

Performance, degradation, and safety modeling for battery systems

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November 21, 2014



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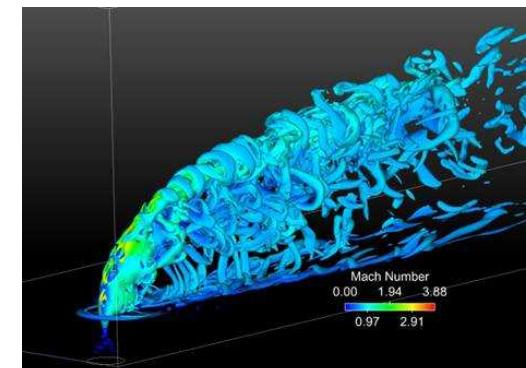
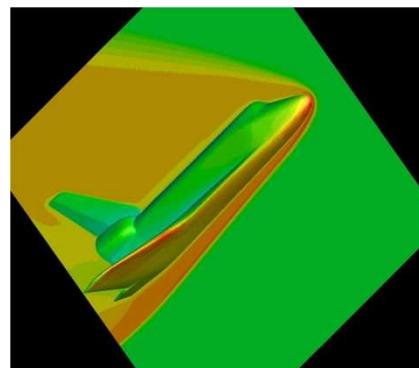
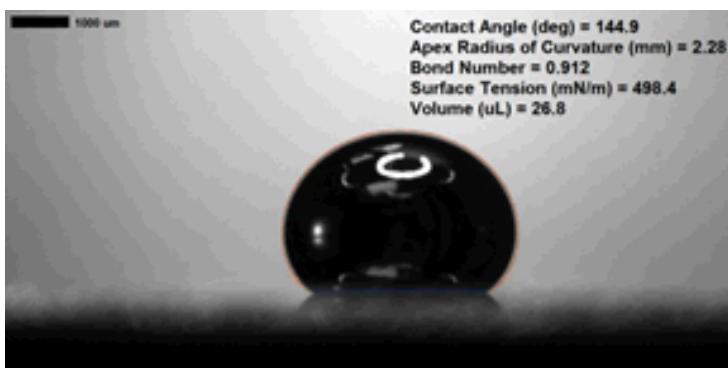
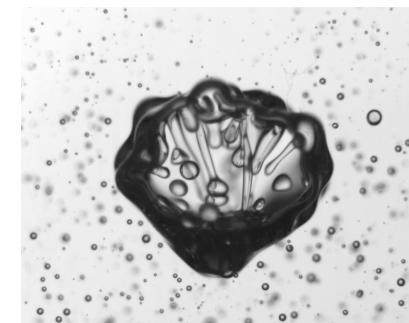
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Unclassified Unlimited Release: SAND2014-XXXXX



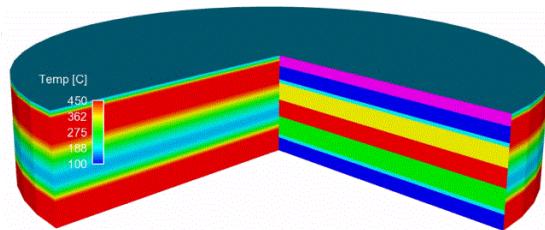
Engineering Sciences Center:

- Engineering analysis
- Environmental simulation and test
- Engineering science physical phenomena
- Computational simulation technology

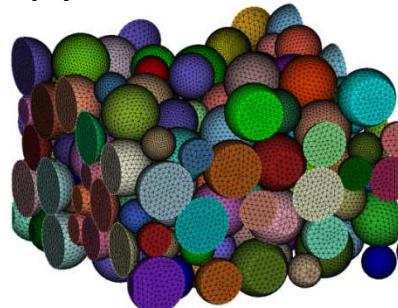


Who am I?

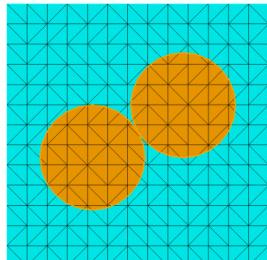
- B.S. Chemical Engineering – University of Kansas
- Ph.D. Chemical Engineering – University of Minnesota
- Joined Sandia National Laboratories in 2010



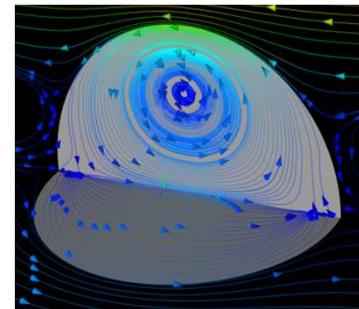
Battery performance modeling



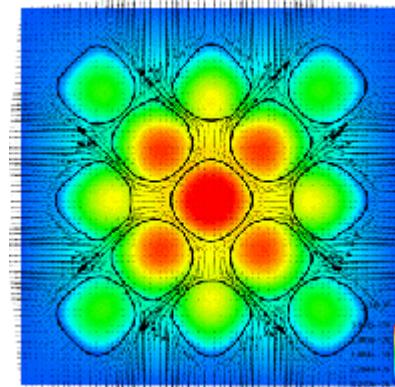
Li-Ion battery degradation



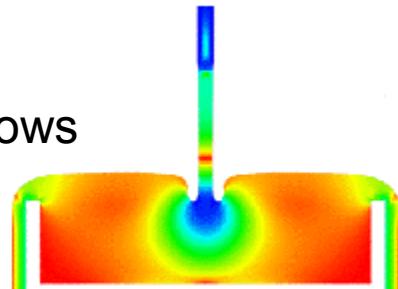
GOMA and
Sierra code
development



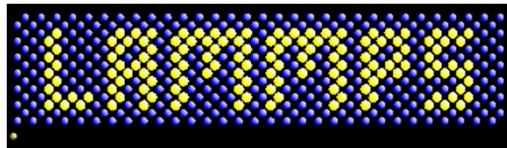
Microfluidics



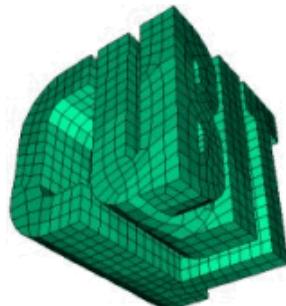
Free surface flows



Nanomanufacturing



LAMMPS (SNL, OSS): Particle dynamics, configuration generation



Cubit (SNL, GUN/commercial): Mesh generation



FEI Avizo (commercial): 3D reconstructions, mesh generation, visualization

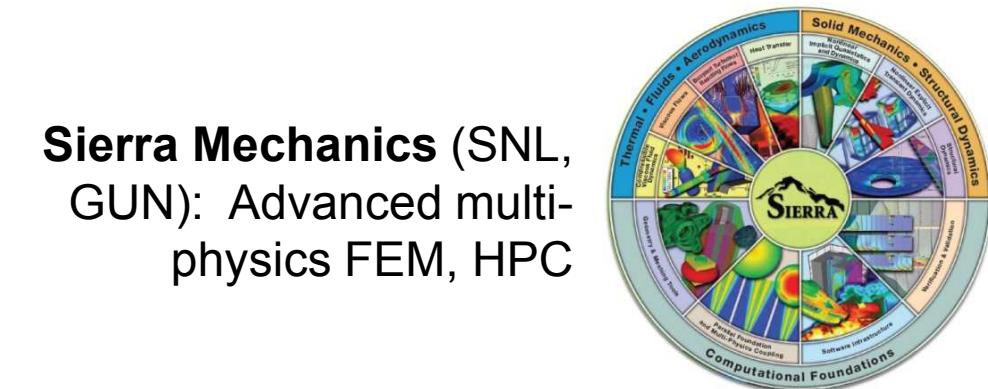


cantera

An object-oriented software toolkit for chemical kinetics, thermodynamics, and transport processes.

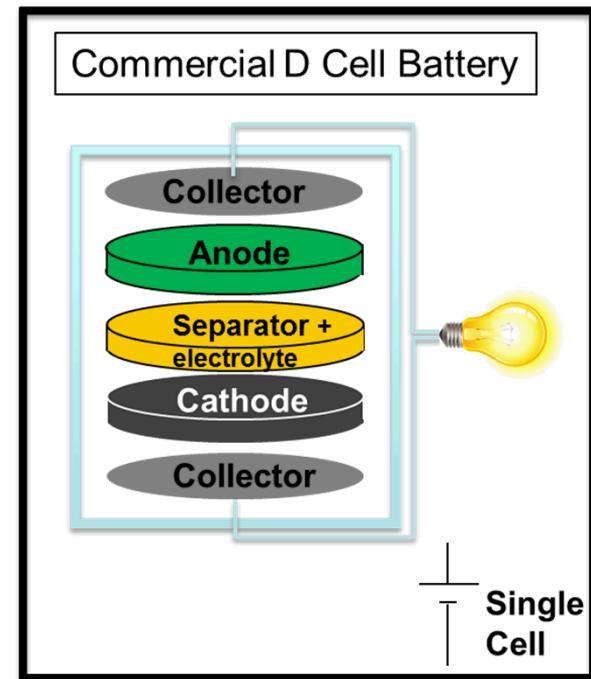


GOMA (SNL, OSS): Multi-physics FEM simulations

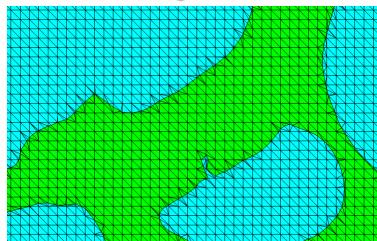
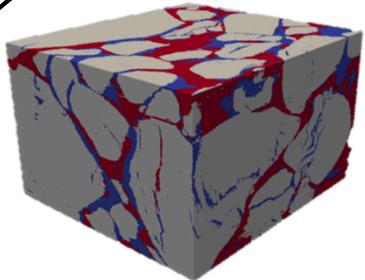


Battery basics

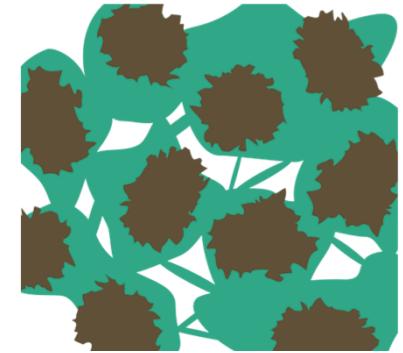
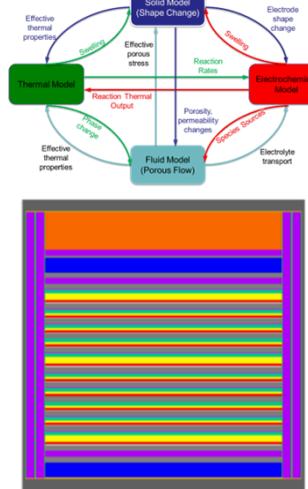
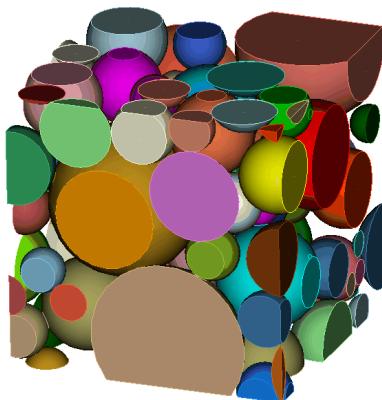
- Batteries consist of thin, porous layers of electroactive and non-electroactive materials
- During use, electrons flow from the negative electrode (anode), through the circuit, to the positive electrode (cathode)
- Electrochemical reactions at the anode/cathode release/absorb electrons while generating charged ions
- The separator layer allows ions to transport through the electrolyte to the cathode while keeping the cathode and anode from shorting
- Common problems: Capacity fade, energy density, current density
- Models can provide insight into the physical mechanisms that cause these problems and suggest solutions



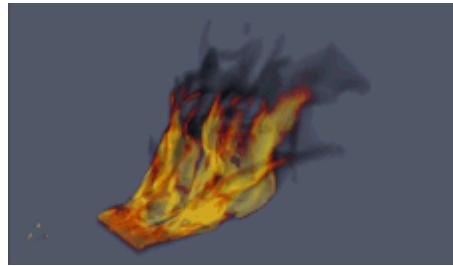
Outline



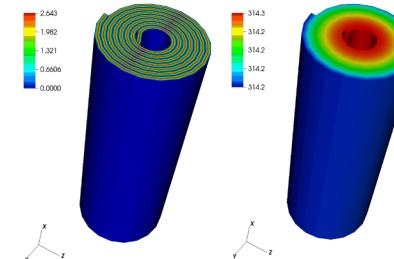
Lithium-Ion battery mesoscale
degradation simulations



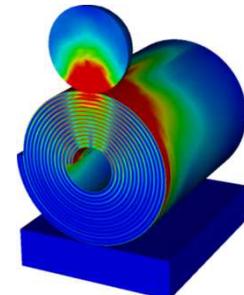
Performance models of
molten salt batteries



Grid storage

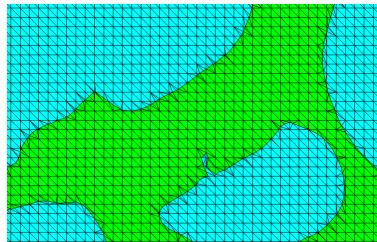
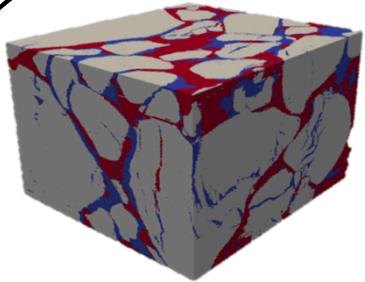


Alkaline batteries

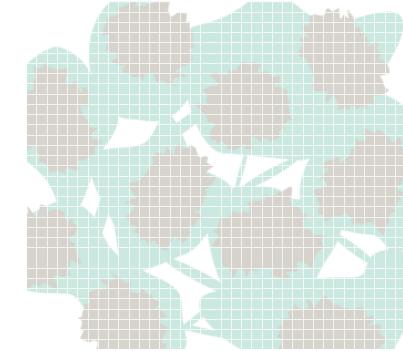
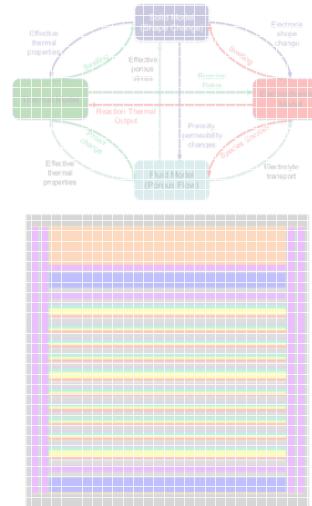
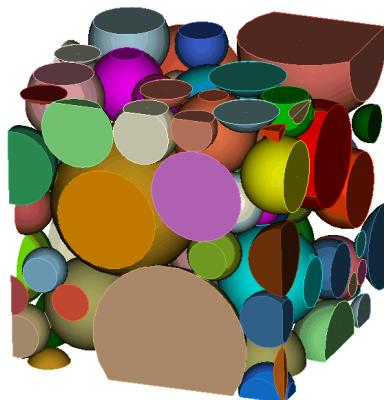


CAEBAT

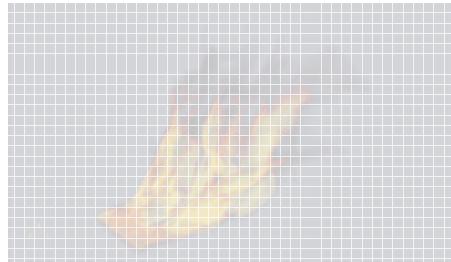
Outline



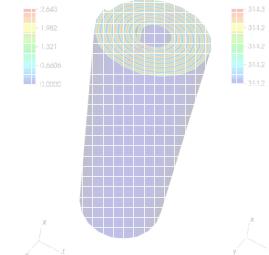
Lithium-Ion battery mesoscale
degradation simulations



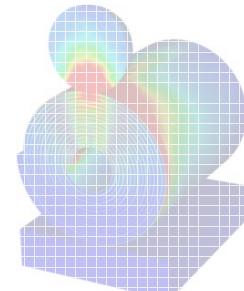
Performance models of
molten salt batteries



Grid storage



Alkaline batteries



CAEBAT

THREE-DIMENSIONAL MESOSCALE MODELING OF MECHANICAL DEFORMATION IN LI-ION ELECTRODES DURING CYCLING

Scott A. Roberts, Hector Mendoza, Victor E. Brunini, Kevin N. Long,
Farid El Gabaly, Chelsea Ehlert, Christopher A. Apblett, Anne M. Grillet

F3052

Journal of The Electrochemical Society, **161** (11) F3052-F3059 (2014)



JES Focus Issue on Mechano-Electro-Chemical Coupling in Energy Related Materials and Devices

**A Framework for Three-Dimensional Mesoscale Modeling
of Anisotropic Swelling and Mechanical Deformation
in Lithium-Ion Electrodes**

Scott A. Roberts,^{*^z} Victor E. Brunini, Kevin N. Long, and Anne M. Grillet^{*}

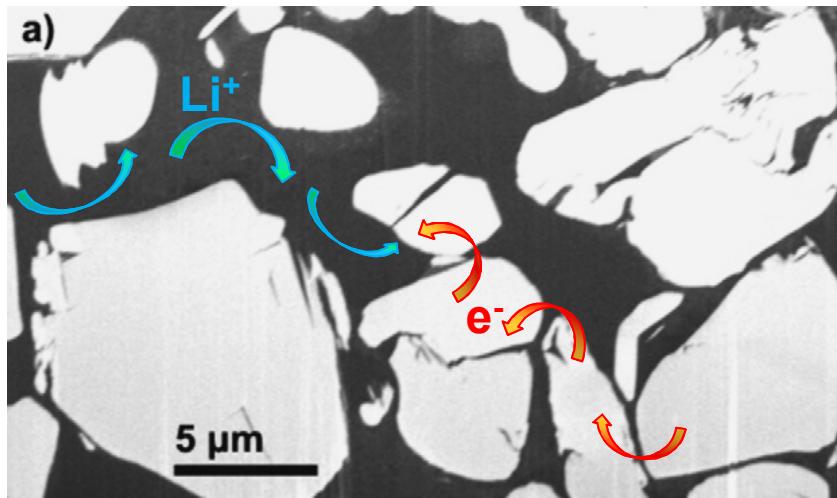
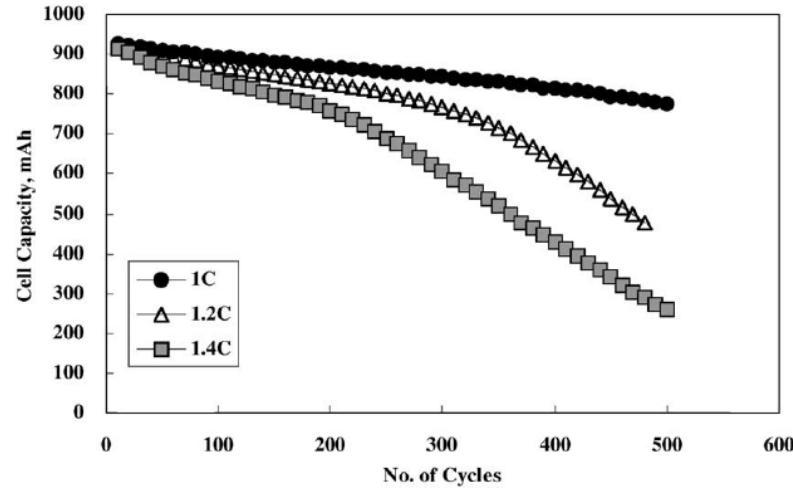
Sandia National Laboratories, Albuquerque, New Mexico 87185-0836, USA

Lithium-ion battery electrodes rely on a percolated network of solid particles and binder that must maintain a high electronic conductivity in order to function. Coupled mechanical and electrochemical simulations may be able to elucidate the mechanisms

Capacity fade in Lithium Ion batteries

Capacity fade – irreversible processes that reduce available battery capacity

- Increases expense of Li-Ion implementation
- Limits depth of discharge in production
- Tied to power fade – limits useful current
- Reduces reliability and performance margin
- Limits adoption in other applications



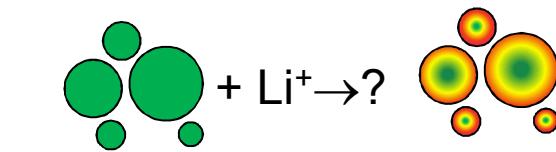
Mechanisms at the mesoscale

- Electrochemistry requires electronic and ionic conductivity
- Transport relies on a 3D bicontinuous percolated network
- Network heterogeneities cause gradients, altering the local potential

Hypothesis: Degradation of the 3D electrode percolated structure is a primary mechanism for capacity fade

Grain Scale Mechanisms

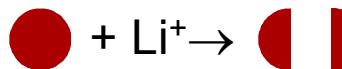
Lithiation progression



Anisotropic particle swelling



Electrochemical Shock



Solid Electrolyte
Interphase

Binder
relocation

Modulus changes
 $E + \text{Li}^+ \rightarrow 3E$

Electrode Impacts

CAPACITY FADE

- Electrode swelling
- Macroscopic Strain
- Porosity changes
- Tortuosity changes
- Particle isolation
- Stress-lithiation coupling
- Non-uniform lithiation

Experimental Discovery

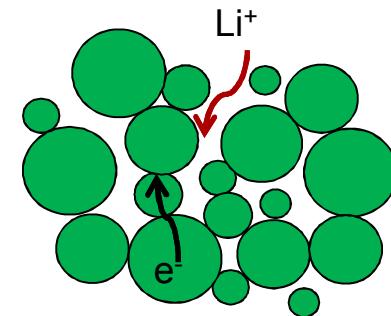
- Structure evolution
- Binder mechanics & conductivity
- State of charge & connectivity

Network Model Development

- Lithium ion and electron conductivity
- Particle swell models
- Mechanics of structure
- Coupling lithiation potential and mechanical stress

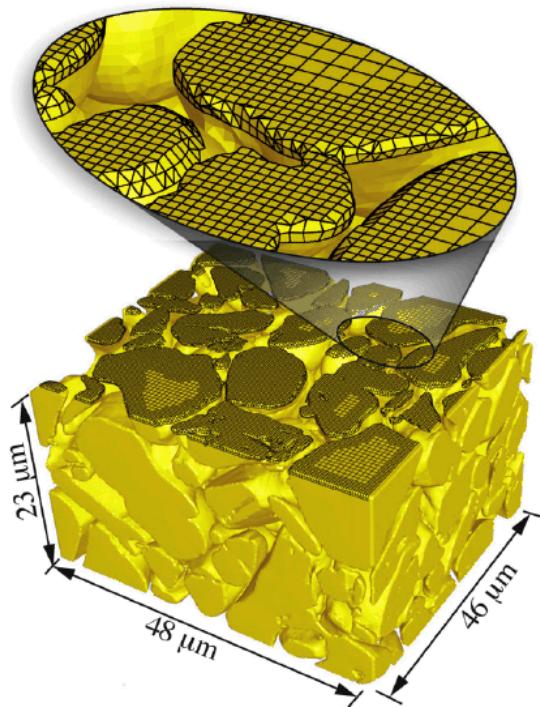
Margin Prediction

- Transport in porous materials
- Heterogeneous degree of (dis)charge
- Heterogeneous structure evolution
- Capacity fade mechanisms

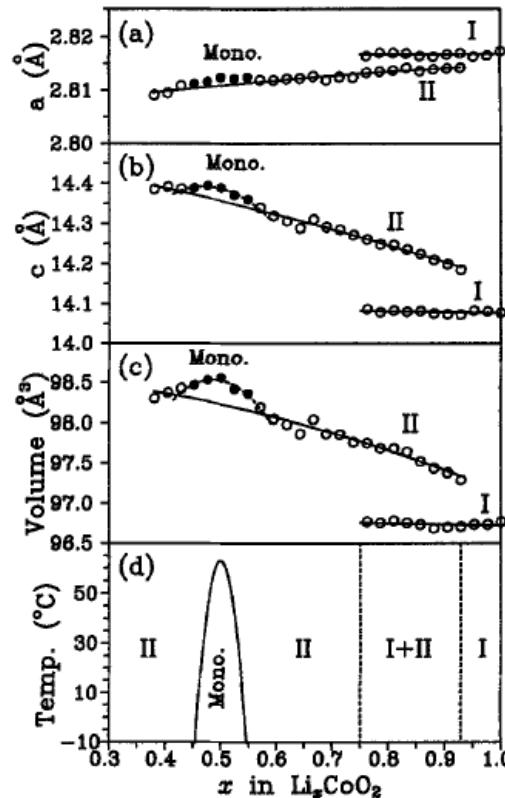


- New and improved multiphysics models for electrochemical systems
- New techniques for understanding mesoscale electrochemical phenomena
- Elucidate effect of mesoscale structure on safety and reliability of chemical energy storage systems.

