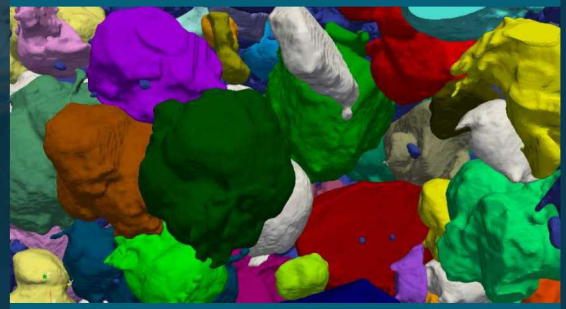
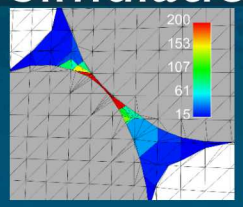
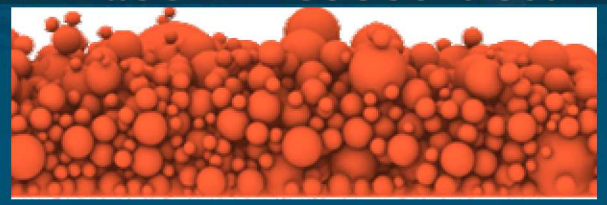
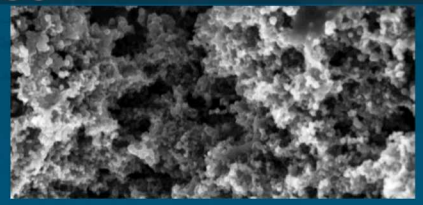
SAND2018-10021C

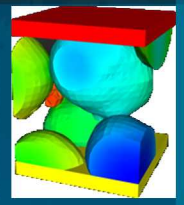
Application of the Conformal Decomposition Finite Element Method for Rapid Turnaround Analysis of Tomographic Imaging and Particle Simulation Based Mesostructures











PRESENTED BY

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Co-authors:

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- Mark E. Ferraro
- Jeremy B. Lechman
- David R. Noble
- Ishan Srivastava
- Bradley L. Trembacki

USACM Thematic Conference on Meshfree and Particle Methods: Applications and Theory
September 11, 2018

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Motivation for understanding electrode mesoscale morphology

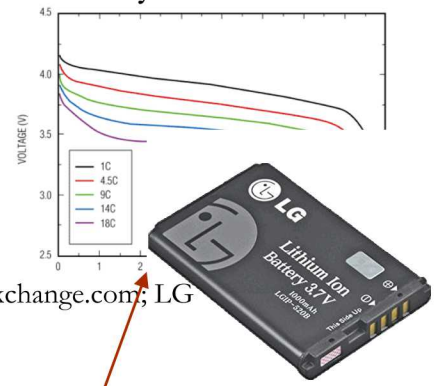
Length scale

Processing

Manufacturing

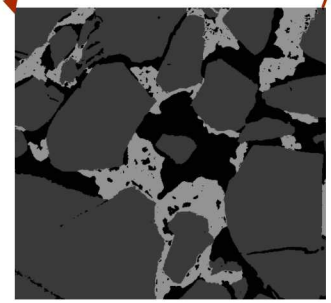
www.targray.com

Battery Performance



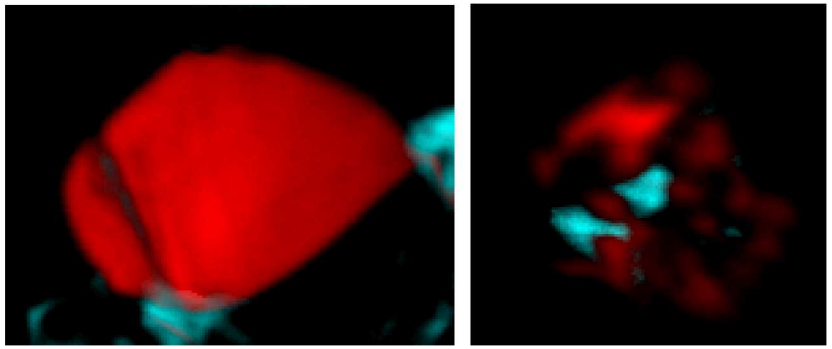
stackexchange.com; LG

Mesostructure



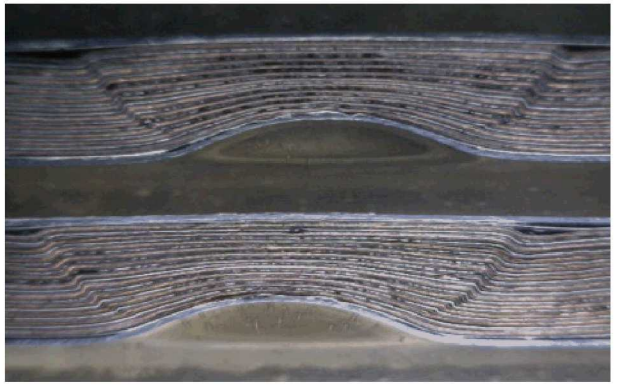
Hutzenlaub (2012)

Lithiation-Induced Fracture

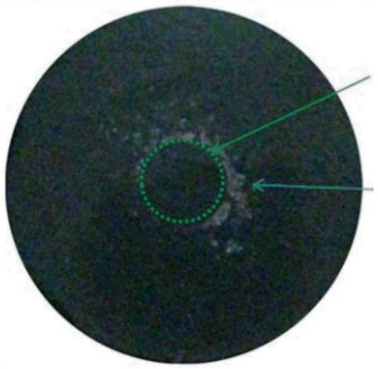


LiCoO2 STXM, Farid El Gabaly Marquez (Sandia)

Mechanical Abuse → Electrochemistry / Mesostructure



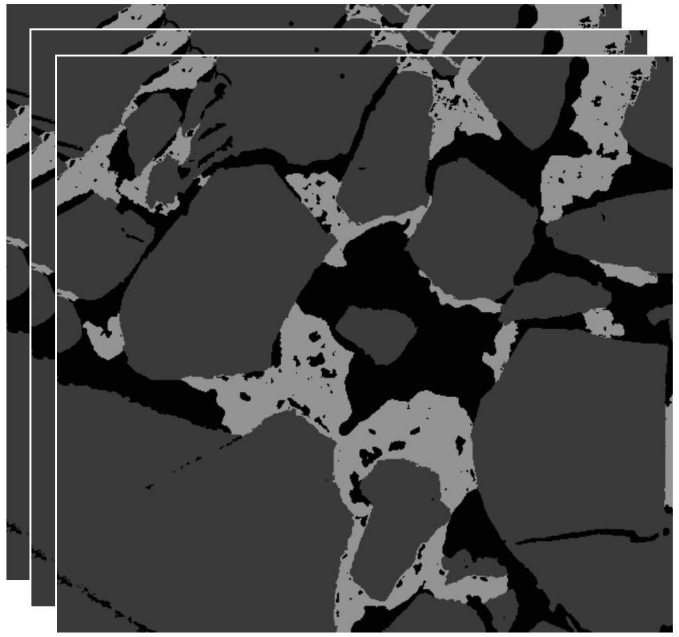
NMC/graphite pouch, H. Wang (ORNL)



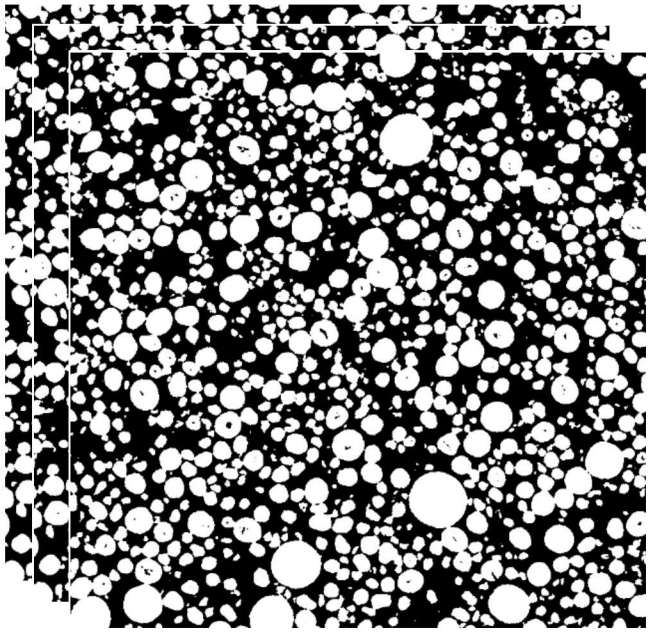
Cannarella/Arnold (2015)

Mesoscale morphology is critical link between manufacturing and performance

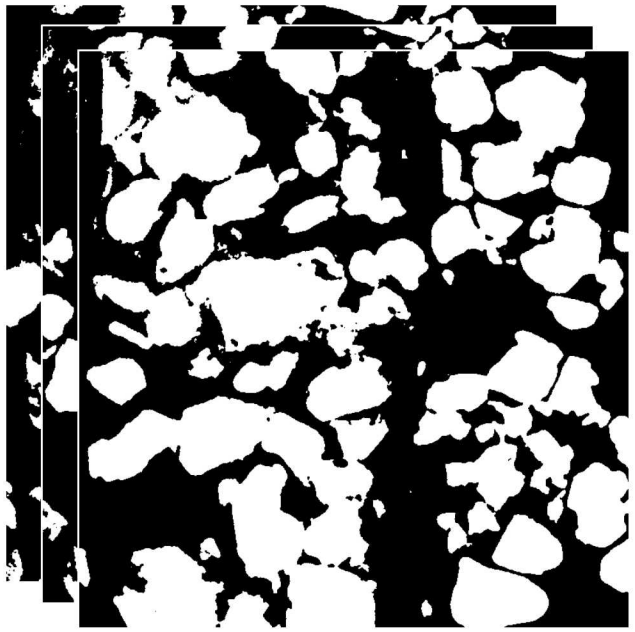
Imaging of cathode mesostructures



LCO with binder from FIB/SEM,
35 nm resolution,
20 μm domain.
Hutzenlaub (2012)



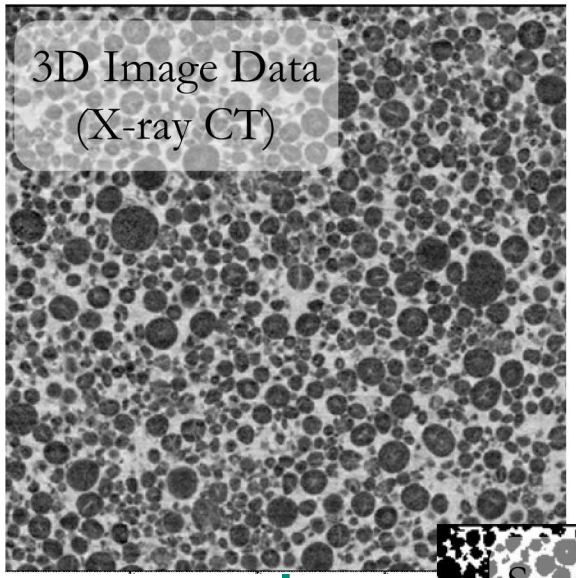
NMC from XRCT,
370 nm resolution,
757 μm domain.
Ebner (2013)

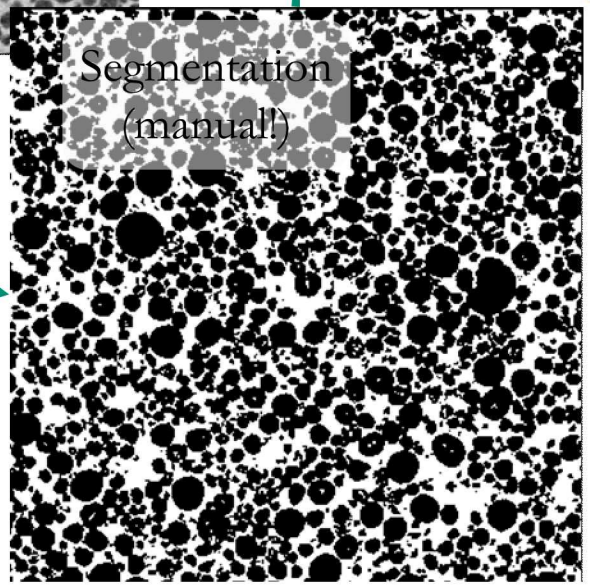


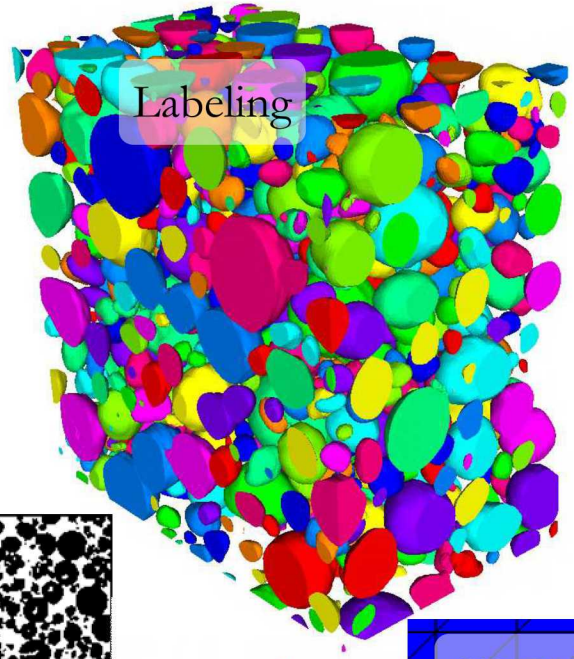
LCO from XRCT,
64 nm resolution,
22 μm domain.
Yan (2012)

