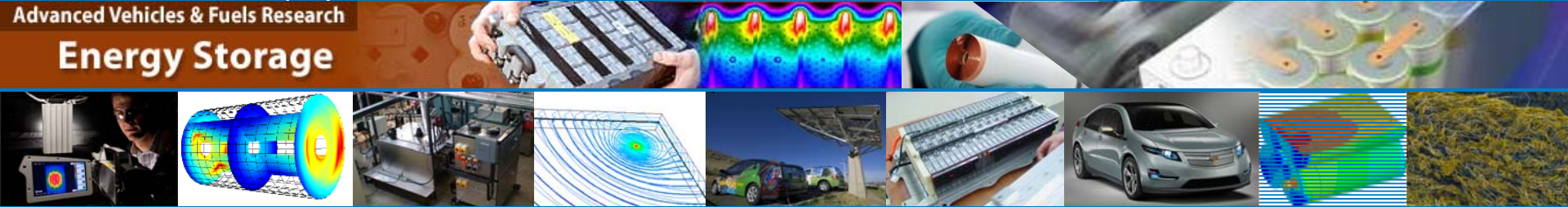


Computer-Aided Engineering of Batteries for Designing Better Li-Ion Batteries

Advanced Vehicles & Fuels Research
Energy Storage



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

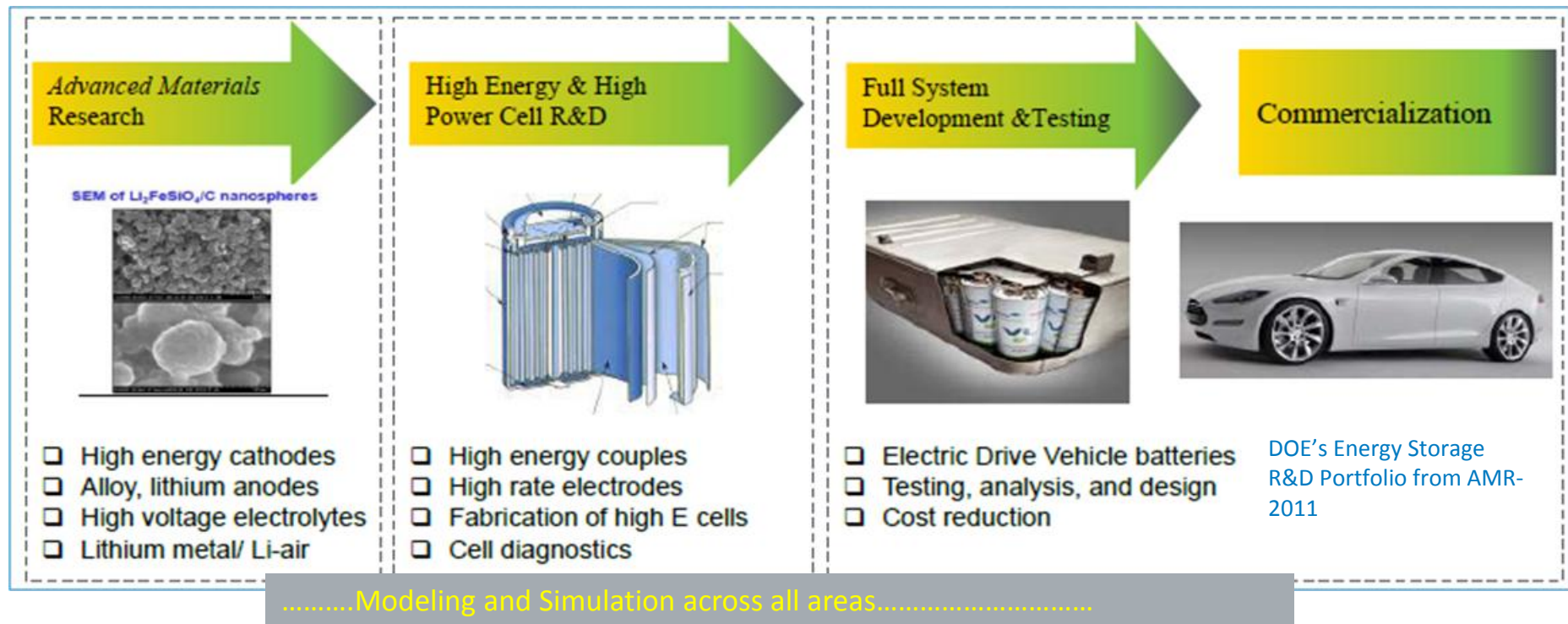
Advanced Automotive Battery Conference
Battery Modeling Software and Applications Workshop
Orlando, Florida, February 6, 2012

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.



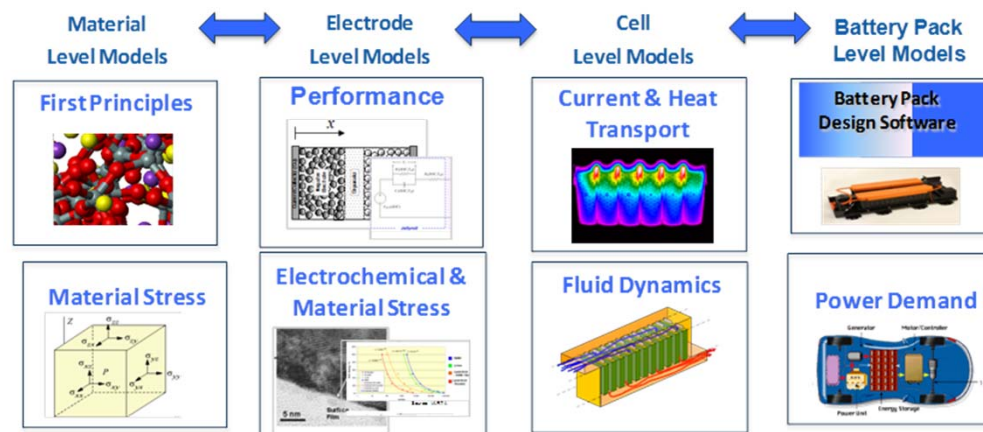
- NREL ES Objective: Support DOE and industry to achieve energy storage targets through research and development, testing, analysis, design, and modeling.

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

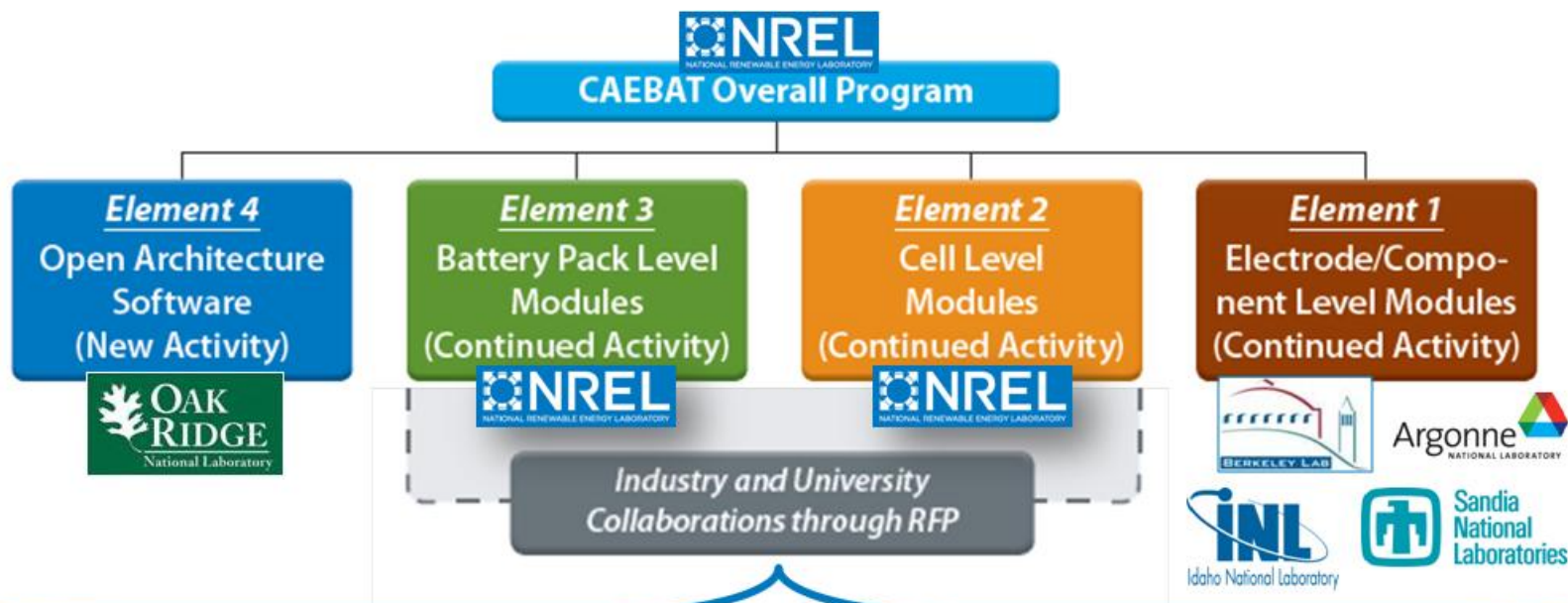
- **There are a number of battery models in academia, national labs, and industry, but they either**
 - Include relevant physics details, but mostly neglect engineering complexities, or
 - Include relevant macroscopic geometry and system conditions in 3D, but use too many simplifications in fundamental 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.