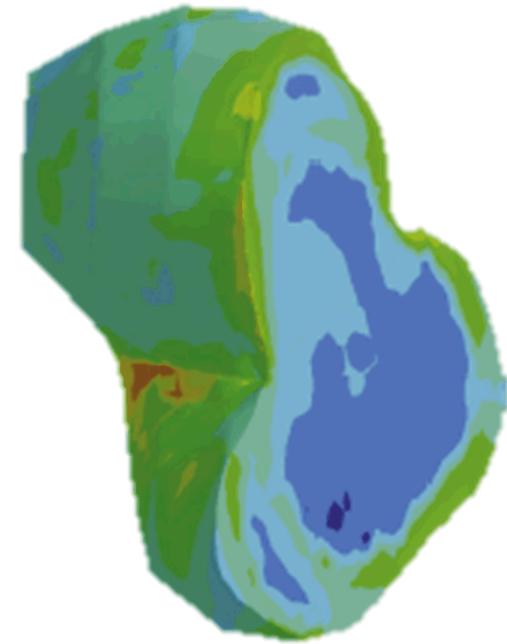
Previous efforts in understanding network structures



3D reconstruction and meshing of cathode. Transport, electrochemistry studies.
Wiedemann *et al* (2013)



Anisotropic stress-strain relationships on lithiation.
Reimers and Dahn (1992)

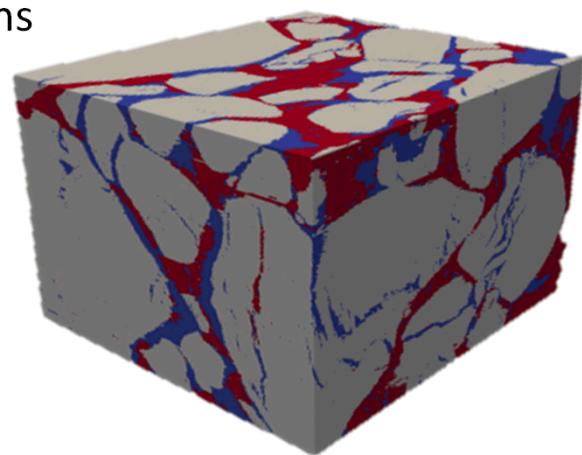


Simulations of anisotropic particle swelling coupled with electrochemistry. Malave *et al* (2014).

To date, no computational studies have addressed the effect of lithiation-induced swelling on network structure, capacity fade.

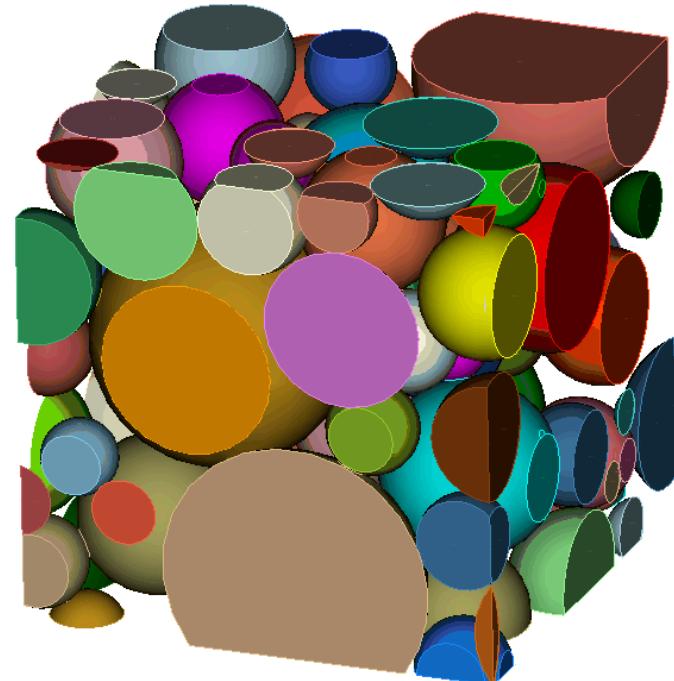
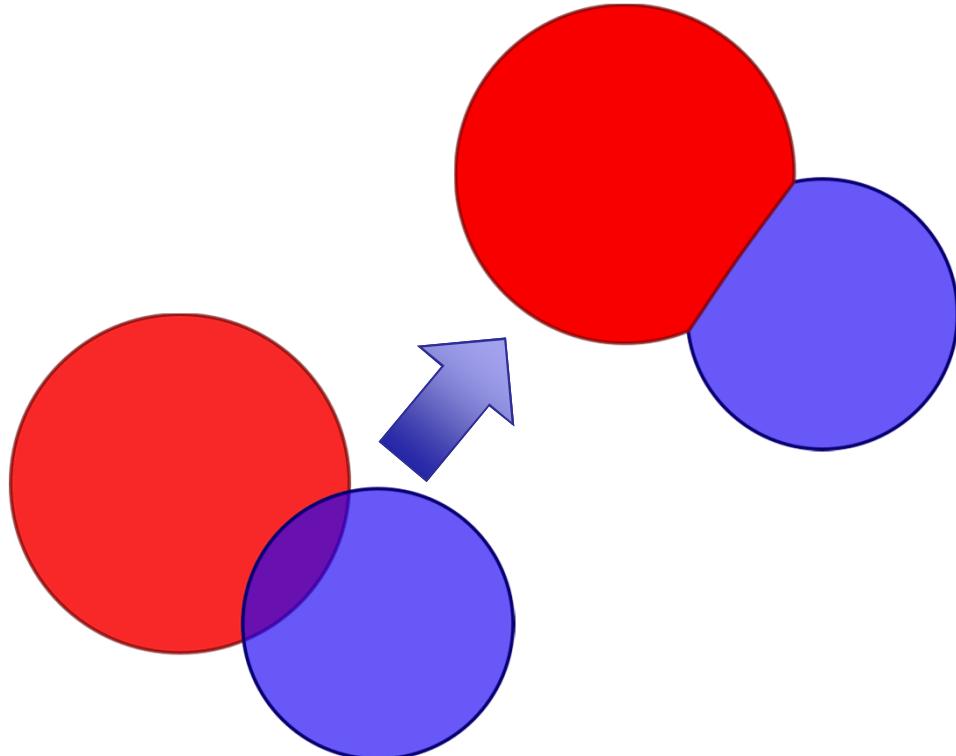
Network model development

- Primary goal: Develop a computational tool to study capacity fade caused by degradation of the percolated network
 - Coupled electrochemistry, thermal transport, and mechanical deformation
 - Realistic network structure through 3D reconstruction
 - Validation through experimental discovery
 - Understanding of reliability and margin through computational exploration
- In this work:
 - 3D reconstructions of electrode microstructure
 - Mathematical models of relevant physics
 - Computational algorithms enabling mesoscale simulations
 - Demonstrations of computational capability and preliminary analysis



3D microstructure: Simple distribution

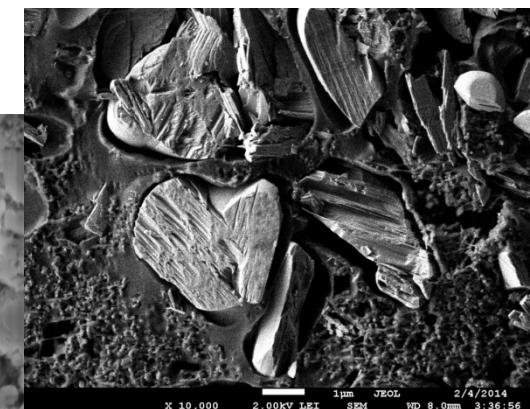
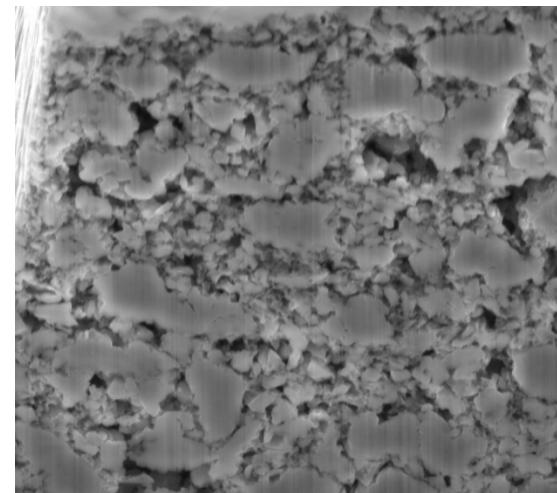
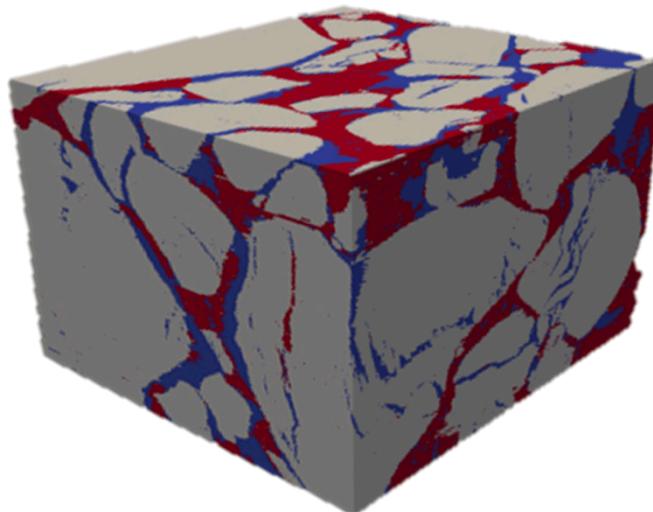
- Easy method: Spherical particle pack from known particle size distribution
 - Create a dilute representation of deformable particles in liquid – LAMMPS
 - “Dry” the coating using a discrete element simulation, evaporating the solvent
 - Draw spherical particles using Cubit primitives
 - Resolve overlaps by cutting intersection midplane



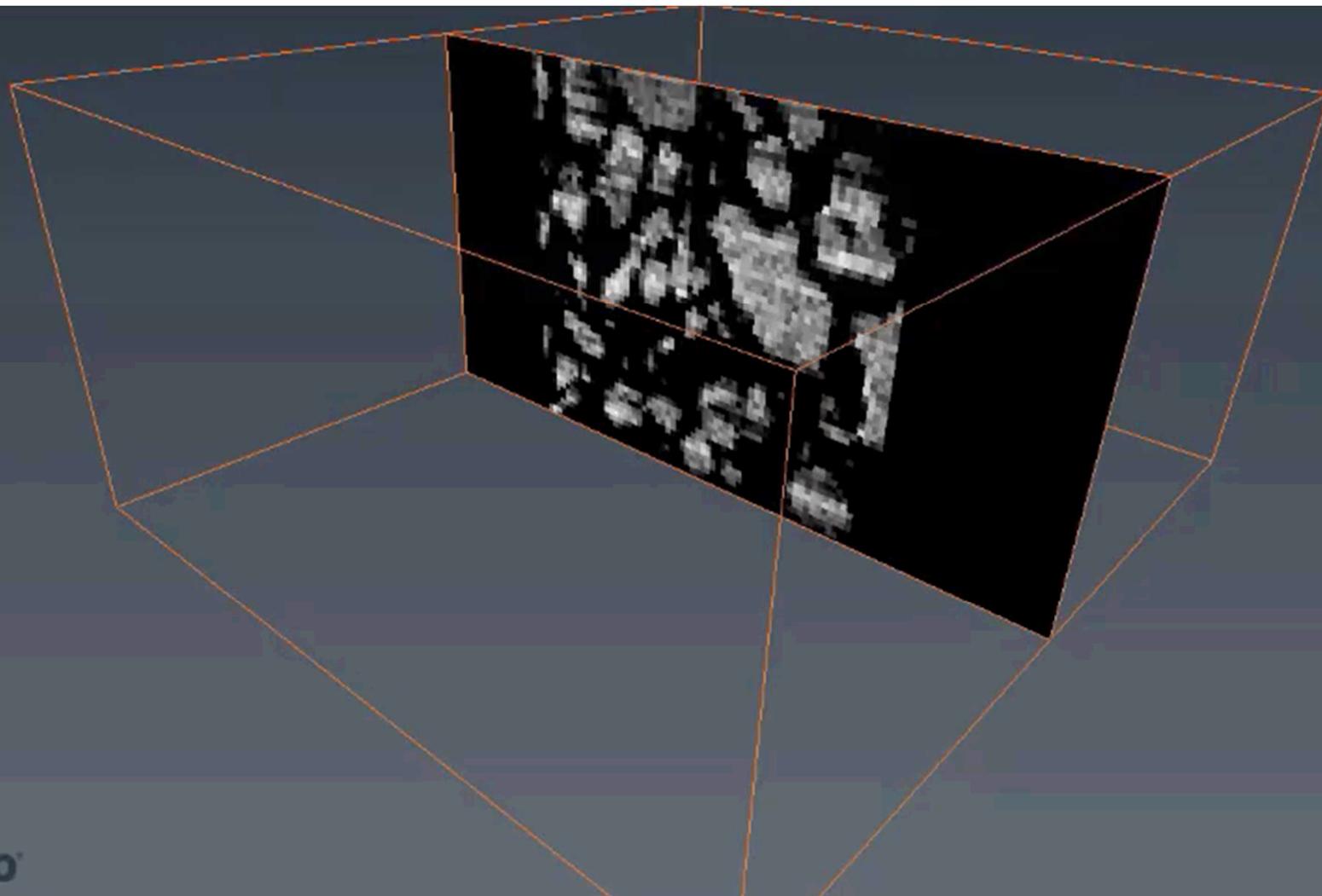
NMC 111 cathode material

3D microstructure: Experimental

- Experimentally based: Reconstruction from FIB/SEM imaging
 - SEM images provided by Hutzelaub *et al* (2012)
 - 3D reconstruction from 2D images using FEI Avizo
 - Create surface mesh of the particles
 - Currently only using particles; future work will include binder in simulations



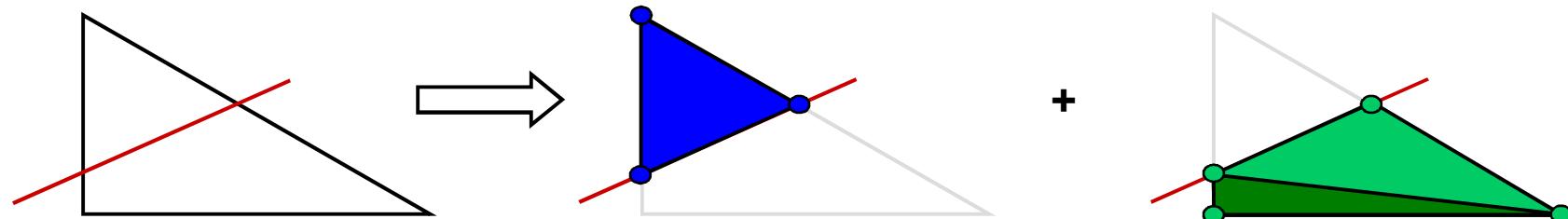
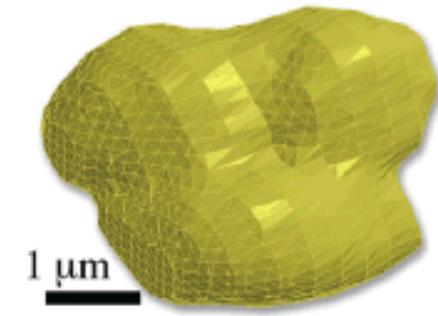
3D microstructure: Experimental



