Image-Based Failure Assessment of Li-ion Batteries

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ASC Conference – San Diego, CA– Oct 22, 2024
NREL/PR-2C00-91494

Heterogeneous Electrode Microstructures and Electro-Chemo-Mechanical Cracking

Electrode Microstructure and Electro-Chemo-Mechanical Cracking

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

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

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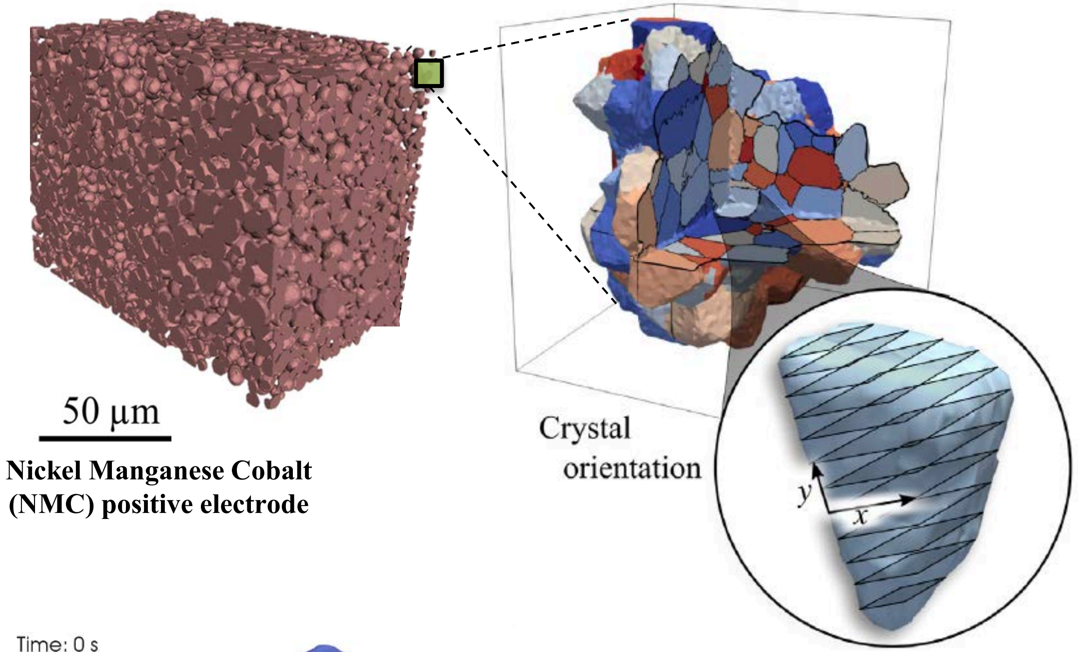
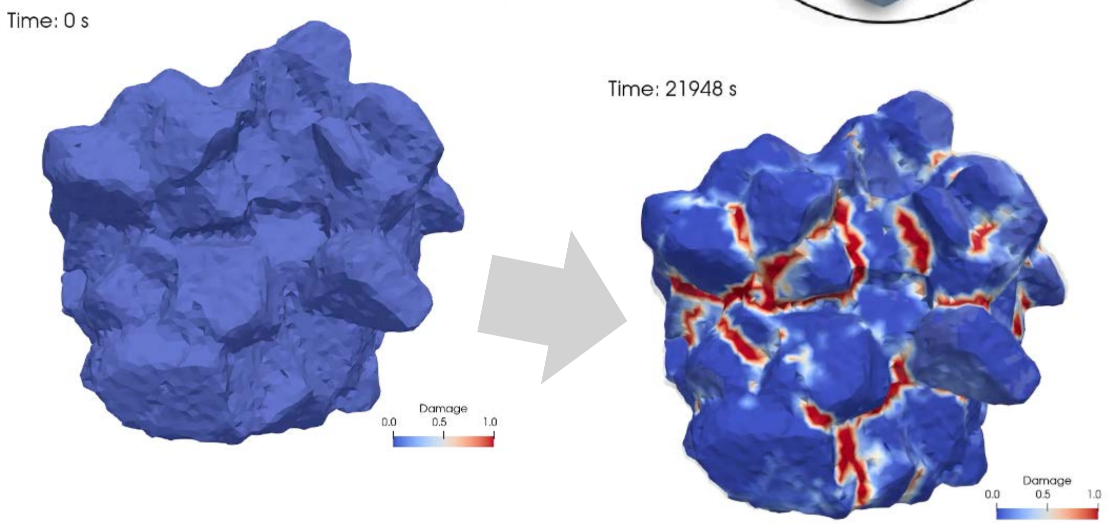
Electro-chemo-mechanical cracking:
- Inhibited lithium flow via tortuous diffusion path
- Reduced battery life





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2. Allen, J., P. Weddle, A. Verma, et al. 2021. “Quantifying the influence of charge rate and cathode-particle architectures on degradation of Li-ion cells through 3D continuum-level damage models.” *J Power Sources*.
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Governing Equations

Electrochemical Model

c

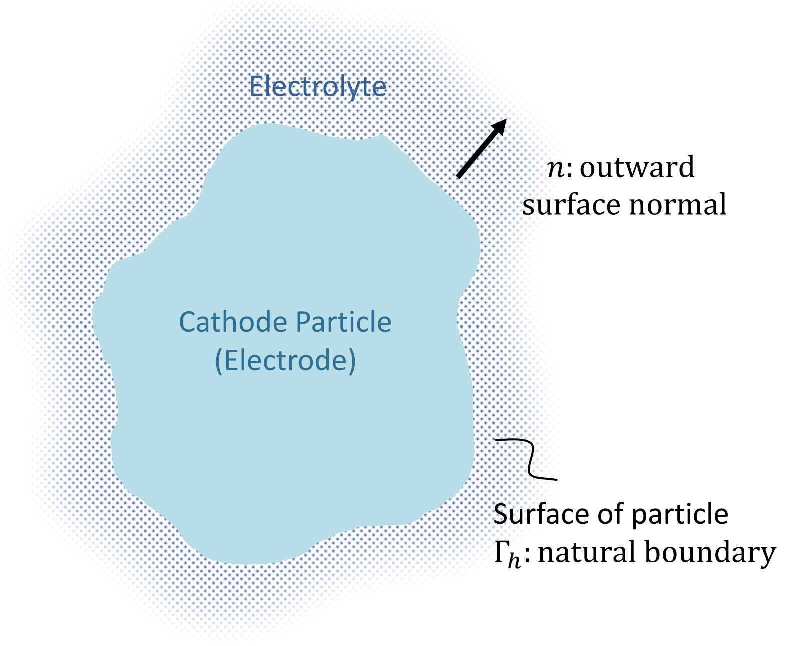
Lithium transport balance → lithium concentration c

$$\dot{c} + \nabla \cdot \boldsymbol{J} = 0 \quad in\ \Omega$$
$$\boldsymbol{J} = -\boldsymbol{D} \cdot \nabla c$$
$$\boldsymbol{D} \cdot \nabla c \cdot \boldsymbol{n} = -\frac{\bar{J}(c, \Phi)}{F} \quad on\ \Gamma_{h_c}$$

