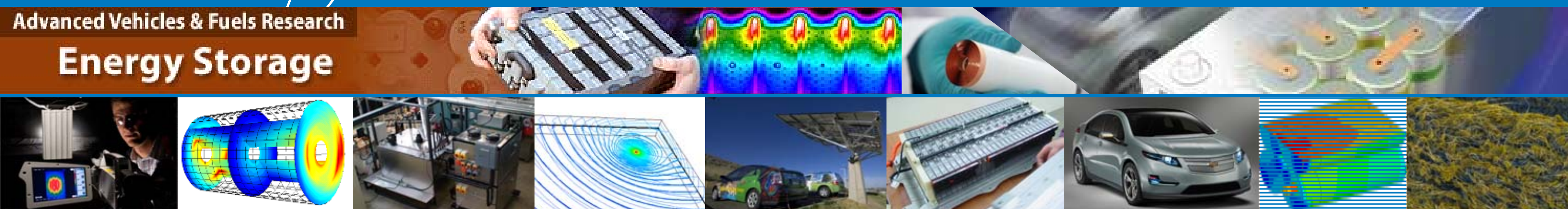
Computer-Aided Engineering of Batteries for Designing Better Li-Ion Batteries



Ahmad Pesaran, Ph.D.
Gi-Heon Kim, Ph.D.
Kandler Smith, Ph.D.
Kyu-Jin Lee, Ph.D.
Shriram Santhanagopalan, Ph.D.

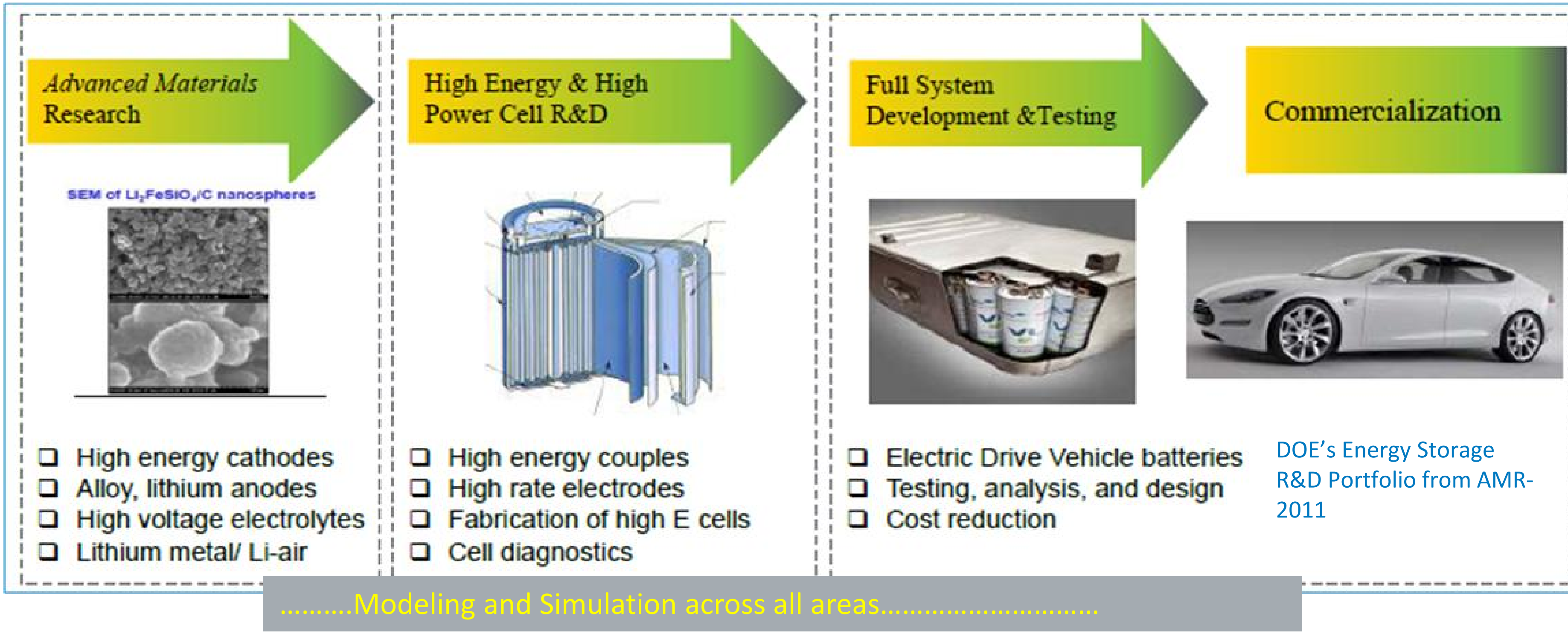
Advanced Automotive Battery Conference
Battery Modeling Software and Applications Workshop
Orlando, Florida, February 6, 2012

NREL/PR-5400-53777

Funded by Energy Storage R&D
Dave Howell and Brian Cunningham
Vehicle Technologies Program
U.S. Department of Energy

Energy Storage R&D Program

- **DOE ES Charter: Advance the development of batteries and electrochemical energy storage devices to enable a large market penetration of hybrid and electric vehicles.**
- **DOE ES Focus: Increase performance at lower cost while meeting weight, volume, and safety targets.**

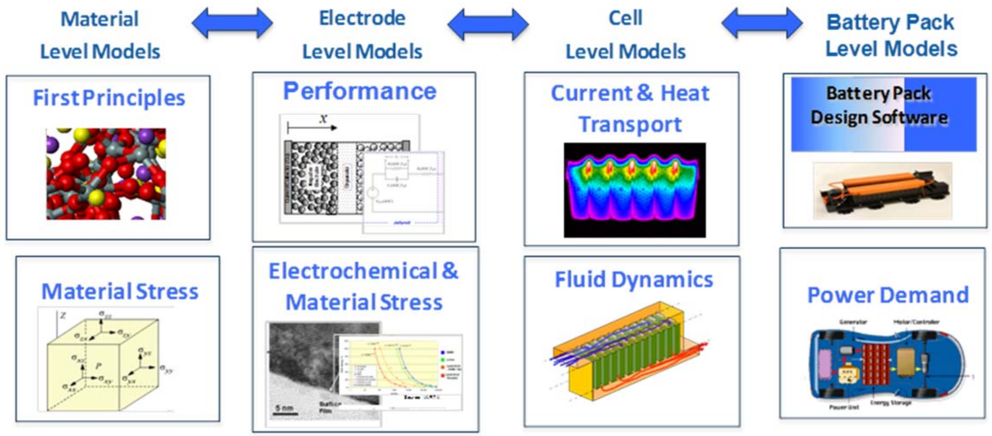


- **NREL ES Objective: Support DOE and industry to achieve energy storage targets through research and development, testing, analysis, design, and modeling.**

Modeling and Design Tools

> Most models are wrong, but some are useful…..
>
> anonymous

- **Simulation and computer-aided engineering (CAE) tools are widely used to speed up the research and development cycle and reduce the number of build-and-break steps.**
- **Use of CAE tools has enabled the automakers to reduce product development cost and time while improving the safety, comfort, and durability of many components and vehicles.**
- **There is a need to have several user-friendly, 3D, fully-integrated CAE software tools available for the battery community across many scales.**



The Current State of Battery Modeling

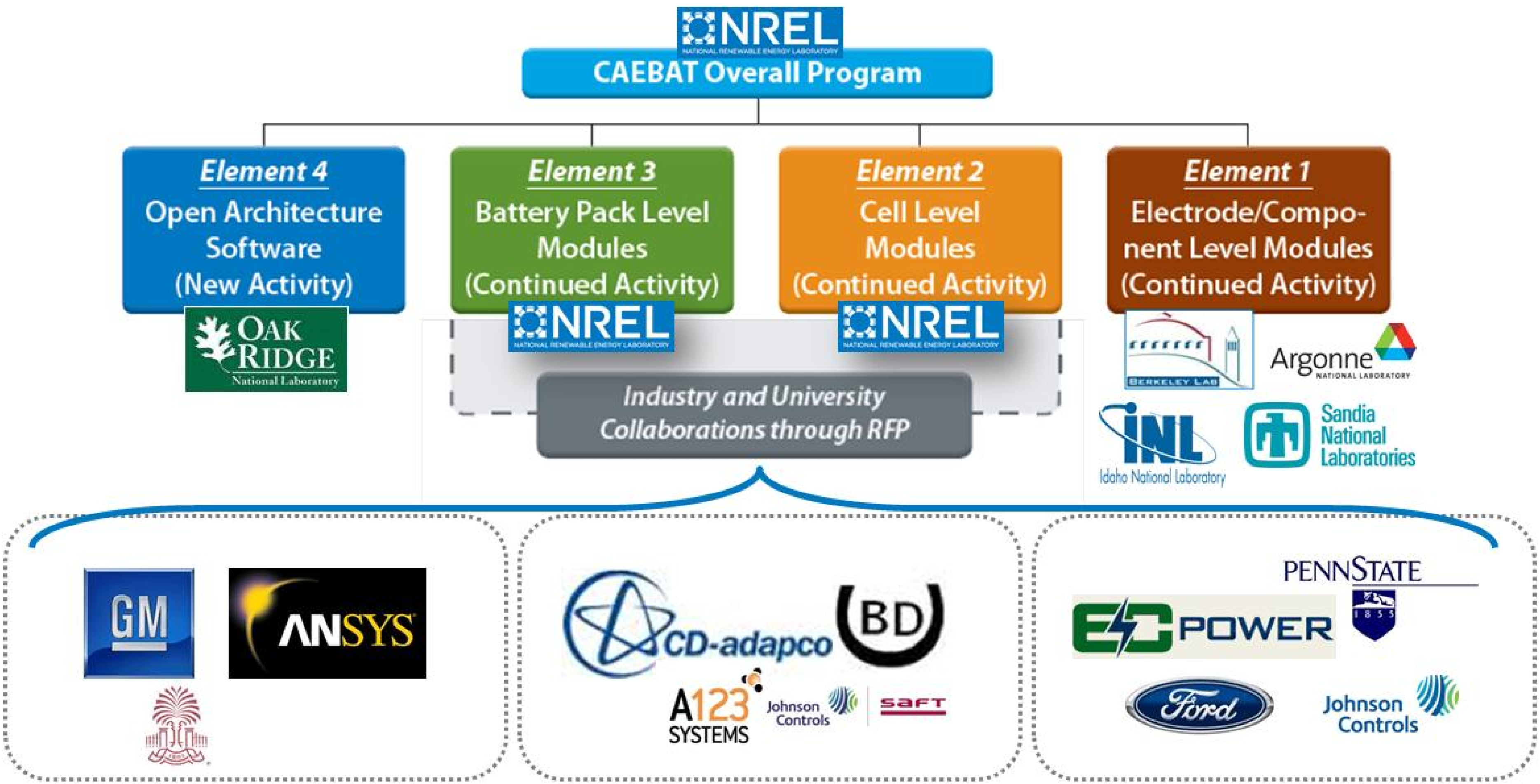
- **There are a number of battery models in academia, national labs, and industry, but they either**
  - Include relevant physics details, but mostly neglect engineering complexities, or
  - Include relevant macroscopic geometry and system conditions in 3D, but use too many simplifications in fundamental physics.
- **There are a number of custom battery codes available; however, they require expert users.**
- **The Battery Design Studio software suite has been in the forefront of battery simulations and now is being integrated into CD-adapco's CAE environment.**
- **Validation of data is the key to building confidence.**

The Current State of Battery Modeling

- **With DOE funding, national laboratories, industry, and universities have developed many models for simulating lithium-ion battery (LIB)**
  - cost,
  - life,
  - performance (electro-thermal, electrochemical), and
  - abuse reactions.
- **So far, these models have not been fully integrated into 3D CAD for design of battery packs and linked with ease, especially for engineering purposes.**
- **Realizing the need, DOE has initiated the CAEBAT project to bring together these battery models to develop suites of battery CAE tools.**

DOE's CAEBAT Program

- **Objective: Incorporate existing and new models into software tools for design of cells and packs.**
- **Goal: Shorten development and design cycles and optimize batteries for improved performance and safety, long life, and low cost.**

