Neural Network Enhanced RKPM for Electrochemical-Mechanical Coupled Damage Modeling of Energy Storage Materials

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NREL Transforming ENERGY

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Li-ion Battery Electrode Microstructures and Chemo-Mechanical Cracking

Electrode Microstructure and Chemo-mechanical Cracking

Cathode Composition:
- Randomly-oriented grains
- Anisotropic grain material properties

+

Charge Cycling:
- Li movement between electrodes causes nonuniform grain expansion and contraction

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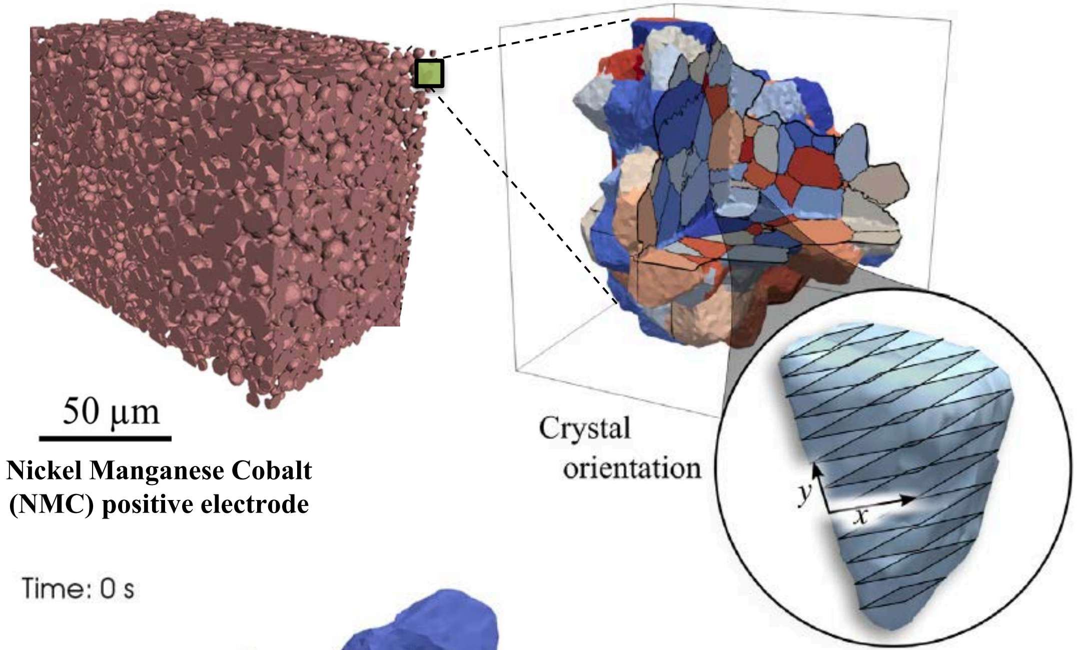
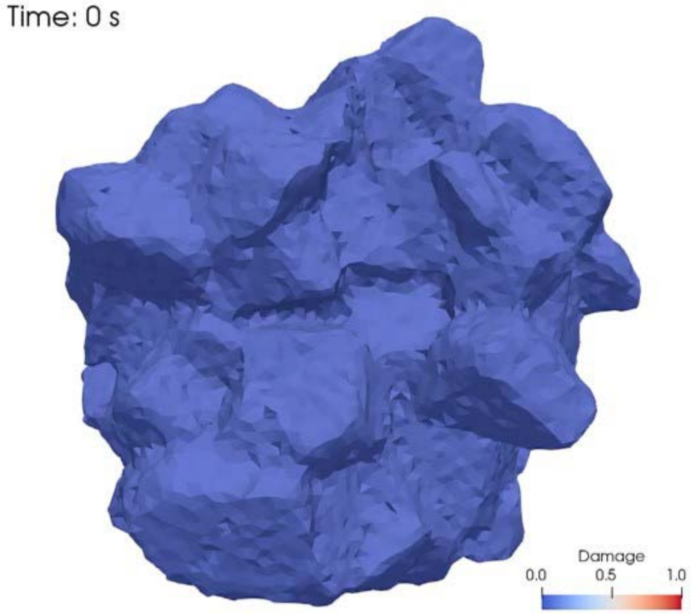
Chemo-mechanical cracking:
- Inhibited Li flow via tortuous diffusion path
- Reduced battery life





1. NREL. “Battery Microstructures Library.” https://www.nrel.gov/transportation/microstructure.html.
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3. Quinn, A., H. Moutinho, F. Usseglio-Viretta, et al. 2020. “Electron Backscatter Diffraction for Investigating Lithium-Ion Electrode Particle Architectures.” *Cell Reports Physical Science* 1, 100137. https://doi.org/10.1016/j.xcrp.2020.100137.

Coupled Electrochemical-Mechanical Formulation

Governing Equations

Electrochemistry Model

$[Li]$

- **Lithium transport → lithium concentration $[\boldsymbol{Li}]$**

$$[\dot{Li}] + J_{j,j} = 0 \quad in\ \Omega \quad (Similar\ to\ a\ transient\ heat\ equation)$$

Fickian diffusion: $J_j = -D_{jk}[Li]_{,k}$

Φ_{NMC}

- **Solid-phase electrostatic potential → $\boldsymbol{\Phi_{NMC}}$**

$$\left(\kappa \Phi_{NMC,j}\right)_{,j} = 0 \quad in\ \Omega \quad (Poisson\ equation)$$

Mechanics Model

$\boldsymbol{u}$

- **Mechanics → $\boldsymbol{u}$**

$$\sigma_{ij,j} = 0 \quad in\ \Omega \quad (Balance\ of\ linear\ momentum)$$

Stress: $\sigma_{ij} = C_{ijkl}\epsilon^{e}_{kl}$

$$\epsilon^{e}_{kl} = \epsilon_{kl} - \epsilon^{[Li]}_{kl}$$

Electrochemistry Boundary Condition (BC): Butler-Volmer Relation

- **Lithium transport → intercalated lithium concentration $[Li]$**

BC: $$\frac{i}{F} = J_k n_k \qquad on\ \Gamma_h$$

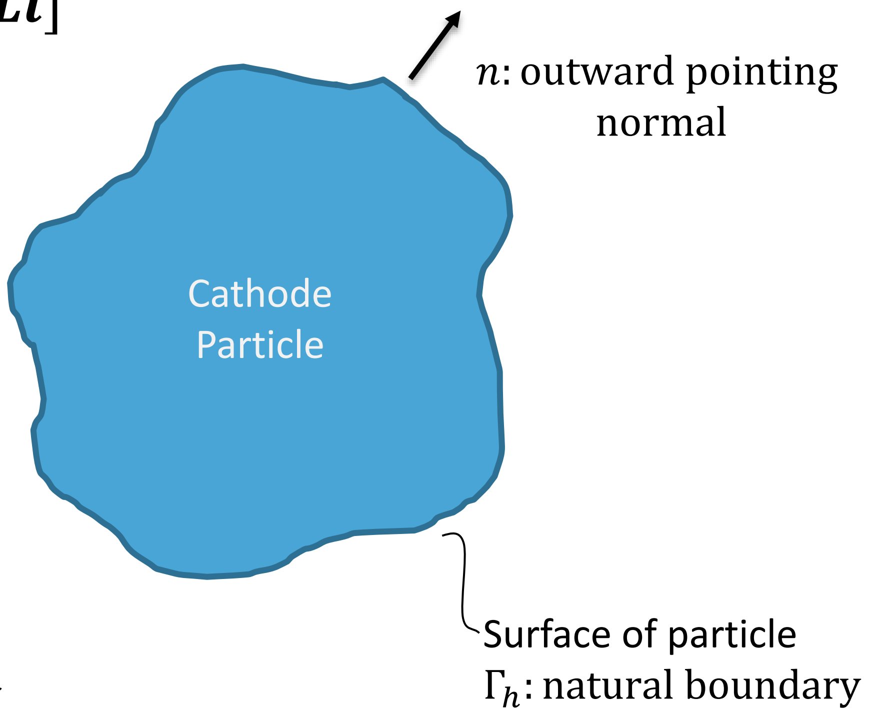
- **Solid-phase electrostatic potential → Φ_{NMC}**

BC: $$i = -\kappa \frac{\partial \Phi_{NMC}}{\partial x_k} n_k \qquad on\ \Gamma_h$$

- **Butler-Volmer coupling**

BC: $$i = i_0 \left[\exp\left(\frac{\alpha_a \eta F}{RT}\right) - \exp\left(-\frac{\alpha_c \eta F}{RT}\right) \right] \qquad on\ \Gamma_h$$

$$\eta([Li], \Phi_{NMC}) = \Phi_{NMC} - \Phi_{el} - E^{eq}\left(\frac{[Li]}{[Li]_{max}}\right)$$

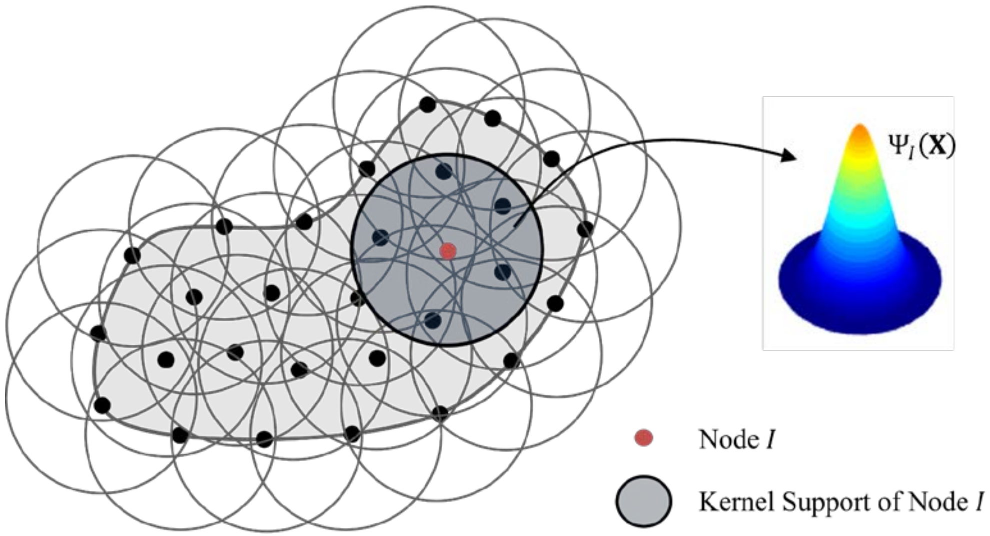


Reproducing Kernel Particle Method (RKPM)