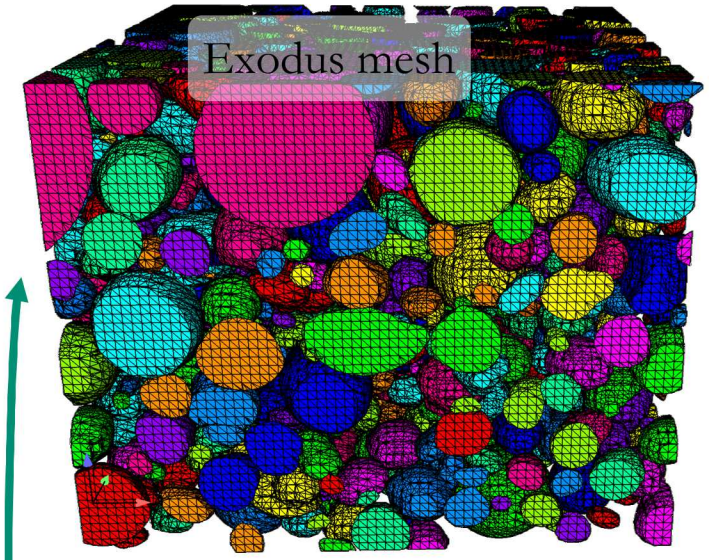
Imaging reveals complex networks; binder can be difficult to detect at scale

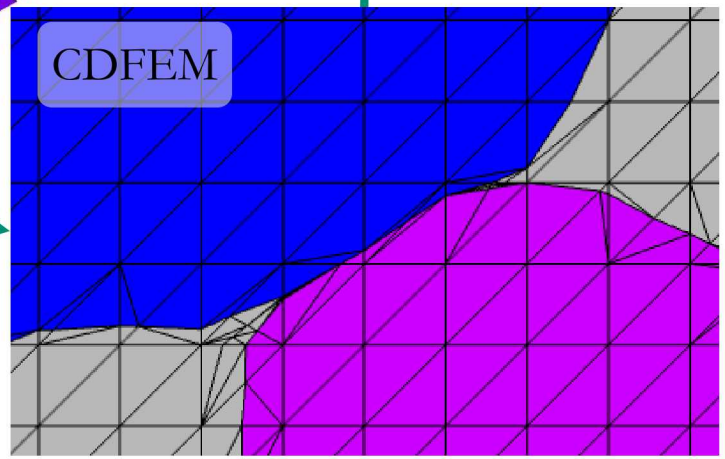
Mesoscale geometry from CT data using CDFEM











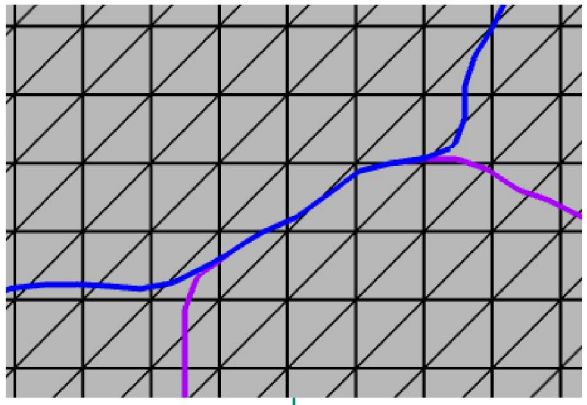
CDFEM is a powerful tool for creating multi-material conformal meshes

Noble (2013); Roberts (2014, 2016, 2018)

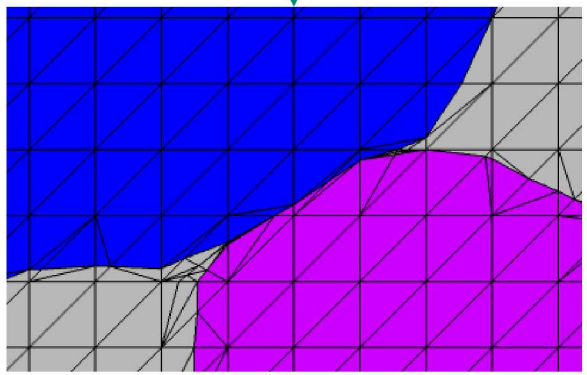
CDFEM for mesostructure mesh generation

Conformal Decomposition Finite Element Method (CDFEM) – Sandia's Sierra/Krino code

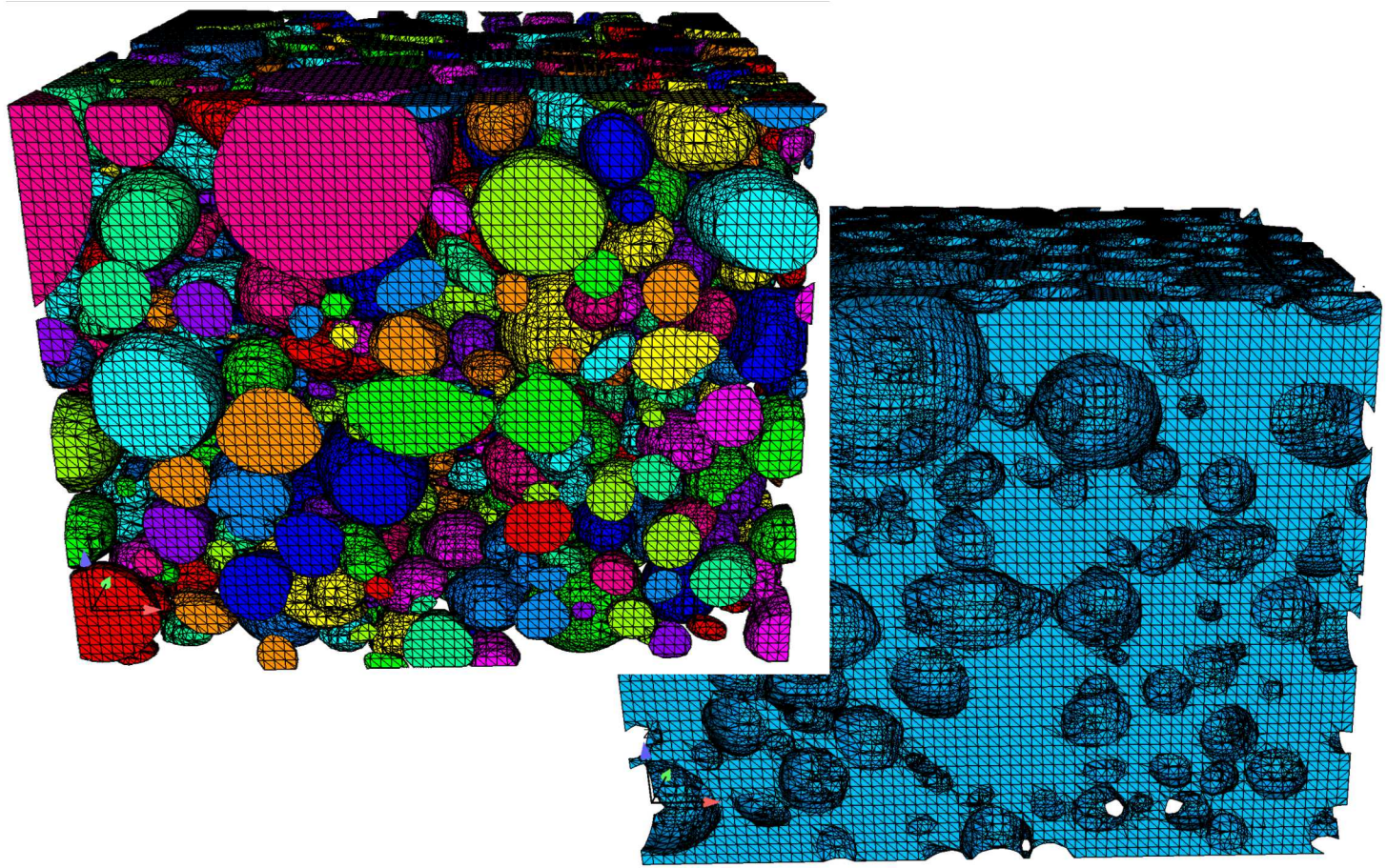
Background mesh + Surface descriptions (STL/analytic)



CDFEM



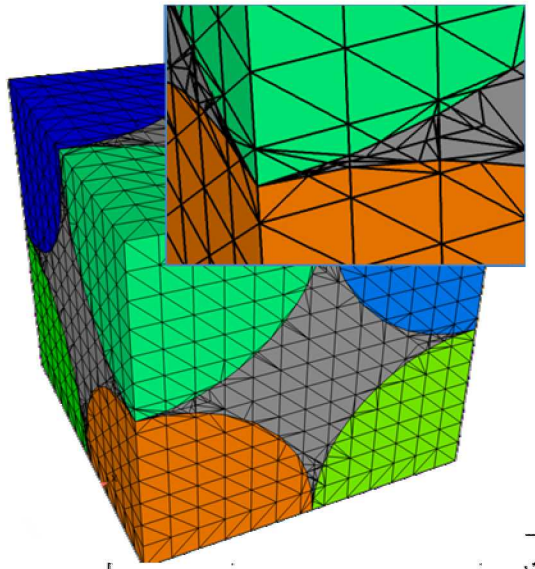
Conformal multi-domain mesh

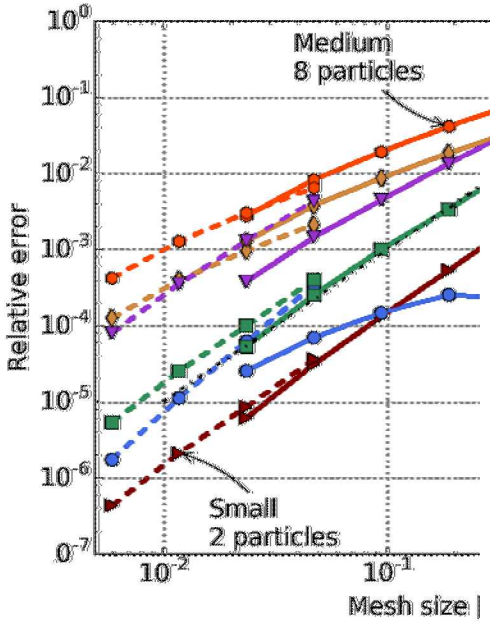


CDFEM enables rapid meshing of many complex domains from various source descriptions

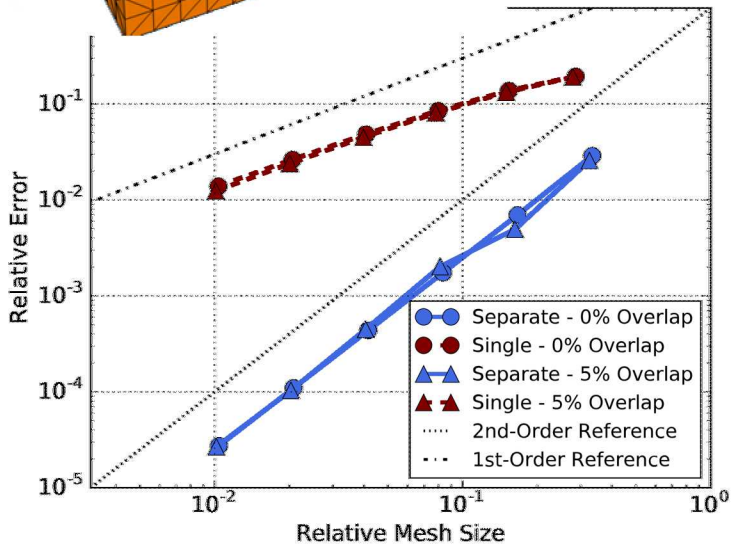
Noble (2013); Roberts (2014, 2016, 2018)

