Correlative modelling of microstructure and stress in Solid Mechanics using Machine Learning

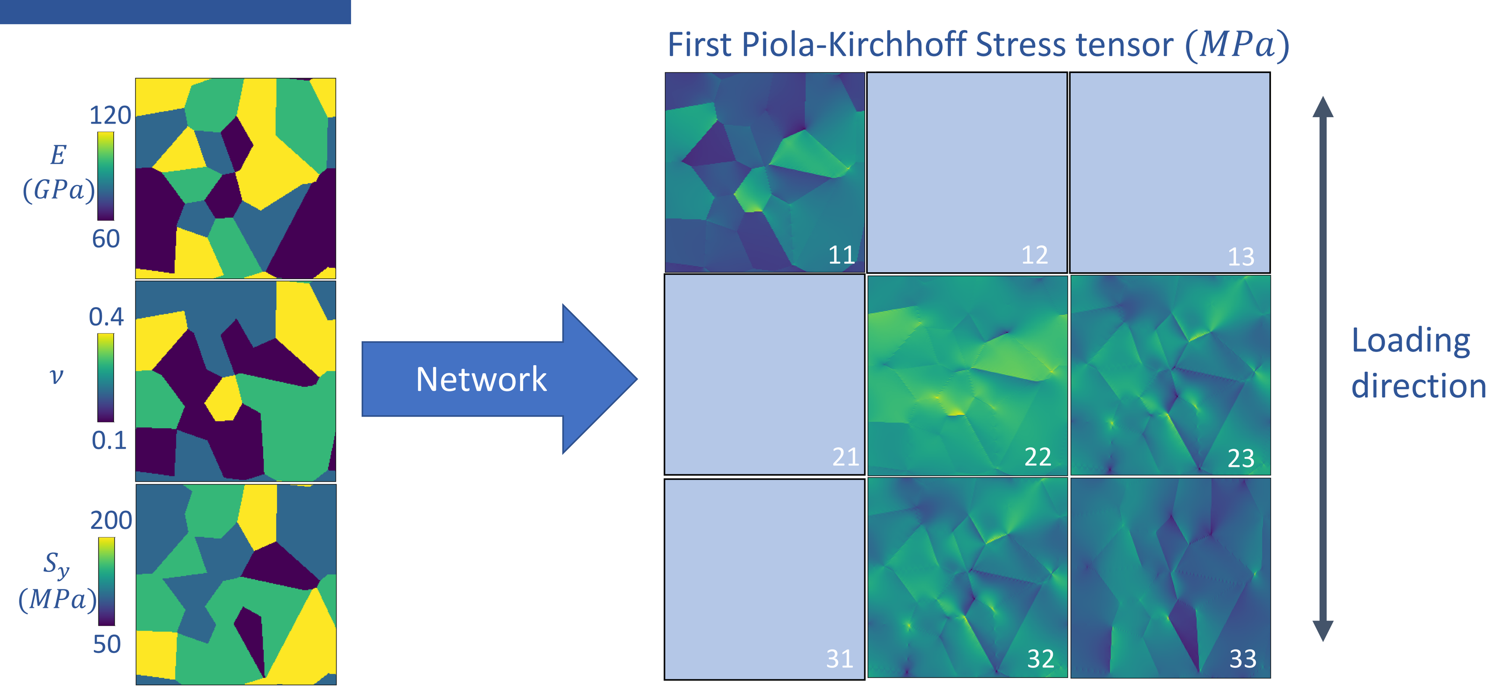
Sarthak Kapoor[1], Jaber Rezaei Mianroodi[2], Bob Svendsen[1,2]

[1]Material Mechanics, RWTH Aachen
[2]Max-Plank Institute for Iron Research, Düsseldorf