Reproducing Kernel (RK) Approximation

RK Approximation:

$$u(\boldsymbol{x}) \approx u^h(\boldsymbol{x}) = \sum_{I=1}^{NP} \Psi_I(\boldsymbol{x}) d_I$$



Shape Function Construction: $\Psi_I(\boldsymbol{x})$

Strategic Correction of Kernel Functions, ϕ_a :

$$\Psi_I(\boldsymbol{x}) = C(\boldsymbol{x}; \boldsymbol{x} - \boldsymbol{x}_I)\phi_a(\boldsymbol{x} - \boldsymbol{x}_I) = \left(\sum_{|\boldsymbol{\alpha}| \le n} (\boldsymbol{x} - \boldsymbol{x}_I)^{\boldsymbol{\alpha}}\, b_{\boldsymbol{\alpha}}(\boldsymbol{x})\right) \phi_a(\boldsymbol{x} - \boldsymbol{x}_I)$$

$$\Psi_I(\boldsymbol{x}) \equiv \boldsymbol{H}^T(\boldsymbol{x} - \boldsymbol{x}_I)\boldsymbol{b}(\boldsymbol{x})\phi_a(\boldsymbol{x} - \boldsymbol{x}_I)$$

$$\boldsymbol{H}^T(\boldsymbol{x} - \boldsymbol{x}_I) = [1, (x_1 - x_{1I}), (x_2 - x_{2I}), (x_3 - x_{3I}), \ldots, (x_3 - x_{3I})^n]$$

Reproducing Conditions:

$$\sum_{\mathrm{I}=1}^{NP} \Psi_I(\boldsymbol{x})\boldsymbol{x}_I^{\boldsymbol{\alpha}} = \boldsymbol{x}^{\boldsymbol{\alpha}}, \quad |\boldsymbol{\alpha}| \le n \quad OR \quad \sum_{I=1}^{NP} \Psi_I(\boldsymbol{x})(\boldsymbol{x} - \boldsymbol{x}_I)^{\boldsymbol{\alpha}} = \delta_{0\boldsymbol{\alpha}}, |\boldsymbol{\alpha}| \le n$$

$$\boldsymbol{b}(\boldsymbol{x}) = \boldsymbol{M}^{-1}(\boldsymbol{x})\boldsymbol{H}(\boldsymbol{0}), \ \ \textit{where}\ \mathbf{M}(\boldsymbol{x}) = \sum_{I=1}^{NP} \mathrm{H}(\boldsymbol{x} - \boldsymbol{x}_I)\mathrm{H}^{\mathrm{T}}(\boldsymbol{x} - \boldsymbol{x}_I)\phi_a(\boldsymbol{x} - \boldsymbol{x}_I)$$

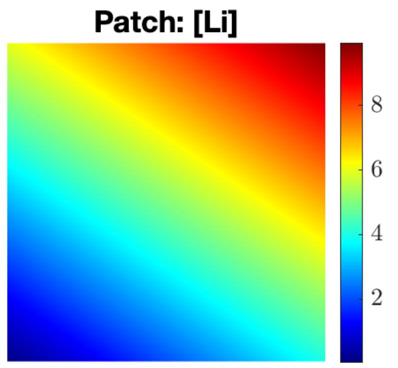
$$\Psi_I(\boldsymbol{x}) = \boldsymbol{H}^T(\boldsymbol{0})\boldsymbol{M}^{-1}(\boldsymbol{x})\boldsymbol{H}(\boldsymbol{x} - \boldsymbol{x}_I)\phi_a(\boldsymbol{x} - \boldsymbol{x}_I)$$

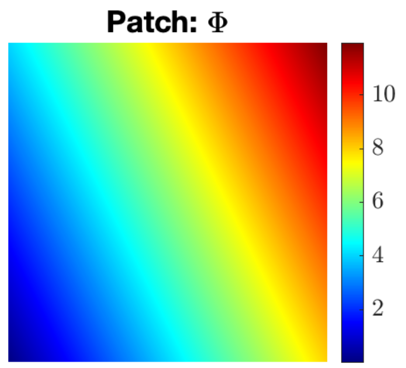
4. Liu, W.K., S. Jun, S. Li, J. Adee, T. Belytschko. 1995. "Reproducing kernel particle methods for structural dynamics." *Int J Numer Methods Eng* 38(10): 1655-1679. https://doi.org/10.1002/nme.1620381005.
5. Chen, J.S., C. Pan, C-T Wu, W.K. Liu. 1996. "Reproducing kernel particle methods for large deformation analysis of non-linear structures." *Comput Methods Appl Mech Eng* 139(96): 195-227. https://doi.org/10.1016/S0045-7825(96)01083-3.

Linear Patch Test for Coupled Problem

Formulating Linear Patch Test for Coupled Problem

- Considerations:
  - Assume arbitrary linear fields:
    - $[Li]^p = a_0 + a_1 x_1 + a_2 x_2$
    - $\Phi^p = a_4 + a_5 x_1 + a_6 x_2$
  - Must design coupled BCs that satisfy governing equations.





- Designing Mixed BCs (applied as Natural BCs)
  - $\mathrm{BC}_{[\mathrm{Li}]}$: $i_{[Li]} = -D_{kj}\dfrac{\partial [Li]}{\partial x_j} n_k \quad on\ \Gamma_h$

    $$\Rightarrow\ i_{[Li]}^{\nu+1} = -D_{kj}\frac{\partial [Li]^p}{\partial x_j} n_k + \Phi^p - \Phi^{\nu+1}$$
  - BC_{Φ}: $i_{\Phi} = -\kappa\dfrac{\partial \Phi_{NMC}}{\partial x_j} n_j \quad on\ \Gamma_h$

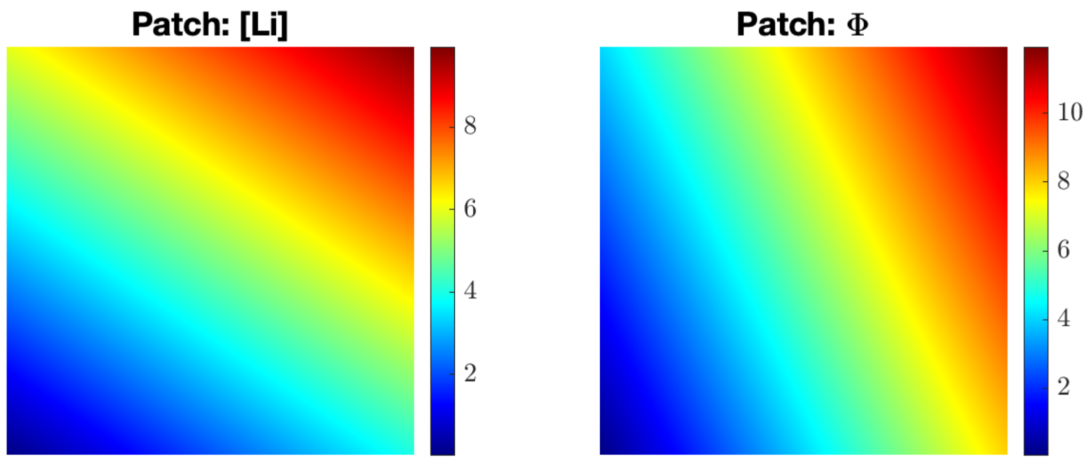
    $$\Rightarrow\ i_{\Phi}^{\nu+1} = -\kappa\frac{\partial \Phi^p}{\partial x_j} n_j + [Li]^p - [Li]^{\nu+1}$$

Note: We **recover the original governing equations** once convergence is reached (i.e. $\Phi^{(\nu+1)} = \Phi^p$, $[\mathrm{Li}]^{(\nu+1)} = [\mathrm{Li}]$).

Note: A **mixed type boundary condition** is used (i.e. if solving for $[Li]$, then $\nabla[Li]^p$ and Φ^p are used in the traction BC).

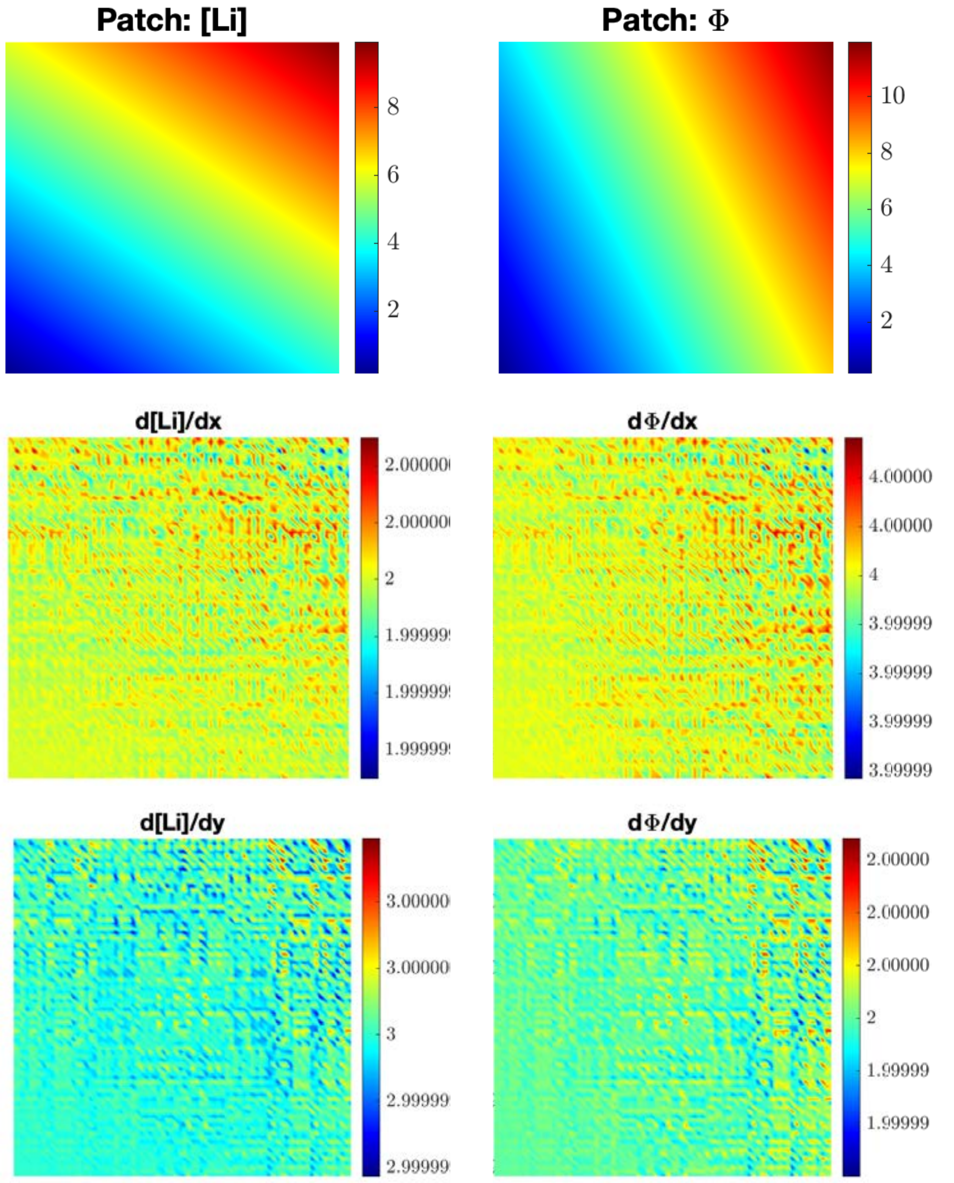
Implementing Linear Patch Test for Coupled Problem

- Analytical Linear Fields:



$$[Li]^p = 5 + 2x_1 + 3x_2 \qquad \Phi^p = 6 + 4x_1 + 2x_2$$

- Formulation **passes coupled linear patch test**.



