2012 Automotive Simulation World Congress

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Accelerating Development of EV Batteries Through Computer-Aided Engineering

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Summary

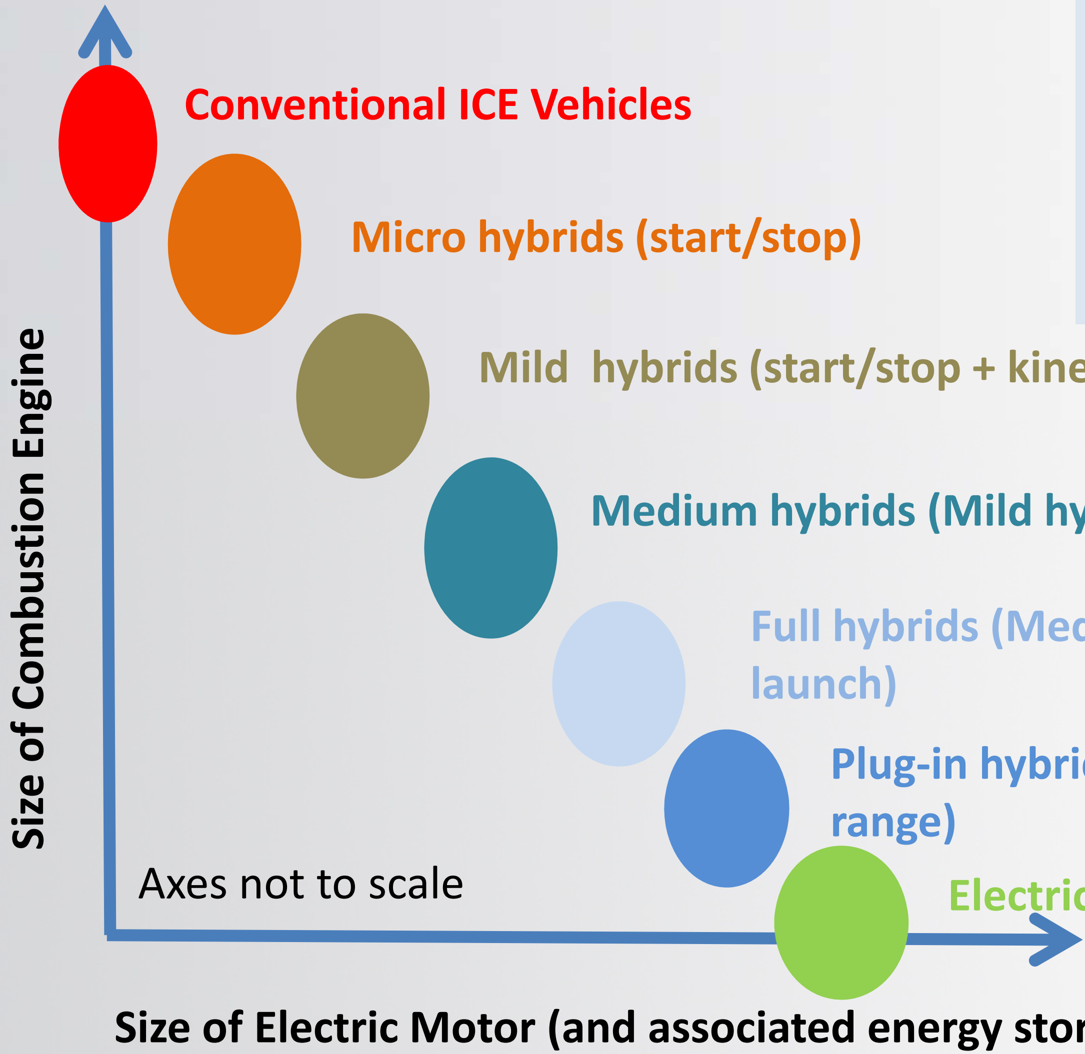
- The Department of Energy's Vehicle Technology Program has launched the Computer-Aided Engineering for Automotive Batteries (CAEBAT) project to work with national labs, industry and software venders to develop sophisticated software.
- As coordinator, NREL has teamed with a number of companies to help improve and accelerate battery design and production.
- This presentation provides an overview of CAEBAT, including its predictive computer simulation of Li-ion batteries known as the Multi-Scale Multi-Dimensional (MSMD) model framework.
- The MSMD’s modular, flexible architecture connects the physics of battery charge/discharge processes, thermal control, safety and reliability in a computationally efficient manner.
- This allows independent development of submodels at the cell and pack levels.

Outline

- Background – Vehicle Electrification
- Batteries for Electric Drive Vehicles (EDVs)
- Battery Development for EDVs
- Role of Simulation
- Computer-Aided Engineering for EDV Batteries Project
  - Background
  - Progress
- NREL Battery Simulation Activities
- Summary

Spectrum of EDV Technologies

New Fuel Economy Standards
Petroleum Use Reduction
Reducing Imported Oil
Reducing Gaseous Emissions
Switch to Electricity
Renewable Energy



Conventional ICE Vehicles

Micro hybrids (start/stop)

Mild hybrids (start/stop + kinetic energy recovery)

Medium hybrids (Mild hybrid + engine assist)

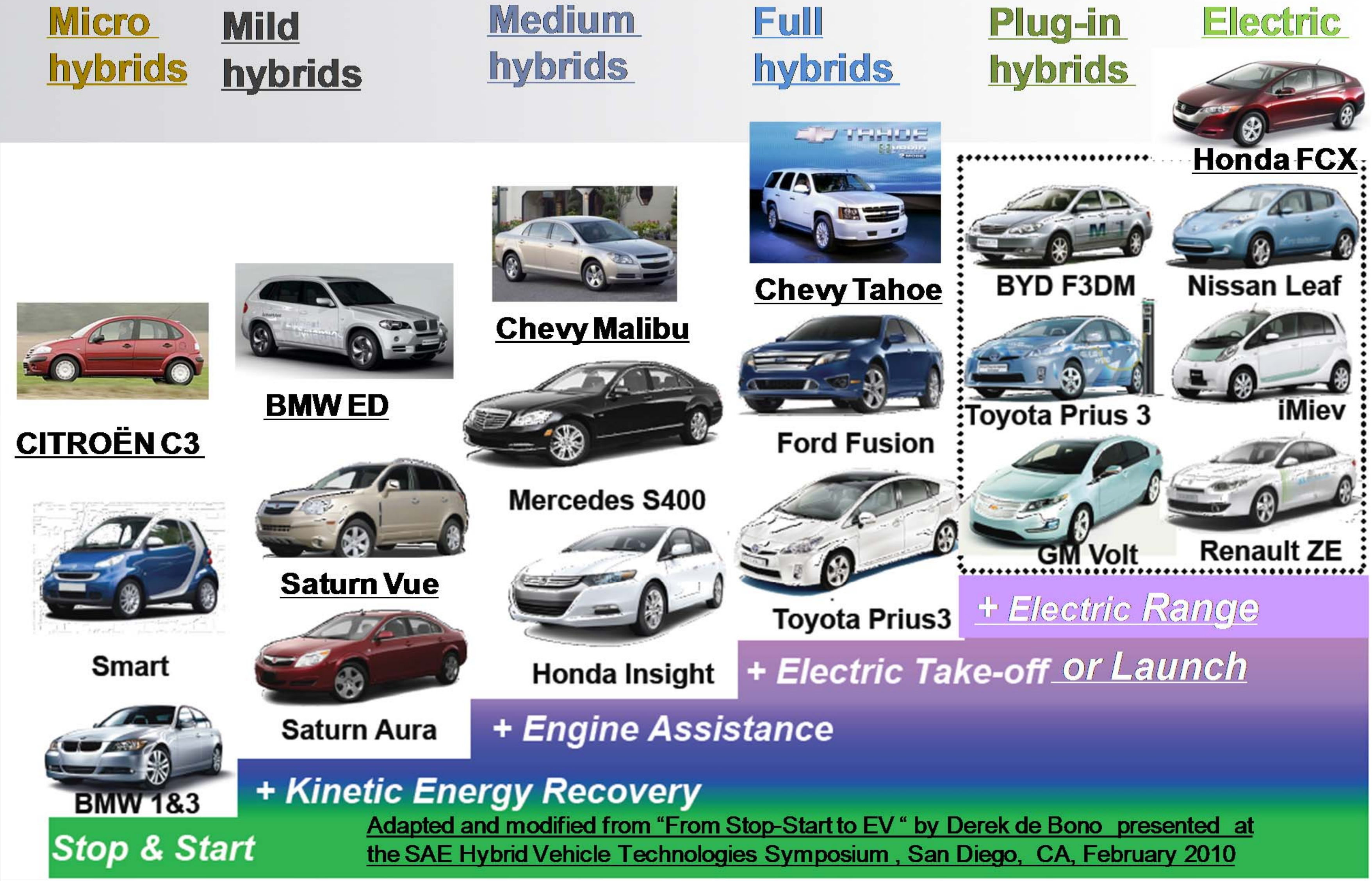
Full hybrids (Medium hybrid capabilities + electric launch)

Plug-in hybrids (Full hybrid capabilities + electric range)

Electric Vehicles (battery or fuel cell)