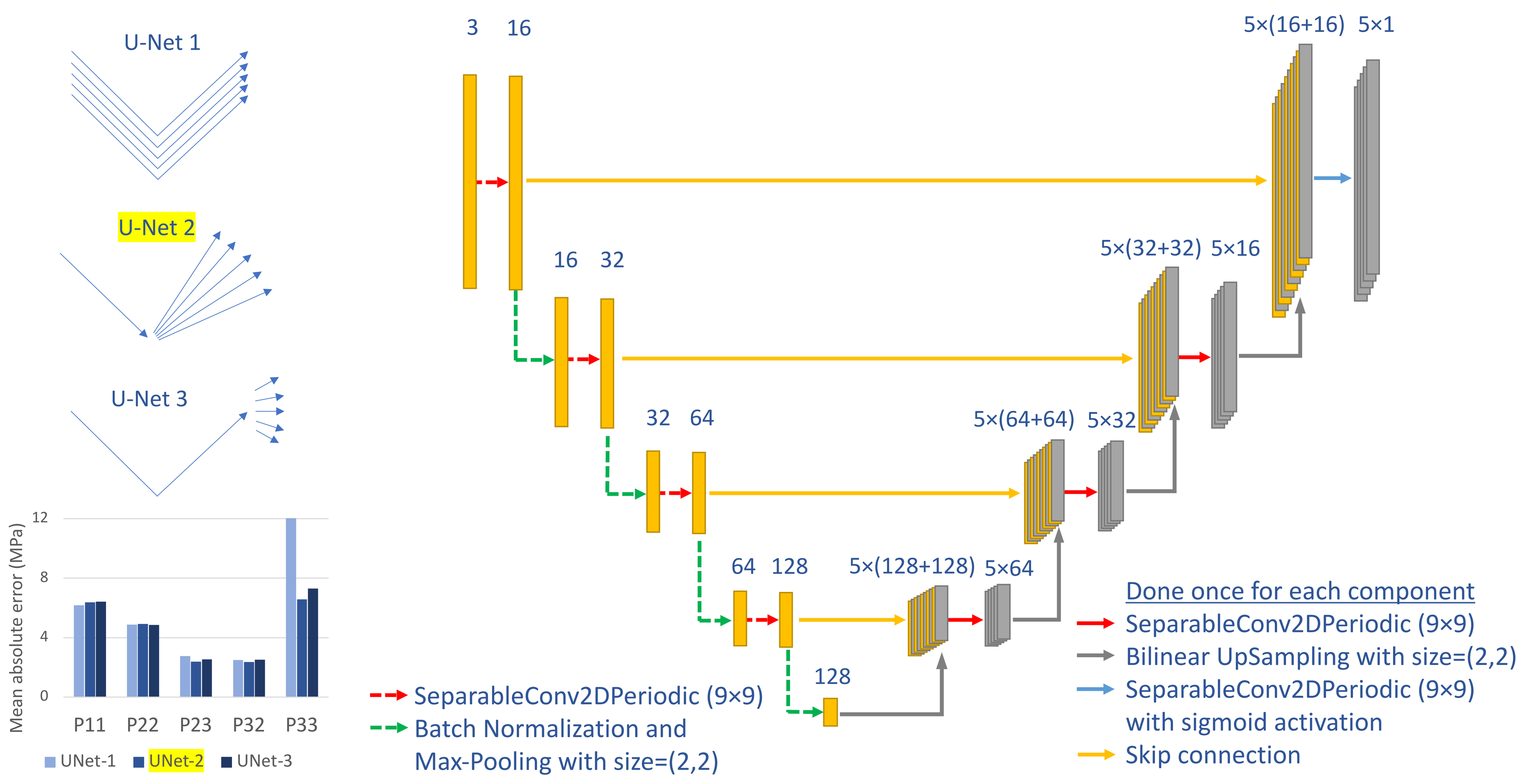
Goals

- Learn mapping between material properties and stress fields for given boundary condition and loading.
- Predict full stress tensor (First Piola-Kirchhoff) with expected speedups
- Study the generalizability of the trained network