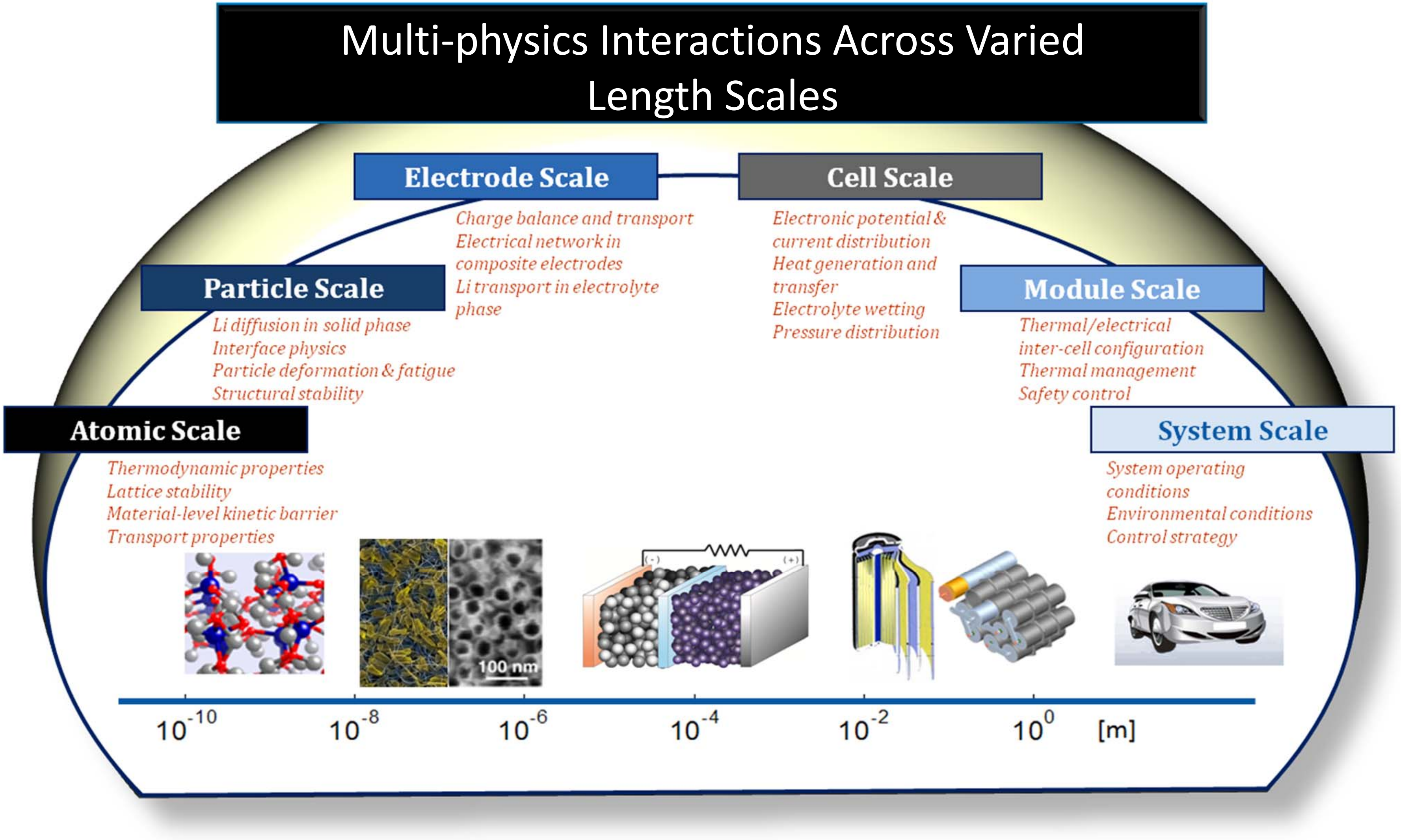


NREL's Role in the CAEBAT Project

1. **As project coordinator, NREL supports DOE to achieve the CAEBAT objectives:**
   - Provide input/support to DOE for the CAEBAT project plan
   - Coordinate activities among national laboratories
   - Support industry and universities through competitively-placed subcontracts
     - 50%-50% cost sharing with three teams
     - Work started in June 2011 to develop CAE tools
2. **Enhance and further develop existing electrochemical, thermal, abuse reaction, and internal short circuit models for use by industry and CAEBAT participants.**

Model	Length Scale μm --- mm --- m	Geometry	Physics / Application
Electro-thermal (FEA) & Fluid-dynamics (CFD)		1-D, 2-D, & 3-D	• Electrical, thermal & fluid flow • Performance, detailed cooling design • Commercial software (restrictive assumptions)
Electrochemical-thermal ("MSMD")		1-D, 2-D & 3-D	• Electrochemical, electrical & thermal • Performance, design
Electrochemical-thermal-degradation ("MSMD-life")		1-D, 2-D & 3-D	• Electrochemical, electrical & thermal • Cycling- & thermal-induced degradation • Performance, design, life prediction
Thermal abuse reaction kinetics		Thermal network, 2-D & 3-D	• Chemical & thermal • Safety evaluation
Internal short circuit		3-D	• Chemical, electrical, electrochem. & thermal • Safety evaluation

Battery Performance, Durability and Safety

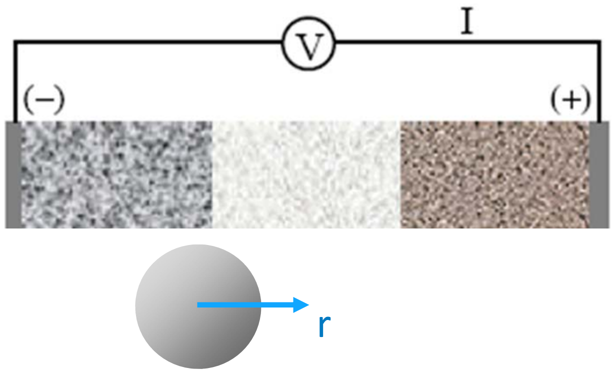


Porous Electrode Model – Commonly Used

Charge Transfer Kinetics at Reaction Sites

$$j^{Li} = a_s i_o \left\{ \exp\left[\frac{\alpha_a F}{RT}\eta \right] - \exp\left[-\frac{\alpha_c F}{RT}\eta \right] \right\}$$

$$i_0 = k(c_e)^{\alpha_a}(c_{s,\max} - c_{s,e})^{\alpha_a}(c_{s,e})^{\alpha_c} \qquad \eta = (\phi_s - \phi_e) - U$$



Species Conservation

$$\frac{\partial c_s}{\partial t} = \frac{D_s}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial c_s}{\partial r} \right)$$

$$\frac{\partial(\varepsilon_e c_e)}{\partial t} = \nabla \cdot \left(D_e^{eff} \nabla c_e \right) + \frac{1 - t_+^o}{F} j^{Li} - \frac{\mathbf{i}_e \cdot \nabla t_+^o}{F}$$

Charge Conservation

$$\nabla \cdot \left(\sigma^{eff} \nabla \phi_s \right) - j^{Li} = 0$$

$$\nabla \cdot \left(\kappa^{eff} \nabla \phi_e \right) + \nabla \cdot \left(\kappa_D^{eff} \nabla \ln c_e \right) + j^{Li} = 0$$

Energy Conservation

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + q'''$$

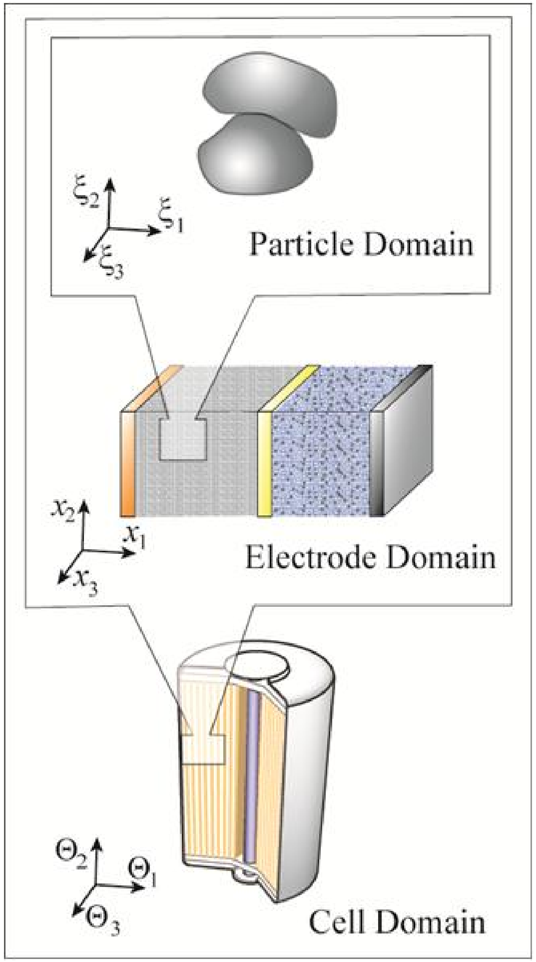
$$q''' = j^{Li}\left(\phi_s - \phi_e - U + T\frac{\partial U}{\partial T} \right) + \sigma^{eff} \nabla \phi_s \cdot \nabla \phi_s + \kappa^{eff} \nabla \phi_e \cdot \nabla \phi_e + \kappa_D^{eff} \nabla \ln c_e \cdot \nabla \phi_e$$

- **Pioneered by John Newman's group at the University of Berkeley (*Doyle, Fuller, and Newman 1993*)**
- Captures *lithium diffusion dynamics* and *charge transfer kinetics*
- Predicts *current/voltage response* of a battery
- Provides design guide for thermodynamics, kinetics, and transport across electrodes

- Difficult to apply in large-format batteries where *heat* and *electron current* transport critically affect the battery responses

NREL's MSMD Model Framework

*Through the multi-year effort supported by DOE, NREL has developed a modeling framework for predictive computer simulation of LIBs known as the **Multi-Scale Multi-Dimensional (MSMD)** model that addresses the interplay among the physics in varied scales.*



- **Introduce *multiple computational domains* for corresponding length scale physics**
- ***Decouple LIB geometries* into separate computation domains**
- ***Couple physics* using the predefined inter-domain information exchange**
- **Selectively resolve higher spatial resolution for smaller characteristic length scale physics**
- **Achieve high computational efficiency**
- **Provide flexible & expandable modularized framework**

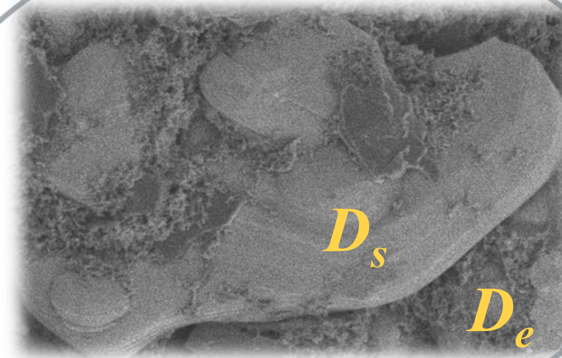
Kim et al., "Multi-Domain Modeling of Lithium-Ion Batteries Encompassing Multi-Physics in Varied Length Scales," *J. of Electrochemistry*, 2011, Vol. 158, No. 8, pp. A955–A969

Segregation of Time and Length Scales

Self-Balancing Nature

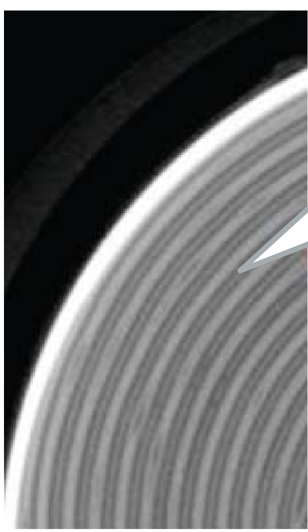
→ Continuum approach with thermodynamic representation for sub-domain system

Kinetic/dynamic representation



Lithium transport is much faster in liquid electrolyte than in solid particles

e.g., $D_s << D_e$

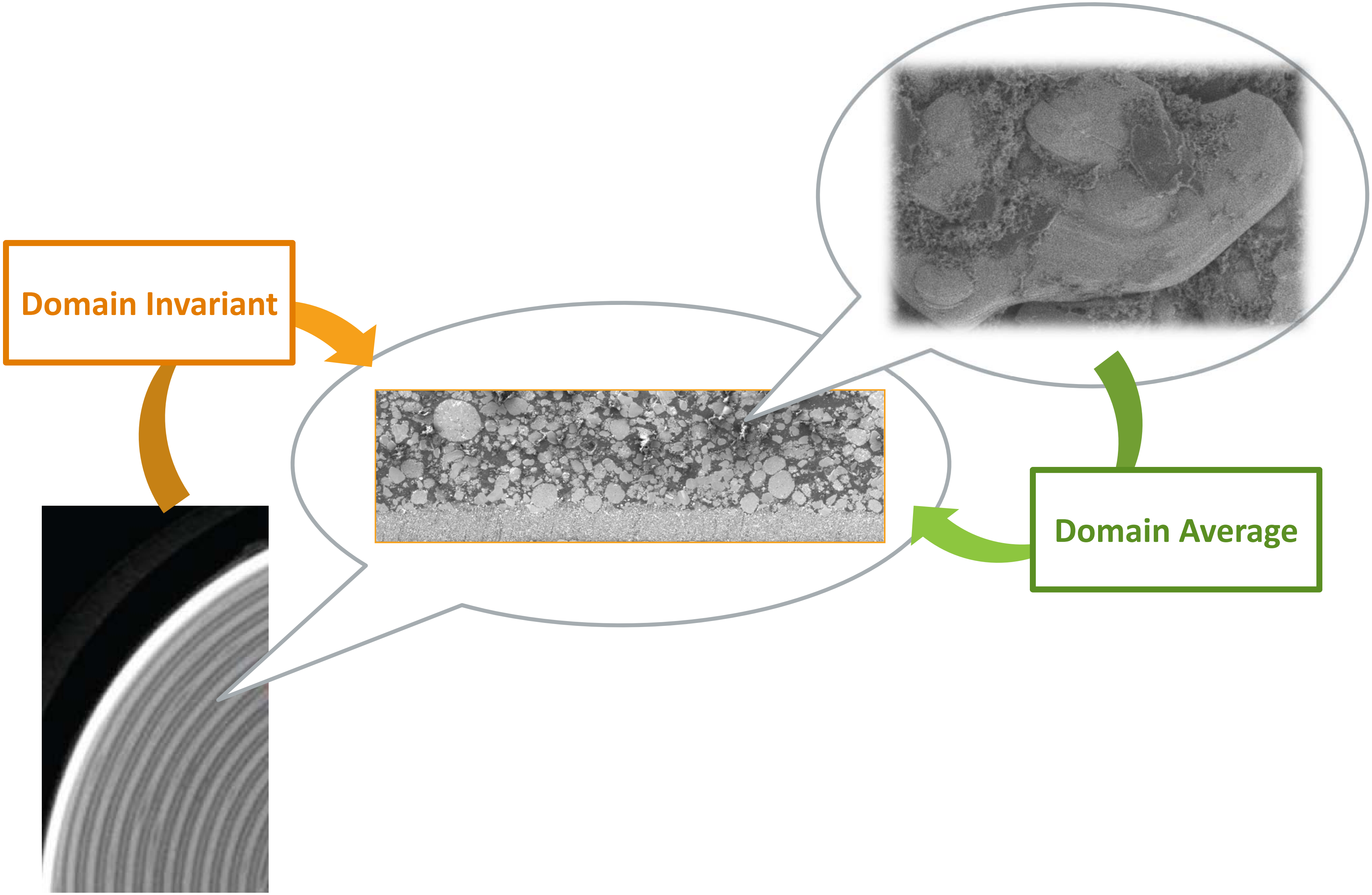


Electronic conductivity is much higher in metal current collectors than in composite electrode matrix