Introducing Weak and Strong Discontinuities to the RK Approximation Space

Kernel Function Modifications for Grain Boundaries: $\max[\tanh(dist), 0]$

Case 1: Standard RKPM

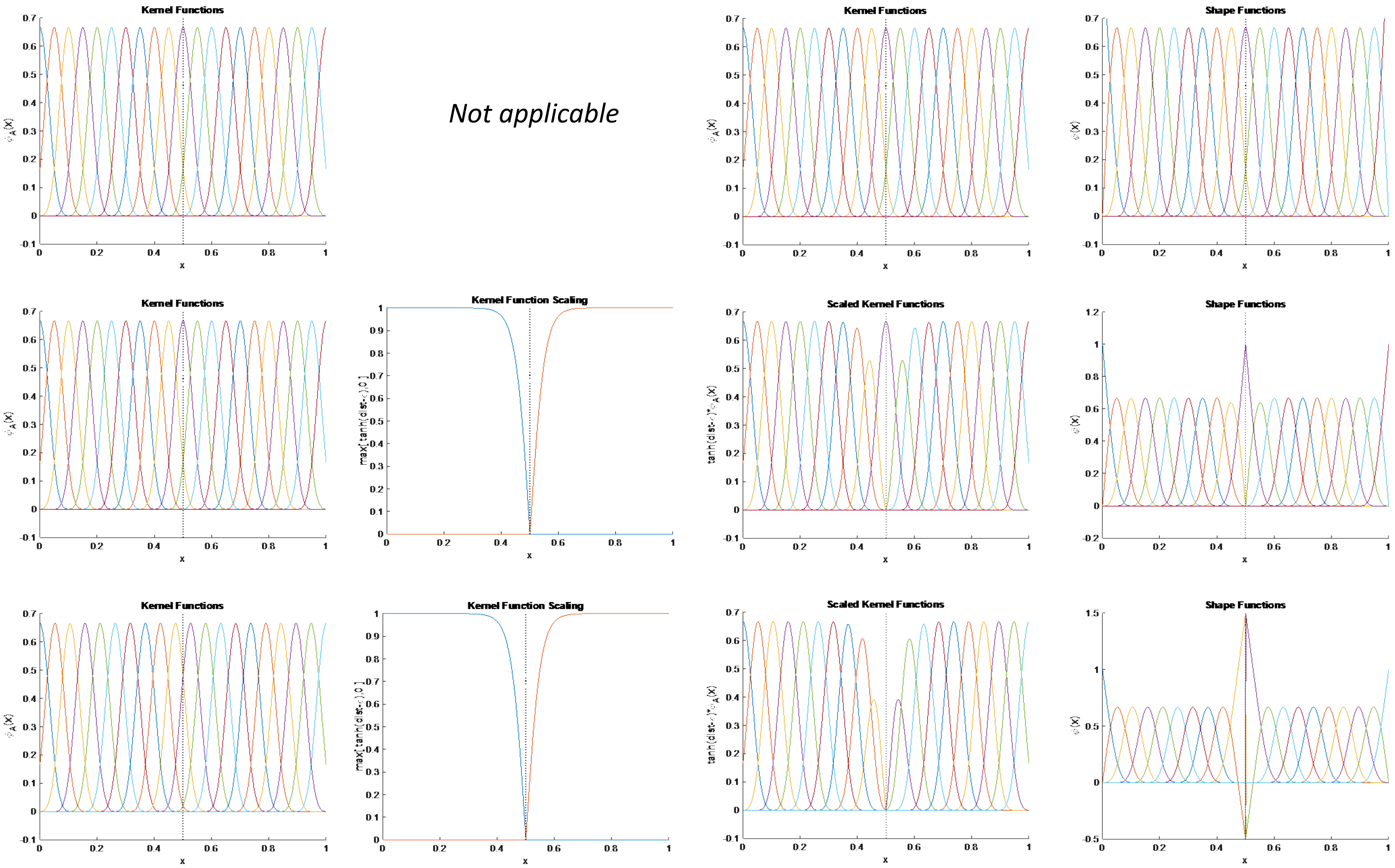
Smooth Ψ everywhere

Case 2: Scaling with node on boundary

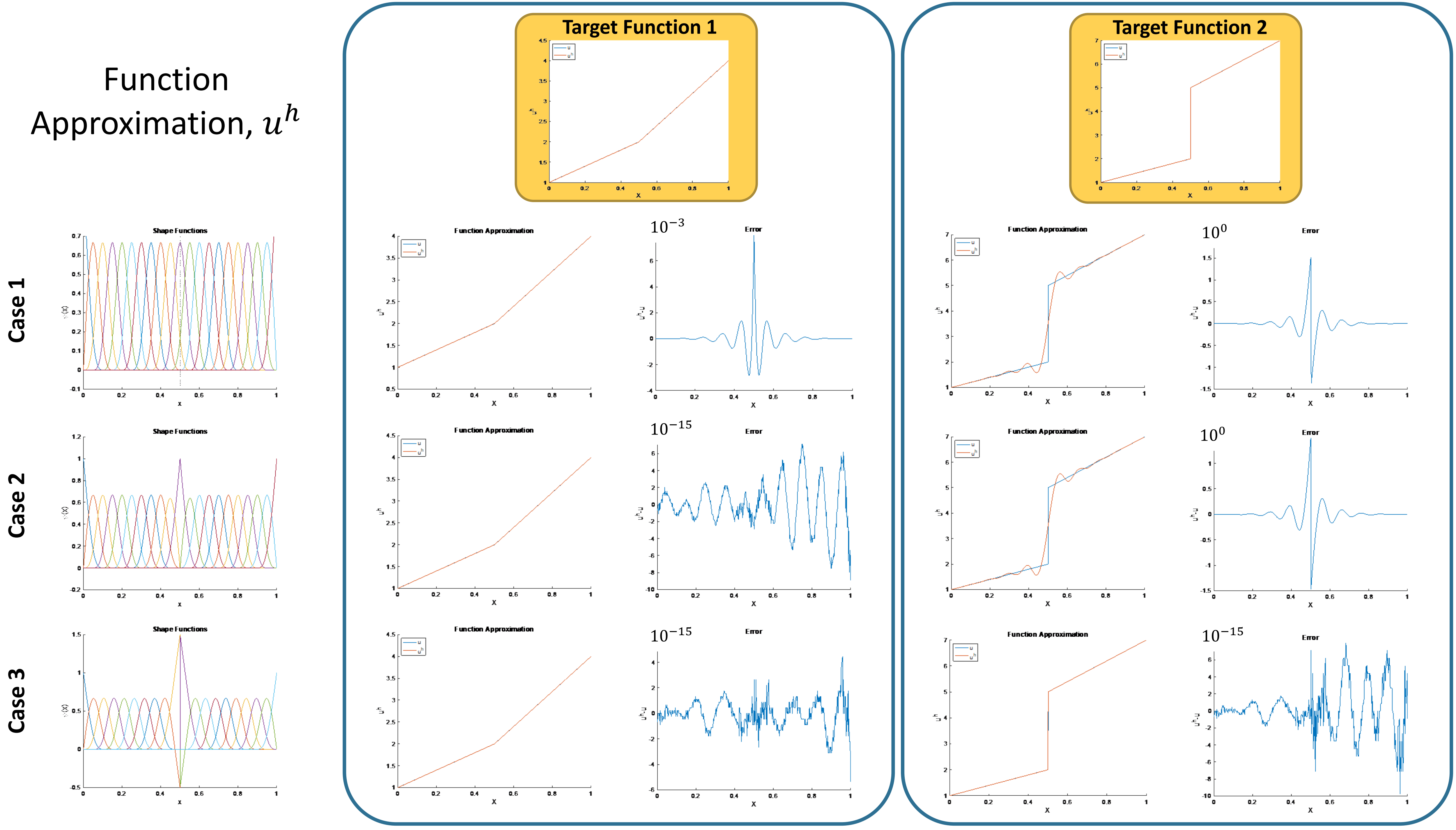
Weak discontinuity introduced only for $\Psi_{Boundary}$

