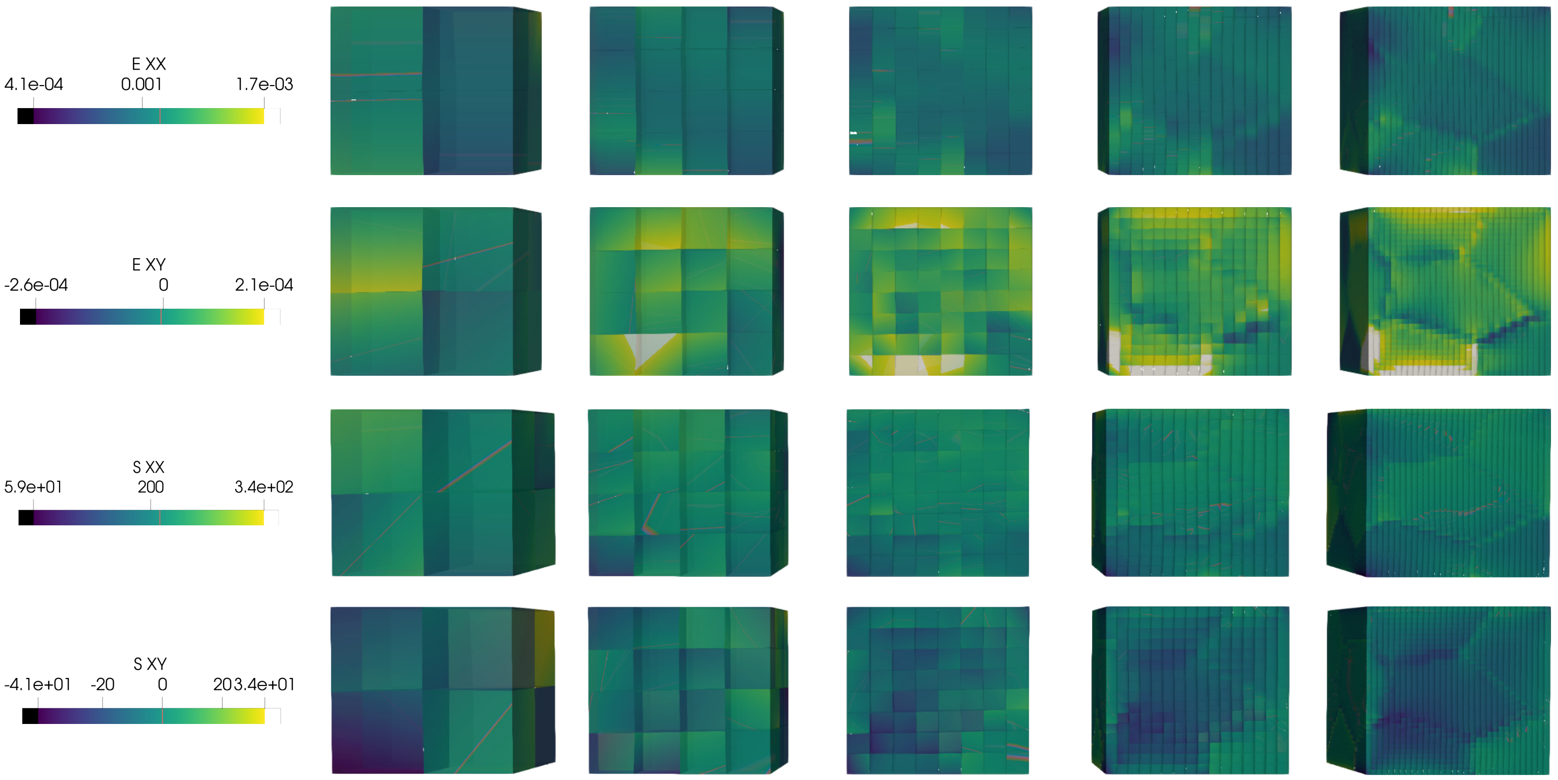


Weight update:

