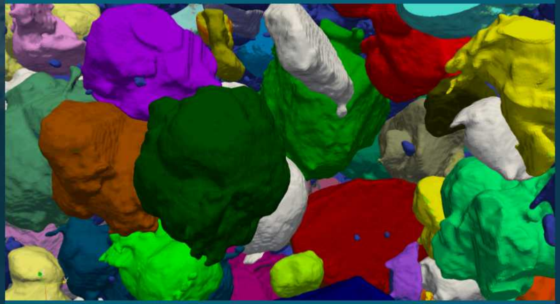
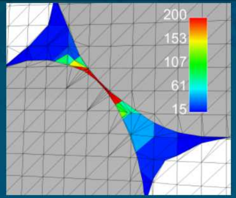
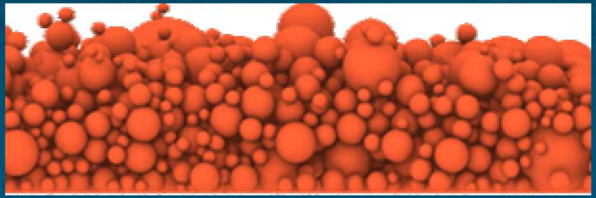
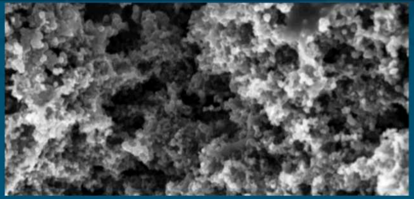
SAND2018-11974PE

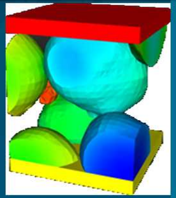
Modeling Mesoscale Coupled Physics using Image Data: Batteries, Composites, and More











PRESENTED BY

Scott A. Roberts, Ph.D.

October 2018

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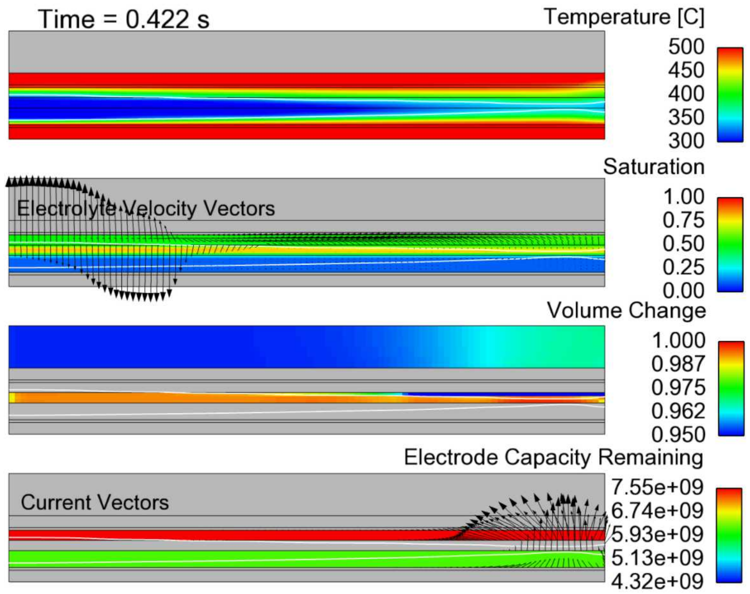
Roberts research efforts

Multi-physics, multi-scale applied modeling & simulation
- Lead teams comprised of 14 PhD staff members, 3 post-docs, 2 graduate students, and numerous summer interns
- $3.4M in FY19 research funding



Thermal batteries

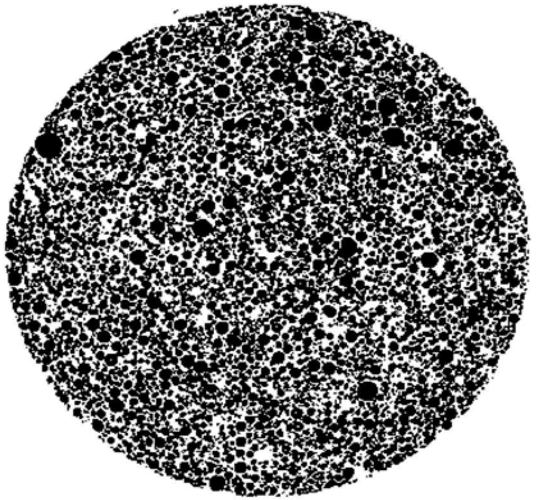
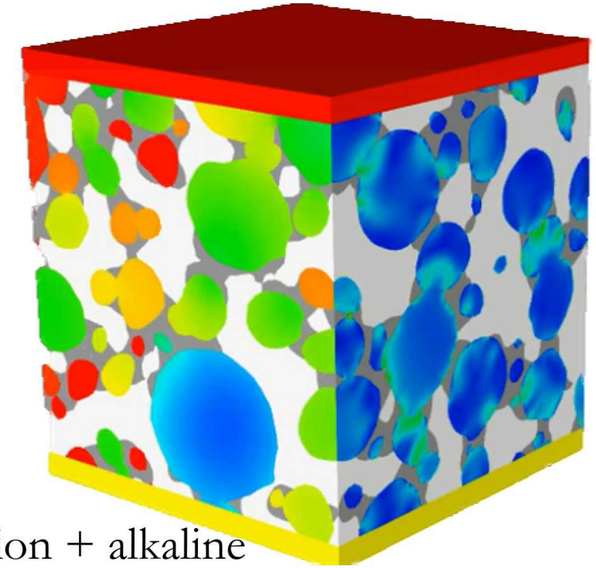
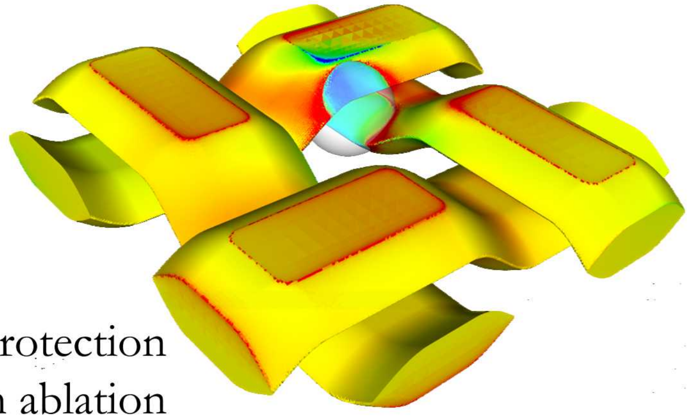


Image-to-mesh with ML/UQ

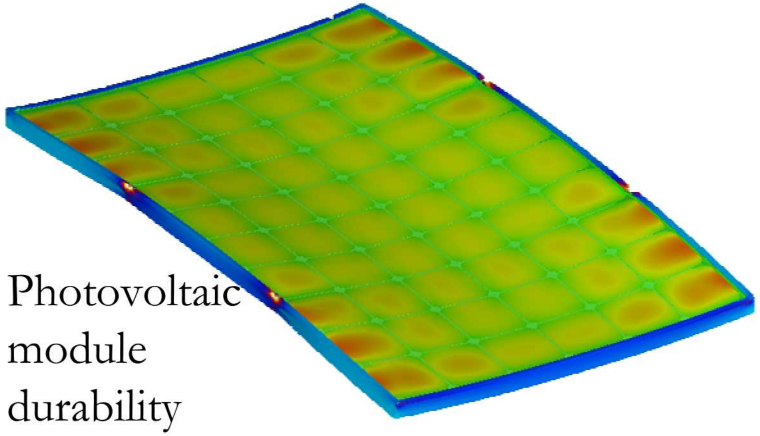


Li-ion + alkaline battery mesoscale

EM railgun launcher performance

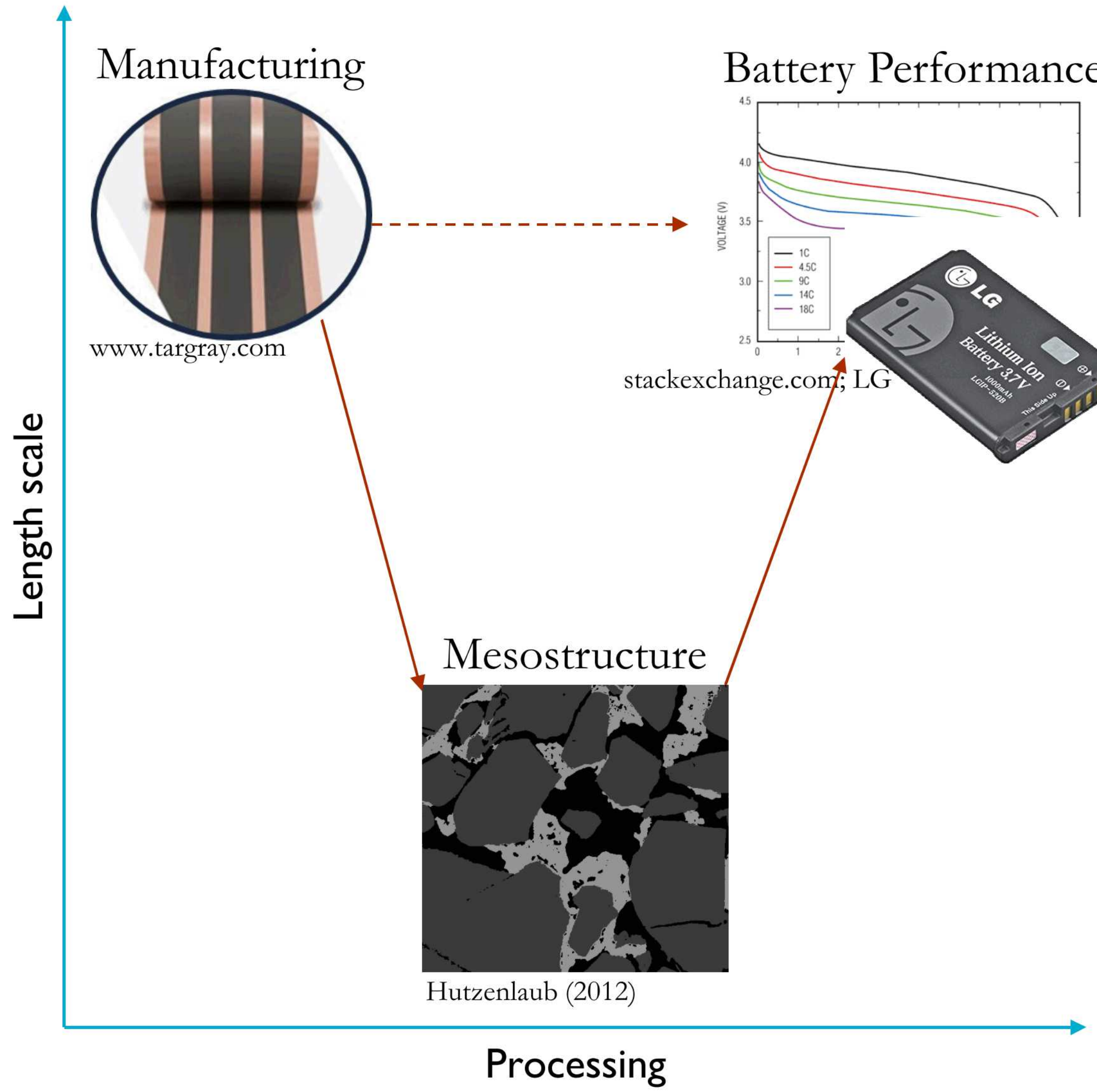


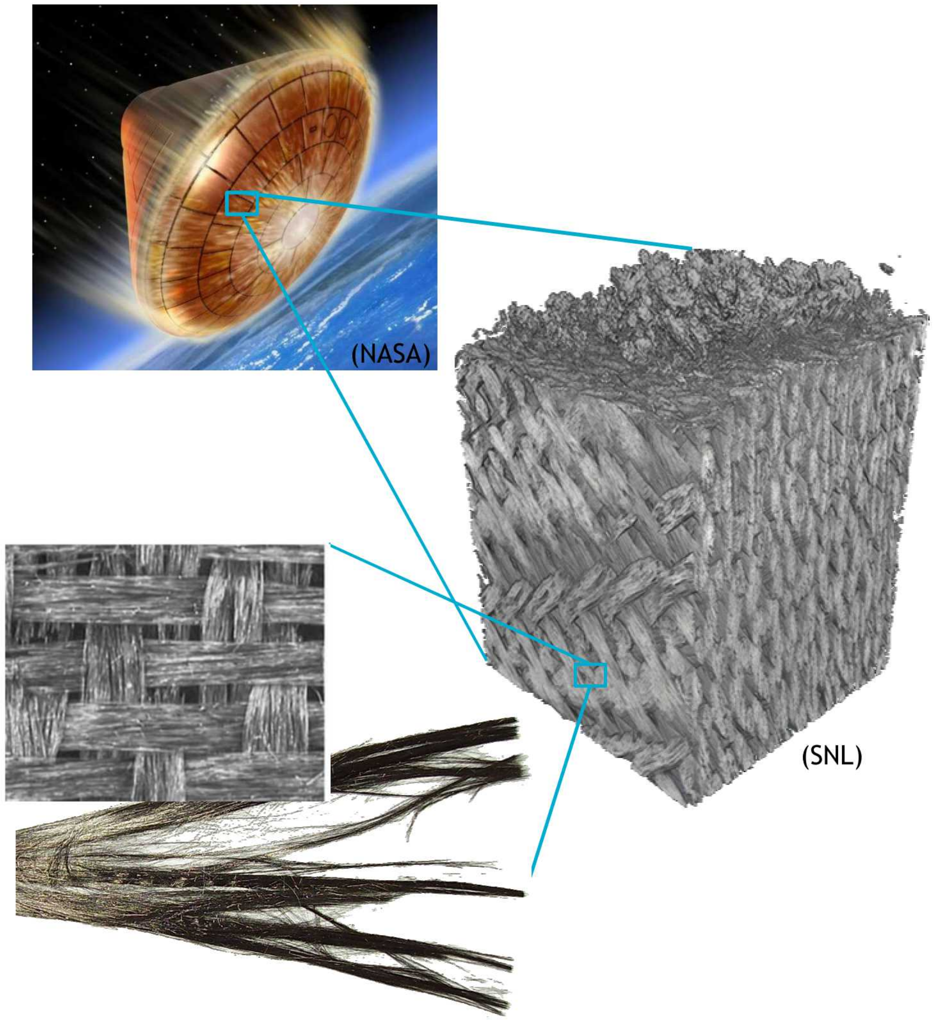
Thermal protection system ablation



Photovoltaic module durability

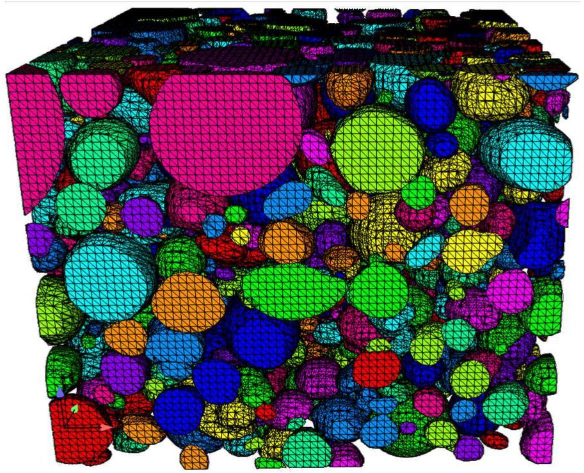
Motivation



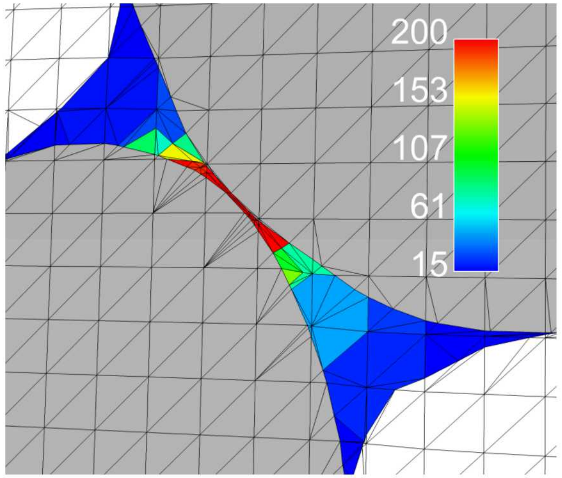


Coupled multi-physics effects at the mesoscale connect component manufacturing to performance

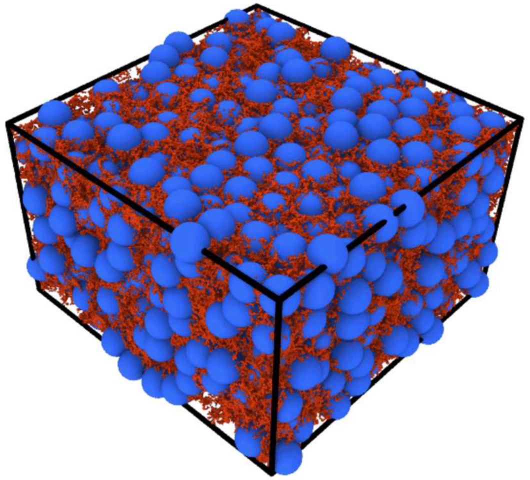
Outline



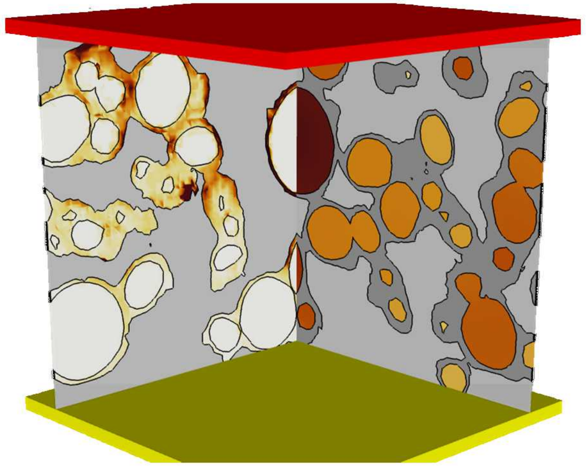
Computational representation of electrode mesostructures