Solution verification for credible mesostructure simulations

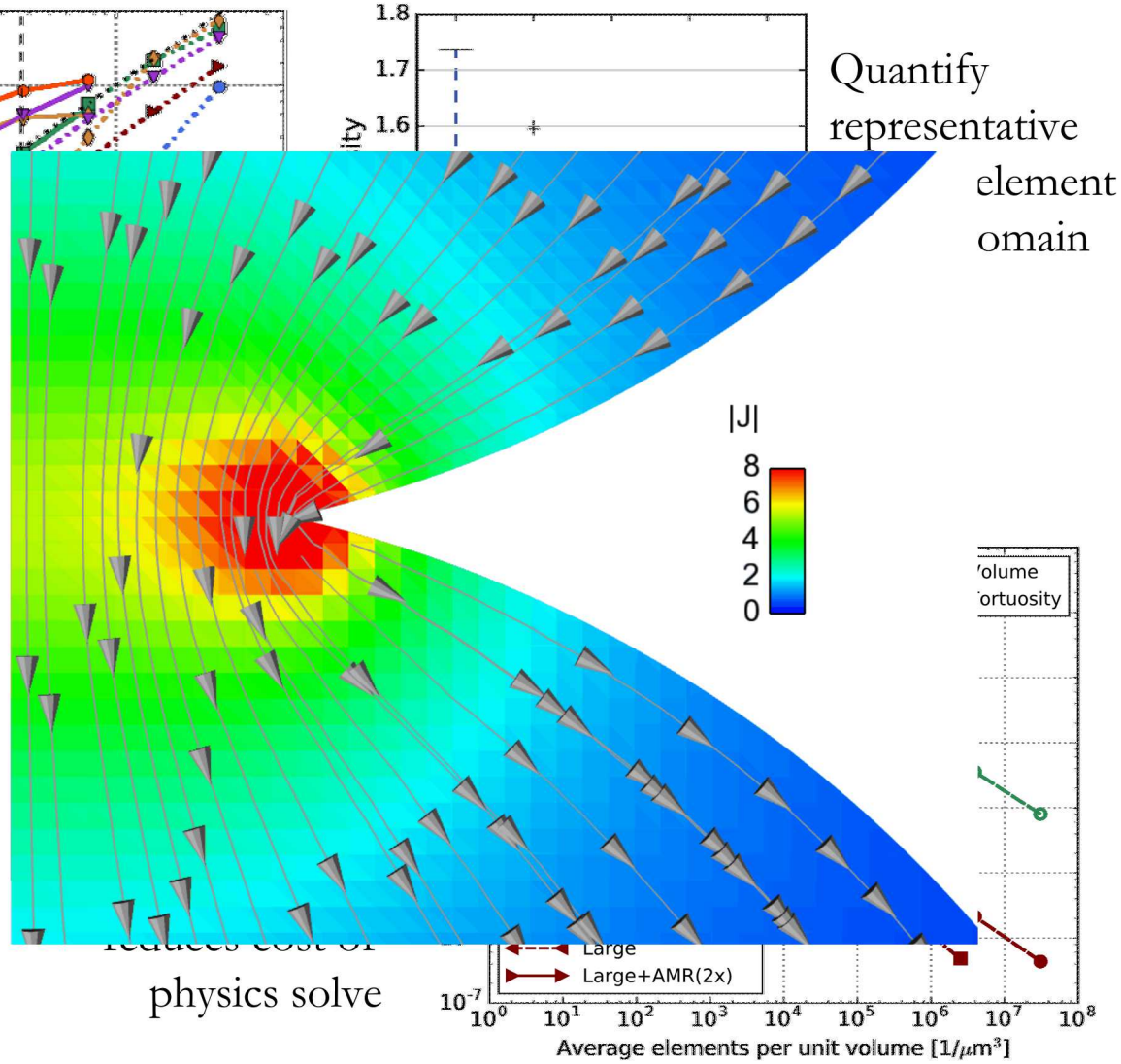




Understand mesh resc
for accurate pred



Separate particle representations required for optimal convergence



Quantify representative element omain

reduces cost of physics solve

Solution verification establishes simulation correctness and domain/mesh size requirements

Roberts (2018)

What about the conductive binder?

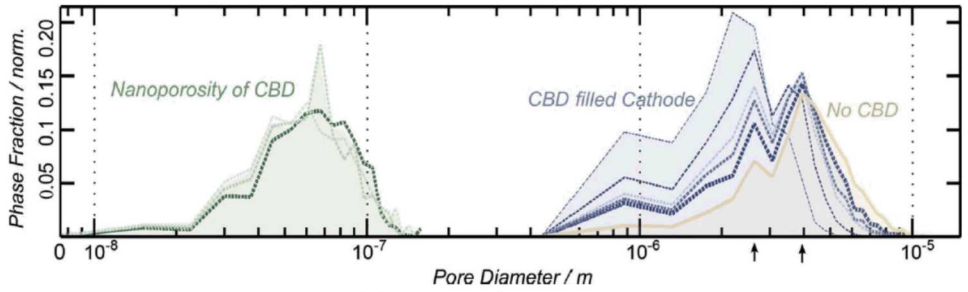
Resolving conductive binder in 3D imaging difficult

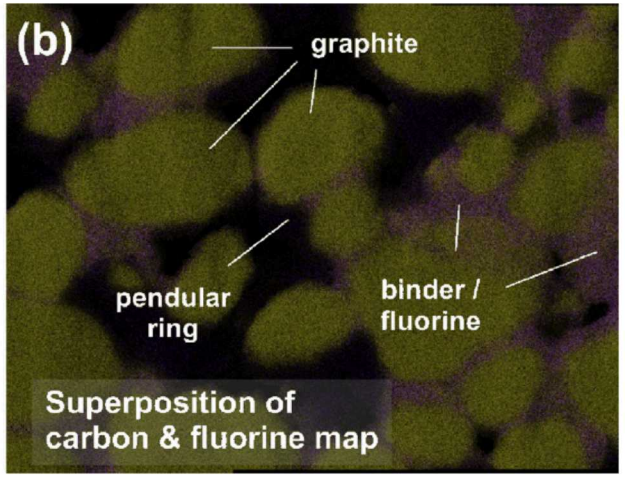
- Binder often neglected, assuming non-active void space is electrolyte
- Limited imaging results can hint at binder location

Amorphous binder is significantly nanoporous

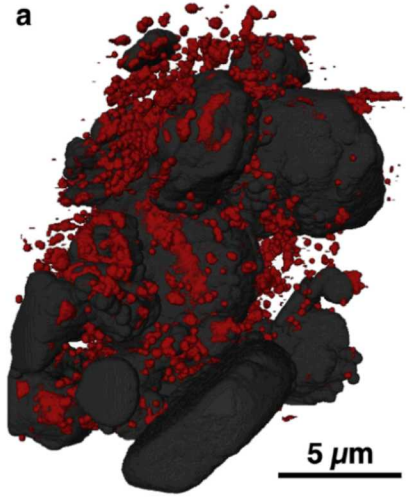
- 47% Zielke (2015); 45% Grillet (2016)
- 5% ionic conductivity of pure electrolyte

Binder weight fraction	Dense volume binder:particle	Porous volume binder:particle
0.04	0.10	0.15
0.06	0.16	0.23
0.08	0.22	0.31
0.10	0.28	0.40

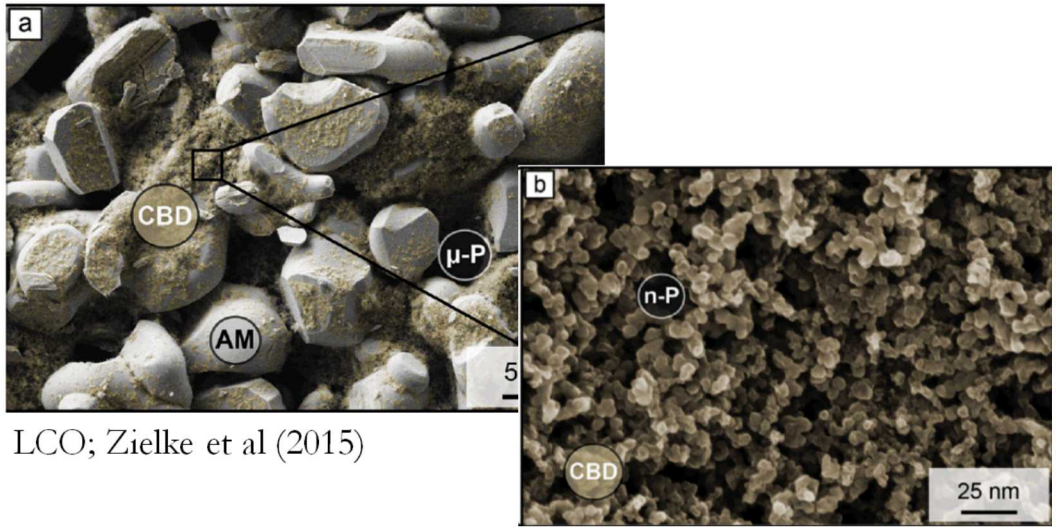




Graphite; Jaiser et al. (2017)



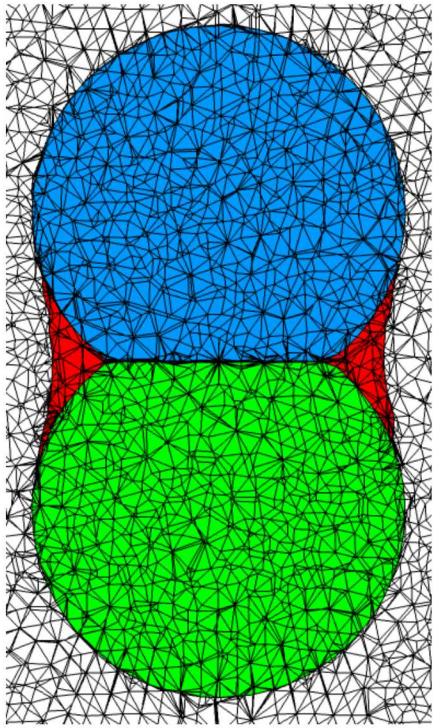
LCO; Komini Babu et al (2015)



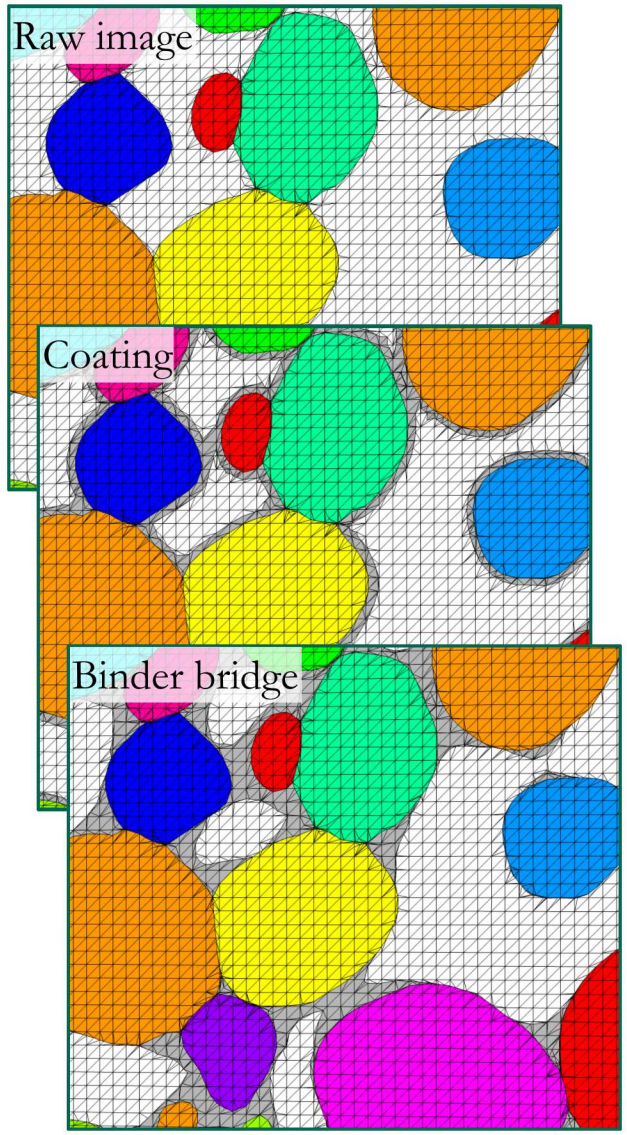
LCO; Zielke et al (2015)

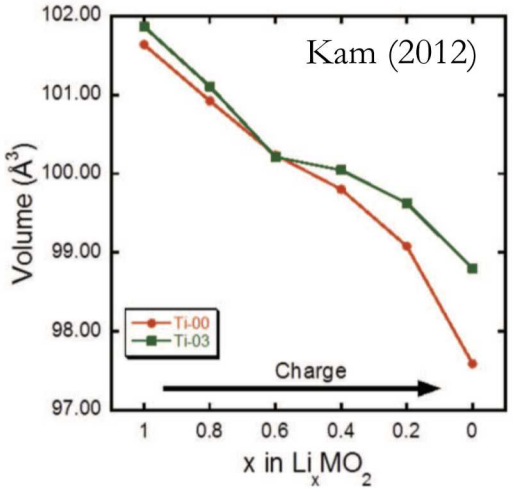
How are electrode-scale properties affected by the inclusion of binder? How does the morphology matter?