Axes not to scale

Examples of Light-Duty EDVs in the Market



Micro hybrids

Mild hybrids

Medium hybrids

Full hybrids

Plug-in hybrids

Electric

CITROËN C3

Smart

BMW 1&3

BMW ED

Saturn Vue

Saturn Aura

Chevy Malibu

Mercedes S400

Honda Insight

Chevy Tahoe

Ford Fusion

Toyota Prius3

BYD F3DM

Toyota Prius 3

GM Volt

Honda FCX

Nissan Leaf

iMiev

Renault ZE

+ Electric Range

+ Electric Take-off or Launch

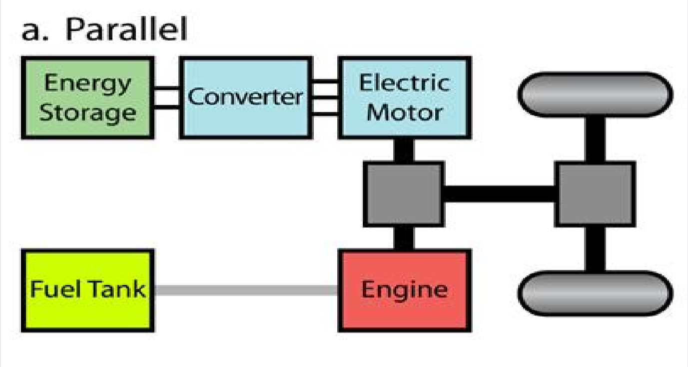
+ Engine Assistance

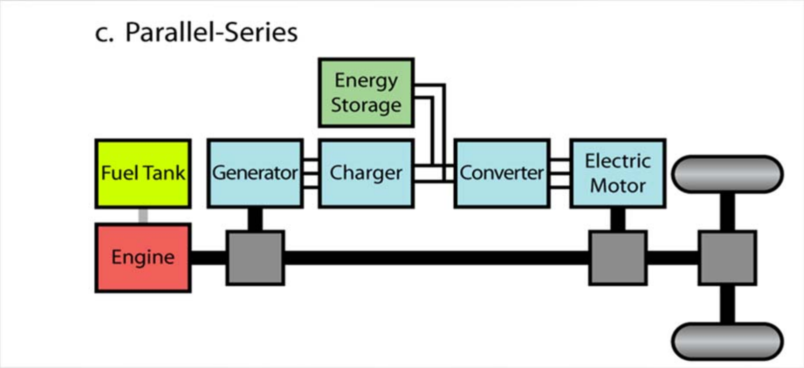
+ Kinetic Energy Recovery

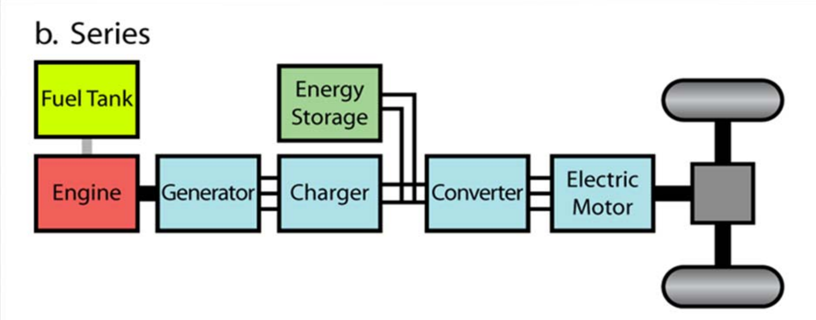
Stop & Start

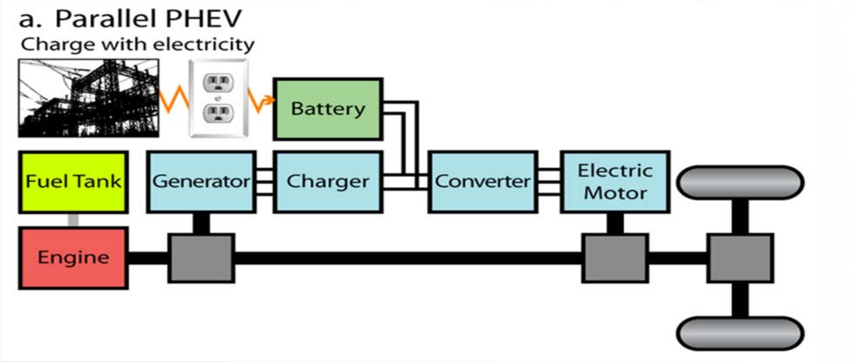
Adapted and modified from "From Stop-Start to EV" by Derek de Bono presented at the SAE Hybrid Vehicle Technologies Symposium, San Diego, CA, February 2010

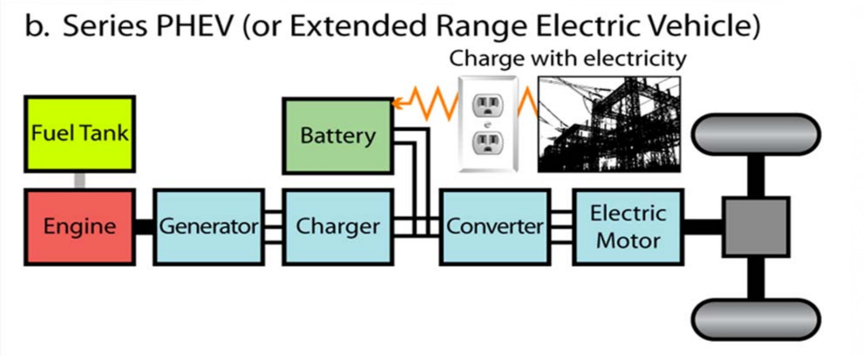
Many Powertrain Configurations and Battery Systems

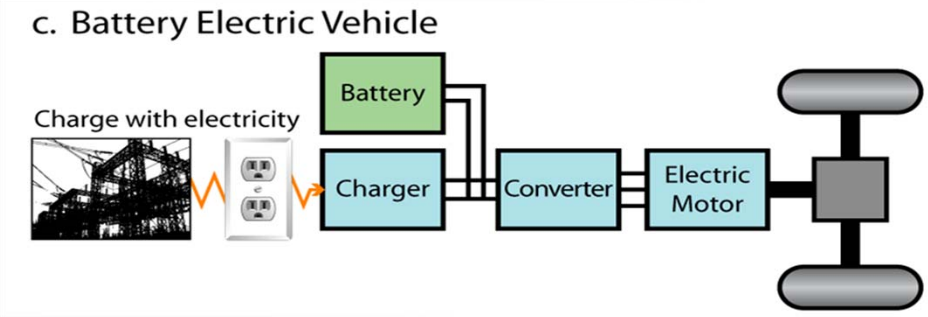

a. Parallel


c. Parallel-Series


b. Series

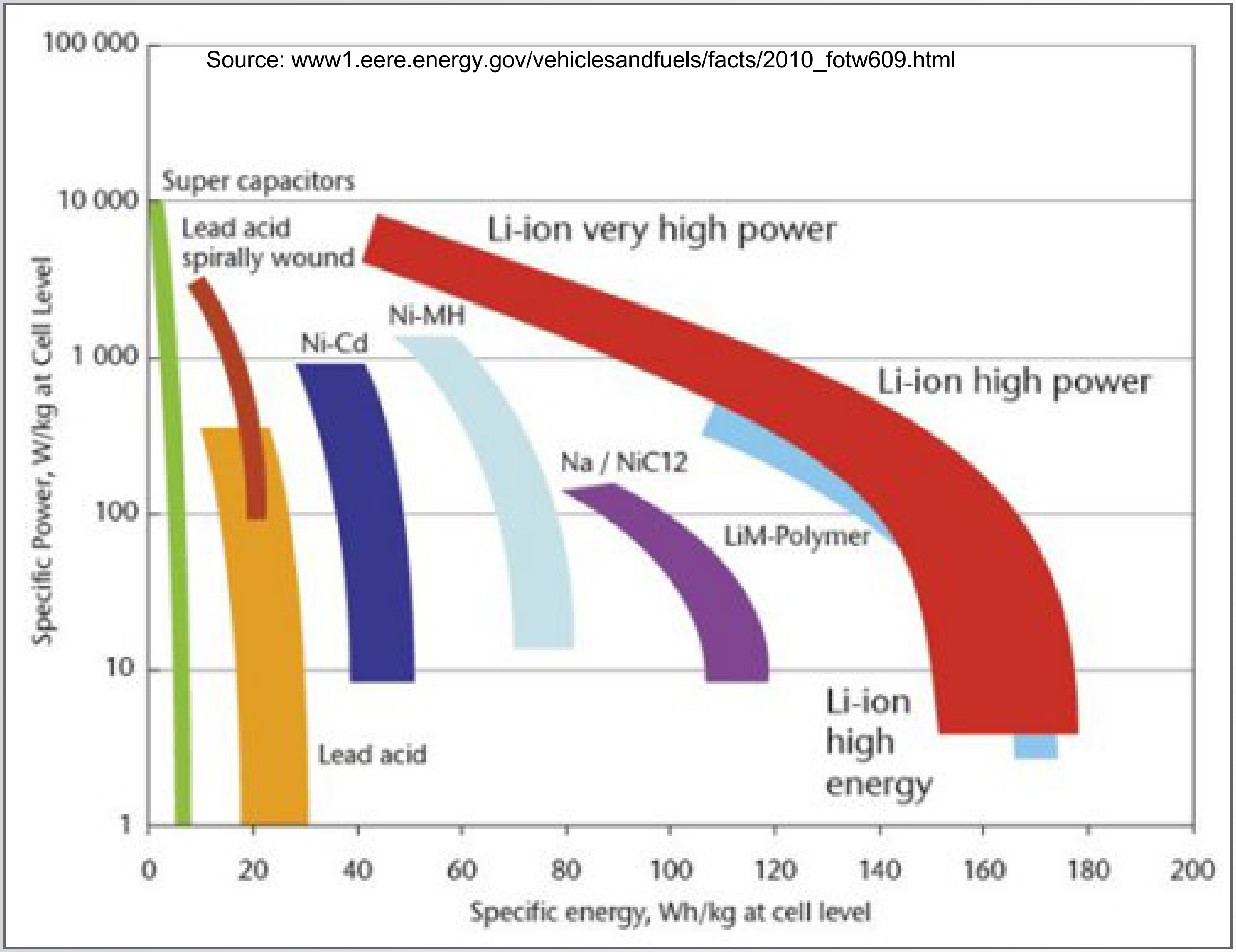

a. Parallel PHEV


b. Series PHEV (or Extended Range Electric Vehicle)


c. Battery Electric Vehicle

http://en.wikipedia.org/wiki/Hybrid_vehicle_drivetrain

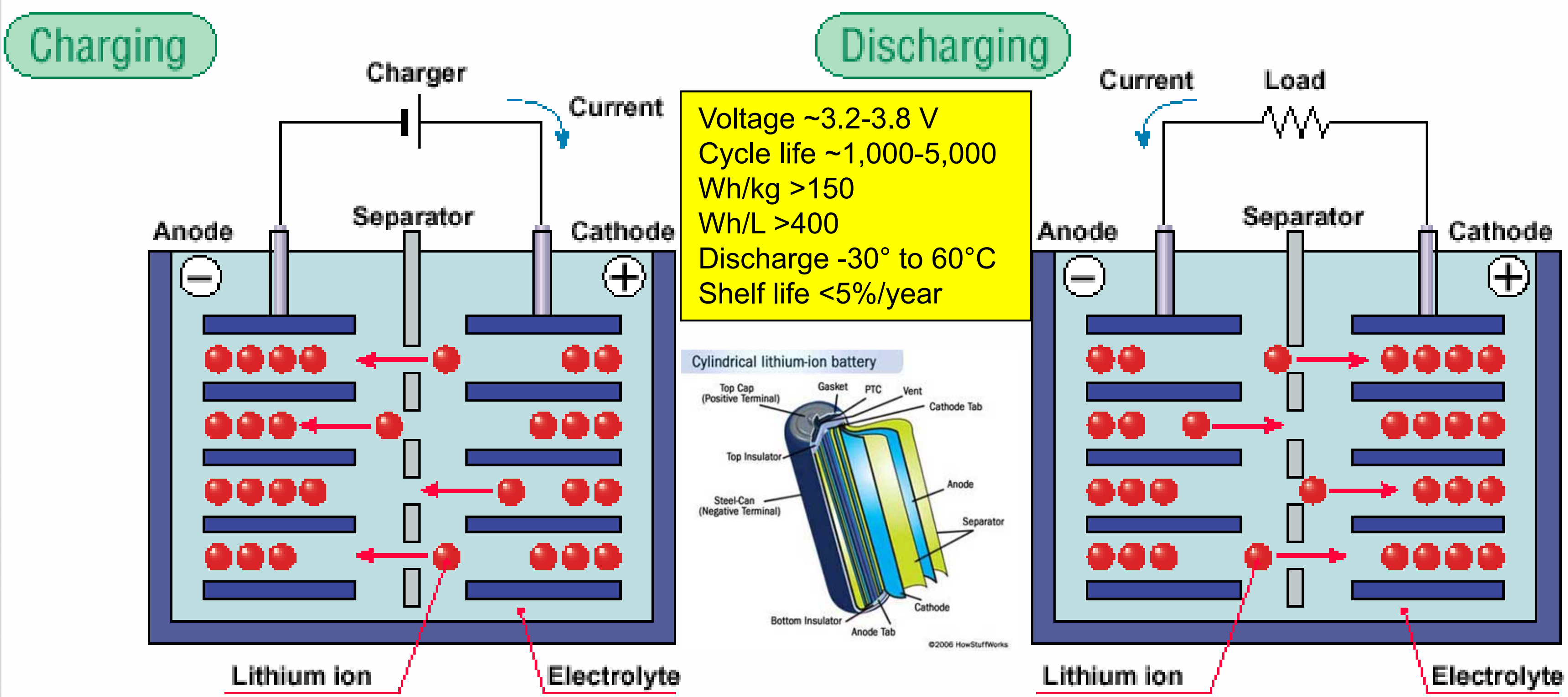
Battery Technology Critical for EDVs : Energy &Power


Source: www1.eere.energy.gov/vehiclesandfuels/facts/2010_fotw609.html

NiMH proven sufficient for many HEVs. Still recovering early factory investments.