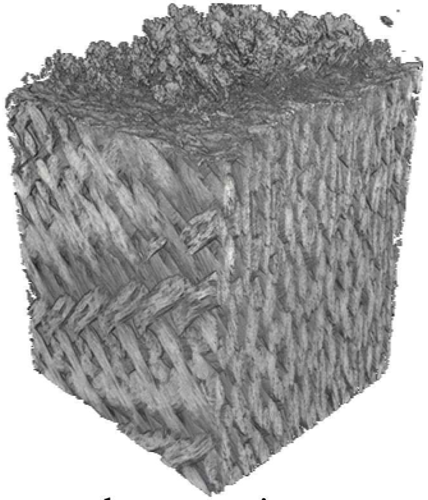
Representation and role of conductive binder morphology



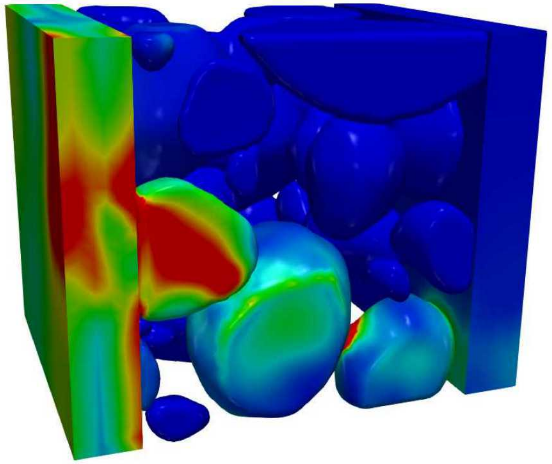
Discrete element method mesostructure generation



Electrochemical-mechanical discharge simulations



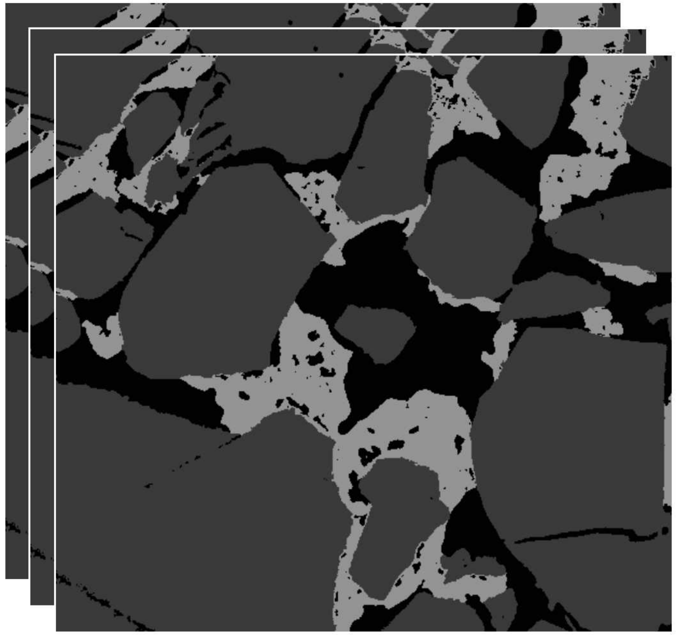
Thermal protection systems



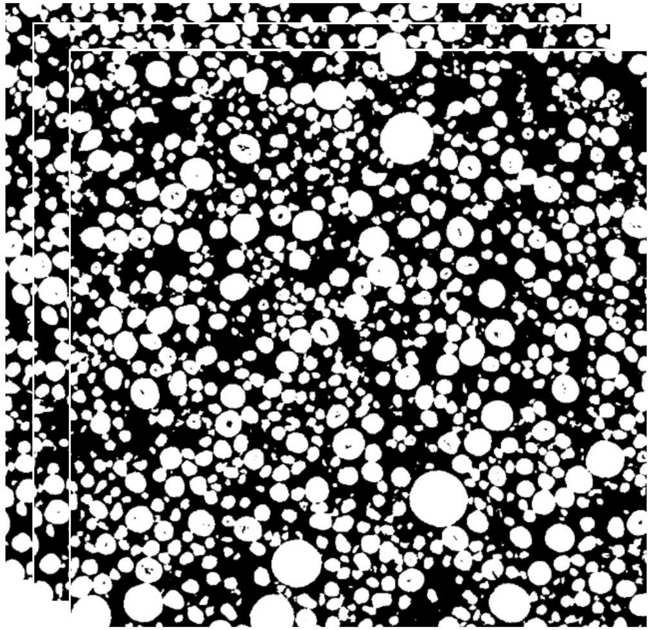
Future directions in credible image-based simulation

Computational representation of electrode mesostructures

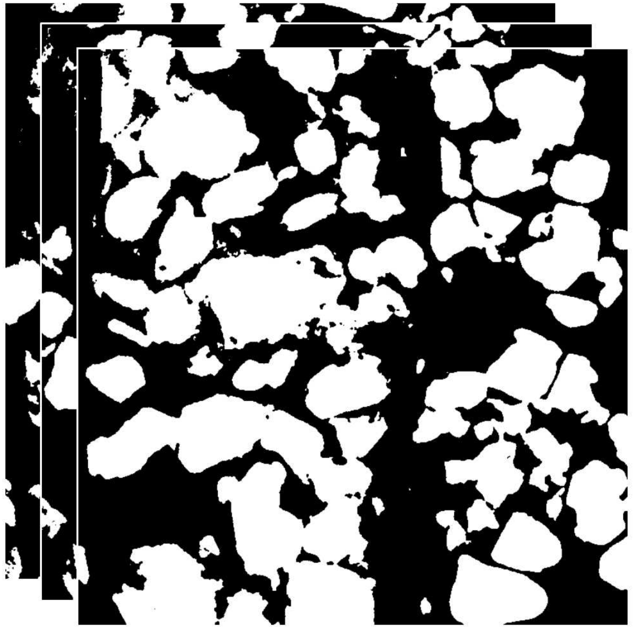
Imaging of cathode mesostructures



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



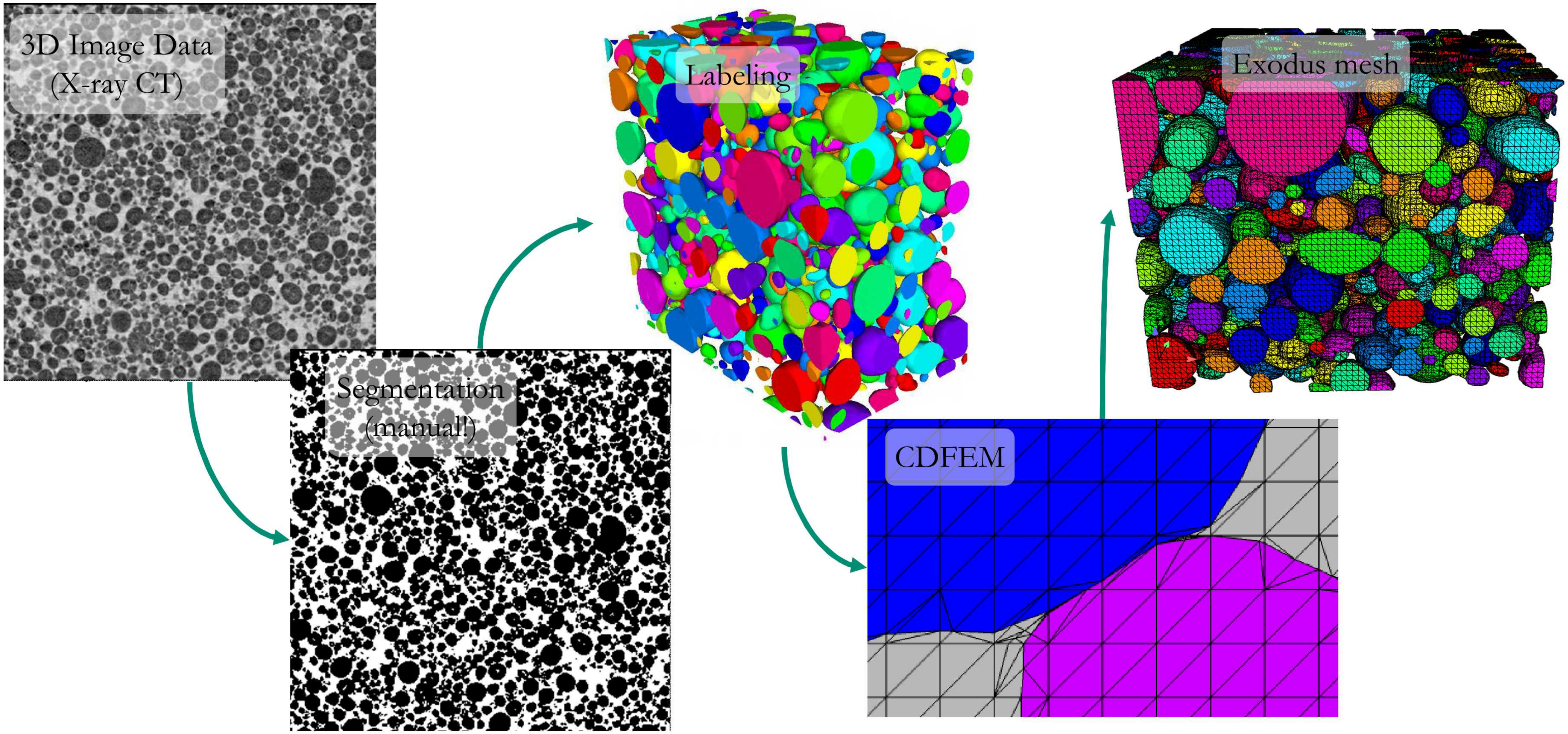
NMC from XRCT,
370 nm resolution,
757 μm domain.
Ebner (2013)



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

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

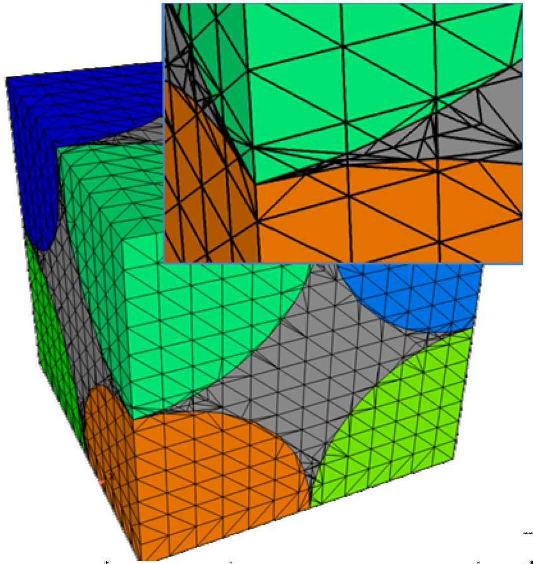
Mesoscale geometry from CT data using CDFEM

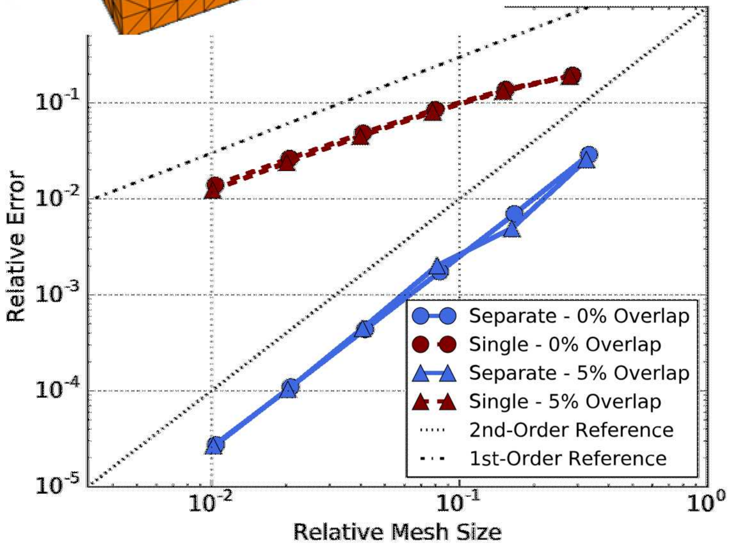


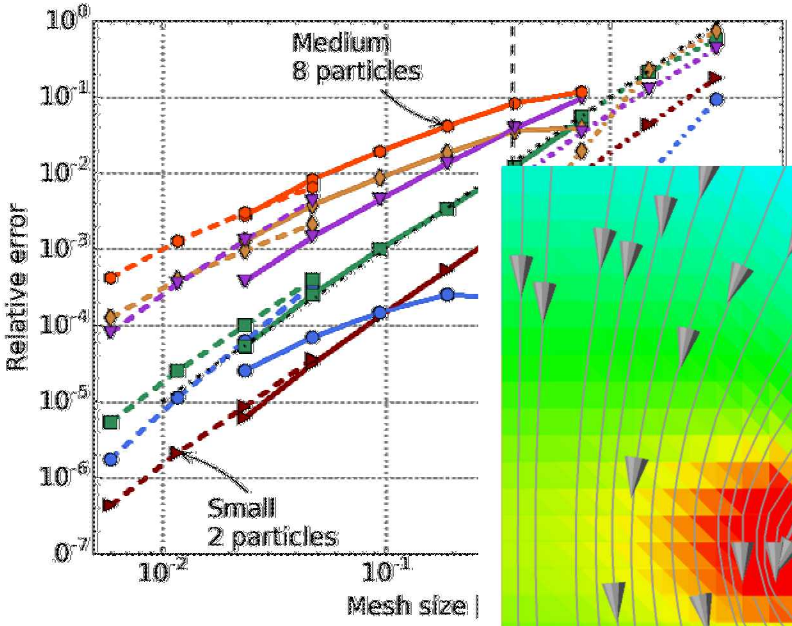
Detailed 3D reconstruction and image processing necessary to get usable mesostructure data

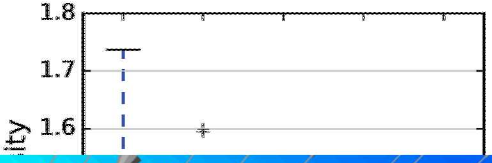
Roberts JES (2014), Roberts JEECS (2016), Roberts JCP (2018)

Solution verification for credible mesostructure simulations

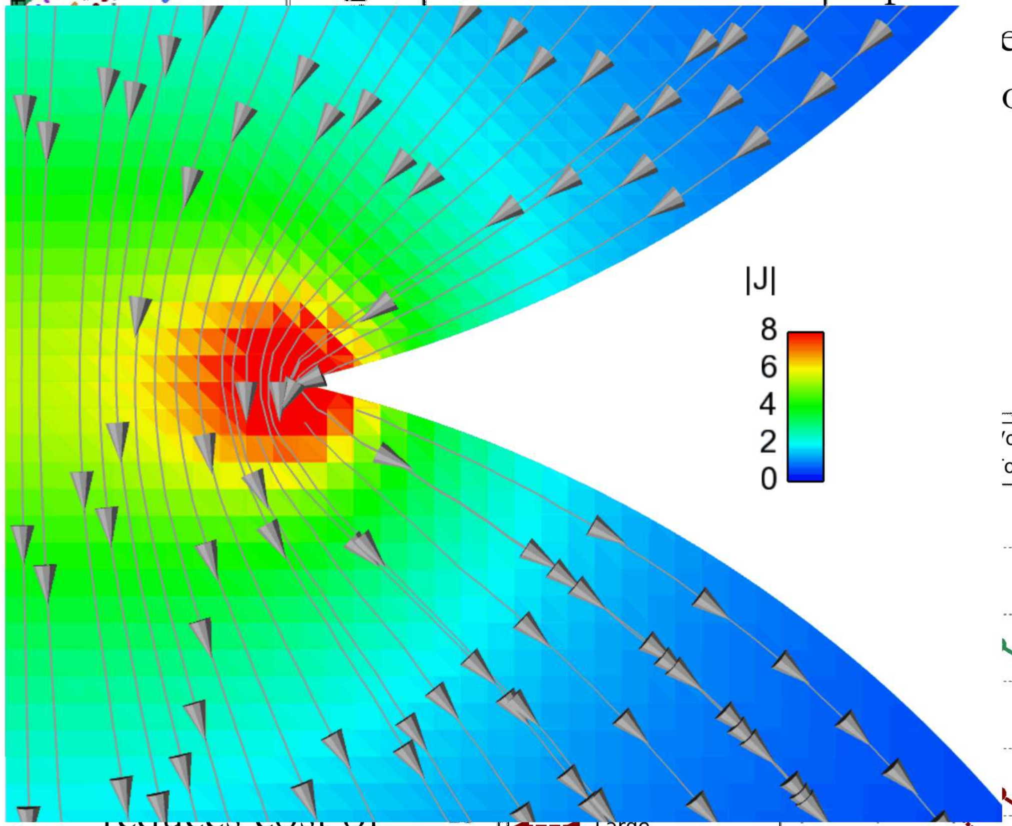








Quantify representative
element
omain



Understand mesh resc
for accurate pred

Separate particle representations required for optimal convergence

reduces cost of physics solve

Solution verification establishes simulation correctness and domain/mesh size requirements

Roberts JCP (2018)

Representation and role of conductive binder morphology

What about the conductive binder?