Case 3: Scaling with no node on boundary

Strong discontinuity introduced only for $\Psi_{Boundary}$



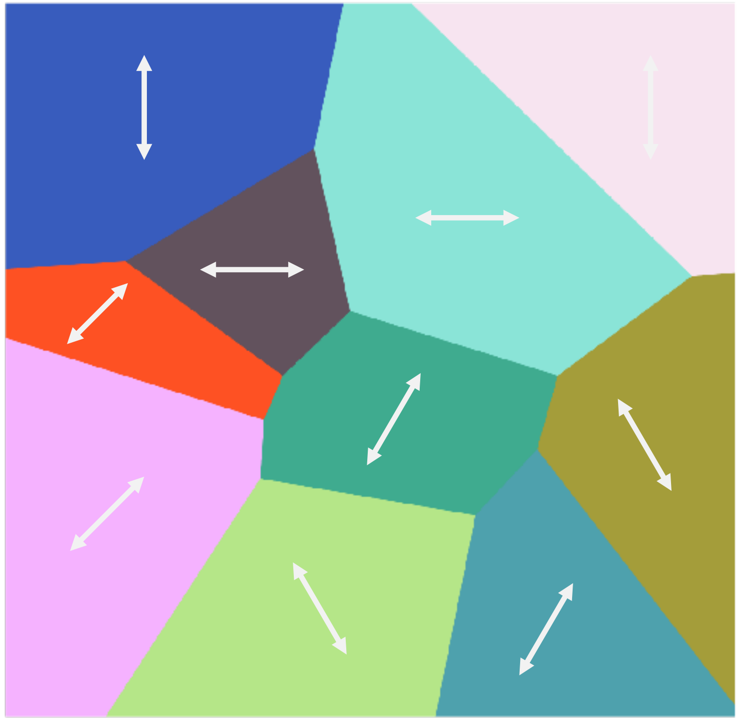
Function Approximation, u^h

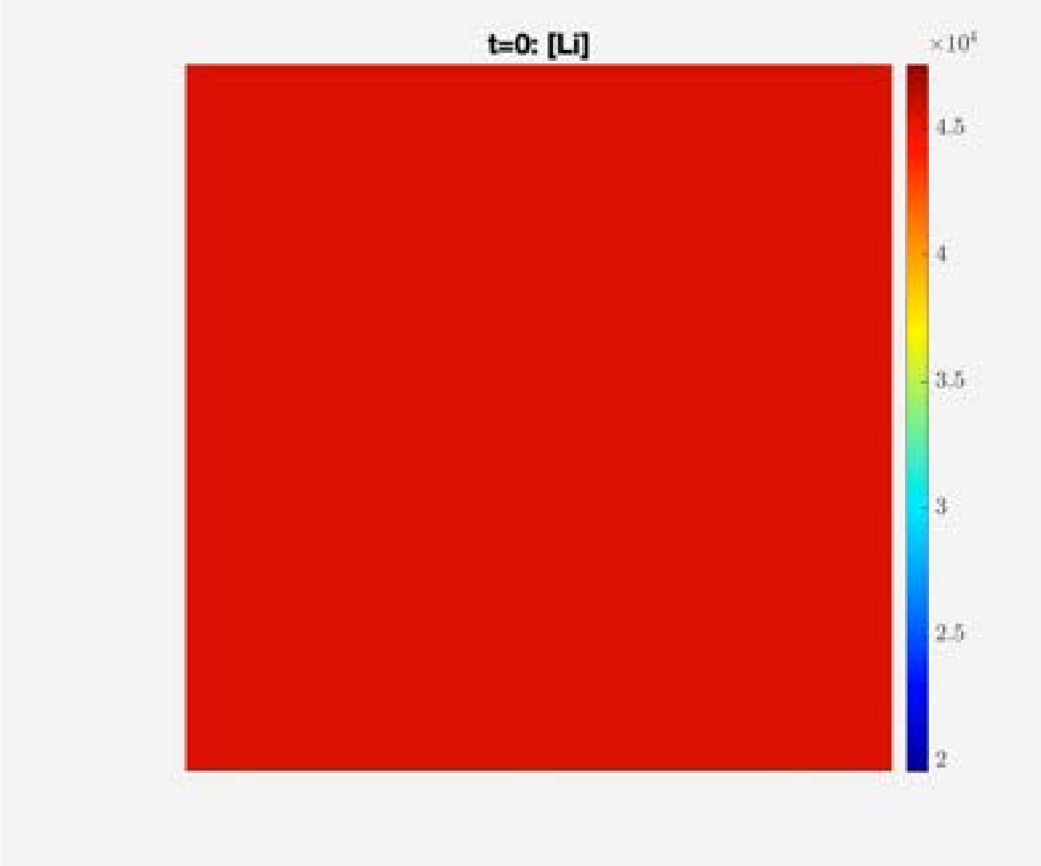


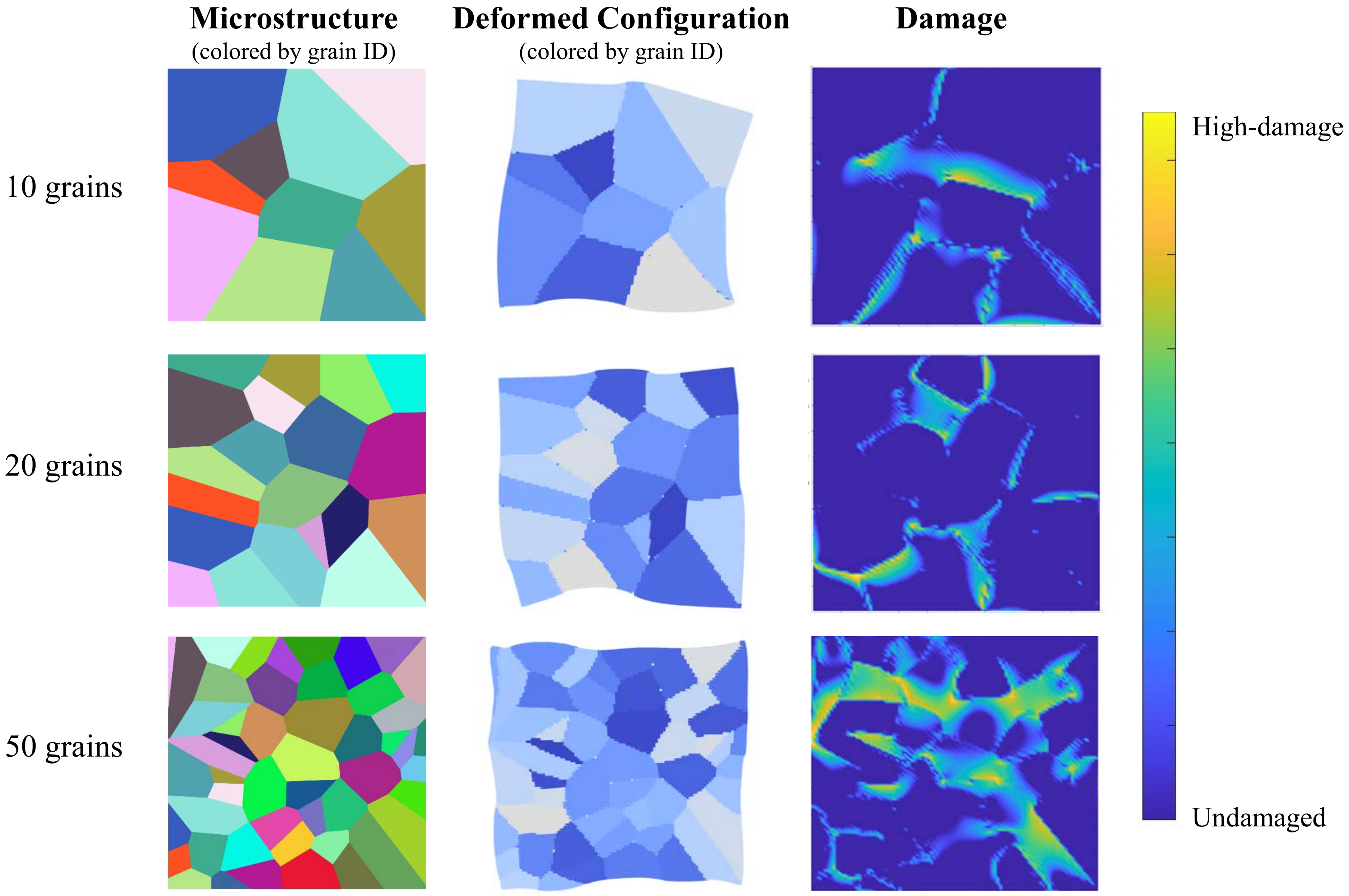
Multiple Grain Demonstration Problem

10 Voronoi Grains with Anisotropic Diffusion

Grain Orientations:



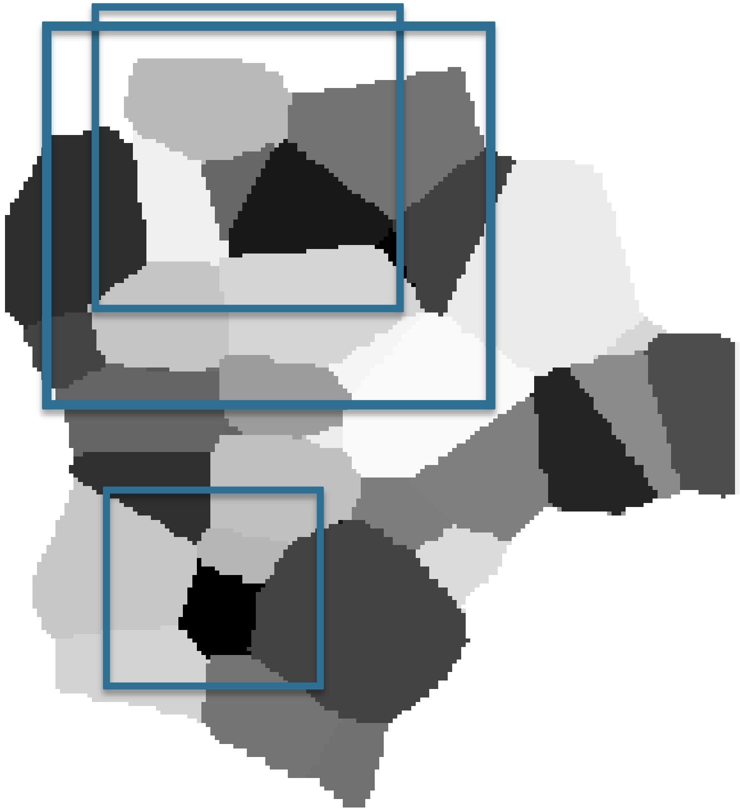


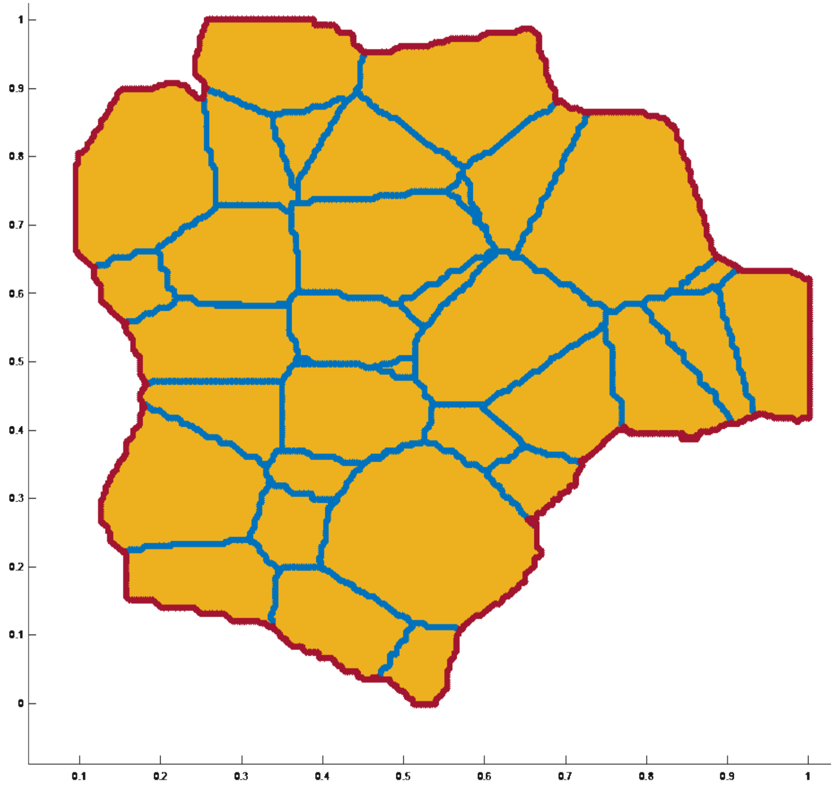


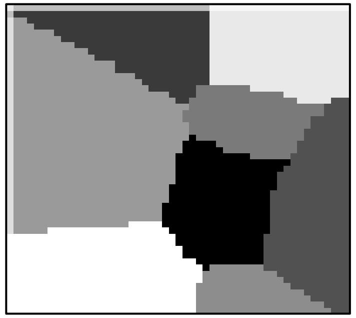
Microstructure
(colored by grain ID)
Deformed Configuration
(colored by grain ID)
Damage
10 grains
20 grains
50 grains
High-damage
Undamaged