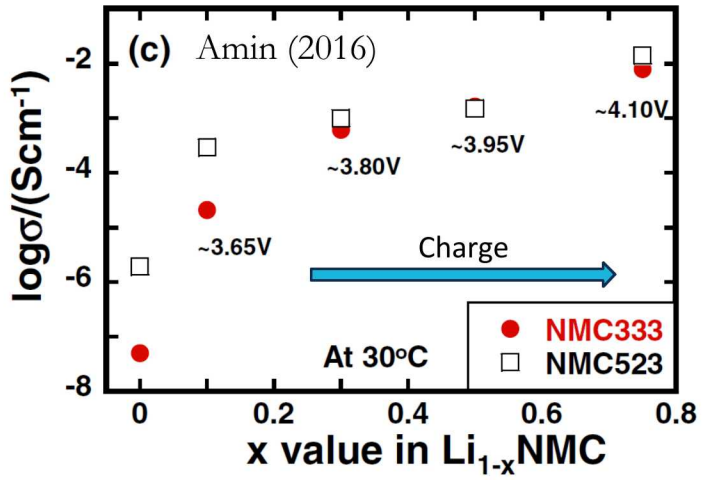
Binder bridge morphology approach



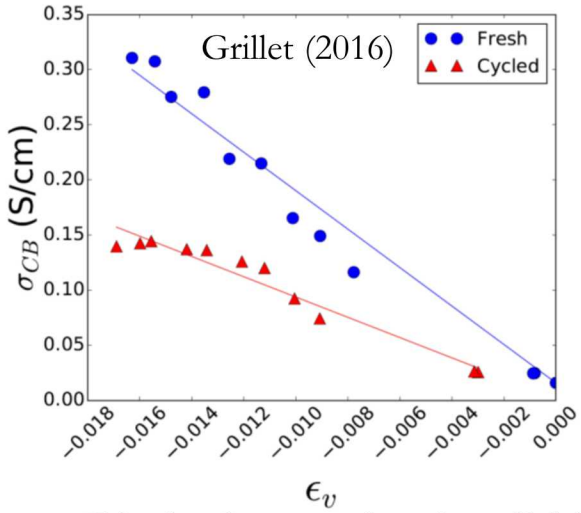
Mathematical description of "binder bridges"

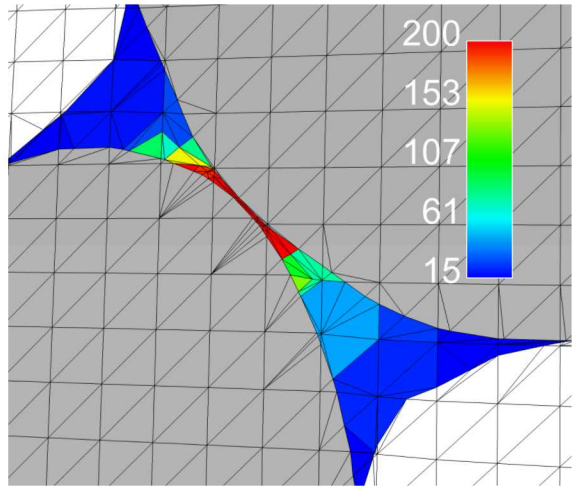






NMC has lithiation-dependent properties



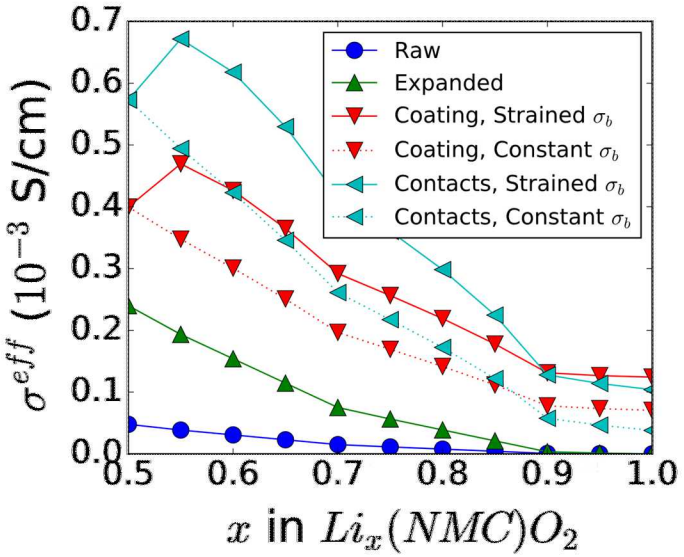


Binder has strain- (e.g. lithiation-) dependent properties

Binder bridge mimics experimental observations; properties are lithiation-dependent

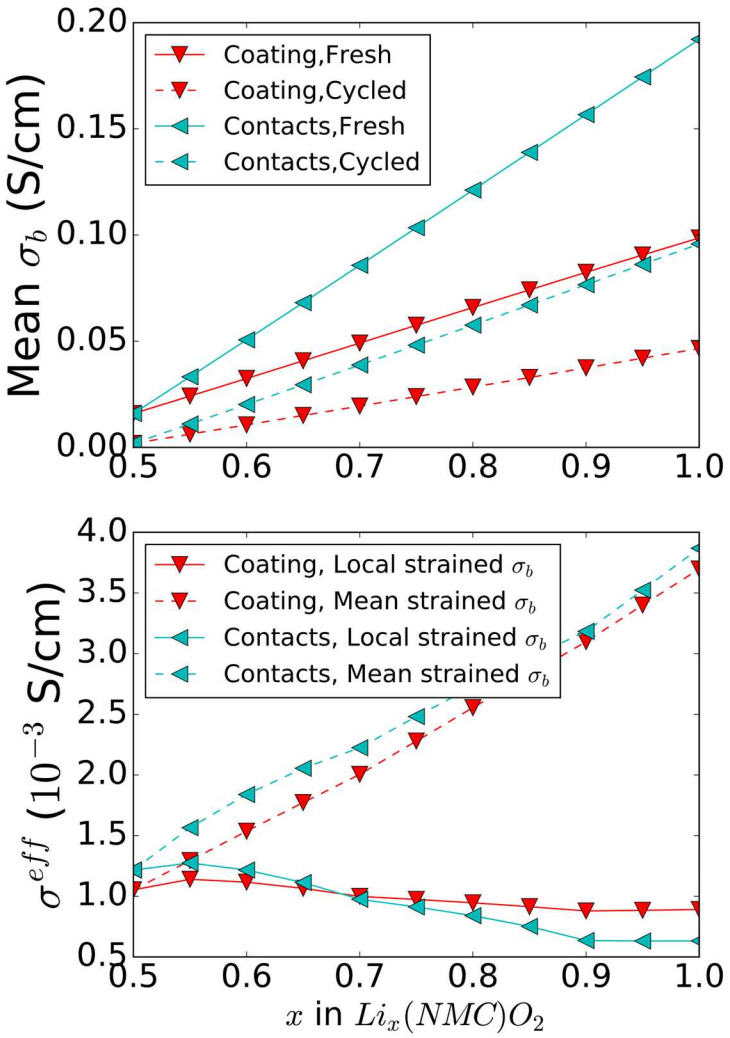
Trembacki (2017)

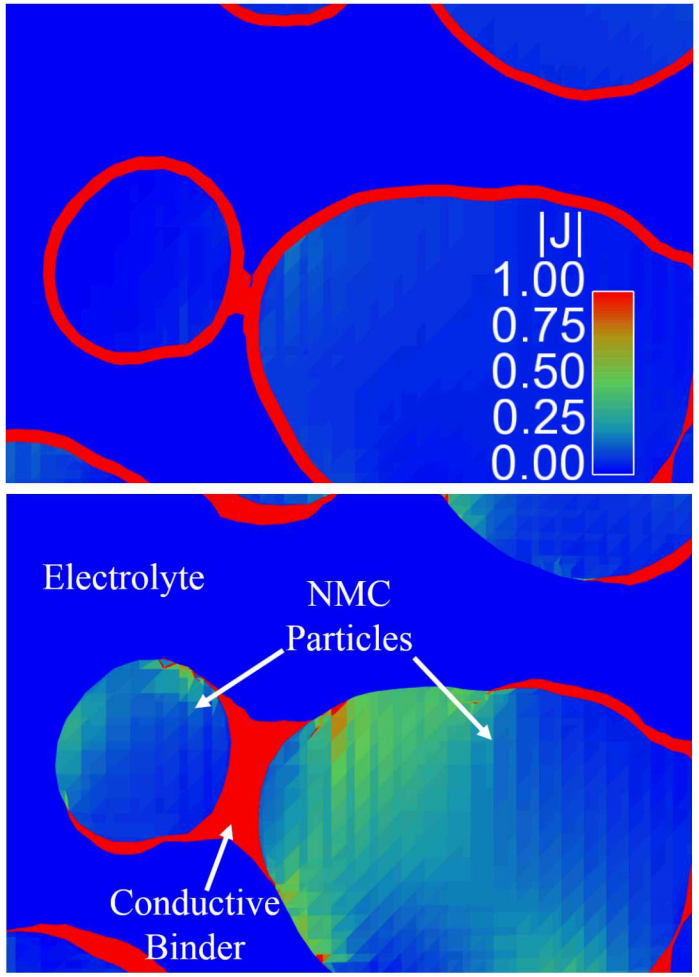
Effect of including binder on effective properties



Presence of binder increases electrical conductivity. Mechanics further increase conductivity.

Binder morphology and current localization matters. Binder bridge forces current flow through particles.