Lithium ion technology believed to be viable for most EDVs in the next 10 years.

Many Chemistries of the Lithium Ion Battery Technology

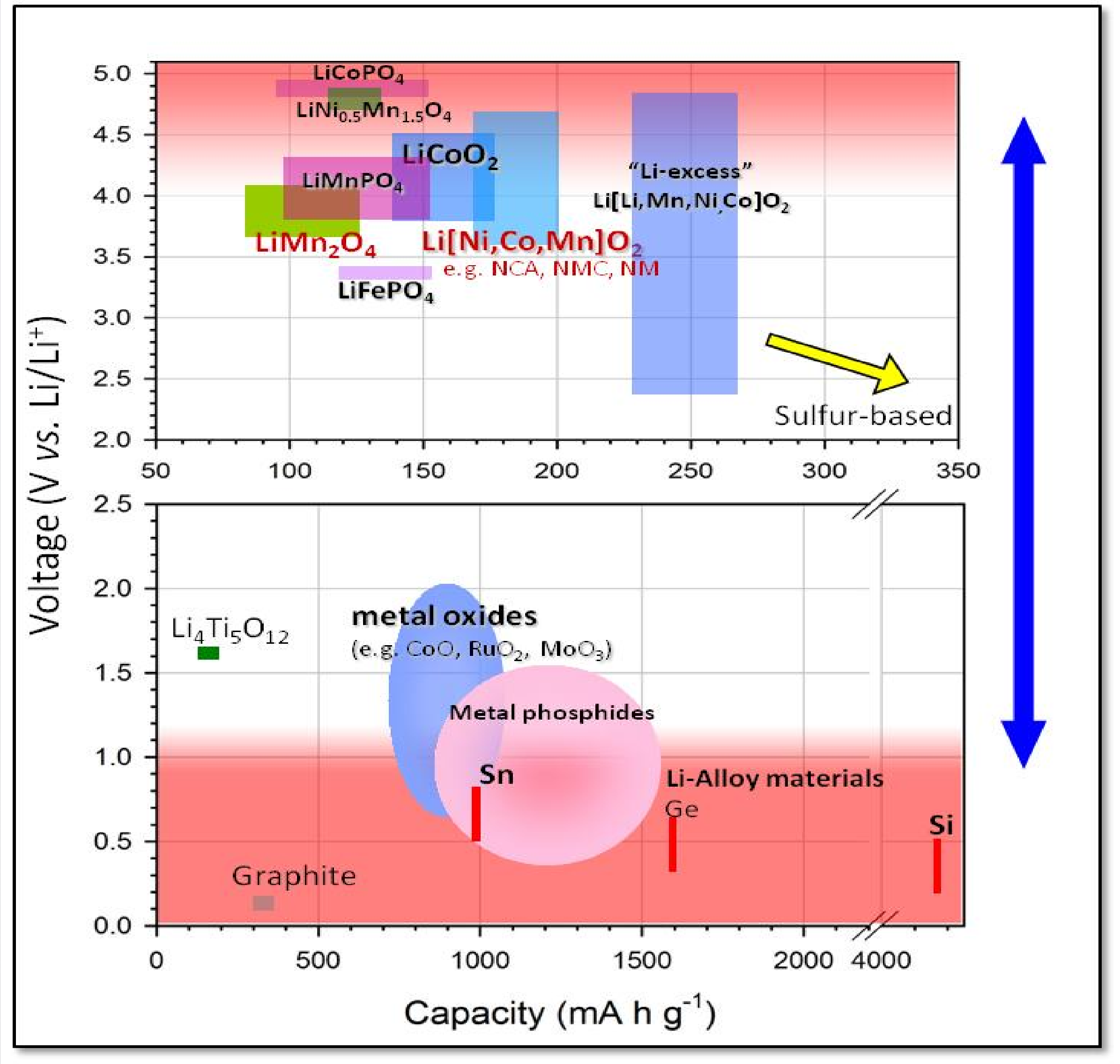


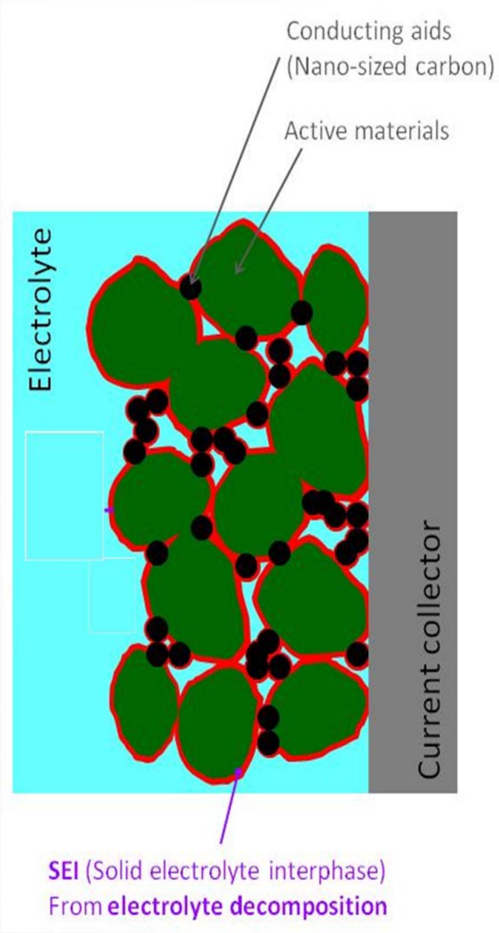
Voltage ~3.2-3.8 V
Cycle life ~1,000-5,000
Wh/kg >150
Wh/L >400
Discharge -30° to 60°C
Shelf life <5%/year

Many anodes are possible	Many electrolytes are possible	Many cathodes are possible
Carbon/Graphite	$LiPF_6$ based	Cobalt oxide
Titanate ($Li_4Ti_5O_{12}$)	$LiBF_4$ based	Manganese oxide
Titanium-oxide based	Various solid electrolytes	Mixed oxides with nickel
Silicon based	Polymer electrolytes	Iron phosphate
Metal oxides	Ionic liquids	Vanadium-oxide based

Source: Robert M. Spotnitz, Battery Design LLC, "Advanced EV and HEV Batteries"

Different Chemistries Leads to Different Behaviors/Needs

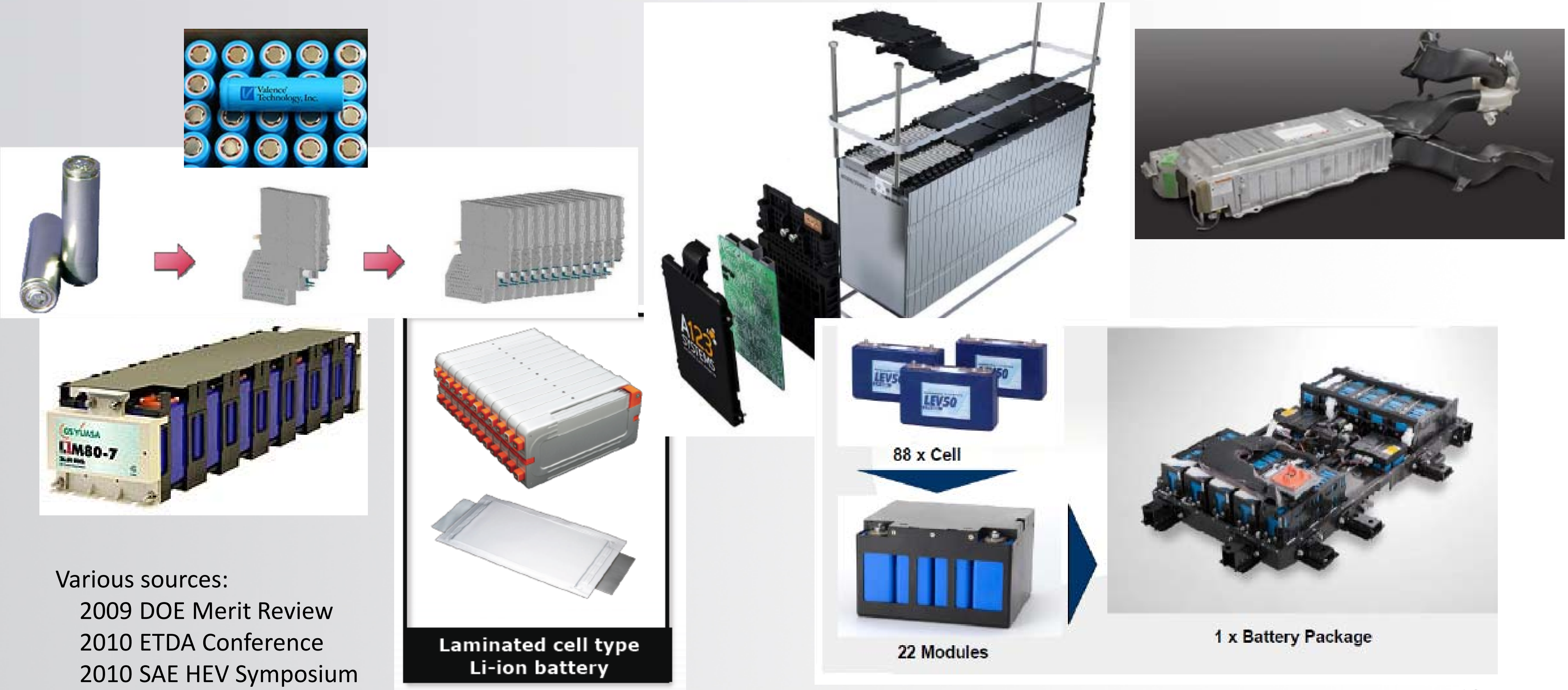




Source: Yoon Seok Jung et. al. Presented at 2011 MRS Spring Meeting, San Francisco, CA

Many Design Choices to Meet Requirements

- **Many chemistries, cell sizes and shapes, module configurations, and pack configurations, but at optimum cost**
- **Integration of the battery system <u>in the vehicle</u> with proper electrical, safety, mechanical, structural, and thermal considerations is the key.**