Methods

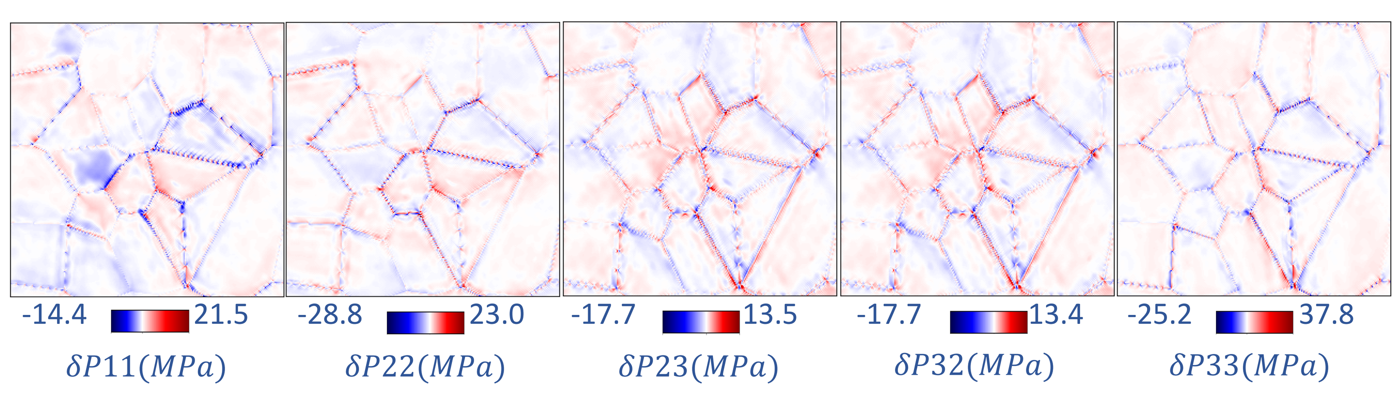


- Spectral Solver (DAMASK)
  - Geometry – 20-seeds Voronoi; square periodic boundary (64px, 256px)
  - Uniaxial tensile loading – gives 5 non-trivial stress fields
  - Material properties at each point picked from defined sets
  - Considerations – Fixed point iterations, convergence, numerical resolution, system size.
- Network (U-Net)
  - Fully-convolutional implementation, MAE loss, Adam optimizer
  - Kernels learned at different resolution, skip connections preserve higher resolution information
  - Multi-output channels start from first decoding stage