PENN STATE



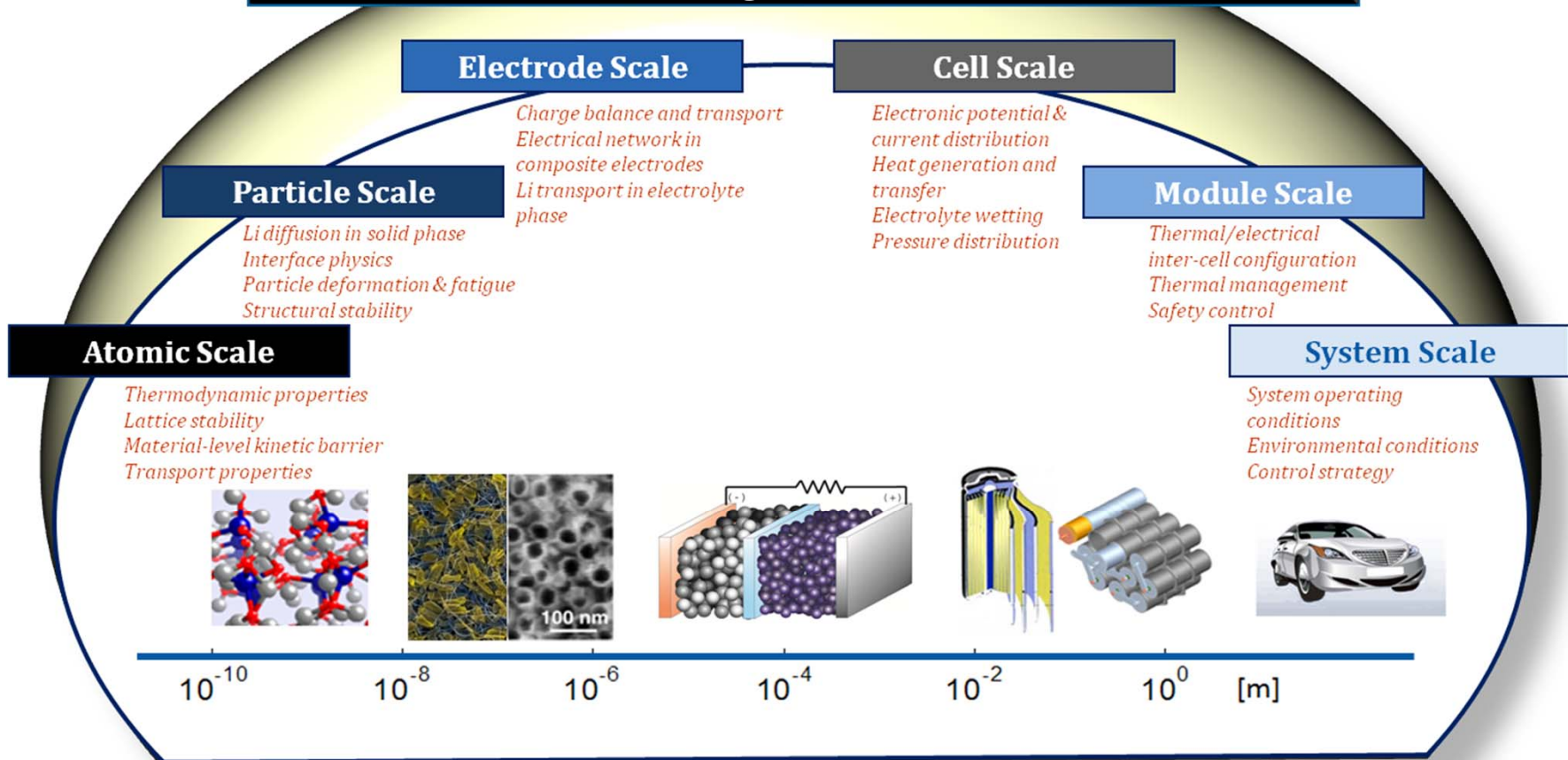
NREL's Role in the CAEBAT Project

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	<ul style="list-style-type: none"> • Electrical, thermal & fluid flow • Performance, detailed cooling design • Commercial software (restrictive assumptions)
Electrochemical-thermal ("MSMD")		1-D, 2-D & 3-D	<ul style="list-style-type: none"> • Electrochemical, electrical & thermal • Performance, design
Electrochemical-thermal-degradation ("MSMD-life")		1-D, 2-D & 3-D	<ul style="list-style-type: none"> • Electrochemical, electrical & thermal • Cycling- & thermal-induced degradation • Performance, design, life prediction
Thermal abuse reaction kinetics		Thermal network, 2-D & 3-D	<ul style="list-style-type: none"> • Chemical & thermal • Safety evaluation
Internal short circuit		3-D	<ul style="list-style-type: none"> • Chemical, electrical, electrochem. & thermal • Safety evaluation

Battery Performance, Durability and Safety

Multi-physics Interactions Across Varied Length Scales

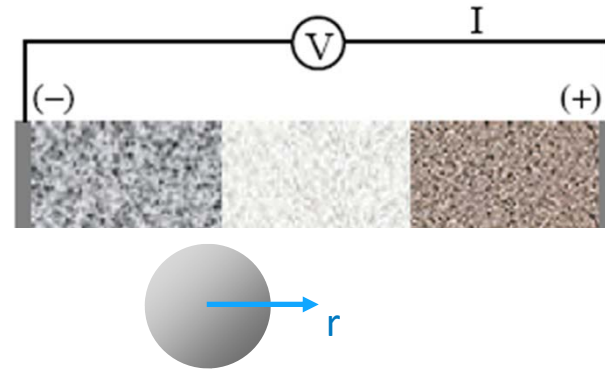


Porous Electrode Model – Commonly Used

Charge Transfer Kinetics at Reaction Sites

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

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



Species Conservation

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

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

Charge Conservation

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

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

Energy Conservation

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

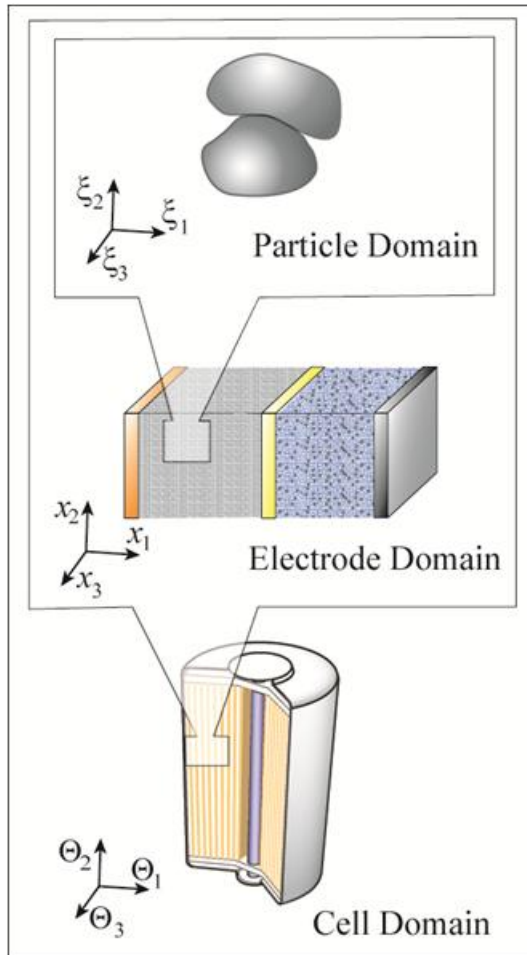
$$q''' = j^{Li} \left(\phi_s - \phi_e - U + T \frac{\partial U}{\partial T} \right) + \sigma^{eff} \nabla \phi_s \cdot \nabla \phi_s + \kappa^{eff} \nabla \phi_e \cdot \nabla \phi_e + \kappa_D^{eff} \nabla \ln c_e \cdot \nabla \phi_e$$

- 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.



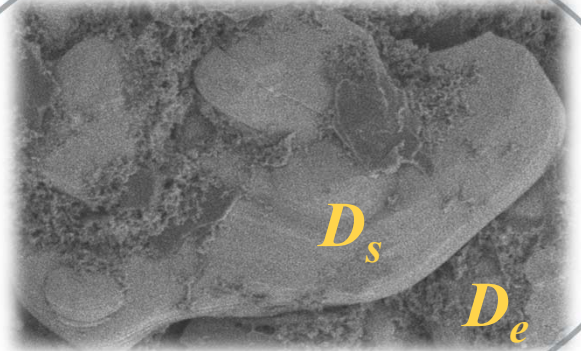
- Introduce **multiple computational domains** for corresponding length scale physics
- **Decouple LIB geometries** into separate computation domains
- **Couple physics** using the predefined inter-domain information exchange
- **Selectively resolve higher spatial resolution** for smaller characteristic 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