Various sources:
2009 DOE Merit Review
2010 ETDA Conference
2010 SAE HEV Symposium

DOE and USABC Battery Requirements

DOE Energy Storage Goals	HEV (2010)	PHEV (2015)	EV (2020)
Equivalent Electric Range (miles)	**N/A**	**10–40**	**200–300**
10-sec Discharge Pulse Power (kW)	**25**	**38–50**	**80**
Regen Pulse Power (10 seconds) (kW)	**20**	**25–30**	**40**
Recharge Rate (kW)	**N/A**	**1.4–2.8**	**5–10**
Cold Cranking Power @ -30°C (2 seconds) (kW)	**5**	**7**	**N/A**
Available Energy (kWh)	**0.3**	**3.5–11.6**	**30–40**
Calendar Life (year)	**15**	**10+**	**10**
Cycle Life (cycles)	**3,000**	**3,000–5,000, deep discharge**	**750+, deep discharge**
Maximum System Weight (kg)	**40**	**60–120**	**300**
Maximum System Volume (L)	**32**	**40–80**	**133**
Operating Temperature Range (ºC)	**-30 to +52**	**-30 to 52**	**-40 to 85**
Selling Price of System (@100K units/year)	**$20/kW**	**$300/kWh**	**$150/kWh**

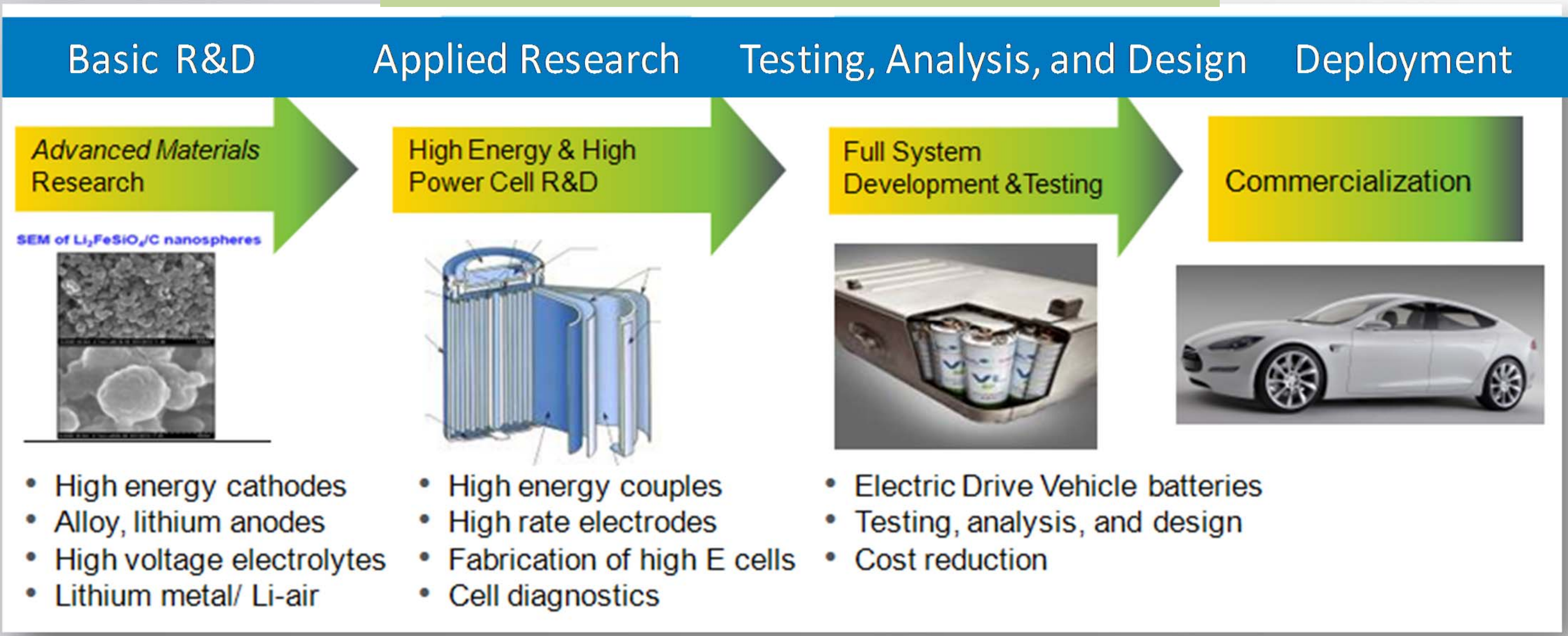
Cost, Performance, Life, and Safe Need Improvements

Source: David Howell, 2011 DOE Vehicle Technologies Annual Merit Review

USABC: United States Advanced Battery Consortium

The Department of Energy's R&D Program To Move the Technology Forward

Low Cost, High Performance, Long Life, Safe



Basic R&D	Applied Research	Testing, Analysis, and Design	Deployment
Advanced Materials Research	High Energy & High Power Cell R&D	Full System Development & Testing	Commercialization

SEM of Li_2FeSiO_4/C nanospheres

- High energy cathodes
- Alloy, lithium anodes
- High voltage electrolytes
- Lithium metal/ Li-air

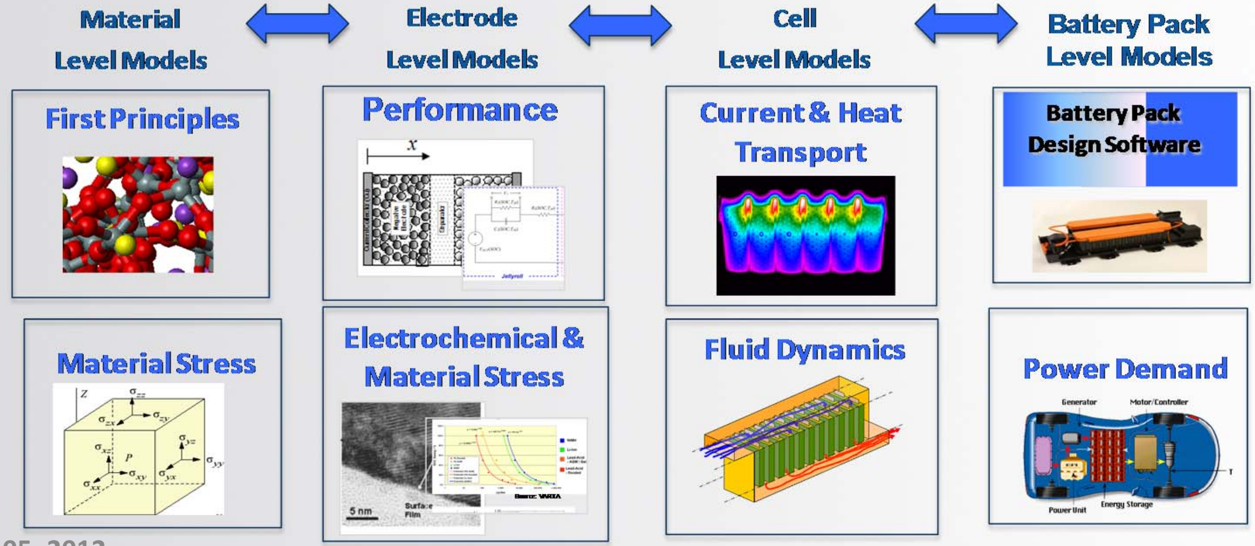
- High energy couples
- High rate electrodes
- Fabrication of high E cells
- Cell diagnostics

- Electric Drive Vehicle batteries
- Testing, analysis, and design
- Cost reduction

- Fundamental modeling under Basic & Applied Battery Research for many years
- Battery component modeling under Analysis and Design for several years
- DOE recognized the need for simulation tools for design & improvement

Need for Battery Simulation and Design Tools

- 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.
- DOE has recognized the need for user-friendly, 3D, fully integrated CAE software tools to be accessible to the battery community

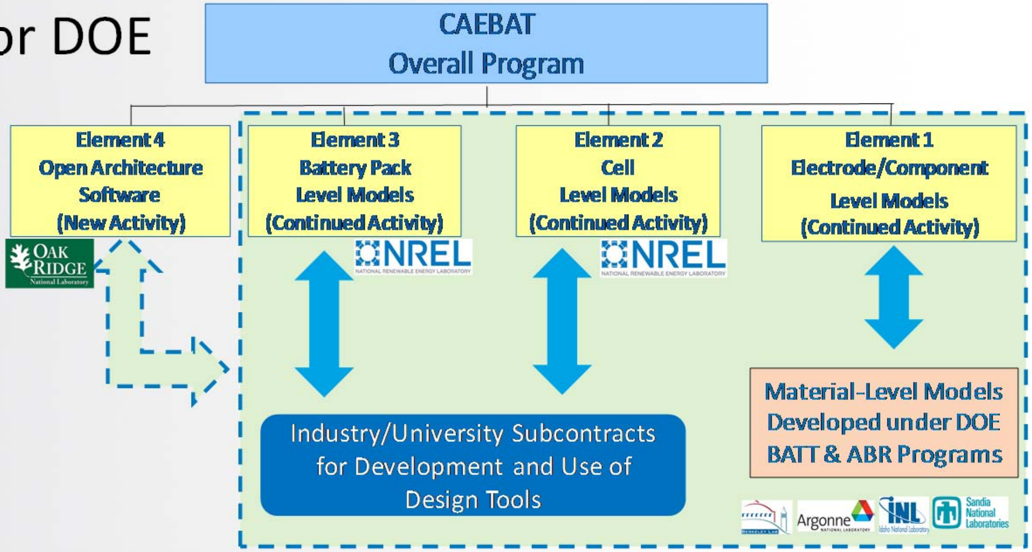


Material Level Models ⟷ Electrode Level Models ⟷ Cell Level Models ⟷ Battery Pack Level Models

Material Level Models	Electrode Level Models	Cell Level Models	Battery Pack Level Models
First Principles	Performance	Current & Heat Transport	Battery Pack Design Software
Material Stress	Electrochemical & Material Stress	Fluid Dynamics	Power Demand

Computer Aided Engineering for EDV Batteries (CAEBAT)

- In April 2010, DOE’s Vehicle Technologies Program launched the CAEBAT activity to develop “validated” battery design software/tools by incorporating existing and new battery models
- The goals of the CAEBAT project are to
  - Shorten design cycles and optimization of batteries
  - Simultaneously address the barriers of cost, performance, life, and safety of lithium-ion with quantitative tools
  - Support meeting the DOE/USABC battery system targets
- NREL is coordinating CAEBAT for DOE
  - Collaborate with industry through competitive solicitations
  - Collaborate with ORNL, who is developing a software platform to link the developed tools



CAEBAT
Overall Program

Element 4
Open Architecture Software
(New Activity)

Element 3
Battery Pack
Level Models
(Continued Activity)

Element 2
Cell
Level Models
(Continued Activity)