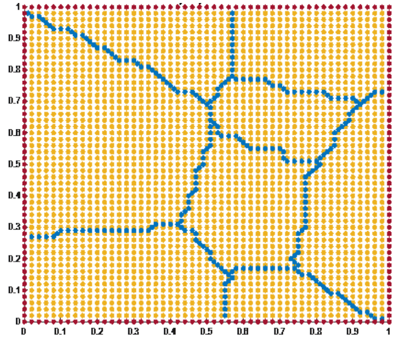
Image-based Modeling

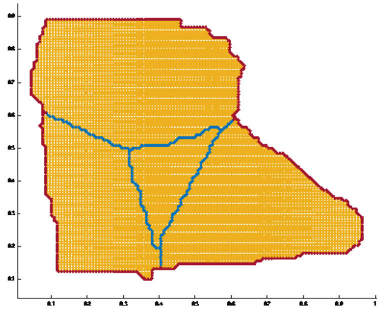
From Pixels to Nodes

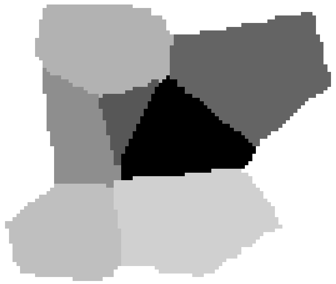


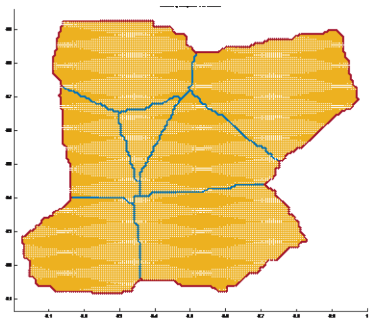


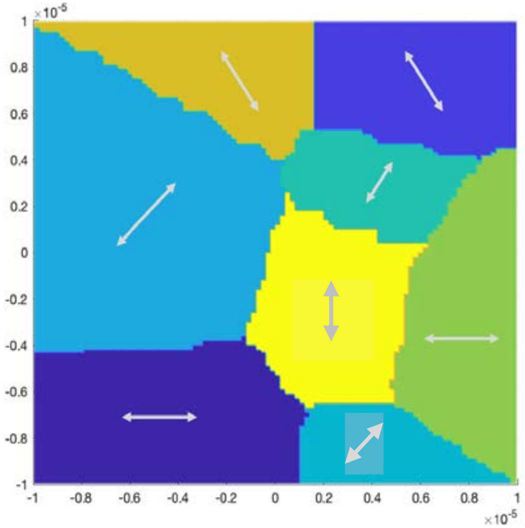






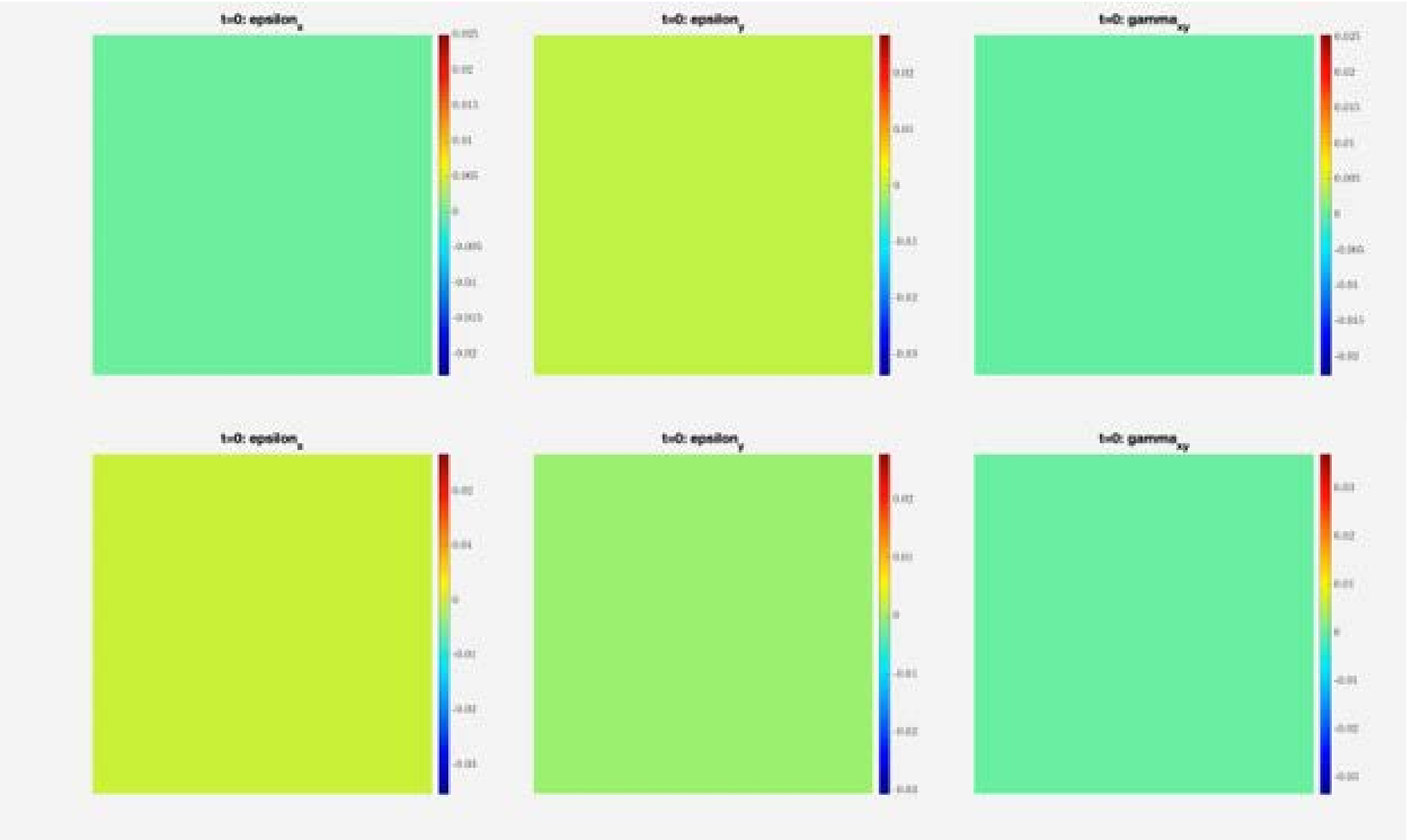






Standard RKPM

RKPM with Kernel Scaling on Grain Boundaries

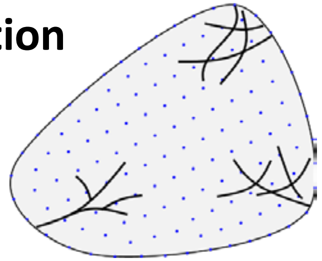


Neural Network Enhanced Reproducing Kernel Approximation

Neural Network Enhanced Reproducing Kernel (NN-RK) Approximation

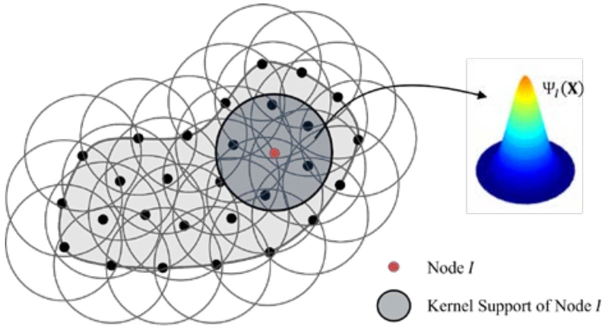
Solution decomposition

$$\mathbf{u}^h = \tilde{\mathbf{u}}^h + \hat{\mathbf{u}}^h$$



<u>Smooth solution approximation</u>

$$\tilde{\mathbf{u}}^h(\mathbf{X}) \approx \mathbf{u}^{RK}(\mathbf{X}) = \sum_{I=1}^{NP} \Psi_I(\mathbf{X})\mathbf{d}_I$$



<u>Neural Network (NN) Enrichment</u>

$$\hat{\mathbf{u}}^h(\mathbf{x}) \approx \mathbf{u}^{NN}(\mathbf{X}) = \sum_{I=1}^{NB} b_I(\mathbf{X}; \mathbf{W})$$

Neural network (NN) approximation

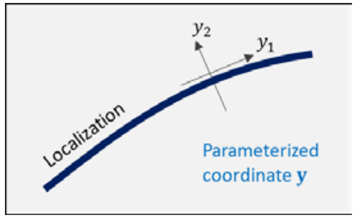
$$u^{NN}(\mathbf{x}) = \sum_{B=1}^{N_B} b_B^{NN}(\mathbf{x}; \mathbf{W}_B)$$

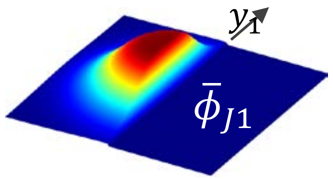
- b_B^{NN}: block-level NN approximation

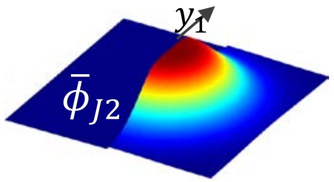
Block-level NN approximation

$$b_B^{NN}(\mathbf{x}; \mathbf{W}) = \sum_{K=1}^{N_K} \hat{\phi}_{KB}\left(\mathbf{y}(\mathbf{x}; \mathbf{W}_B^L), \mathbf{W}_{KB}^S\right) p(\mathbf{x}; \mathbf{W}_{KB}^P)$$

- NK: the number of NN kernels per block







NN Kernel function captures
- Location and orientation of localization
- Shape of solution transition

- $\mathbf{W}^L$: NN weight set controlling the location and orientation of the kernel.
- $\mathbf{W}^S$: NN weight set controlling the shape of transition.