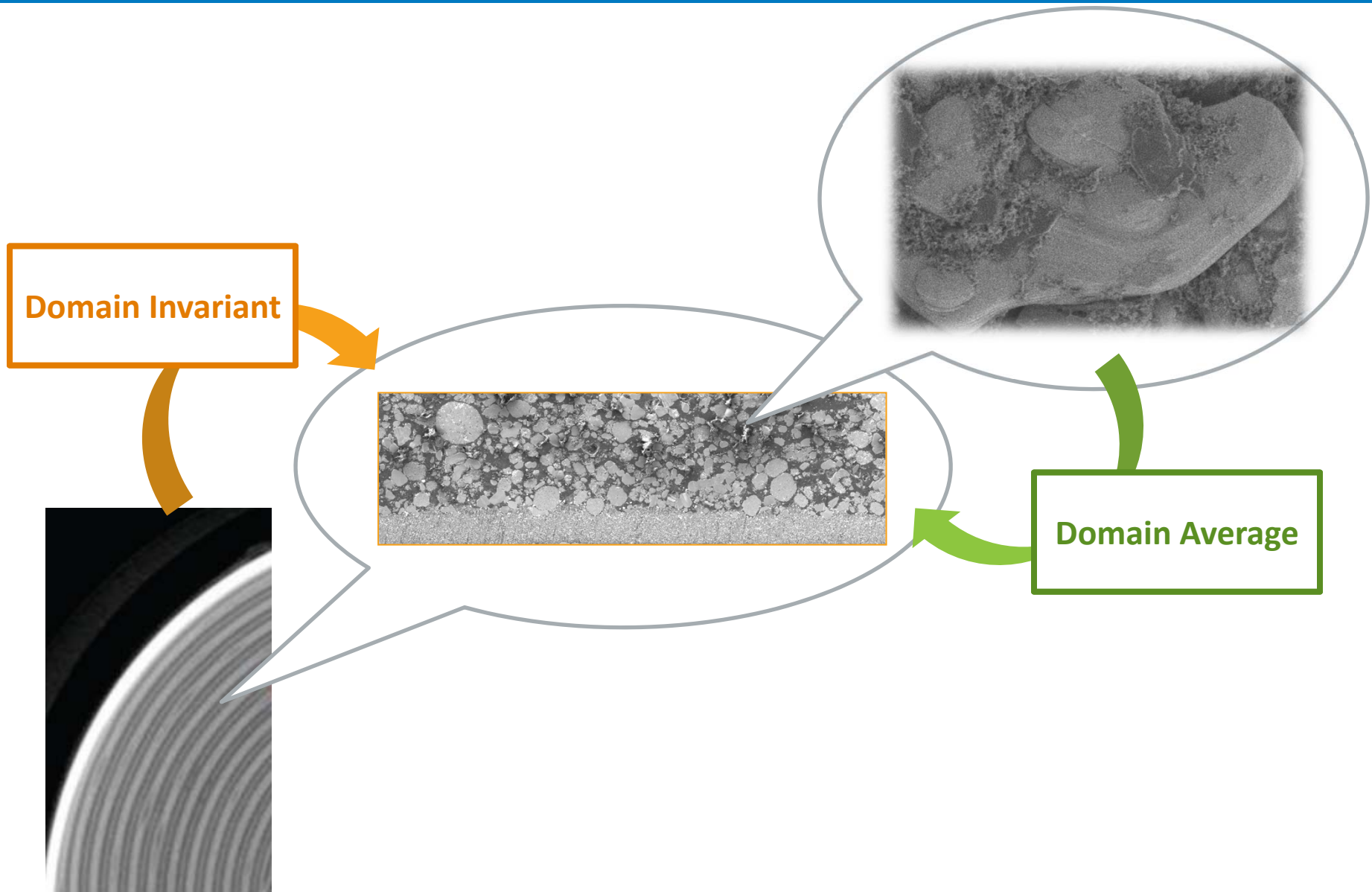
$$\text{e.g., } D_s \ll D_e$$

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

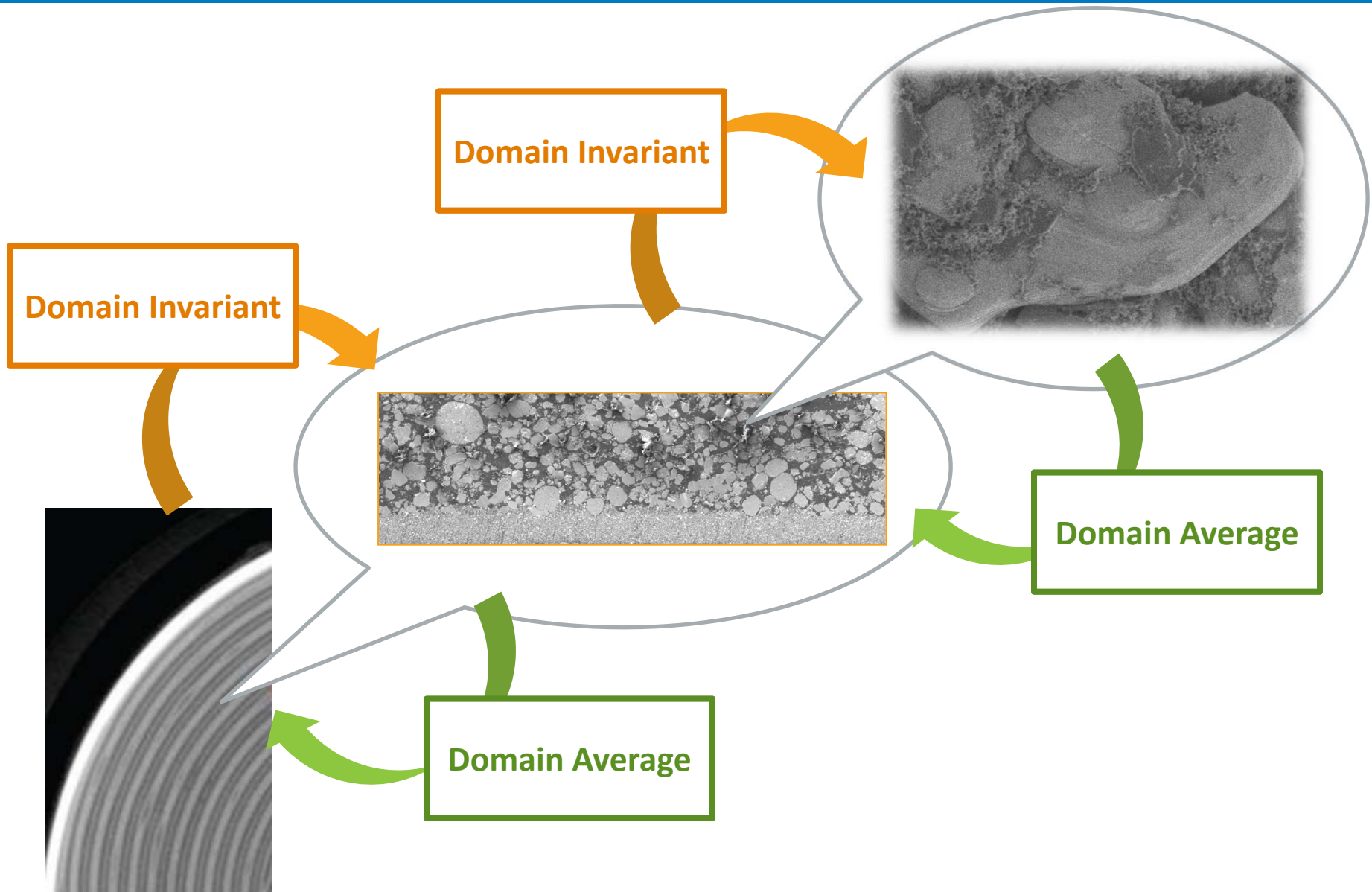
$$\text{e.g., } \sigma_{ce} \ll \sigma_{cc}$$