$$w \leftarrow w - \alpha \frac{\partial L}{dw}$$

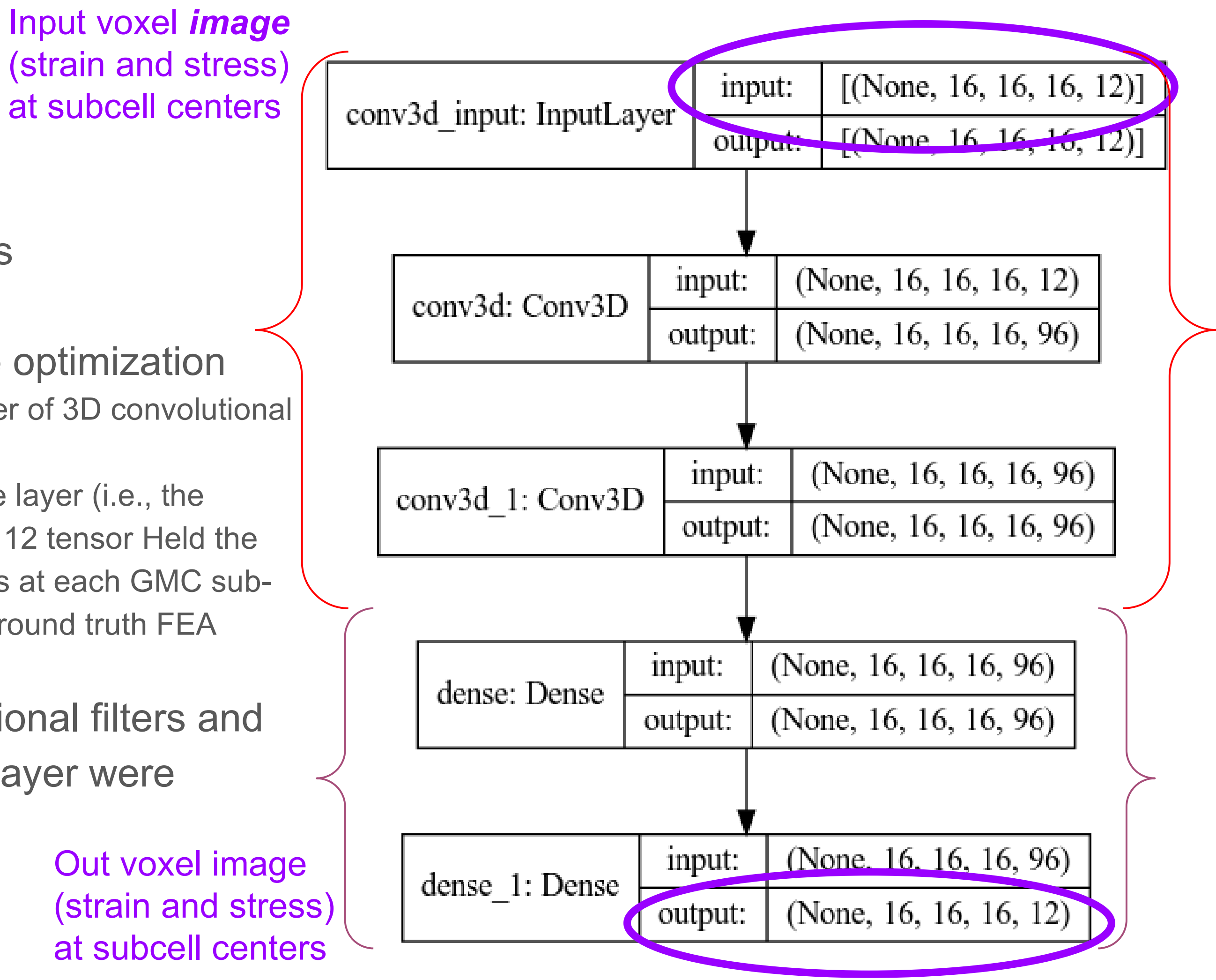
joshua.stuckner@nasa.gov

FEA Stress and strain predictions



Architecture

- # of Convolutional layers
- # of Dense layers
- Grid search architecture optimization
  - Each combining a number of 3D convolutional and dense layers.
  - The input and final dense layer (i.e., the output) was a n x n x n x 12 tensor Held the input stresses and strains at each GMC sub-cell and corresponding ground truth FEA outputs of the same.
- The number of convolutional filters and dense neurons in each layer were integer multiplier of 12.

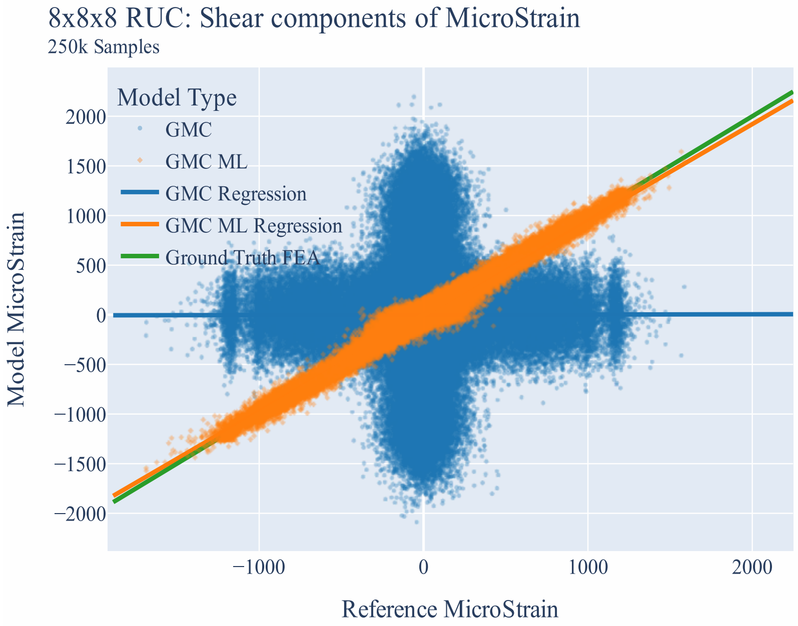


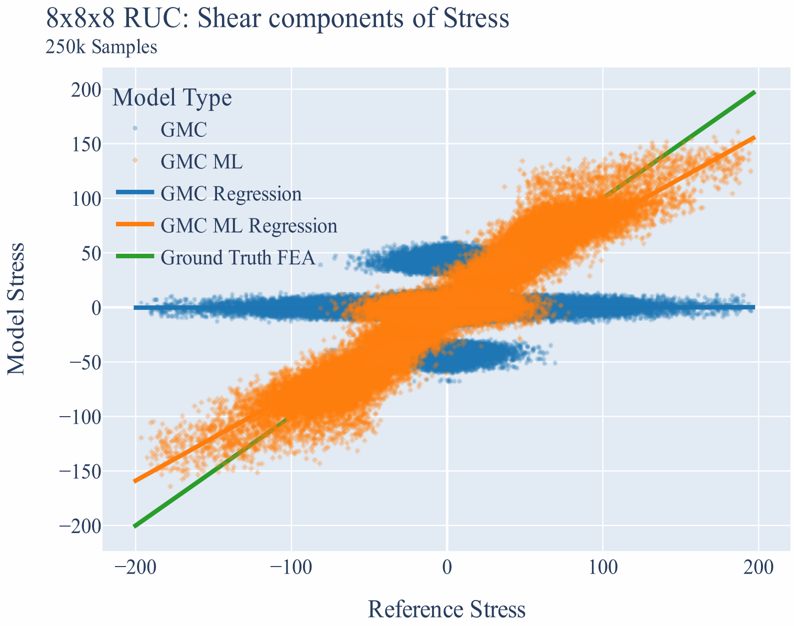
Physical measures of ML model quality?

- Training on minimization of the loss function
  - Hard (for me) to interpret
  - Especially in the context of mixed units on inputs
  - Scaling choices *<u>necessarily impact loss function</u>*
- After training, consider Strain/Stress slopes as a physically meaningful metric
  - Each plotted against the ground truth
    - for each cumulative subcell of each RUC
    - Linear slope and Pearson correlation (r^2) values were also used to assess model quality.
      - Ideal → slope of 1 and an r^2 value of 1
    - Scatter plots for each ML model, visual evaluation

What does the goal look like? What is ideal?