NN Polynomial introduces
- Monomial completeness for further accuracy

- $\mathbf{W}^P$: NN monomial coefficient set

* The NN control parameters $\mathbf{W}^L$, $\mathbf{W}^S$, and $\mathbf{W}^P$ are ***automatically*** determined via loss function minimization.

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6. Baek, J., J.S. Chen, K. Susuki. 2022. "A neural network-enhanced reproducing kernel particle method for modeling strain localization." *Int J Numer Methods Eng* 123(18): 4422-4454. https://doi.org/10.1002/nme.7040.

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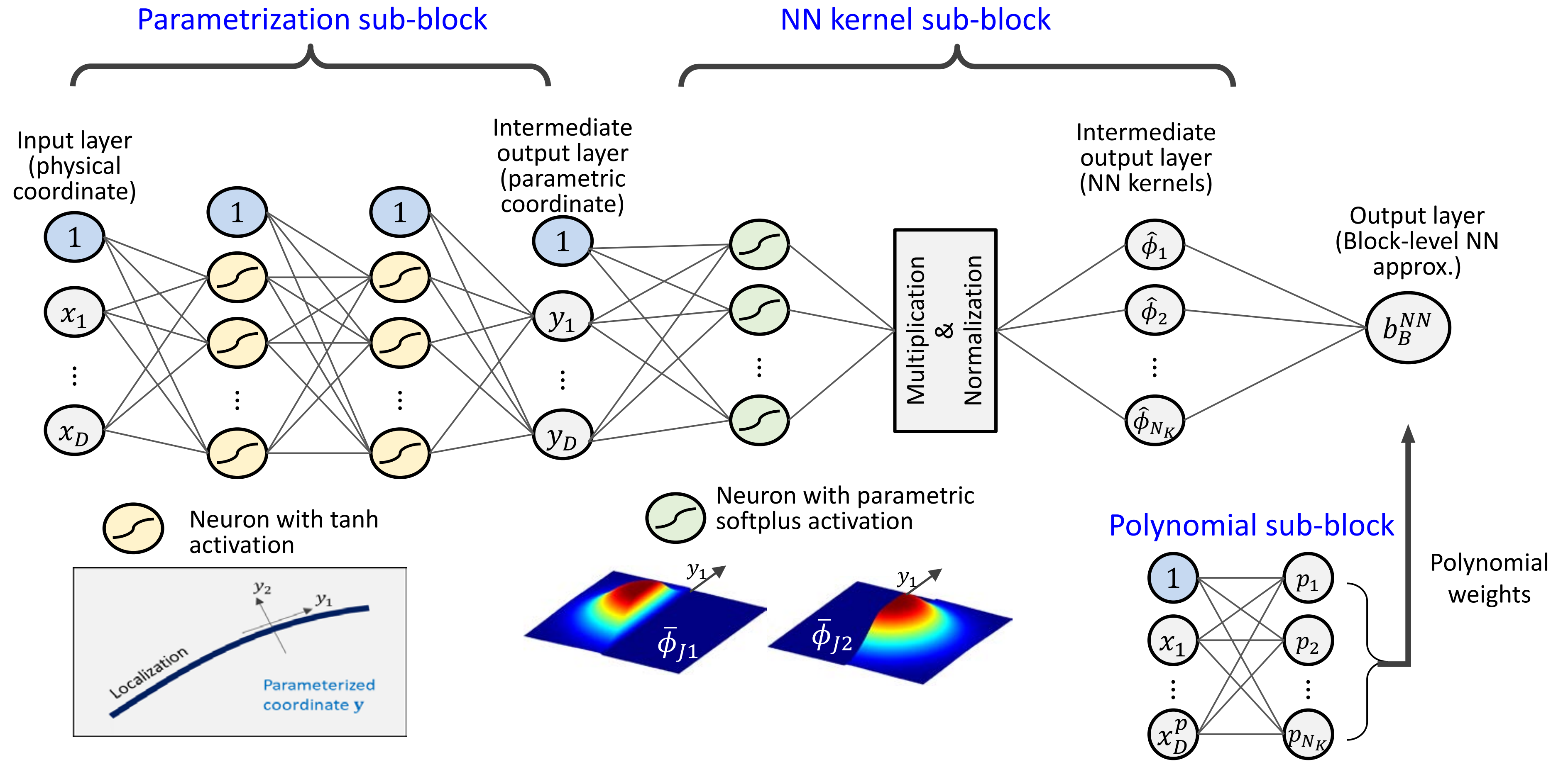
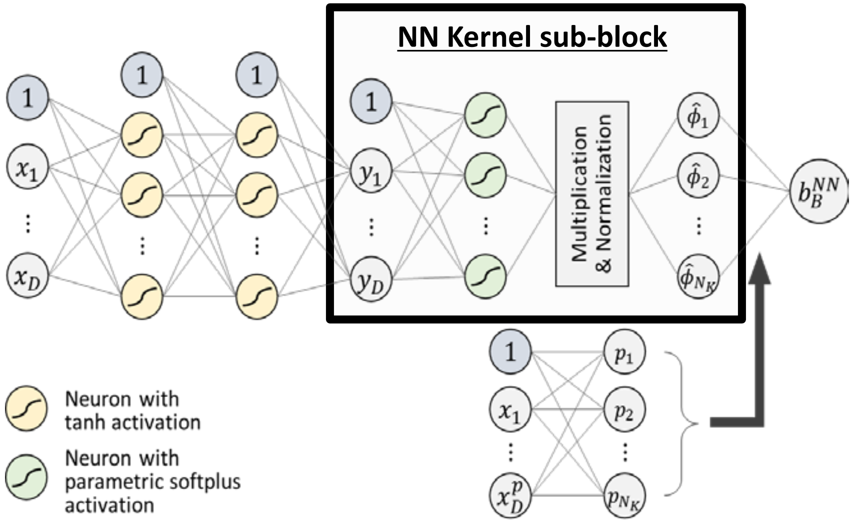
Block-Level Neural Network Architecture

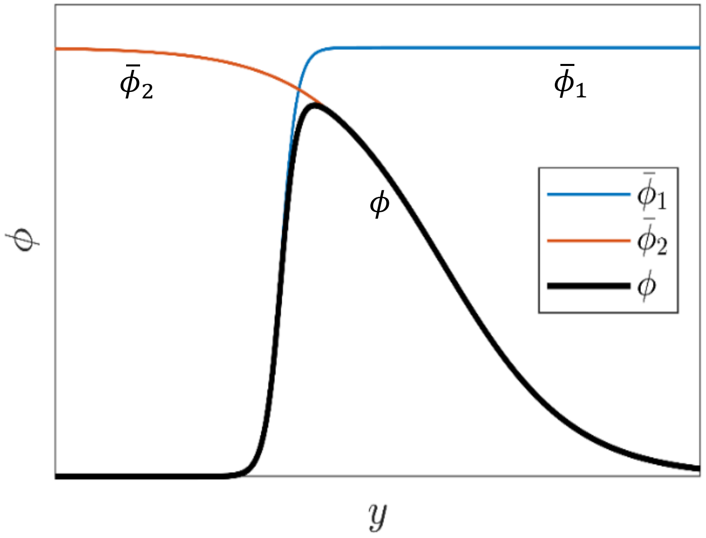
A block-level neural network is a modified deep neural network with ***increased interpretability***.



6. Baek, J., J.S. Chen, K. Susuki. 2022. "A neural network-enhanced reproducing kernel particle method for modeling strain localization." *Int J Numer Methods Eng* 123(18): 4422-4454. https://doi.org/10.1002/nme.7040.

NN Kernel Function Controlled by $\mathbf{W}^S$





NN Kernel Function

$$\phi(y;\mathbf{W}^S_{KB}) = \prod_{i=1}^{2} \underbrace{\bar{\phi}\left(z_i\left(y, \bar{y}_i^{KB}, c_i^{KB}\right); \beta_i^{KB}\right)}_{\text{Regularized step functions}}$$

Regularized Step Functions

$$\bar{\phi}(z_i;\beta_i) \equiv S\left(z_i + \frac{1}{2};\beta_i\right) - S\left(z_i - \frac{1}{2};\beta_i\right)$$

Where $z_i = (-1)^i\,(y - \bar{y}_i)/c_i$, $i = 1, 2$

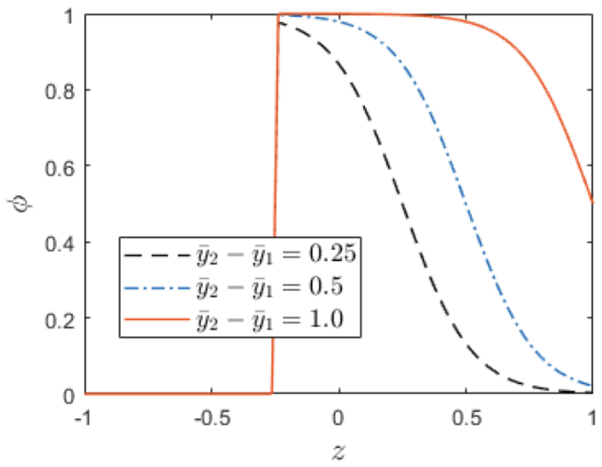
$S(z;\beta) = \frac{1}{\beta}\log\left(1 + e^{\beta z}\right)$

(parametric softplus function)