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

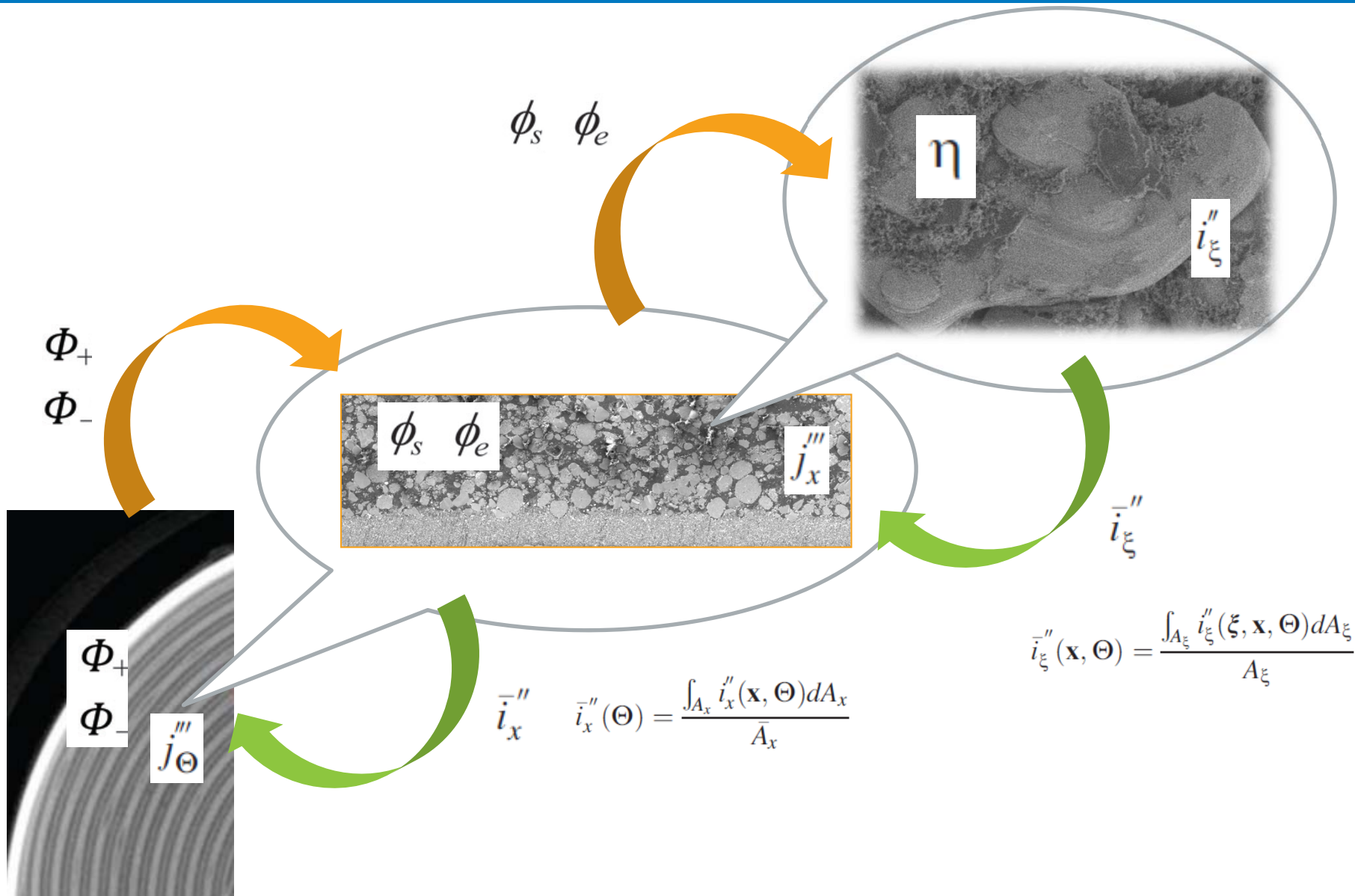
Geometry Decoupling



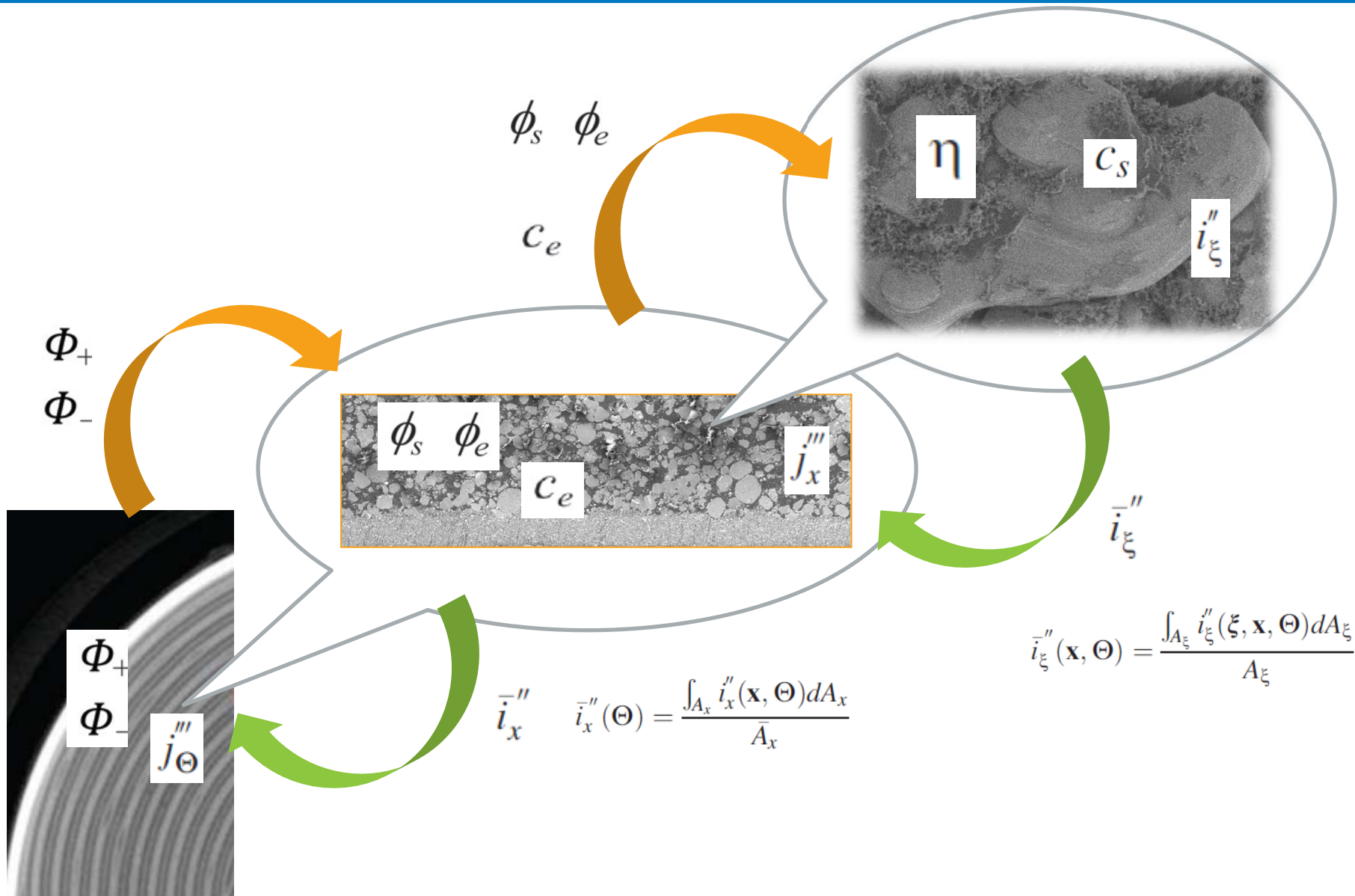
Geometry Decoupling



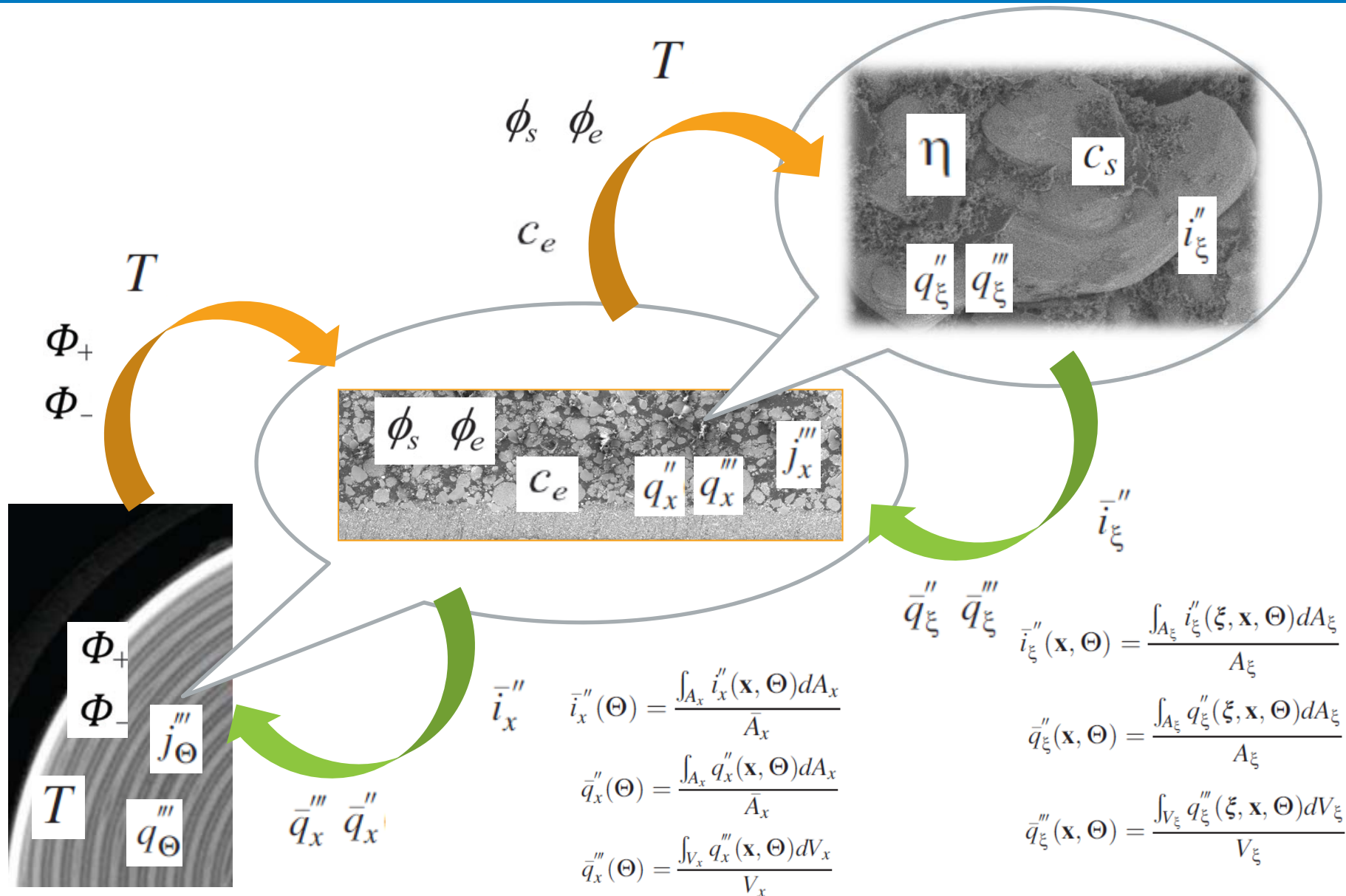
MSMD Protocol for Transferring Information



MSMD Protocol for Transferring Information

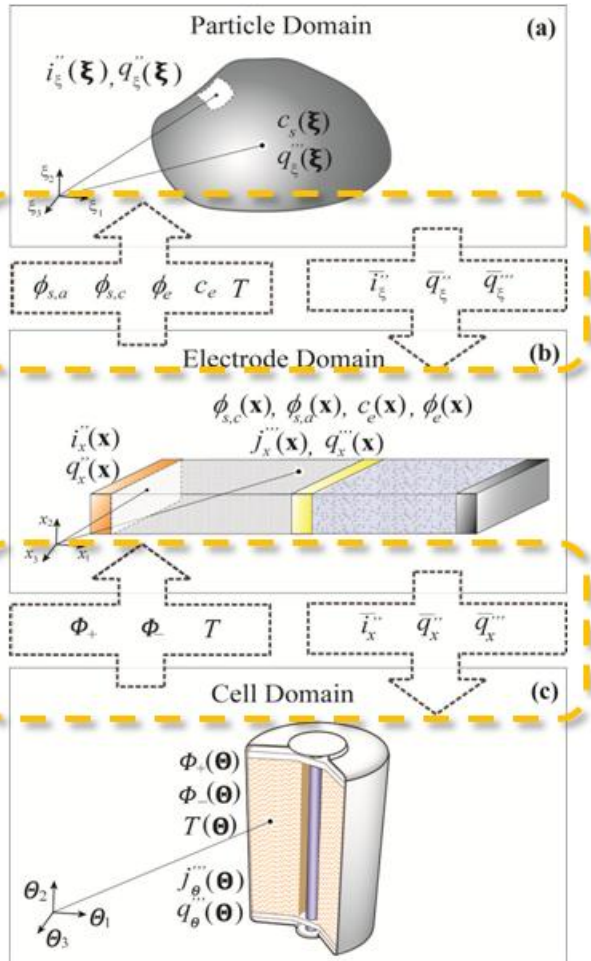


MSMD Protocol for Transferring Information



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
- ...

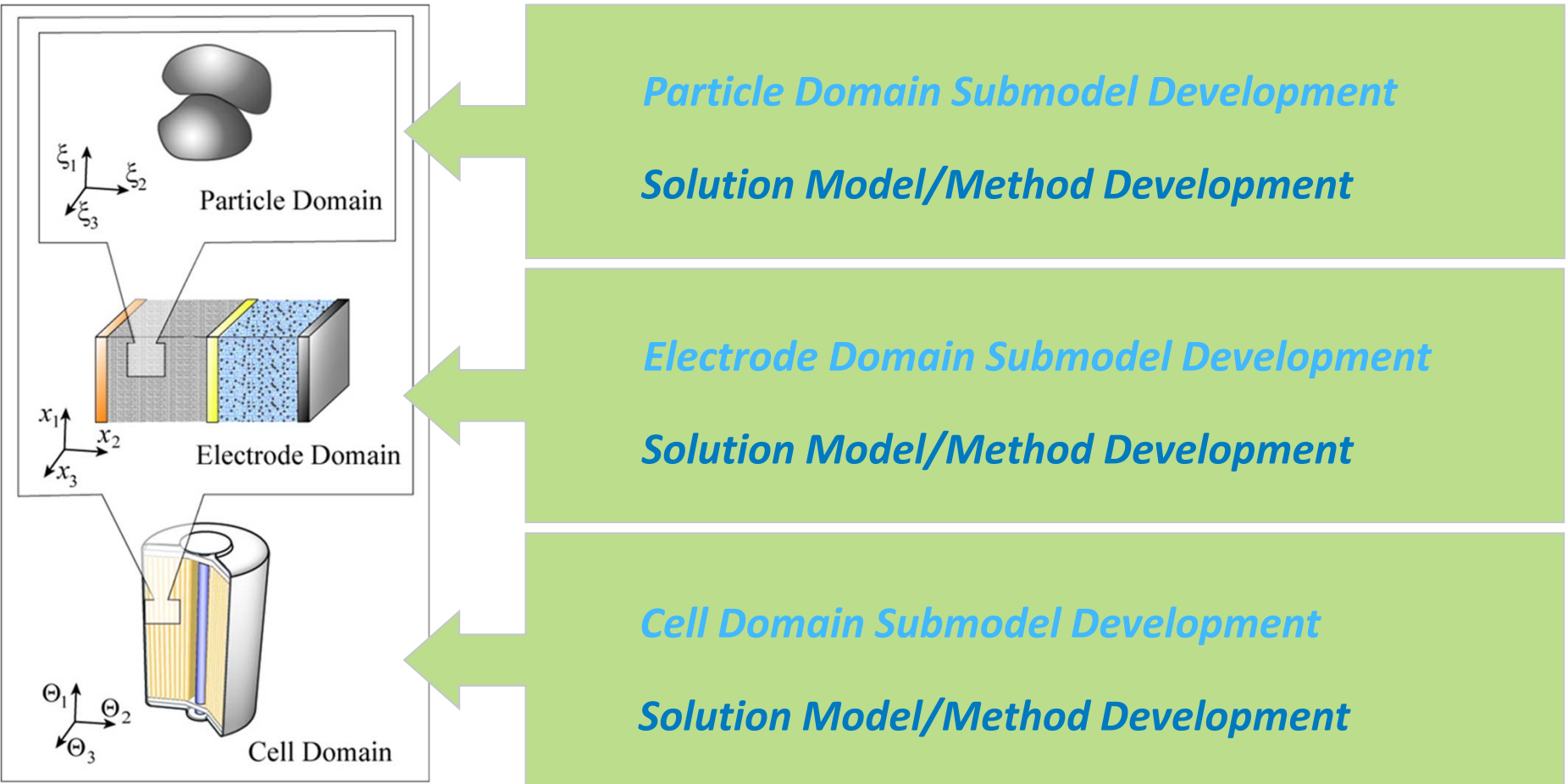
Cell Domain

- 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

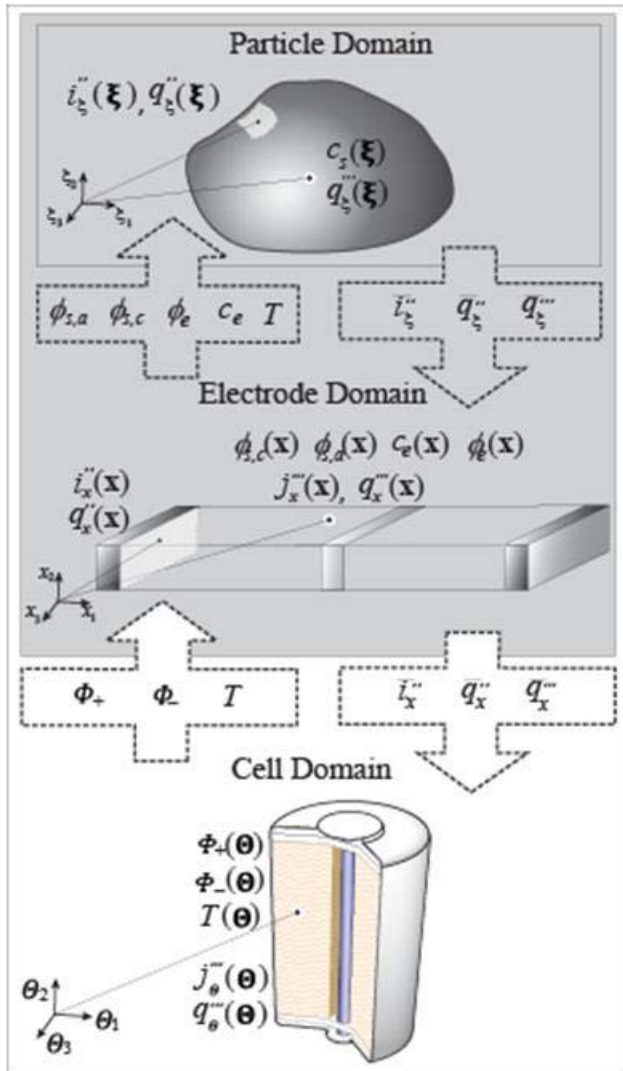
Modularized Development

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



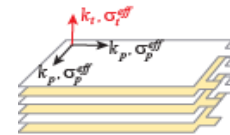
The modularized framework facilitates collaboration with external expertise.