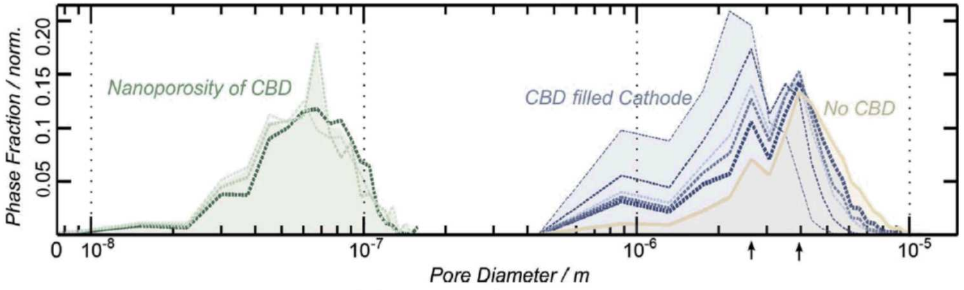
Binder weight fraction	Dense volume binder:particle	Porous volume binder:particle
0.04	0.10	0.15
0.06	0.16	0.23
0.08	0.22	0.31
0.10	0.28	0.40

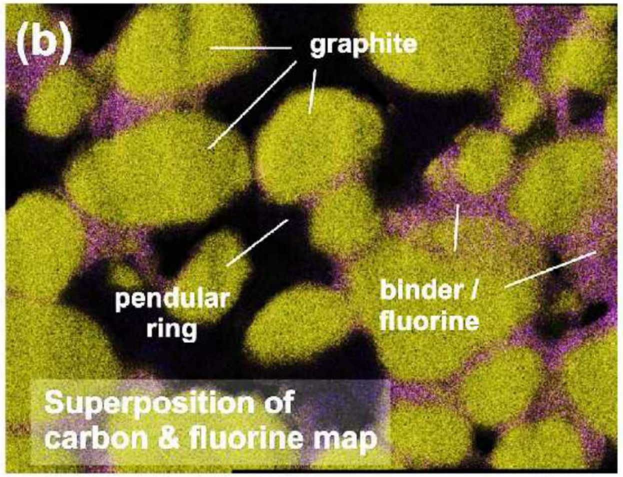
Resolving conductive binder in 3D imaging difficult

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

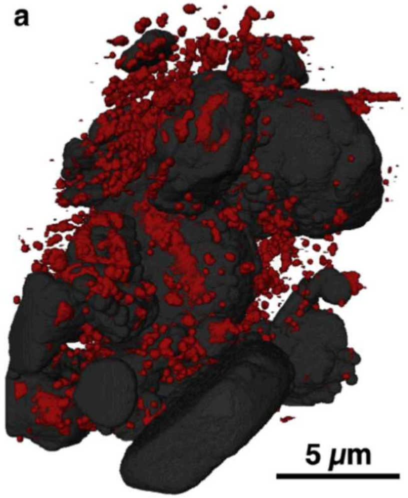
Amorphous binder is significantly nanoporous

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

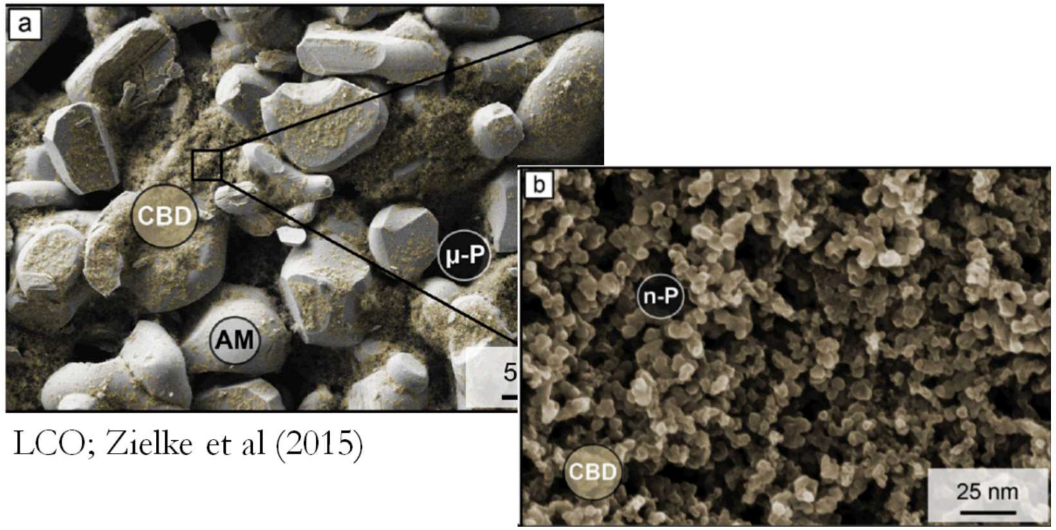




Graphite; Jaiser et al. (2017)



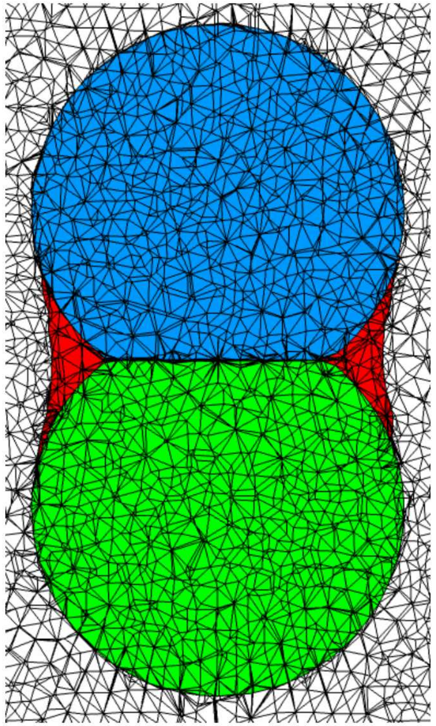
LCO; Komini Babu et al (2015)



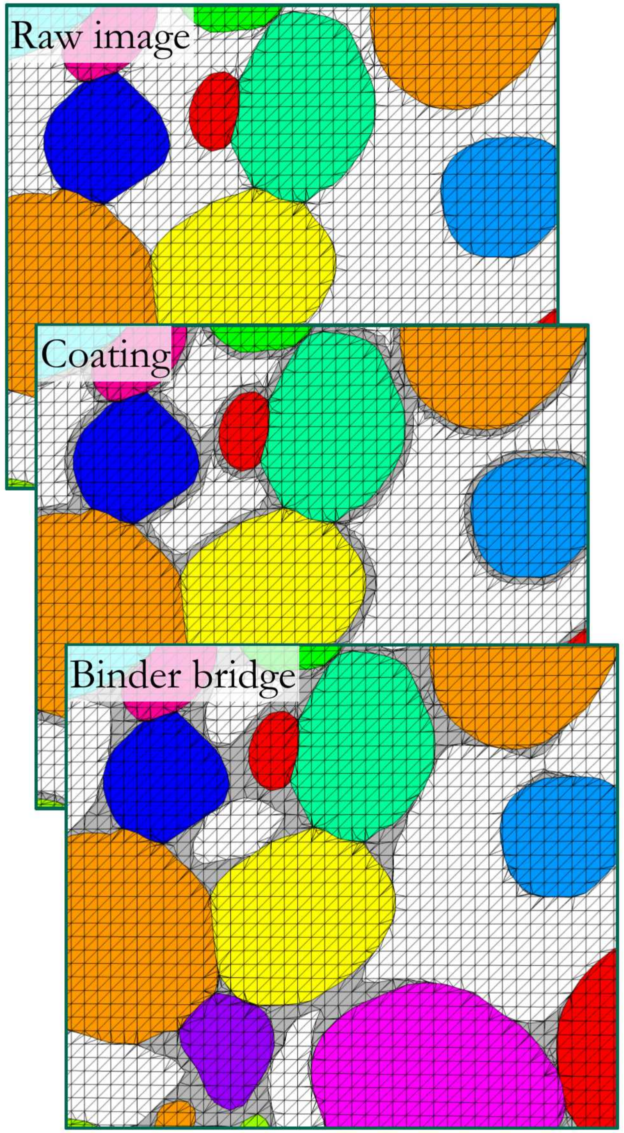
LCO; Zielke et al (2015)

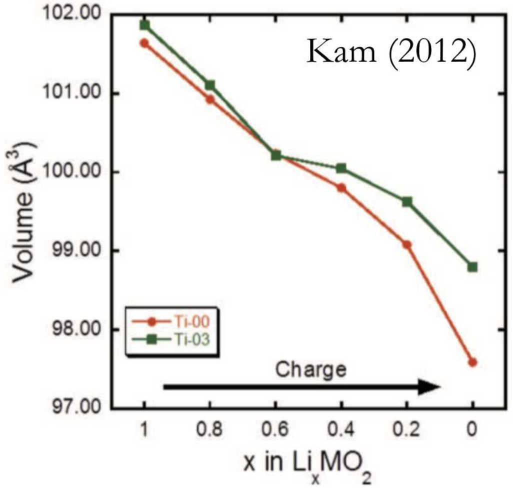
How are electrode-scale properties affected by the inclusion of binder? How does the morphology matter?

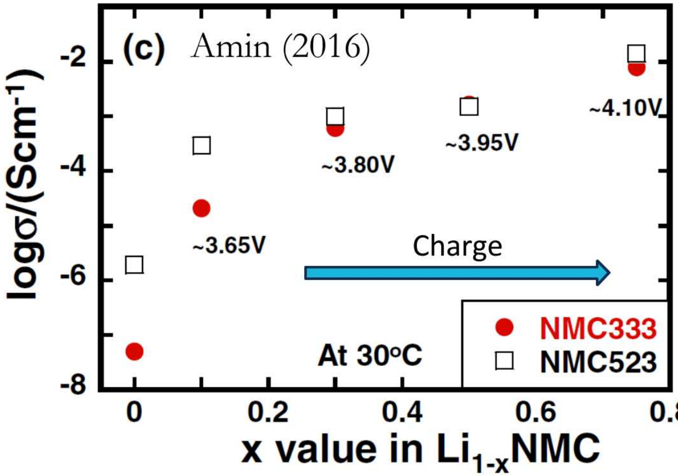
Binder bridge morphology approach



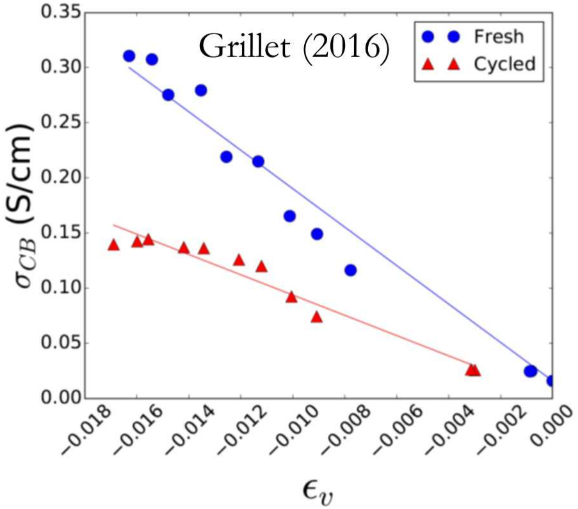
Mathematical description of "binder bridges"

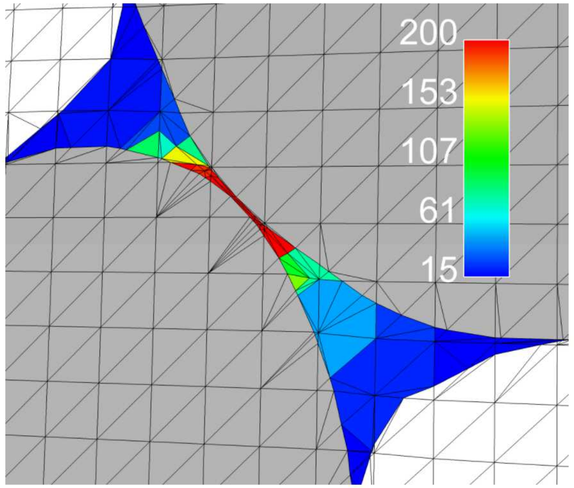






NMC swells on lithiation, compressing binder



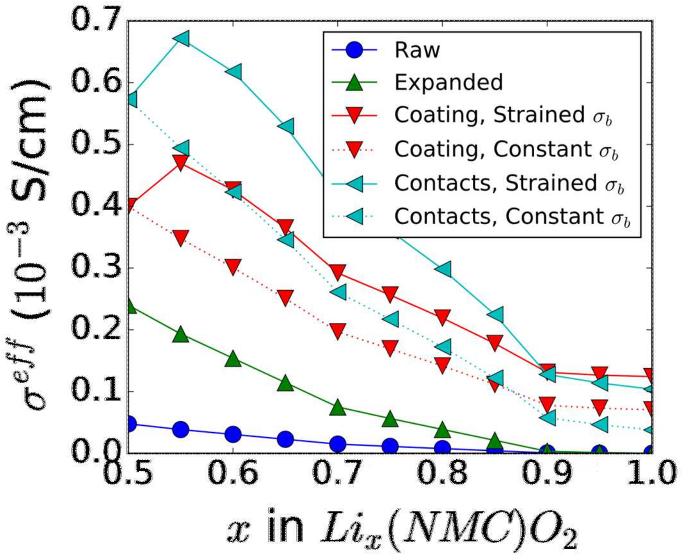


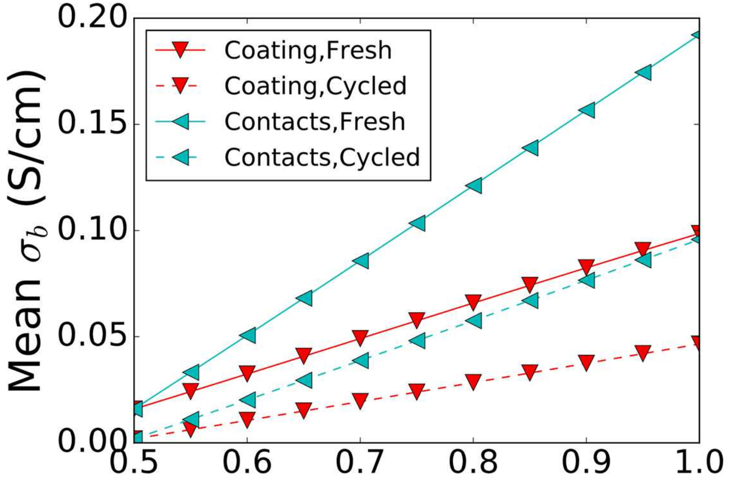
Binder has strain- (e.g. lithiation-) dependent properties

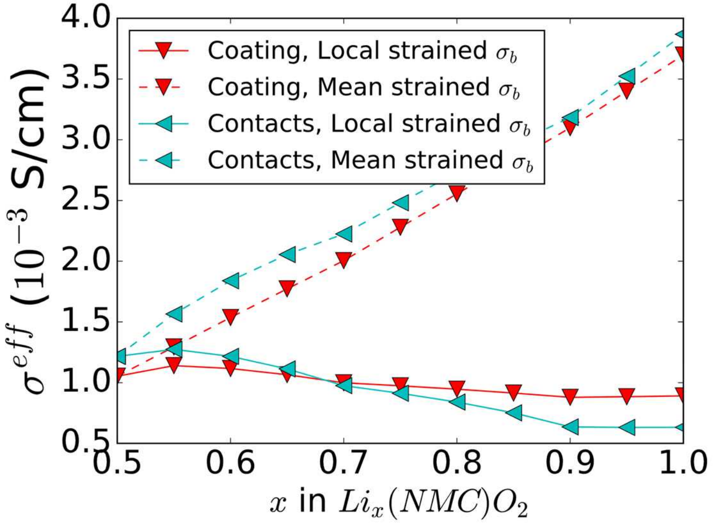
Binder bridge mimics experimental observations; properties are lithiation-dependent

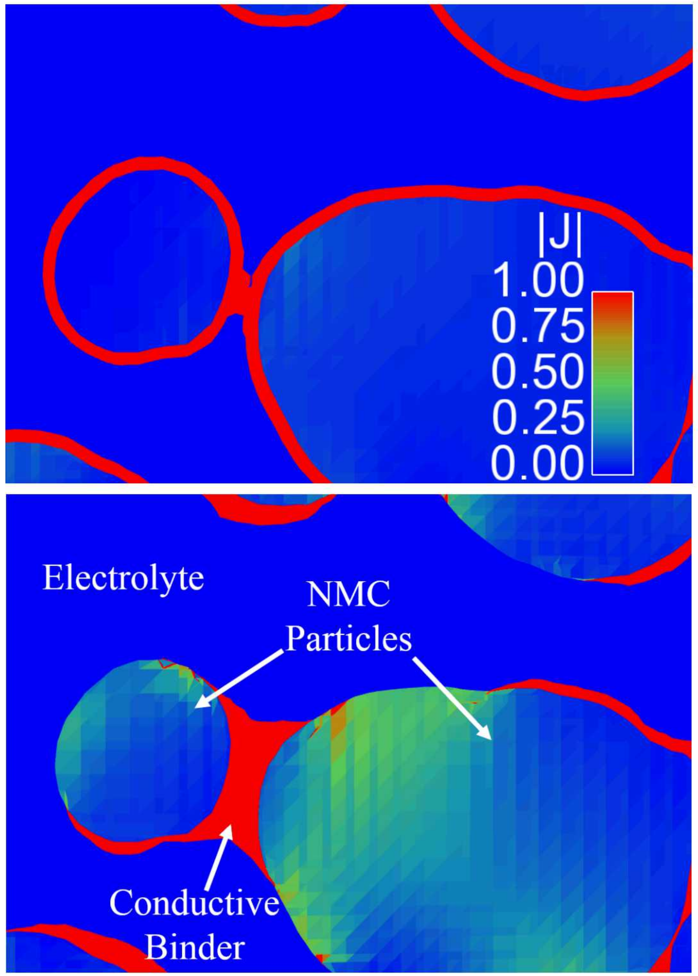
Trembacki JES (2017)

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.