Neural Network Kernel Function Controlled by $\mathbf{W}^S$

NN Control Parameter $\bar{y}$

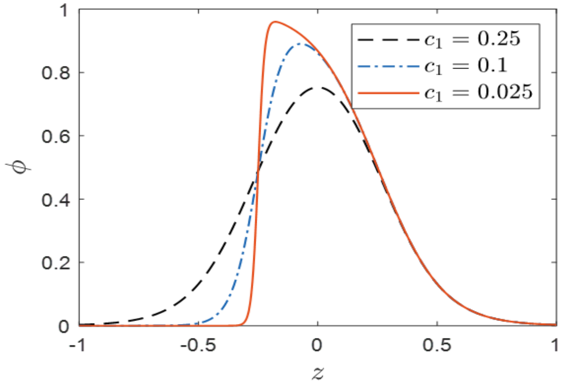
Domain of influence



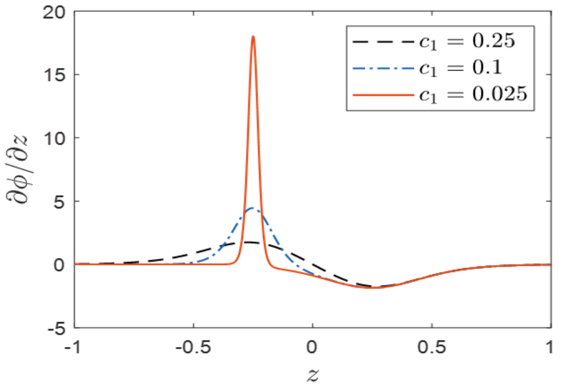
NN Control Parameter c

Transition of NN kernel function

NN kernel function

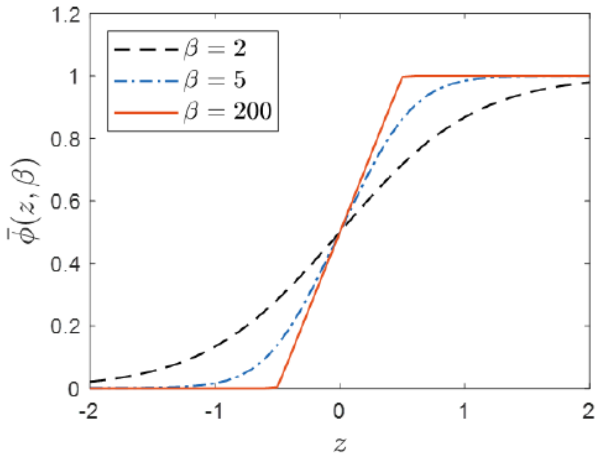


NN kernel function derivatives



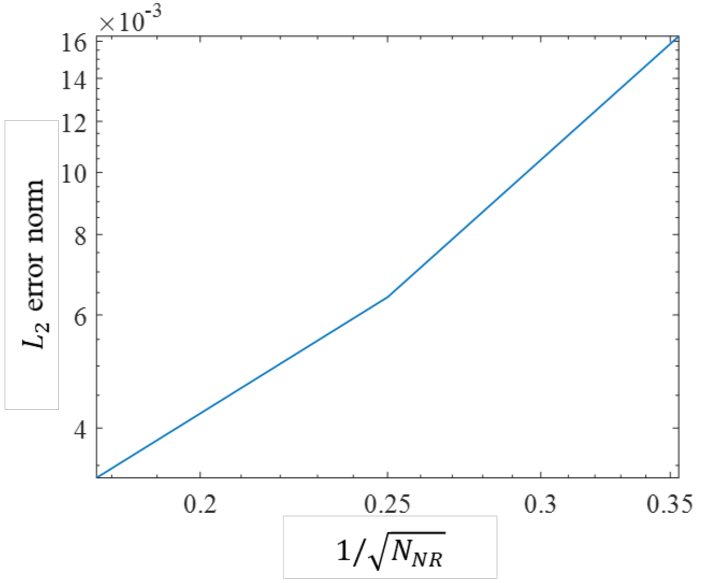
NN Control Parameter β

Transition of NN kernel function derivative



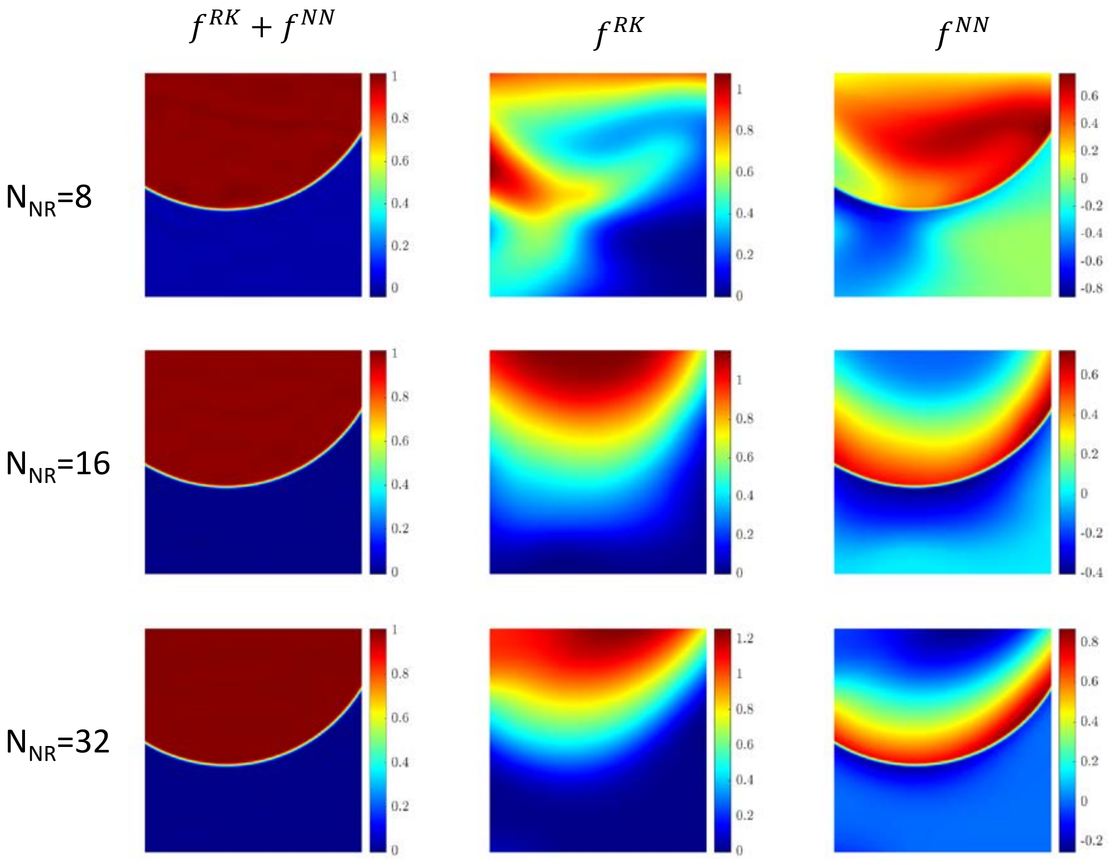
Convergence Performance for Function Evaluation: (1) Influence of the Number of Neurons (N_{NR})

Average rate of convergence: 2.282



Number of block $N_B = 1$

Number of NN kernel per block $N_K = 4$



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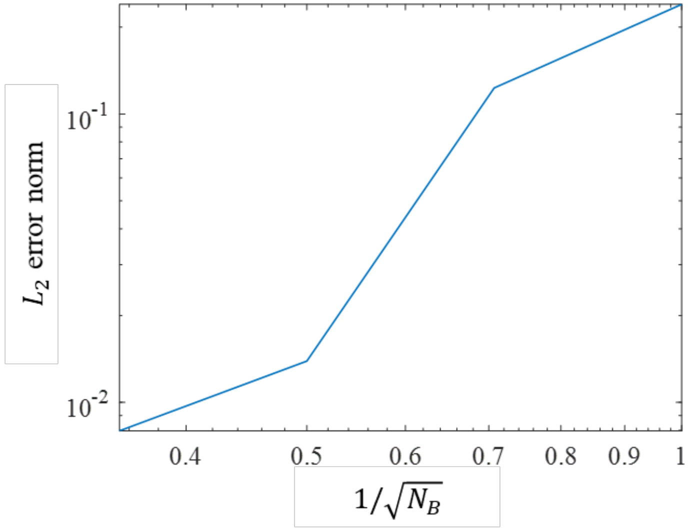
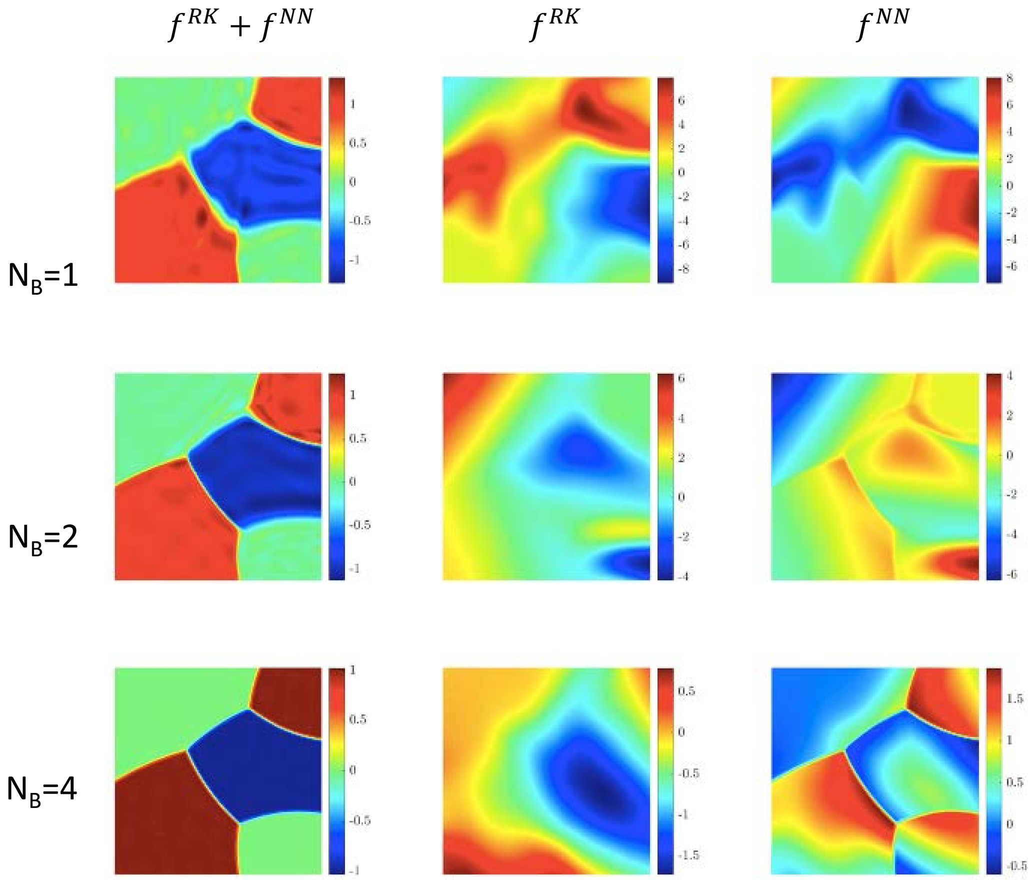
Convergence Performance for Function Evaluation: (2) Influence of the number of NN Blocks (N_B)