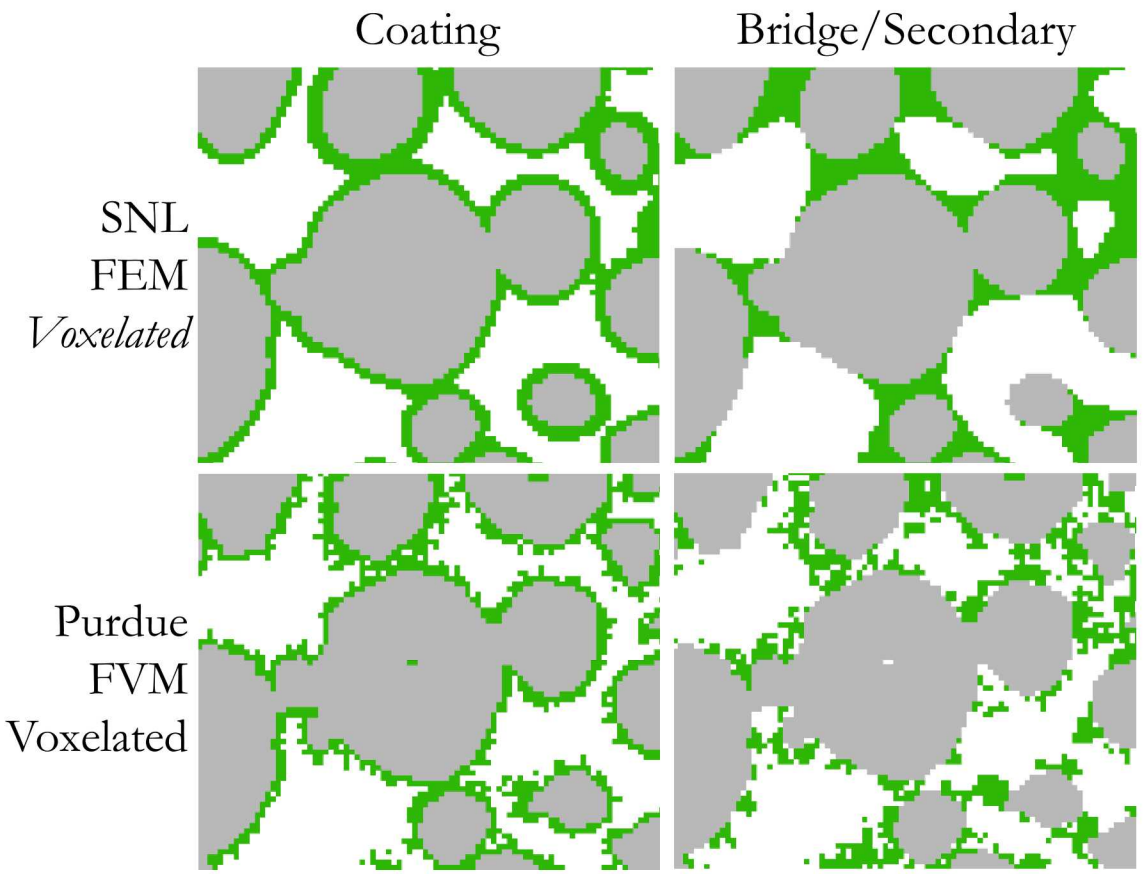


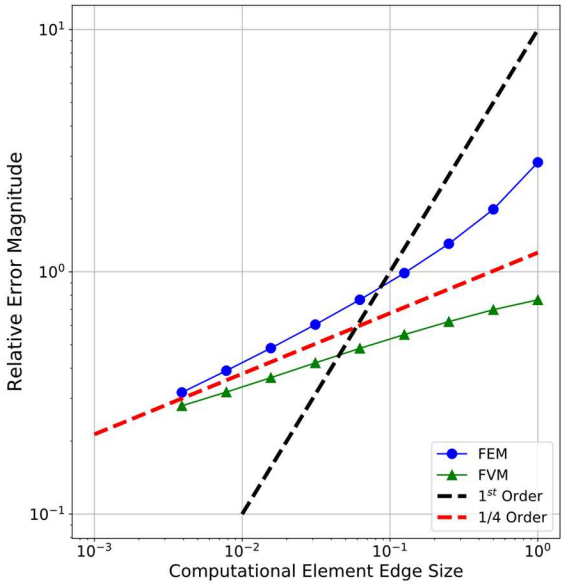


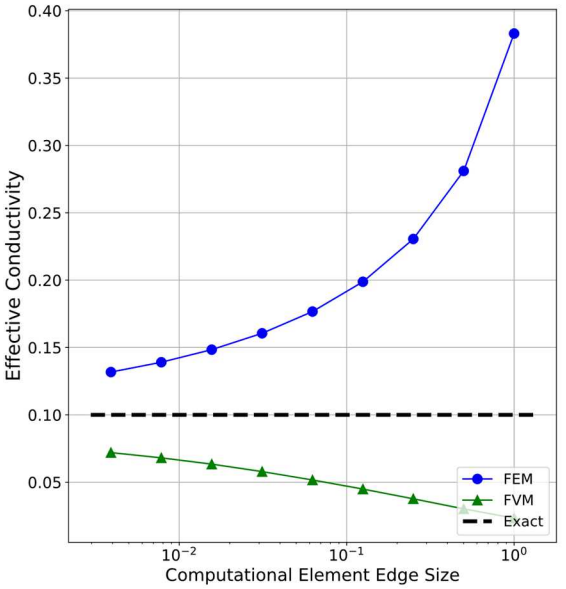
Binder morphology and mechanical coupling have a significant impact on effective properties; localization matters!

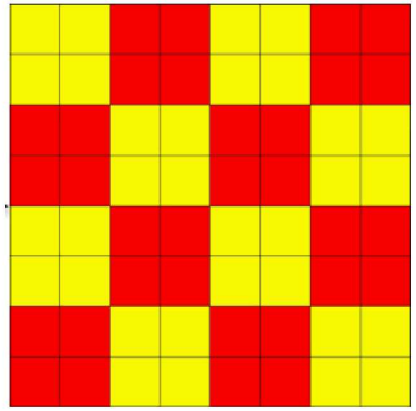
Trembacki (2017)

What about other morphologies and numerical methods









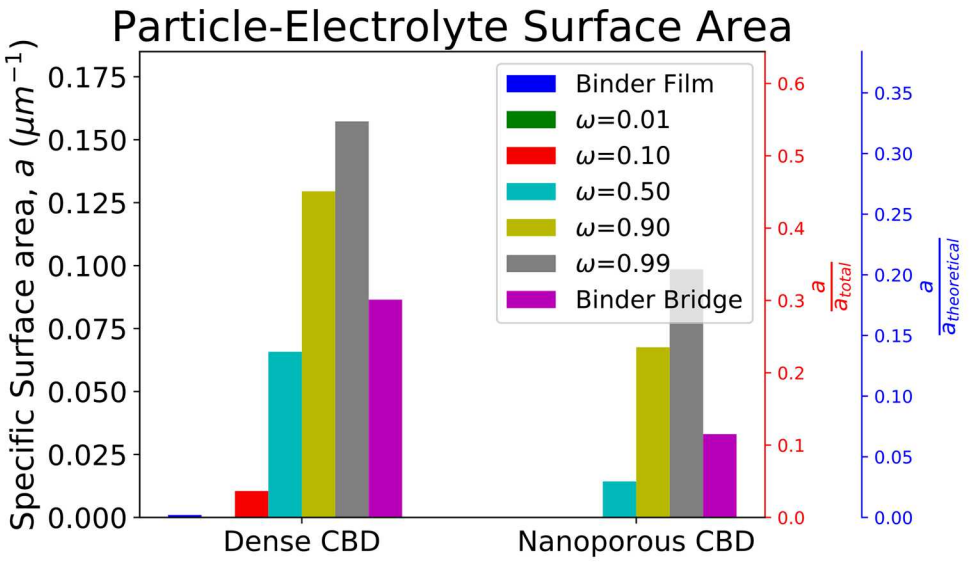
Both methods convergent on voxelated meshes, but:

- At slow rates (1/4-order)
- From different directions
- Unrefined results 10x different

Care must be taken when comparing results generated using different numerical methods; likely not converged!

Trembacki, submitted

Porous binder and morphology considerations



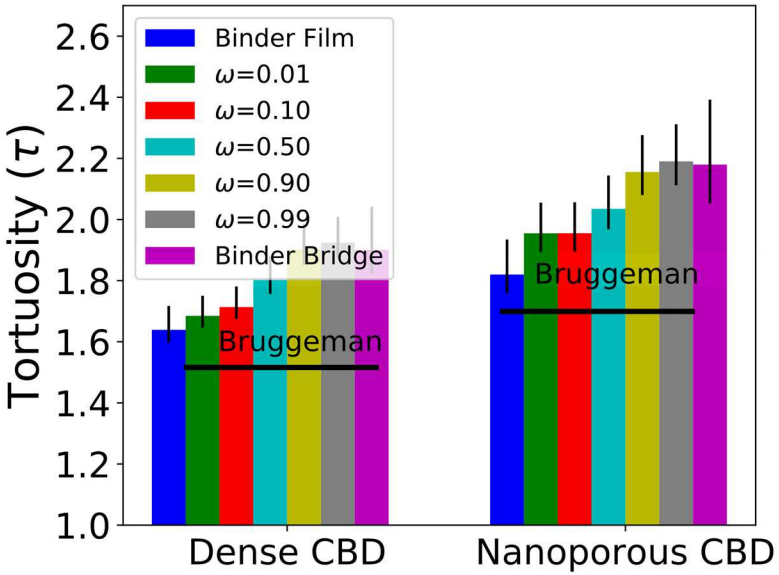
- More particle surface area available with non-uniform morphologies
- Nanoporous binder decreases bare particle surface area, but binder area is porous
- Surface are much less than theoretical

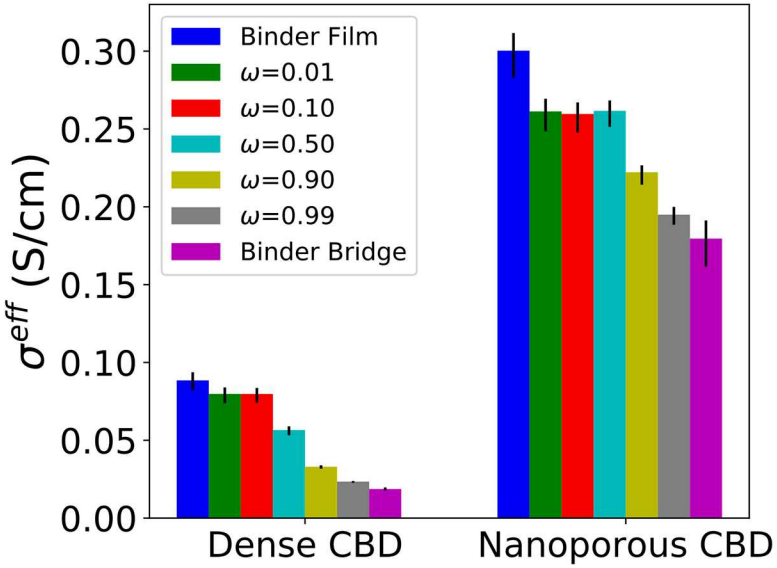
Non-uniform binder:

- Increases tortuosity
- Decreases conductivity

Nanoporosity:

- Increases tortuosity
- Increases conductivity





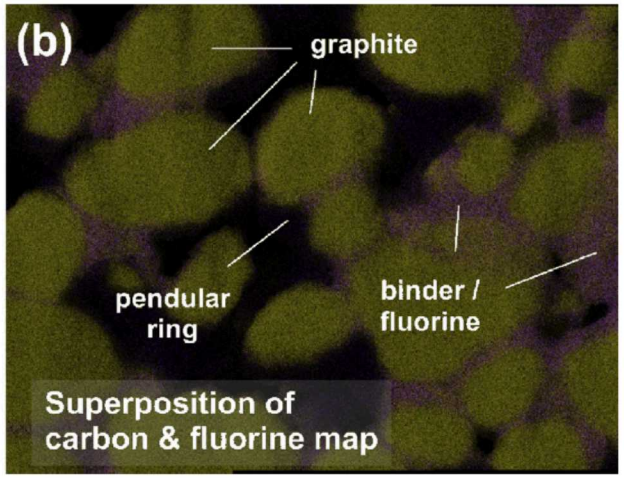
Limiting cases of both morphology methods show similar (but not identical) behavior; nanoporosity is important!

Trembacki, submitted

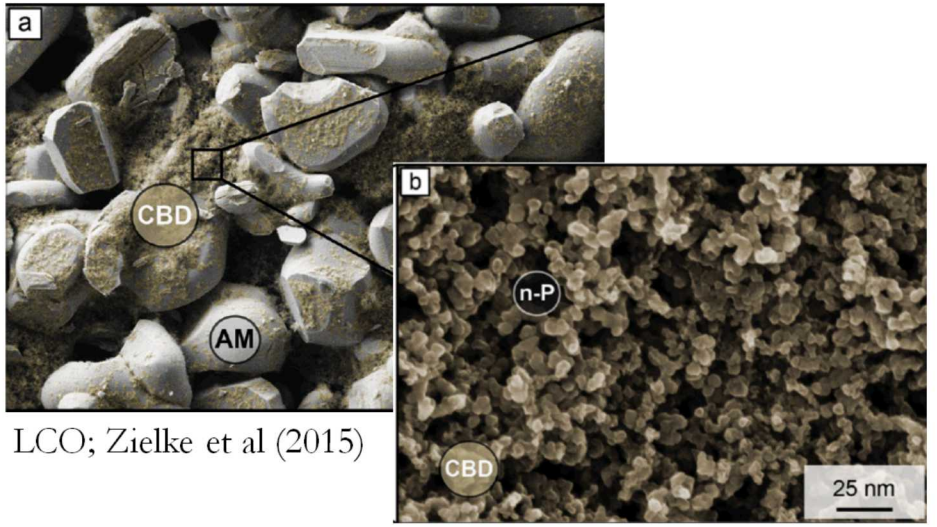
Challenges with using CT mesoscale data

3D CT image data:

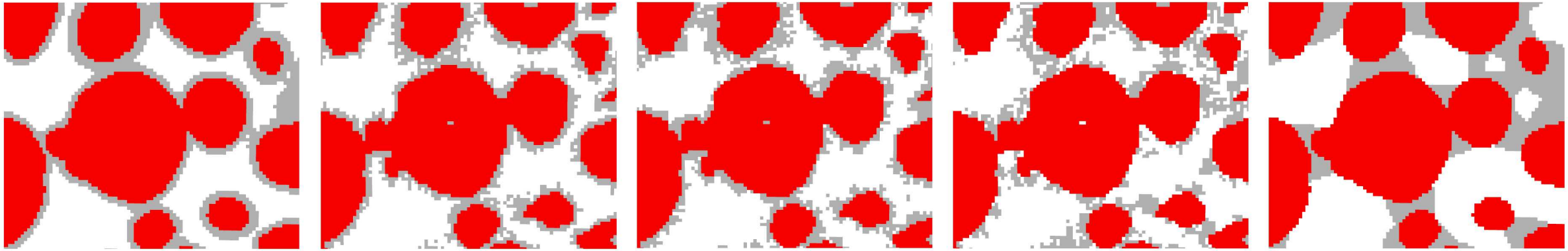
- Expensive
- Time consuming
- Conductive binder not visible



Graphite; Jaiser et al. (2017)



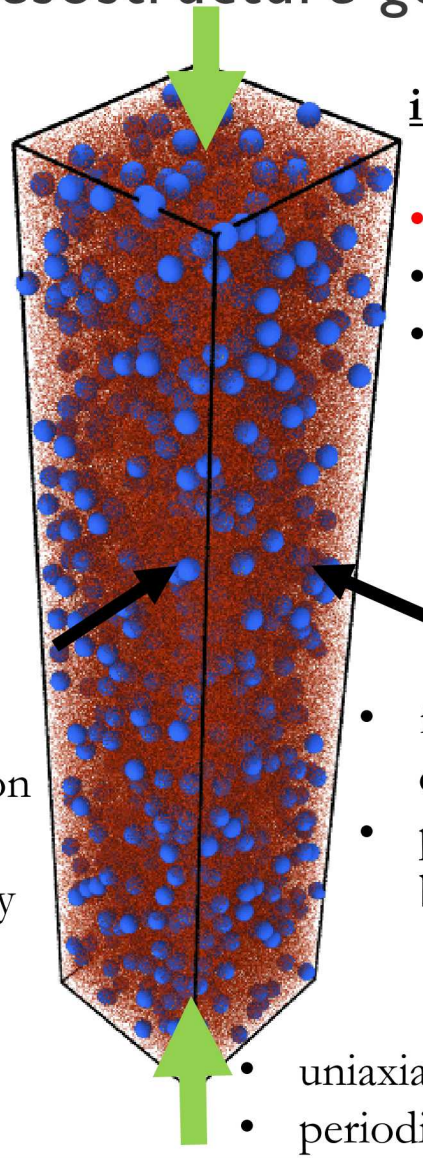
LCO; Zielke et al (2015)



Hypothesis: Use DEM simulations to create AM+CBD mesostructures and CDFEM for physics predictions

Trembacki, submitted

Mesostructure generation: Uniaxial compression



initial microstructure

- **porosity: 90%**
- height: 525 um
- width: 100 um

- fixed dimension
- periodic boundary

- fixed dimension
- periodic boundary

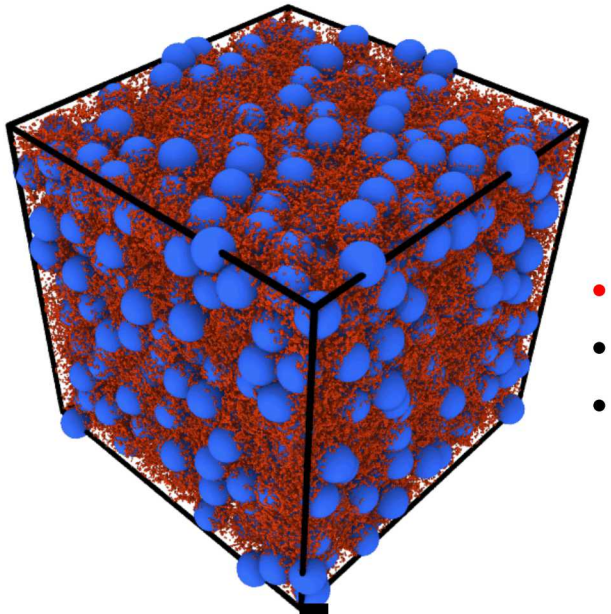
- uniaxial compression
- periodic boundary

compression (drying)

constant strain-rate compression

$$\dot{\gamma} = 4\mathrm{s}^{-1}$$

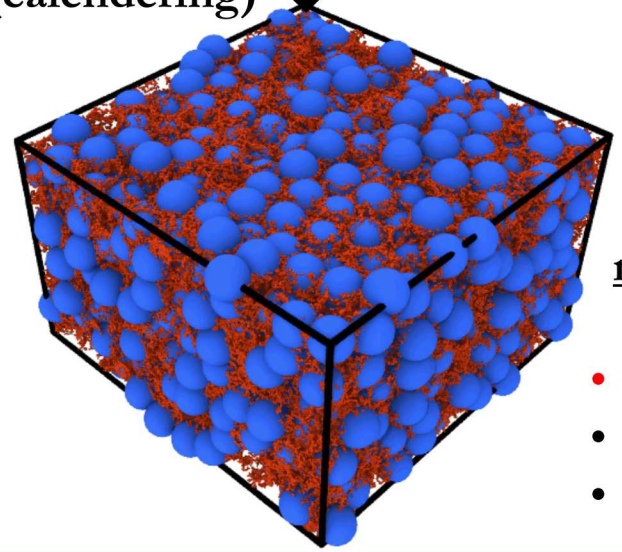
0.4 s physical time
864 cores
~ 12 hours simulation time



intermediate microstructure

- **porosity: 50%**
- height: 100 um
- width: 100 um

compression (calendering)



compressed microstructure

- **porosity: 20%**
- height: 66 um
- width: 100 um

Uniaxial compression represents both drying and calendering

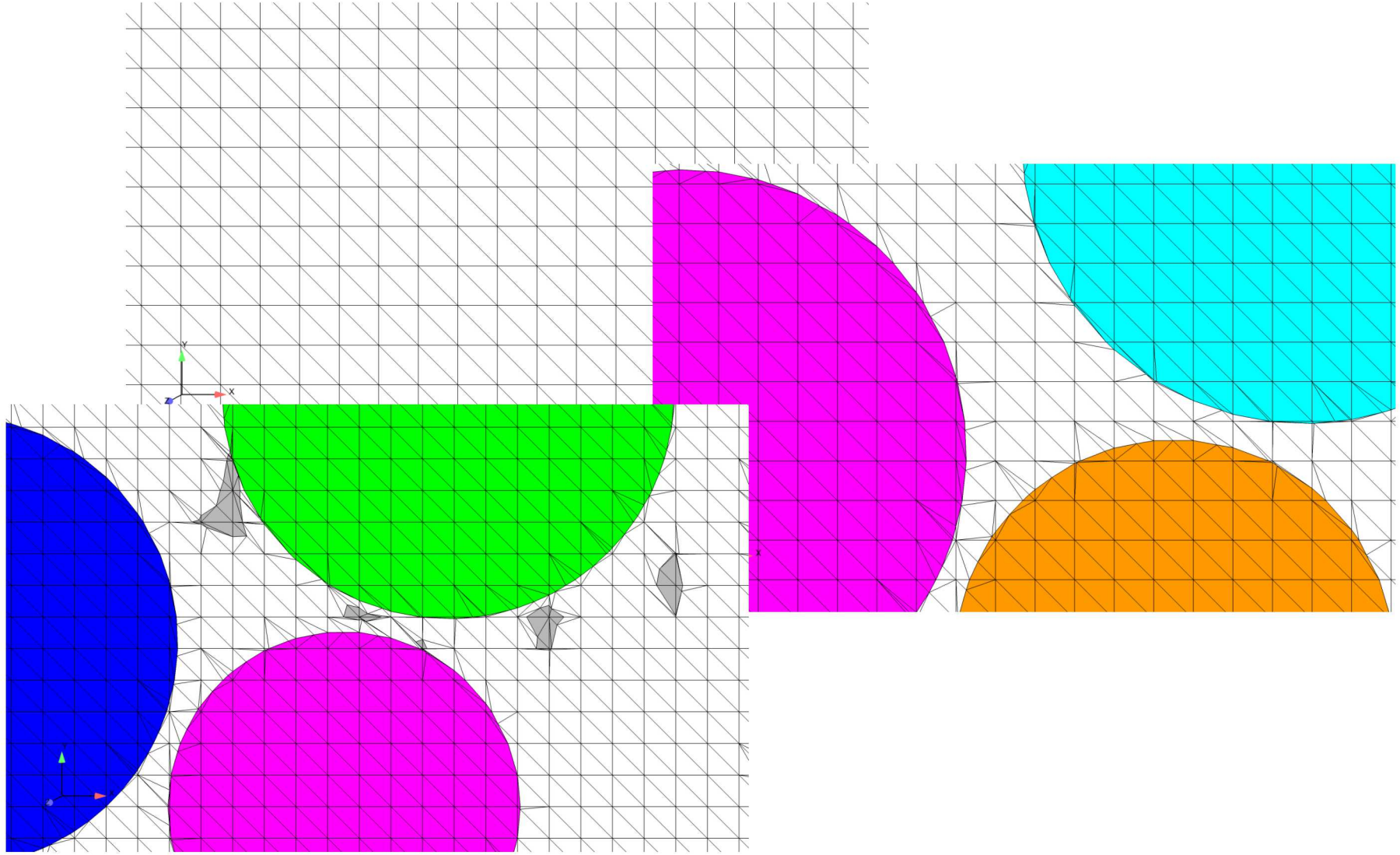
Srivastava, unpublished

Conformal Decomposition Finite Element Method (CDFEM)

Background mesh
- 0.7 μm resolution
- 22M elements

Mesh AM phase
- 39M elements
- 84 cores, 40 s

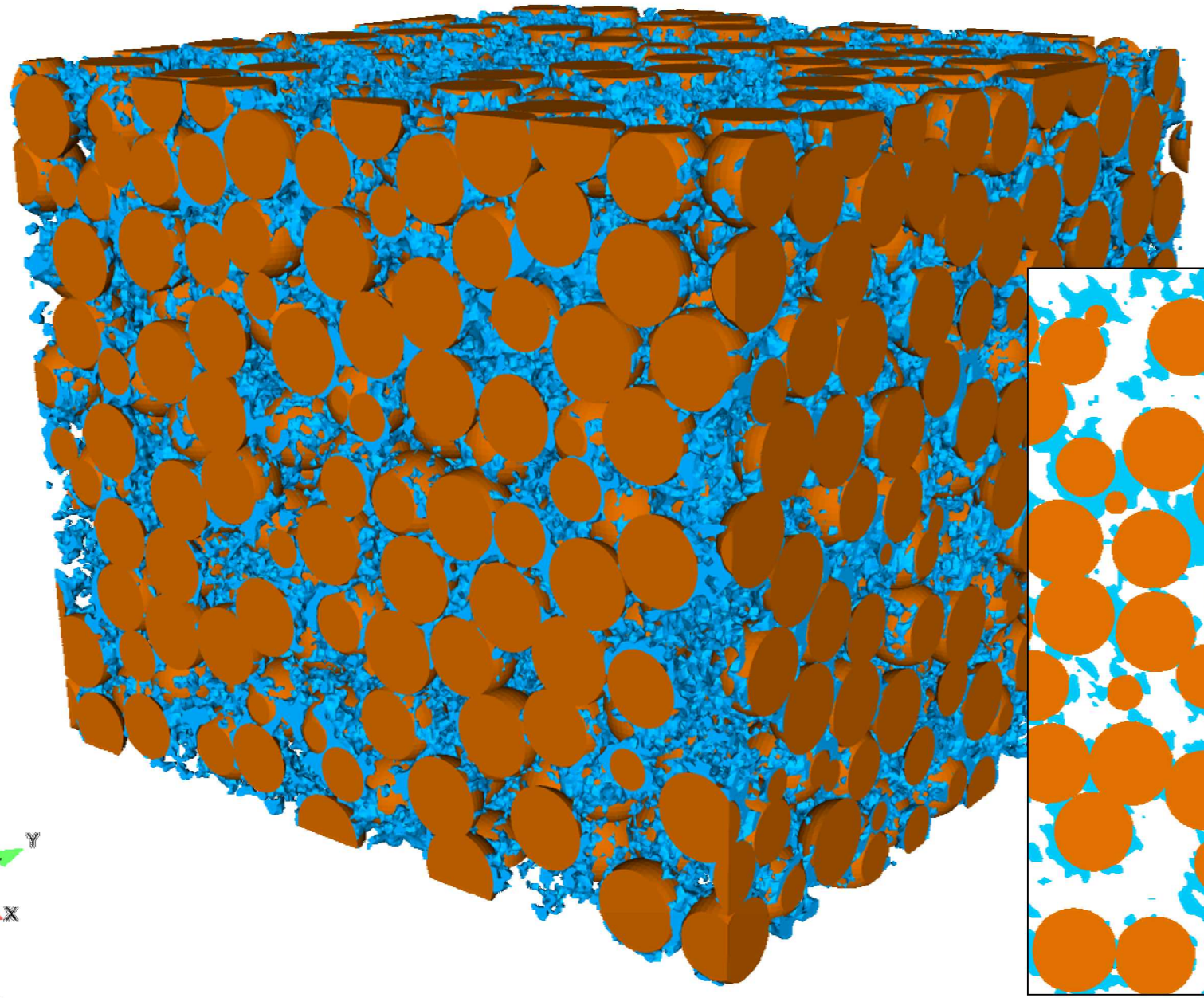
Mesh CBD phase
- 70M elements
- 84 cores, 3 min
- Swell CBD 2x (nano-porous)