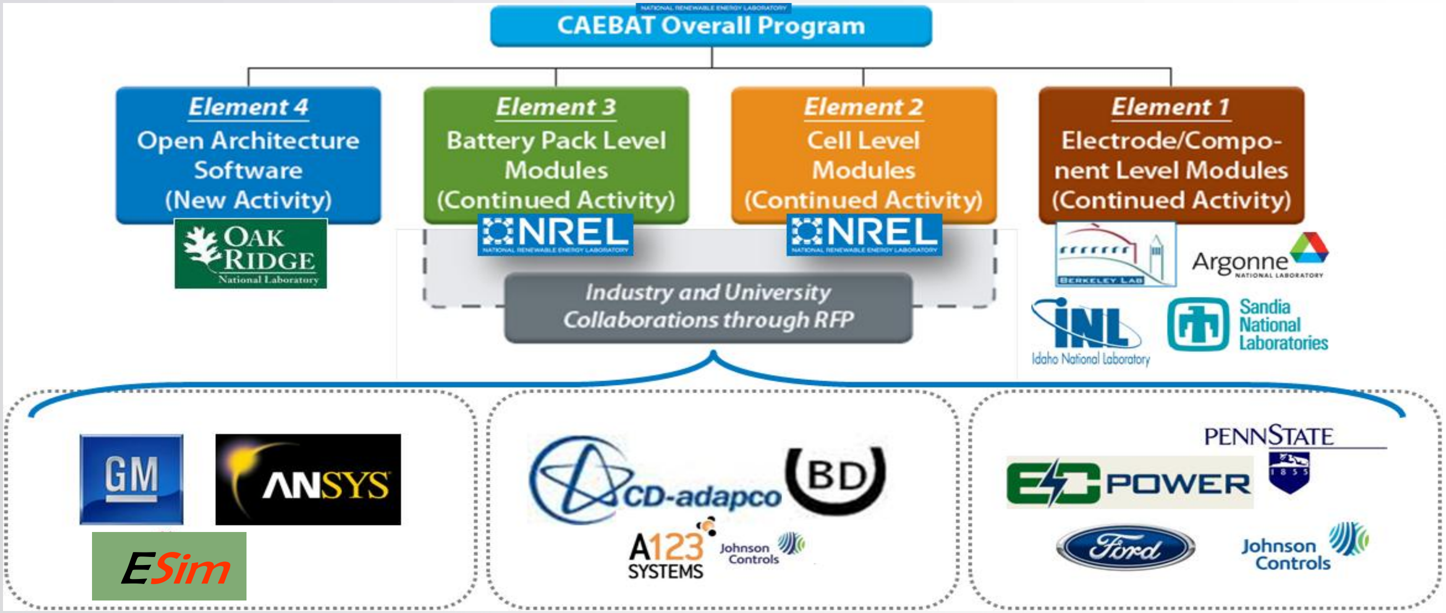
Element 1
Electrode/Component
Level Models
(Continued Activity)

Industry/University Subcontracts for Development and Use of Design Tools

Material-Level Models Developed under DOE BATT & ABR Programs

CAEBAT Progress

- In FY10, NREL issued an RFP to solicit cost-shared proposals from industry
- After a comprehensive review process, three teams were selected to develop CAEBAT software tools
- In June of FY11 negotiations were completed; three teams initiated their 50-50 cost-shared projects and significant progress has been made
  - Please see the presentation by Taeyoung Han, Gi-Heon Kim and Lewis Collins in this Congress



CAEBAT Overall Program

Element 4
Open Architecture Software
(New Activity)

Element 3
Battery Pack Level Modules
(Continued Activity)

Element 2
Cell Level Modules
(Continued Activity)

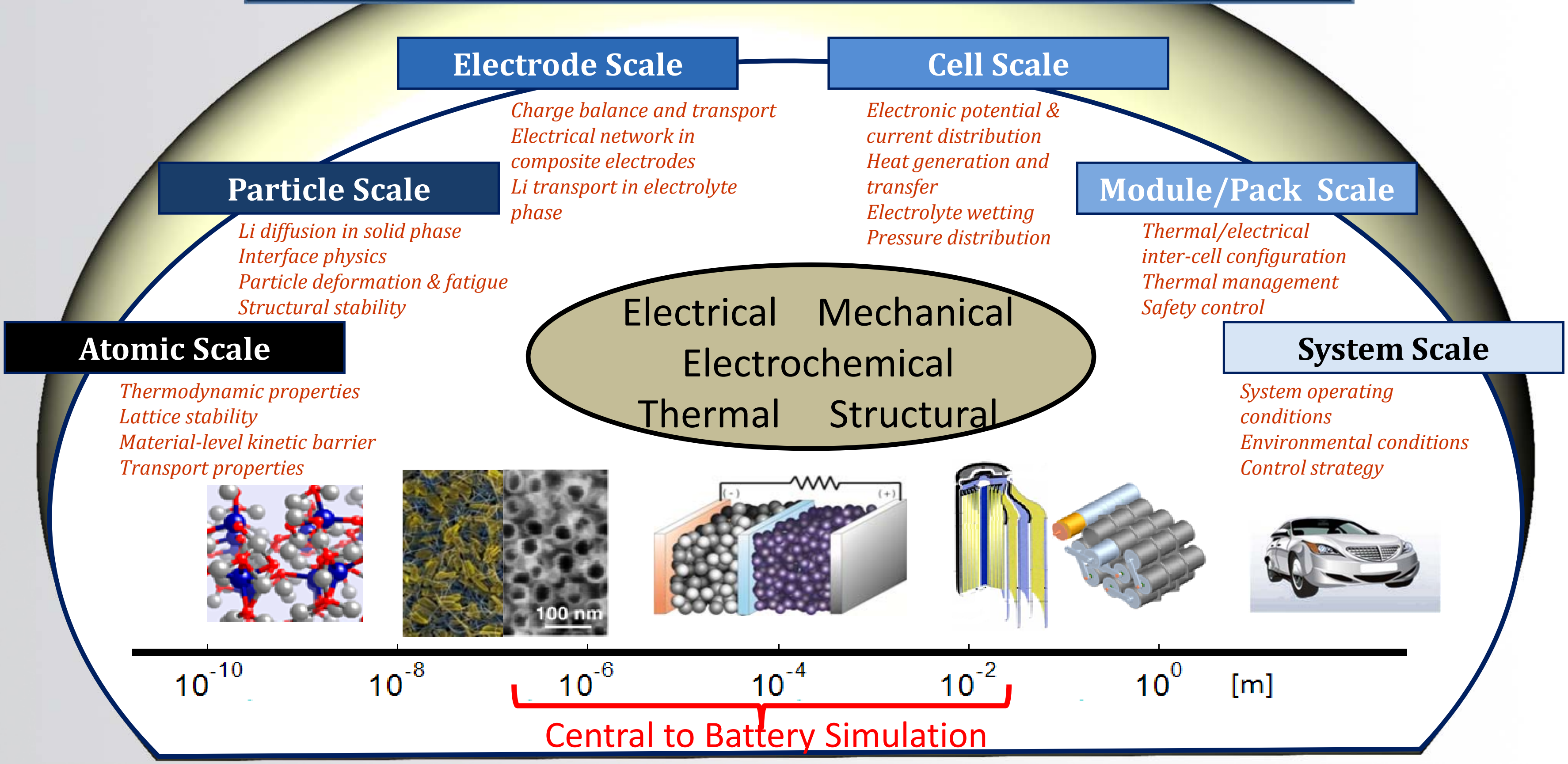
Element 1
Electrode/Component Level Modules
(Continued Activity)

Industry and University Collaborations through RFP

- NREL has performed R&D to enhance and further develop the existing electrochemical-thermal (MSMD) models for use by CAEBAT participants

Battery Performance, Durability & Safety – Multi-physics Interactions Across Varied Length Scales

Physics of Li-Ion Battery Systems in Different Length Scales



Atomic Scale

Thermodynamic properties
Lattice stability
Material-level kinetic barrier
Transport properties

Particle Scale

Li diffusion in solid phase
Interface physics
Particle deformation & fatigue
Structural stability

Electrode Scale

Charge balance and transport
Electrical network in composite electrodes
Li transport in electrolyte phase

Cell Scale

Electronic potential & current distribution
Heat generation and transfer
Electrolyte wetting
Pressure distribution

Module/Pack Scale

Thermal/electrical inter-cell configuration
Thermal management
Safety control

System Scale

System operating conditions
Environmental conditions
Control strategy

Electrical Mechanical
Electrochemical
Thermal Structural

Central to Battery Simulation

Li-Ion Porous Electrode Model – Commonly Used

Charge Transfer Kinetics at Reaction Sites

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

$$i_0 = k(c_e)^{\alpha_a}(c_{s,\max} - c_{s,e})^{\alpha_a}(c_{s,e})^{\alpha_c}$$

$$\eta = (\phi_s - \phi_e) - U$$

Species Conservation

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

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

Charge Conservation

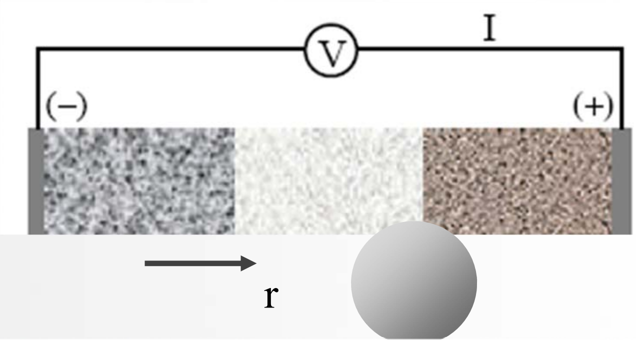
$$\nabla\cdot\left(\sigma^{eff}\nabla\phi_s\right) - j^{\mathrm{Li}} = 0$$

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

Energy Conservation

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

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

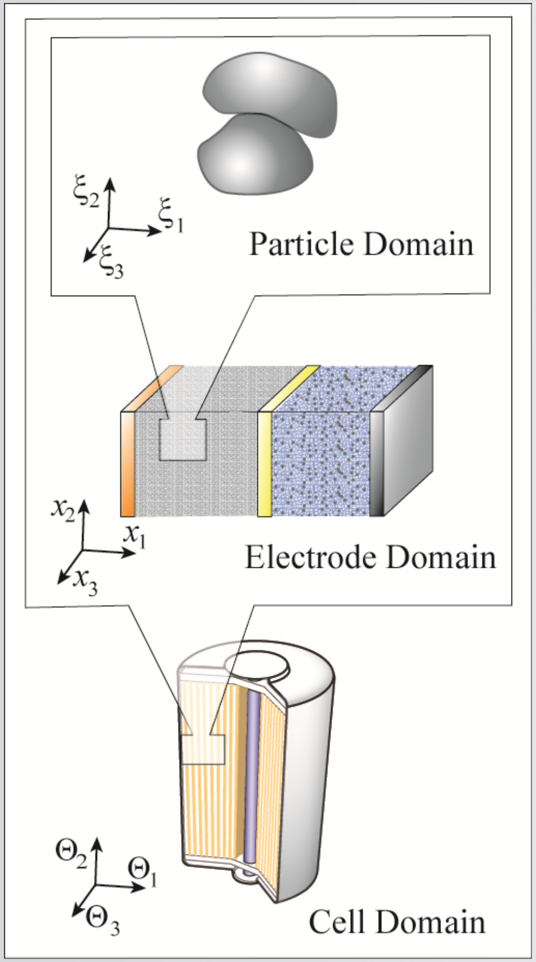


- **Pioneered by John Newman group at University of Berkeley (*Doyle, Fuller, and Newman 1993*)**
- Captures *lithium diffusion dynamics* and *charge transfer kinetics*
- Predicts *current/voltage response* of a battery
- Provides design guide for thermodynamics, kinetics, and transport across electrodes