Φ

Solid-phase electrostatic potential balance → potential Φ

$$\nabla \cdot (\kappa \nabla \Phi) = 0 \quad in\ \Omega$$
$$\kappa \nabla \Phi \cdot \boldsymbol{n} = -\left(\bar{J}(c, \Phi) + \bar{J}_{applied}\right) \quad on\ \Gamma_{h_\Phi}$$



Mechanical Model

$\boldsymbol{u}$

Diffusion-induced mechanical deformation → displacement $\boldsymbol{u}$

$$\nabla \cdot \boldsymbol{\sigma} = \boldsymbol{0} \quad in\ \Omega$$
$$\boldsymbol{\sigma} = \mathbb{C}\boldsymbol{\epsilon}^e$$
$$\boldsymbol{\sigma} \cdot \boldsymbol{n} = 0 \quad on\ \Gamma_{h_u}$$
$$\boldsymbol{\epsilon}^e = \boldsymbol{\epsilon} - \boldsymbol{\epsilon}^D$$
$$\boldsymbol{\epsilon}^D = \boldsymbol{\beta}\Delta c$$

Butler-Volmer interface condition

$$\bar{J}(c, \Phi) = \bar{J}_0 \left[\exp\left(\frac{\alpha_a \eta F}{RT}\right) - \exp\left(-\frac{\alpha_c \eta F}{RT}\right)\right]$$
$$\eta(c, \Phi) = \Phi - \Phi_{el} - E^{eq}\left(\frac{c}{c_{max}}\right)$$

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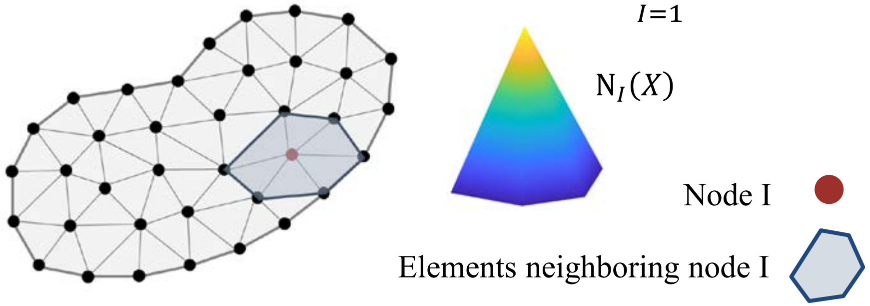
Reproducing Kernel Particle Method (RKPM)

Reproducing Kernel (RK) Approximation

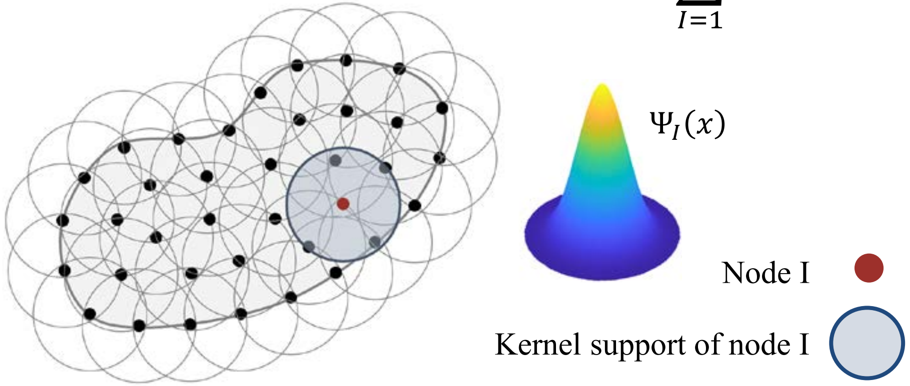
FEM Approximation:

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



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 :

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

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

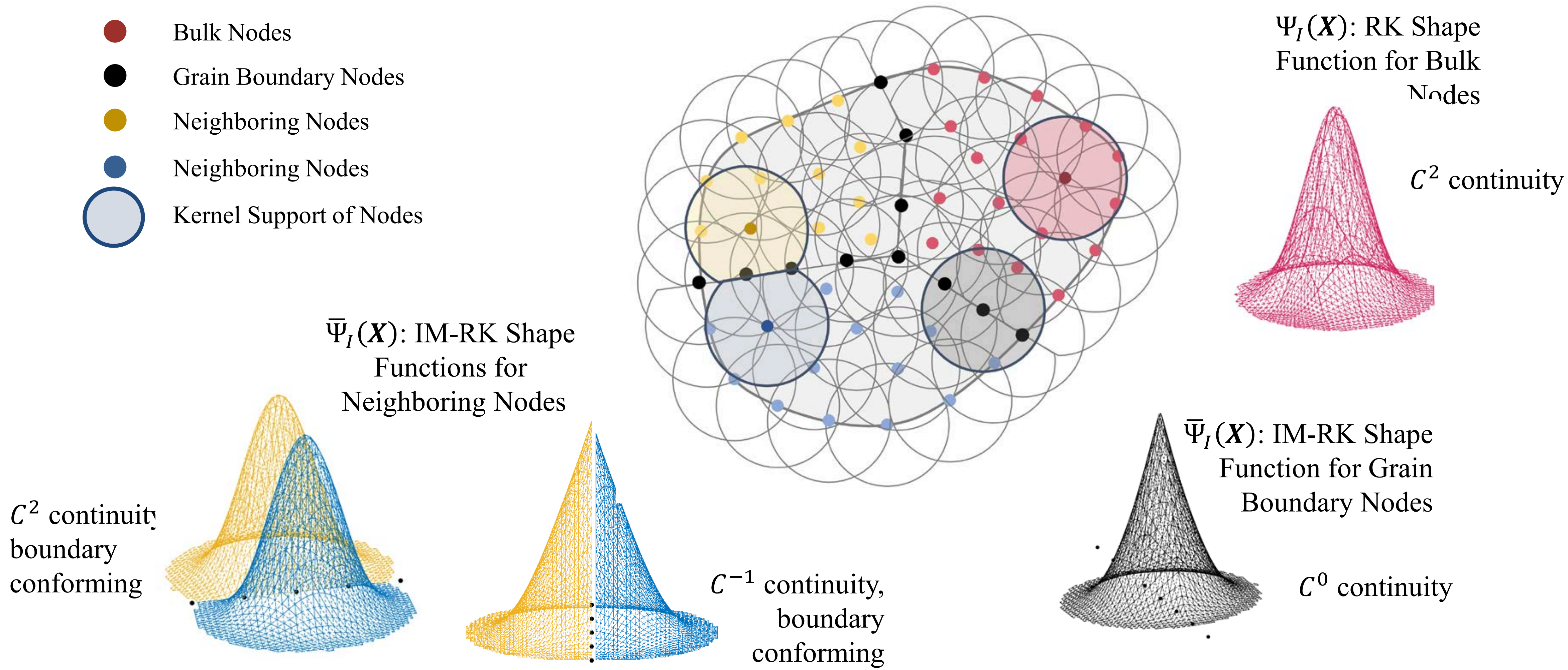
- $\boldsymbol{H}^T(\boldsymbol{x} - \boldsymbol{x}_I)$: controls order of **completeness**
- $\boldsymbol{b}(\boldsymbol{x})$: ensures satisfaction of **polynomial reproducing conditions**
- $\phi_a(\boldsymbol{x} - \boldsymbol{x}_I)$: controls order of **continuity**

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

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

7. 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.
8. 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.