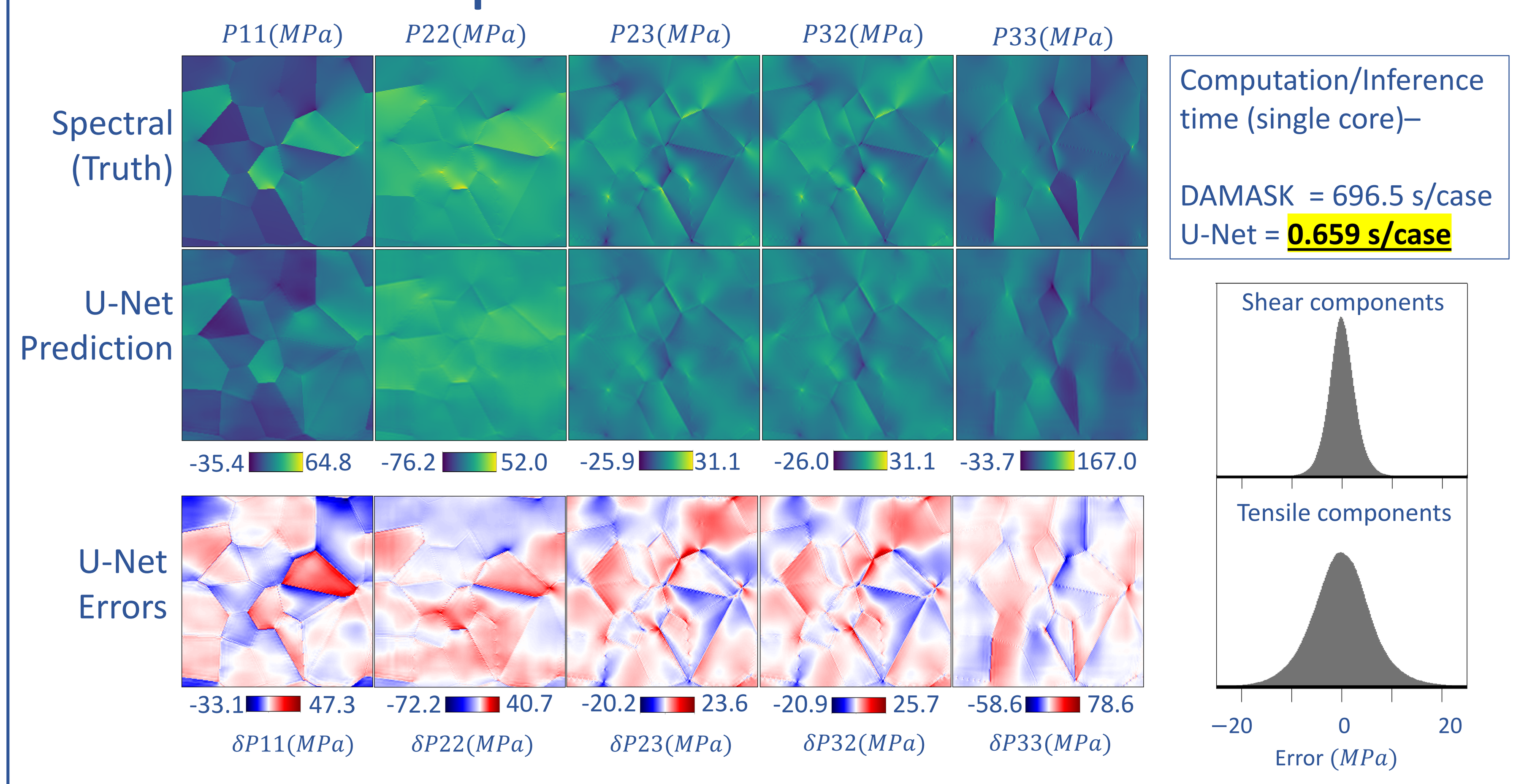
Outlook

- Are the predictions physically correct? Conditions for mechanical equilibrium – PINN
- Another approach – Fourier Neural Operators
  - Lower errors; Discretization-free learning