- 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 U.S. 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*



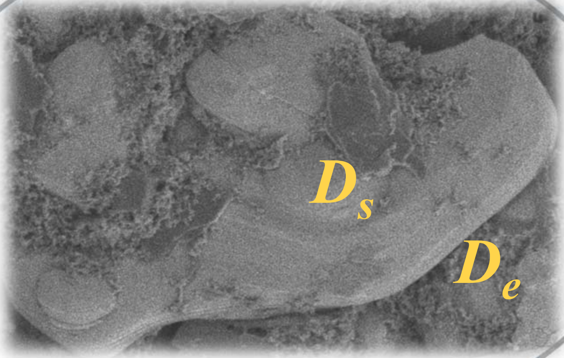
- Introduces multiple computational domains for corresponding length scale physics
- Decouples LIB geometries into separate computational domains
- Couples physics using the predefined inter-domain information exchange
- Selectively resolves higher spatial resolution for smaller characteristic length scale physics
- Achieves high computational efficiency
- Provides 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*



Particle Domain

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

e.g.,

$D_s \ll D_e$

Electrode Domain

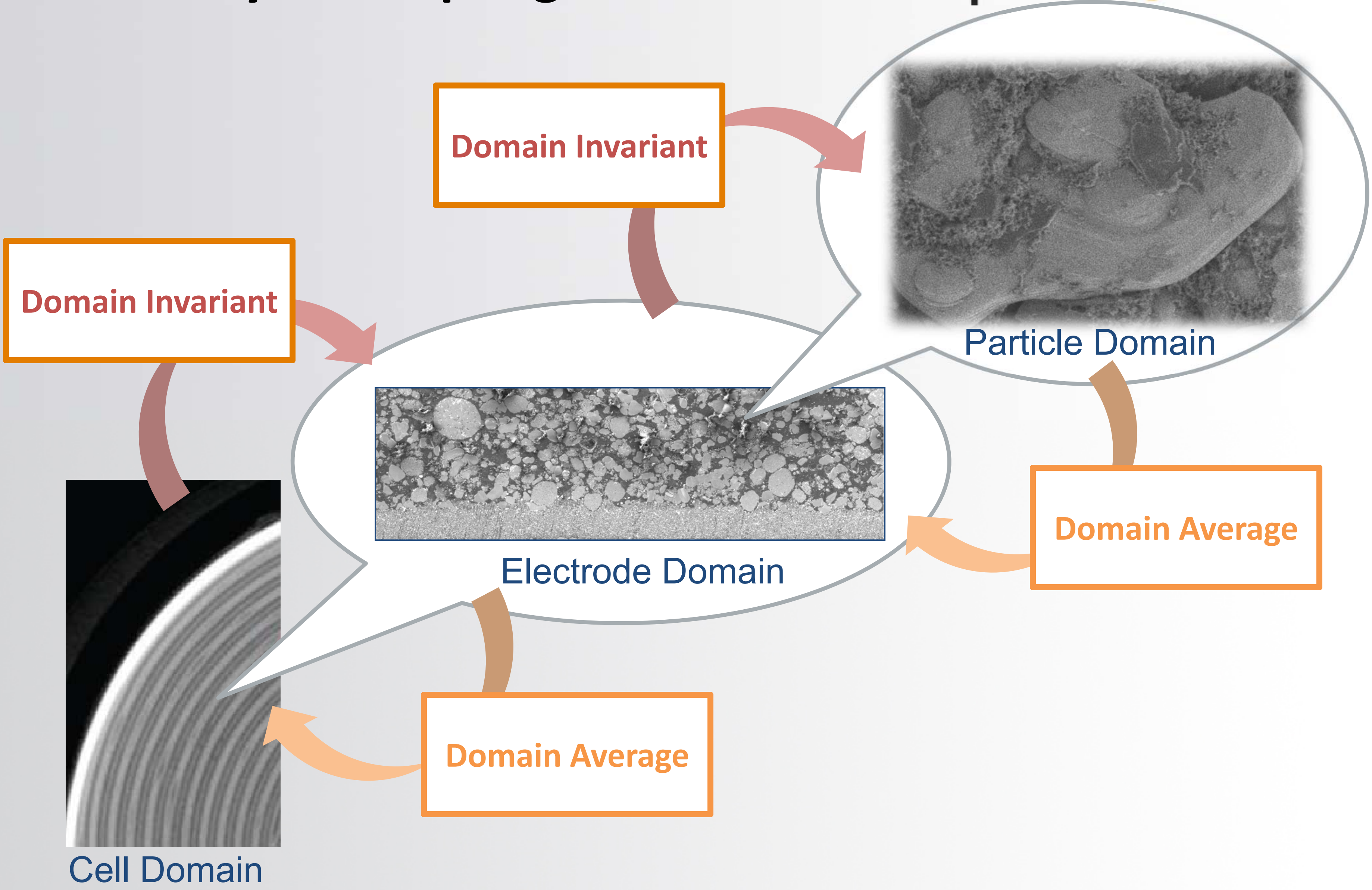
Electronic conductivity is much higher in metal current collectors than in composite electrode matrix

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

Cell Domain

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

Geometry Decoupling



Domain Invariant

Domain Invariant

Particle Domain

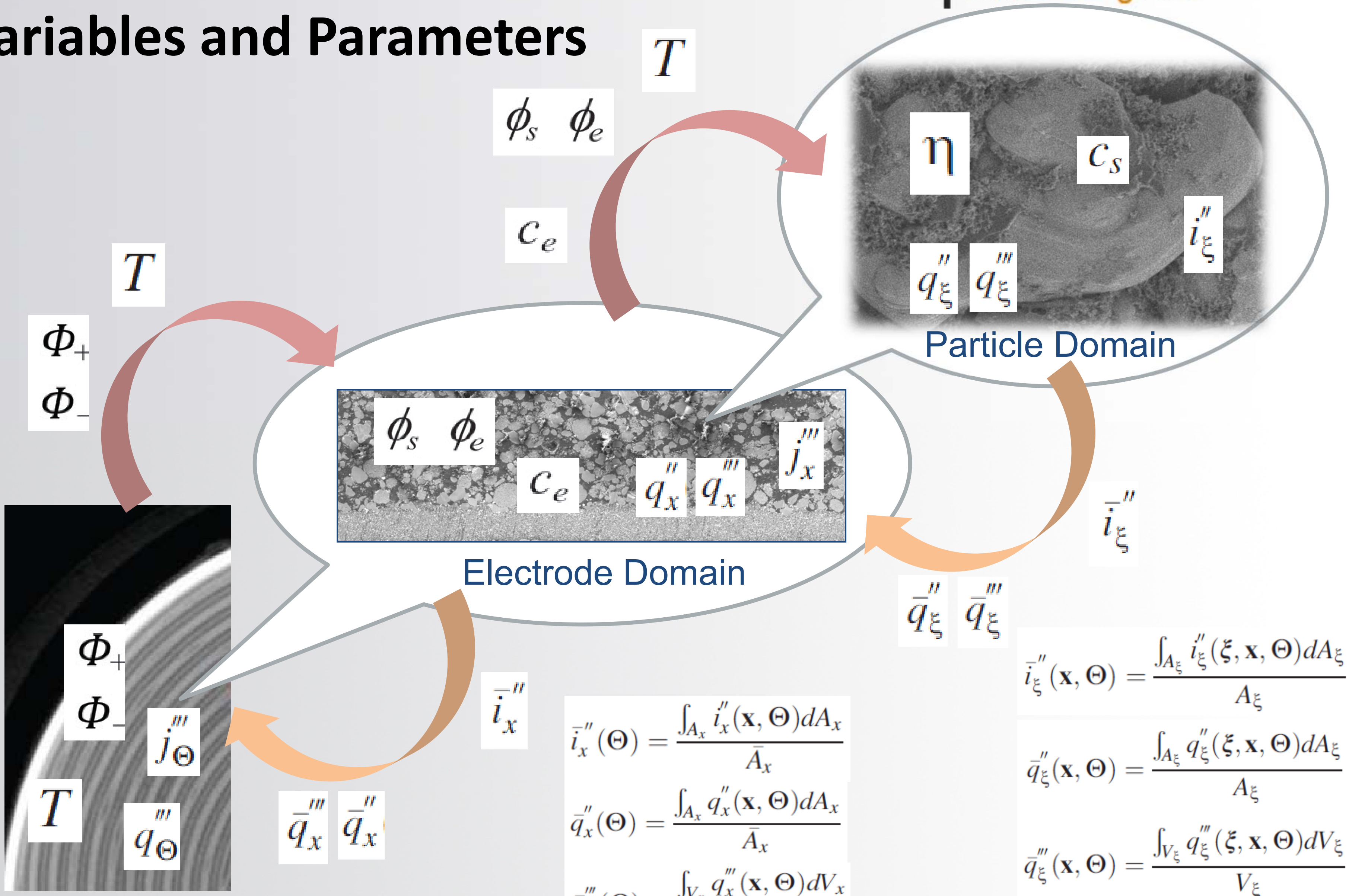
Electrode Domain

Domain Average

Domain Average

Cell Domain

MSMD Protocol For Transferring Variables and Parameters



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

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

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

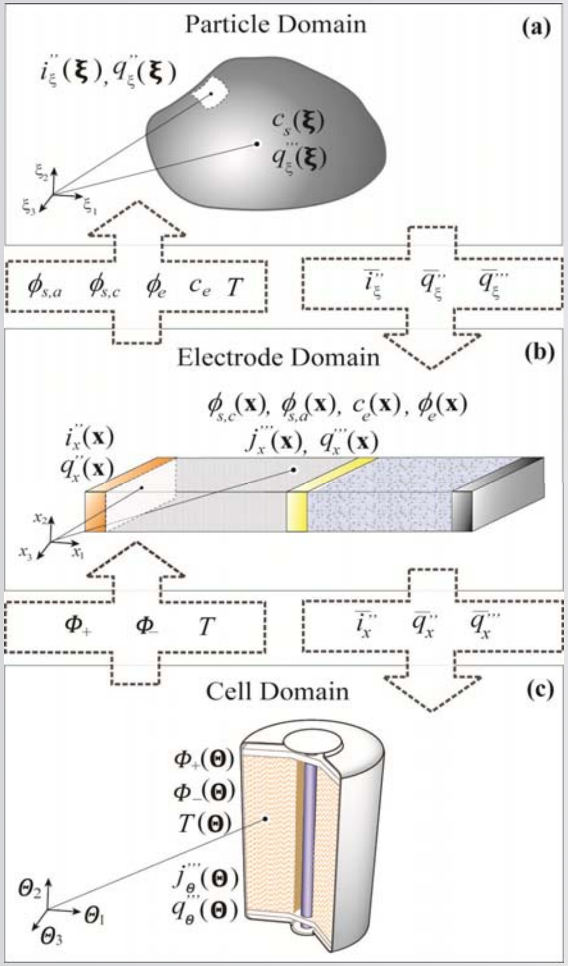
$$\bar{i}''_x(\Theta) = \frac{\int_{A_x} i''_x(\mathbf{x},\Theta)dA_x}{A_x}$$