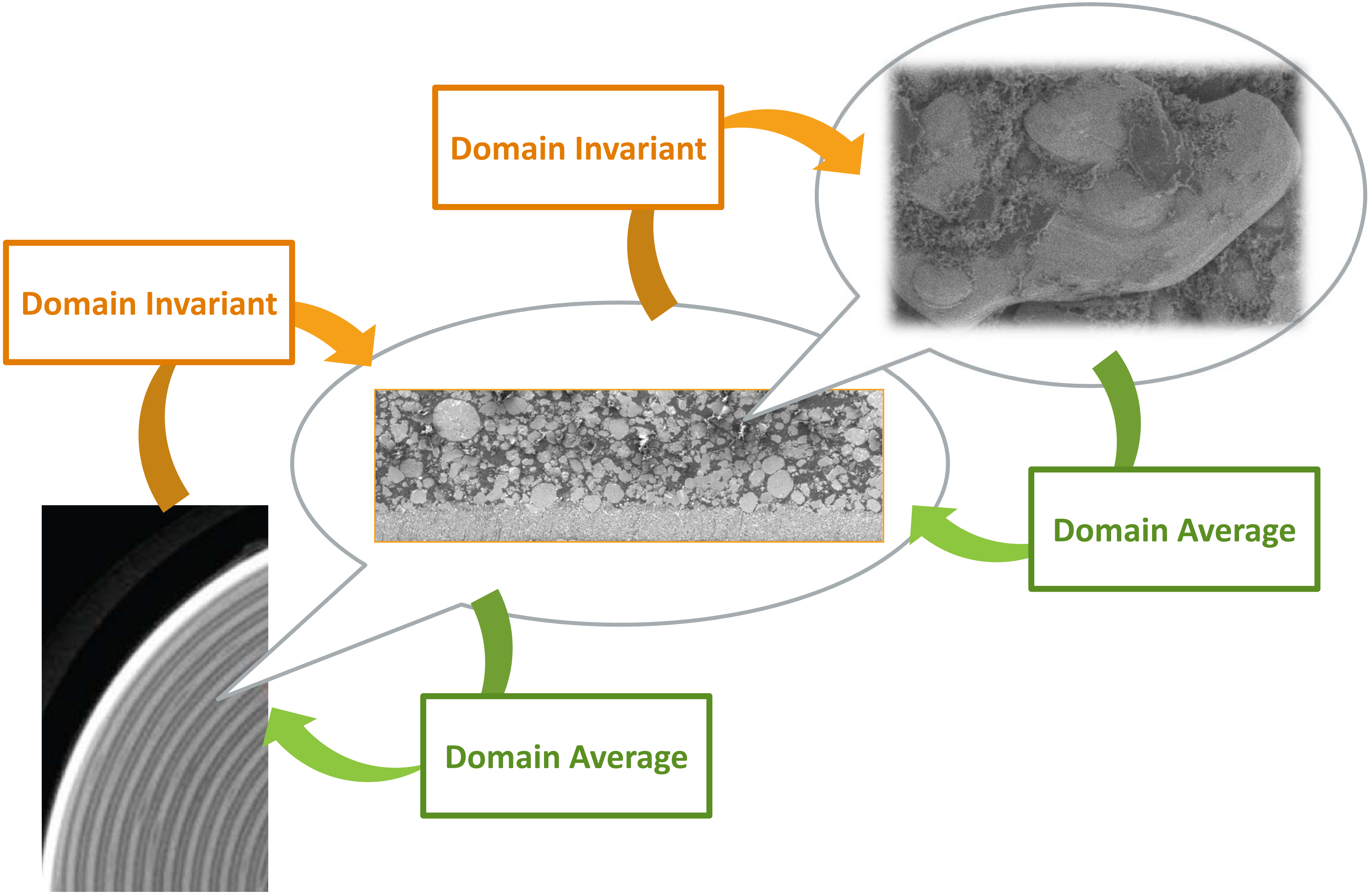
e.g., $\sigma_{ce} << \sigma_{cc}$

Kim et al., "Multi-Domain Modeling of Lithium-Ion Batteries Encompassing Multi-Physics in Varied Length Scales," *J. of Electrochem.*, 2011, Vol. 158, No. 8, pp. A955–A969