Interface-Modified RK (IM-RK) Approximation for Weak and Strong Discontinuities



9. **Susuki, K.**, J. Allen, J.S. Chen. 2024. "Image-based Modeling of Coupled Electro-Chemo-Mechanical Behavior of Li-ion Battery Cathode Using an Interface-Modified Reproducing Kernel Particle Method." *Eng Comput.*

10. Wang, Y., J. Baek, Y. Tang, J. Du, M. Hillman, J.S. Chen. 2023. "Support vector machine guided reproducing kernel particle method for image-based modeling of microstructures", *Comput Mech*.

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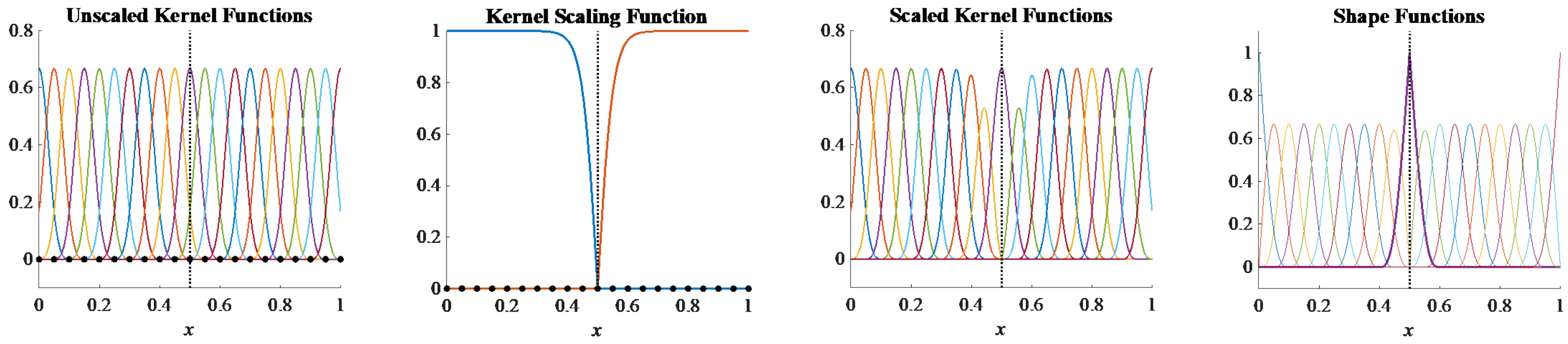
Kernel Function Modifications for Grain Boundaries: $\max[\tanh(dist), 0]$

***IM-RK with Weak Discontinuity**: Scaling with node on interface*

Weak discontinuity introduced only for $\overline{\Psi}_{Interface}$



***IM-RK with Strong Discontinuity**: Scaling with no node on interface*

Strong discontinuity introduced only for $\overline{\Psi}_{Interface}$

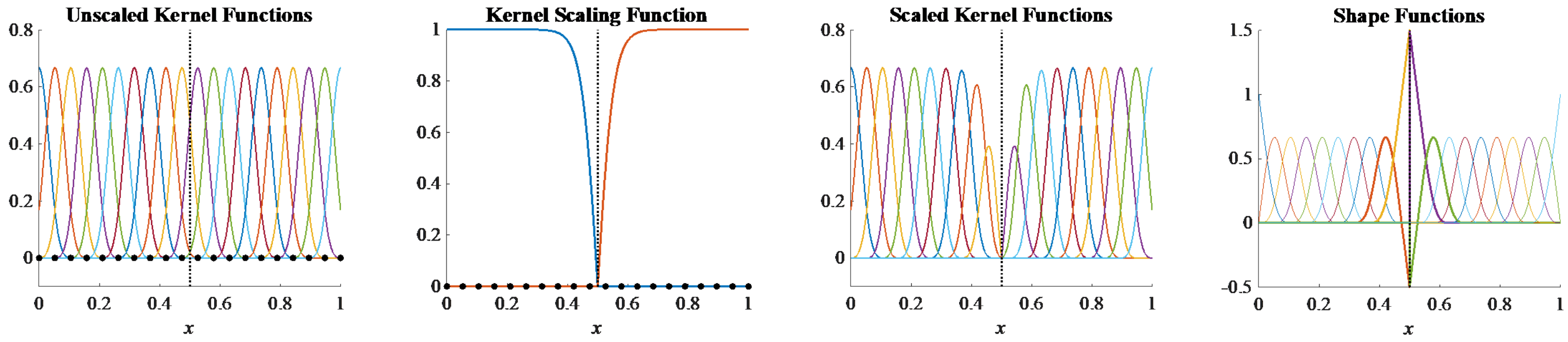


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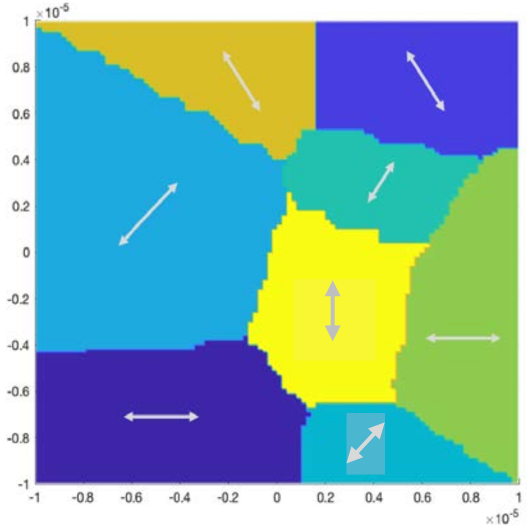
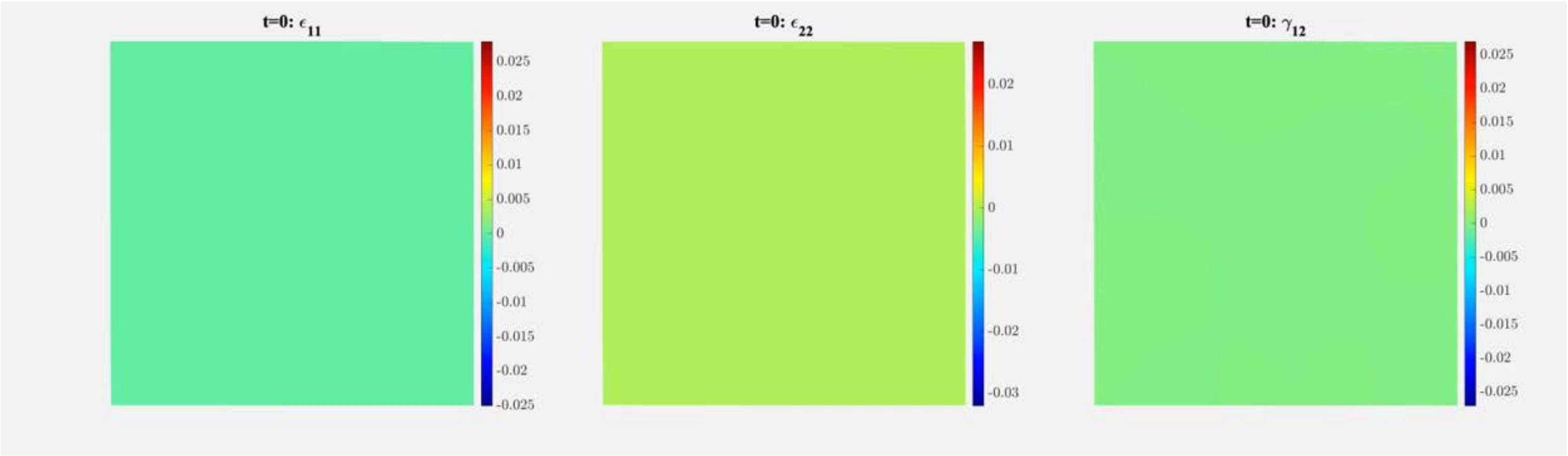
Image-Based Modeling of Statistically-Driven Li-ion Battery Microstructures