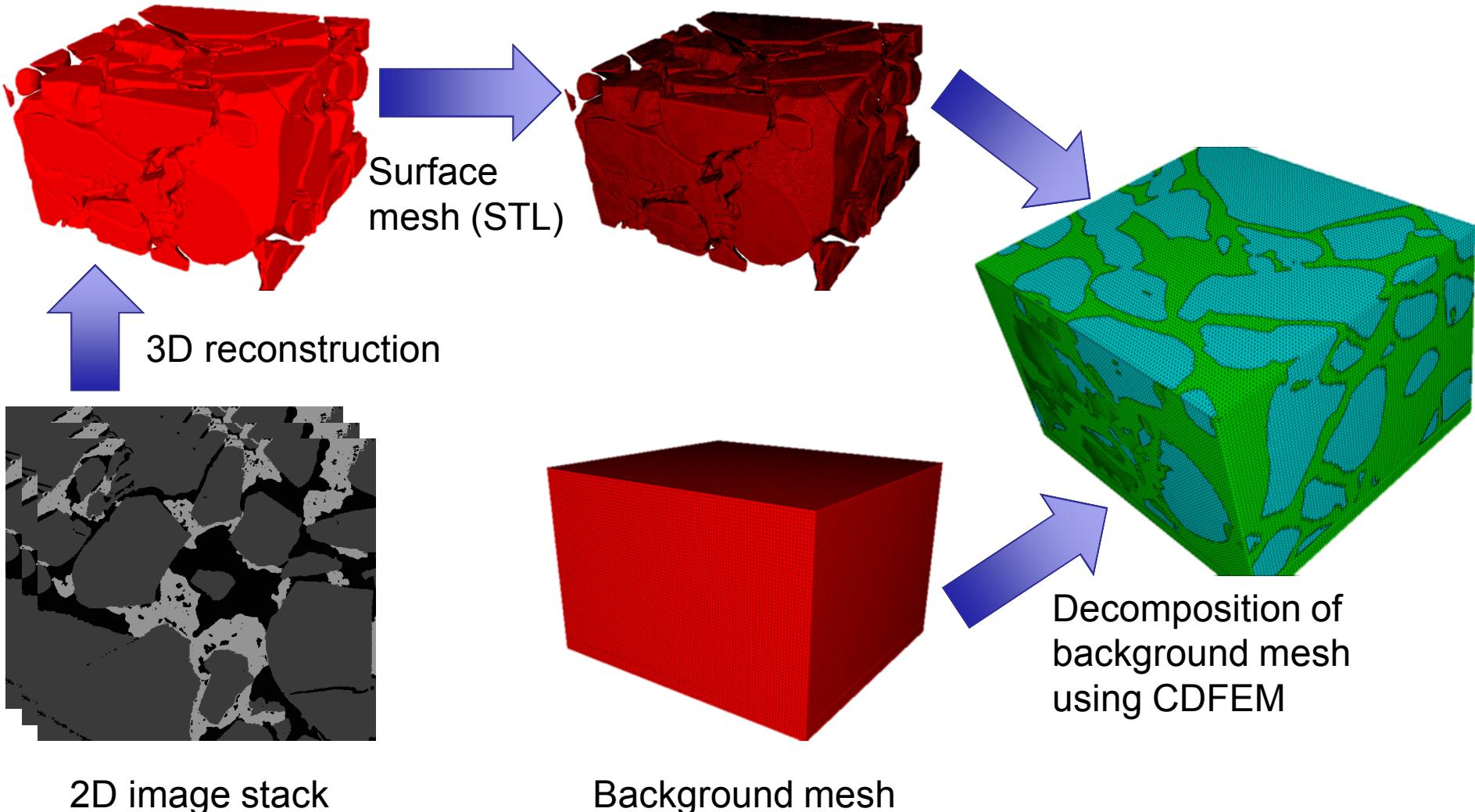
Avizo

Computational approach: CDFEM

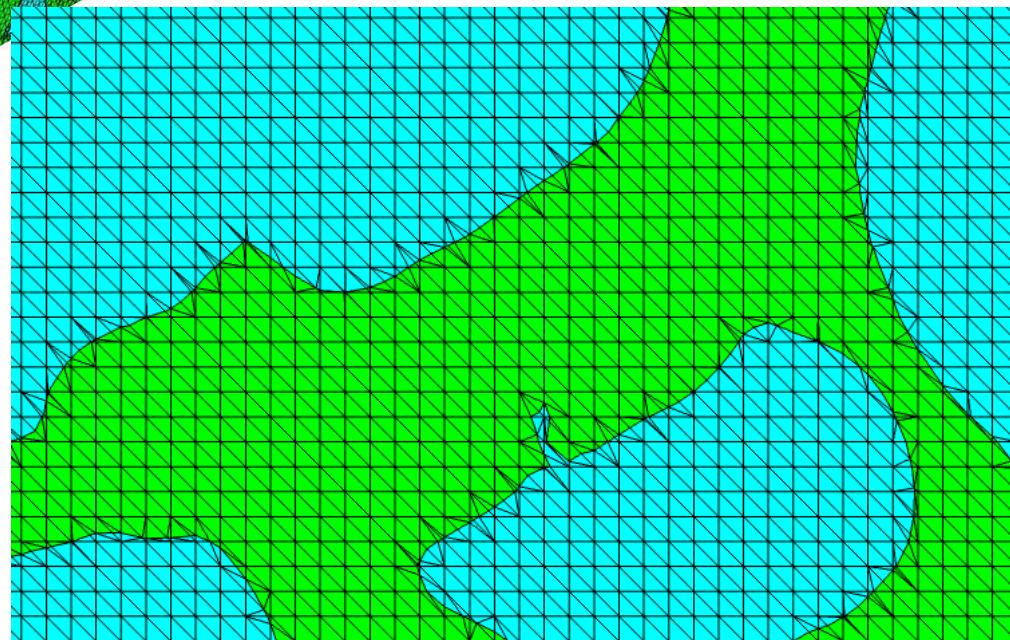
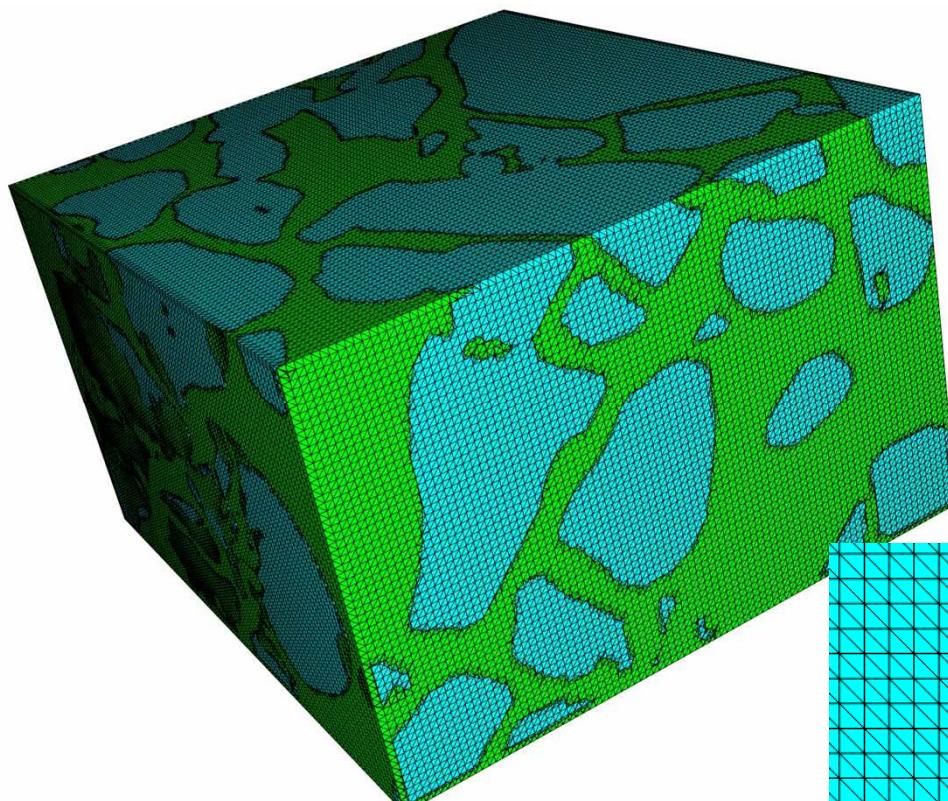
- Sierra/Aria (Sandia's Multiphysics Finite Element Method code)
 - Allows segregated or monolithic solves
- Meshing complex microstructure very difficult
 - Conformal mesh required for interface/surface physics
- Conformal Decomposition Finite Element Method (CDFEM)
 - Begins with a regular or arbitrary background mesh
 - Decomposes mesh along interfaces (STL microstructure description)
 - Additional features:
 - Adaptive mesh refinement for detailed interface representation
 - Support for multiple phases (required for binder)
 - Arbitration of overlapping bodies
 - Guaranteed mesh quality (coming soon!)



Representation of microstructure



Representation of microstructure



In the particle

- Ohm's Law

$$\underline{\nabla} \cdot (\sigma \underline{\nabla} \phi_s) = 0$$

- Intercalated Li conservation

$$\frac{\partial C_{\text{Li}}}{\partial t} + \underline{\nabla} \cdot (-D_{\text{Li}} \underline{\nabla} C_{\text{Li}}) = 0$$

At the interface

- Butler-Volmer reaction rate

$$\underline{J} \cdot \underline{n} = j_0 \left[\exp \left(\frac{\alpha_a F (\phi_s - \phi_l - \phi_{\text{eq}})}{RT} \right) - \exp \left(\frac{-\alpha_c F (\phi_s - \phi_l - \phi_{\text{eq}})}{RT} \right) \right]$$

- Plus, a few other boundary conditions

In the electrolyte

- Current conservation

$$\underline{\nabla} \cdot \left[F \left(\underline{J}_{\text{Li}^+} - \underline{J}_{\text{PF}_6^-} \right) \right] = 0$$

- Nernst-Planck fluxes

$$\underline{J}_i = -D_i \left(z_i C_i \frac{F}{RT} \underline{\nabla} \phi_l + \underline{\nabla} C_i \right)$$

- Li⁺ conservation

$$\frac{\partial C_{\text{Li}^+}}{\partial t} + \underline{\nabla} \cdot \underline{J}_{\text{Li}^+} = 0$$

- Electroneutrality

$$C_{\text{PF}_6^-} = C_{\text{Li}^+}$$

Physics models: Mechanics

- Intercalation-induced swelling causes a volumetric strain

$$\begin{aligned}\underline{\underline{E}} &= \underline{\underline{E}}_{\text{elastic}} + \underline{\underline{E}}_{\text{swelling}} \\ &= \underline{\underline{E}}_{\text{elastic}} + \underline{\underline{\alpha}} \Delta C_{\text{Li}}\end{aligned}$$

- For a linear elastic constitutive behavior, swelling is converted to stress
 - Similar to standard “coefficient of thermal expansion” approach

$$\begin{aligned}\underline{\underline{\sigma}} &= \underline{\underline{\underline{C}}} : \underline{\underline{E}}_{\text{elastic}} \\ &= \underline{\underline{\underline{C}}} : \underline{\underline{E}} - \underline{\underline{\underline{C}}} : \underline{\underline{\alpha}} \Delta C_{\text{Li}} \\ &= \underline{\underline{\underline{C}}} : \underline{\underline{E}} - \underline{\underline{\beta}} \Delta C_{\text{Li}}\end{aligned}$$

- Generally, volumetric strain is isotropic

$$\underline{\underline{\beta}} = \underline{\underline{\beta}} \underline{\underline{\delta}}$$

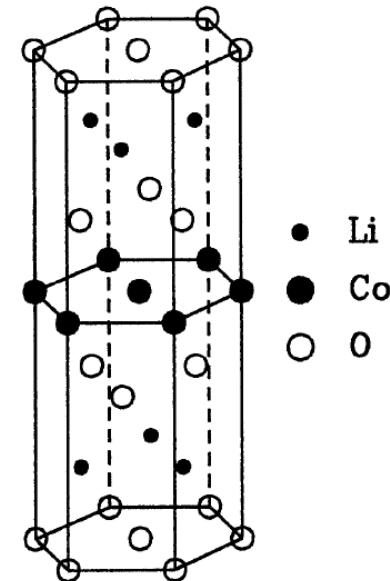
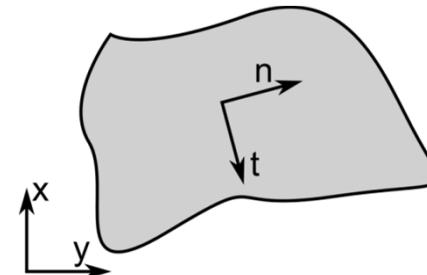
- Stress governed by quasi-static momentum conservation

$$\nabla \cdot \underline{\underline{\sigma}} + \underline{\underline{F}} = \underline{\underline{0}} \quad \rightarrow \quad \underline{\underline{E}}_{\text{elastic}} = \underline{\underline{E}} - \underline{\underline{E}}_{\text{swelling}}$$

Physical models: Anisotropic swelling

- Anisotropic expansion of the crystal lattice on lithiation
 - Transversely Isotropic – crystal plane tangent vs. normal
- Tensorial form for β
 - Define β in directions normal and tangential to crystal plane

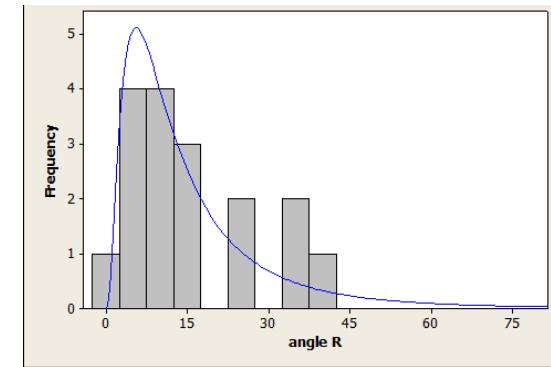
$$\hat{\underline{\underline{\beta}}} = \begin{bmatrix} \beta_n & 0 & 0 \\ 0 & \beta_t & 0 \\ 0 & 0 & \beta_t \end{bmatrix}$$



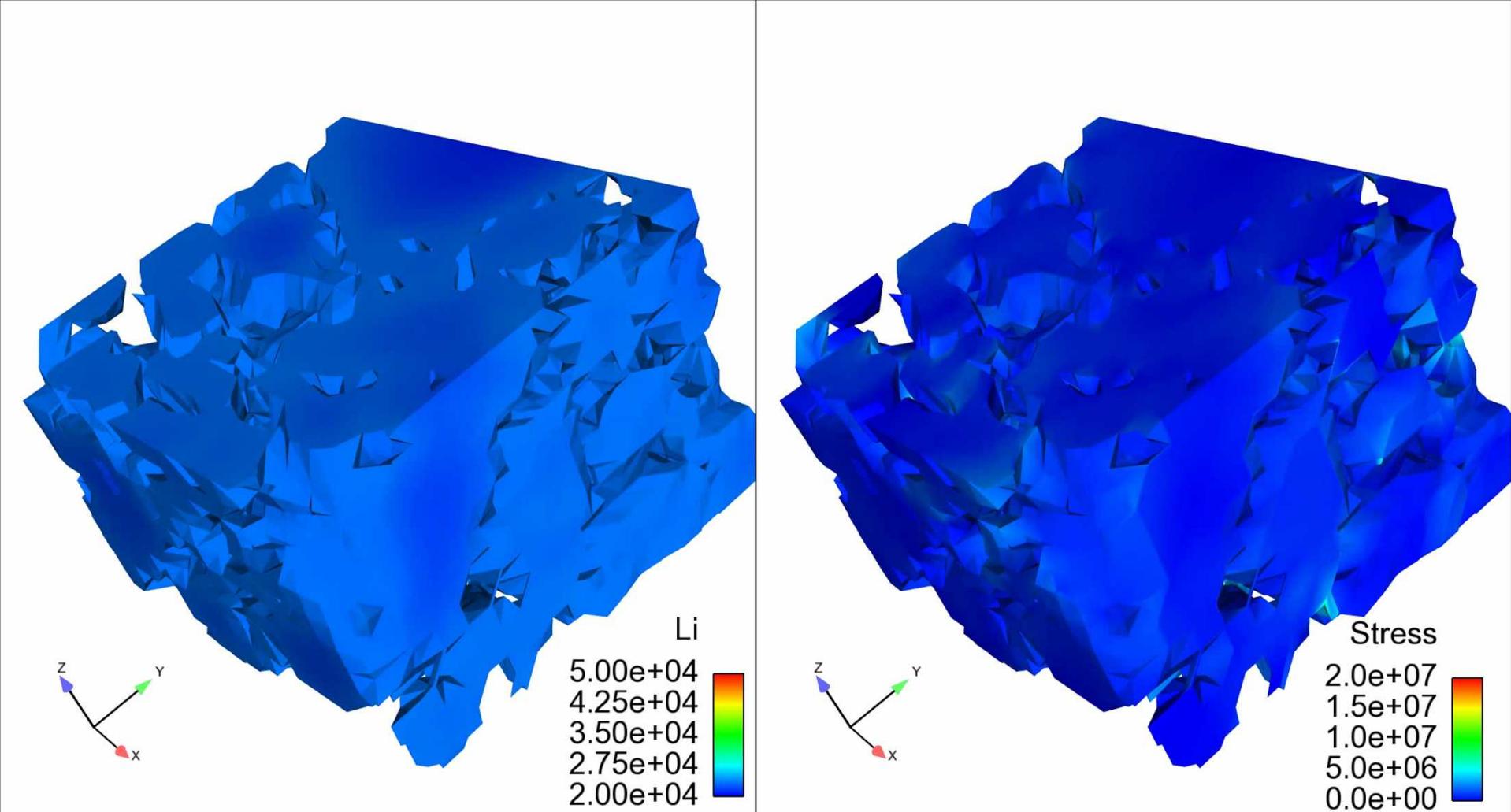
- Rotate into the crystal plane orientation of the particle

$$\underline{\underline{\beta}} = \underline{\underline{R}} \cdot \hat{\underline{\underline{\beta}}} \cdot \underline{\underline{R}}^T$$

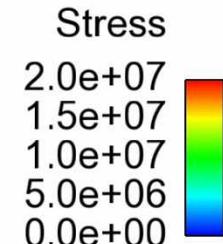
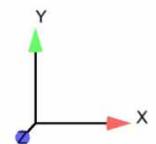
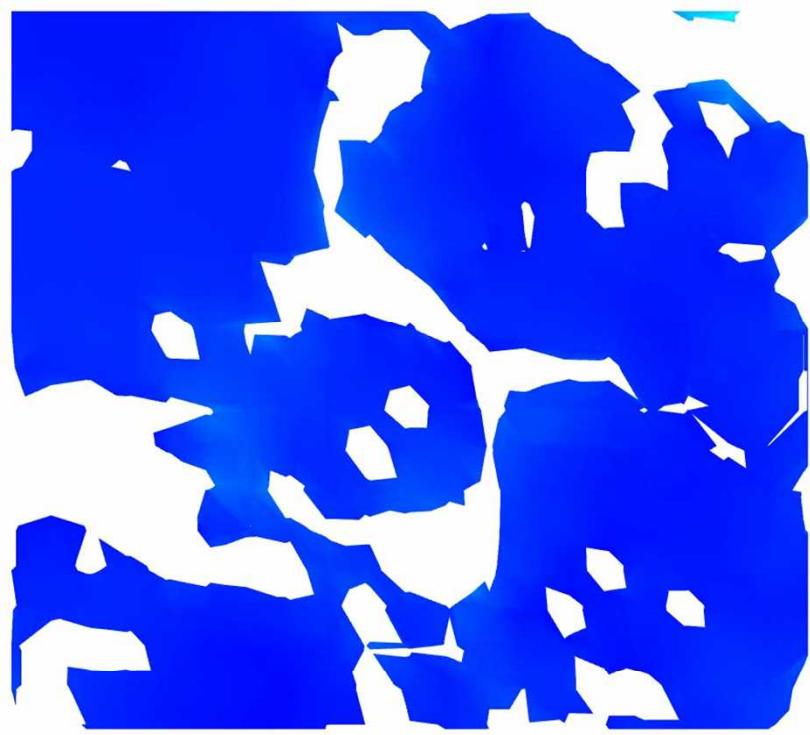
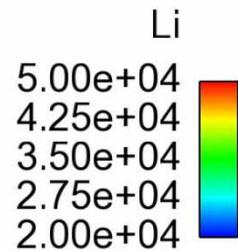
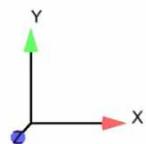
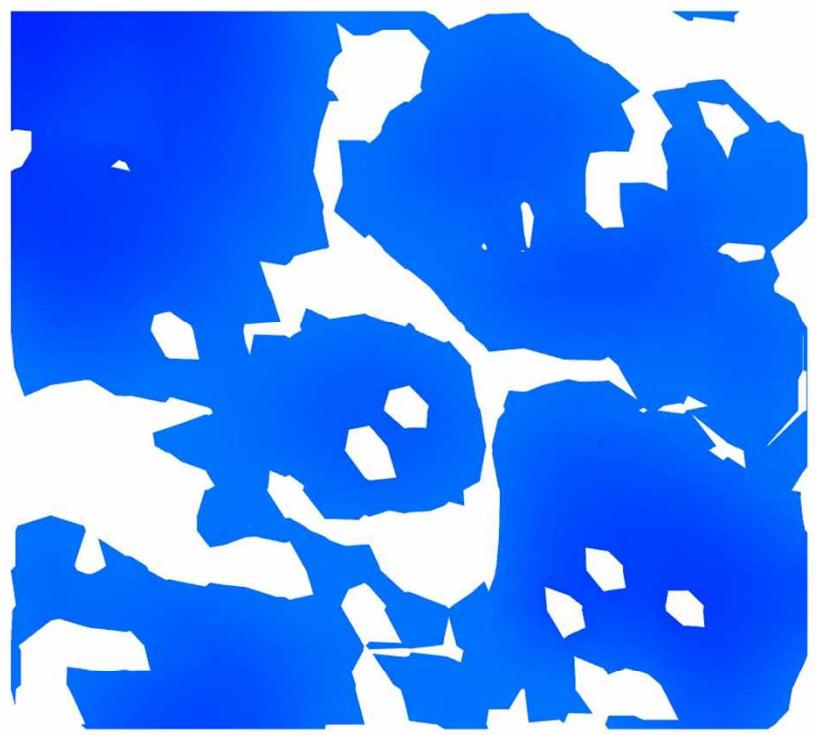
- How to initialize particle orientation?
 - Stochastically (current work)
 - Based on measurements



Results: Isotropic stress, 3D reconstruction

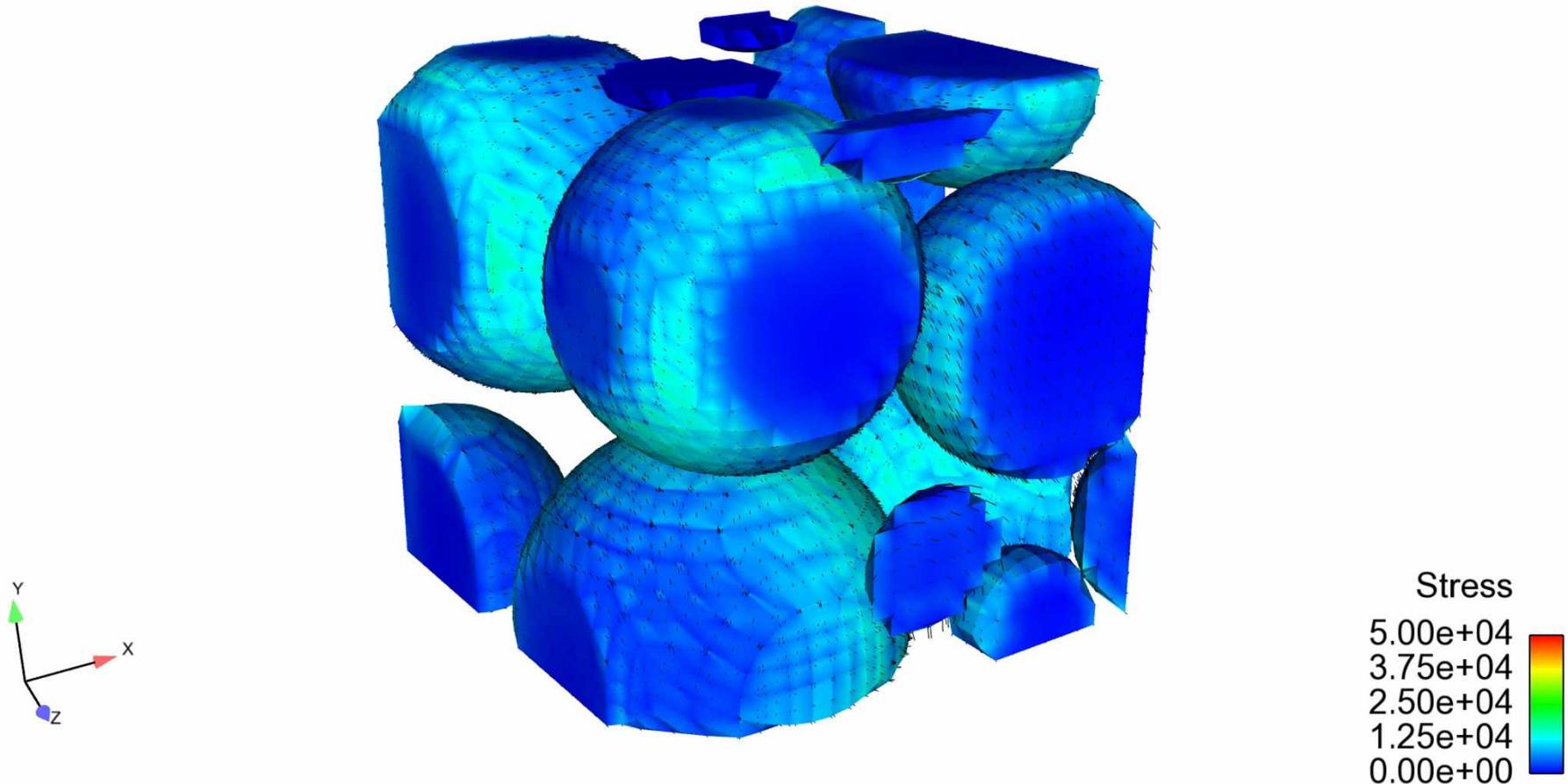


Results: Isotropic stress, 3D reconstruction



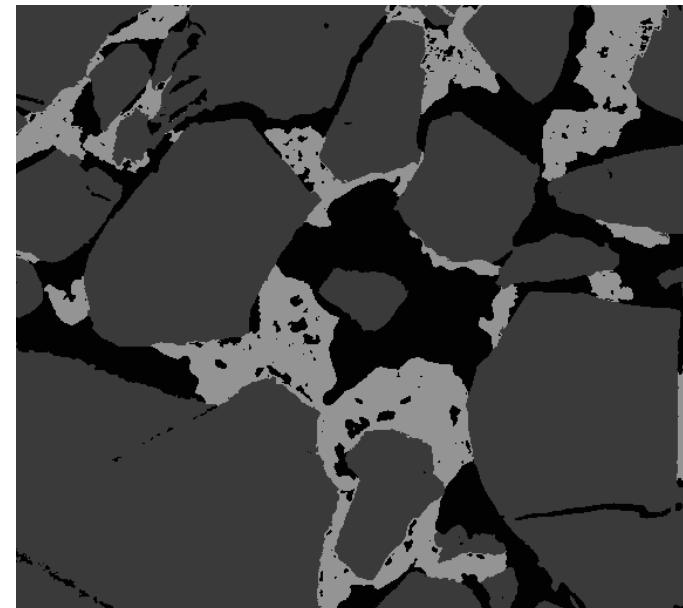
Stress concentrations highest in regions with fine features and sharp corners