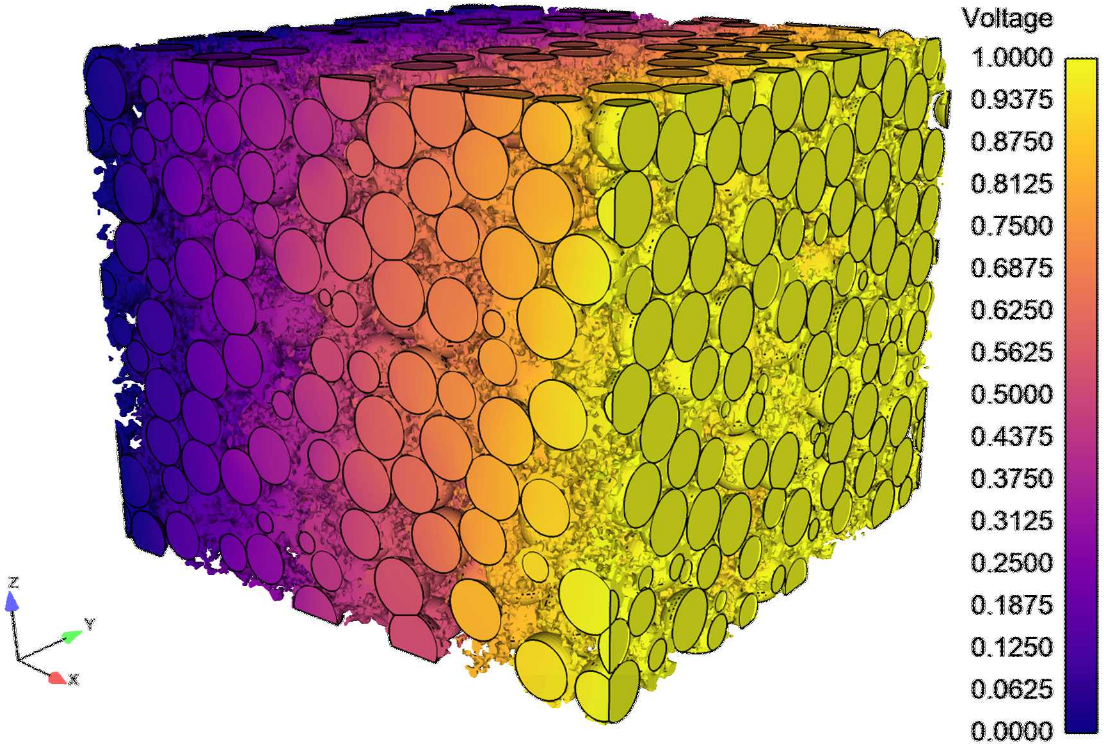
Binder morphology and mechanical coupling have a significant impact on effective properties; localization matters!

Trembacki JES (2017)

Effective electrode property calculations

Calculate effective transport properties for upscaling
- Particle specific surface area
- Electrical conductivity
- Tortuosity

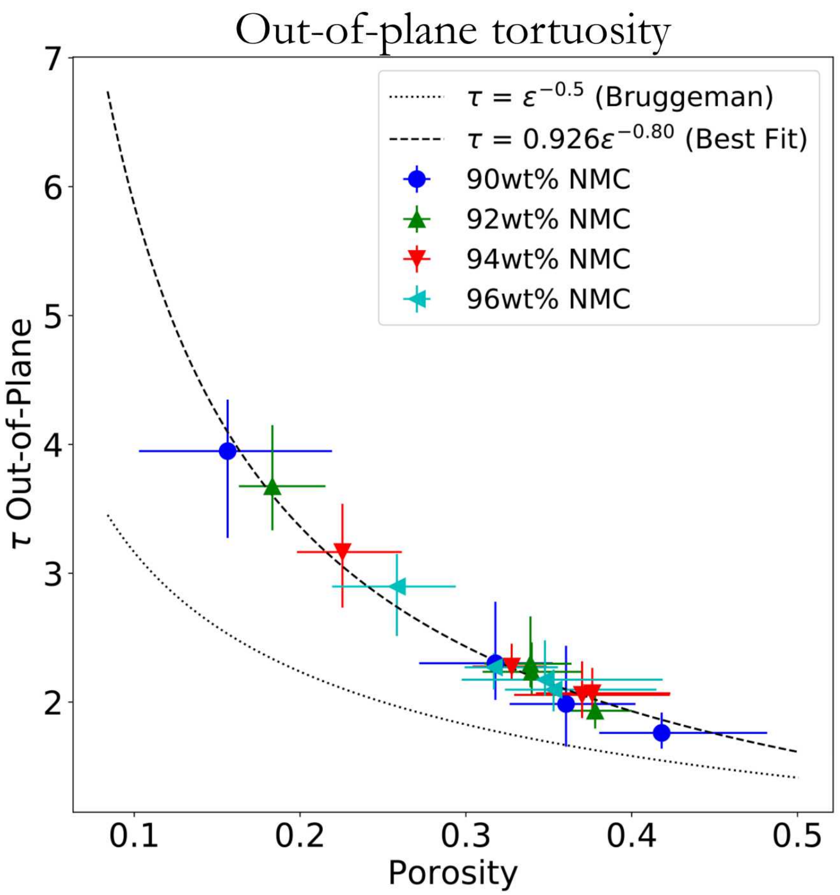
NMC image data from Ebner (2013)
- 90, 92, 94, 96 wt% NMC (remainder 1:1 CB:PVDF)
- 0, 300, 600 & 2000 bar calendering
- 100 μm x 100 μm x 60 μm domain (20 realizations eac
- Binder bridge (porous) morphology approach

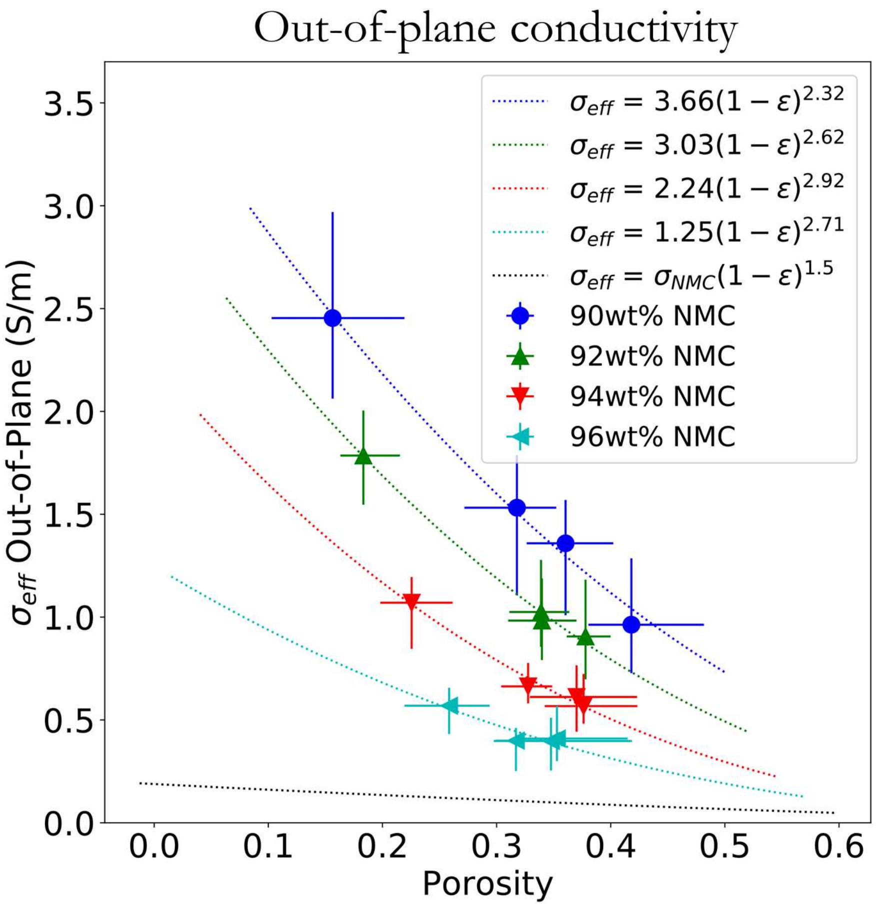


Effective properties are an important first step for upscaling mesoscale data

Trembacki, in preparation

Effective electrode property calculation results – Transport

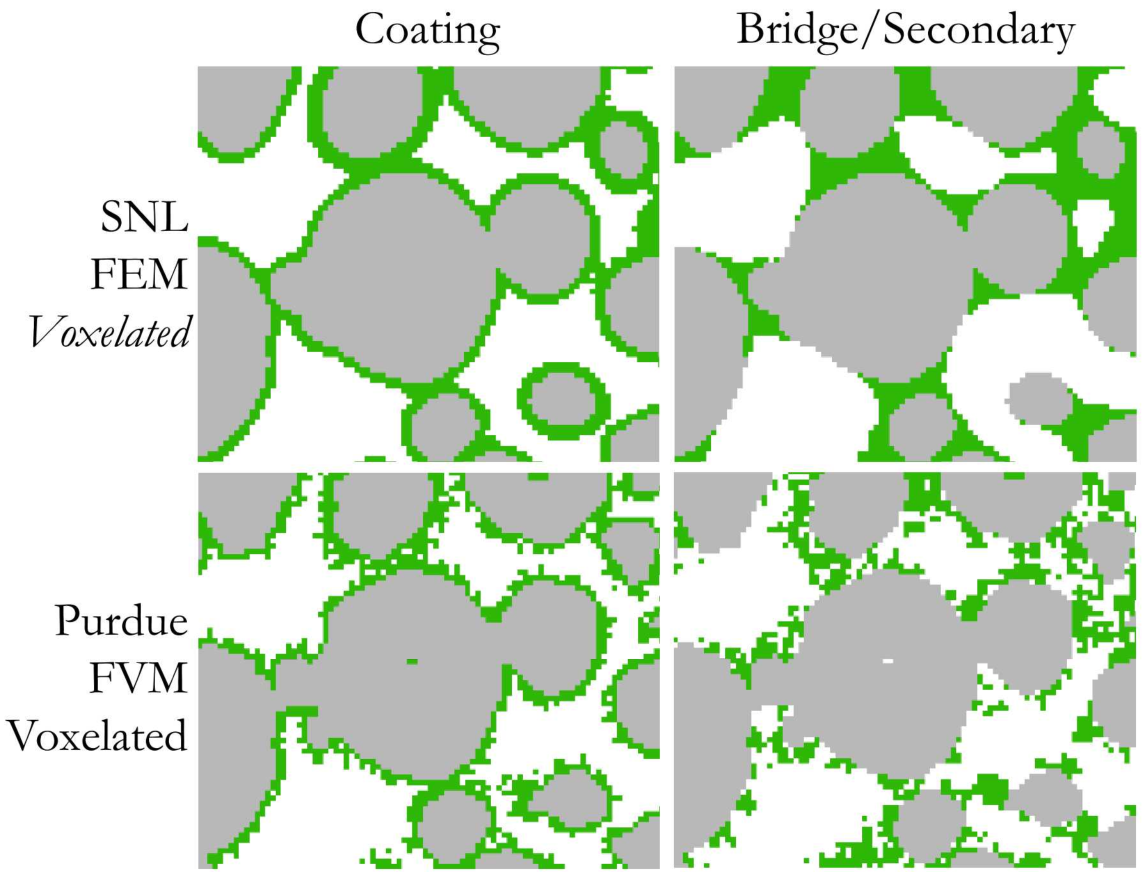


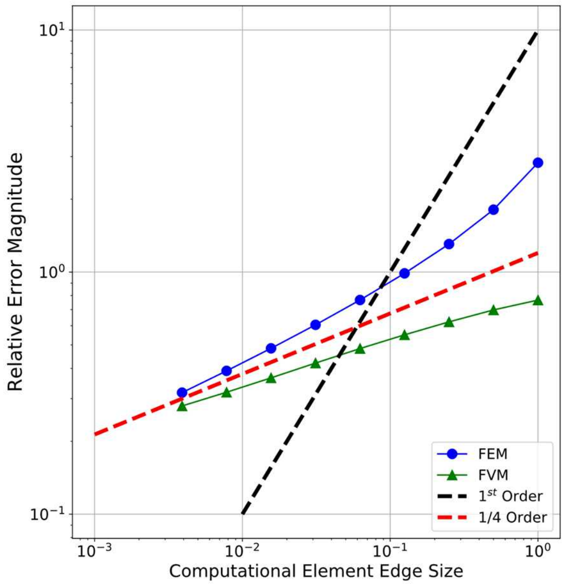


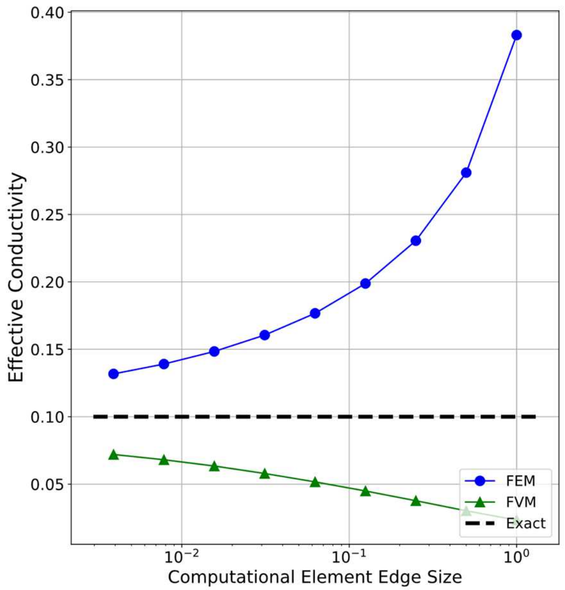
Bruggeman relationships must be re-calibrated to fit simulated data

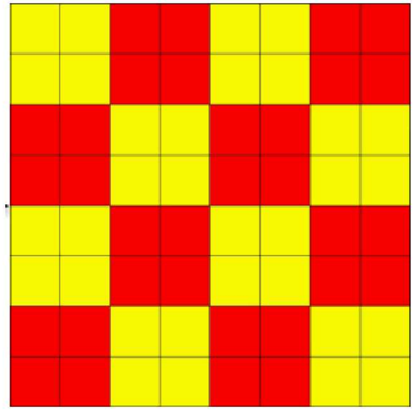
Trembacki, in preparation

What about other morphologies and numerical methods?









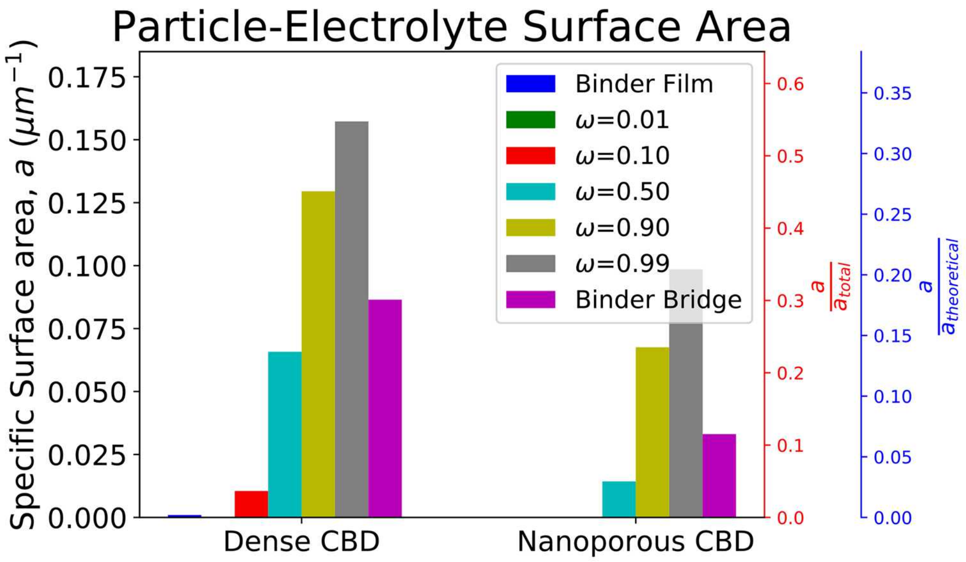
Both methods convergent on voxelated meshes, but:

- 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 JES (2018)

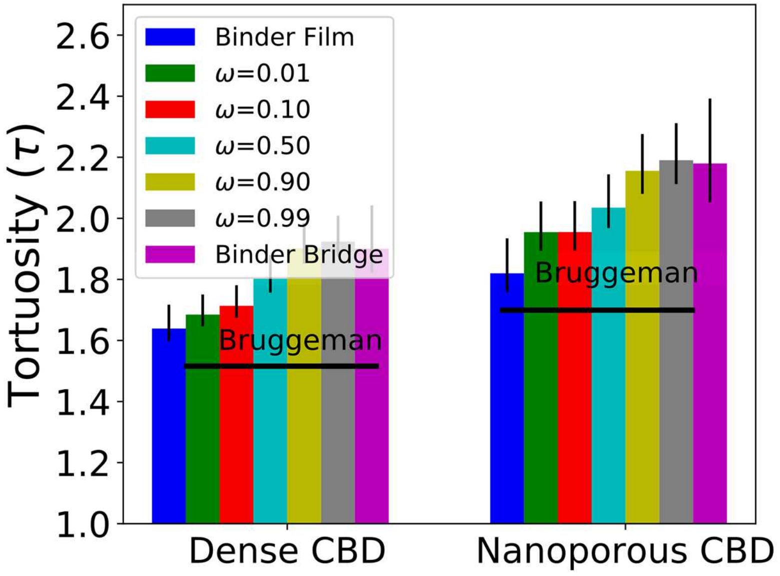
Porous binder and morphology considerations

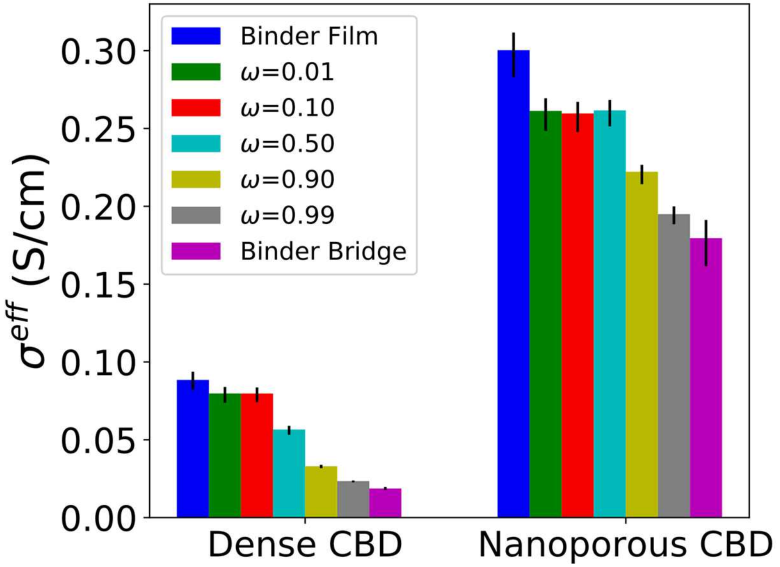


- More particle surface area available with non-uniform morphologies
- Nanoporous binder decreases bare particle surface area, but binder area is porous
- Surface are much less than theoretical

Non-uniform binder:
- Increases tortuosity
- Decreases conductivity

Nanoporosity:
- Increases tortuosity
- Increases conductivity





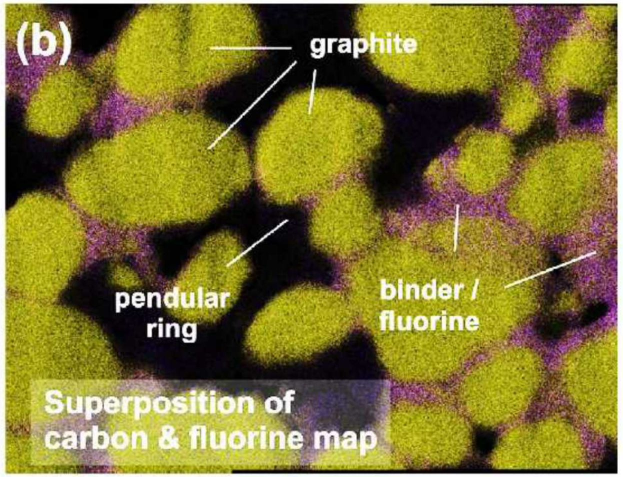
Limiting cases of both morphology methods show similar (but not identical) behavior; nanoporosity is important!