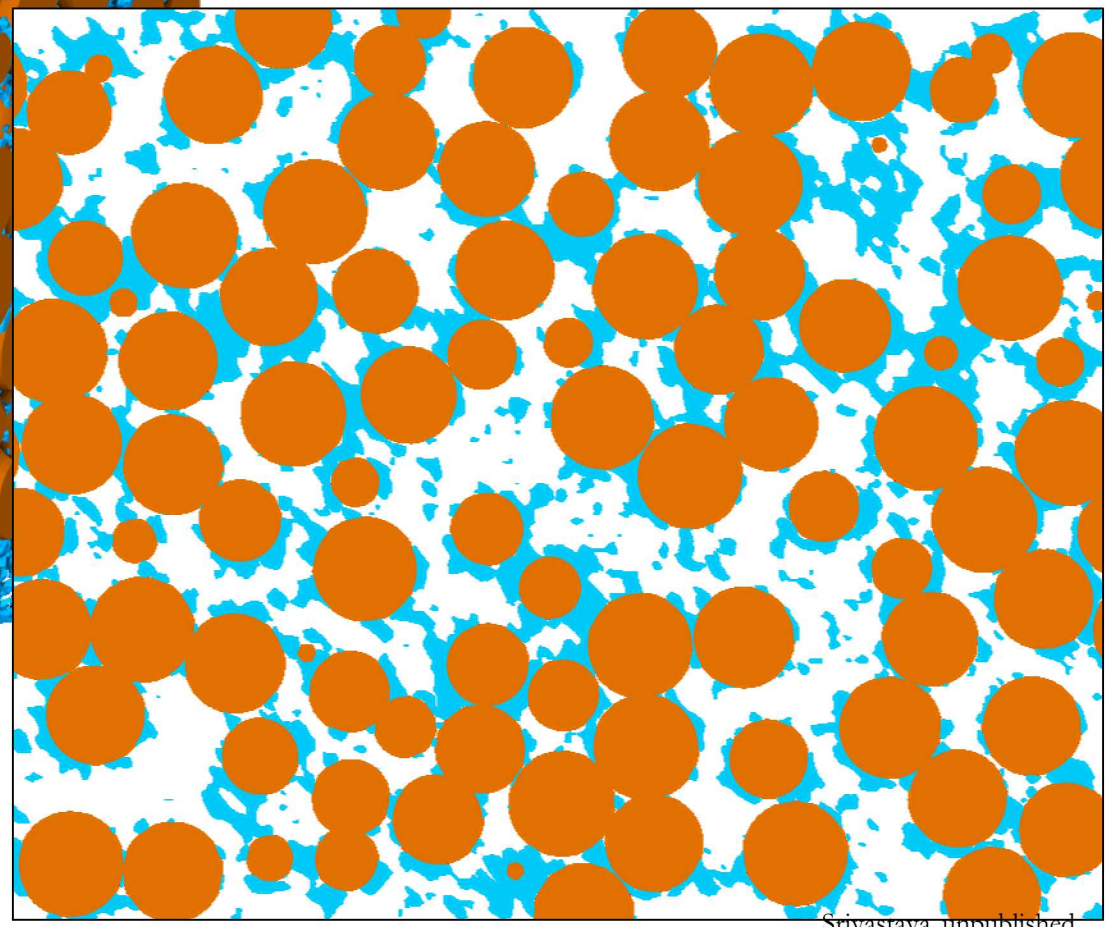


CDFEM efficiently meshes results of DEM simulations

Srivastava, unpublished

Conformal Decomposition Finite Element Method (CDFEM)

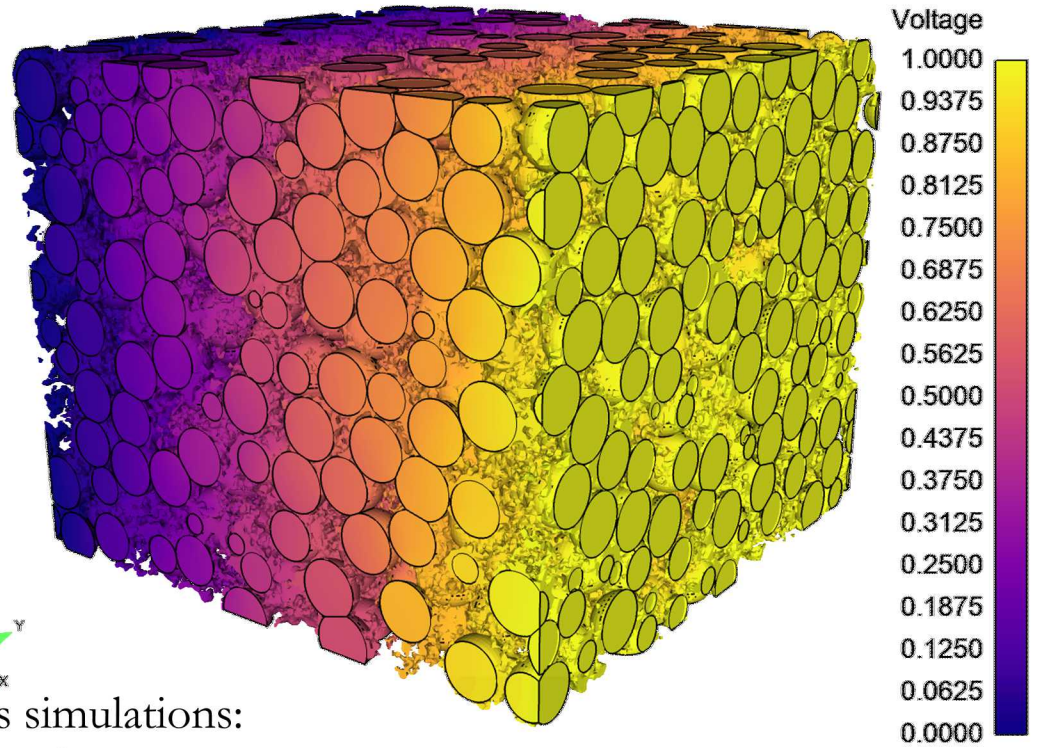




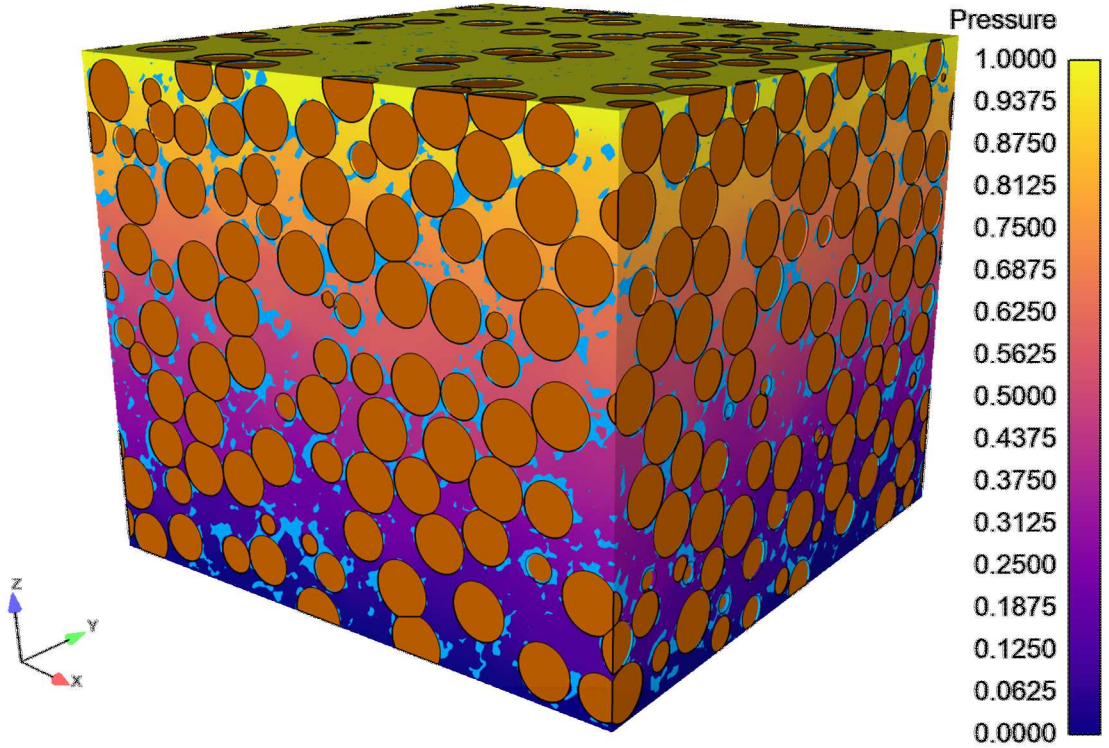
Srivastava, unpublished

Composite effective properties

Electrical conductivity



Tortuosity (ionic conductivity)



Physics simulations:

- Sierra/Aria

Timing:

- 6 solves
- 216 cores
- 16 min

$$\nabla \cdot (\sigma \nabla V) = 0$$

$$\sigma_{\text{eff}} = \left(\frac{L}{\Delta V}\right)\left(\frac{1}{A}\right)\int_A \boldsymbol{n} \cdot \boldsymbol{J}\, dS$$