Time = 0.464000



The mysteriously invisible binder - PVDF

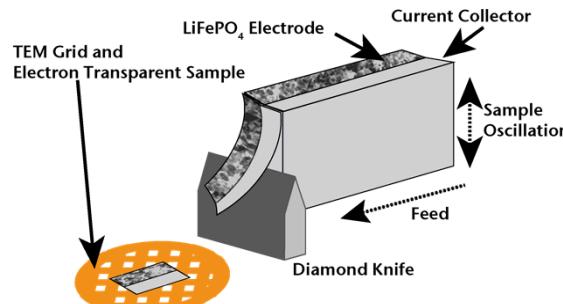
- Polyvinylidene Fluoride (PVDF) - Standard binder
 - Used because it is stable at electrochemical potentials of lithium ion battery
 - Generally neglected
 - NOT ionically conductive
 - NOT electrically conductive
 - Maintains cohesion of composite electrode
- Literature suggests that **mechanical contact between particles is mediated by binder** (not hard contact)
 - Characterize binder mechanics, swelling in contact with electrolyte and ionic conductivity
 - In situ imaging of binder in swollen state
 - Ex situ imaging for high resolution imaging to track rearrangements using SEM
- Determine appropriate constitutive model for binder and resultant impact on **network rearrangements, porosity evolution and ionic transport**
 - Initial guess is low modulus 'compliant' elastic material due to separation of time scales



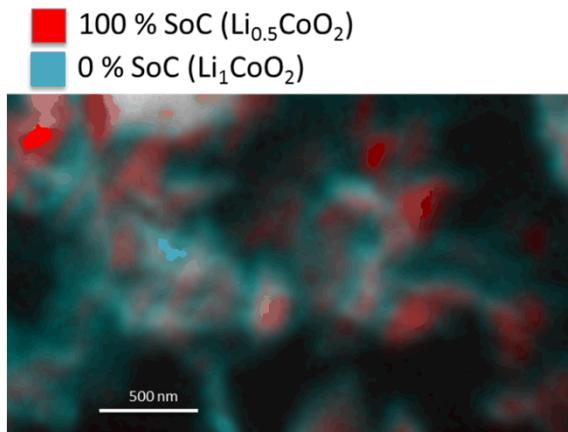
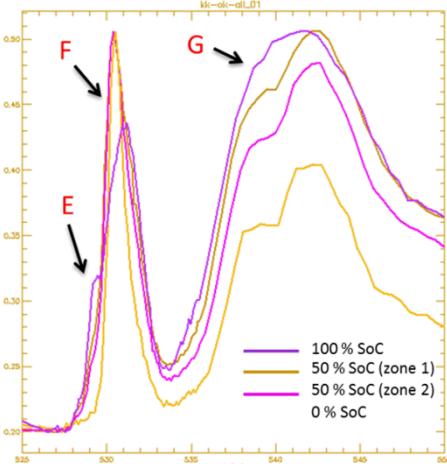
Cathode: LiCoO_2 Binder Void

Lithiation progression – localized state of charge

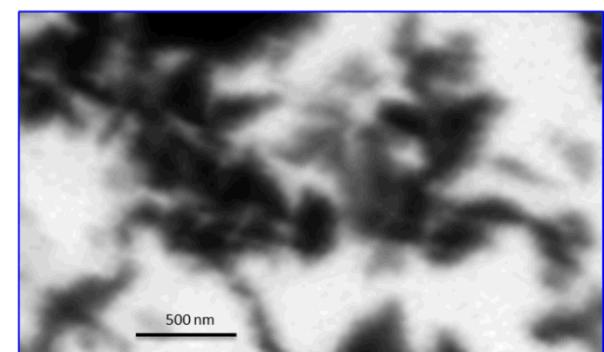
- Ultramicrotoming creates thin slices while preserving microstructure
 - Sections as thin as 100 nm



- Scanning Transmission X-ray Microscopy (STXM) at the Advanced Light Source
 - Produces localized maps of chemical spectra that identify chemical makeup



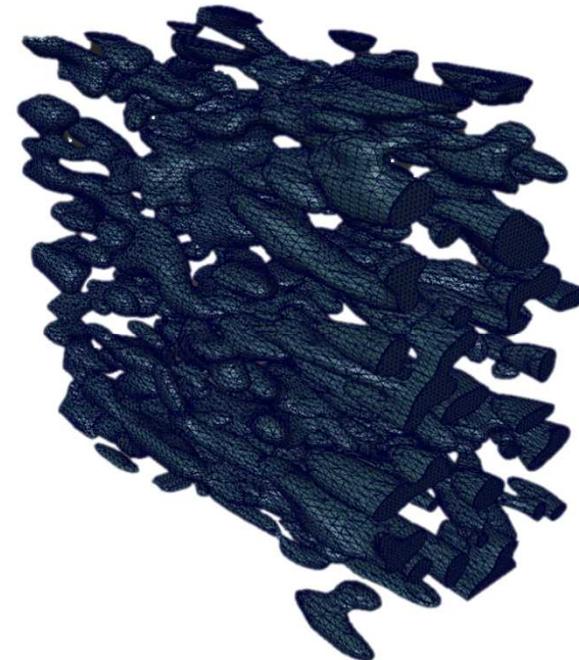
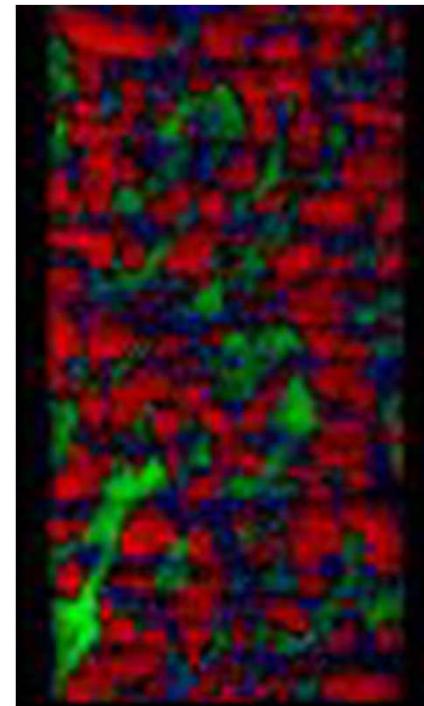
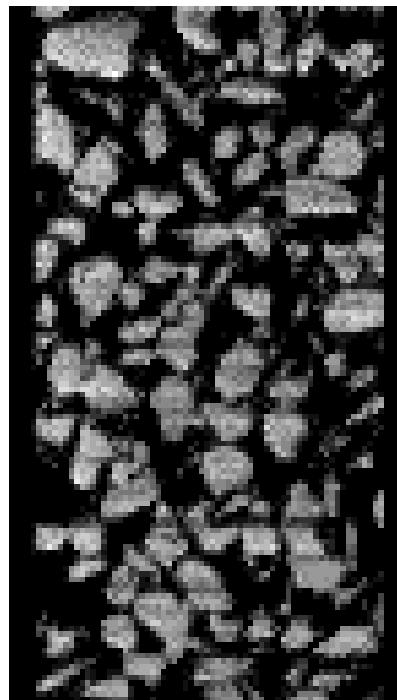
STXM chemical map
(103-energy fit)



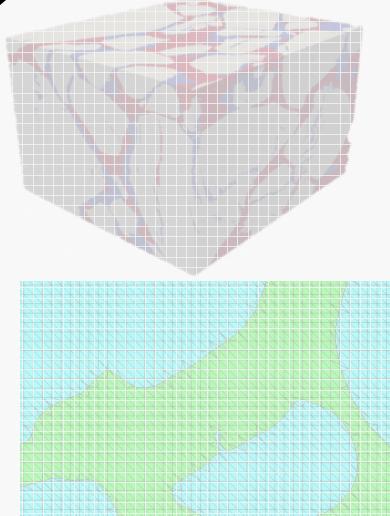
STXM Topography

3D microstructure: Experimental

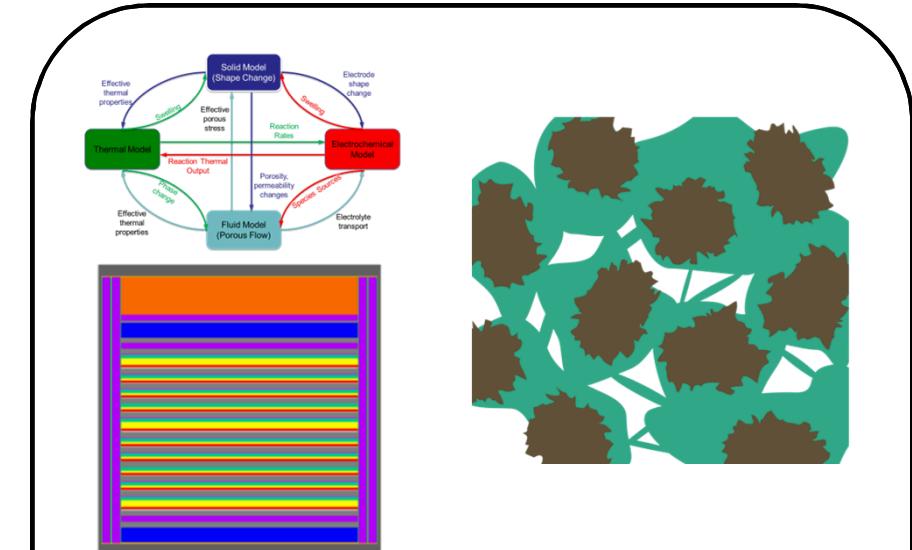
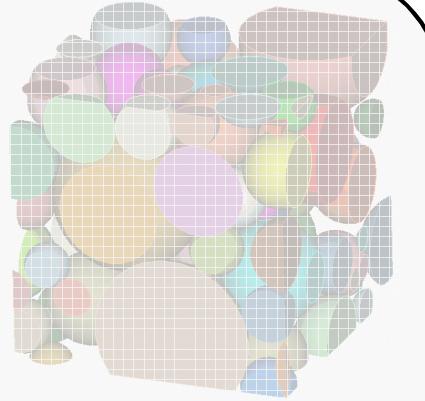
- Current experimental program to generate our own FIB/SEM images
 - Image at various states of charge/discharge, multiple cycles
 - Use for simulation initial conditions and for validation
 - Energy-dispersive X-ray spectroscopy (EDS) used to identify components



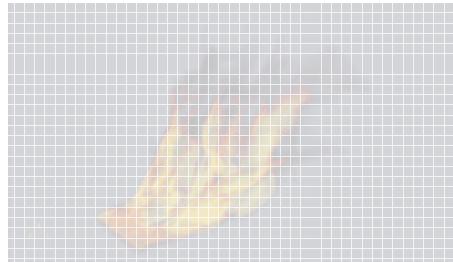
Outline



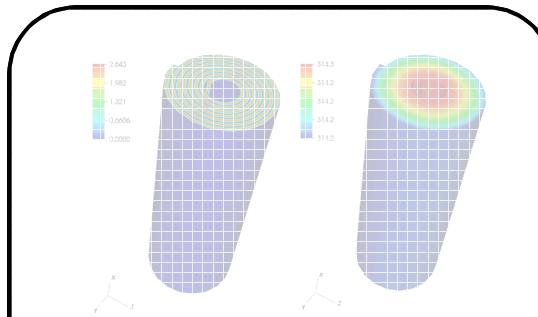
Lithium-Ion battery mesoscale degradation simulations



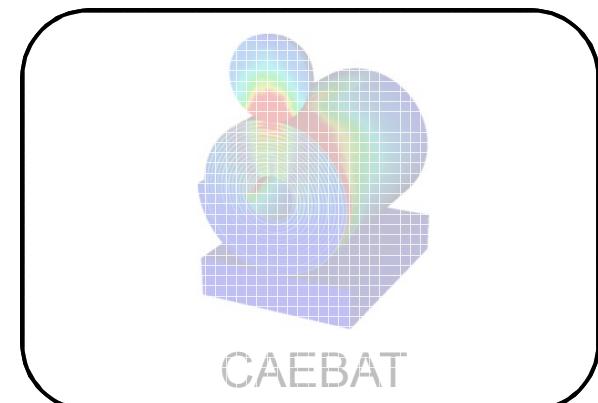
Performance models of molten salt batteries



Grid storage



Alkaline batteries



CAEBAT

TOWARDS A COUPLED MULTI-PHYSICS MODEL OF MOLTEN SALT BATTERY PERFORMANCE

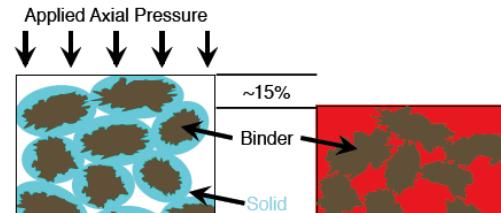
Scott A. Roberts, Christine C. Roberts, Anne M. Grillet, Kevin N. Long, Jonathan R. Clausen, Mario J. Martinez, Harry K. Moffat, John C. Hewson, Victor E. Brunini, Lindsay C. Erickson, Tyler Voskuilen

Proceedings of the 46th Power Sources Conference (2014)
Towards a Coupled Multiphysics Model of Molten Salt Battery Mechanics

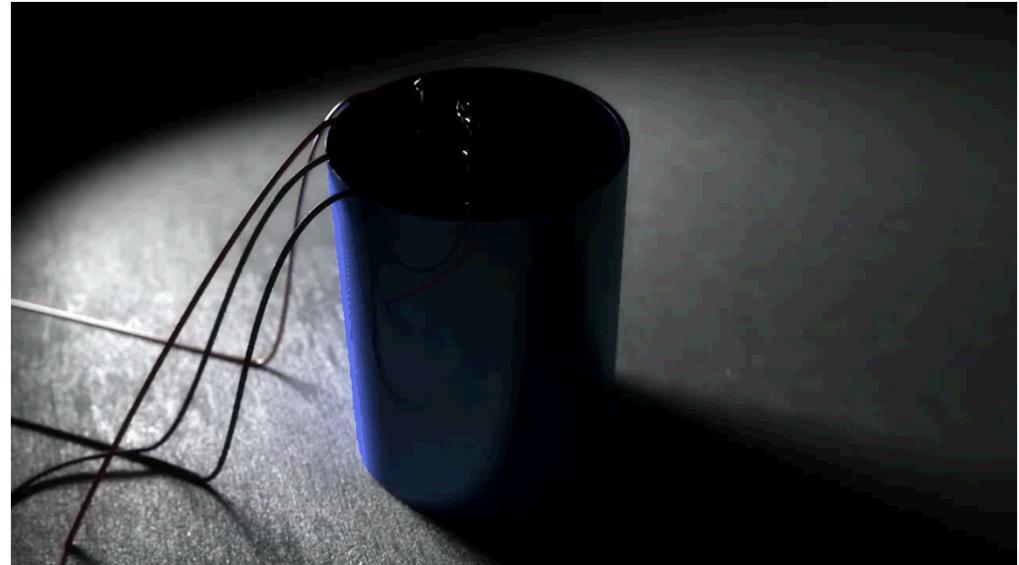
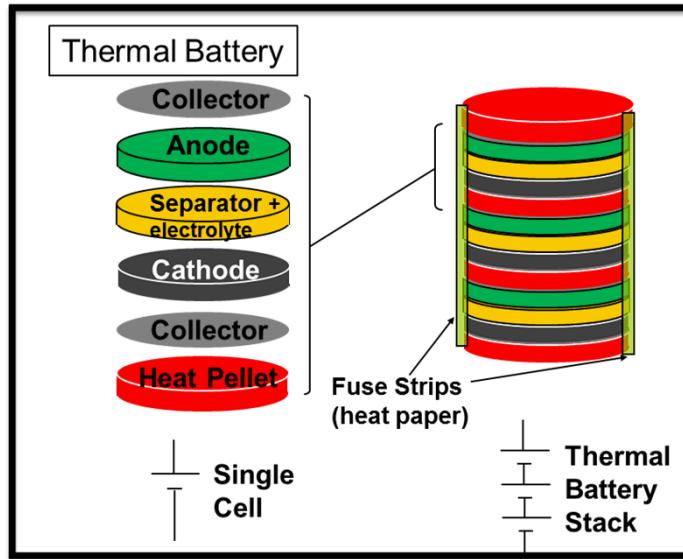
*Scott A. Roberts, Kevin N. Long, Jonathan R. Clausen, Mario J. Martinez,
Edward S. Piekos, and Anne M. Grillet*

Sandia National Laboratories
P.O. Box 5800, MS-0836, Albuquerque, NM 87185-0836

Abstract: When molten salt batteries activate, a number of mechanical processes take place over a very short time span. First, electrolyte that is originally located in the separator wicks into the porous anode and cathode materials under capillary forces, enabling the electrochemical activation of the battery. Second, typically the stack axially compresses by 10 to 20 percent due to the melting of the electrolyte and rearrangement of the solid network, also leading to additional



What is a molten salt battery, and why?