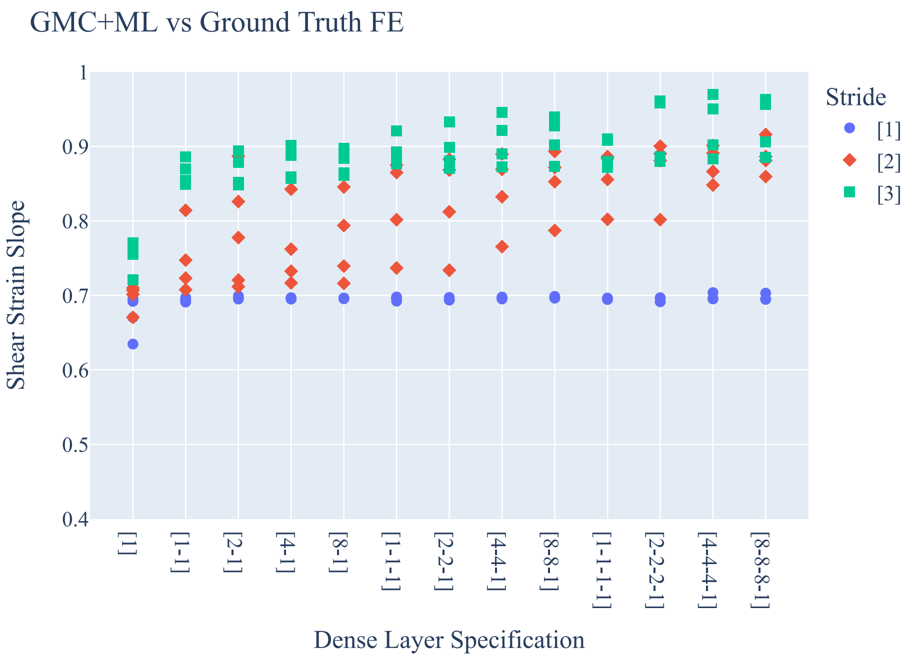
- This example, nearly ideal strain correction
- Similar stress correction (though not as good here)

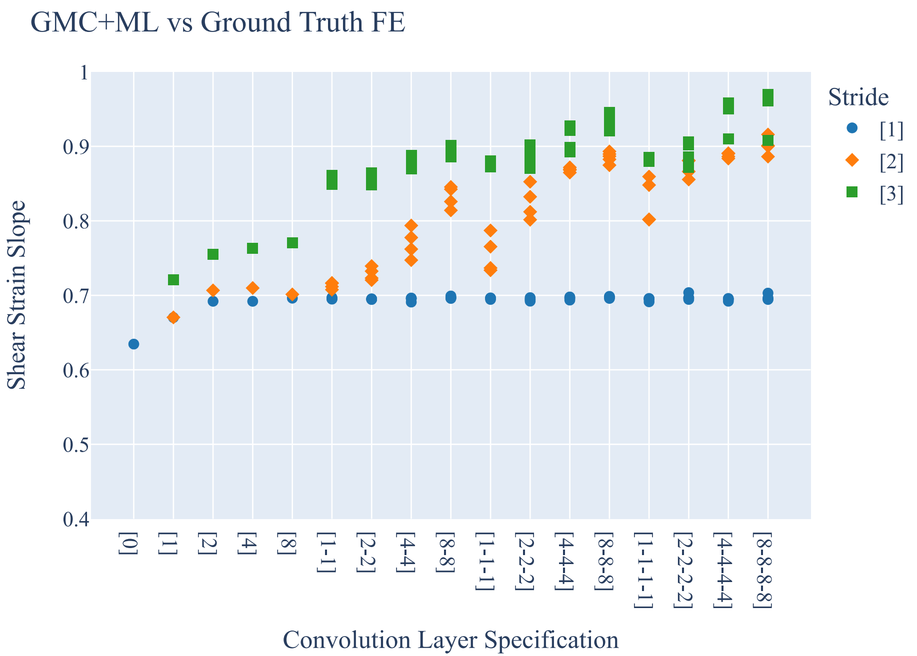




(overfitting a factor?)

ML architecture feature exploration
Layers vs Slope (**Accuracy**)
(Up is more accurate, right is more complex)