	σ	κ
AM	0.743	0.0
CBD	10.6	0.05
E-lyte	0.0	1.0

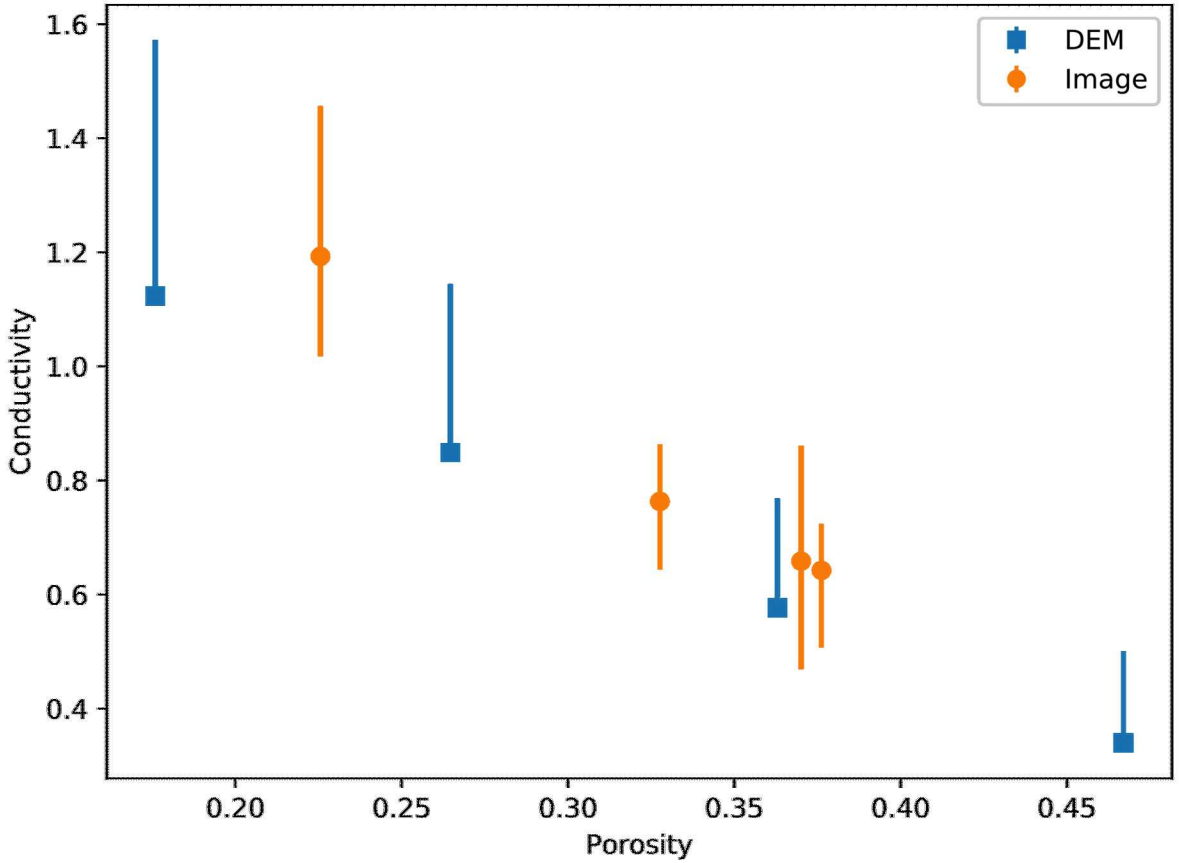
$$\nabla \cdot (\kappa \nabla C) = 0$$

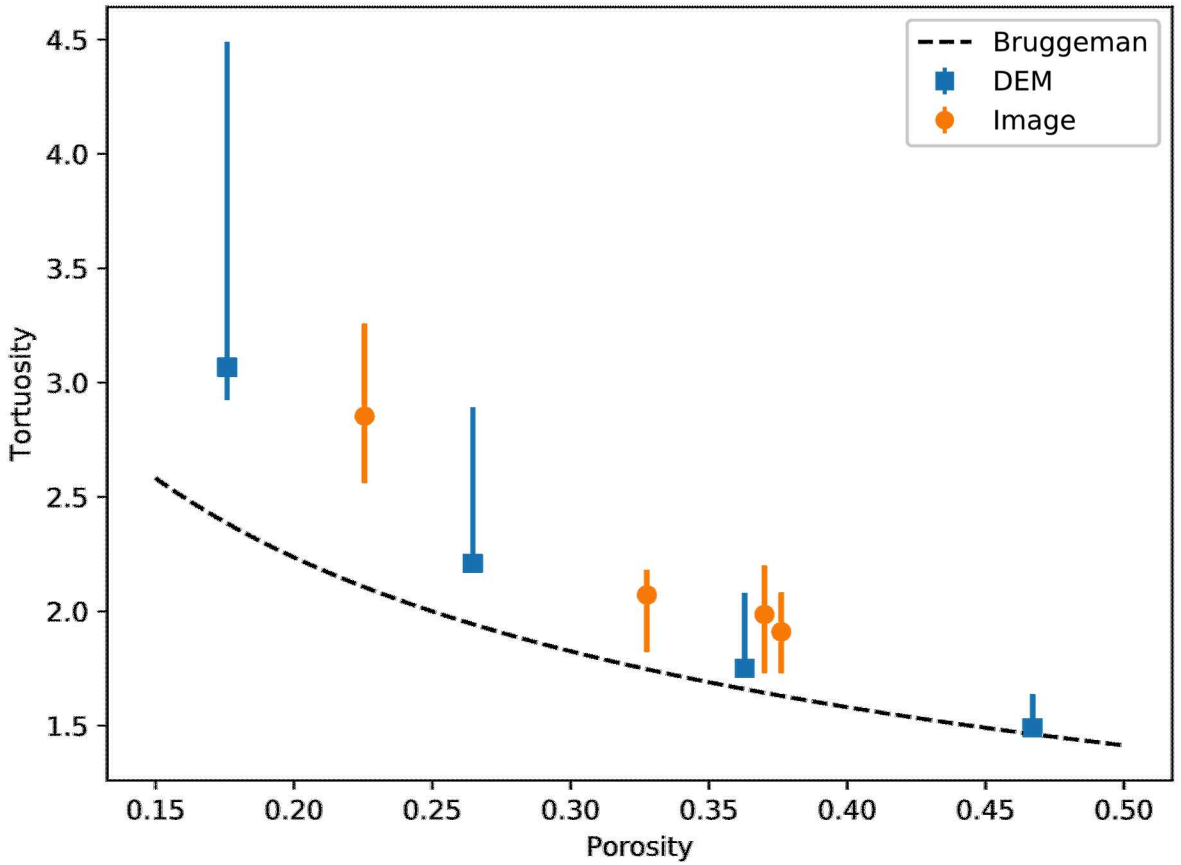
$$\kappa_{\text{eff}} = \left(\frac{L}{\Delta V}\right)\left(\frac{1}{A}\right)\int_A \boldsymbol{n} \cdot \boldsymbol{J}\, dS \qquad \tau = \frac{\phi}{\kappa_{\text{eff}}}$$

Effective properties are simple yet appropriate characterizations of electrode performance

Srivastava, unpublished

Porosity/calendaring comparisons





All simulations for T=600, $\gamma=10^{-5}$

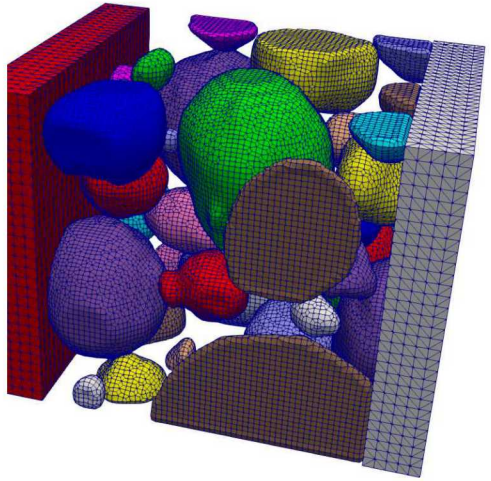
Calendaring → lower porosity → more CBD connectivity → higher conductivity and tortuosity

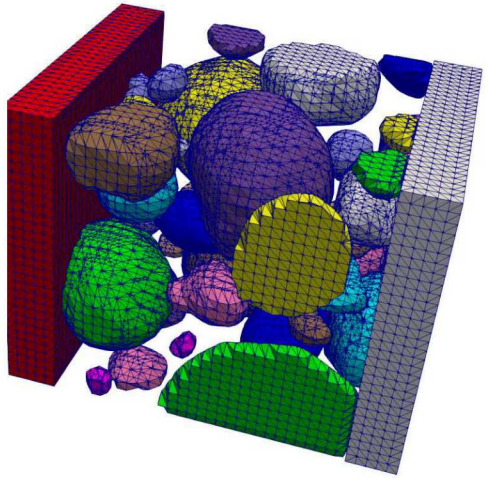
Srivastava, unpublished

Next steps: Large deformation multi-physics formulation

Concept:

- Solid mechanics c
- Transport/electro
- Transfer displacer

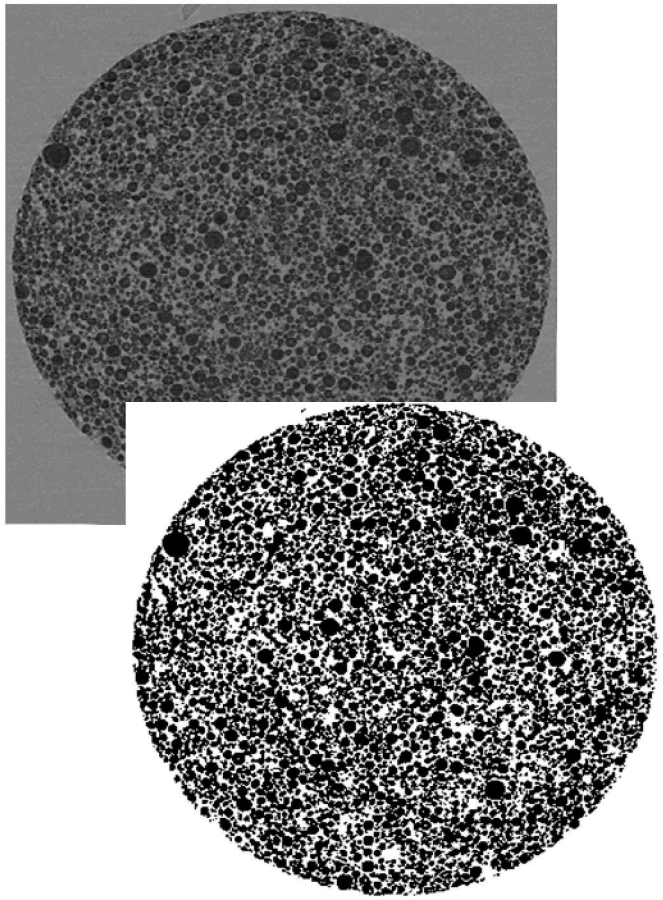




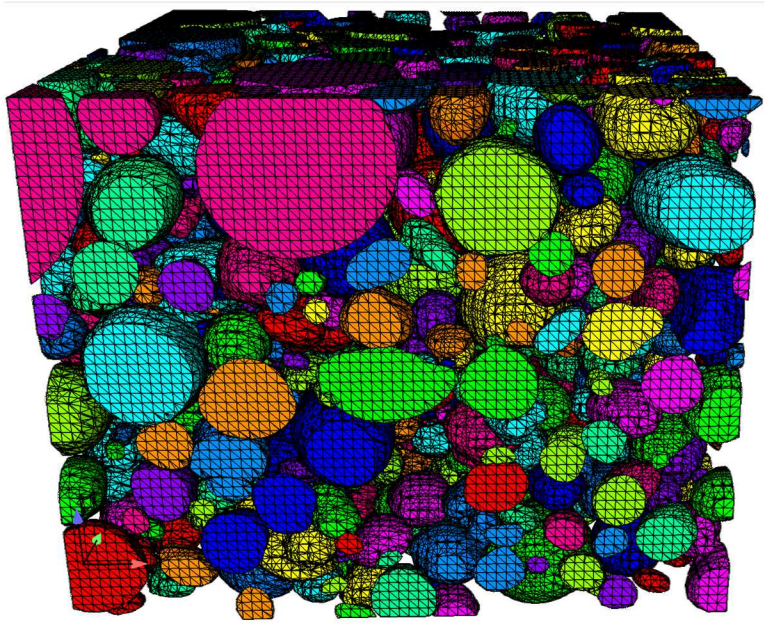
Demonstrated two-way coupling between mechanics and transport codes; developing robust particle contact

Brunini, unpublished

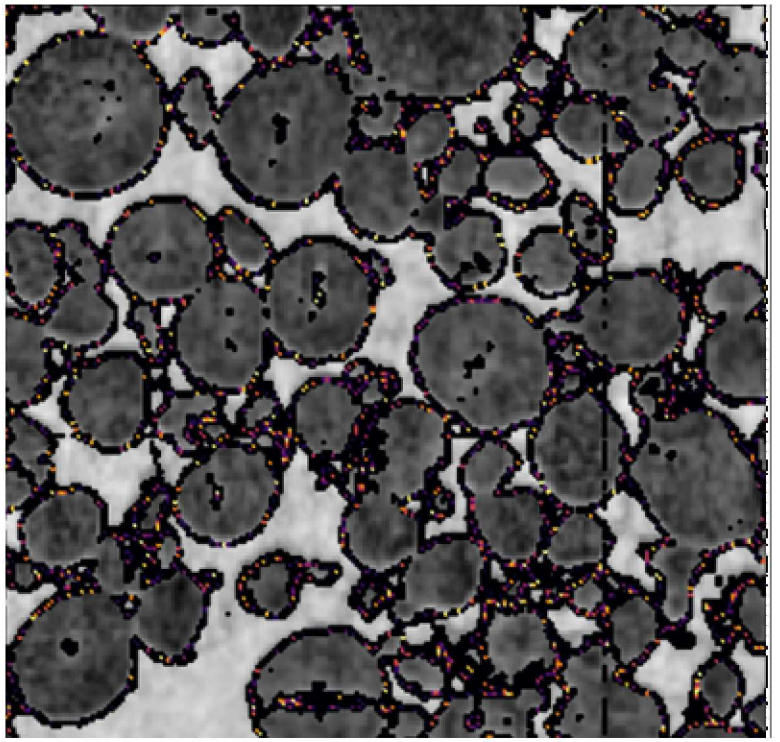
Next Steps: Credible Automated Meshing of Images (CAMI) LDRD



Segmentation using deep CNNs
Labeling, feature detection (CV)



Smooth, low anisotropy
conformal meshing (CDFEM,
morph, sculpt, omega_h)



UQ and propagation
(per voxel, geometric perturbation)

Automatically, efficiently, and reproducibly create conformal meshes from 3D tomography with quantified uncertainty

References and acknowledgments

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Questions?

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