Trembacki JES (2018)

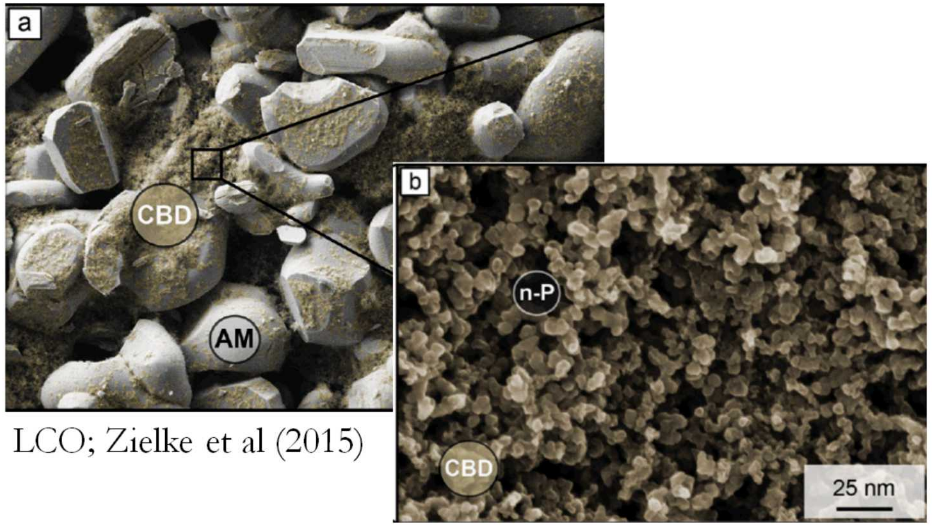
Discrete Element Method Mesostructure Generation

Challenges with using CT mesoscale data

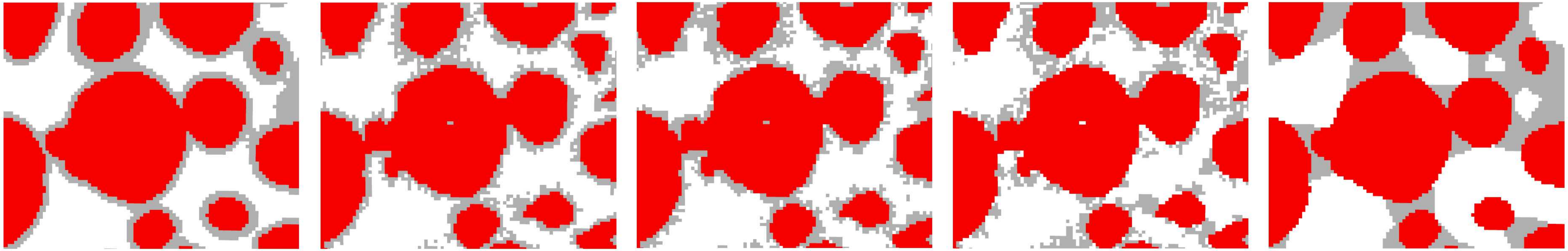
3D CT image data:
- Expensive
- Time consuming
- Conductive binder not visible



Graphite; Jaiser et al. (2017)



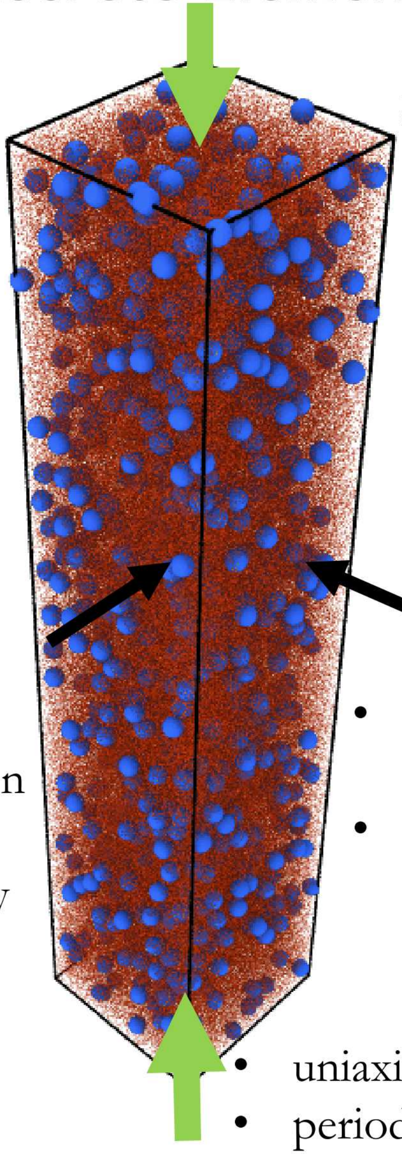
LCO; Zielke et al (2015)



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

Trembacki JES (2018)

Discrete Element Method (DEM) mesostructure



initial microstructure

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

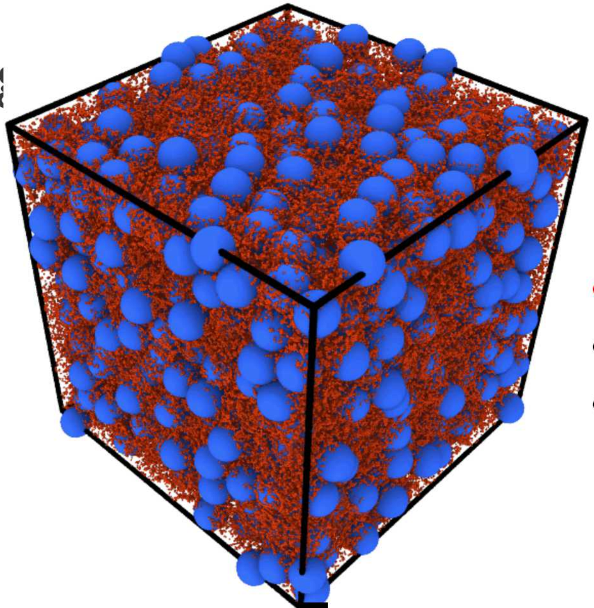
compression (drying)

- fixed dimension
- periodic boundary

- fixed dimension
- periodic boundary

- uniaxial compression
- periodic boundary

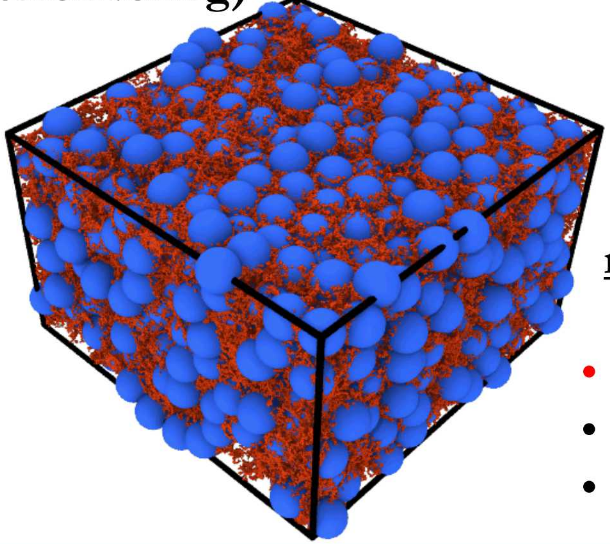
94% AM electrode
- ~1k AM particles (10 μm)
- ~1M CBD coarse grained particles (0.5 μm)



intermediate microstructure

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

compression (calendering)

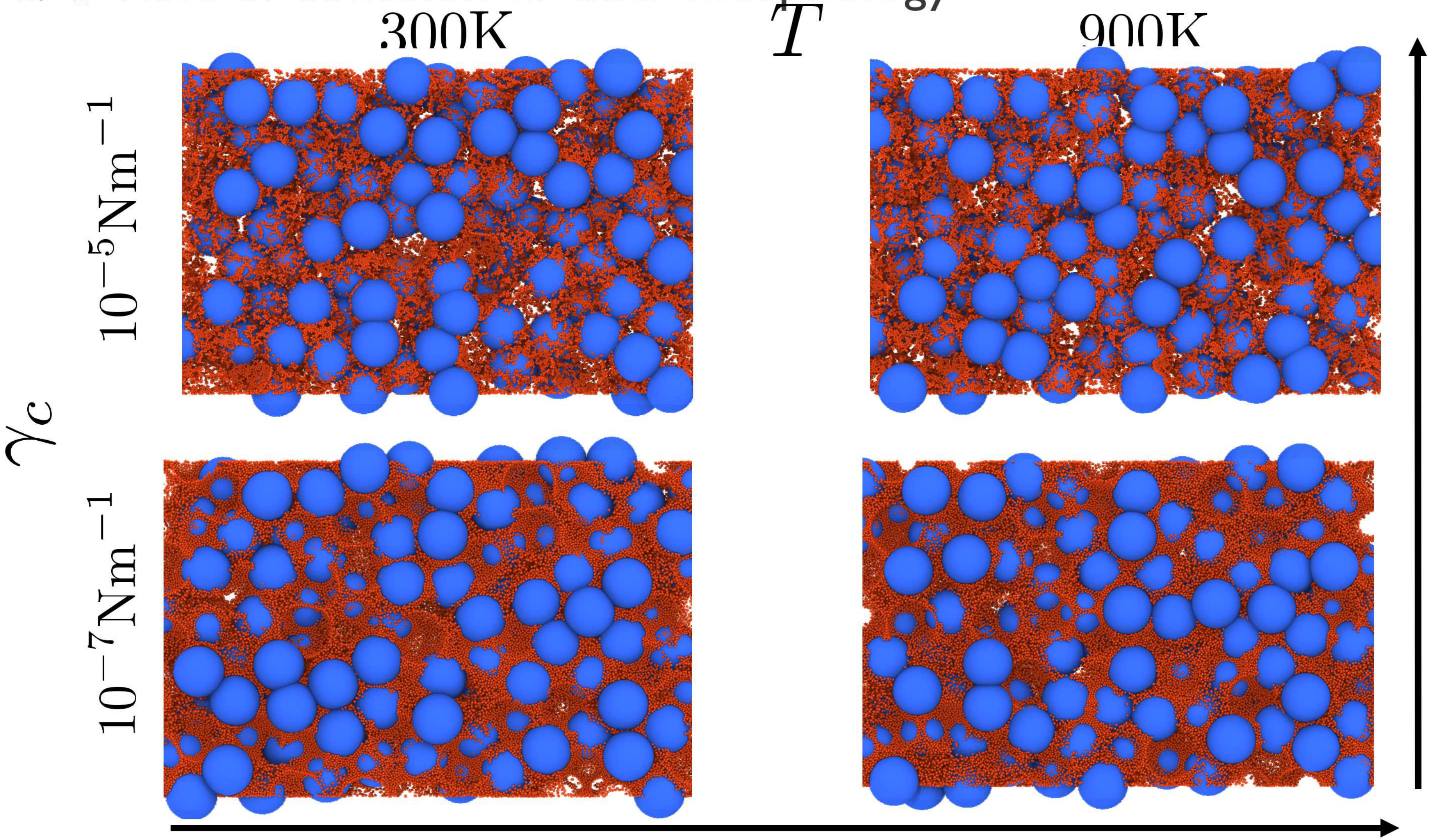


compressed microstructure

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

Uniaxial compression with granular and Brownian forces enable study of AM consolidation and CBD aggregation