Average rate of convergence: 3.578



Number of neurons $N_{NR} = 32$
Number of NN kernel per block $N_K = 4$



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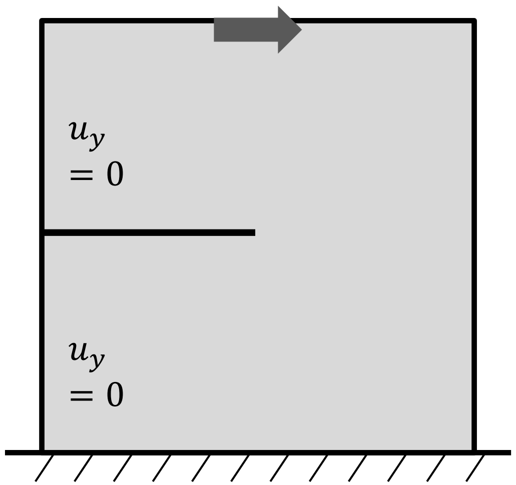
Damage Evolution



$$\min \Pi = \frac{1}{2}\int_{\Omega} g(\eta)\psi^{+} + \psi^{-} d\Omega + \frac{p}{2}\int_{\Omega} \eta^{2} d\Omega + \Pi^{ebc}$$

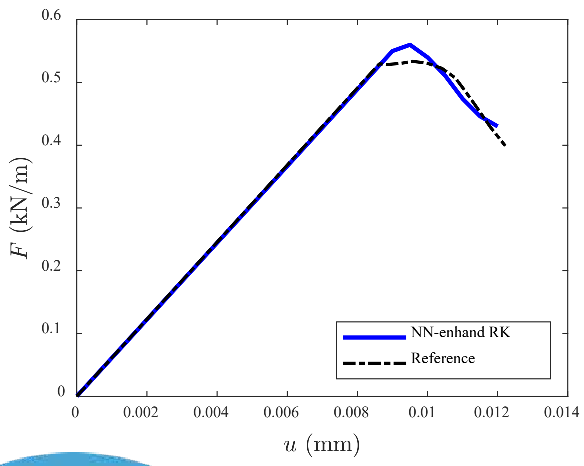
Damage $\eta = \dfrac{\kappa}{\kappa + p}$ $\kappa = \psi^{+} - \psi^{c}$

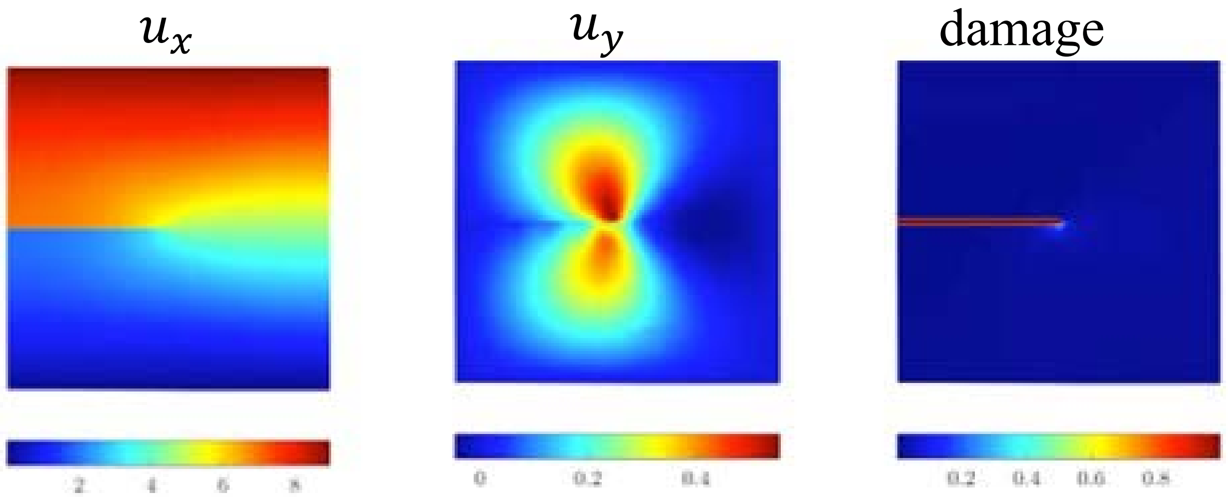
$$\psi^{+} = \frac{1}{2}\lambda\langle tr\varepsilon_i\rangle^2 + \mu\varepsilon_i^{+}\varepsilon_i^{+}$$

$$\psi^{-} = \frac{1}{2}\lambda((tr\varepsilon_i)^2 - \langle tr\varepsilon_i\rangle^2) + \mu\varepsilon_i^{-}\varepsilon_i^{-}$$

$$\langle\cdot\rangle = \max(0,\cdot)$$

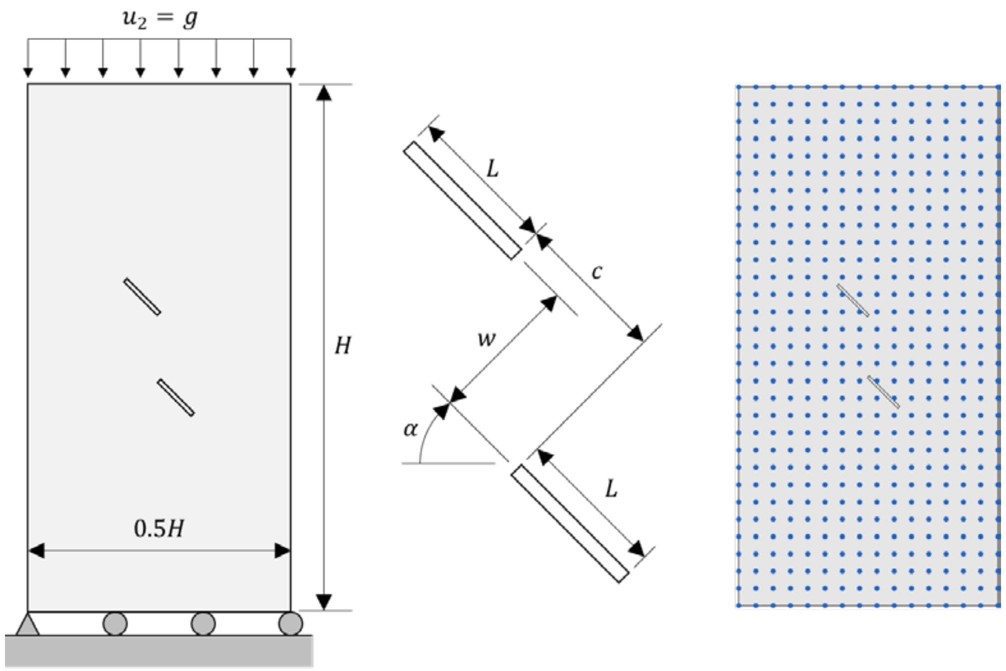
- 256 RK particles (16X16) are used with 512 RK coefficients.
- 3 NN blocks are used with 540 total unknown weights and biases.
- Visibility criteria with diffraction is applied to the RK shape functions around the area of pre-existing crack.



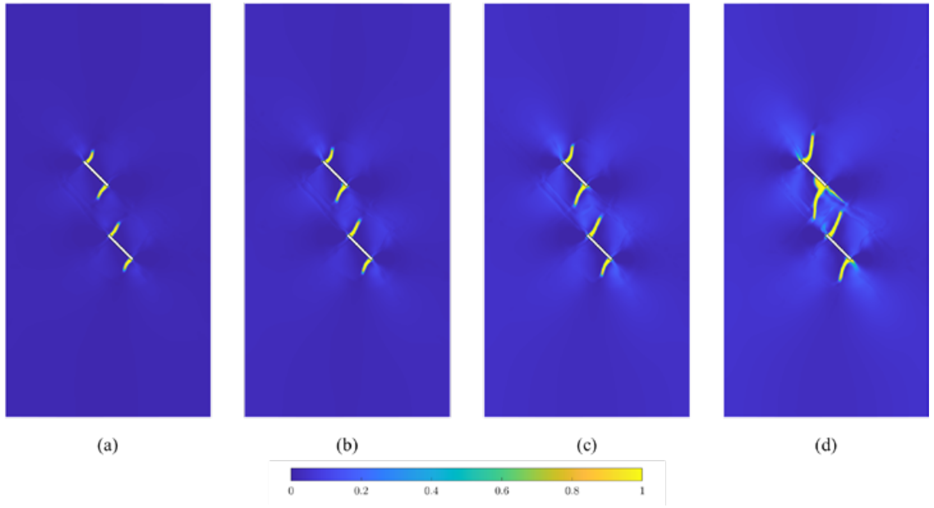


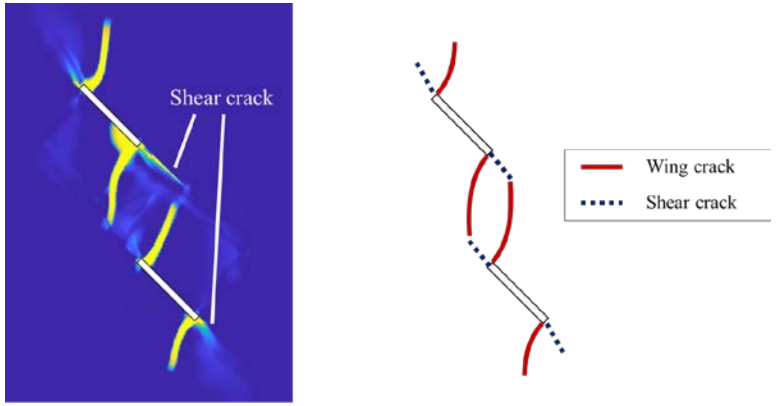
6. Baek, J., J.S. Chen, K. Susuki. 2022. “A neural network-enhanced reproducing kernel particle method for modeling strain localization.” *Int J Numer Methods Eng* 123(18): 4422-4454. https://doi.org/10.1002/nme.7040.

Mixed-mode Fracture of a Doubly Notched Crack Branching



(a) (b) (c)


(a) (b) (c) (d)



(a) (b)

NN-RKPM

Experiment (reference)

Conclusions and Future Work

Conclusions:

- A coupled linear patch test was designed and passed for the electrochemical model.
- Through kernel function scaling and strategic RK node placement, weak and strong discontinuities along grain boundaries were introduced in a flexible manner.
- Image-based modeling techniques were leveraged for realistic model construction.
- NN enhancement increased localization accuracy in homogeneous materials without extensive model refinement.

Future Work:

- Input non-rectangular exterior geometries to fully-coupled simulation.
- Extend NN-RK damage capture to heterogeneous electrode materials.

Thank you

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