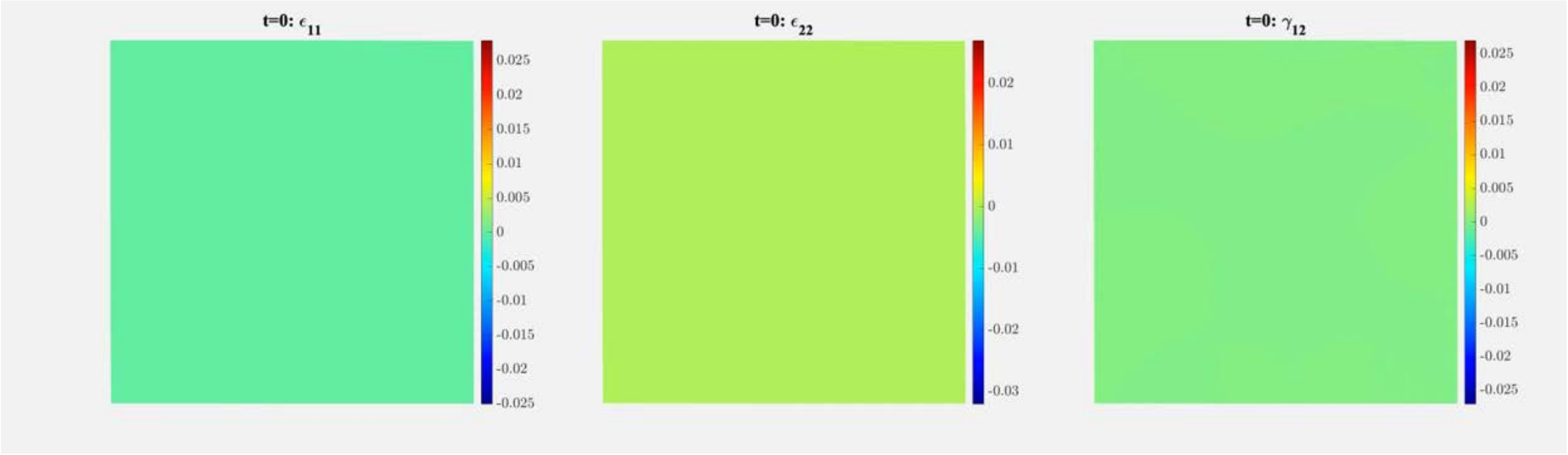
Strain Evolution Under Multiphysics Loading



Standard RKPM



Weak IM-RKPM



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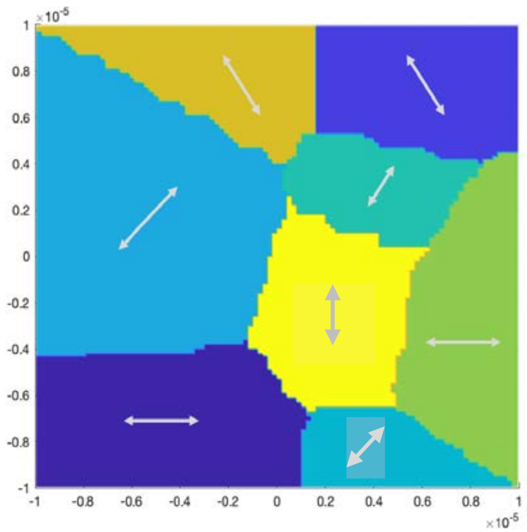
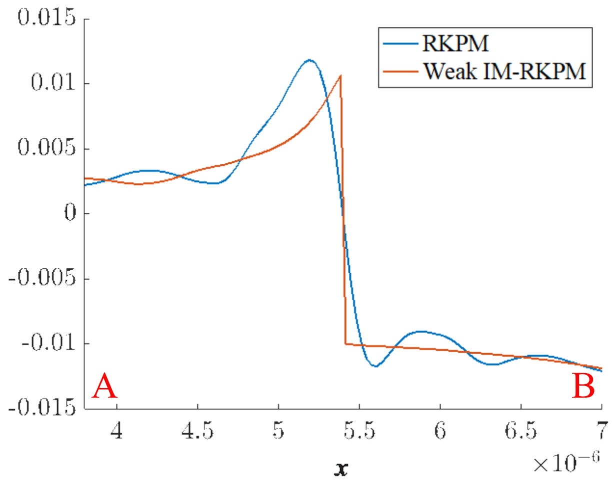
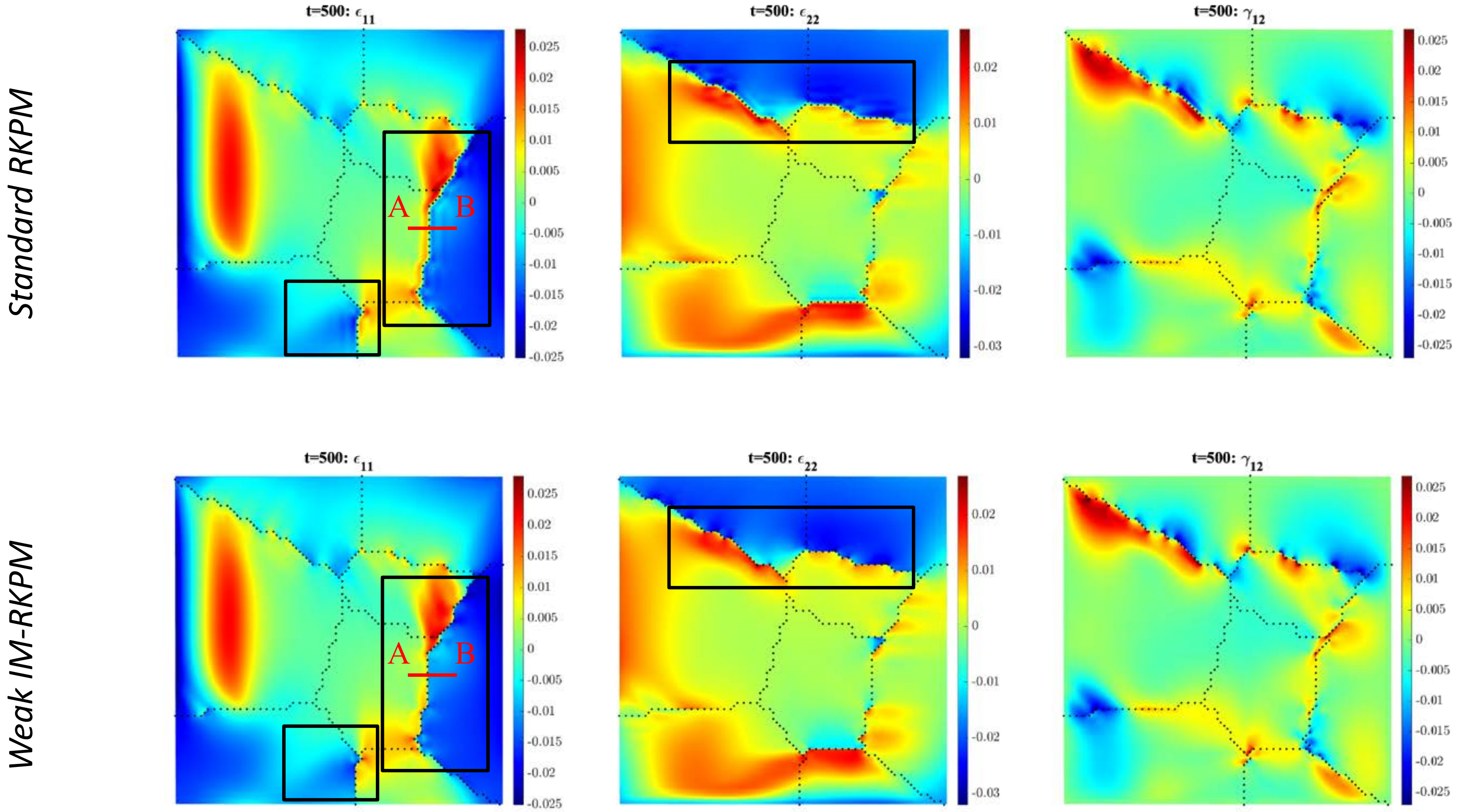
Strain Evolution Under Multiphysics Loading