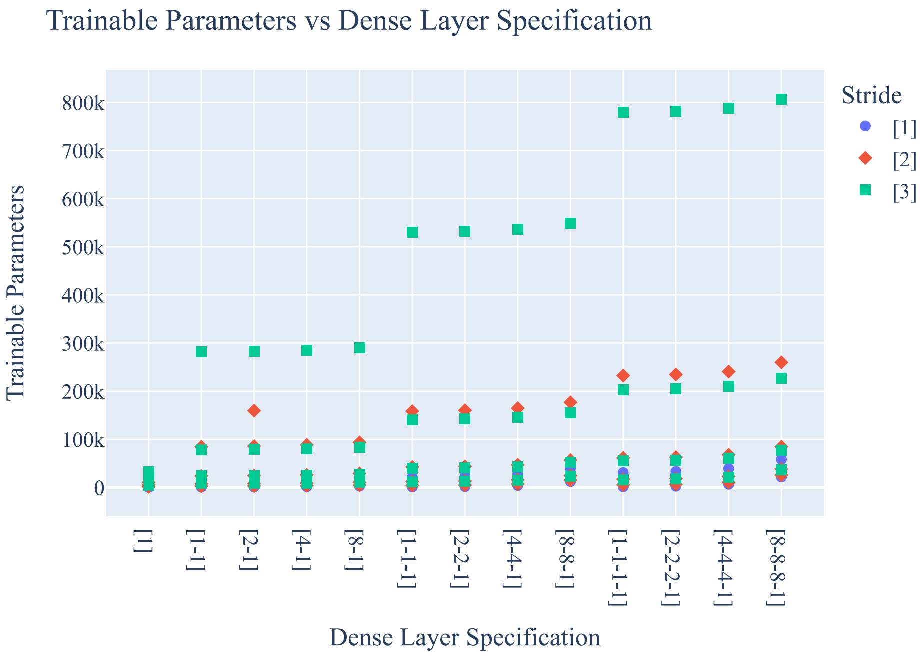


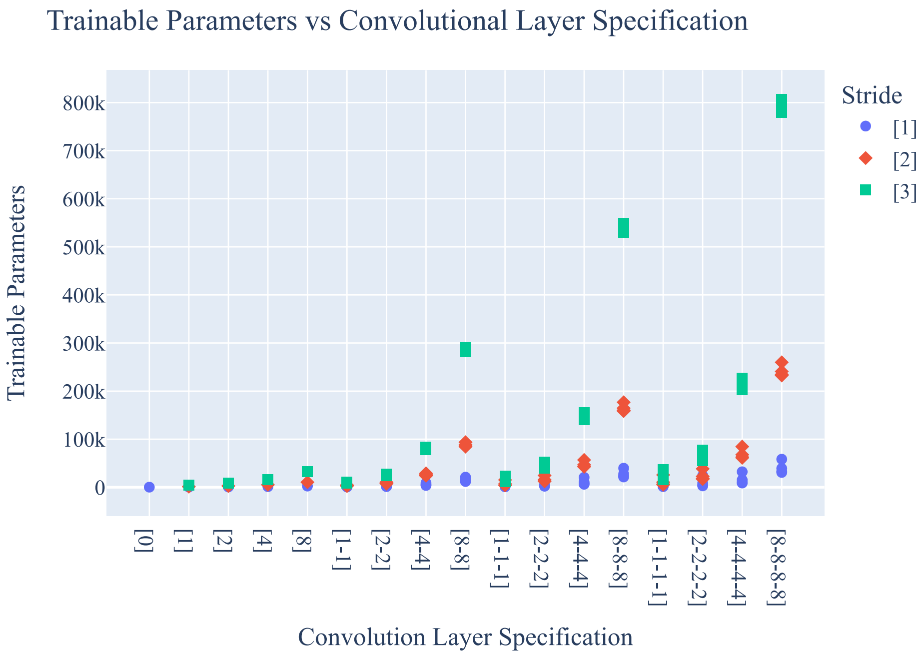


ML architecture feature exploration

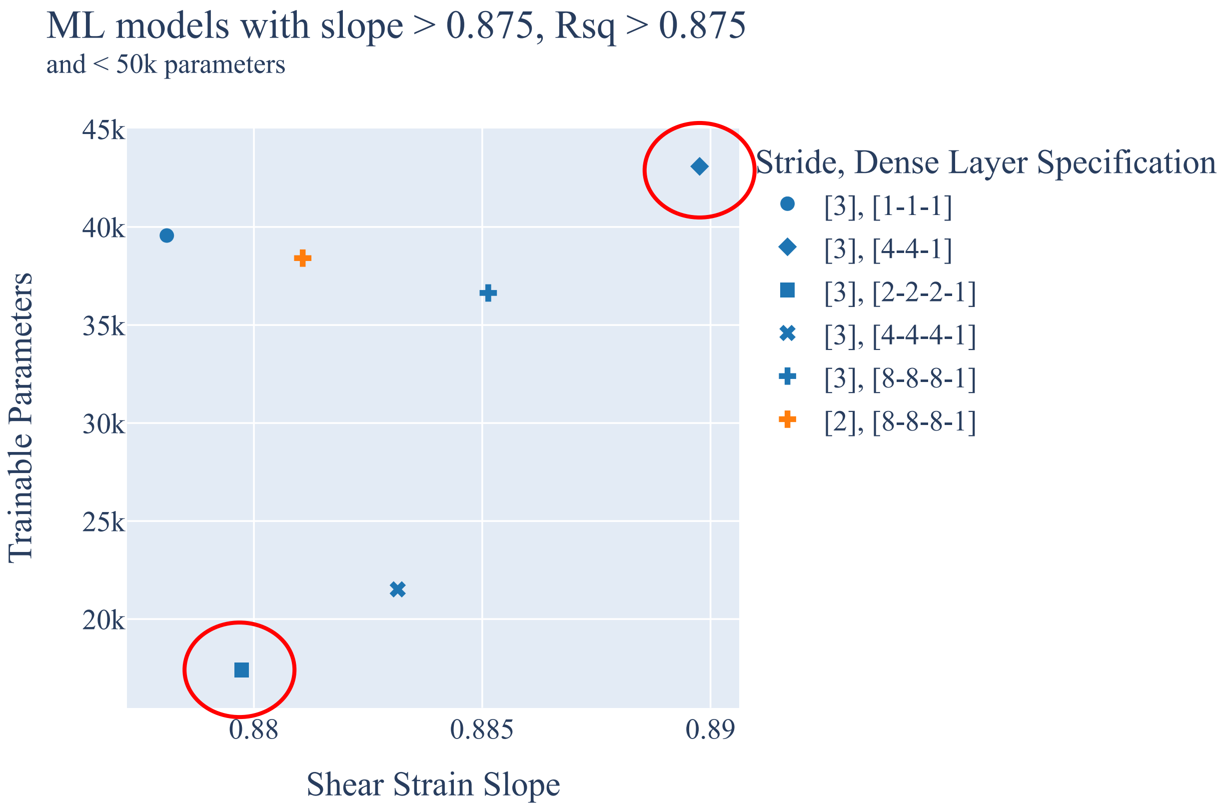
Layers vs **Cost** (Trainable Parameters)
(Up is more costly, right is more complexity of layers)

Cost of training and use





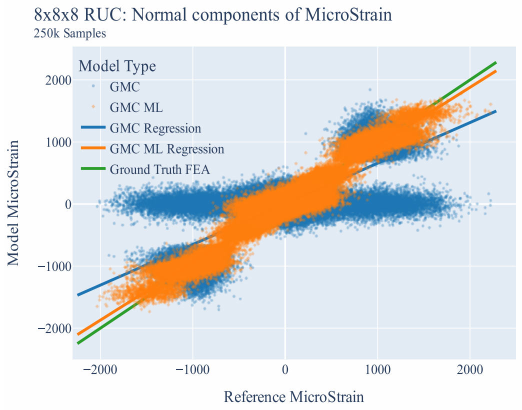
Fast and accurate models

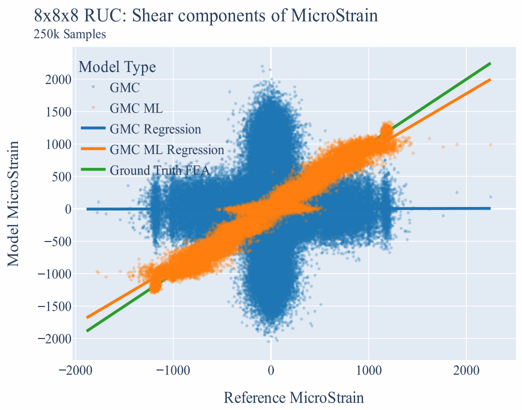


Fast Model: 4 Convolutional Layers [1-1-1-1], 4 dense layers [2-2-2-1], and stride=3 (17,412 parameter model)