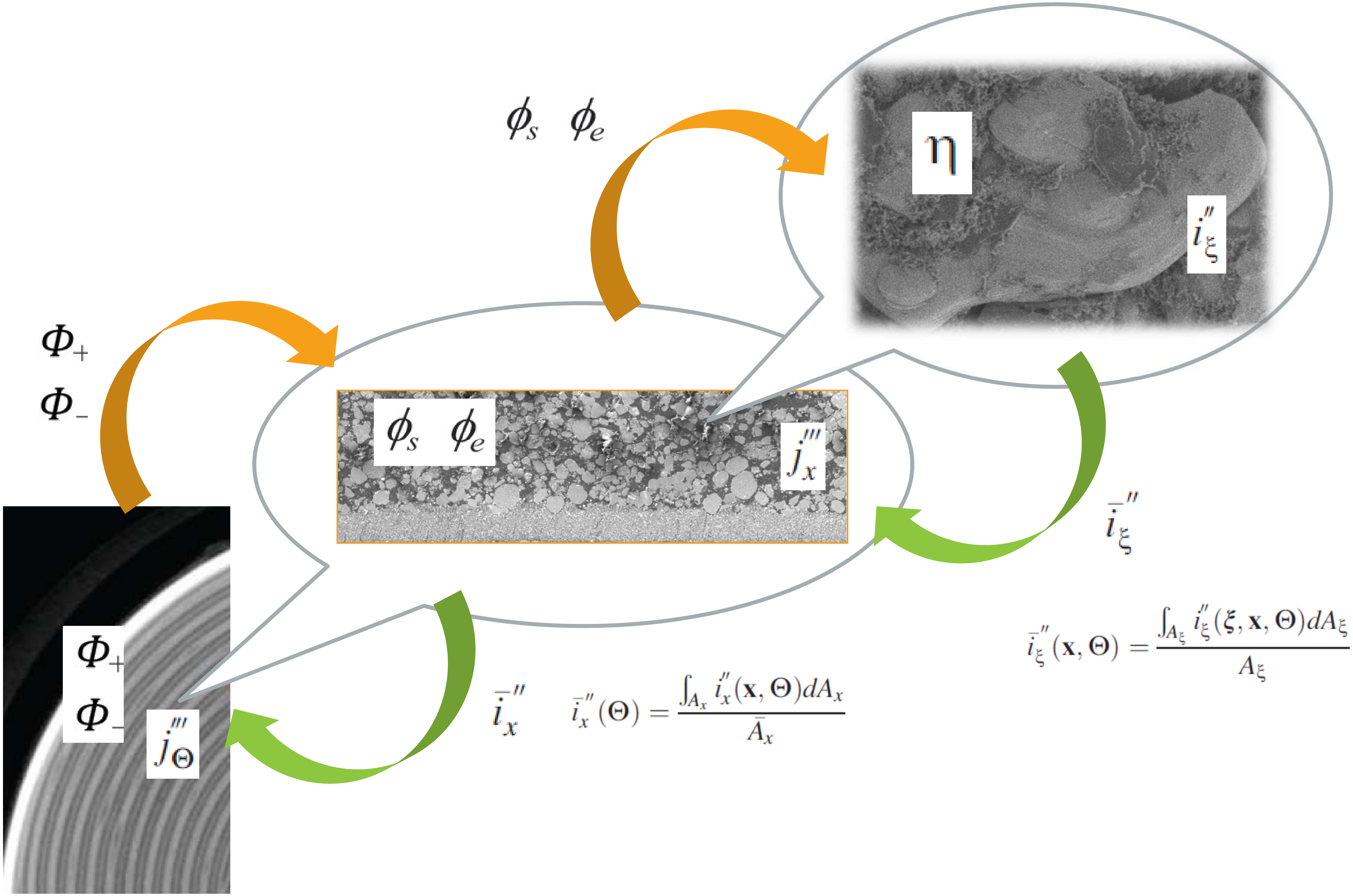
Geometry Decoupling



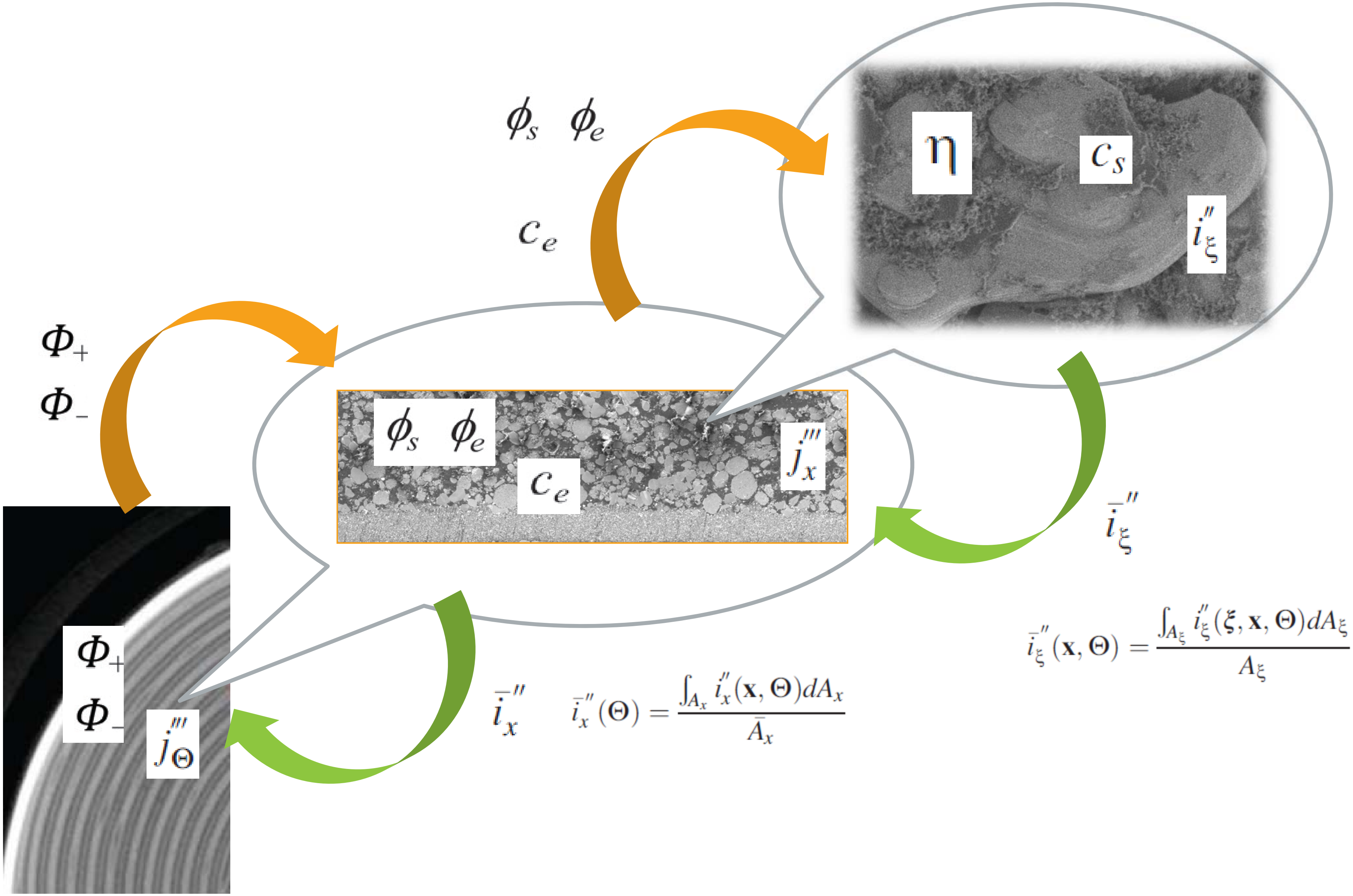
Geometry Decoupling



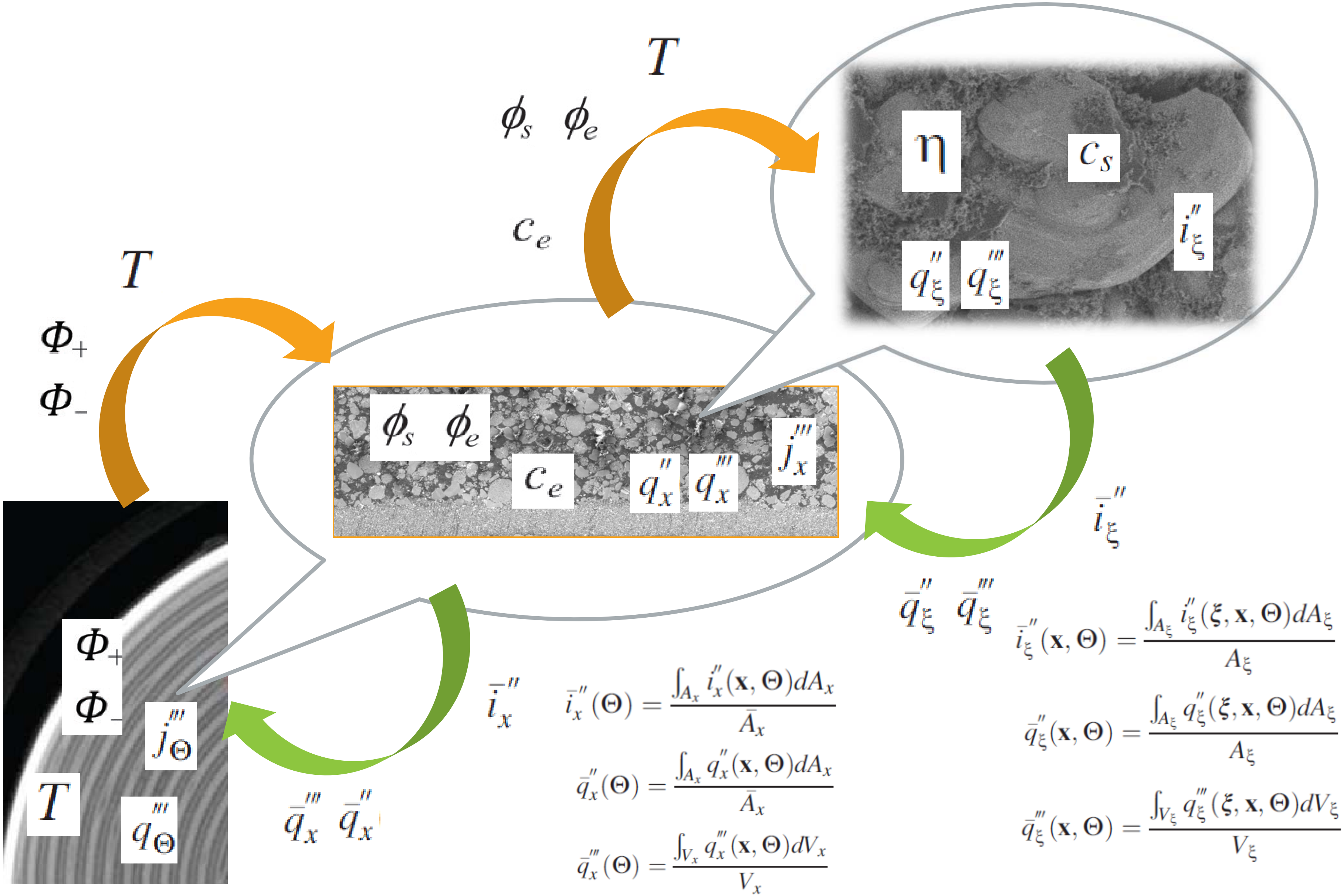
MSMD Protocol for Transferring Information



MSMD Protocol for Transferring Information



MSMD Protocol for Transferring Information



$$\bar{i}''_x(\Theta) = \frac{\int_{A_x} i''_x(\mathbf{x},\Theta)dA_x}{A_x}$$

$$\bar{q}''_x(\Theta) = \frac{\int_{A_x} q''_x(\mathbf{x},\Theta)dA_x}{A_x}$$

$$\bar{q}'''_x(\Theta) = \frac{\int_{V_x} q'''_x(\mathbf{x},\Theta)dV_x}{V_x}$$

$$\bar{i}''_\xi(\mathbf{x},\Theta) = \frac{\int_{A_\xi} i''_\xi(\xi,\mathbf{x},\Theta)dA_\xi}{A_\xi}$$

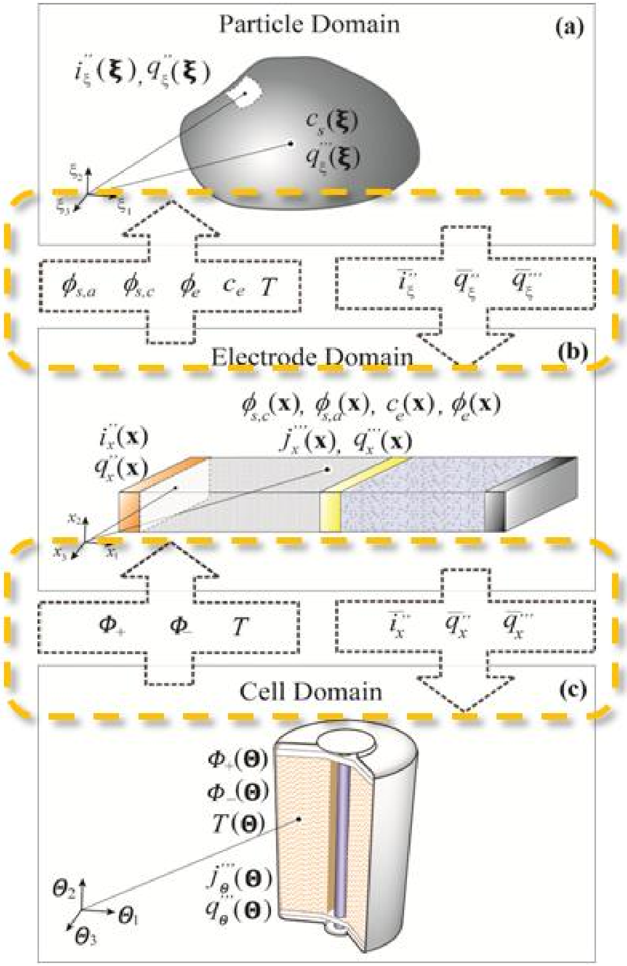
$$\bar{q}''_\xi(\mathbf{x},\Theta) = \frac{\int_{A_\xi} q''_\xi(\xi,\mathbf{x},\Theta)dA_\xi}{A_\xi}$$

$$\bar{q}'''_\xi(\mathbf{x},\Theta) = \frac{\int_{V_\xi} q'''_\xi(\xi,\mathbf{x},\Theta)dV_\xi}{V_\xi}$$

Hierarchical Architecture of MSMD

- ***Modularized flexible framework*** for multi-scale multi-physics battery modeling
- ***Expandable development platform*** providing "pre-defined but expandable communication protocol"

- Charge transfer kinetics
- Li diffusion dynamics in electrode particulates and in electrolyte
- Charge balance
- Energy conservation
- …



Particle Domain

- Charge transfer kinetics
- Li transport in active particles
- …

Electrode Domain

- Charge balance in solid composite electrode matrix
- Charge balance in liquid pore channels
- Li transport in electrolyte
- …

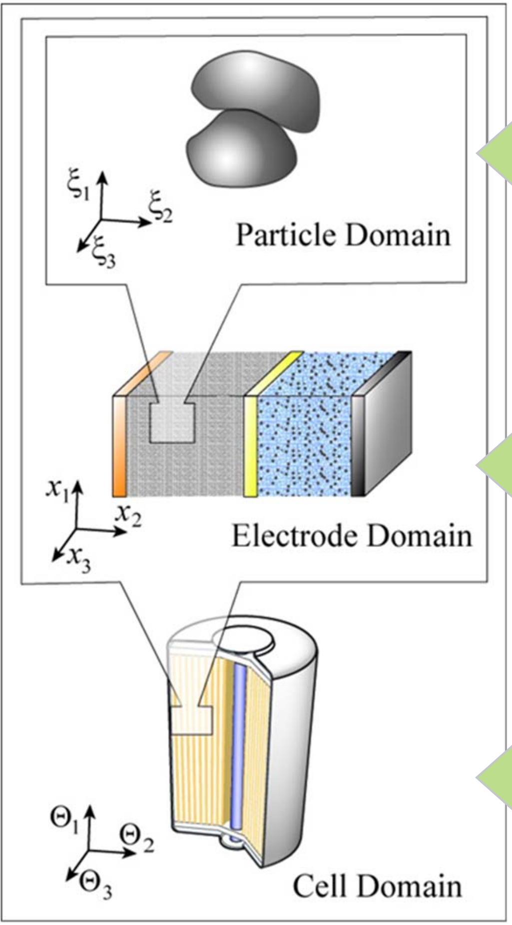
Cell Domain

- Energy conservation
- Charge conservation in current collectors
- …

Kim et al., "Multi-Domain Modeling of Lithium-Ion Batteries Encompassing Multi-Physics in Varied Length Scales," *J. of Electrochemistry*, 2011, Vol. 158, No. 8, pp. A955–A969

Modularized Development

Modularized hierarchical architecture of the MSMD model allows *independent development of submodels* for physics captured in each domain.



Particle Domain Submodel Development

Solution Model/Method Development

Electrode Domain Submodel Development

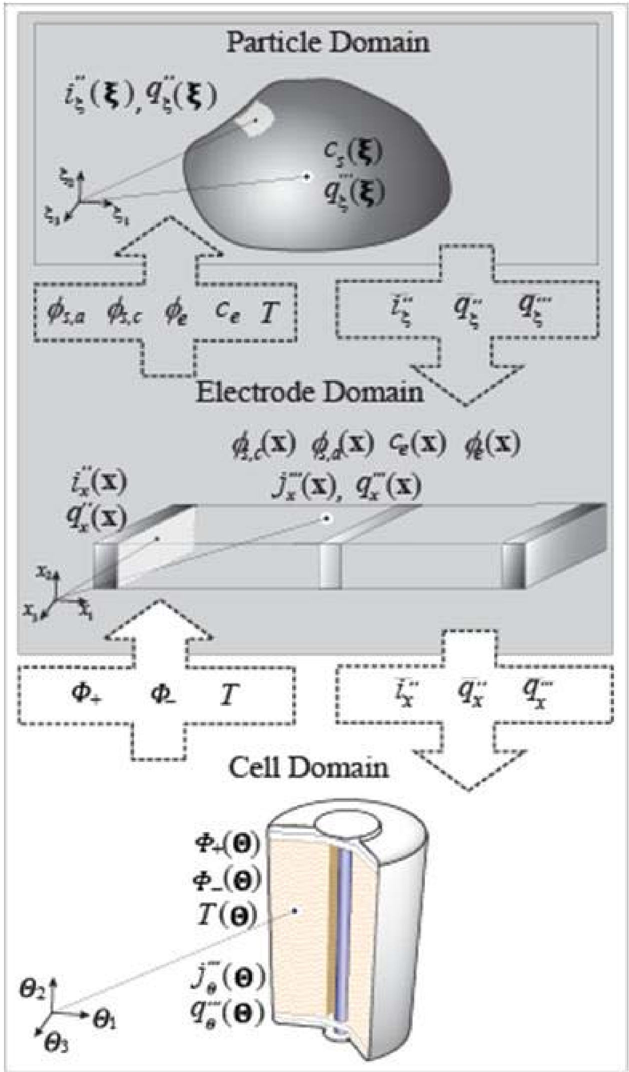
Solution Model/Method Development

Cell Domain Submodel Development

Solution Model/Method Development

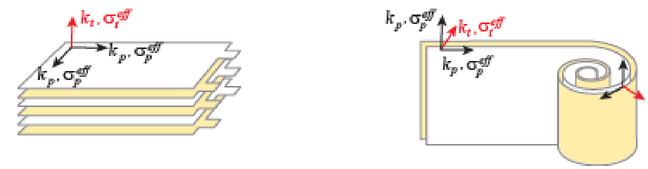
The modularized framework facilitates collaboration with external expertise.