Role of cohesion in CBD morphology



increased CBD diffusion results in a more uniform coating around AM particles

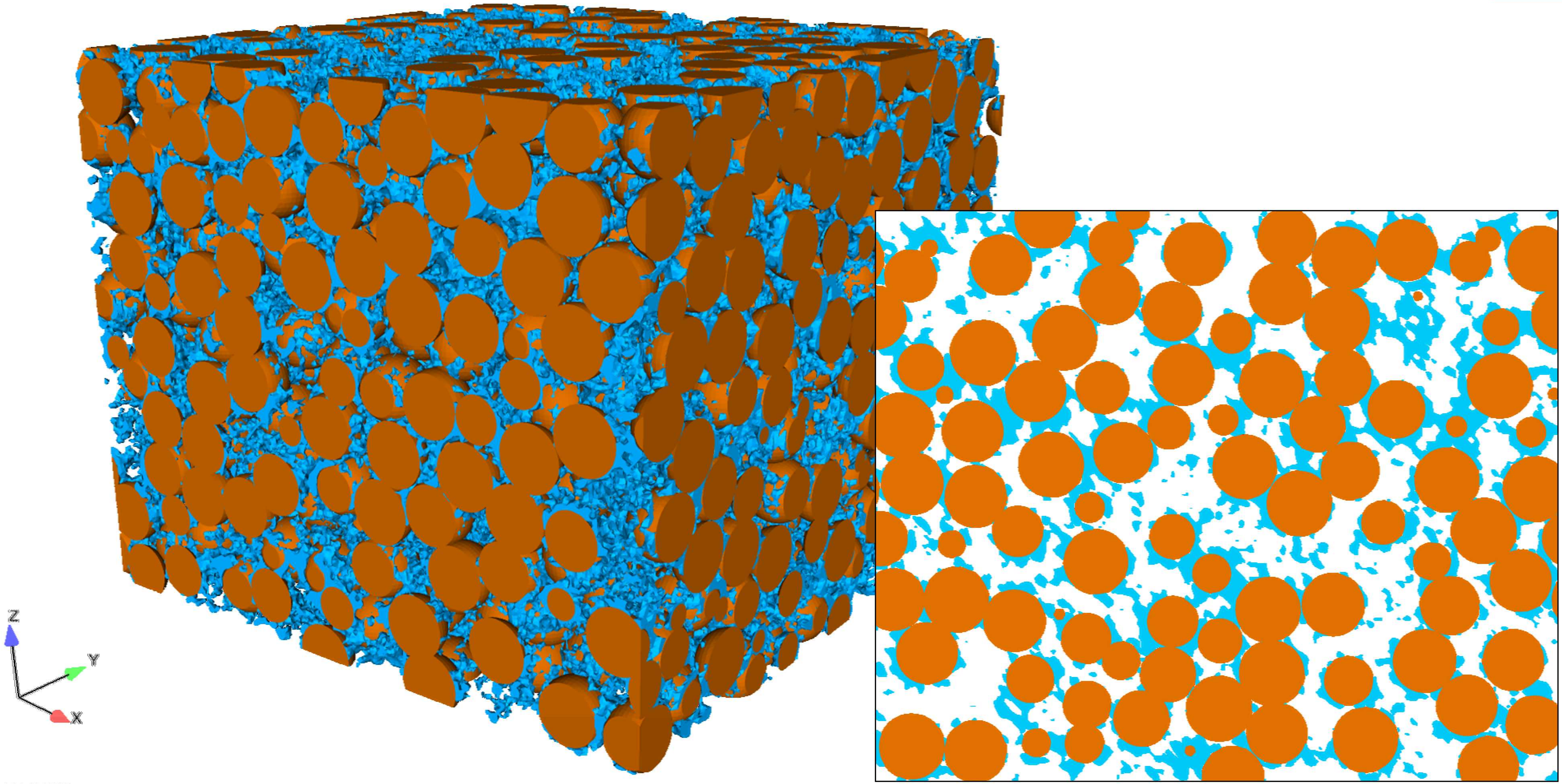
governing parameter

$$\frac{\gamma_c a^2}{kT}$$

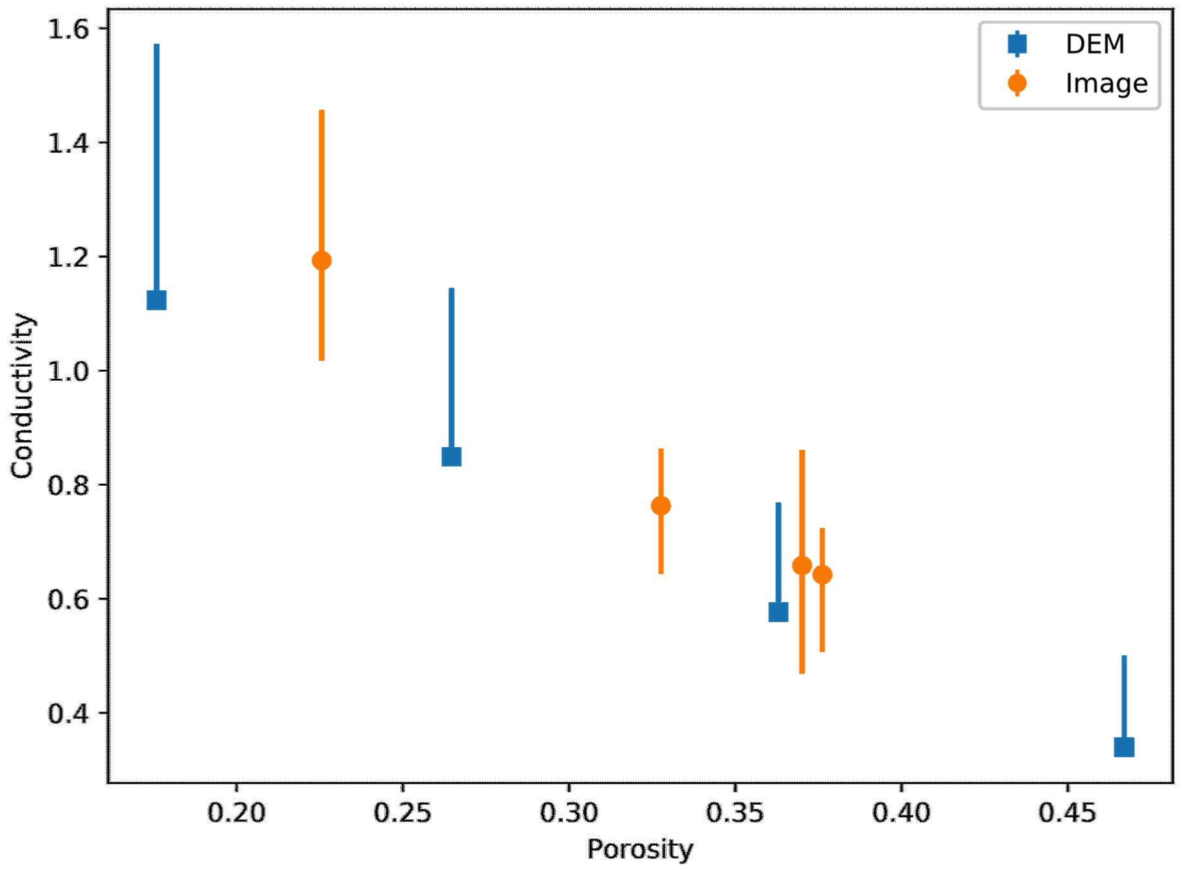
increased string-like fractal microstructure of CBD particles resulting in non-uniform coating around AM particles. CBD phase behaves like a sticky fluid

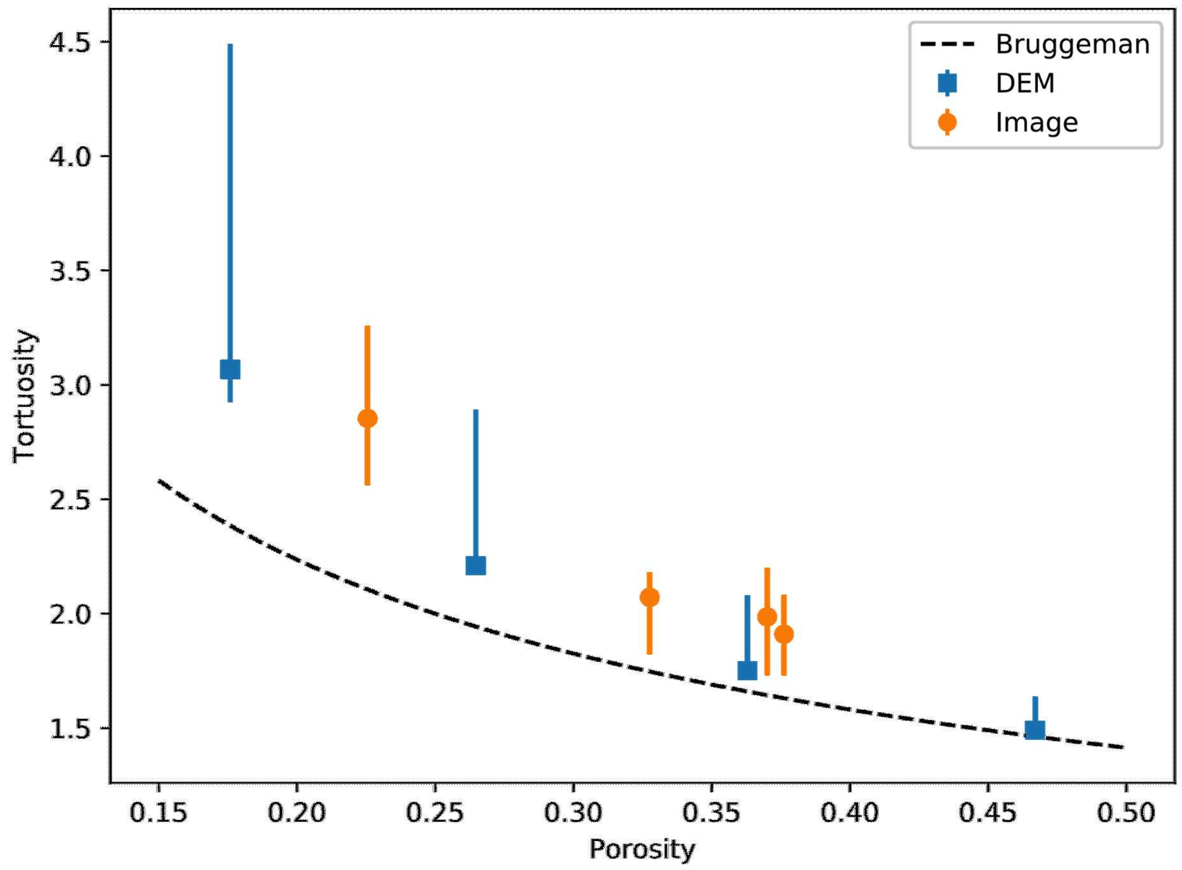
Cohesive surface energy drastically alters CBD morphology

Conformal Decomposition Finite Element Method (CDFEM)



Comparison of image- and DEM-based mesostructures





All simulations for T=600, $\gamma=10^{-5}$, AM=94 wt%, 0 bar calendaring

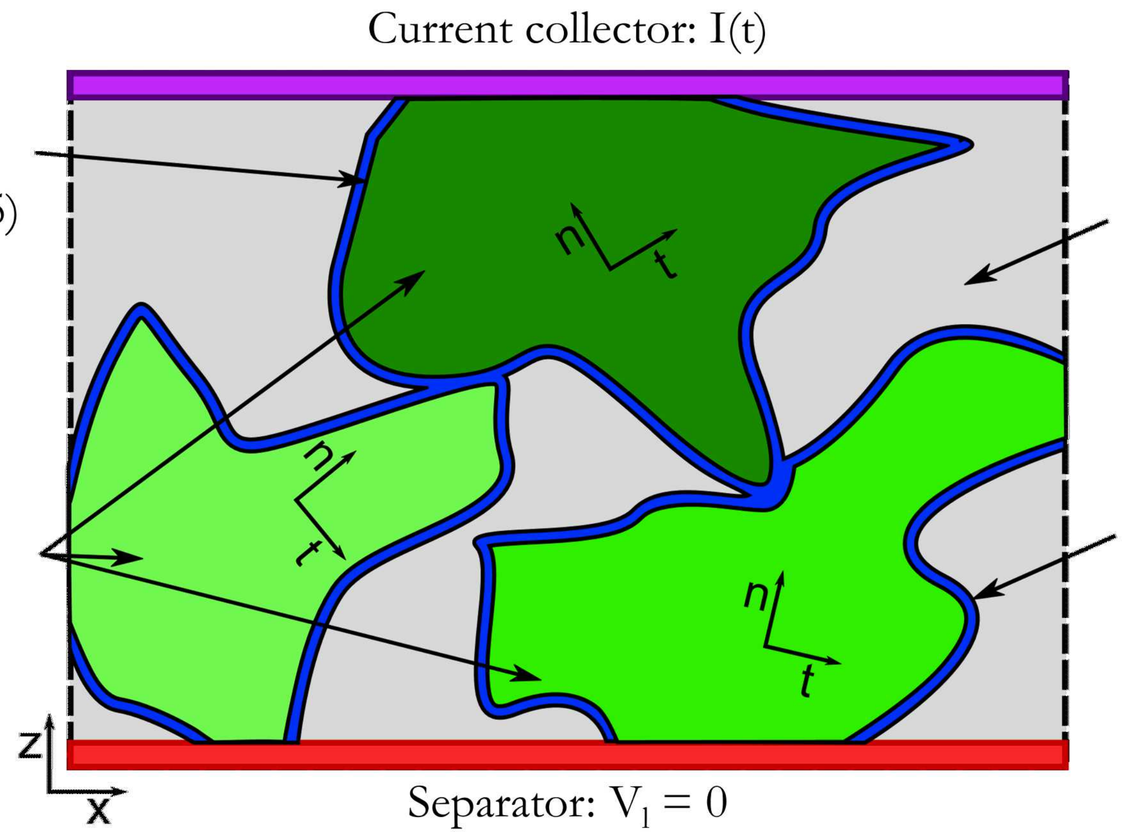
Calendaring → lower porosity → more CBD connectivity → higher conductivity and tortuosity

Electrochemical-mechanical discharge simulations of NMC half-cells

Coupled electrochemical-mechanical half-cell discharge simulations

Particle Interface:
- Butler-Volmer reaction
- OCV from Smekens (2015)

Particles:
- Species – Li tr
  - Chemica
  - Stress pc
- Electrical – O
- Mechanics - E
  - Li-induc



Electrolyte:
- Species – Li^+ transport
  - Nernst-Planck fluxes
  - Electroneutrality for PF_6^-
- Current conservation

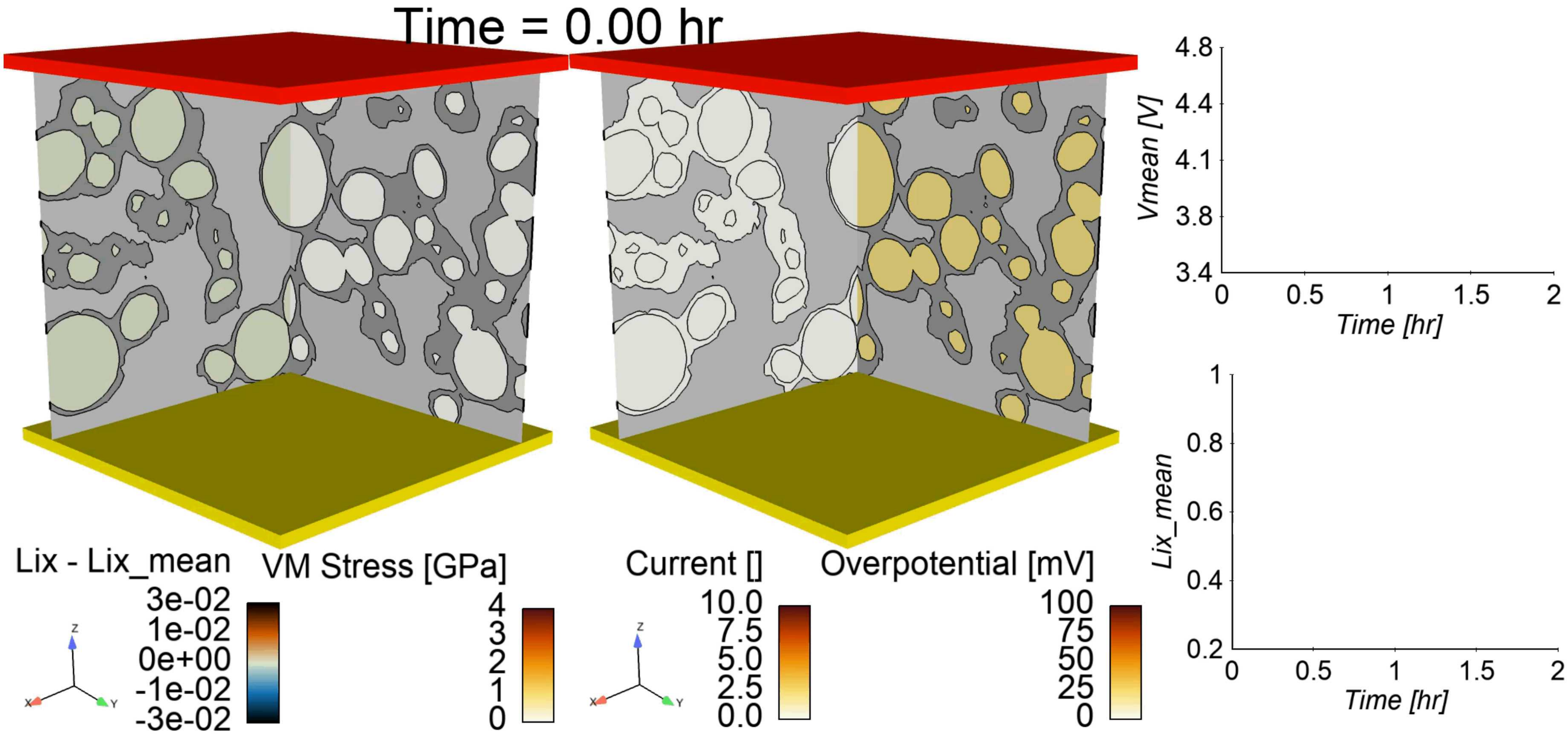
Conductive binder:
- Species – Porous Li^+ transport
- Electrical
  - Solid: Porous Ohm's law
    - Strain-dependent electrical conductivity
  - Liquid: Ionic conservation & electroneutrality
- Mechanics – Elastic

Mathematical formulation builds off of Mendoza (2016) LCO studies

Predictions of discharge curves, effects of mechanics, rate effects, and spatial variations in performance

Ferraro, in preparation

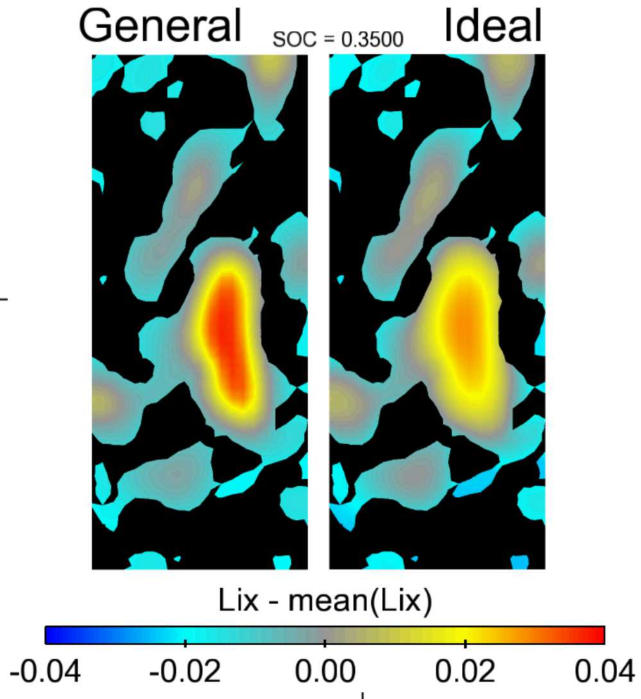
Demonstration of NMC half-cell discharge simulation at C/2

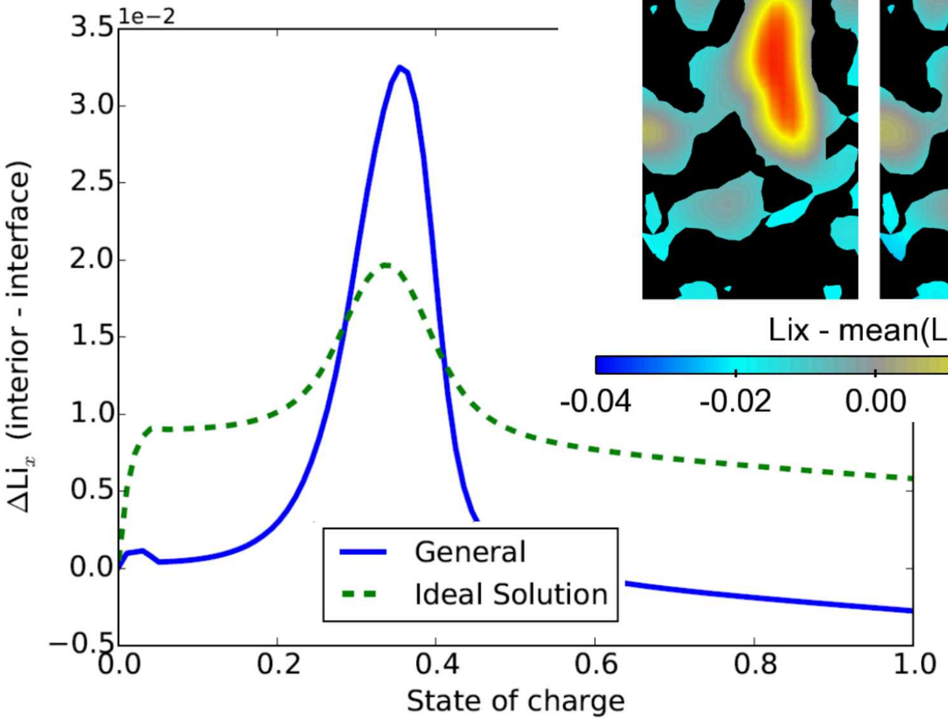


Coupled electrochemical-mechanical simulation yields detailed insight, predicts electrode-scale response