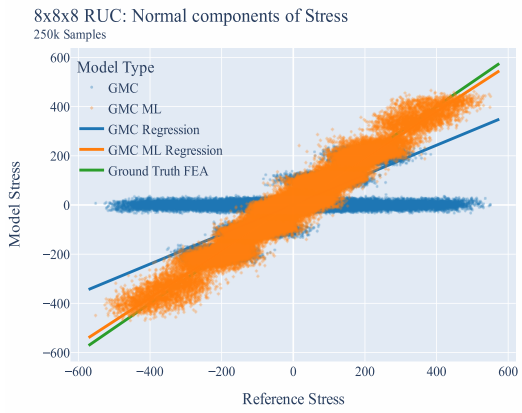
Normal | Shear

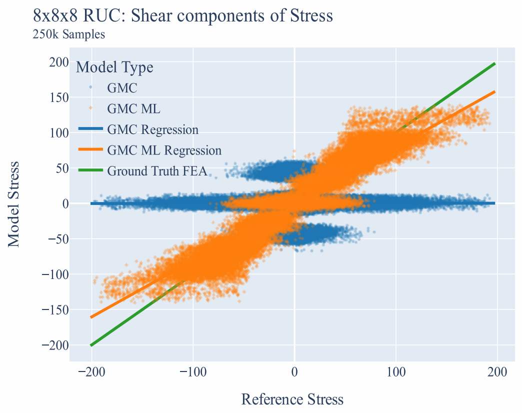
Strain





Stress



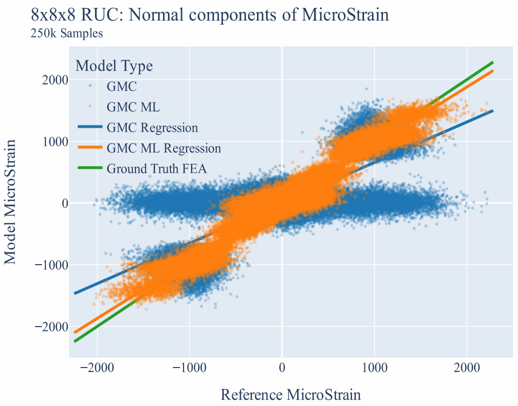


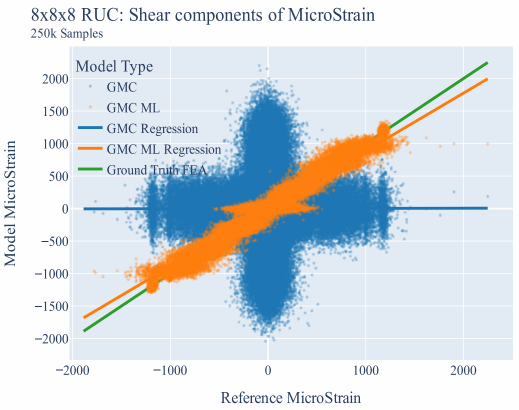
Fast Model: 3 Convolutional Layers [2-2-2], 3 dense layers [4-4-1], and stride=3 (43,092 parameter model)

Normal

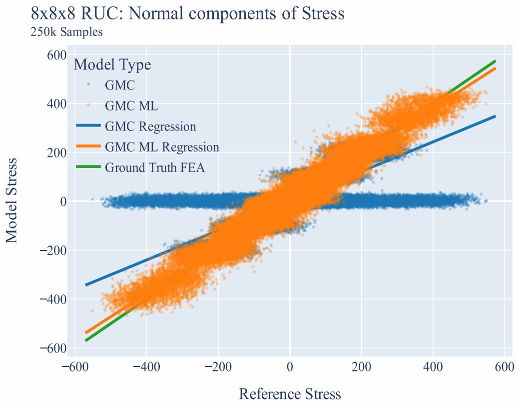
Shear

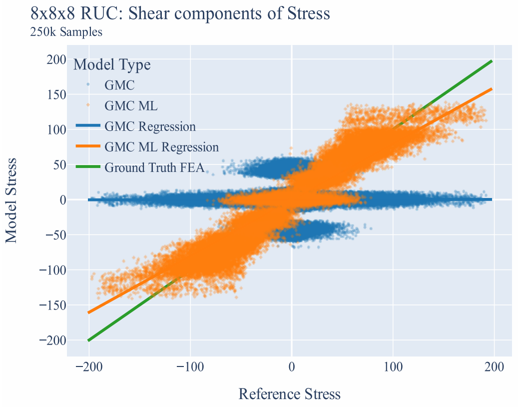
Strain





Stress



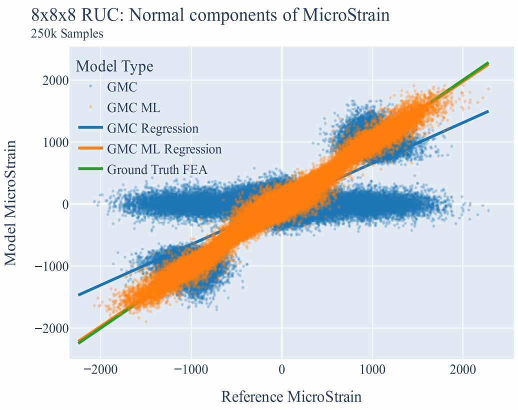


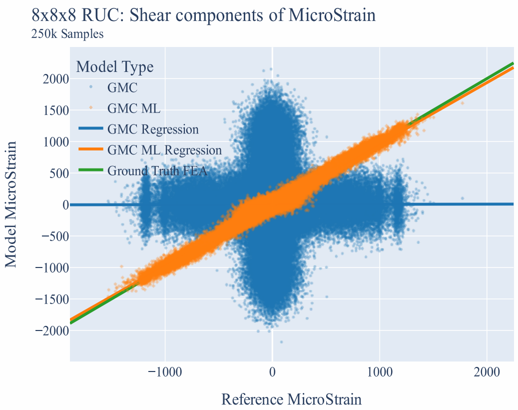
Best Shear Strain Matching: 4 Convolutional Layers [8-8-8-8], 4 dense layers [4-4-4-1], and stride=3 (787,932 parameter model)