NREL's Cell-Domain Models: Orthotropic Continuum Model

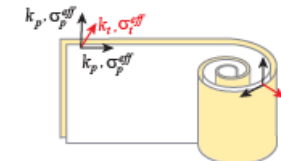


Cell Domain Models

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

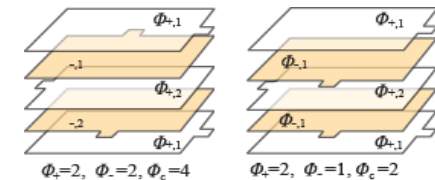


Stacked cell



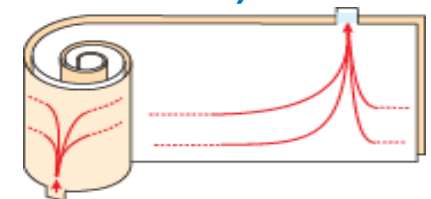
Wound cell with continuous tab

- **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

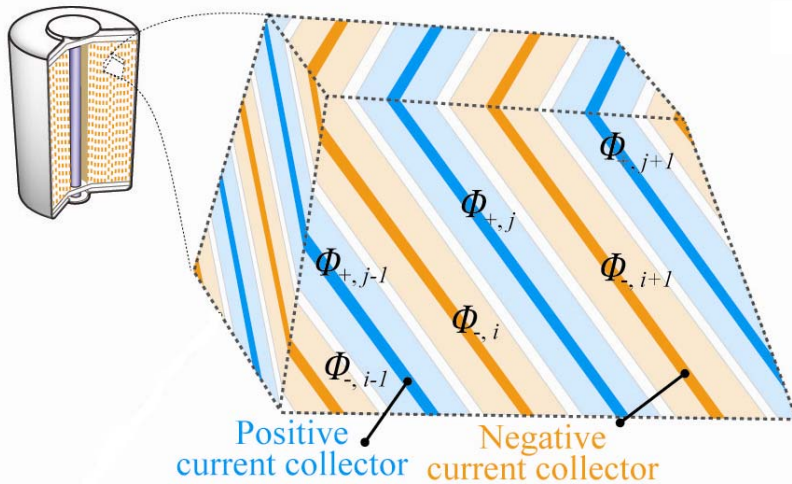
- **Lumped model:** applicable to small cells

✓ Discussed in this presentation

SPPC: Single Potential-Pair Continuum

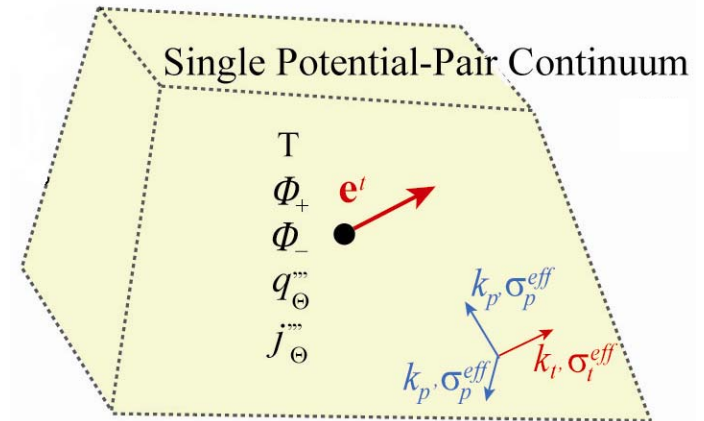
Cell Composite

Arbitrary finite volume of cell composite



Positive current collector
Negative current collector

Orthotropic Continuum Model

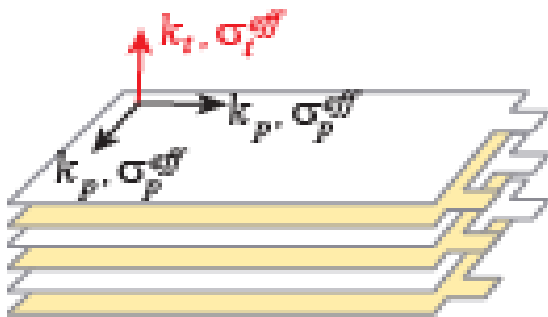


$a_{S,\Theta}$
 $\varepsilon_- \varepsilon_+$

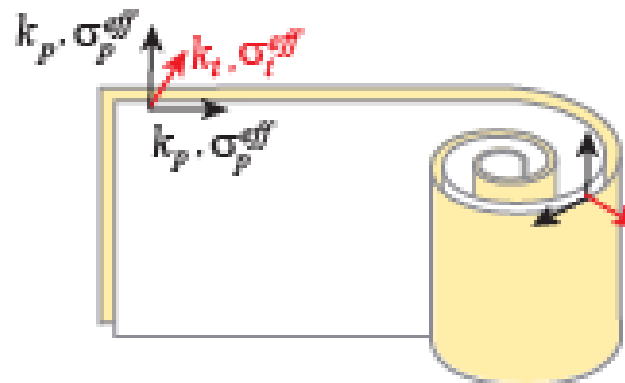
$$k_{ij} = (k_t - k_p) e_i^t e_j^t + k_p \delta_{ij}$$

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

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

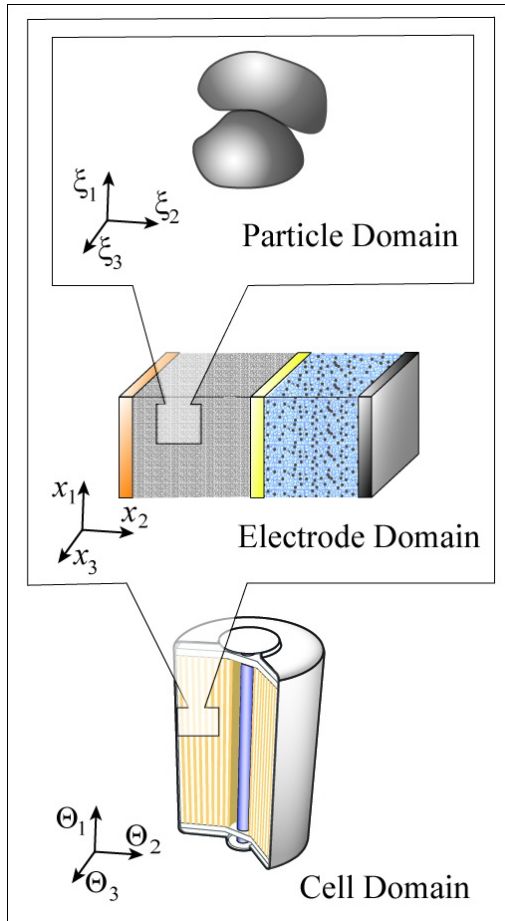


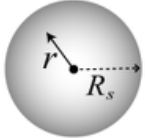
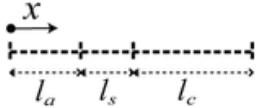
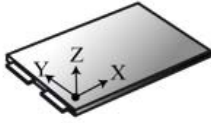
Stacked cell



Wound cell with continuous tab

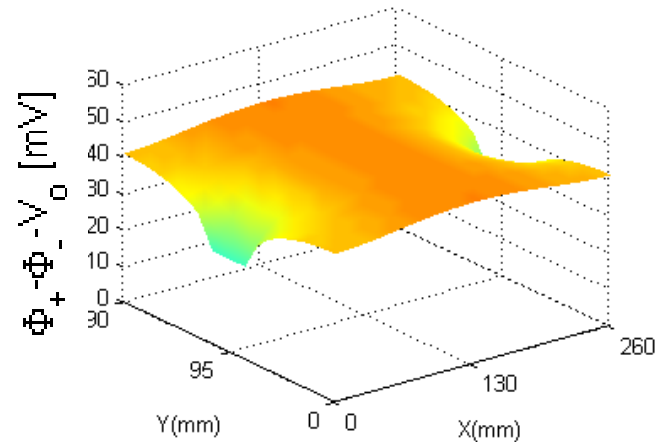
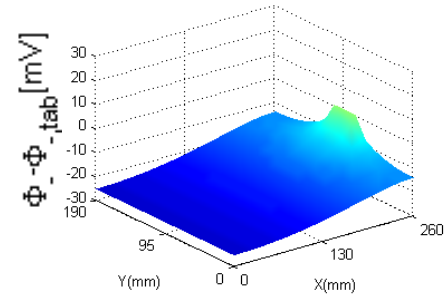
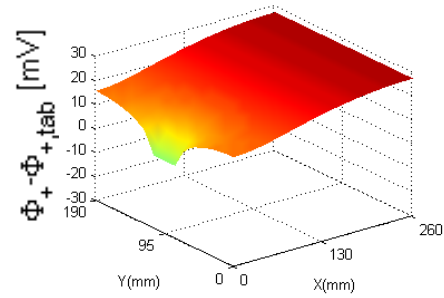
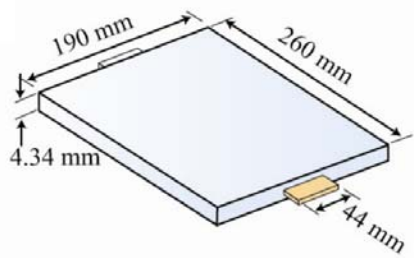
MSMD Application to Prediction of Large Stacked Prismatic Cell Behavior



<i>Submodel Choice</i>	<i>Solution Method</i>
<i>Submodel in the Particle Domain</i>	
 <ul style="list-style-type: none"> • <i>1D spherical particle model</i> 	<ul style="list-style-type: none"> • <i>SVM (state variable method)</i>
<i>Submodel in the Electrode Domain</i>	
 <ul style="list-style-type: none"> • <i>1D porous electrode model</i> 	<ul style="list-style-type: none"> • <i>SVM</i>
<i>Submodel in the Cell Domain</i>	
 <ul style="list-style-type: none"> • <i>3D Single Potential-Pair Continuum Model (SPPC)</i> 	<ul style="list-style-type: none"> • <i>FV-LSM finite volume – linear superposition methods</i>

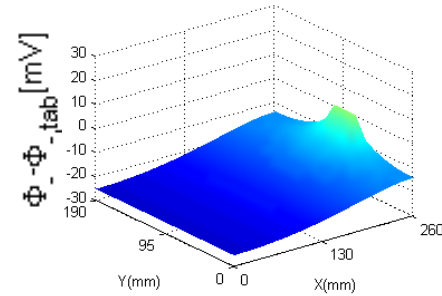
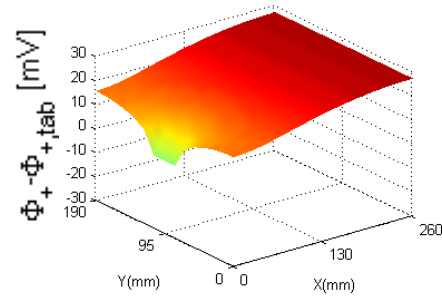
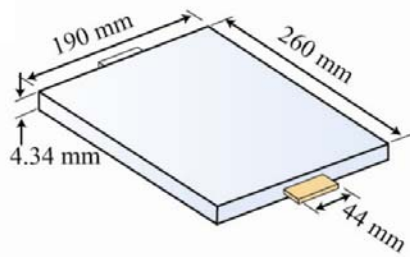
Electric Current Transport