NREL's Cell-Domain Models: Orthotropic Continuum Model



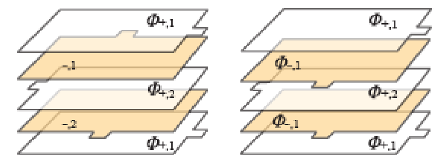
Cell Domain Models

- ***SPPC (Single Potential-Pair Continuum) model:*** applicable to stack prismatic cells, tab-less wound cylindrical/(prismatic) cells:



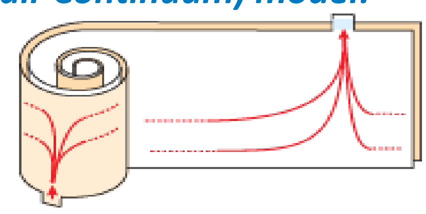
Stacked cell   Wound cell with continuous tab

- ***MPPC (Multi Potential-Pair Continuum) model:*** applicable to alternating stacked prismatic cells:



Alternating stacked cells

- ***WPPC (Wound Potential-Pair Continuum) model:*** applicable to spirally wound cylindrical/ (prismatic) cells:



Cell with discrete tabs

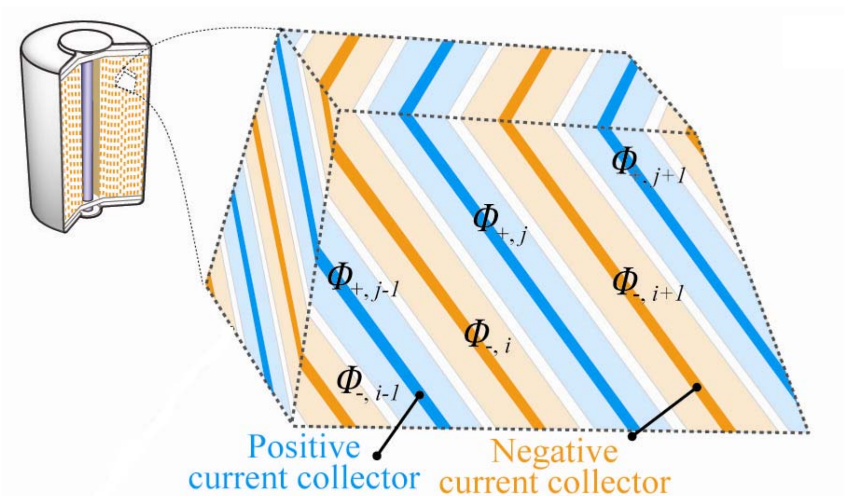
- ***Lumped model:*** applicable to small cells

√ Discussed in this presentation

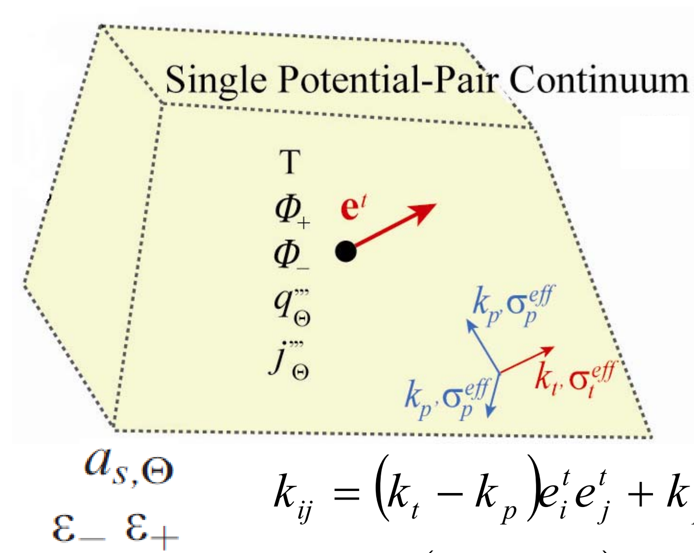
SPPC: Single Potential-Pair Continuum

Cell Composite

Arbitrary finite volume of cell composite



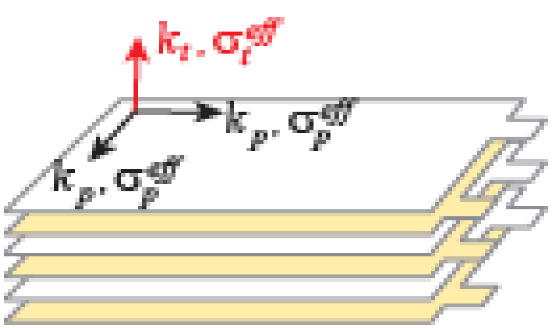
Orthotropic Continuum Model



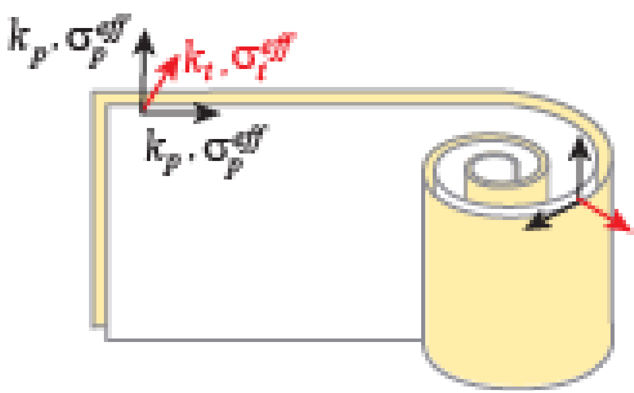
$$k_{ij} = \left(k_t - k_p\right) e_i^t e_j^t + k_p \delta_{ij}$$

$$\sigma_{-\,ij}^{eff} = \left(\delta_{ij} - e_i^t e_j^t\right) \varepsilon_- \sigma_-$$

$$\sigma_{+\,ij}^{eff} = \left(\delta_{ij} - e_i^t e_j^t\right) \varepsilon_+ \sigma_+$$

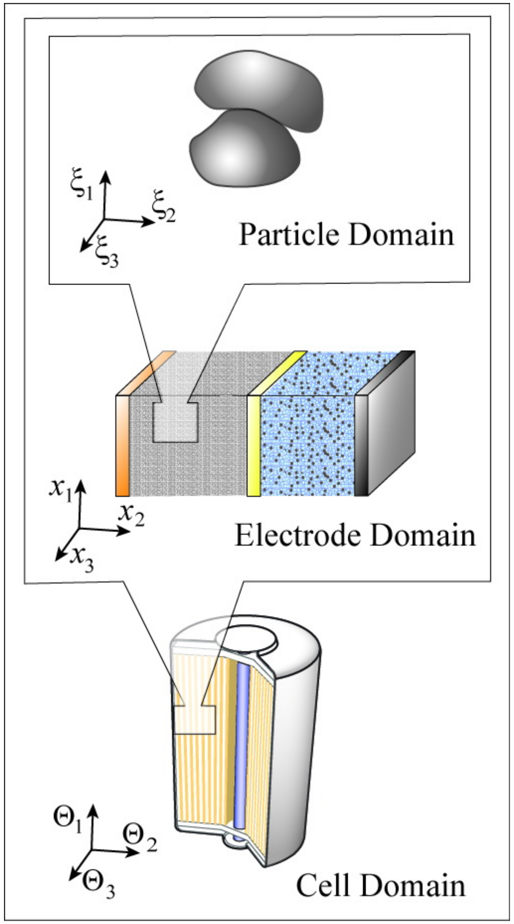


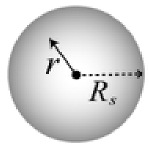
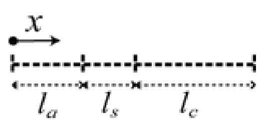
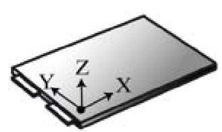
Stacked cell



Wound cell with continuous tab

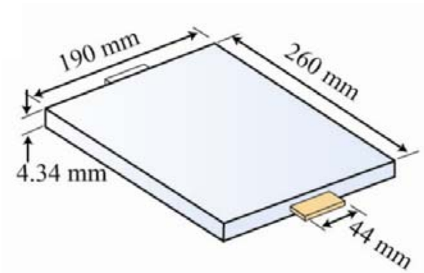
MSMD Application to Prediction of Large Stacked Prismatic Cell Behavior

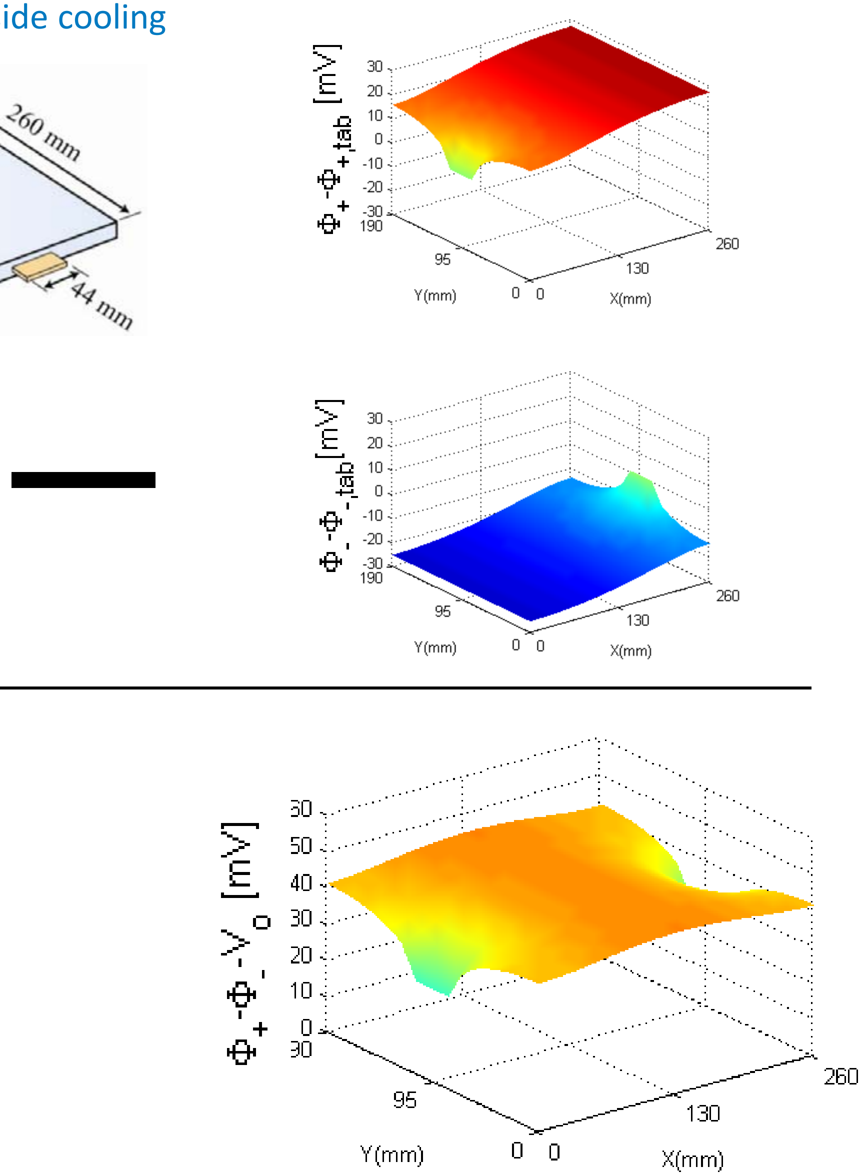


	Submodel Choice	*Solution Method*
Submodel in the Particle Domain		
	• *1D spherical particle model*	• *SVM (state variable method)*
Submodel in the Electrode Domain		
	• *1D porous electrode model*	• *SVM*
Submodel in the Cell Domain		
	• *3D Single Potential-Pair Continuum Model (**SPPC**)*	• *FV-LSM finite volume – linear superposition methods*