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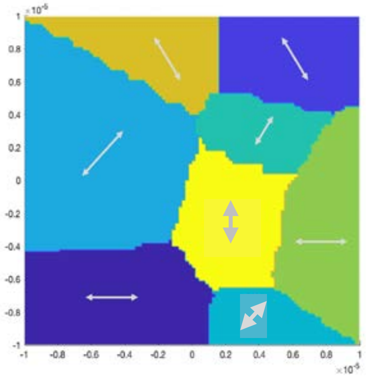
11. **Susuki, K.**, J. Allen, J.S. Chen. 2024. “Image-based Failure Assessment of Li-ion Batteries.” *ASC Technical Conference Proceedings*.

Multiphysics Damage Evolution with Evolving IM-RKPM
(Weak IM-RKPM → Strong IM-RKPM)



Damage

$$f\left(\epsilon_{eq}^{e}, \kappa\right) = \epsilon_{eq}^{e} - \kappa$$

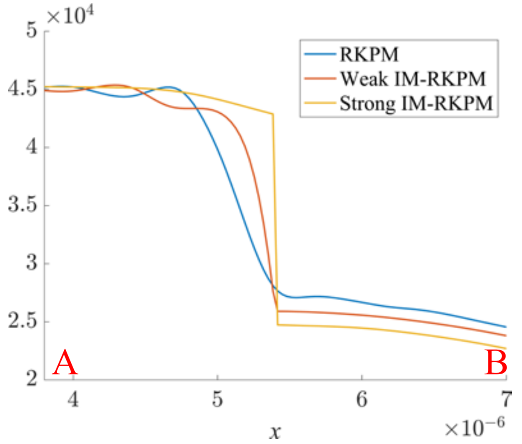
$$D_k(\kappa) = \begin{cases} 0 & if\ \kappa \le \kappa_i \\ \dfrac{\kappa_f}{\kappa}\dfrac{\kappa - \kappa_i}{\kappa_f - \kappa_i} & if\ \kappa_i < \kappa \le \kappa_f \\ 1 & if\ \kappa \ge \kappa_f \end{cases}$$

$$\epsilon_{eq}^{e} = \sqrt{\Sigma_i\left(\langle \epsilon_i^e \rangle\right)^2} \qquad \langle\cdot\rangle = \max(0,\cdot)$$

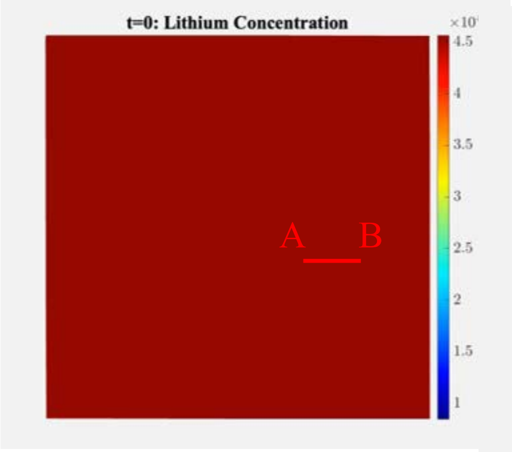
Kuhn-Tucker Conditions

$$f \ge 0\,; \quad \frac{d\kappa}{dt} \ge 0\,; \quad f\frac{d\kappa}{dt} = 0$$

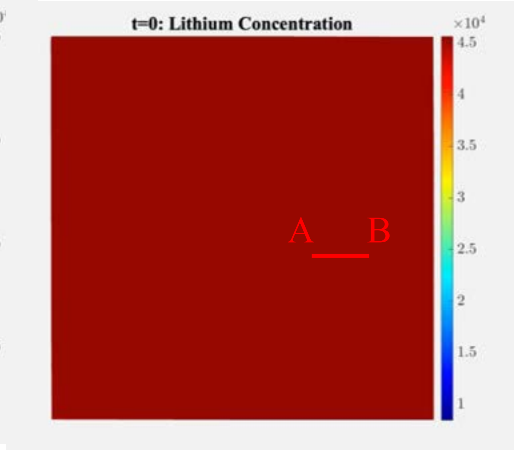
If ***sufficient grain boundary damage*** is detected, interface nodes are removed so ***IM-RKPM discontinuity adaptively evolves***



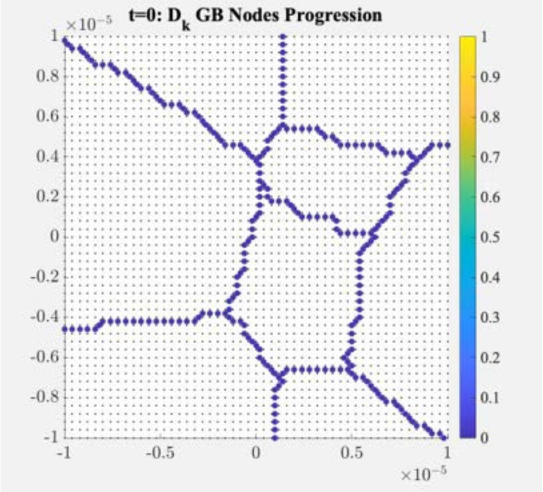
Standard RKPM



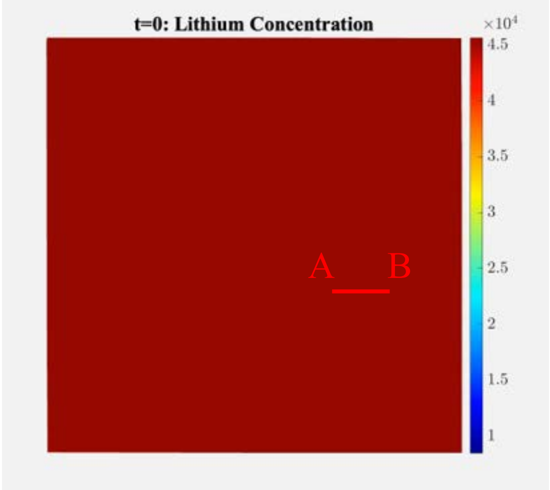
Weak IM-RKPM



Damaged nodes turn yellow



Evolving IM-RKPM



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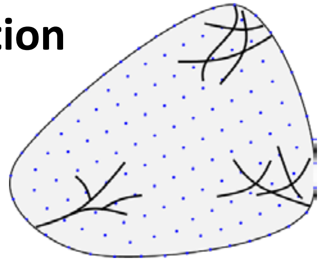
Neural Network-Enhanced RKPM