4C discharge / Single-side cooling



Electric Current Transport

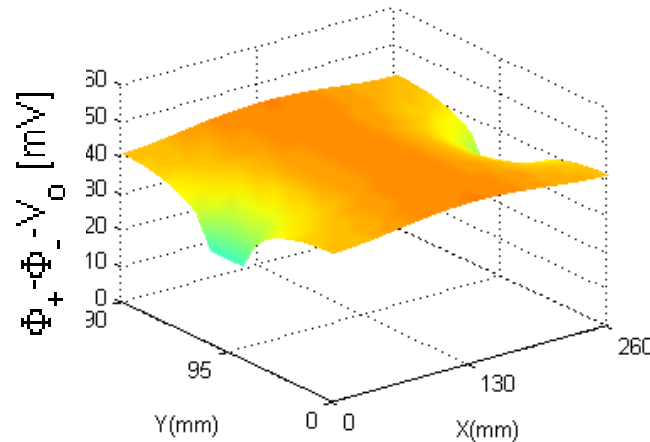
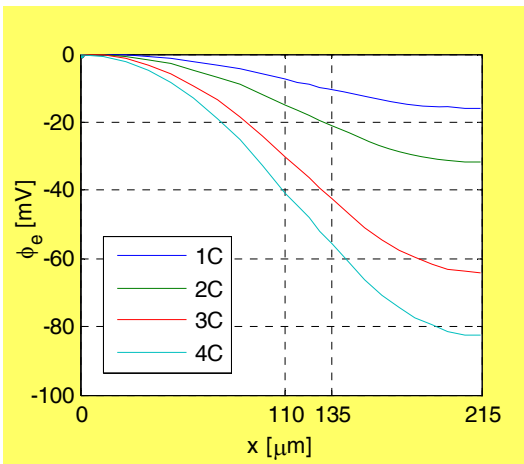
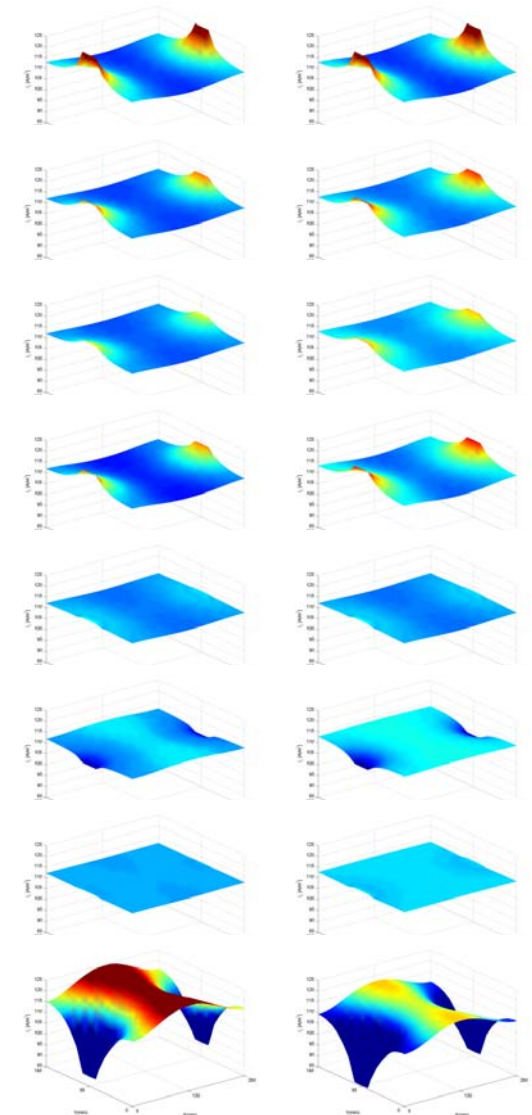
4C discharge / Single-side cooling



i_x''

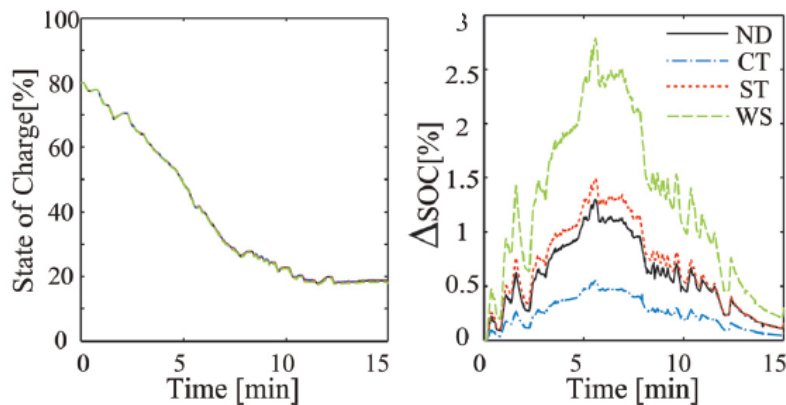
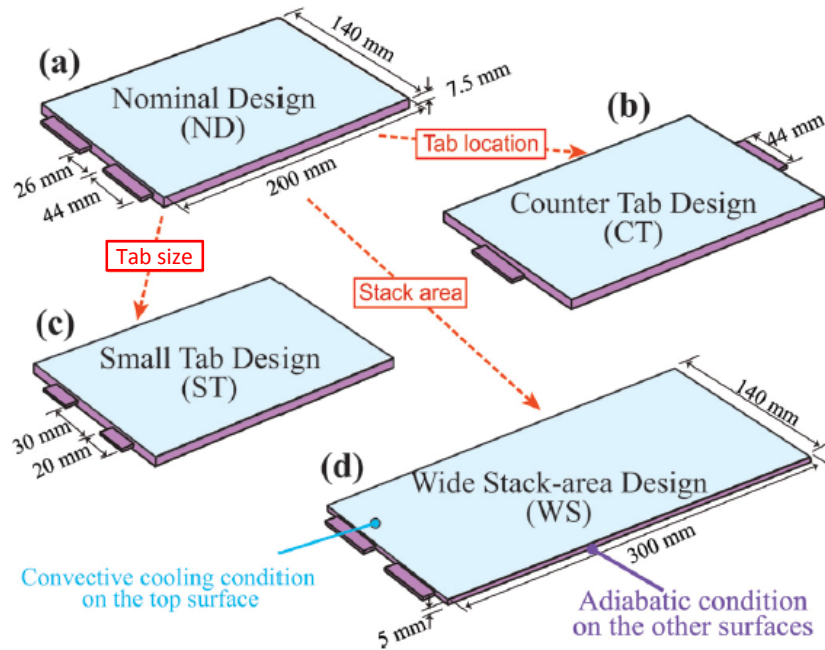
cooled top

bottom

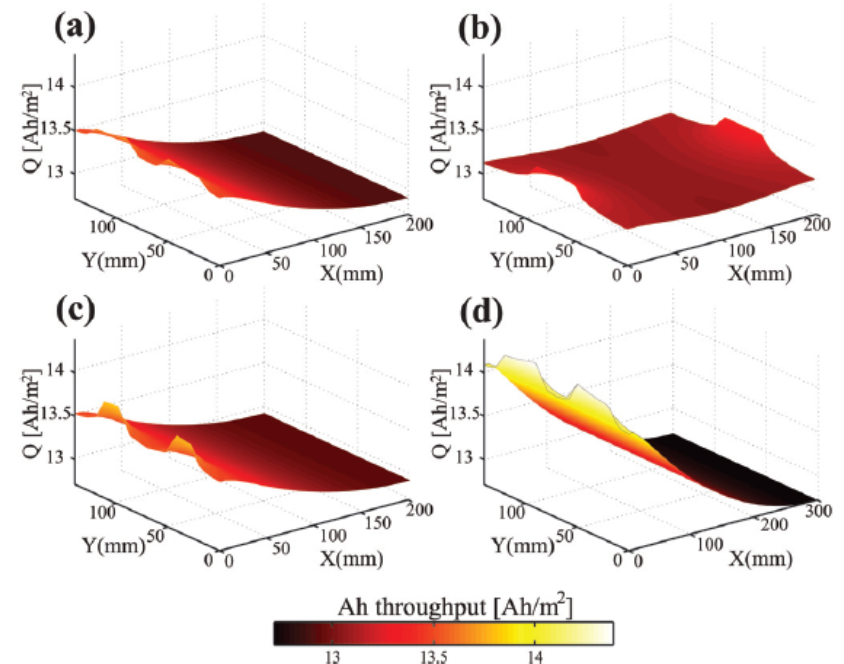
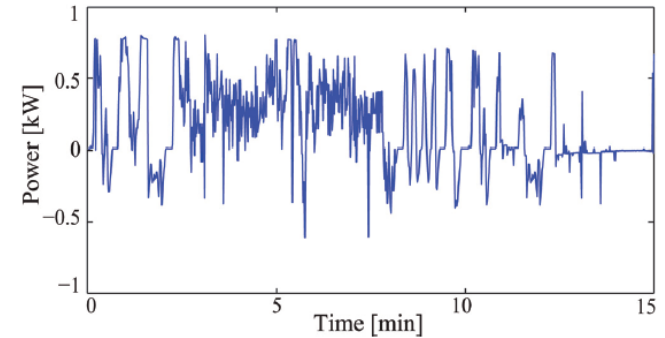