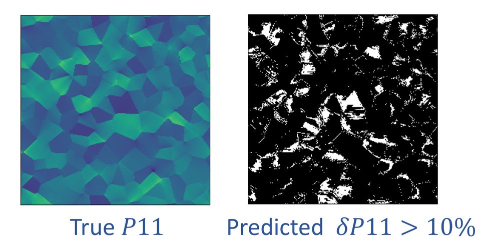
Results

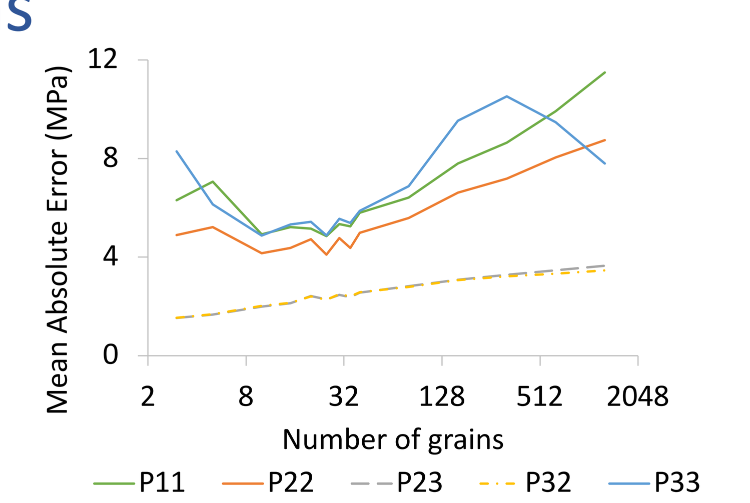
- Stress field predictions and errors



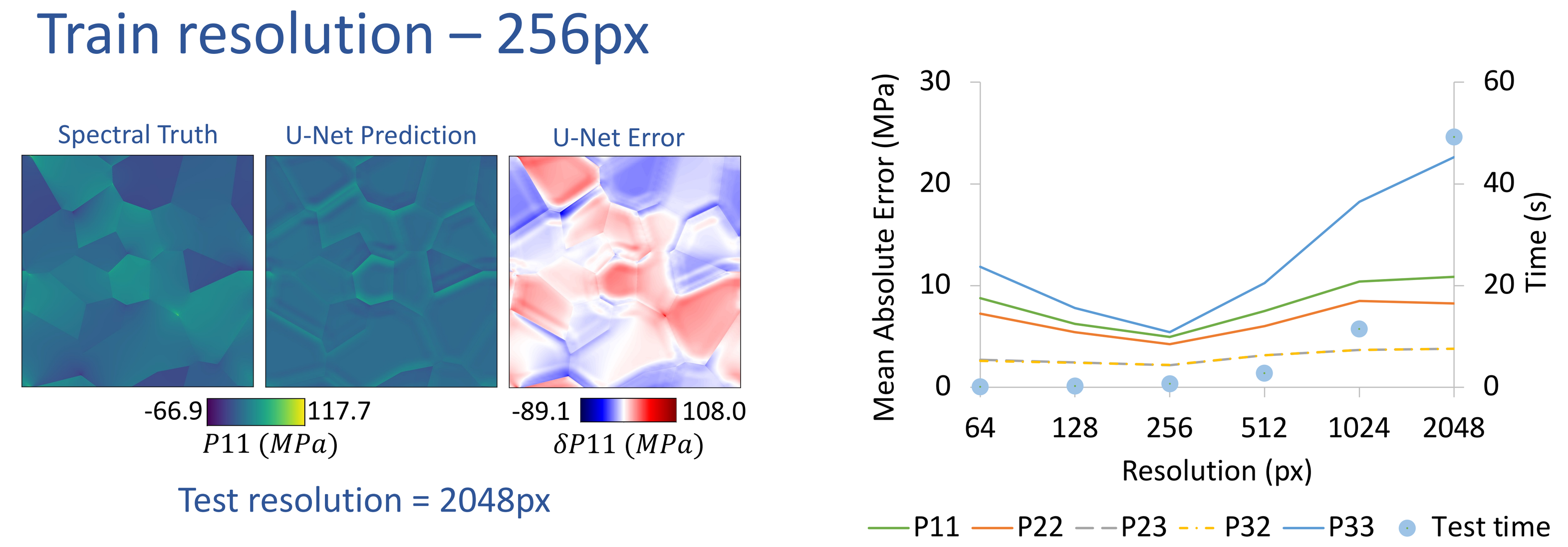
- Generalization
  - Varying the number of grains
    - Train+Test resolution – 256px
    - Errors not only influenced by boundaries