Neural Network Enhanced Reproducing Kernel (NN-RK) Approximation

Solution decomposition

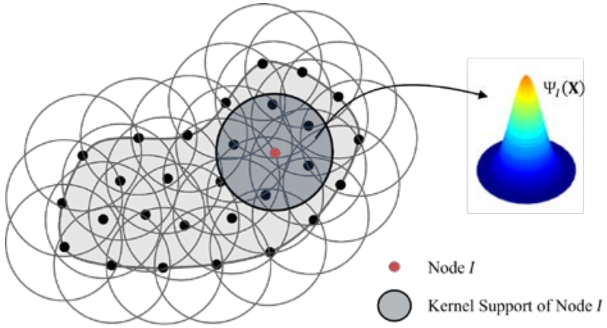
$$\mathbf{u}^h = \tilde{\mathbf{u}}^h + \hat{\mathbf{u}}^h$$

smooth background solution + rough local solution



Smooth solution approximation

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



Neural Network (NN) Enrichment

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

Neural network (NN) approximation

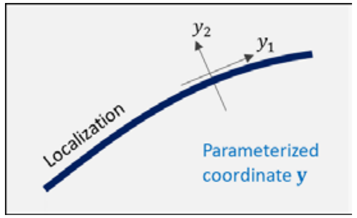
$$u^{NN}(\mathbf{x}) = \sum_{B=1}^{N_B} b_B^{NN}(\mathbf{x}; \mathbf{W}_B)$$

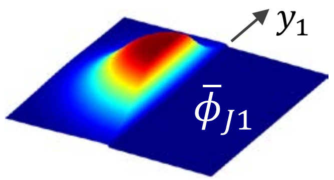
- b_B^{NN}: block-level NN approximation

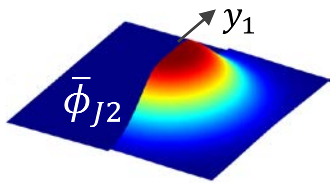
Block-level NN approximation

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

- NK: the number of NN kernels per block







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

NN Polynomial introduces
- Monomial completeness for further accuracy

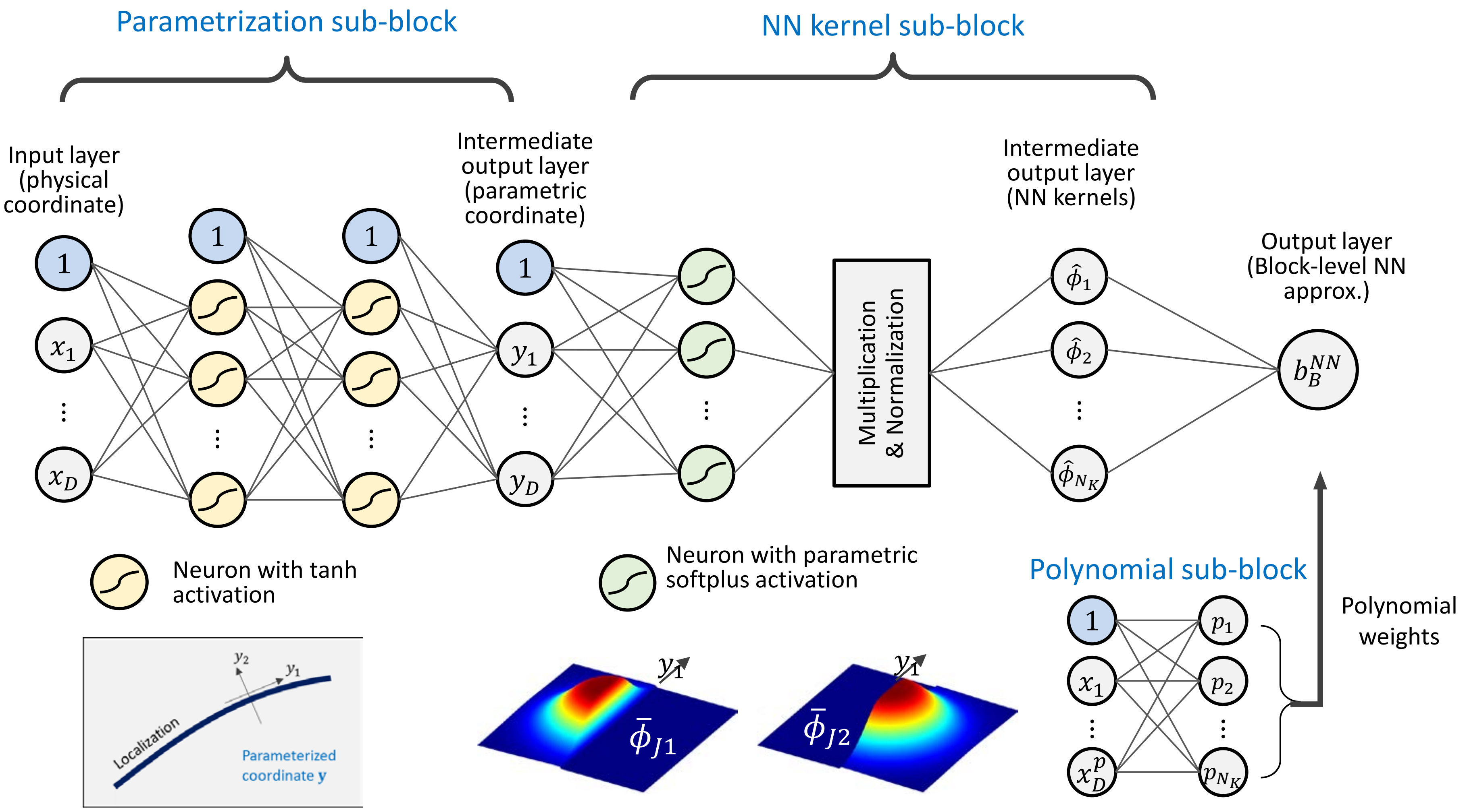
- $\mathbf{W}^L$: NN weight set controlling the location and orientation of the kernel.
- $\mathbf{W}^S$: NN weight set controlling the shape of transition.
- $\mathbf{W}^P$: NN monomial coefficient set