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

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

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*
- *…*

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

Hierarchical Architecture of MSMD

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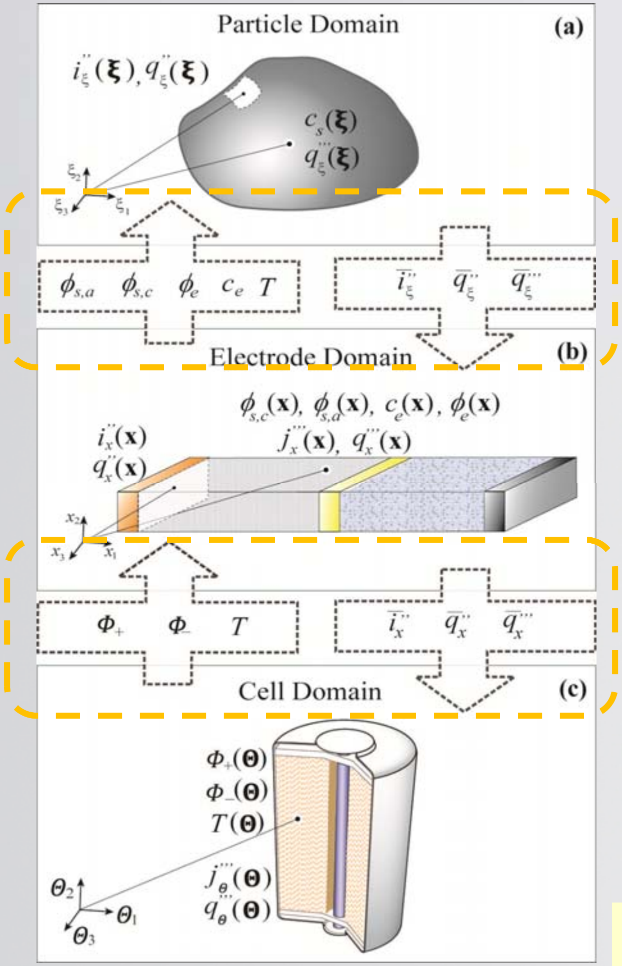


Particle Domain

- *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*
- *…*

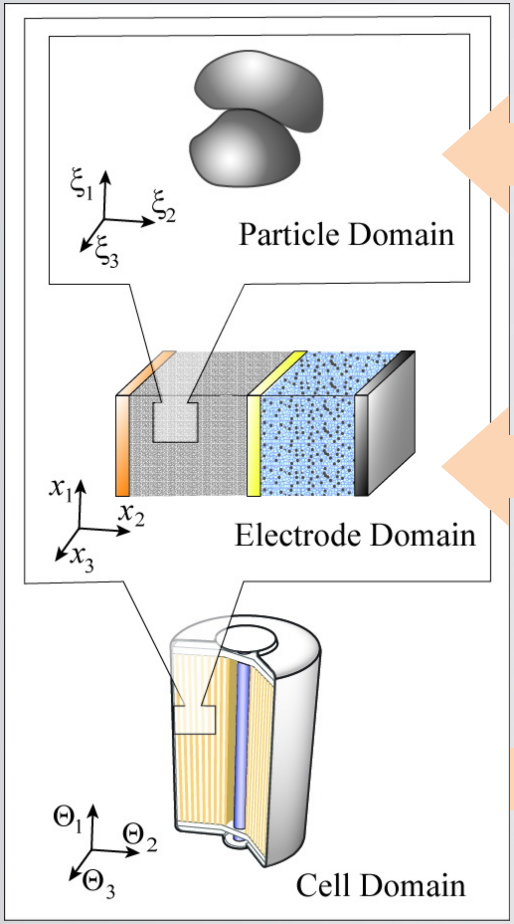
Cell Domain

- *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 Models & Method/Algorithms

1D Spherical particle model

Finite Element

Electrode Domain Submodel Development

Solution Models & Method/Algorithms

Reduced Order Approximation

Cell Domain Submodel Development

Solution Models & Method/Algorithms

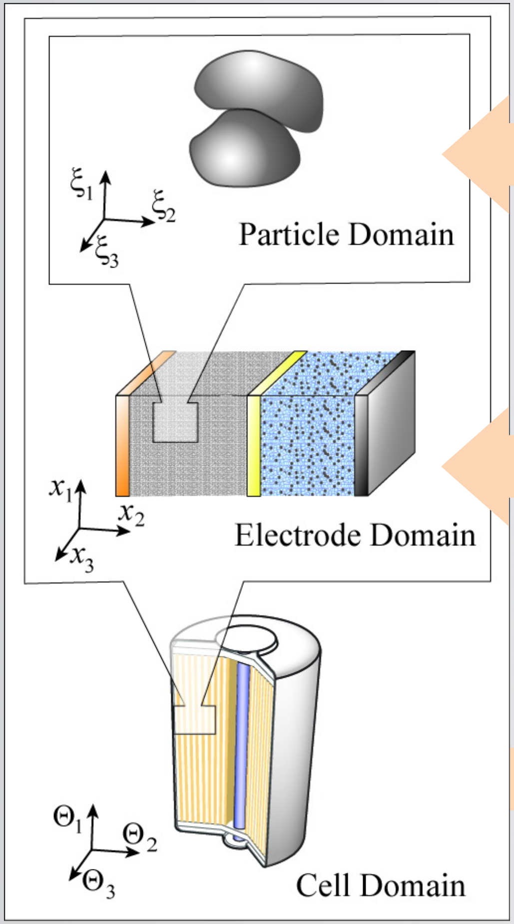
3D Single potential pair continuum model

Finite Volume – Linear superposition

The modularized framework facilitates collaboration with experts across organizations

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 Models & Method/Algorithms

2D Cylindrical particle model

Reduced Order Method

Electrode Domain Submodel Development

Solution Models & Method/Algorithms

1D Porous electrode model

Finite Element Method

Cell Domain Submodel Development

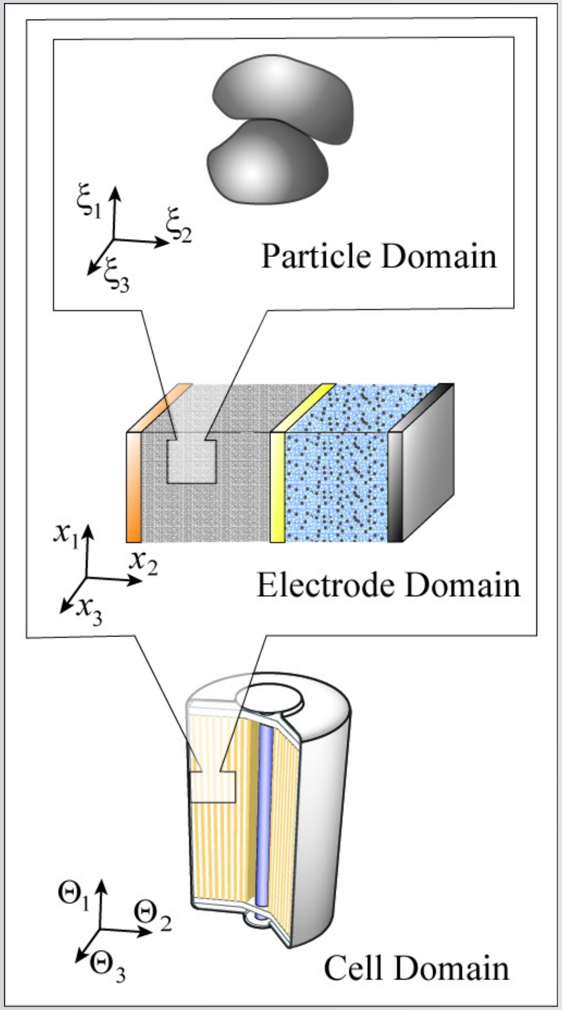
Solution Models & Method/Algorithms

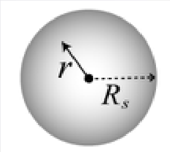
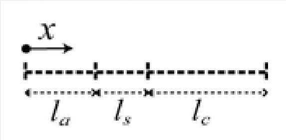
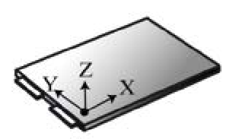
3D Wound potential pair continuum model

Finite Volume Method

The modularized framework facilitates collaboration with experts across organizations

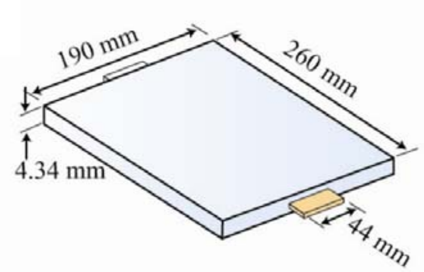
MSMD Application to Prediction of Large Stacked Prismatic Cell Behavior

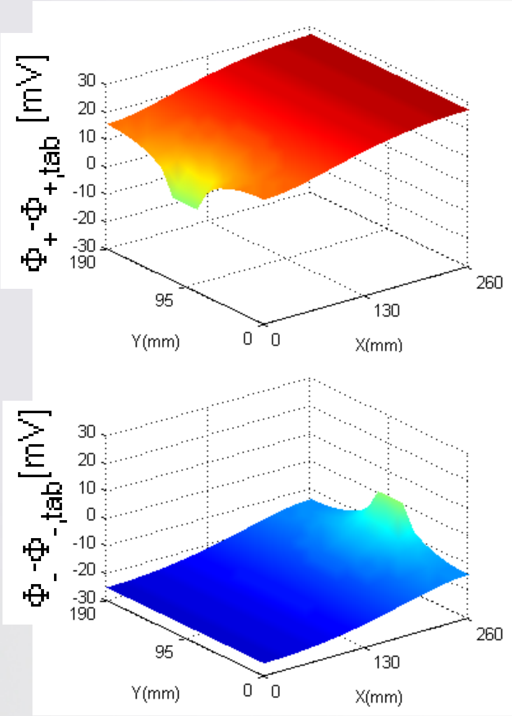


	Submodel Choice	Solution Method
Submodel in the Particle Domain		
	- 1D spherical particle model	- SVM (state variable method)
Submodel in the Electrode Domain		
	- 1D porous electrode model	- SVM
Submodel in the Cell Domain		
	- 3D Single Potential-Pair Continuum Model (**SPPC**)	- FV-LSM (finite volume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