Normal

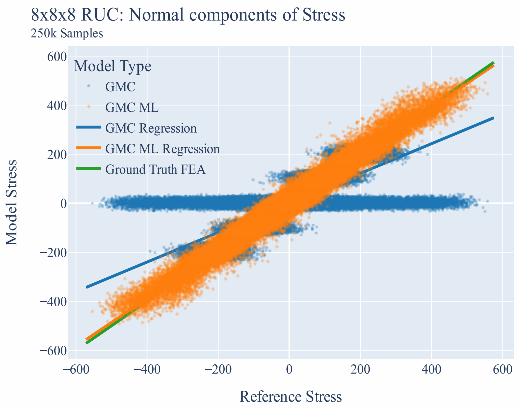
Shear

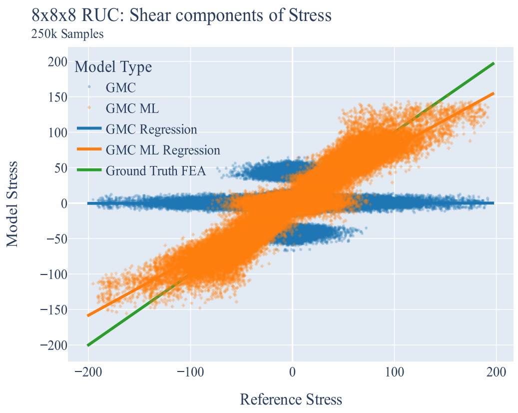
Strain





Stress



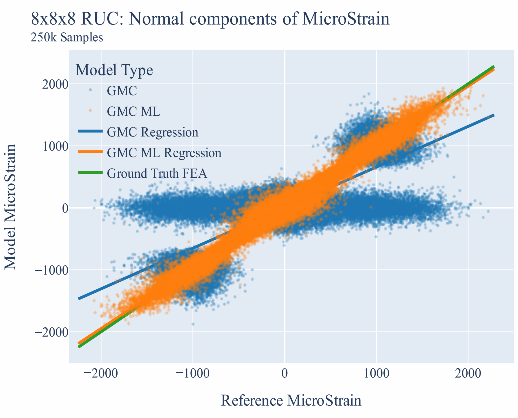


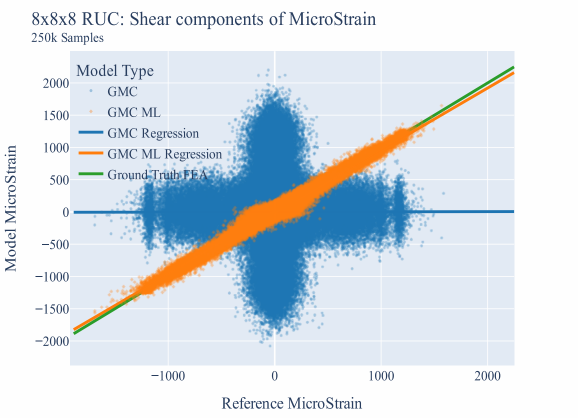
Best Pearson Correlation Coef (r2) for Shear Strain: Predictions with 4 Convolutional Layers [8-8-8-8], 4 dense layers [8-8-8-1], and stride=3 (807,084 parameter model)