Requirements

- Thermal management: Rise time, life time, avoid thermal decomposition
- Electrochemical: Steady voltage through variable current loads
- Mechanical: Stable performance under environments

Physical mechanisms in molten salt battery activation

- Battery activation is a complicated, multi-step process

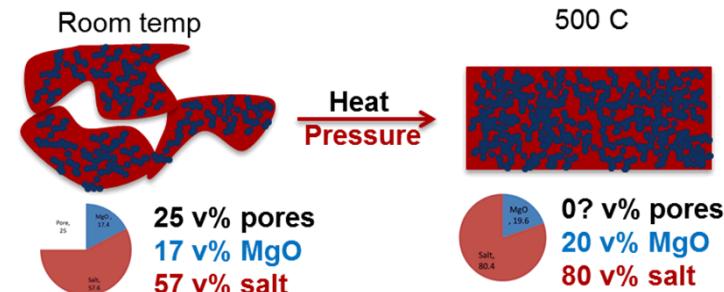
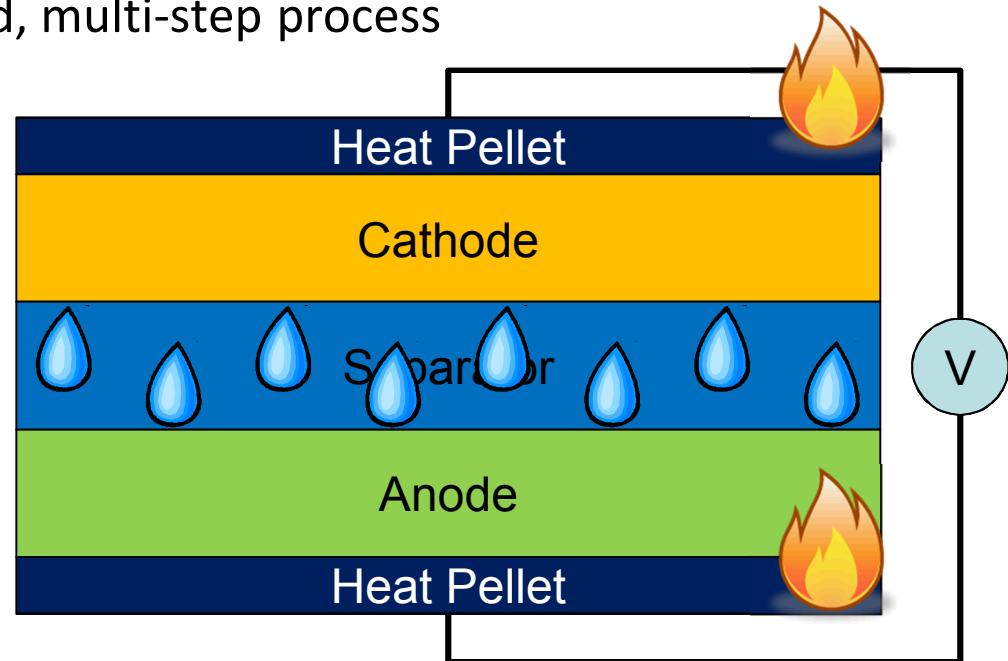
- Heat pellet burning
- Thermal diffusion
- Melting of the electrolyte
- Deformation of the separator
- Flow of the electrolyte
- Activation

- A true multi-physics problem

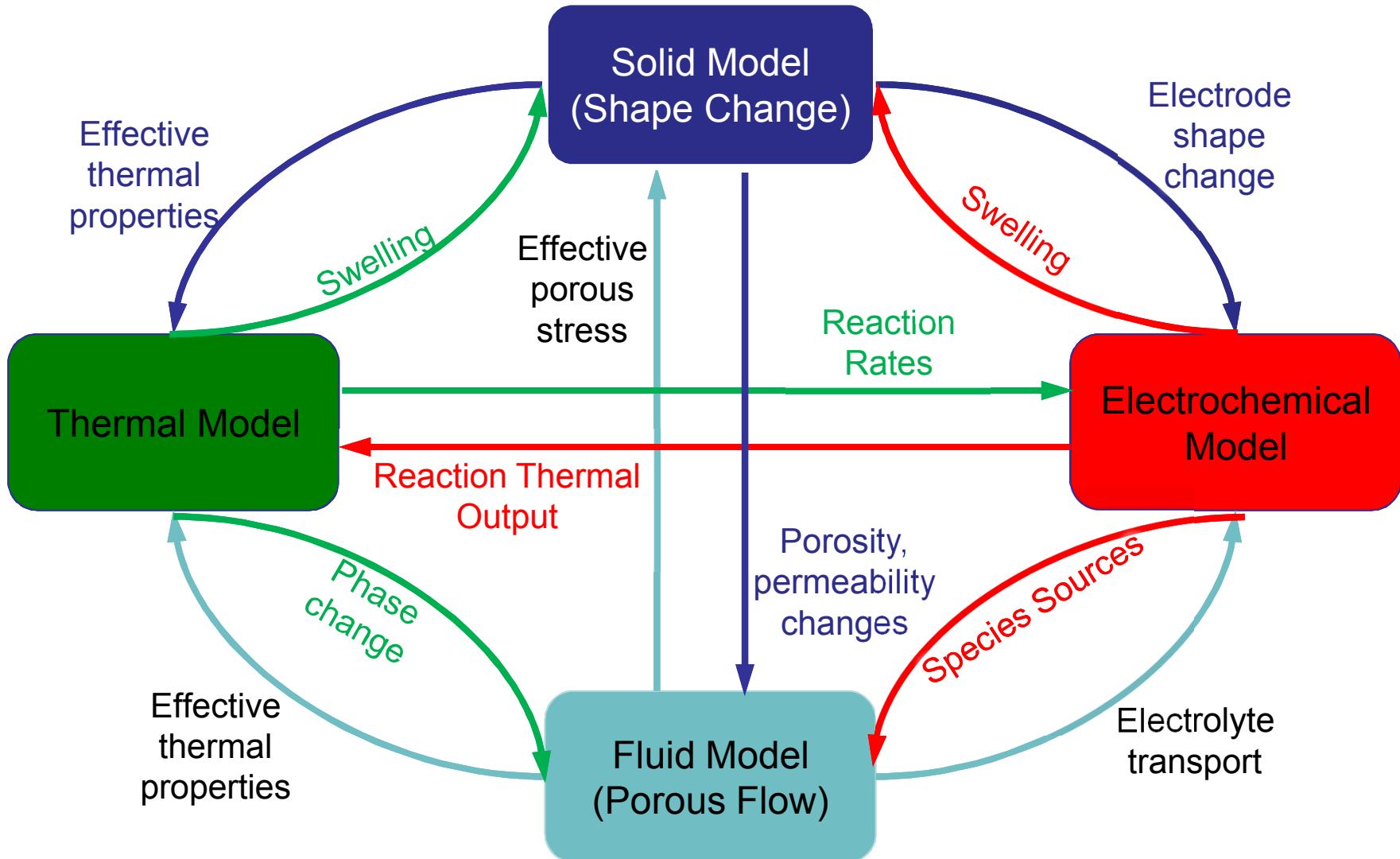
- Thermal
- Mechanical
- Fluid
- Electrochemical

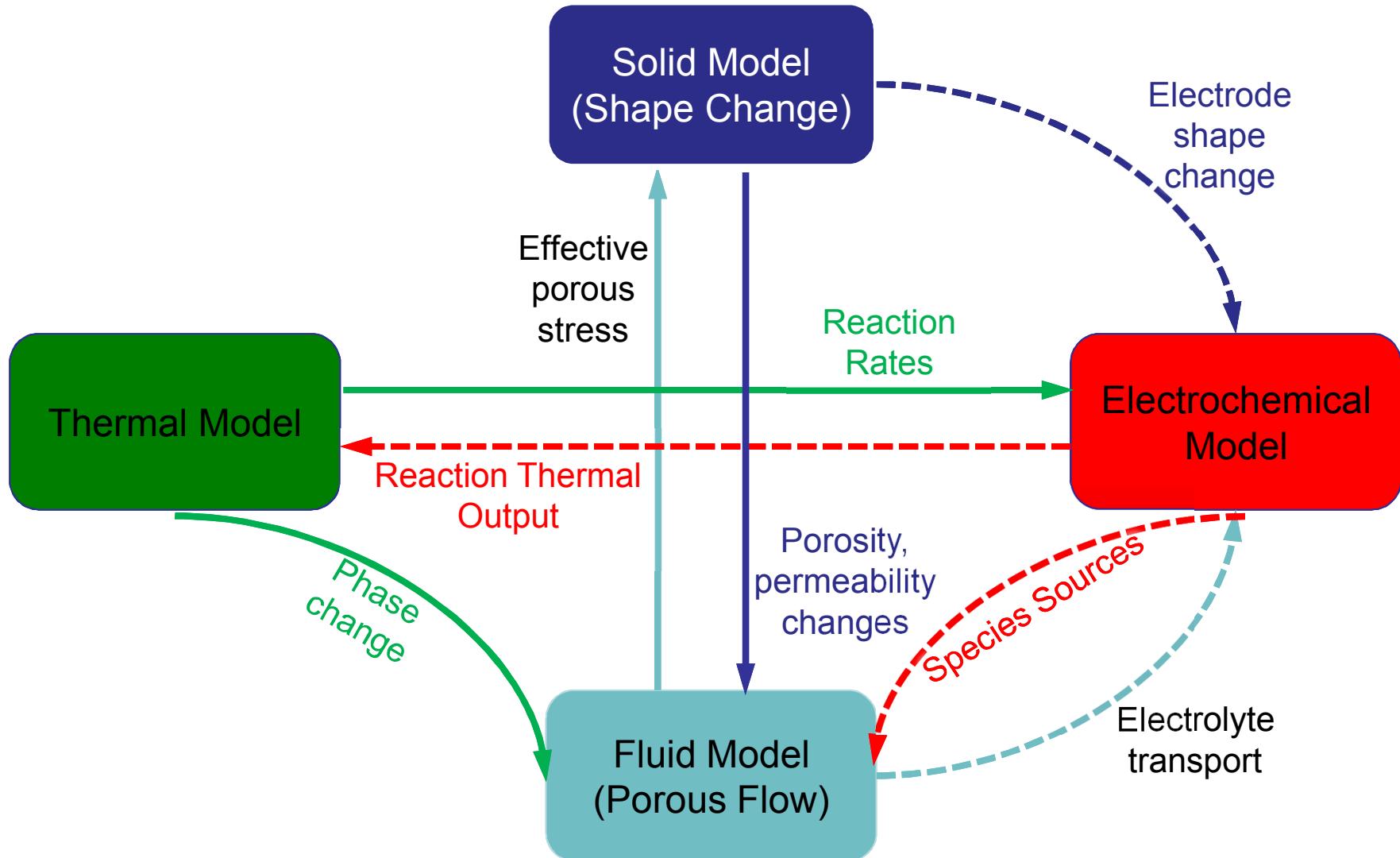
- Why performance models of thermal batteries?

- Predict activation times, electrochemical performance
- Optimize volume, insulation, manufacturing



Physical models and couplings



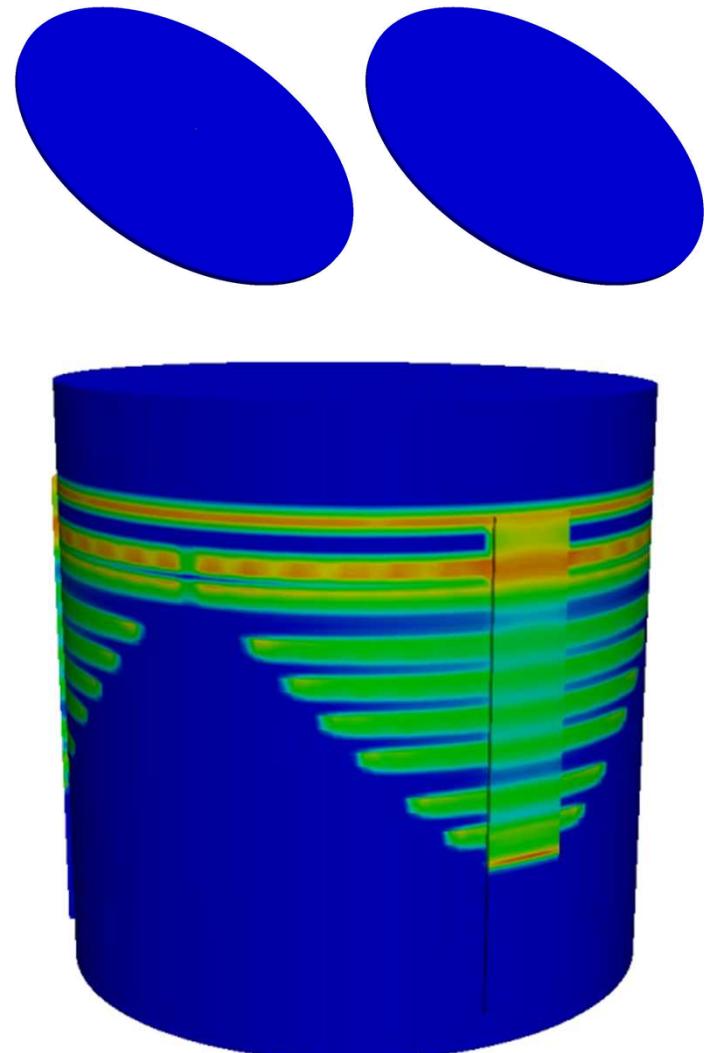


Models: Thermal transport

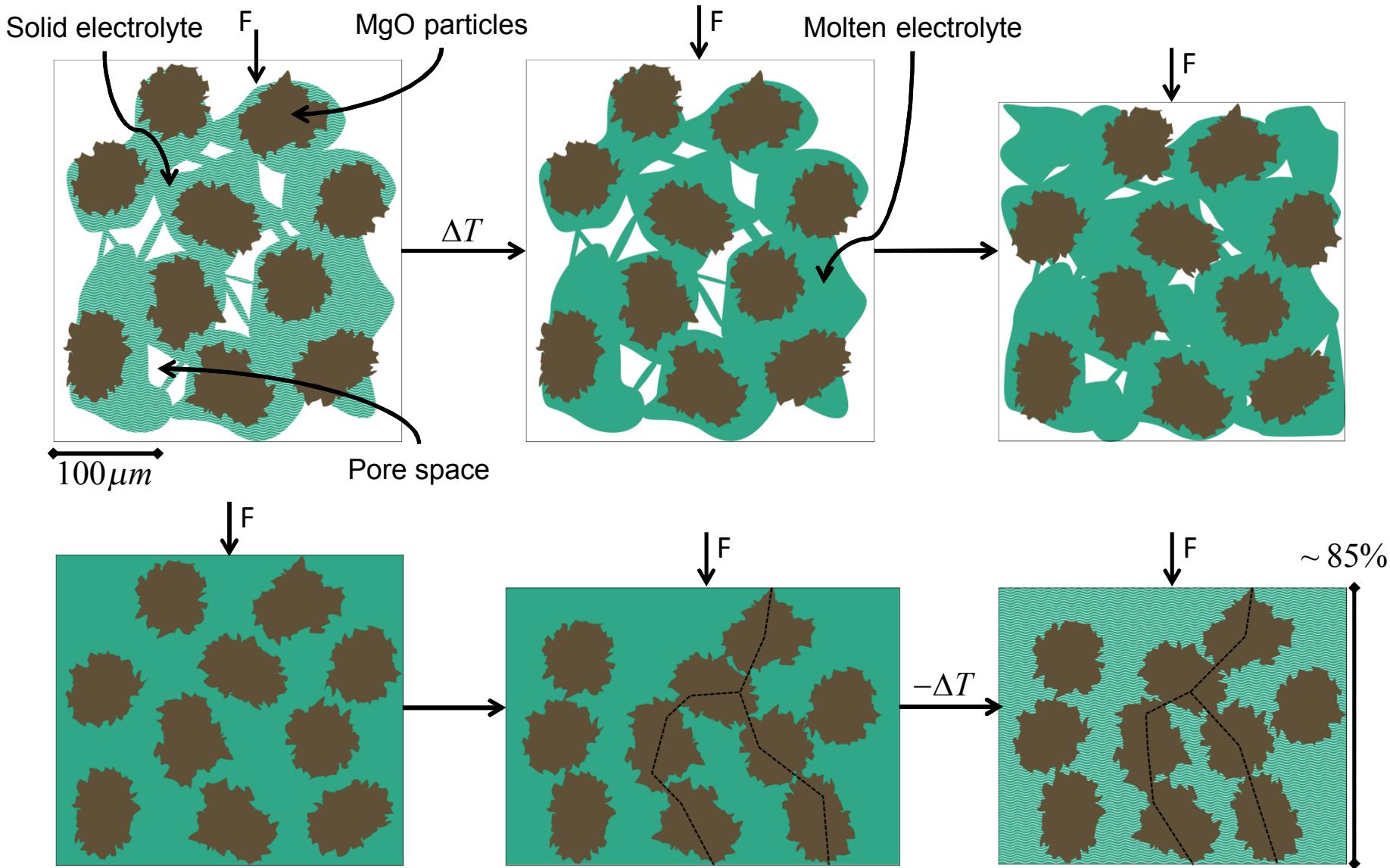
- Based on standard heat conduction model

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T + Q$$

- Source term Q applies to heat pellet, paper
- Enhanced activation model
 - Based on the level-set method, with known propagation speed of the burn front through paper and heat pellets
 - Allows differentiation of temperatures and rise times across the diameter of pellets and through battery height



Separator pellet activation process



Models: Mechanical deformation

- Custom constitutive model for separator
 - Capture the inelastic volumetric and isochoric deformation of the MgO skeleton before, during, and after activation
 - Isotropic, thermal-elastic-plasticity
 - Plasticity governs activation deformation
 - Kinematic split of deformations

$$\underline{\mathbf{F}} = \underline{\mathbf{F}}^e \underline{\mathbf{F}}^p \underline{\mathbf{F}}^T$$

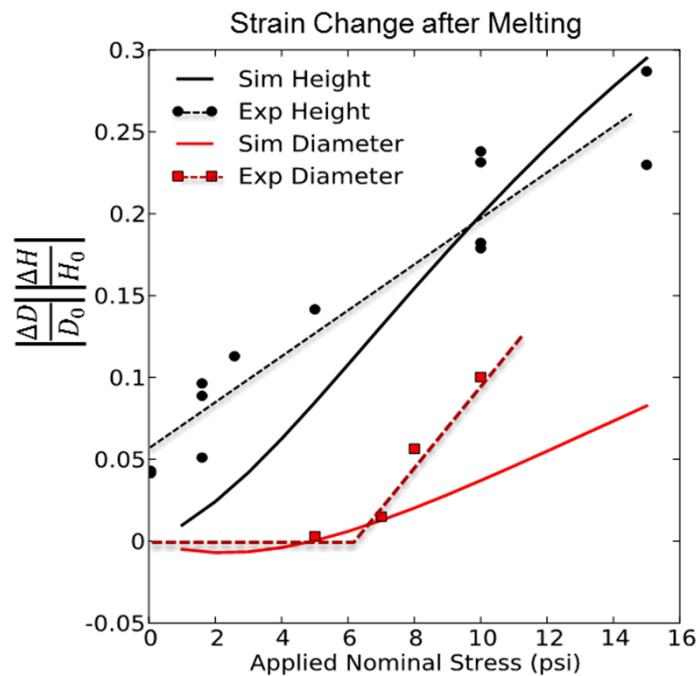
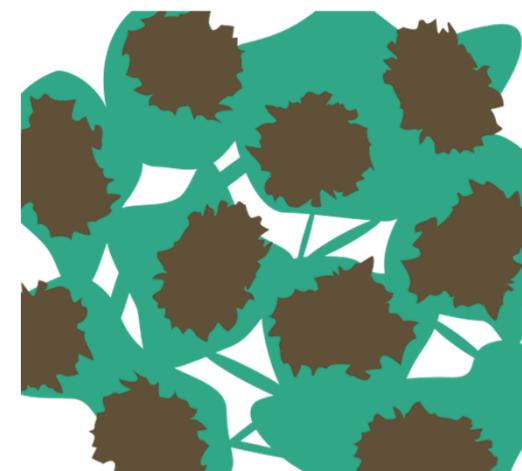
- Rule of mixtures for phase decomposition

$$\chi = \frac{T - (T - T_w/2)}{T_w}$$

- Stress tensor:

$$\underline{\underline{\tau}} = \mu_x(T) \text{dev}(\underline{b}^3) + \frac{\kappa_x(T)}{2} (J_e^2 - 1) \underline{\underline{\delta}}$$

- Conservation of momentum with porous effective stress: $\nabla \cdot (\hat{\underline{\underline{\sigma}}} - \underline{\underline{p}} \underline{\underline{\delta}}) = 0$



Models: Porous flow

- Electrolyte and gas form two immiscible phases upon melting

$$\frac{\partial(\rho_w \phi S_w)}{\partial t} = \nabla \cdot \left(\rho_w \frac{k_{rw}}{\mu_w} \underline{\underline{K}} \cdot (\nabla p_w - \rho_w \underline{g}) \right) + Q_w$$

$$\frac{\partial(\rho_n \phi S_n)}{\partial t} = \nabla \cdot \left(\rho_n \frac{k_{rn}}{\mu_n} \underline{\underline{K}} \cdot (\nabla p_n - \rho_n \underline{g}) \right) + Q_n$$

- Saturation and capillary pressure related to DOFs (wetting and non-wetting pressures) through model relations

$$S = S(p_c); \quad p_c = p_n - p_w$$

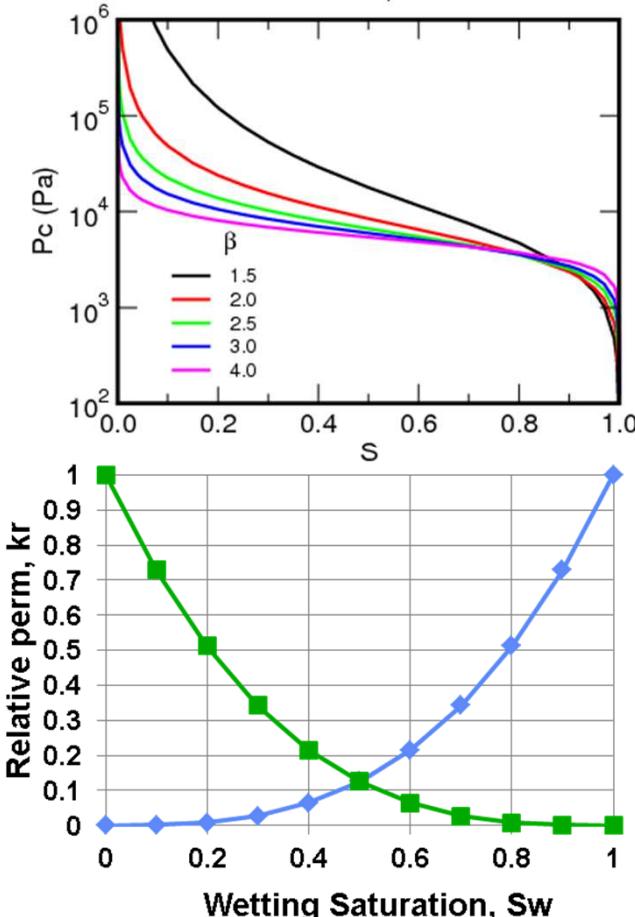
- Coupling to other physics important!