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

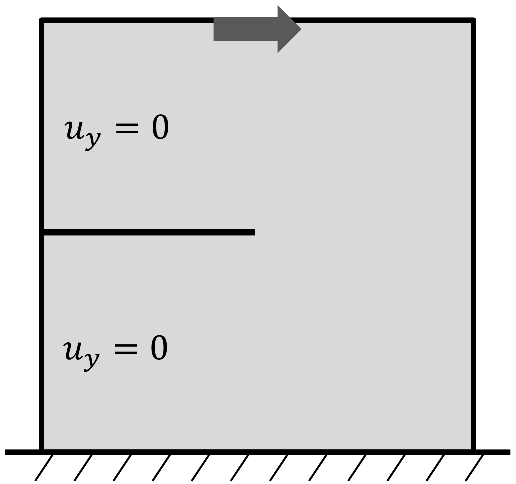
13. Baek, J., J.S. Chen, **K. Susuki**. 2022. "A neural network-enhanced reproducing kernel particle method for modeling strain localization." *Int J Numer Methods Eng.*

Block-Level Neural Network Architecture

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



Damage Evolution with Simple Shear Loading



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

Damage

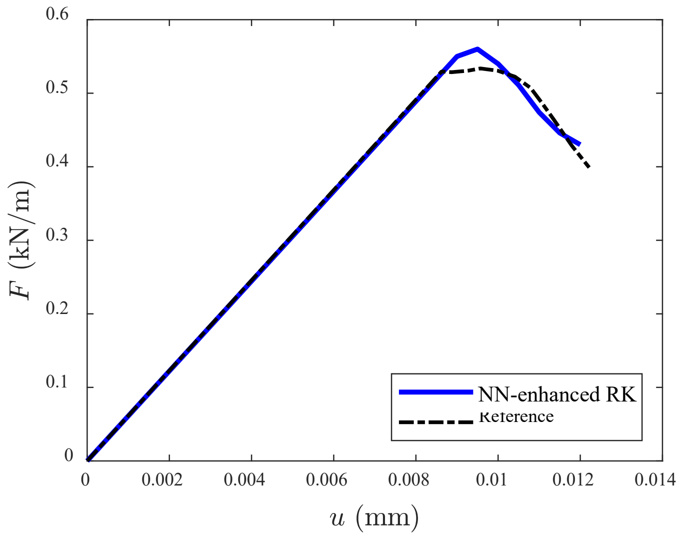
$$\eta = \frac{\kappa}{\kappa + p} \qquad \kappa = \psi^{+} - \psi^{c} \qquad p = G_c/\ell$$

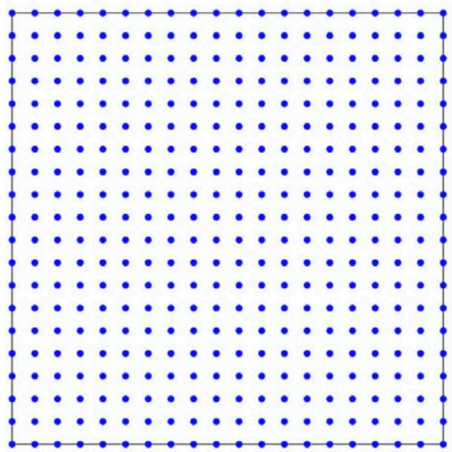
$$g(\eta) = (1-\eta)^2$$

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

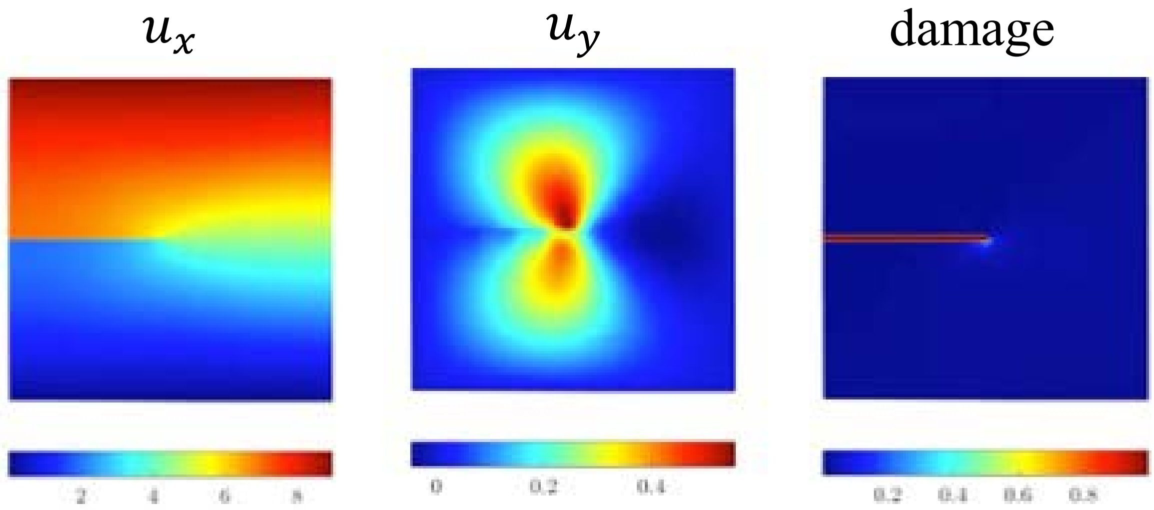
$$\psi^{-} = \frac{1}{2}\lambda((tr\varepsilon_i)^2 - \langle tr\varepsilon_i\rangle^2) + \mu\varepsilon_i^{-}\varepsilon_i^{-}$$

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





- 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.



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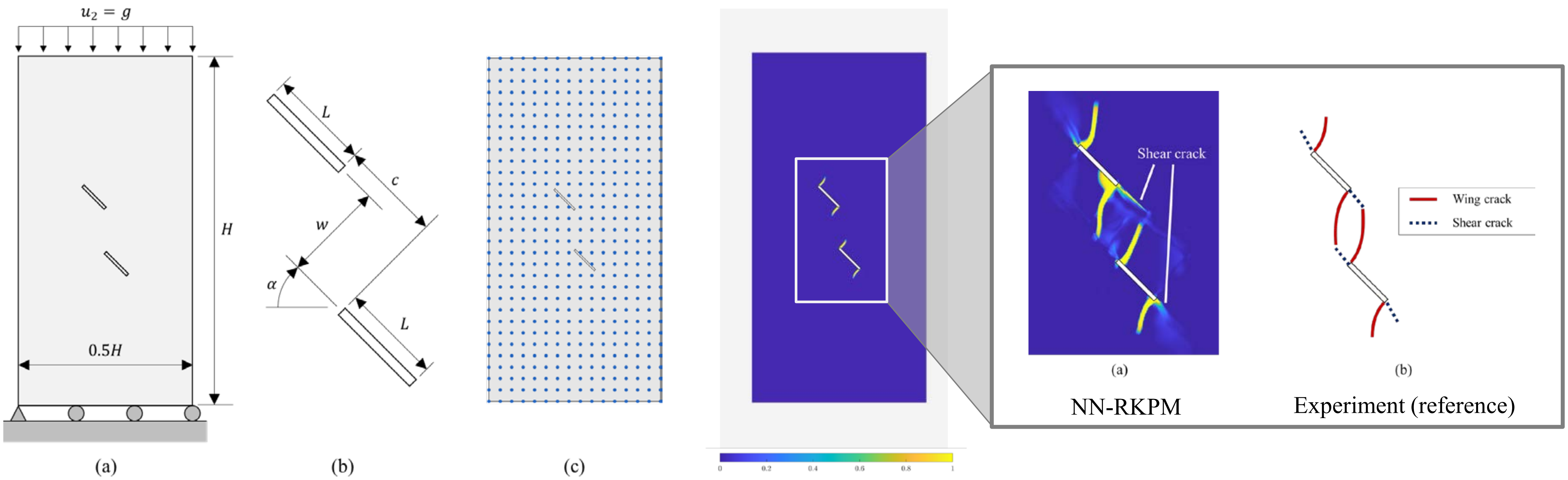
14. Miehe, C., M. Hofacker, F. Welschinger. 2010. “A phase field model for rate-independent crack propagation: robust algorithmic implementation based on operator splits.” *Comput Methods Appl Mech Eng.*