160 grains –

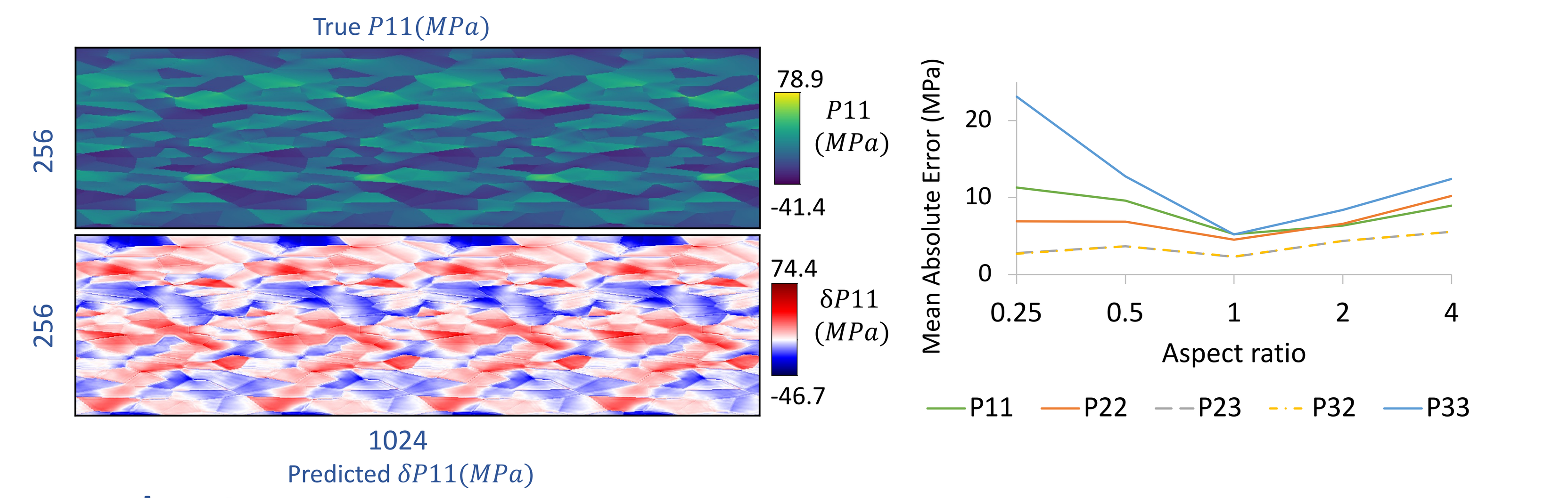




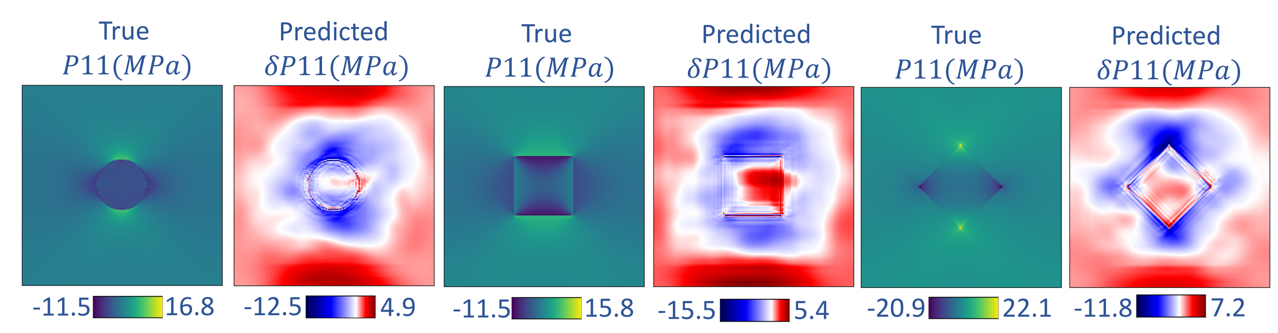
  - Varying the numerical resolution
    - Train resolution – 256px



  - Varying the boundary box aspect ratio



  - Inclusions
    - Two-phase matrix-inclusion



References

1. J. R. Mianroodi et al. Teaching solid mechanics to artificial intelligence-a fast solver for heterogeneous materials. *npj Computational Materials,* 2021.
2. F. Roters et al. DAMASK – the Dusseldorf Advanced Material Simulation Kit for modeling multi-physics crystal plasticity, thermal, and damage phenomena from the single crystal up to the component scale. Computational Materials Science, 2019.
3. Zongyi Li et al. Fourier neural operator for parametric partial differential equations. *CoRR*, abs/2010.08895, 2020.

Materials Mechanics