Electric Current Transport

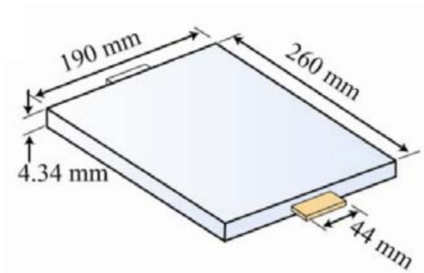
4C discharge / Single-side cooling

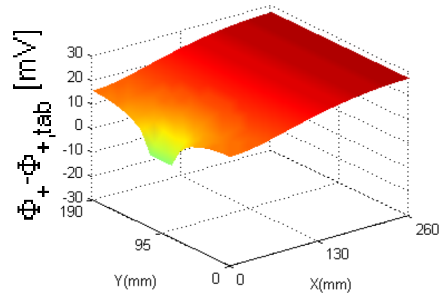


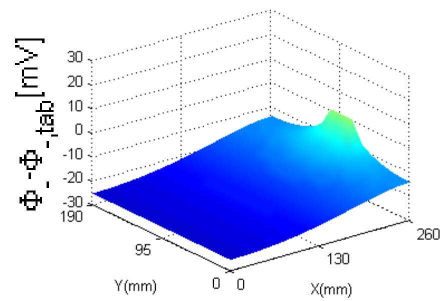


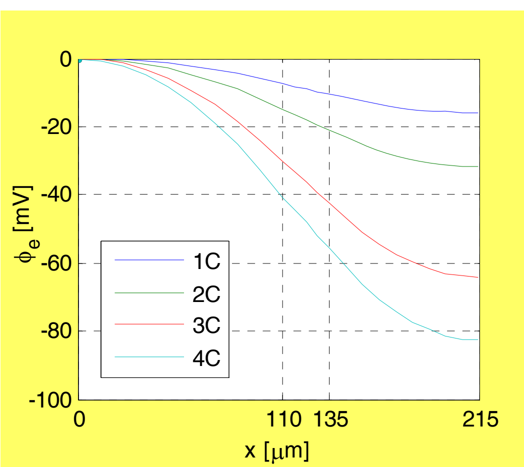
Electric Current Transport

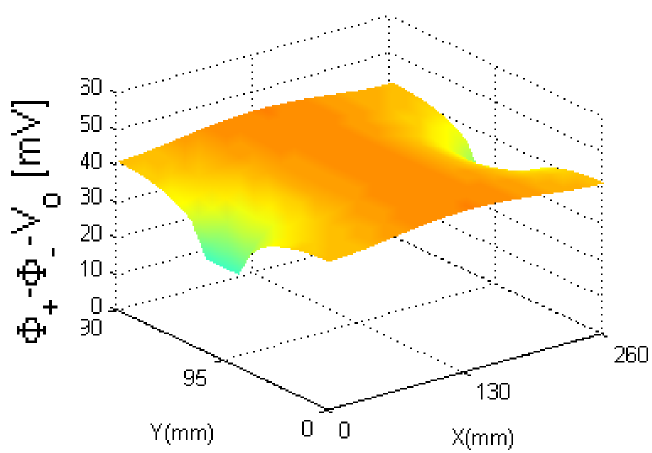
4C discharge / Single-side cooling



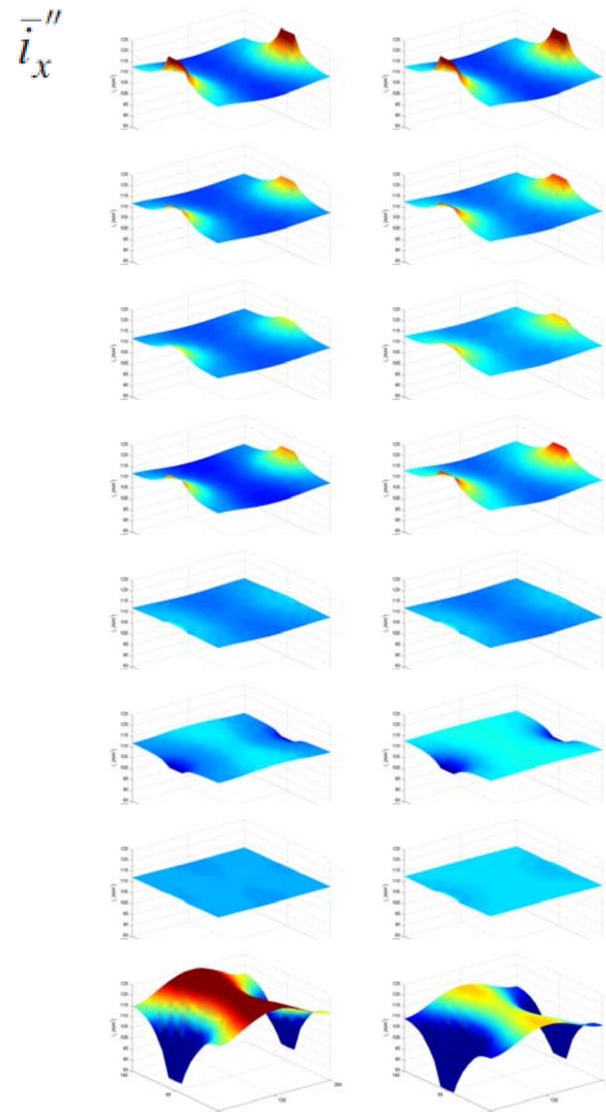






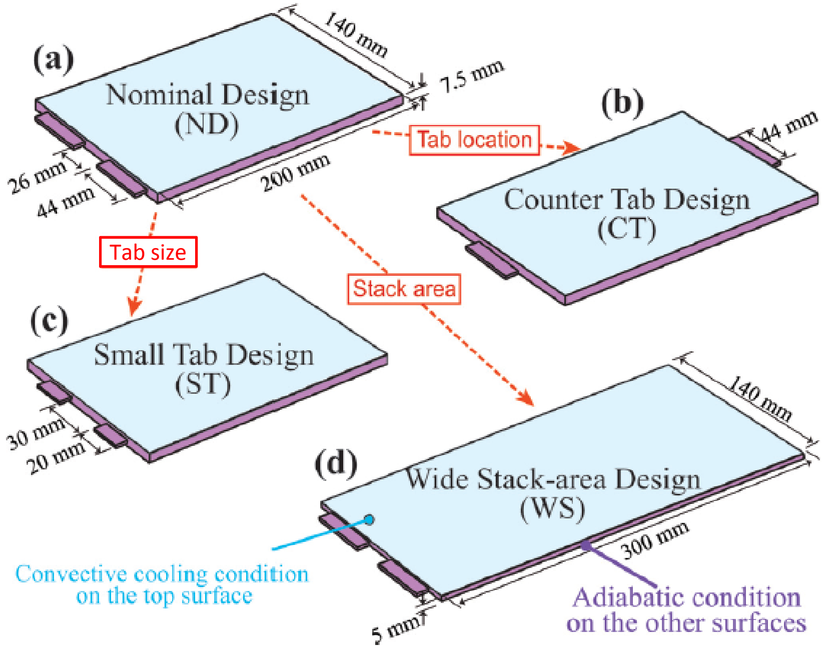


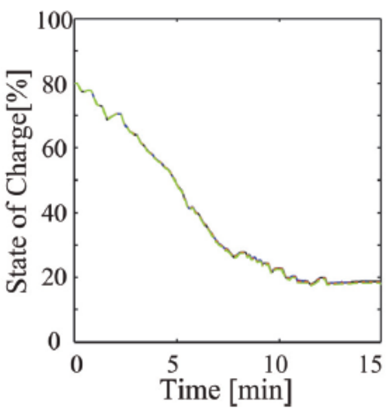
cooled top   bottom

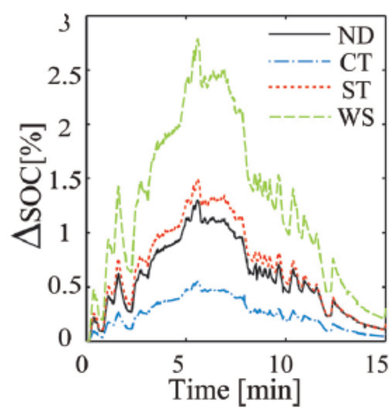


Non-Uniform Utilization

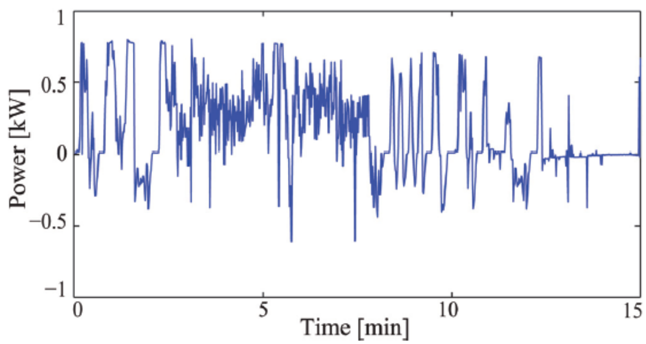
Kim et al., "Multi-Domain Modeling of Lithium-Ion Batteries Encompassing Multi-Physics in Varied Length Scales," *J. of Electrochem.*, 2011, Vol. 158, No. 8, pp. A955–A969

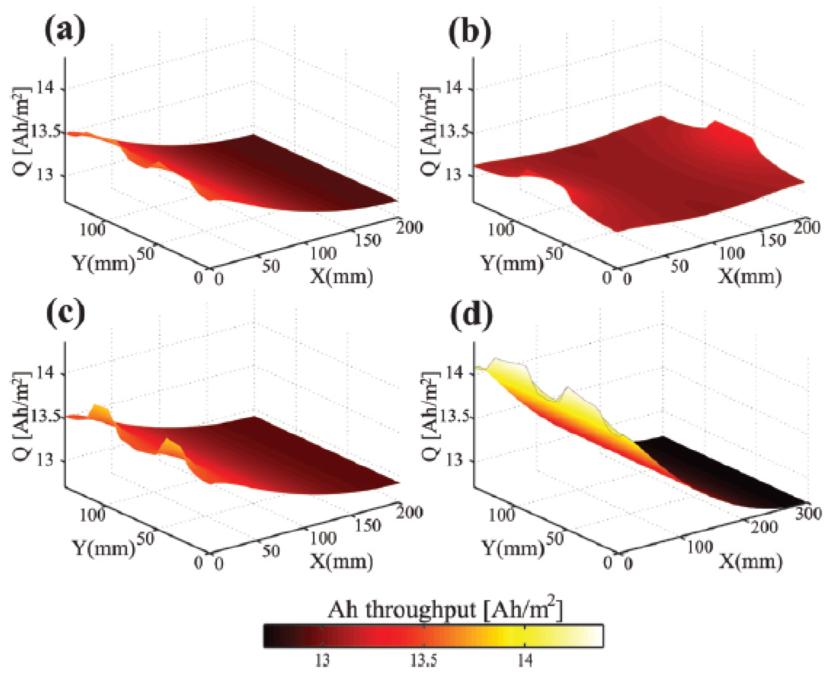






Mid-size sedan PHEV10 US06

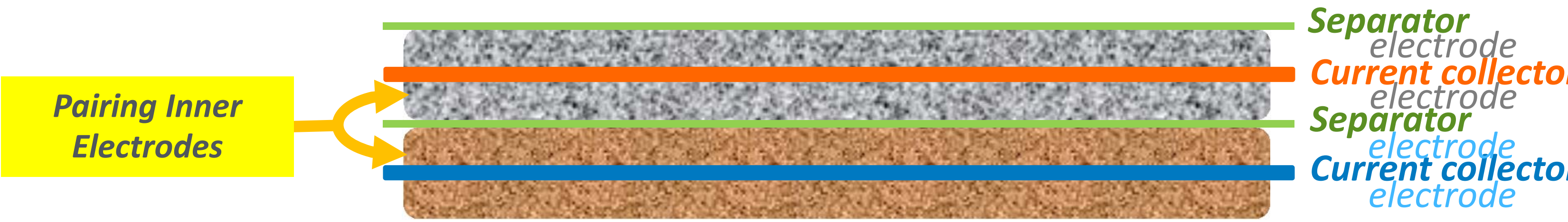




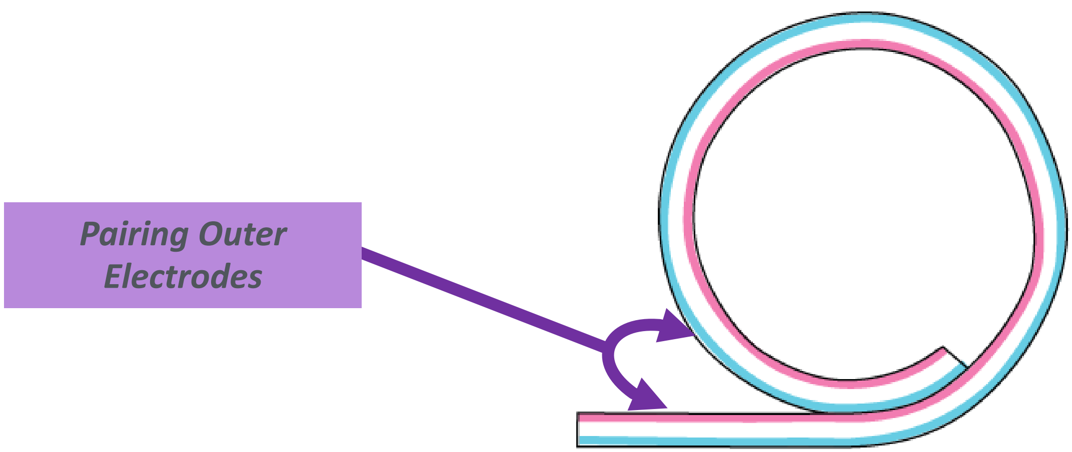
Wound Cells

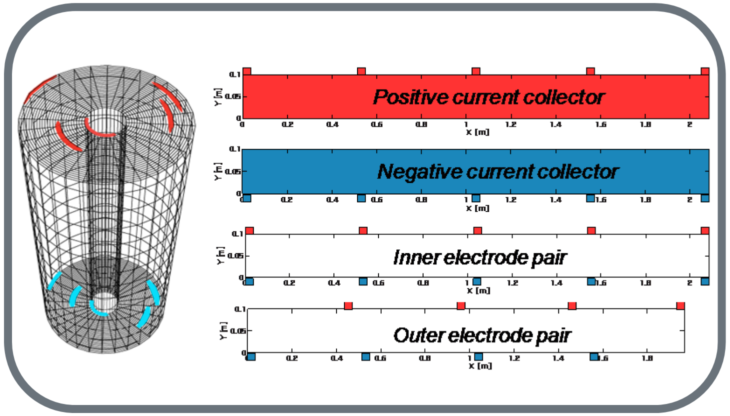
- A pair of ***wide*** current collectors
- Two electrode pairs
- Cylindrical or prismatic cells