Non-Uniform Utilization

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



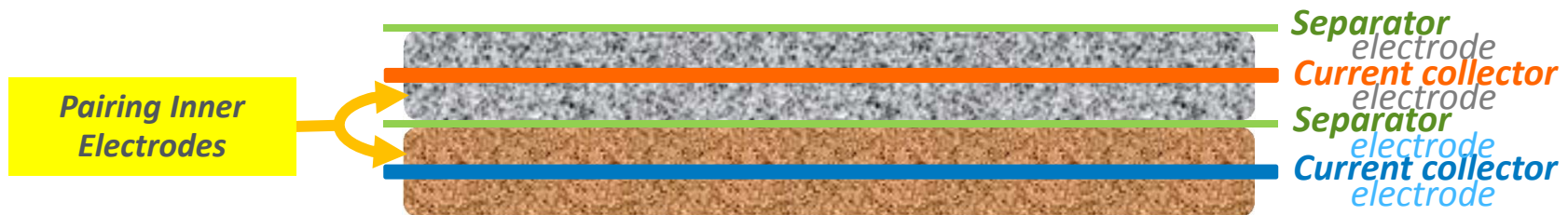
Mid-size sedan PHEV10 US06



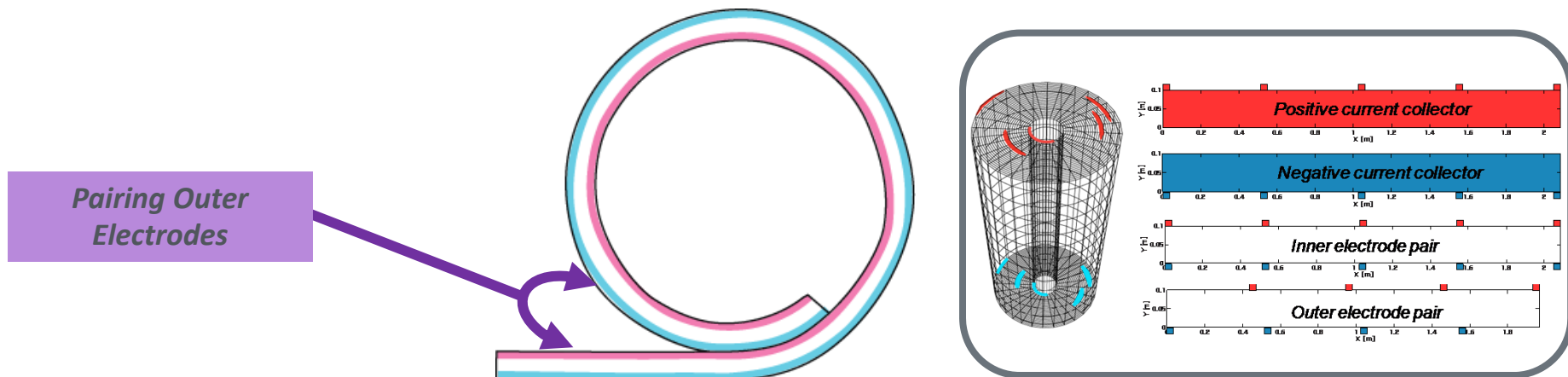
Wound Cells

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

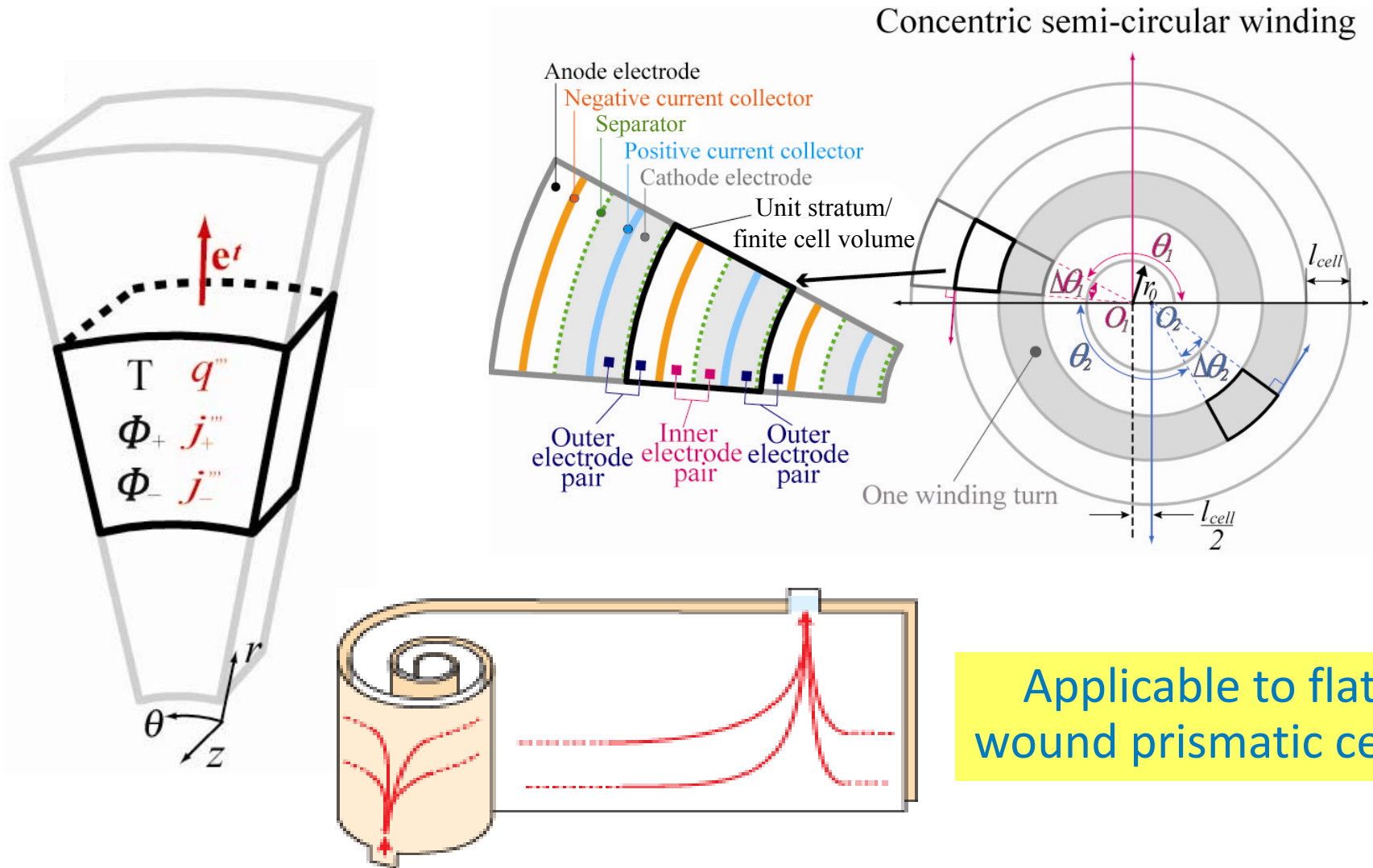
Stacking : Forming the first pair between inner electrodes



Winding : Forming the second pair between outer electrodes



WPPC (Wound Potential-Pair Continuum)

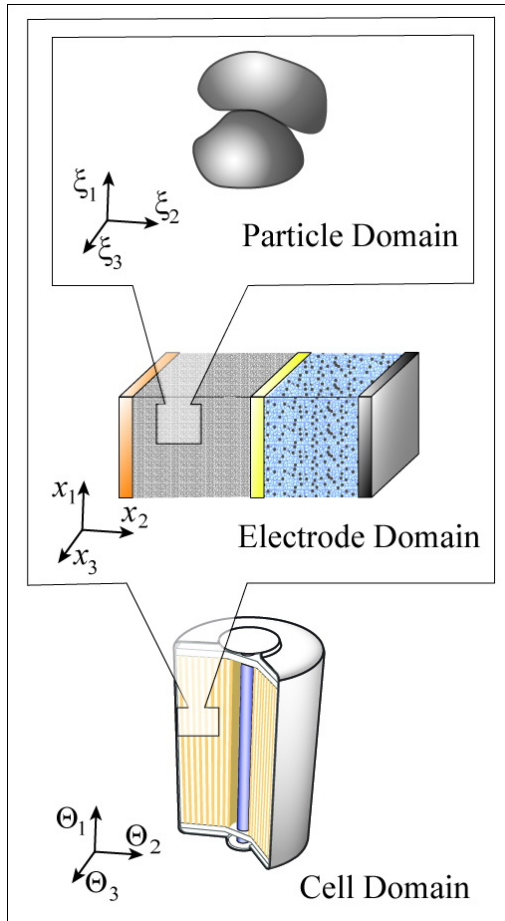


Concentric semi-circular winding

Applicable to flat wound prismatic cells

Cell with discrete tabs

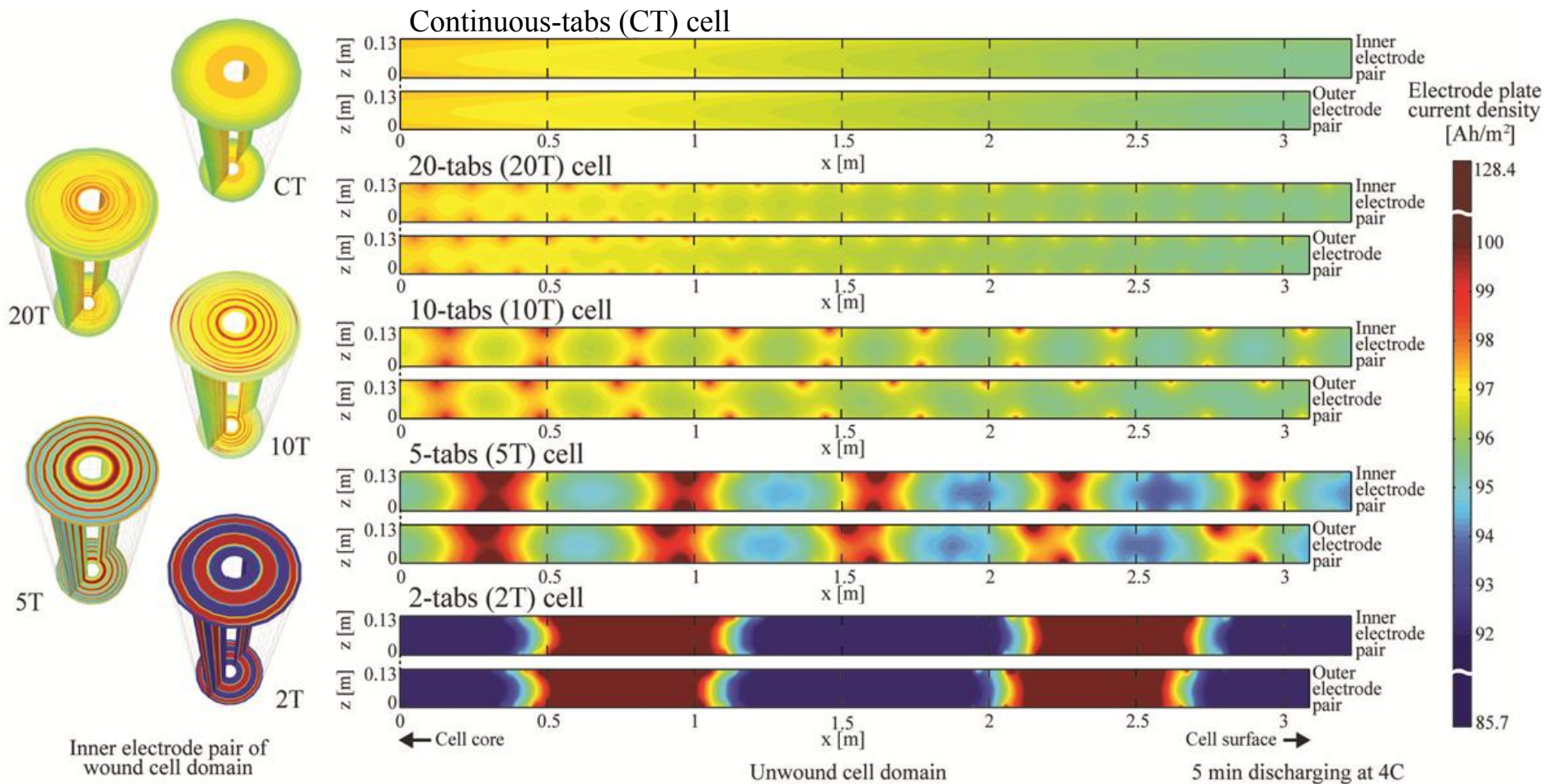
MSMD Application to Prediction of Wound Cylindrical Cell Behavior



<i>Submodel Choice</i>	<i>Solution Method</i>
<i>Submodel in the Particle Domain</i>	
<ul style="list-style-type: none"> • <i>1D spherical particle model</i> 	<ul style="list-style-type: none"> • <i>SVM (state variable method)</i>
<i>Submodel in the Electrode Domain</i>	
<ul style="list-style-type: none"> • <i>1D porous electrode model</i> 	<ul style="list-style-type: none"> • <i>SVM</i>
<i>Submodel in the Cell Domain</i>	
<ul style="list-style-type: none"> • <i>3D Wound Potential-Pair Continuum Model (WPPC)</i> 	<ul style="list-style-type: none"> • <i>FV-LSM finite volume – linear superposition methods</i>