Normal

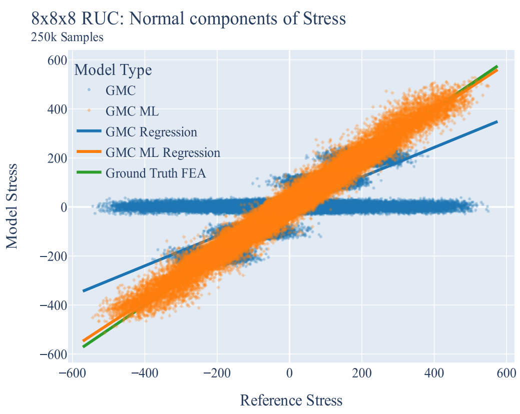
Shear

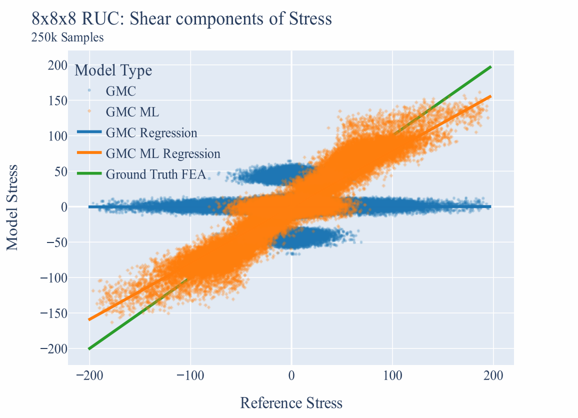
Strain





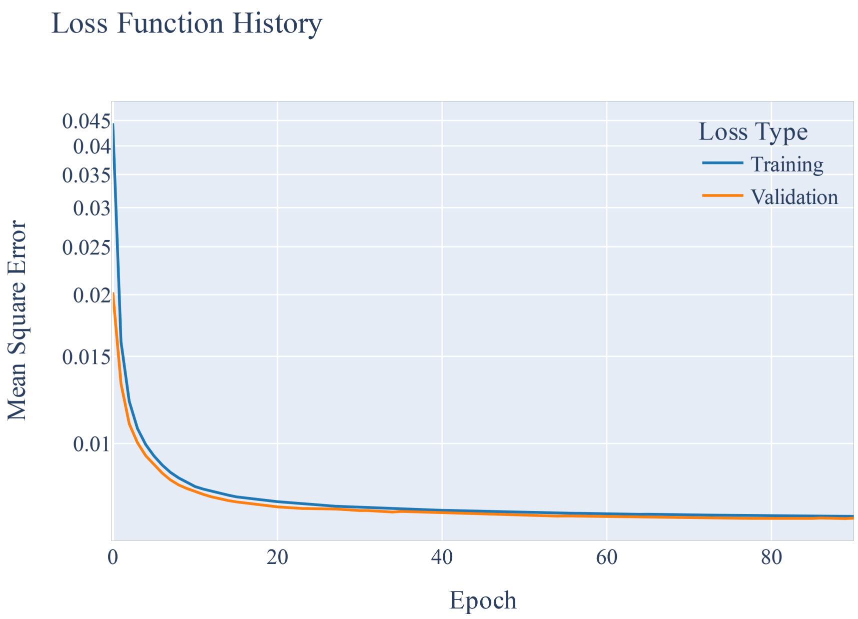
Stress

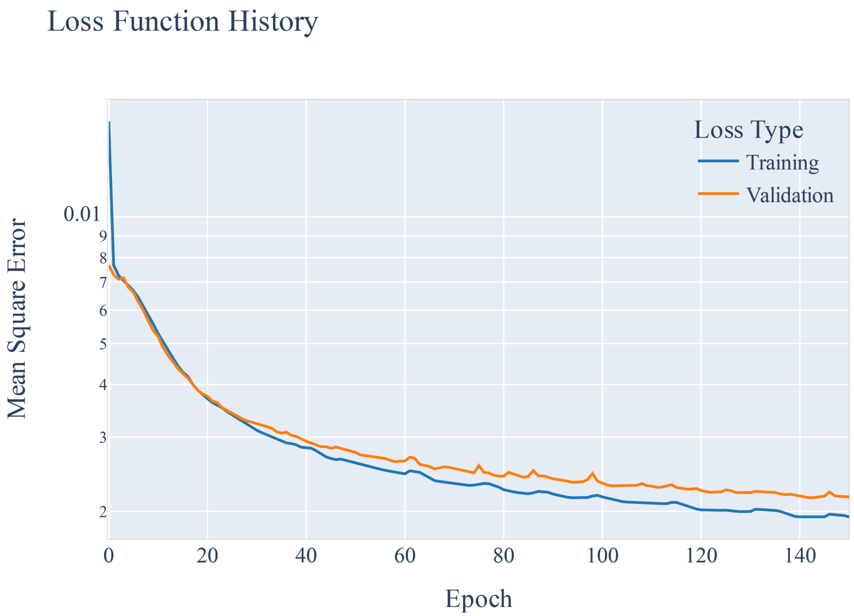




Representative Fast vs Best Loss functions

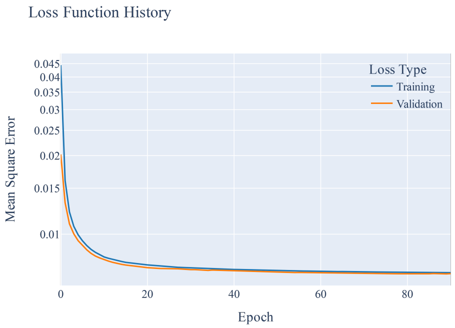
- Successful training exhibits a decreasing loss function for both training and validation loss as training proceeds.

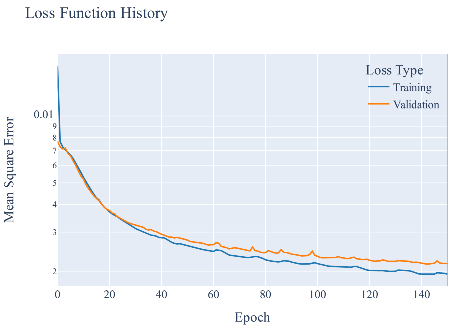




Note scale is different!

Overfit and underfit?





- The fast models:
  - Training and validation curves decrease and converge asymptotically with validation loss near training loss
  - **Thus: accurate, well behaving, and do not exhibit overfitting.**
- Large parameter models (i.e., the best slope and best r^2)
  - Validation loss is somewhat larger than the training loss after approximately 20 epochs.
    - Validation loss still decreasing
    - Suggests more training necessary
    - **Overfitting may be a concern**

Speed and computational cost

Method	Calculation Time (milliseconds)
GMC: Single CPU, Single Load (Optimized MAC/GMC)	**27.00**
GMC: Single CPU, Single Load (Unoptimized NASMAT)	603.00
CalculiX: Single CPU, Single Load (Hex Mesh)	374.24
CalculiX: Single CPU, Single Load (Tet Mesh)	708.81

Speed and computational cost

Method	Convolutional Layer Spec	Dense Layer Spec	Stride	Calculation Time (milliseconds)	Correction Cost %
ML Correction: Parallelized corrections, GPU	[1-1-1-1]	[2-2-2-1]	3	1.84	6.8%
ML Correction: Parallelized corrections, GPU	[2-2-2]	[4-4-1]	3	1.40	5.2%
ML Correction: Parallelized corrections, GPU	[8-8-8-8]	[4-4-4-1]	3	10.58	39.2%
ML Correction: Parallelized corrections, GPU	[8-8-8-8]	[8-8-8-1]	3	11.66	43.2%

Limitations

- Surrogates are trained only on randomly generated metallic microstructures
  - One randomly oriented constitutive description and one grain size
  - Likely can be generalized
- Timing is apples to oranges
  - Call overhead not well accounted
  - Parallelization of GMC in NASMAT not accounted

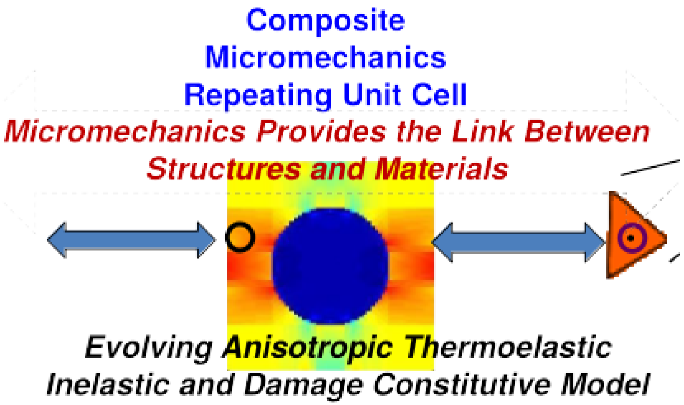
- Despite the limitations noted
  - Demonstrated **fidelity correction** using machine learning.
  - Addresses one of the *most significant criticisms* of the generalized method of cells
    - i.e., addresses lack of coupling of normal and shear through shear lag

Conclusions

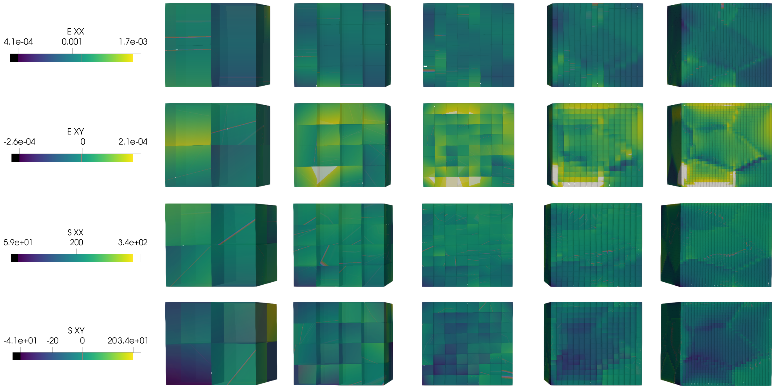
- Strains/Stress were enhanced using machine learning and FE ground truth strain/stress
- GMC+ML Shear improved from inaccurate and uncorrelated (slope=0.003, r^2=0.000) to accurate and well correlated (slope=0.890, r^2=0.882) relative to ground truth.
  - (Ideal slope =1.0, r^2 = 1.0).
- Shear stresses yielded a similar accurate and well correlated result (slope=0.782, r^2=0.800).
- Enhancement was relatively fast, estimated to be a small fraction of computational cost