Mixed-mode Fracture of Doubly Notched Crack Branching in Isotropic Media



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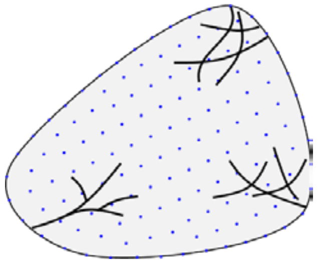
16. Bobet, A., H.H. Einstein, "Numerical modeling of fracture coalescence in a model rock material." *Int. J. Fract*.

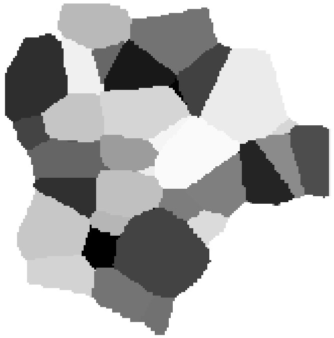
Future Work: Multi-scale NN-RK for Degradation Modeling of Li-ion Batteries

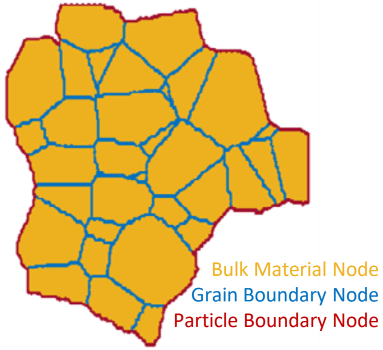
Coarse discretization for $\tilde{\mathbf{u}}^h$ with bulk material pixel point subset

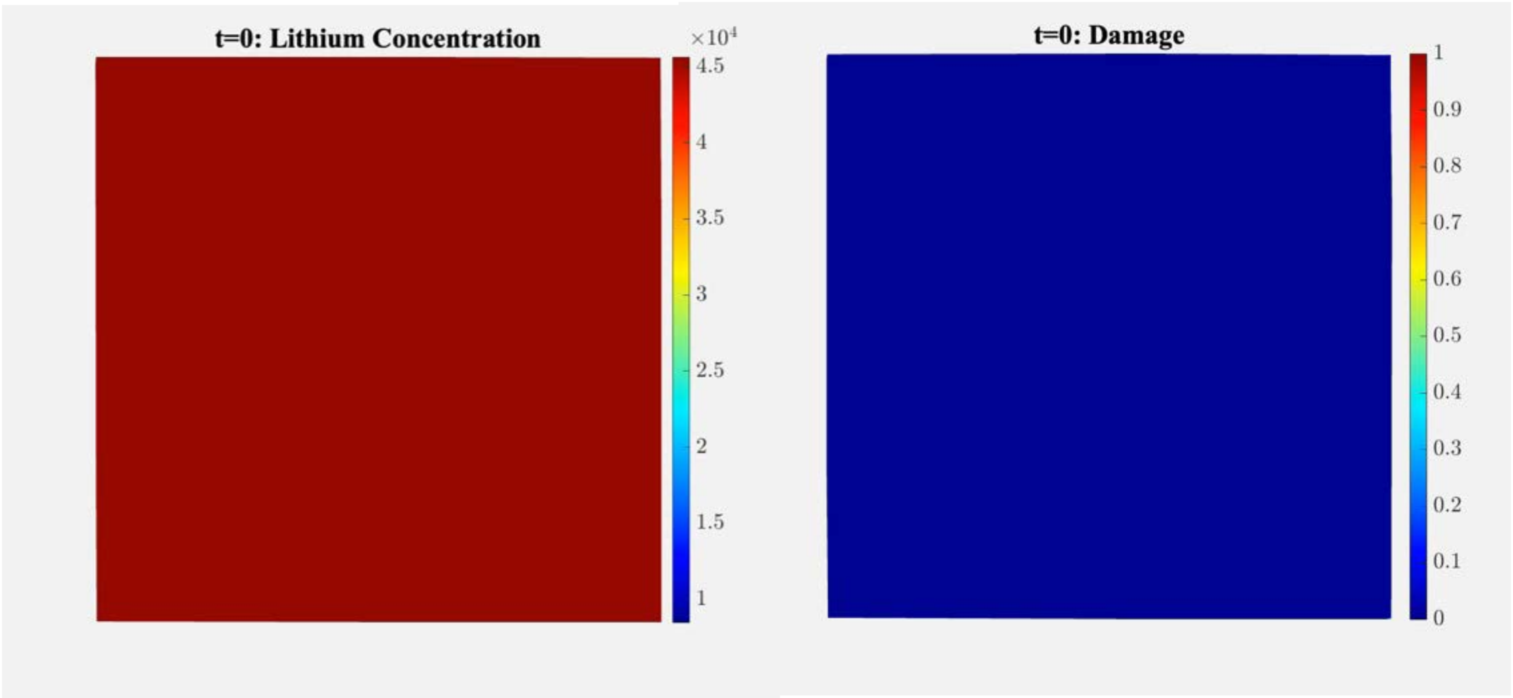
Solution decomposition

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









Conclusions

- Interface-modified RK (**IM-RK) discontinuity** shows significant **Gibbs oscillation reduction** and **sharper solution transitions** with **no additional degrees of freedom**.
- **Evolving IM-RK** approximation can **adaptively** incorporate various discontinuities by leveraging **kernel scaling** and strategic **interface node placement**.
- Neural network-enhanced RK (**NN-RK**) approximation is **designed to be computationally efficient** by superimposing a coarse background solution with a localized NN enrichment for fine/localized features.
- **NN block-level approximations** are designed to capture low order topology but can be **superimposed to capture complex topological geometries**.

Thank you

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- 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.

This work was authored in part by the National Renewable Energy Laboratory, operated by Alliance for Sustainable Energy, LLC, for the U.S. Department of Energy (DOE) under Contract No. DE-AC36-08GO28308. Funding provided by U.S. Department of Energy Office of Energy Efficiency and Renewable Energy. The views expressed in the article do not necessarily represent the views of the DOE or the U.S. Government. The U.S. Government retains and the publisher, by accepting the article for publication, acknowledges that the U.S. Government retains a nonexclusive, paid-up, irrevocable, worldwide license to publish or reproduce the published form of this work, or allow others to do so, for U.S. Government purposes.