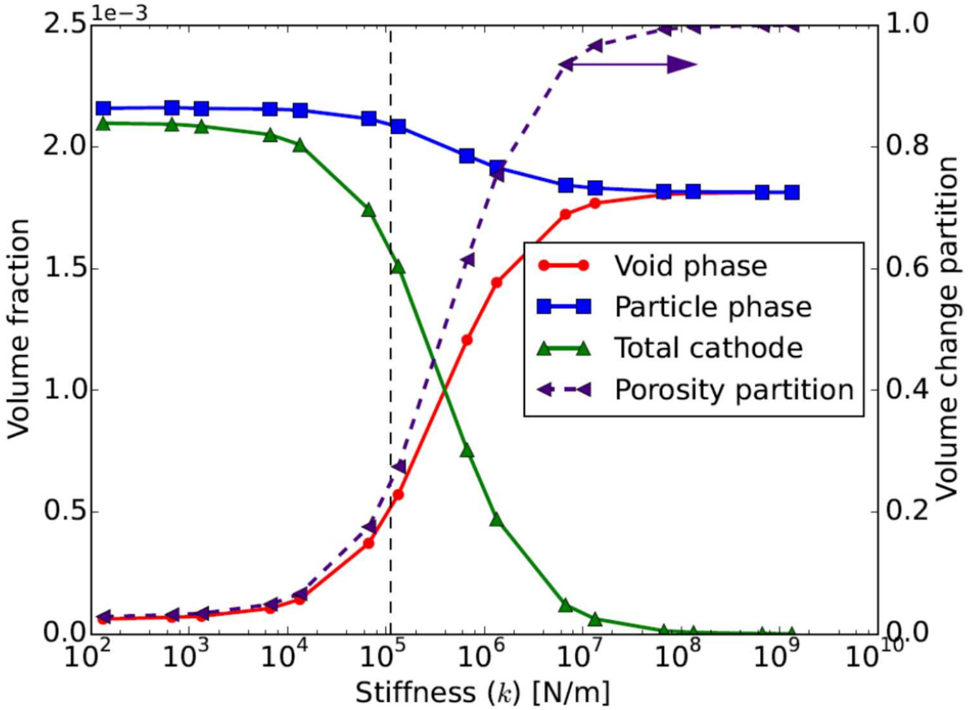
Ferraro, in preparation

What can you learn from coupled half-cell simulations? LCO





LCO is a non-ideal solution, gradients not as dominant as some believe



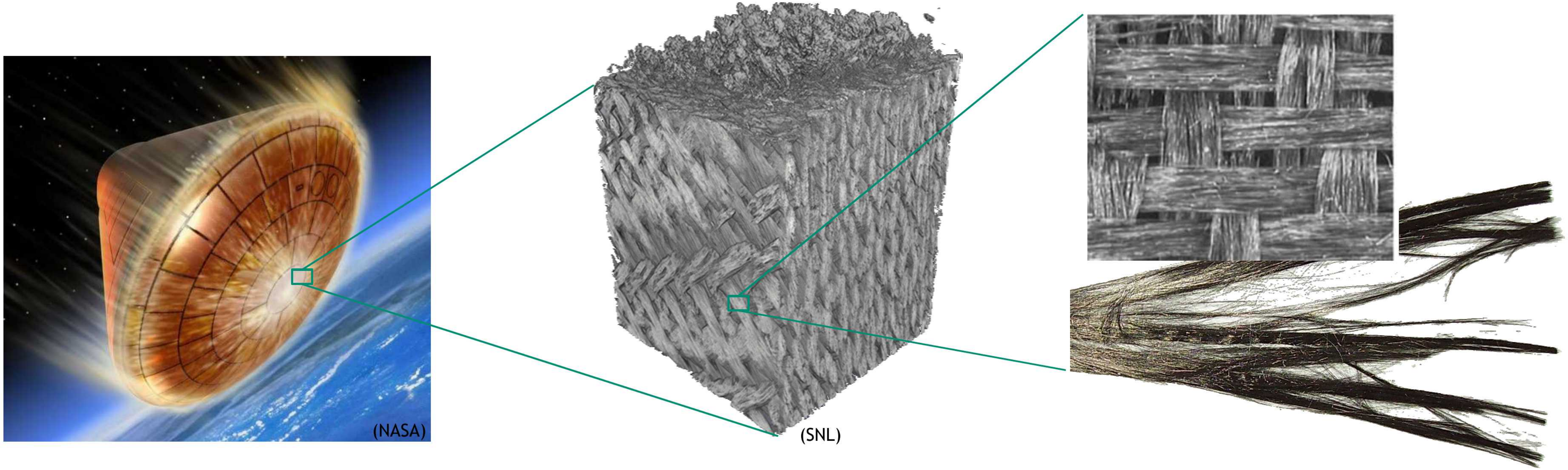
Separator/collector stiffness/boundary conditions influence electrode mesostructure evolution

Details at the mesoscale influence cell performance … and vice versa!

Mendoza (2016)

Mesoscale modeling of TPS materials: Effective property calculations and sensitivity analysis

TPS materials are hierarchical, multi-scale composites



Macroscale
Typical performance assessments and modeling.
Composite properties required.

Mesoscale
Woven fiber surrounded by phenolic resin. Governed by weave geometry, resin/tow properties.

Microscale
Individual fiber filaments spun into yarns, impregnated with resin. Fiber arrangement affects tow properties.

TPS performance governed at the mesoscale and microscale, modeling those scales gives flexibility to CMA etc.

Bulk properties depend on constituents

Constituents

Fiber properties
- Anisotropy

Resin properties

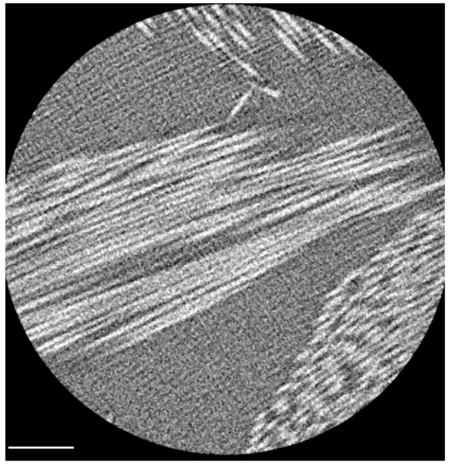
Filler properties
- Size distribution
- % mass

Void space
- % vol.

Microscale

Yarn model
- Filament packing
- Filament count
- Twist
- Shape/length

Matrix model
- Effective medium
  - Bruggeman etc.
- Void/filler shape/size

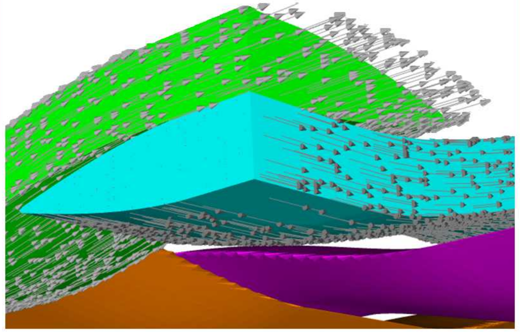


Mesoscale

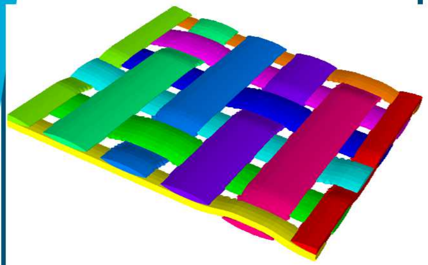
Fabric geometry
- Yarn Count
- Thickness
- Gaps in fabric
- "Waviness"

Yarn properties

Matrix properties



RVE Model
+
FEM Model



Macroscale

Composite Effective Properties

Properties
- K
- C_p
- ϱ
- E, G
- ν
- CTE

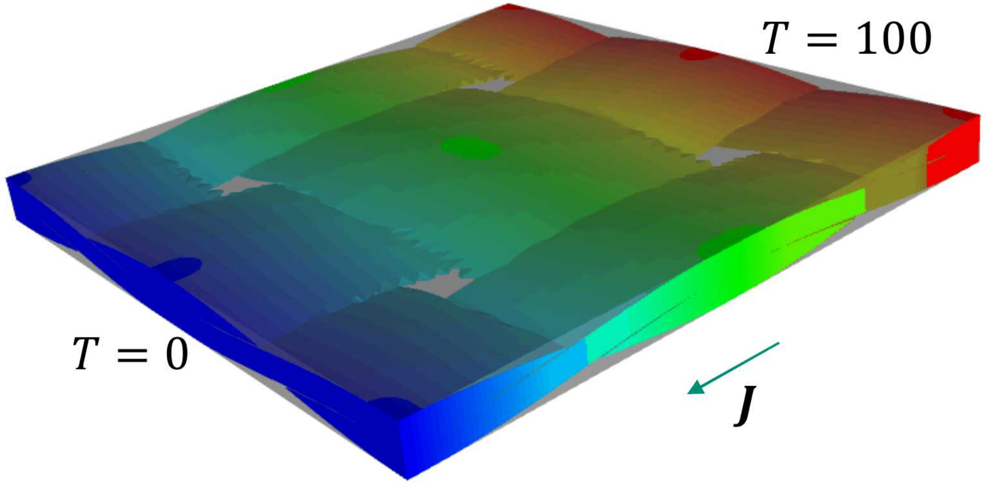
Trends in thermal conductivity and distributions

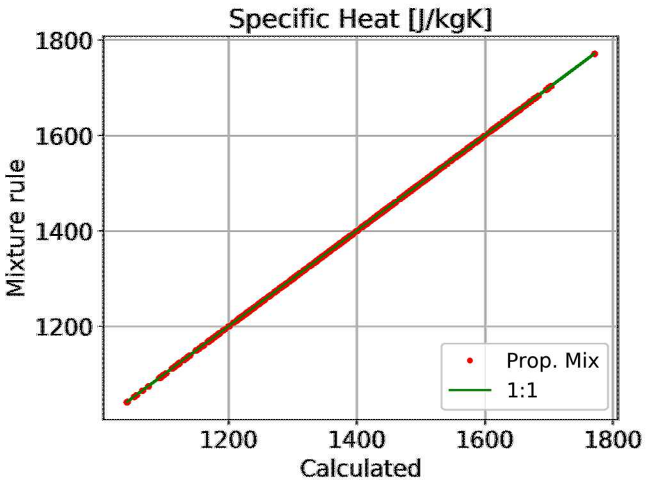
Proportional mixture rule (axial, upper bound):

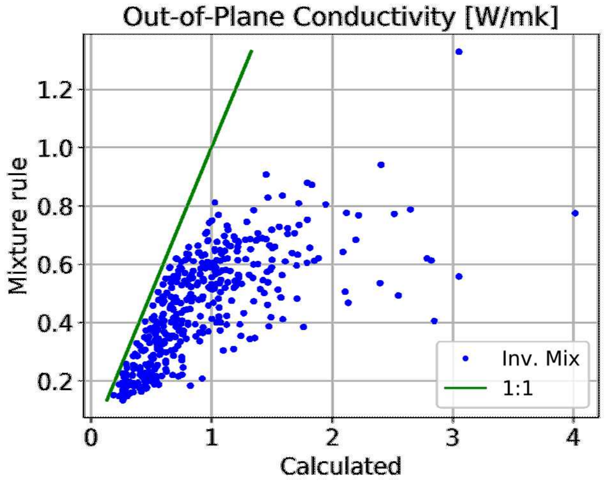
$$E_{\mathrm{v}}^{*} = v_f E_f + (1 - v_f) E_m$$

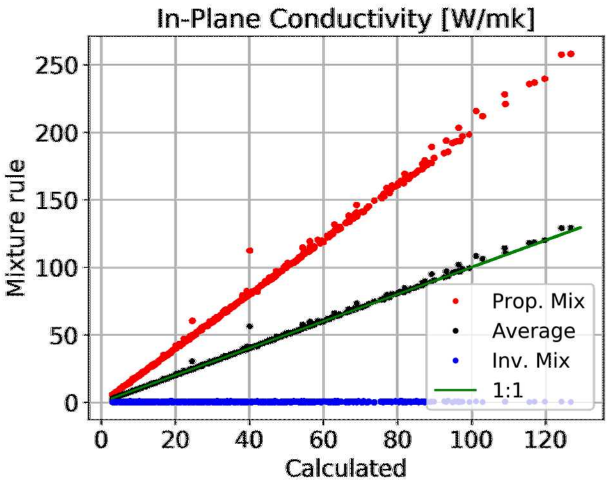
Inverse mixture rule (transverse, lower bound):

$$E_{\mathrm{r}}^{*} = \left(\frac{v_f}{E_f} + \frac{1 - v_f}{E_m} \right)^{-1}$$









Effect medium approximations are applicable only in certain situations

Ablation is a transient process

Mesoscale is *not* static during ablation

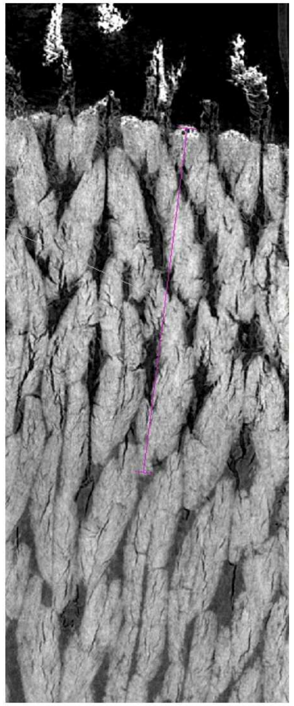
- Surfaces recede
- Phases evolve (resin→ char)
- Phases melt
- Phases deposit (coking)