Kinetics Response

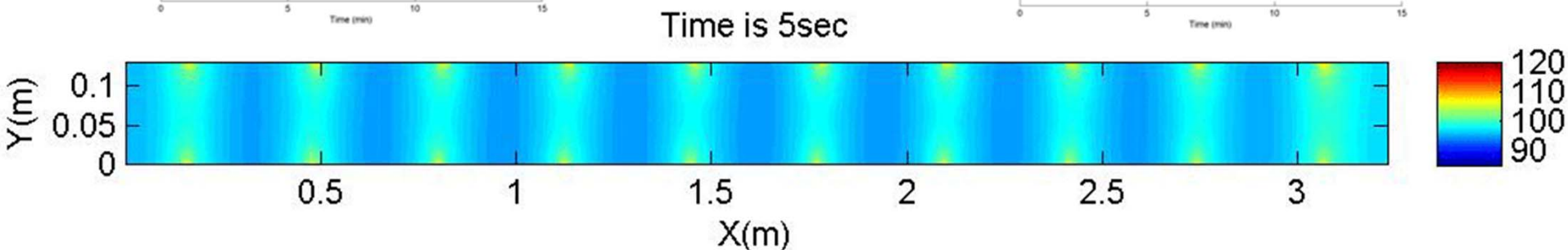
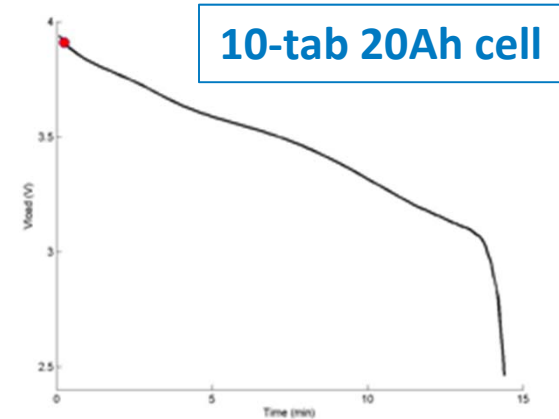
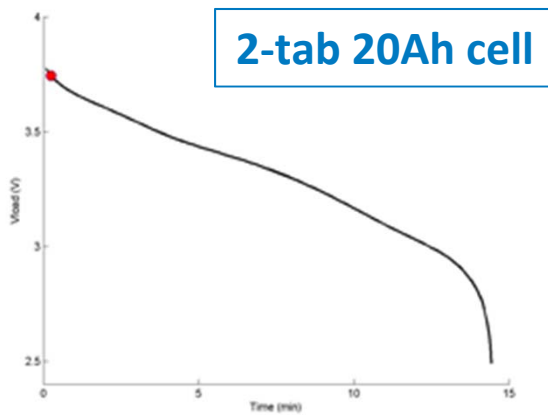
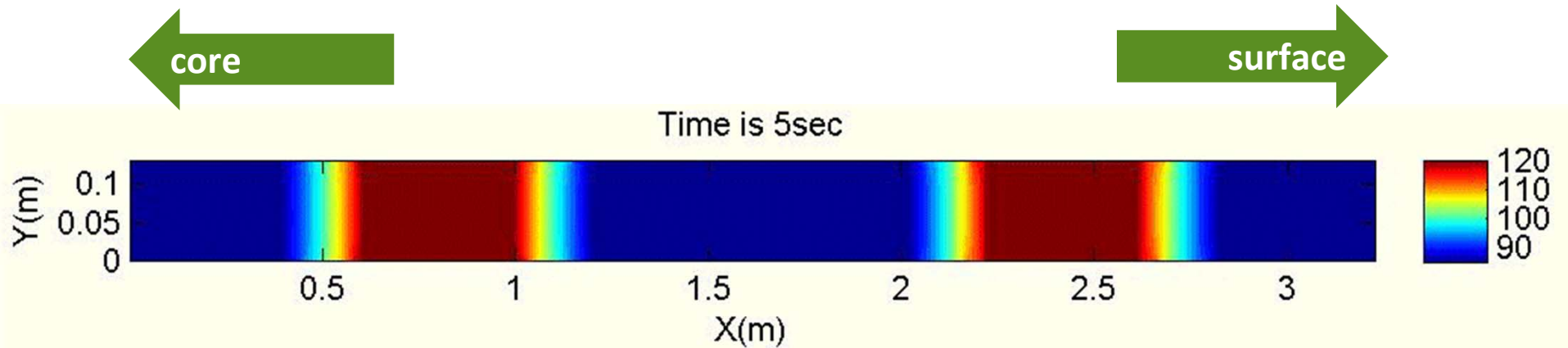
Impact of electrical current transport design



Kyu-Jin Lee, et al., April 2011

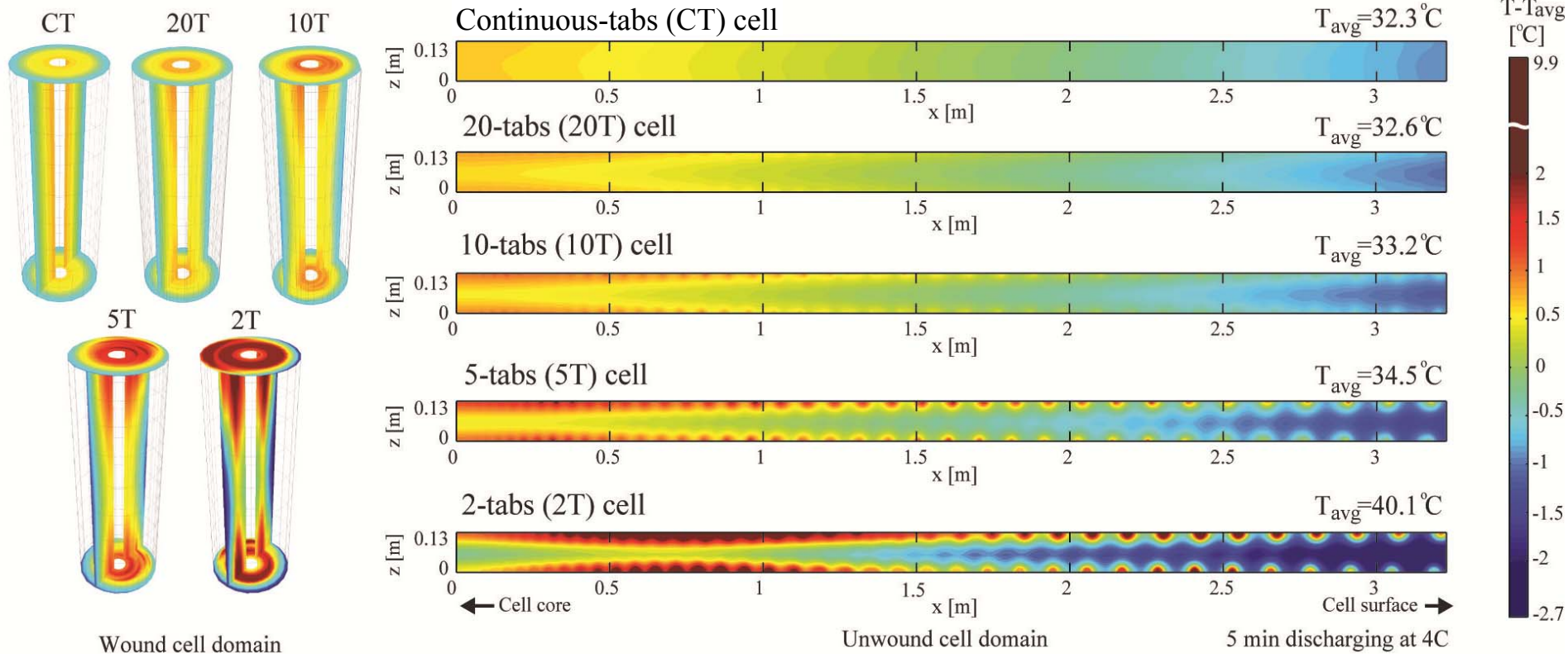
Non-uniform Kinetics during 4C Discharge

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



Thermal Response

Impact of electrical current transport design



Kyu-Jin Lee, et al., April 2011

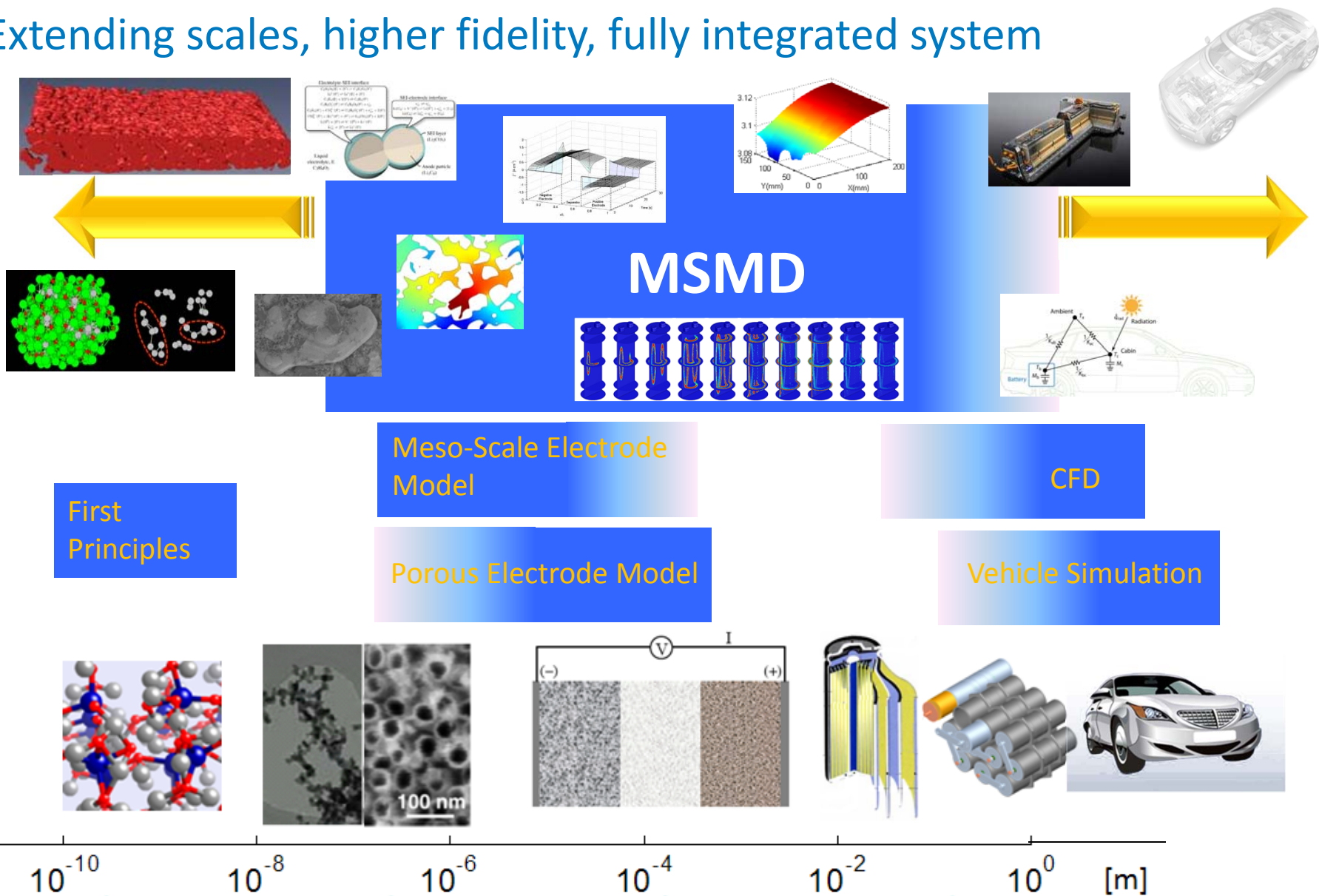
Thermal Evolution during 4C Discharge

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