***Stacking* : Forming the first pair between inner electrodes**

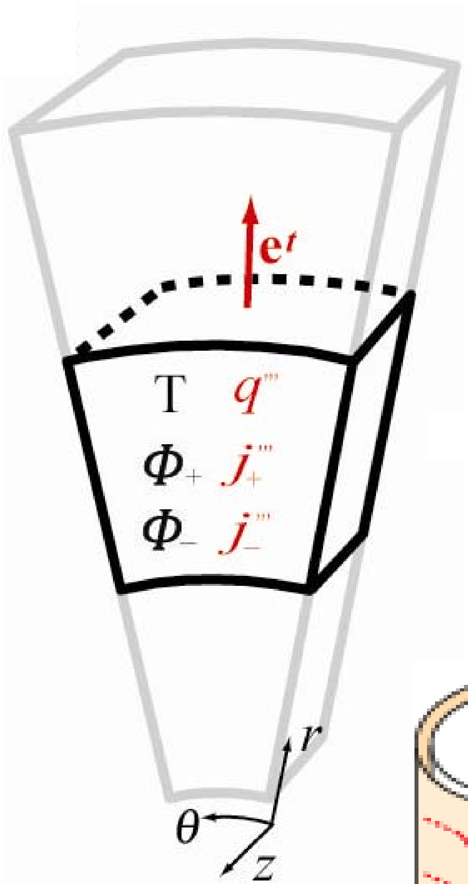


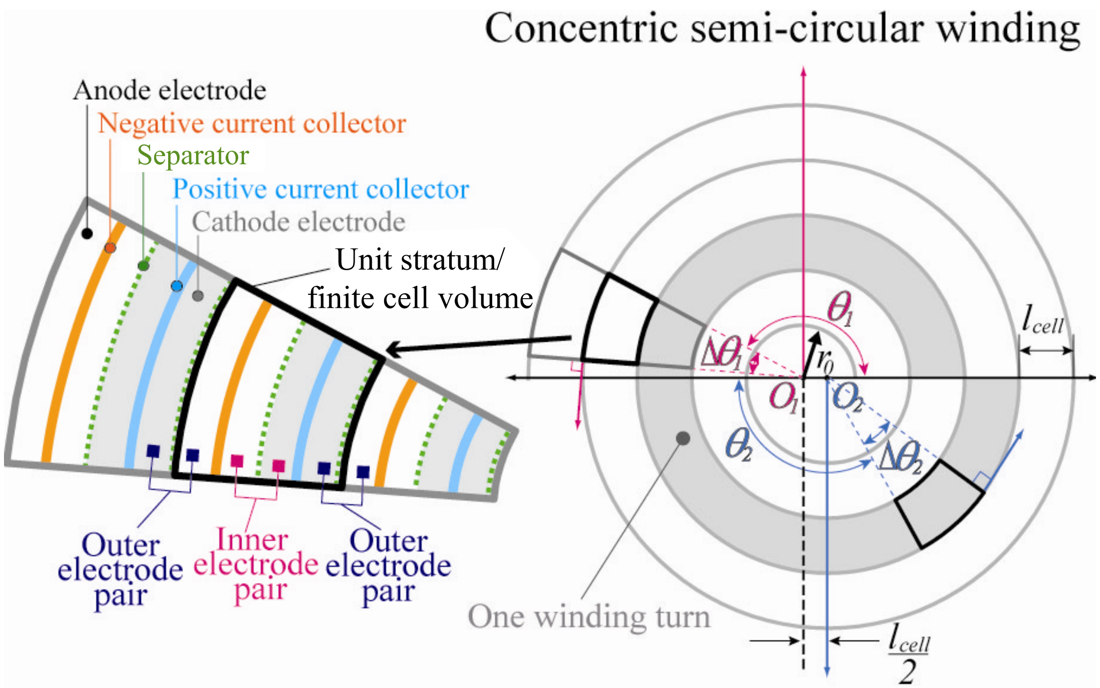
***Winding* : Forming the second pair between outer electrodes**

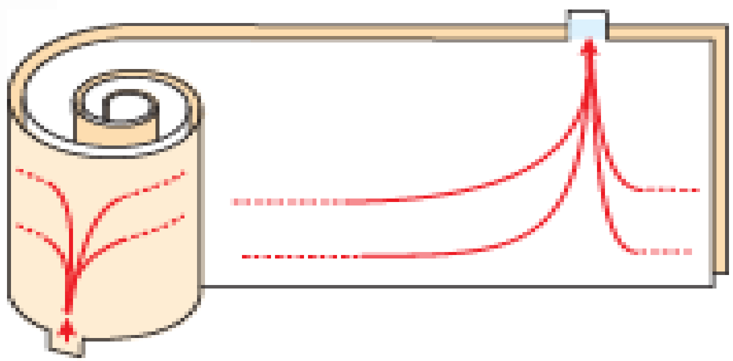




WPPC (Wound Potential-Pair Continuum)



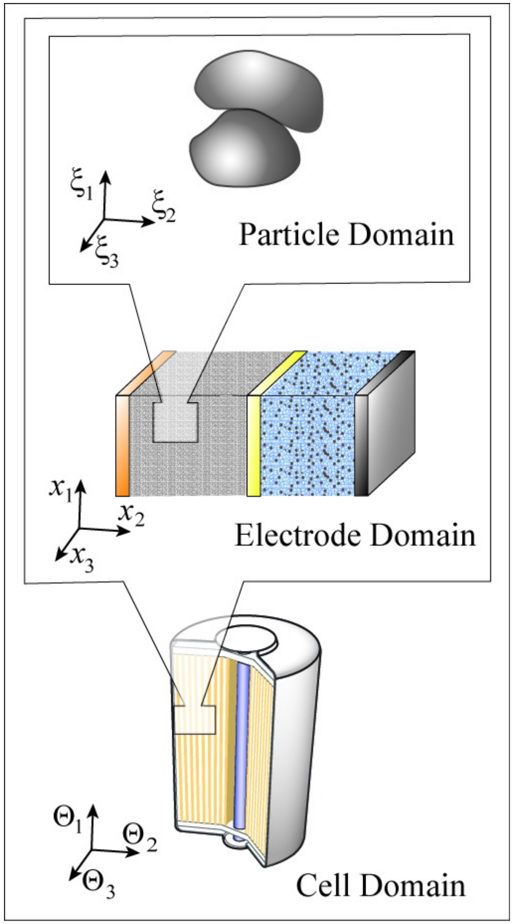


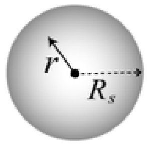
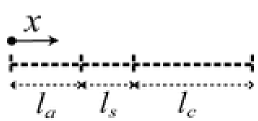


Cell with discrete tabs

Applicable to flat wound prismatic cells

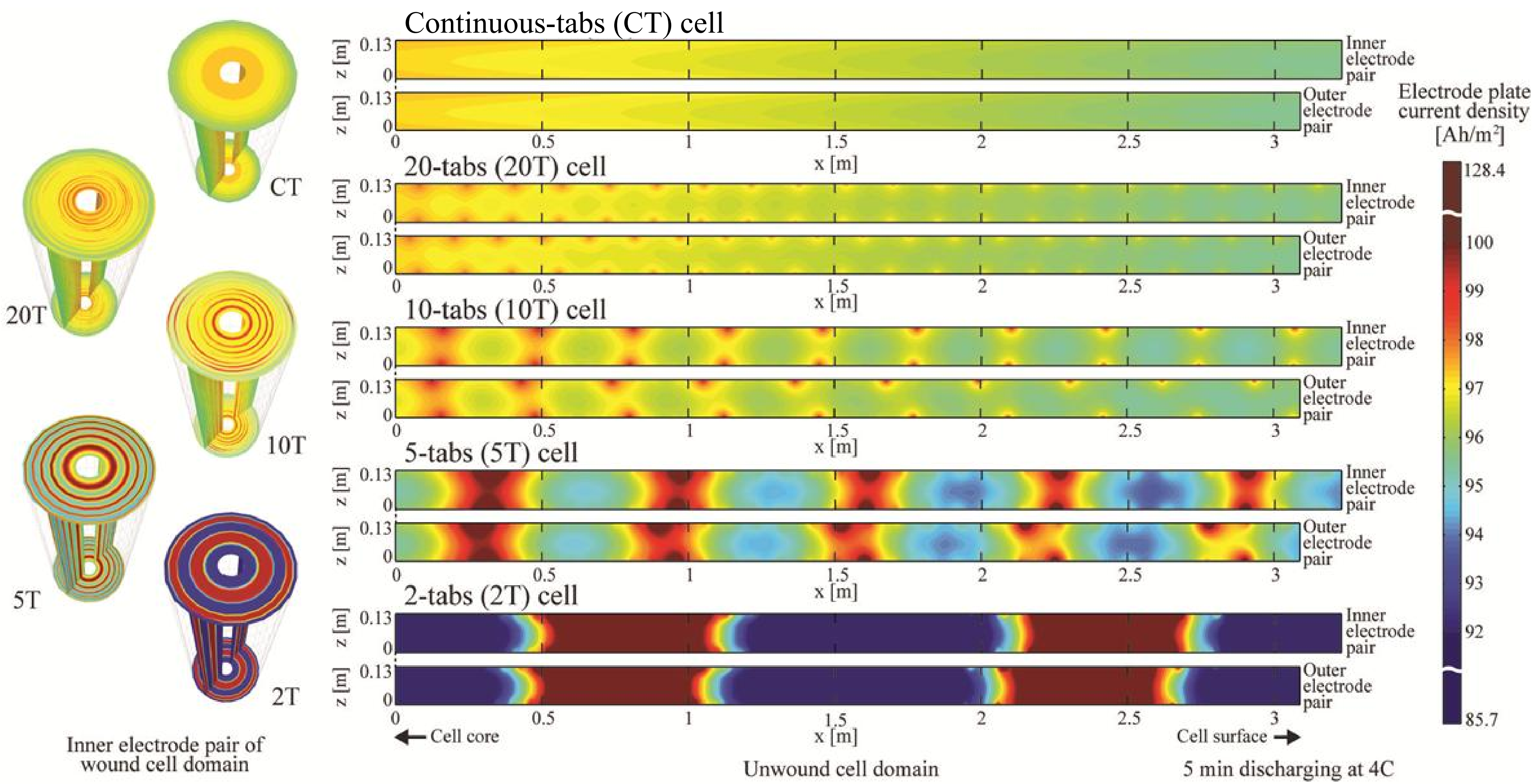
MSMD Application to Prediction of Wound Cylindrical Cell Behavior



	Submodel Choice	*Solution Method*
Submodel in the Particle Domain		
	• *1D spherical particle model*	• *SVM (state variable method)*
Submodel in the Electrode Domain		
	• *1D porous electrode model*	• *SVM*
Submodel in the Cell Domain		
	• *3D Wound Potential-Pair Continuum Model (**WPPC**)*	• *FV-LSM finite volume – linear superposition methods*

Kinetics Response

Impact of electrical current transport design



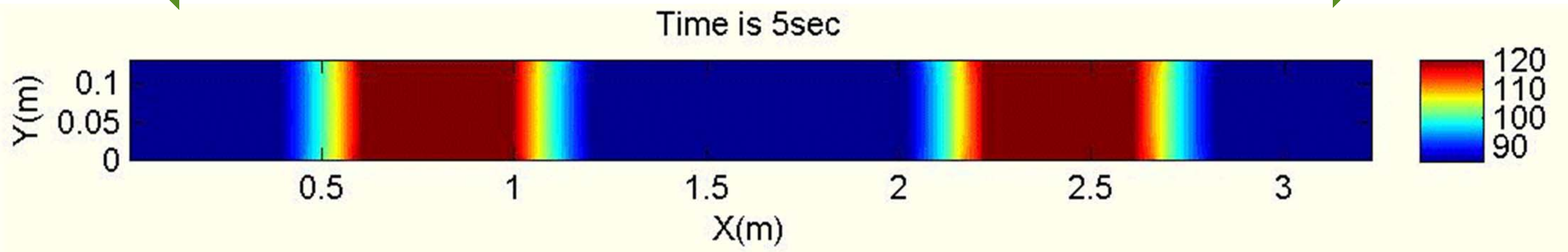
Kyu-Jin Lee, et al., April 2011

Non-uniform Kinetics during 4C Discharge

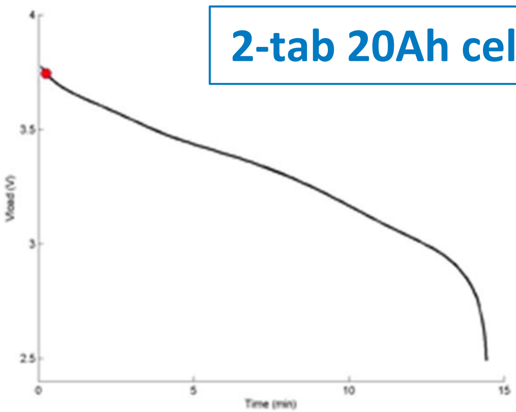
Electrode plate current density [A/m^2] at inner-electrode pair