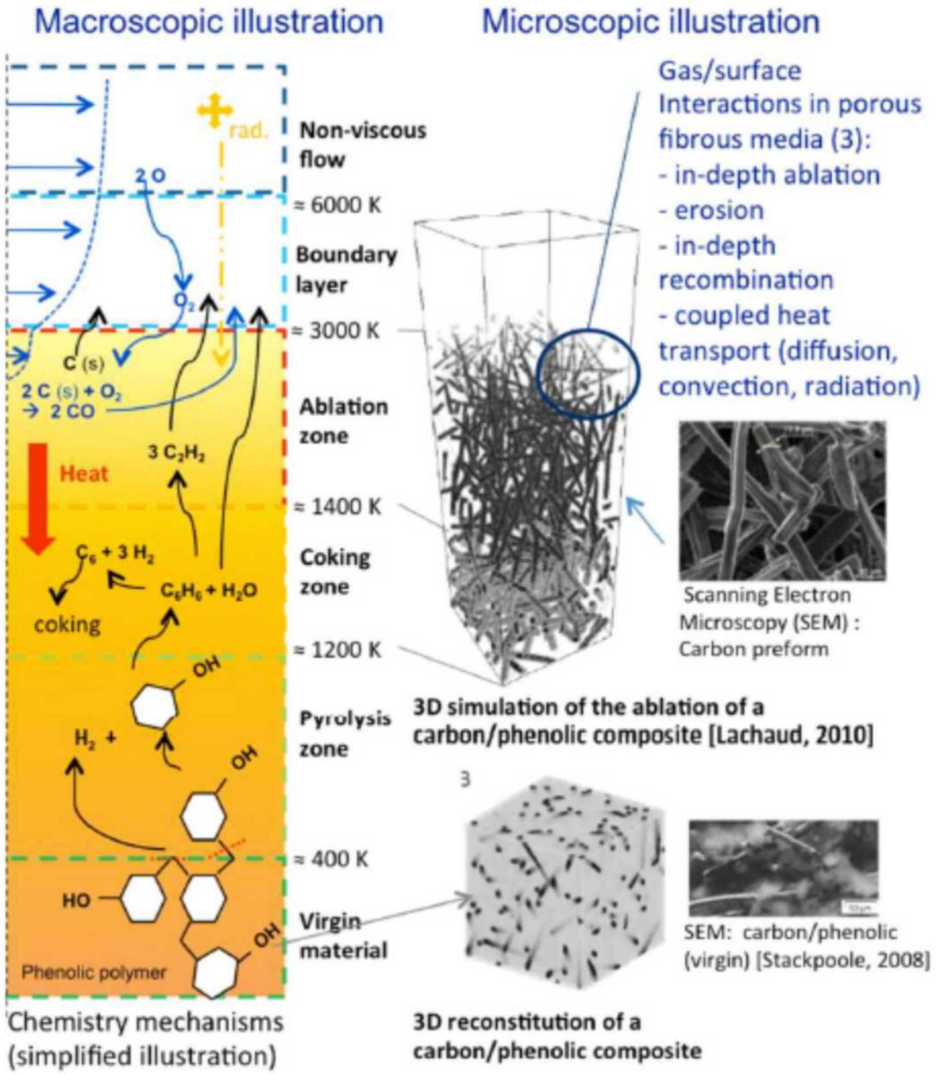
Evolving geometries are necessary

Analytic background
- System of sinusoid fabric descriptions

Moving resin interface
- Transient level set

Ablation modeling

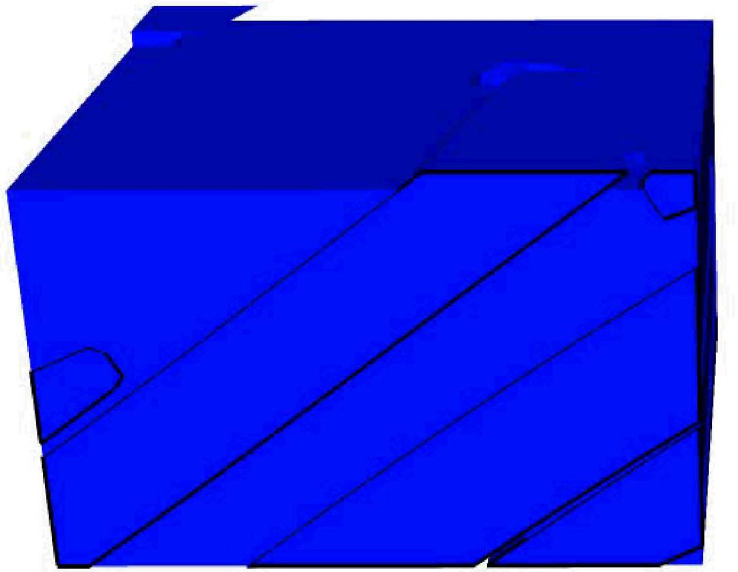


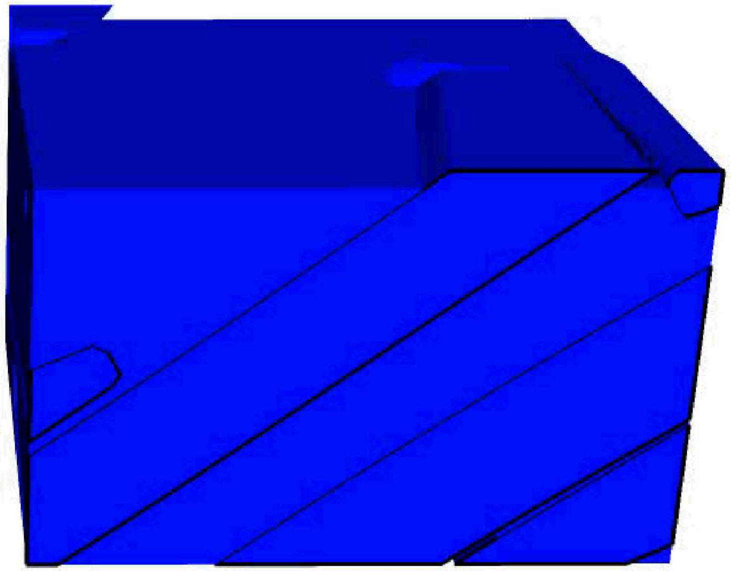


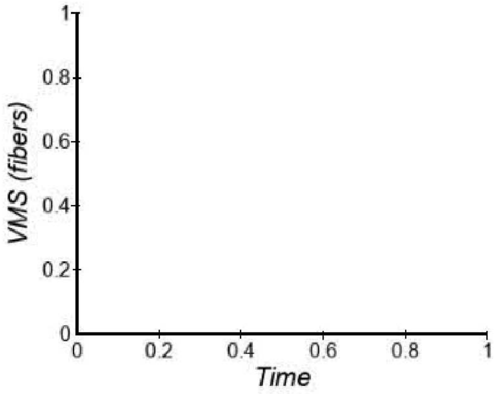
(Lachaud, 2014)

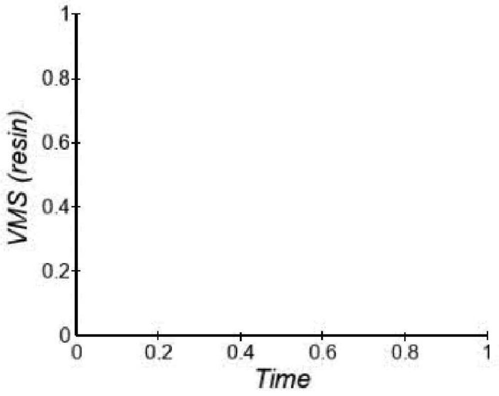
Dynamic geometry is necessary to model ablation

Transient thermochemical-mechanical demonstration









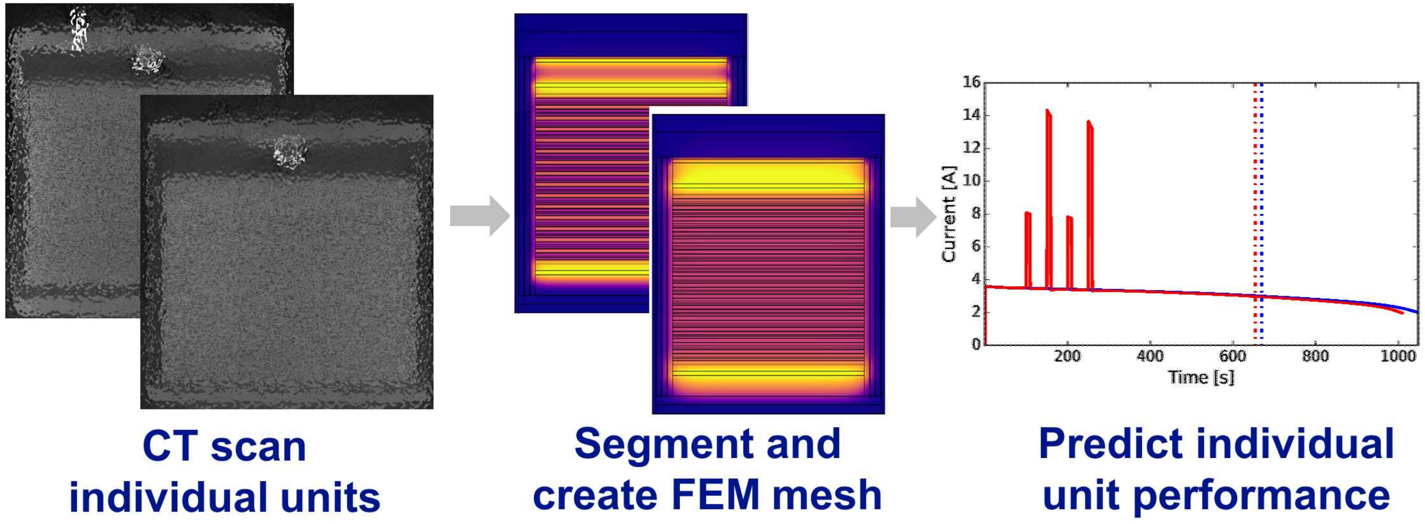
Coupled thermal and mechanical effects can identify failure mechanisms

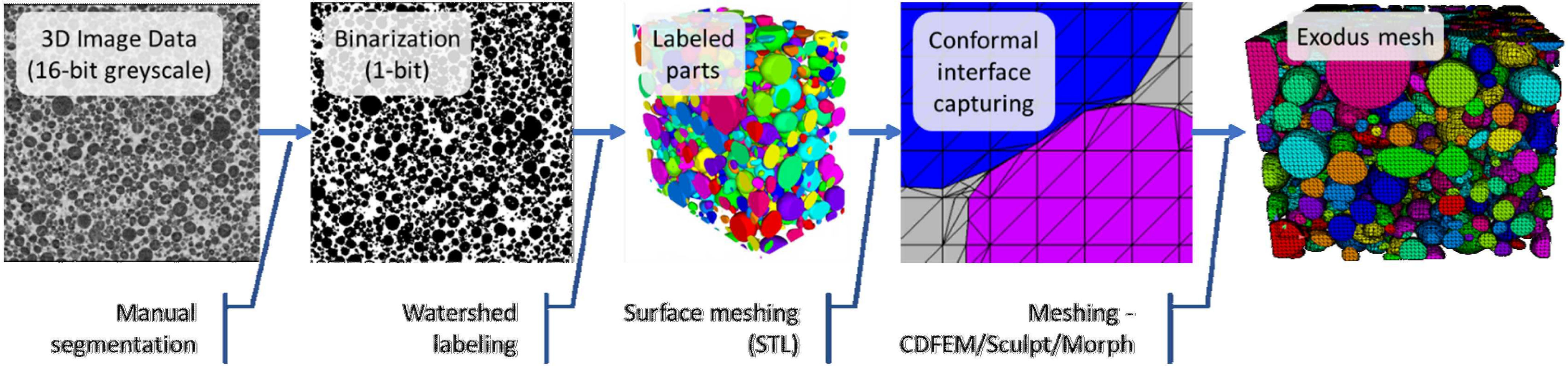
Credible Automated Meshing of Images

Problem statement

Desire to perform FEM simulations directly from 3D tomographic imaging
- Enables "digital-twins"

Recent state-of-the-art processes are:
- Manual, SME-dependent
- Time-consuming
- Unknown credibility
- Don't capture all geometric features





Automated, credible CT-to-mesh would revolutionize engineering analysis workflows!

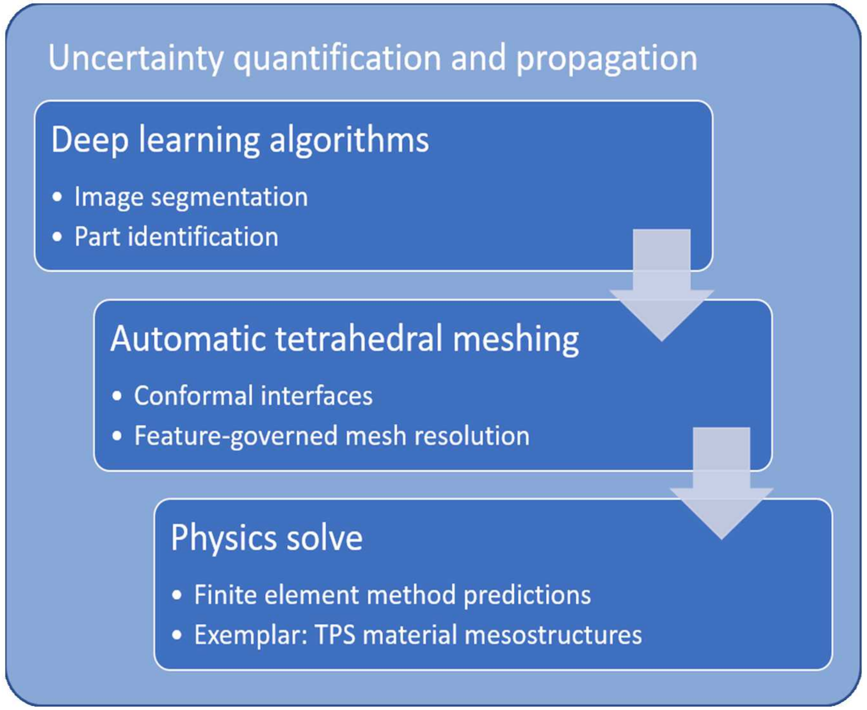
Project overview

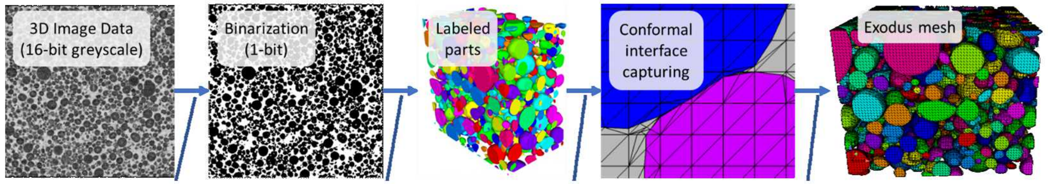
Hypothesis: We can develop an automated and credible image-to-mesh technology that can demonstrate the physics impact of per-unit variability on material, component, or system performance

Objective: We seek to develop a methodology for **automatically**, **efficiently**, and **reproducibly** creating **conformal** finite element meshes from **3D tomography** with **quantified uncertainty**.

Research thrusts – primary science questions:

- Deep machine learning algorithms (ML)
- Automatic conformal tetrahedral mesh creation (ATM)
- Uncertainty quantification and propagation (UQ)
- Application exemplar: Thermal protection system materials (TPS)





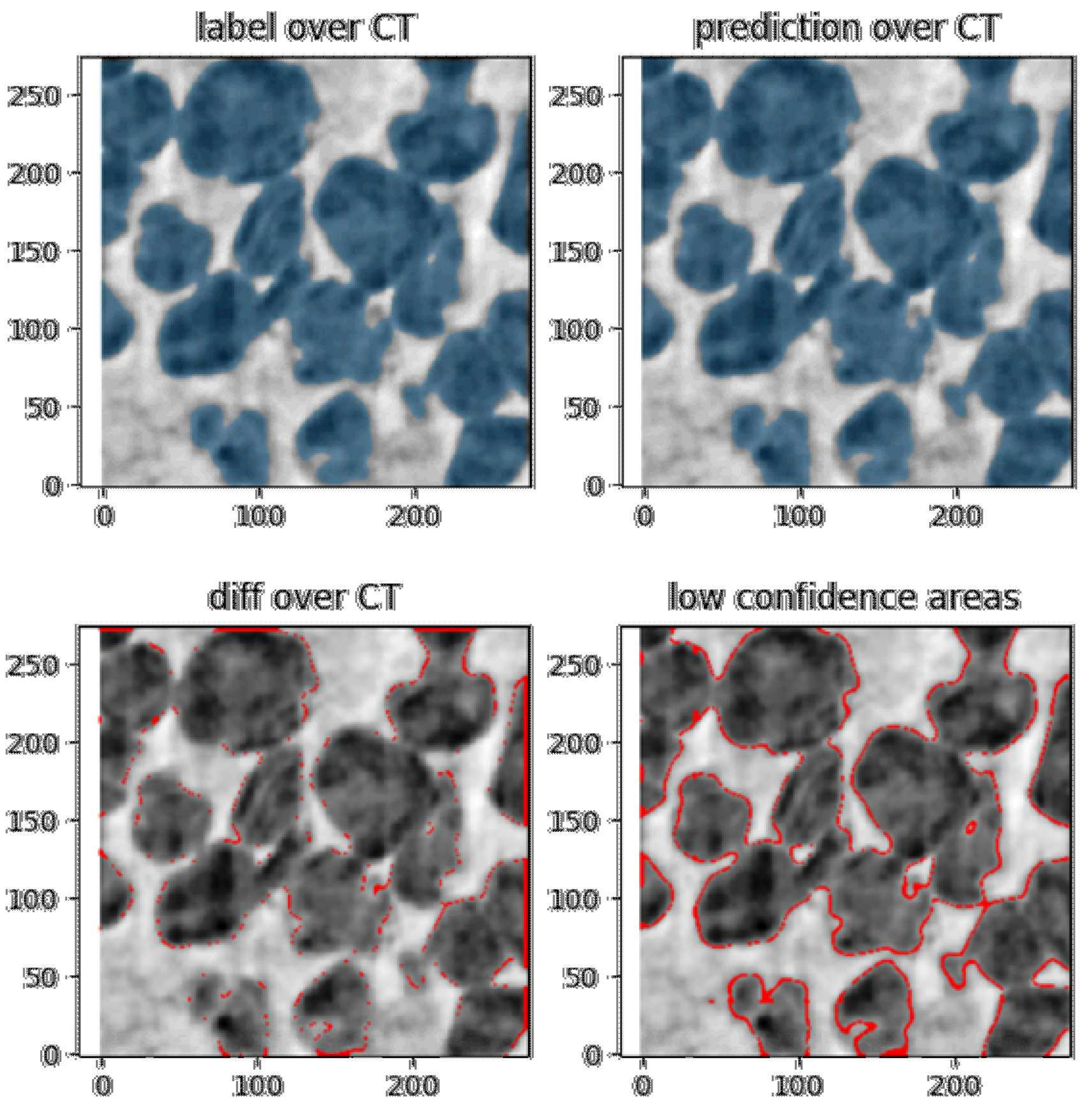
Early demonstration of DL and UQ on graphite electrodes

DL trained with human labels to segment with > 99.9% accuracy

Developing methodology to continuously assess per-voxel confidence in assessment and propagate through mesh

Upcoming challenges:

- Instance segmentation (particle labeling)
- Feature identification (edges/corners)
- Part orientation
- Mesh quality
- Verification of uncertainties (ground truth)

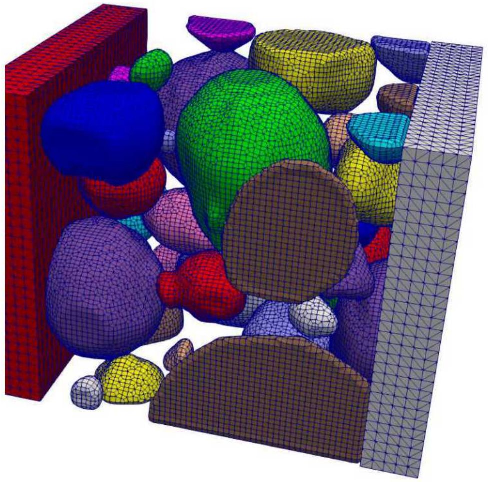


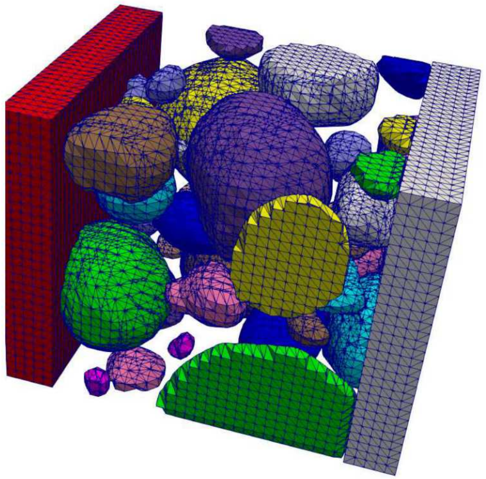
Deep learning shows huge promise in increasing throughput, repeatability, and credibility

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

Summary

We have developed a **unique image-to-mesh capability** to enable rapid analysis of as-manufactured parts

We have carefully **verified this approach**, identifying potential pitfalls and domain/mesh requirements

We have applied this technique to **lithium-ion battery cathode** mesostructures and have:

- Created and characterized the impact of conductive binder morphology
- Calculated and correlated effective properties
- Predicted coupled electrochemical-mechanicals effects during charge/discharge

We are developing **particle simulations** to carefully manufacture realistic mesostructures

We are applying these techniques to woven composites for **thermal protection systems**

We are beginning to improve the **credibility, reproducibility, and time required** to create high-quality meshed from 3D image data

References and acknowledgments

Publications

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Data

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Questions?

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