- Required:

$$\phi = \phi(\underline{d}); \quad \mu_i = \mu_i(T)$$

- Optional?:

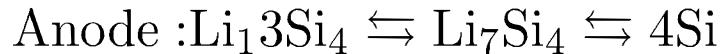
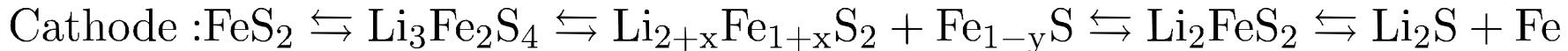
$$S_i = S_i(p_c, \underline{d}); \quad \underline{\underline{K}} = \underline{\underline{K}}(\underline{d})$$



Capillary pressure (top) and relative permeability (bottom) depend on wetting phase saturation and electrode pore structure

Models: Electrochemistry

- Reactions, especially for the cathode, are stoichiometrically complicated

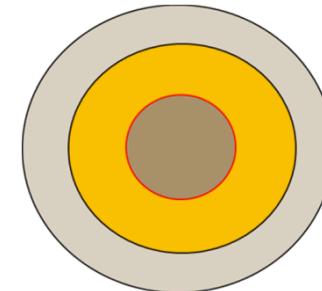


- Cantera's "Electrode Object" deploys multiple sub-grid models

- Infinite capacity
- Multi-plateau
- Newman reaction extend
- Finite capacity

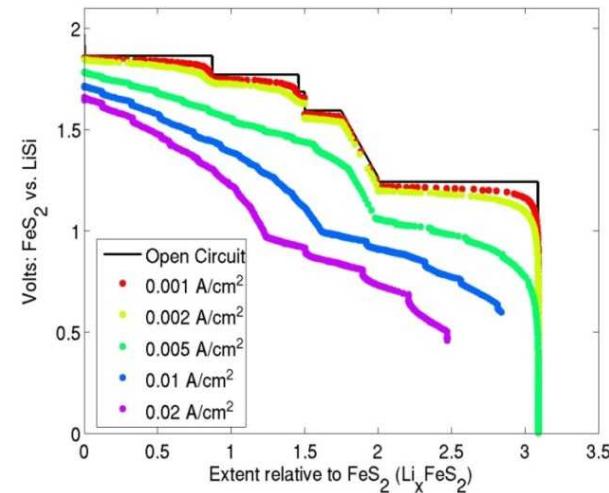
- Primary electrochemical coupling is the temperature
 - Cantera's thermodynamics all **temperature-dependent**

- Future: Use deformed geometry to affect porosity in electrochemical calculations



Shrinking Core Model

- Multiple plateaus can react simultaneously
- Diffusional losses with transport



Demonstration: Thermal transport and validation

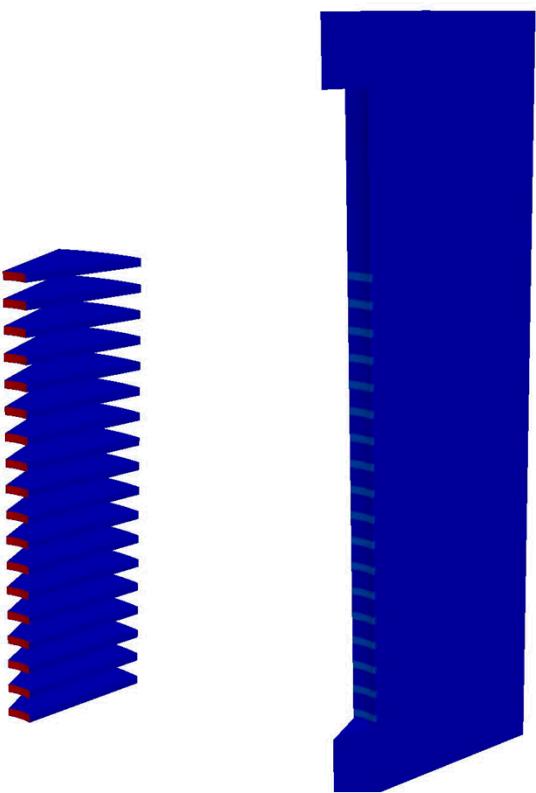
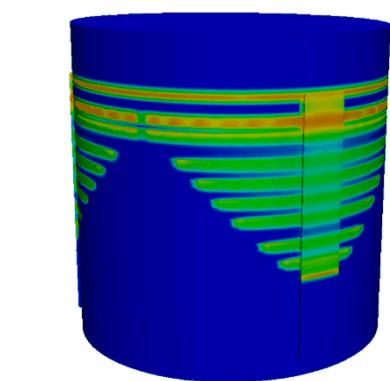
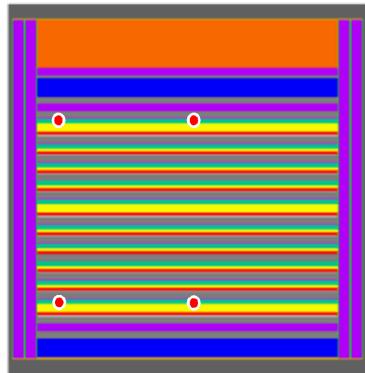
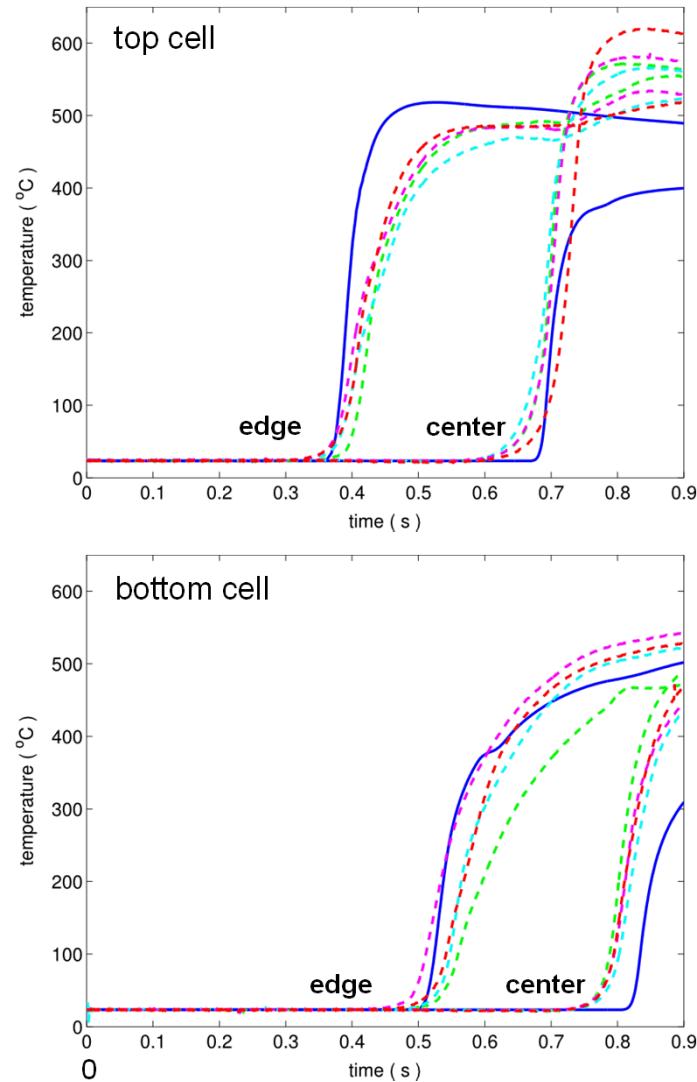


Illustration of center-fired geometry burn front

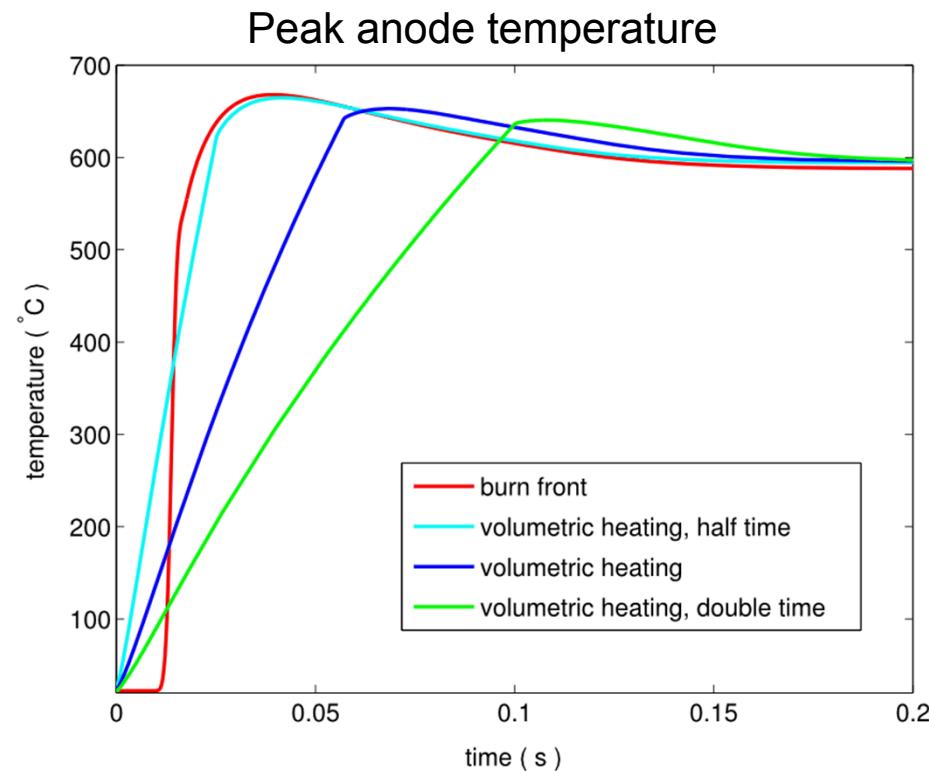
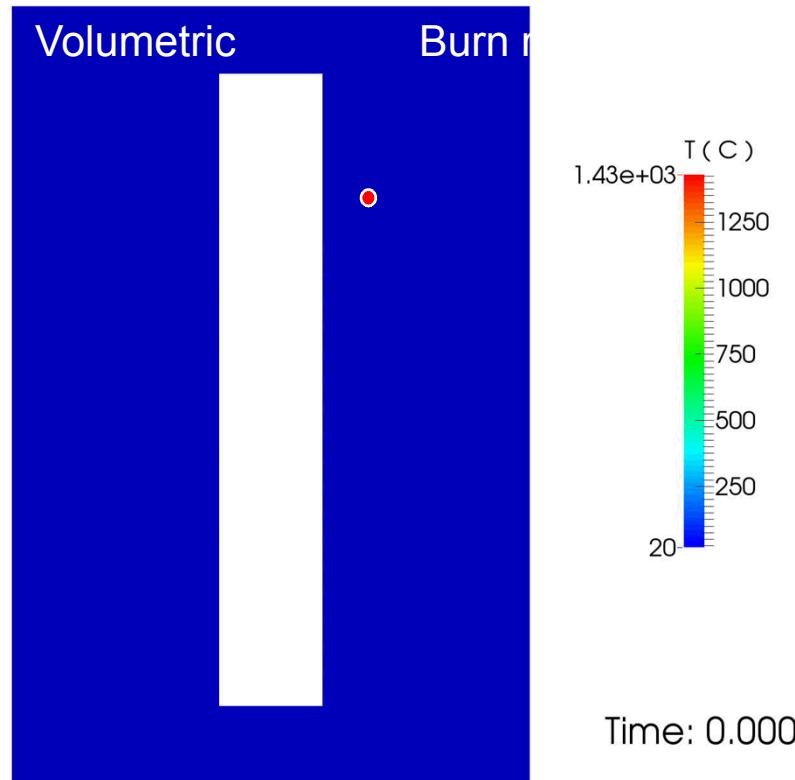


Side-fired experimental validation configuration showing temperature probes



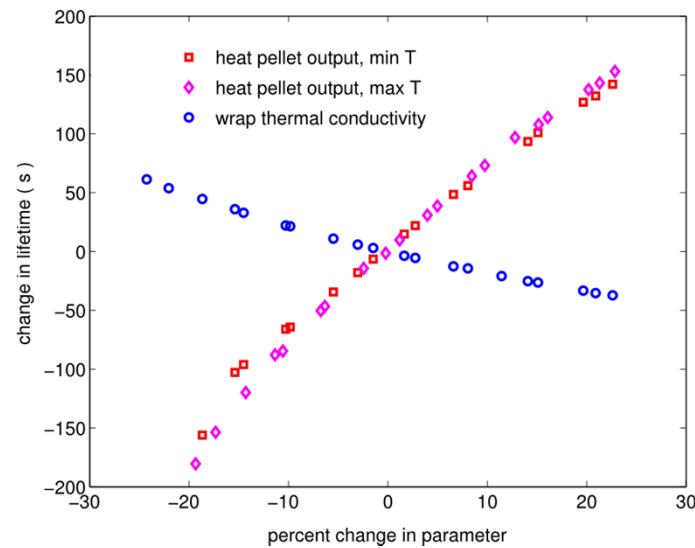
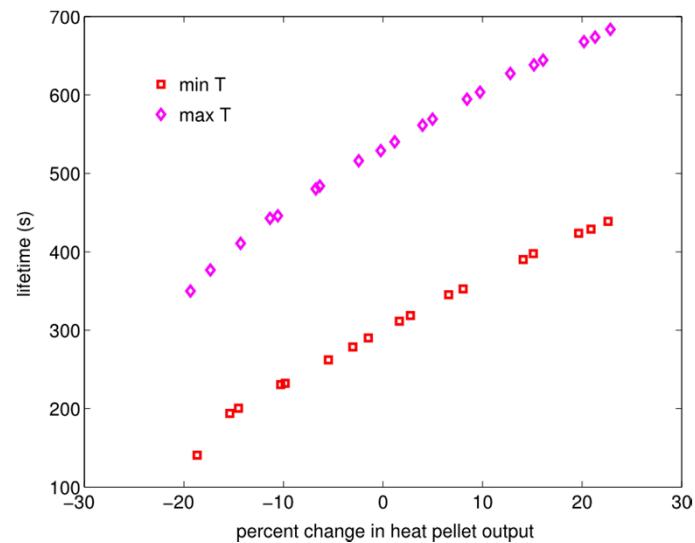
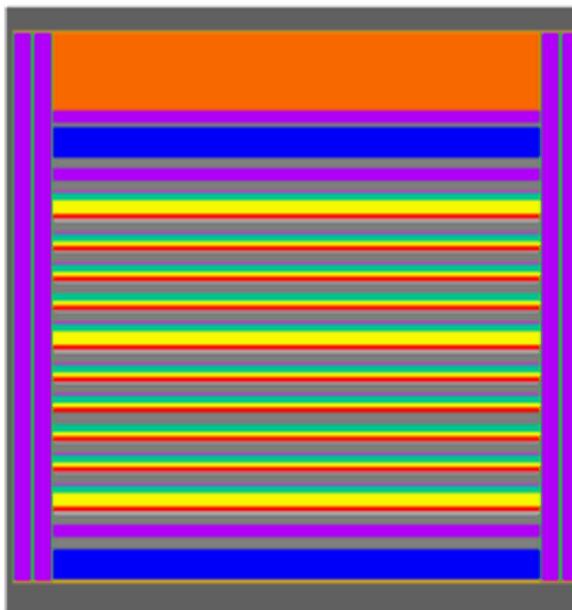
Perhaps improved prediction for thermal runaway

- Overheating of the anode is a proposed mechanism for thermal runaway
 - For volumetric burn times longer than 0.025sec, under-predict the anode temperature overshoot and peak temperature
 - Top anode gets much hotter than center stack
 - Larger batteries can have longer burn times

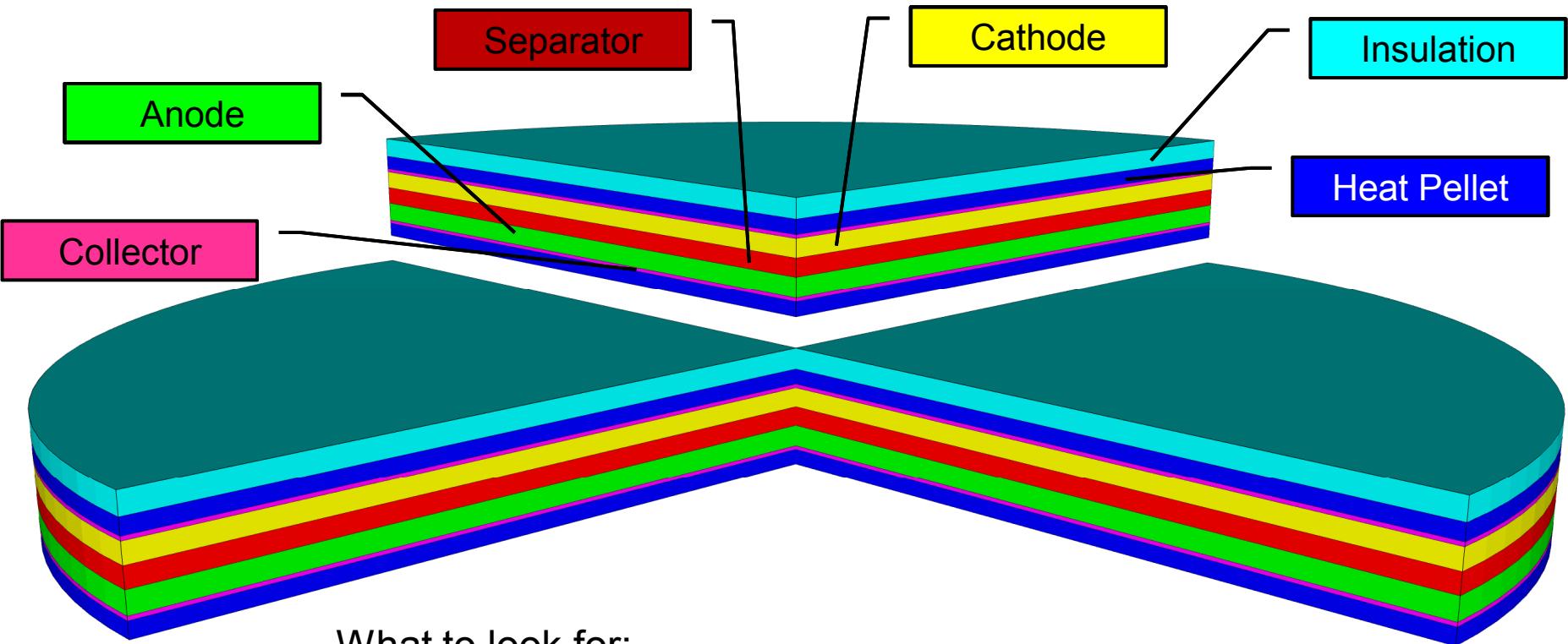


Impact: Lifetime of model validation battery

- Large difference between min temperature and max temperature within the battery
- But when we consider the change relative to the baseline, then the result is not sensitive to choice of temperature
- Lifetime of this battery is strongly dependent on heat pellet output. Wrap thermal conductivity is also important.

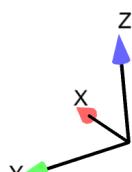


Demonstration: Coupled single cell mechanical simulation



What to look for:

1. Heat pellet burns (bottom left)
2. Electrolyte melts and flows (bottom right)
3. Separator crushes, insulation expands (top)

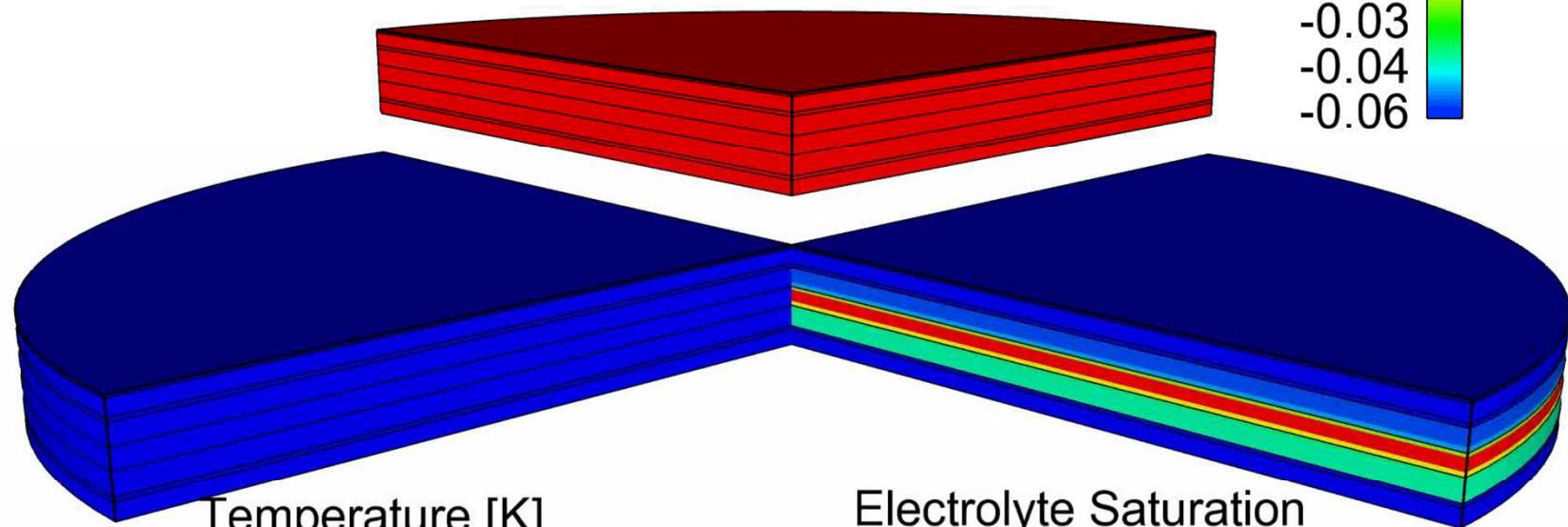
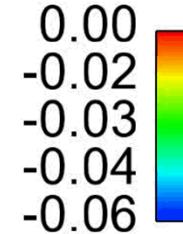


Demonstration: Coupled single cell mechanical simulation

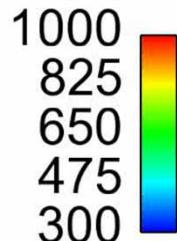
Time = 0.001 s

Deformations magnified 5x

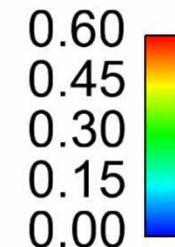
Axial Strain



Temperature [K]