core

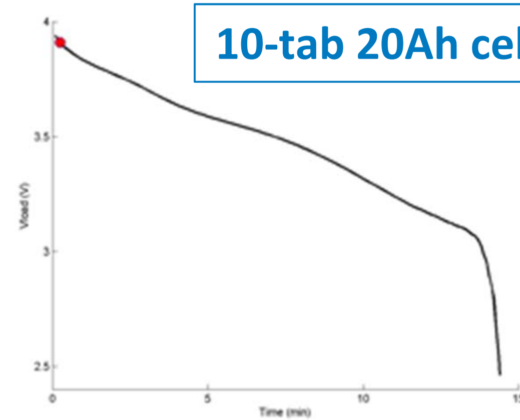
surface

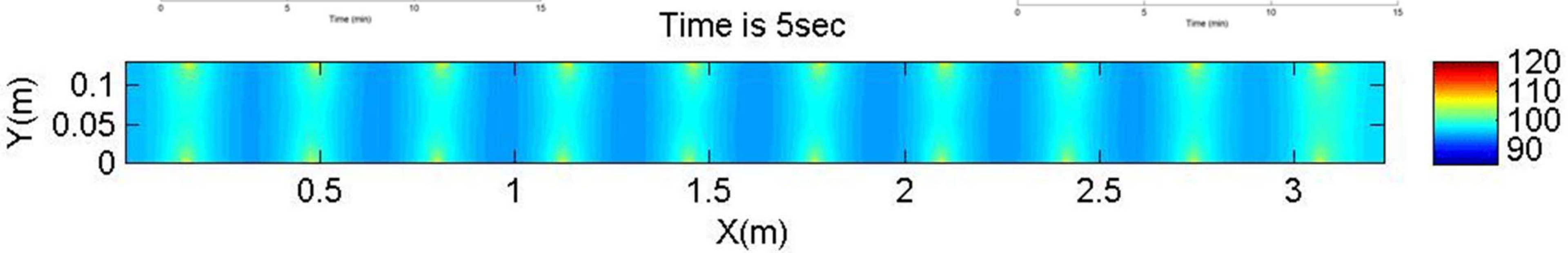


2-tab 20Ah cell



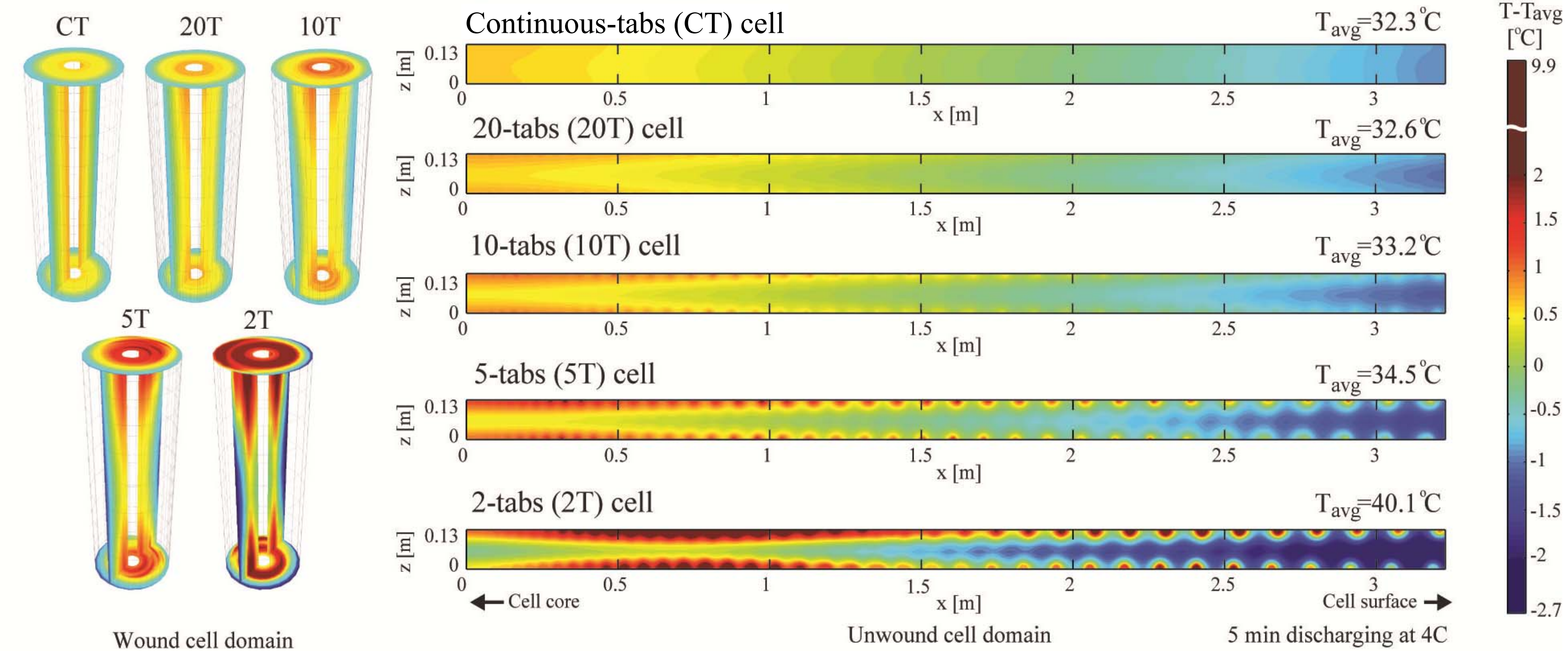
10-tab 20Ah cell





Thermal Response

Impact of electrical current transport design

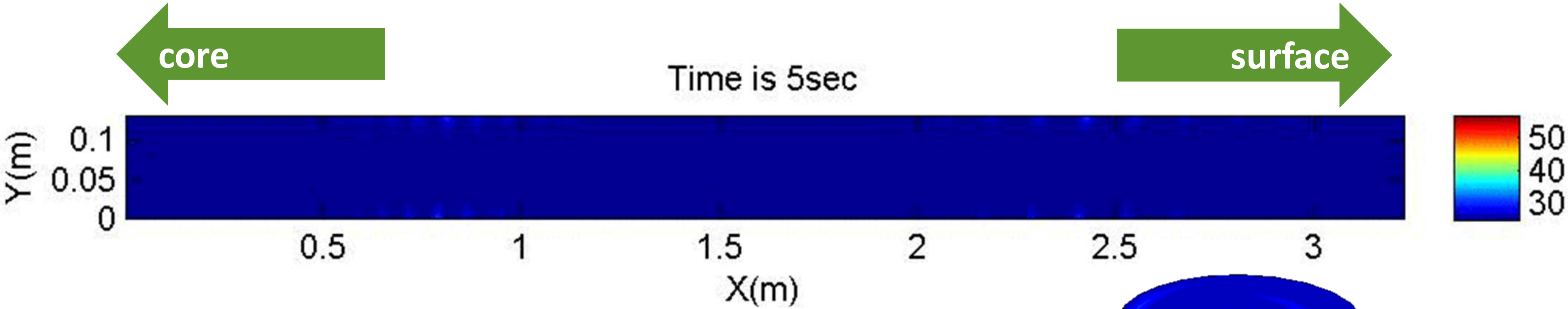


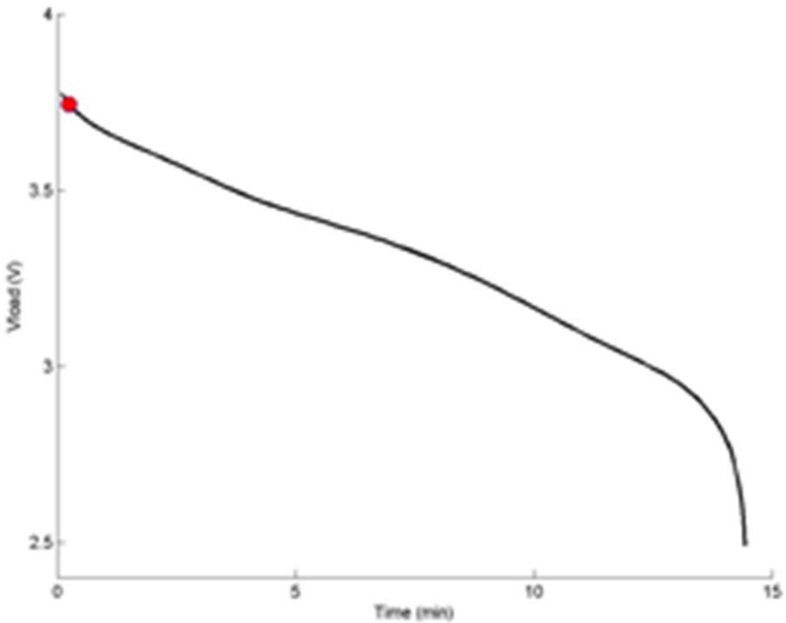
Temperature imbalance at 4C discharge

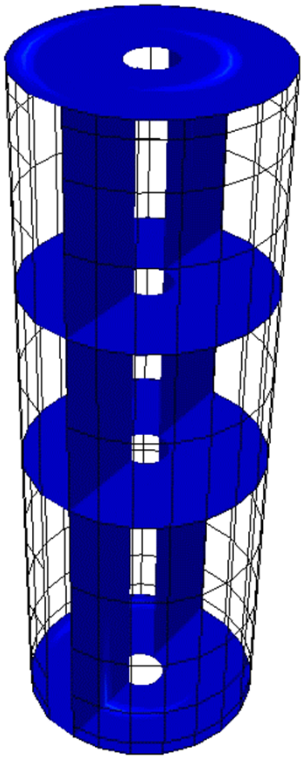
Kyu-Jin Lee, et al., April 2011

Thermal Evolution during 4C Discharge

2-Tab Design

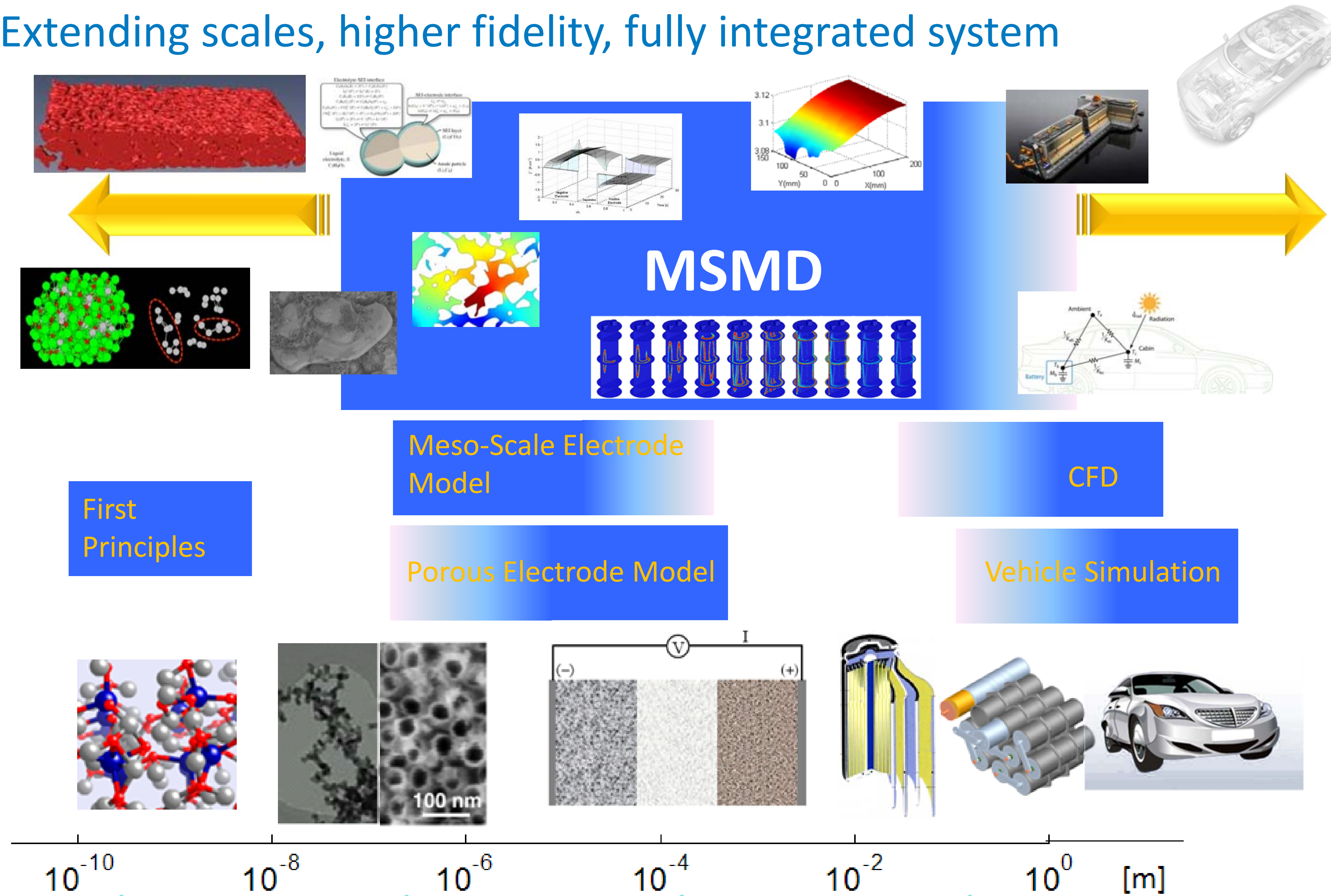






The Road Ahead

Extending scales, higher fidelity, fully integrated system



Acknowledgments

- **Support Provided by the DOE Vehicle Technologies Program**
  - Dave Howell, Hybrid and Electric Systems Team Lead
  - Brian Cunningham, Energy Storage Technology Manager
- **Feedback from CAEBAT Subcontract Technical Leads**
  - Taeyoung Han (General Motors)
  - Steve Hartridge (CD-adapco)
  - Christian Shaffer (EC Power)
- **NREL Support for CAEBAT Implementation**
  - Terry Penney
  - Barbara Goodman
  - Michael Sprague
  - Kathy Roque
  - John Enoch