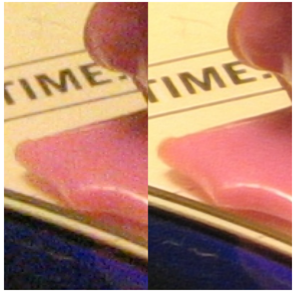
Next Steps (Part 1)

- Examine fibrous composites
  - large differences in local moduli, multiple materials
- Superesolution techniques
  - Efficient prediction of detailed models



Superresolution Enhancement

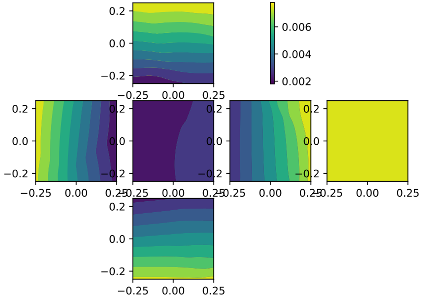




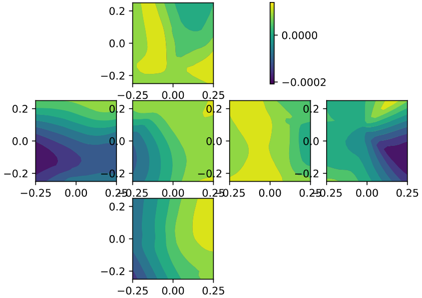
Superresolution Enhancement

Next Steps (Part 2)

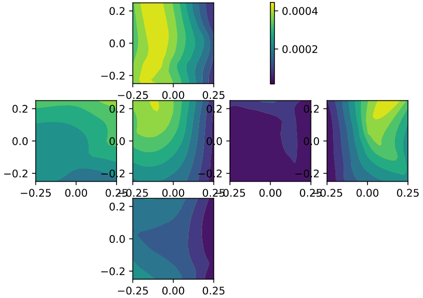
- Effect of boundary conditions
  - Assumption of periodic BCs inconsistent with assumed RUC internal asymmetries
  - Not critical for homogenization, critical for localization



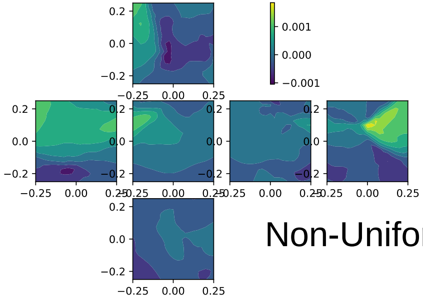
Uniform BC
Displacement (Z)



Non-Uniform BC
Displacement (X)



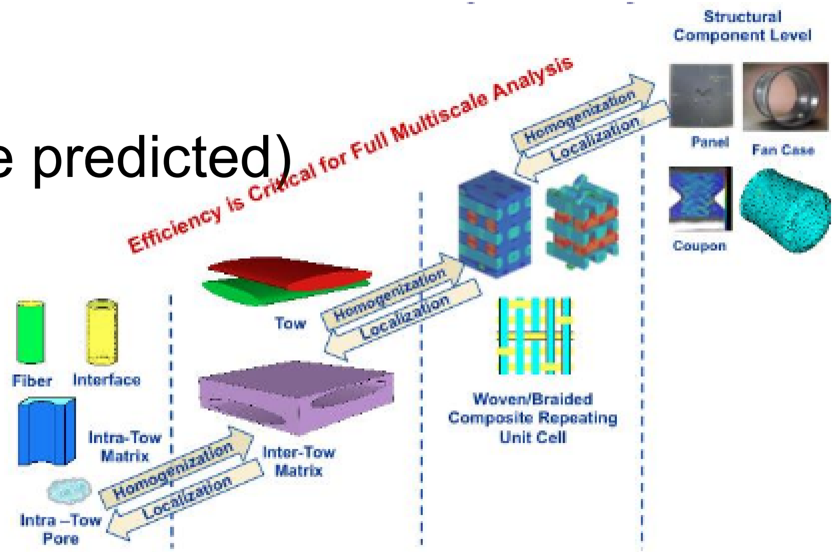
Non-Uniform BC
Displacement (Y)



Non-Uniform Strain (Exx)

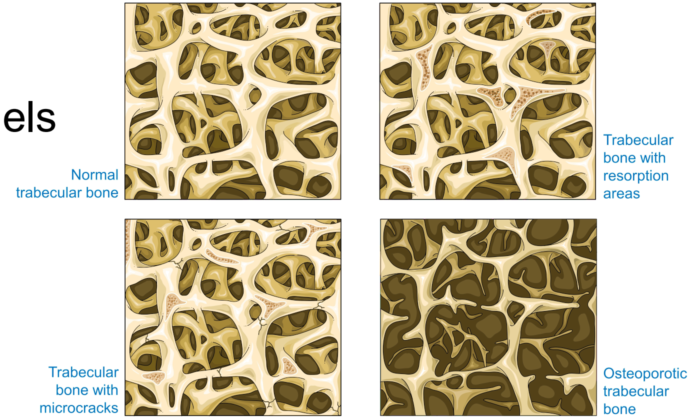
Next Steps (Part 3)

- Multi-scale outcomes
  - Quantify how improved strain/stress predictions cascade through scales
  - Localization is "uniform"
    - (but must also accurately be predicted)

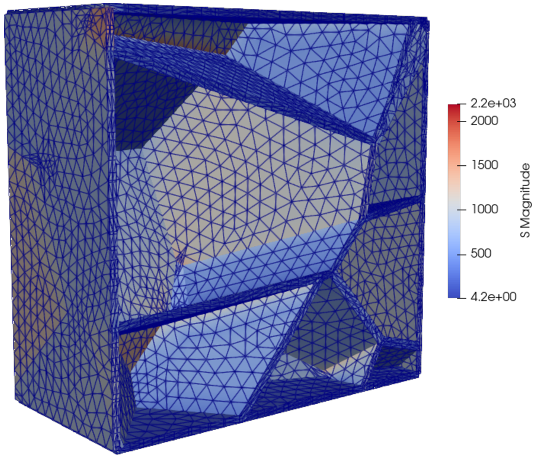


Next Steps (Part 4)

- Damage mechanics, LSTM models
- Localized MLs
  - Train on localized subscales… use for filtering
  - Only calculate lower scales where non-linear damage occurs
- Repeat
  - CMCs
  - thermomechanical models
  - Bone and soft tissue



Laboratoires Servier (Wikipedia)



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- Questions?
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