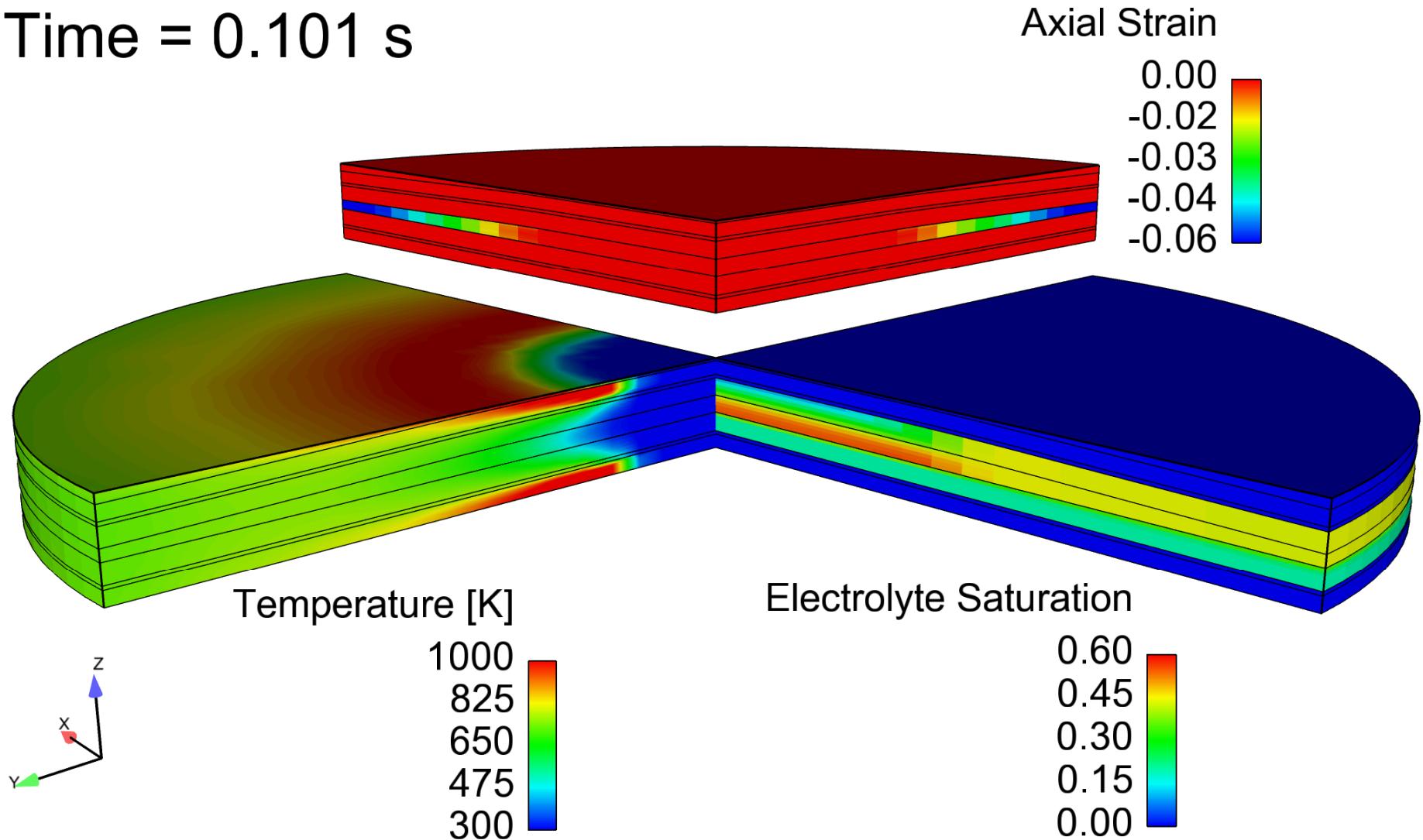


Electrolyte Saturation



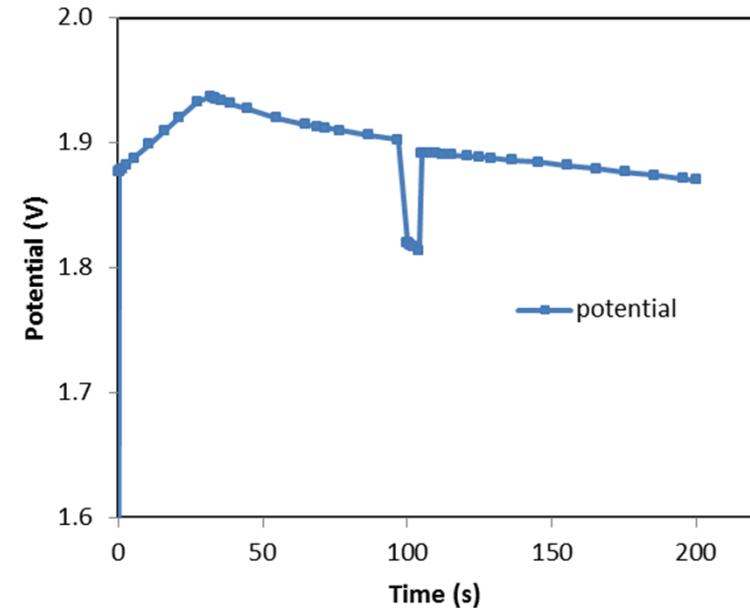
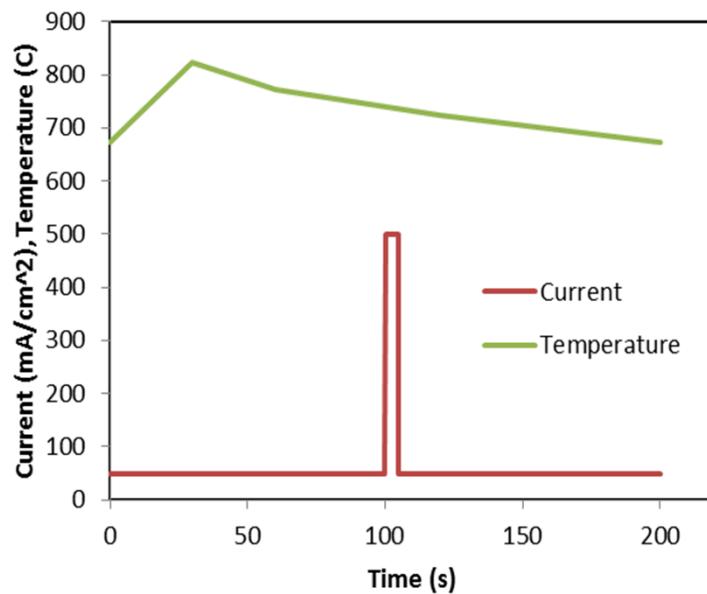
Demonstration: Coupled single cell mechanical simulation

Time = 0.101 s

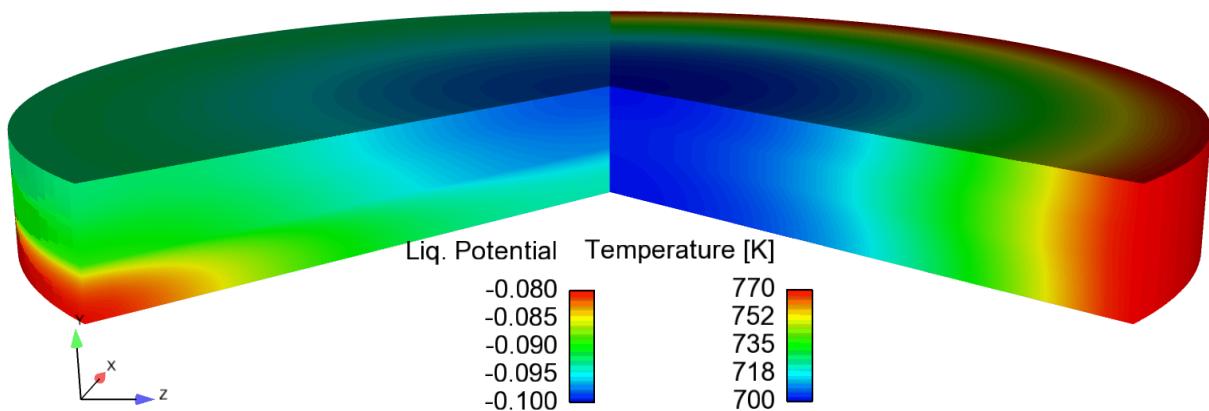


Demonstration: Thermo-electrochemical coupling

- Voltage responds to temperature and current

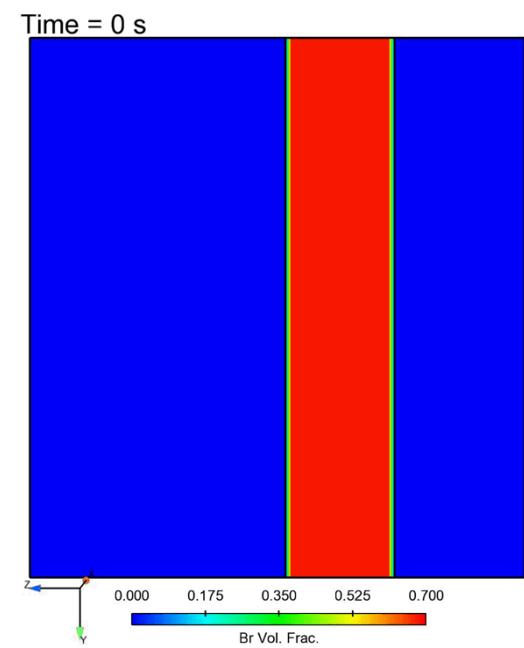
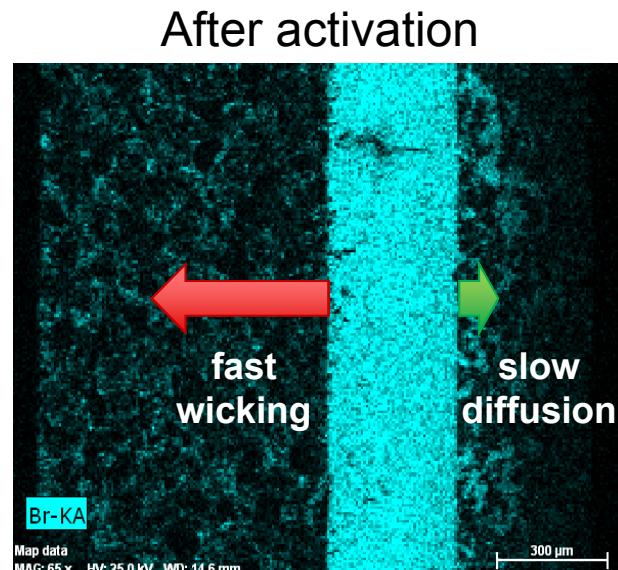
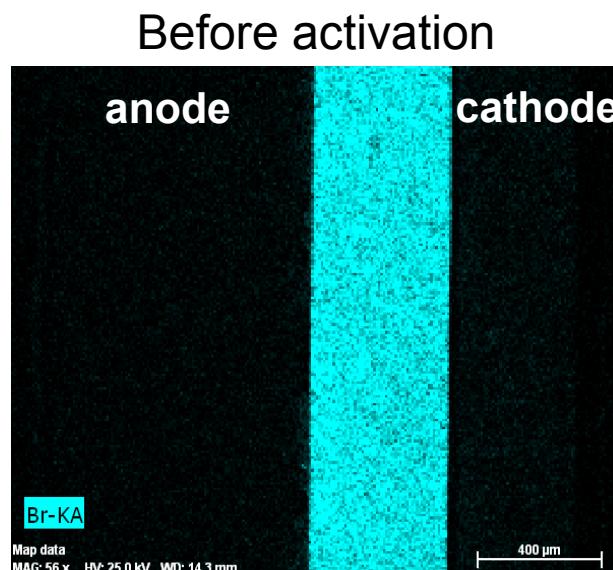
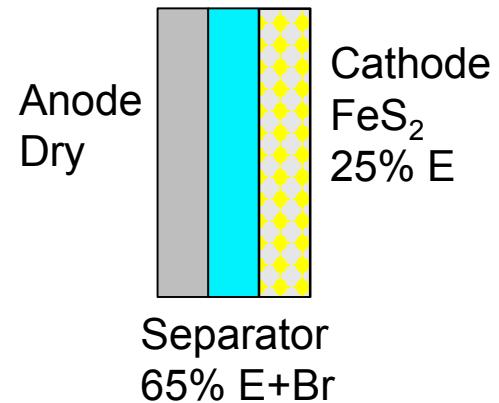


- Spatial temperature variations affect local potentials and current densities



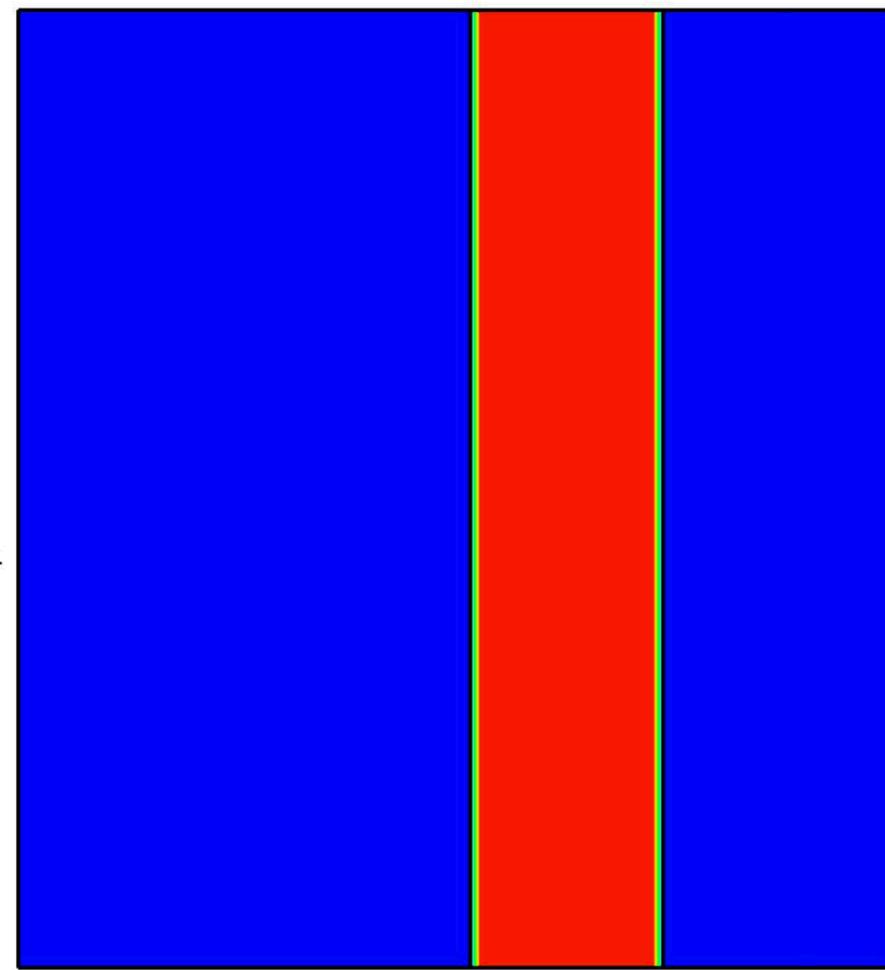
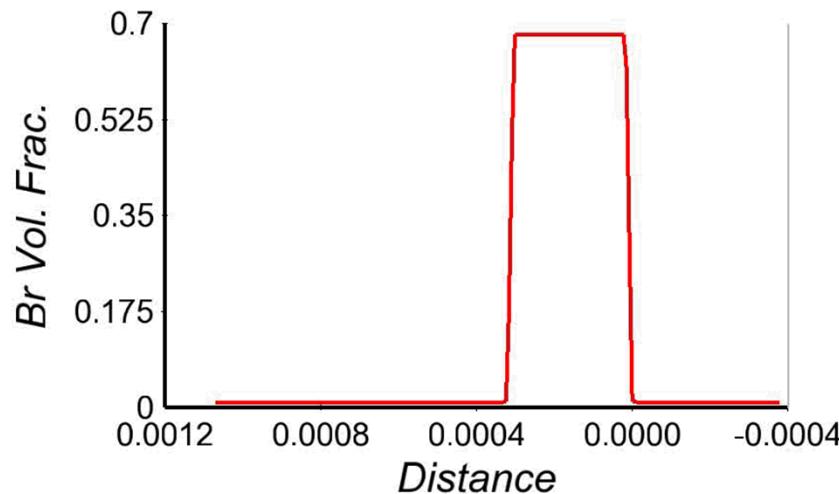
Demonstration: Bromine tracer diffusion permeability experiments

- Electrolyte migration and retention are critical to predicting performance
 - Used electrolyte with bromine tracer in the separator
 - Discover: Two mechanisms for electrolyte transport
 - Understand: Calculate porous flow parameters

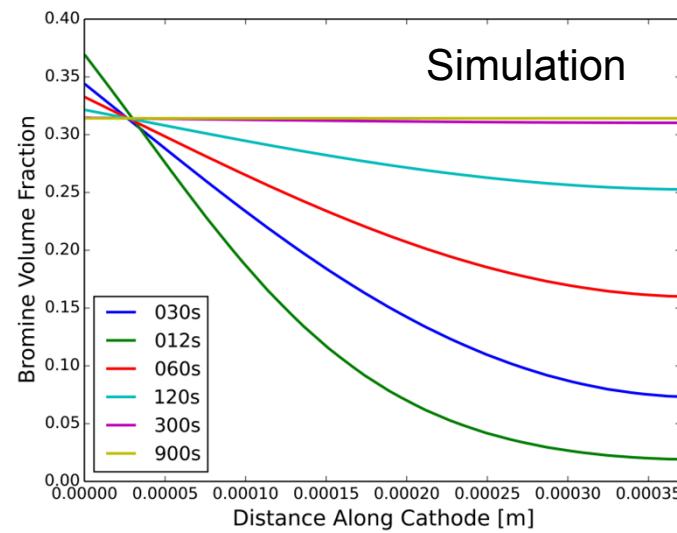
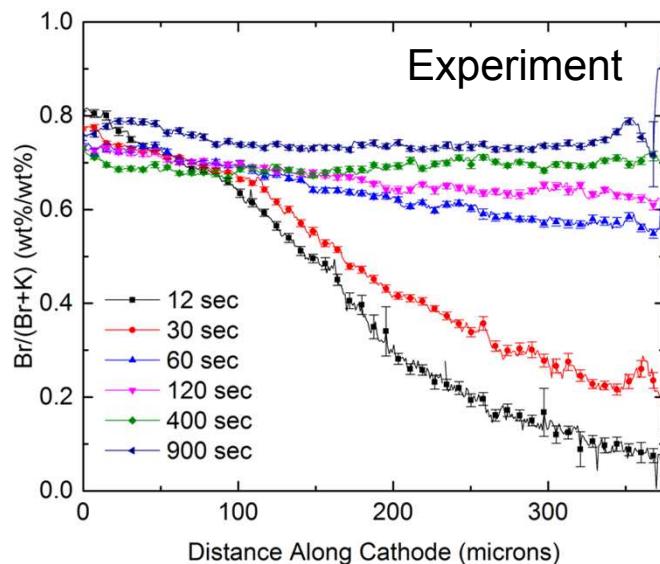
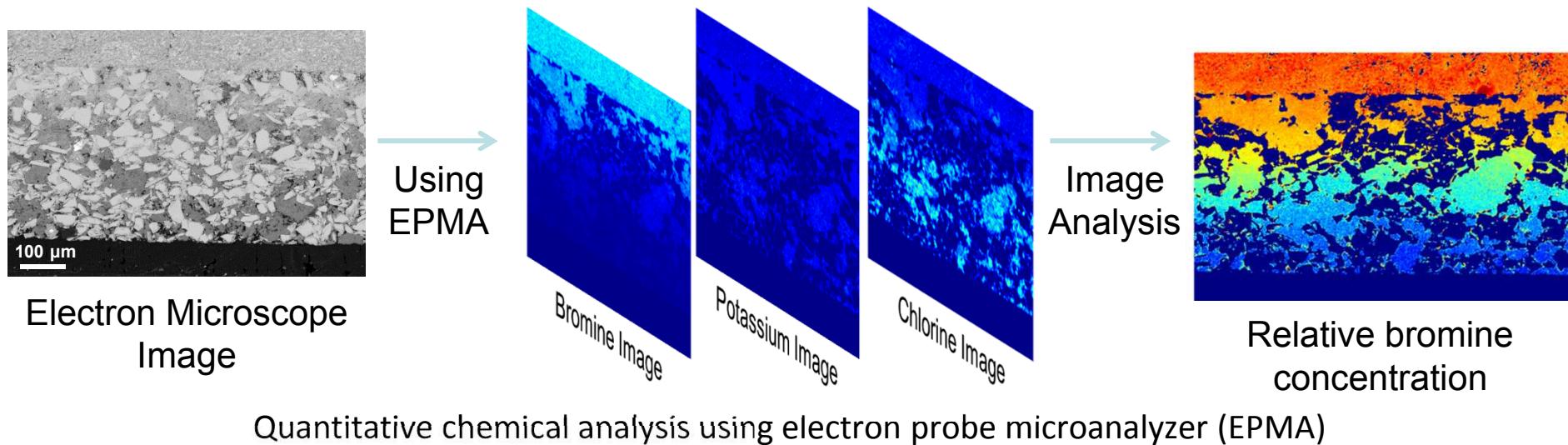


Demonstration: Bromine tracer diffusion permeability experiment

Time = 0 s

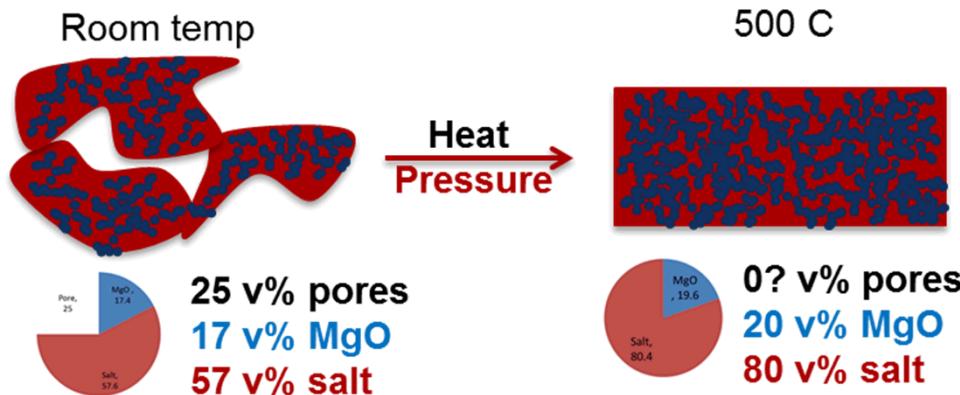
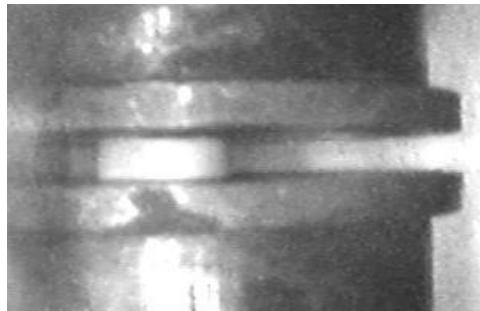


Demonstration: Bromine tracer diffusion permeability experiments

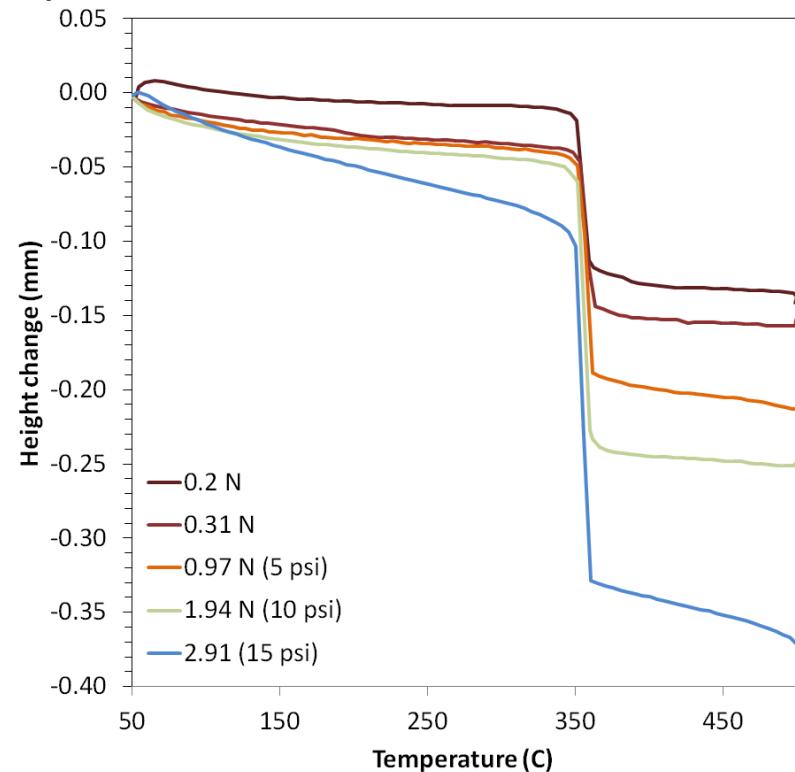


Separator Characterization

- Detailed characterization of how the separator changes on melting of the electrolyte

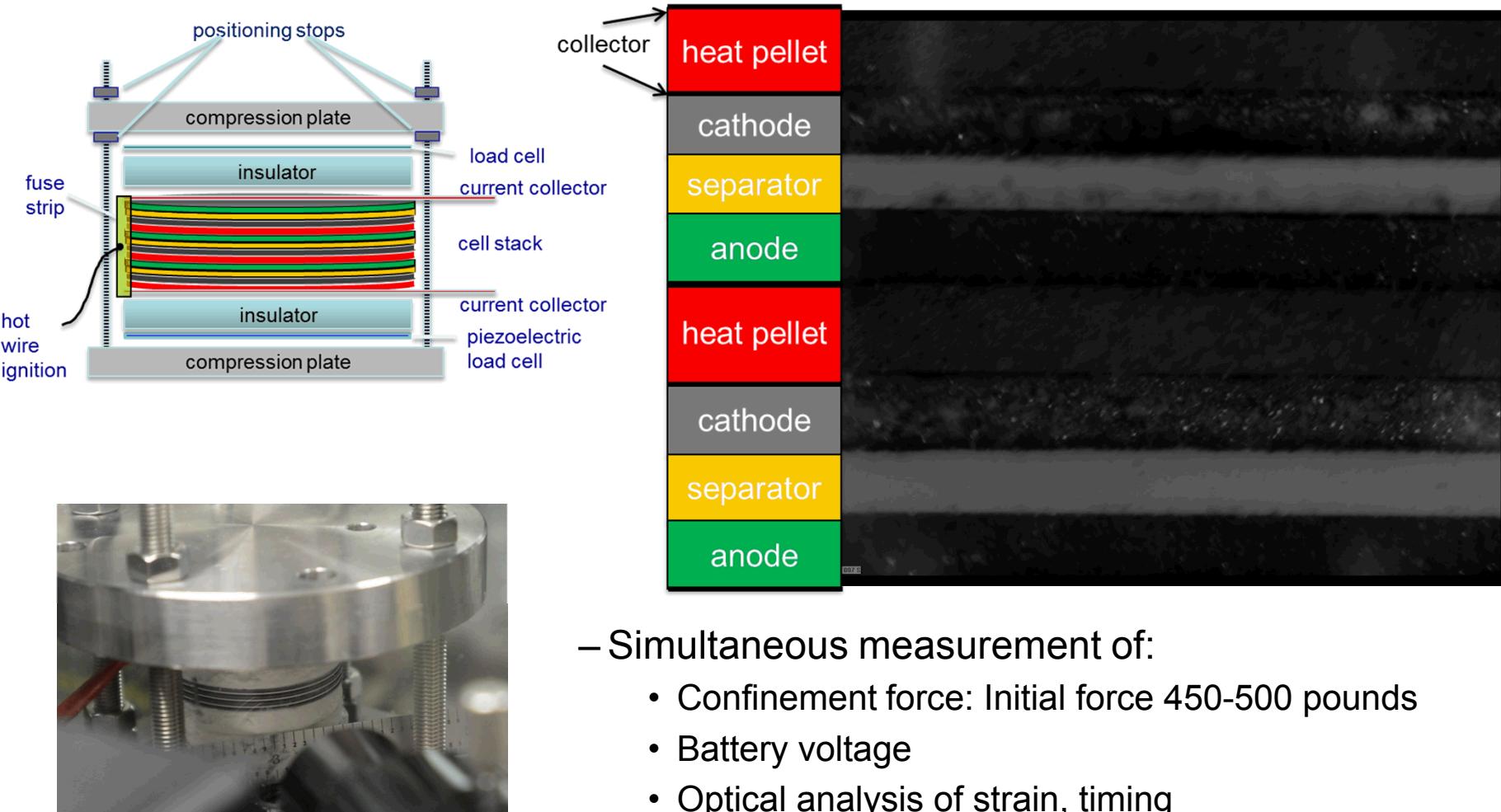


Separator deformation under constant force



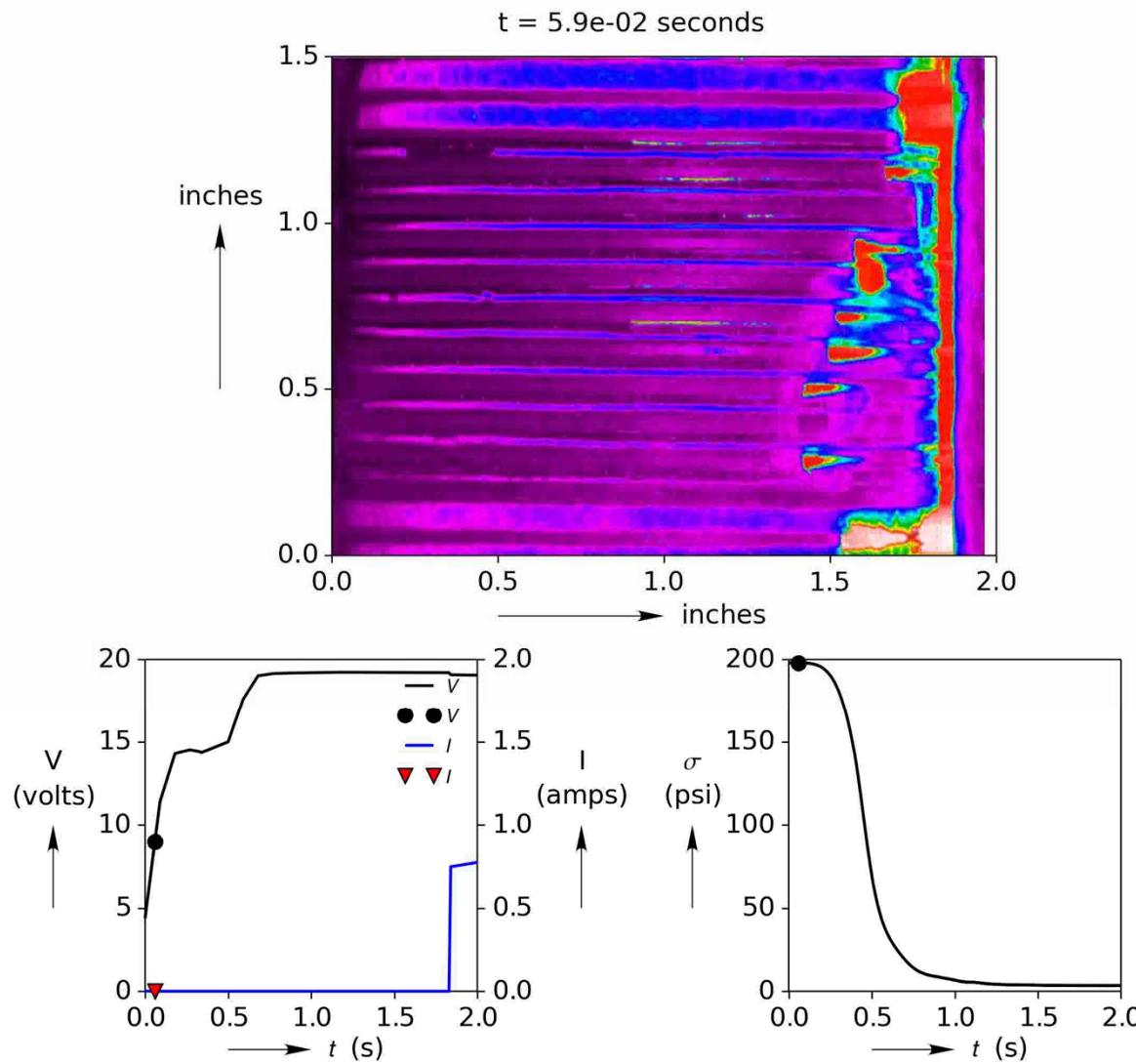
Too Much Deformation: Electrolyte shorts the battery
Too Little: High battery resistance – Poor performance

Working towards mechanical validation: Open stack testing

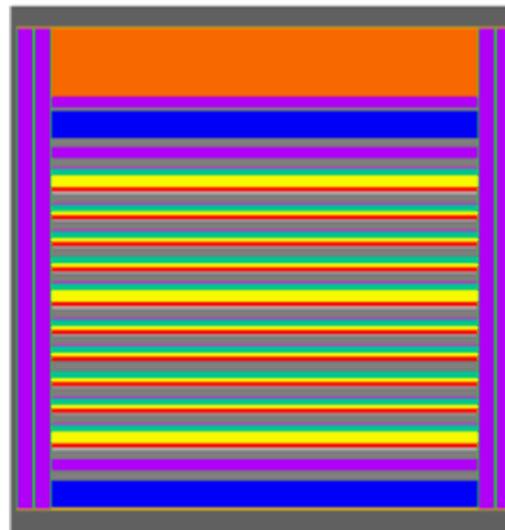


- Simultaneous measurement of:
 - Confinement force: Initial force 450-500 pounds
 - Battery voltage
 - Optical analysis of strain, timing
- Impact of insulation type and stack height

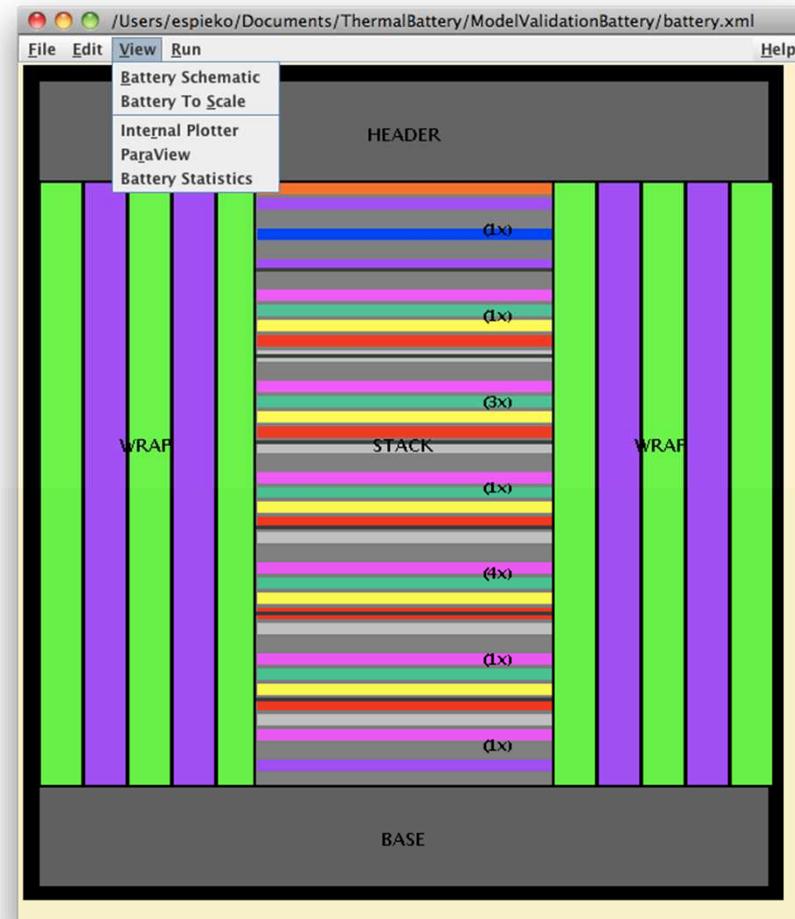
Working towards mechanical validation: Open stack testing



- Design tool to provide high fidelity modeling capability (Sierra) with a user friendly interface
- Thermal models used extensively for battery design and to inform system level thermal models
- New in FY14: electrochemistry prediction and center hole fired geometry support



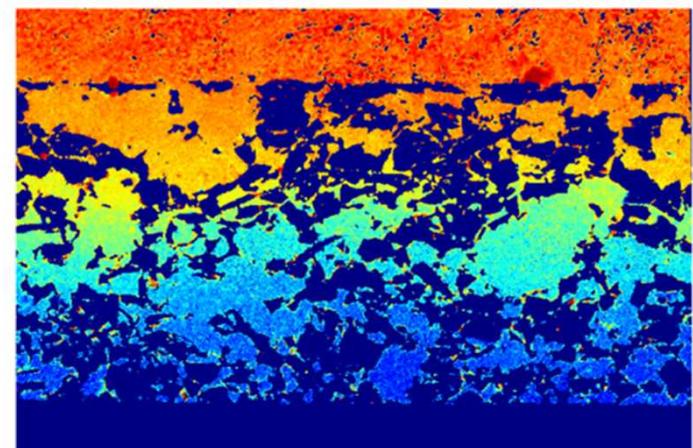
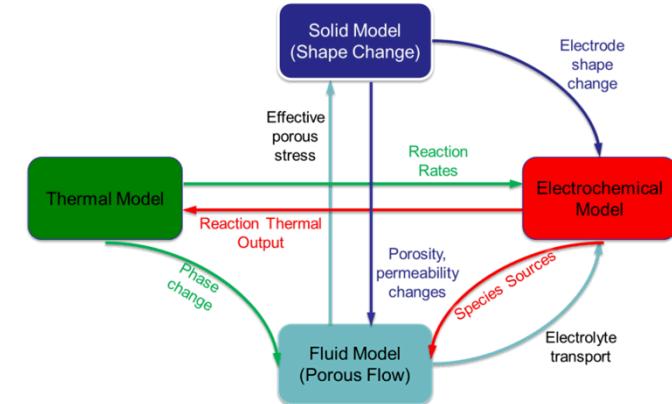
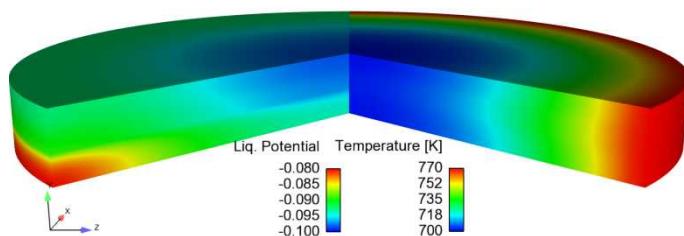
battery to scale



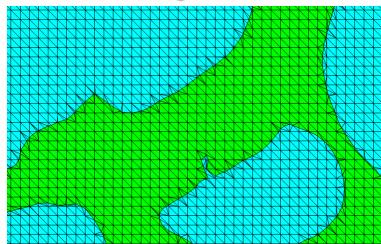
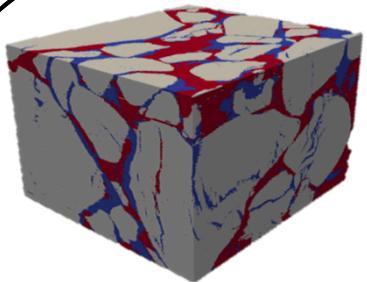
battery schematic

Thermal battery modeling summary

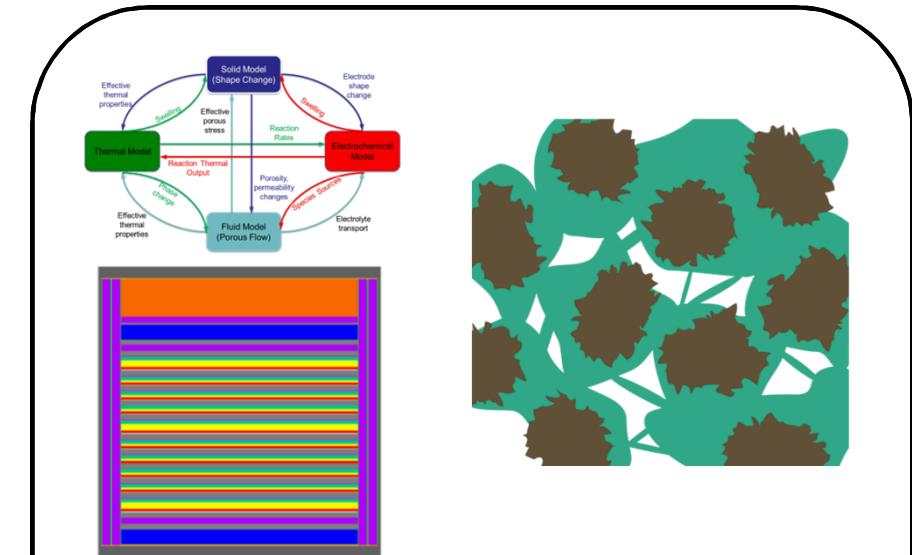
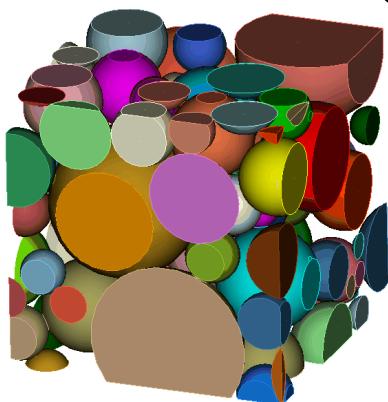
- “Intelligent” coupling of physics can provide significantly higher-fidelity models, with potentially only modest performance penalties.
- Further validation of individual models
- Future investigation of additional couplings:
 - Material properties for physics affected by:
 - Mechanical deformation (change in solid fraction)
 - Saturation (change in liquid fraction)
 - Eventually couple electrochemistry to the thermo-poro-mechanics



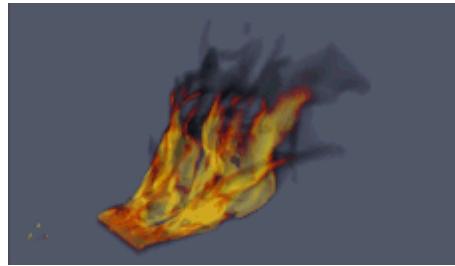
Summary



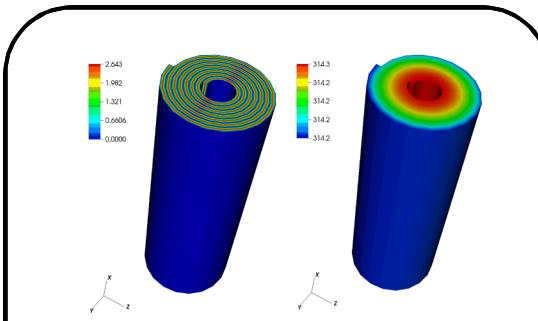
Lithium-Ion battery mesoscale
degradation simulations



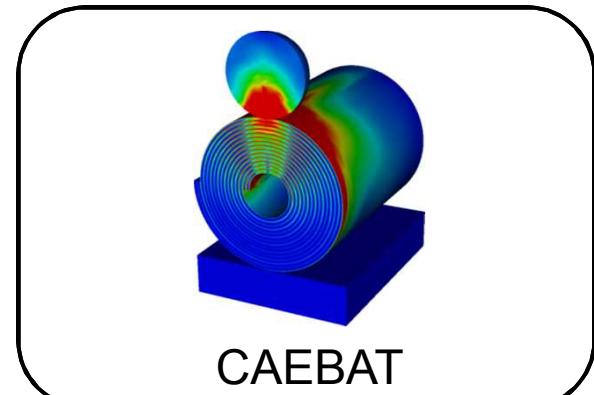
Performance models of
molten salt batteries



Grid storage



Alkaline batteries



CAEBAT

BACKUP SLIDES