Electric Current Transport

4C discharge / Single-side cooling



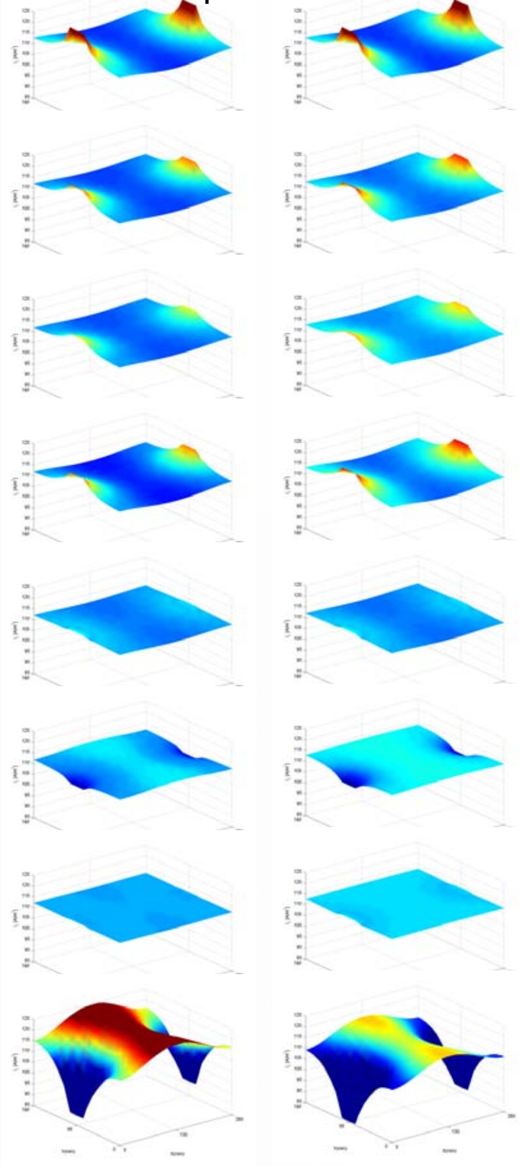


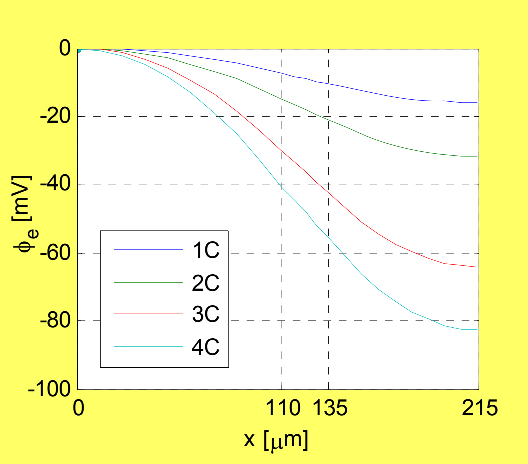
−

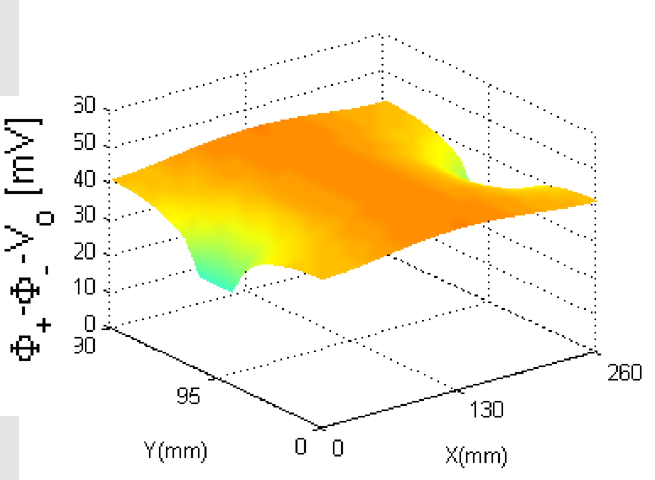
$\bar{i}_x''$

cooled top

bottom







Non-Uniform Utilization

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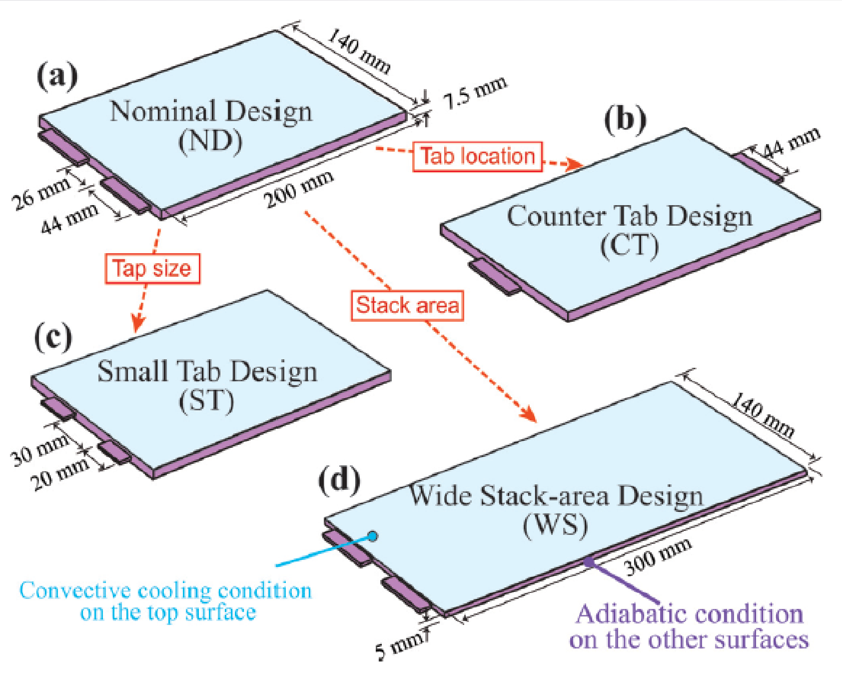
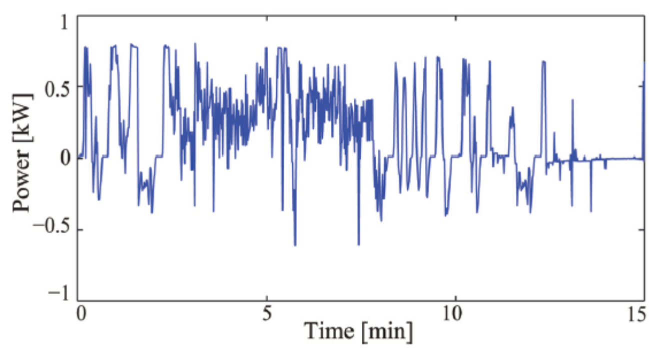
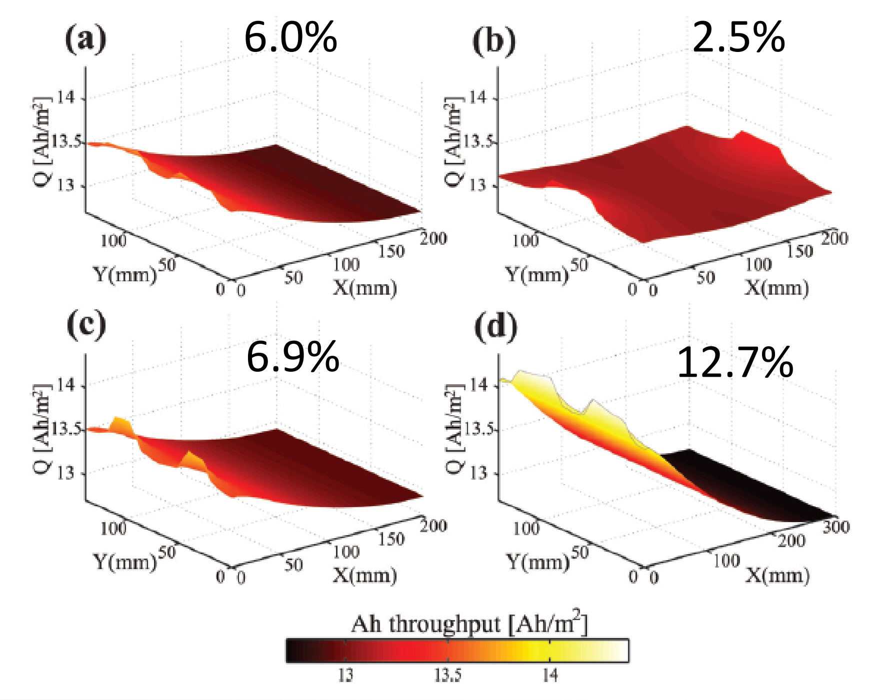
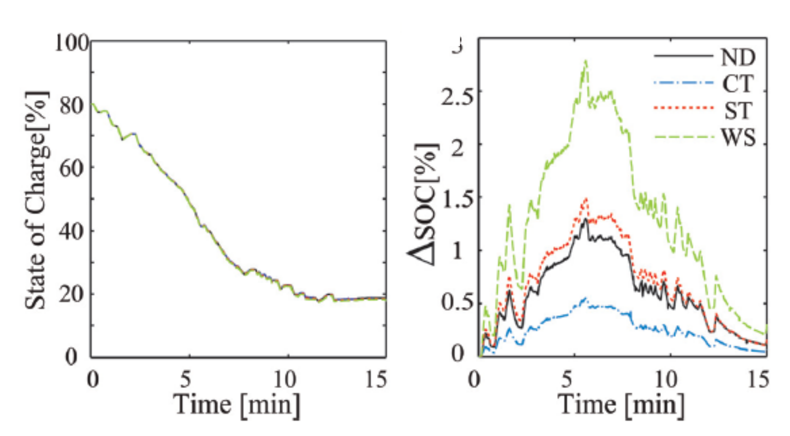


Mid-sized Sedan PHEV10 US06







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

Wound Cells

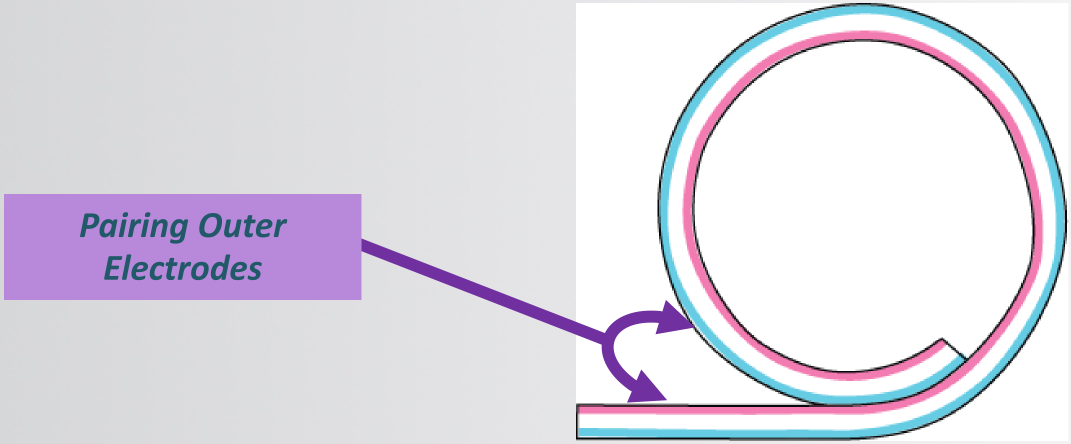
- *A pair of wide current collectors*
- *Two electrode pairs*

Stacking : Forming the first pair between inner electrodes

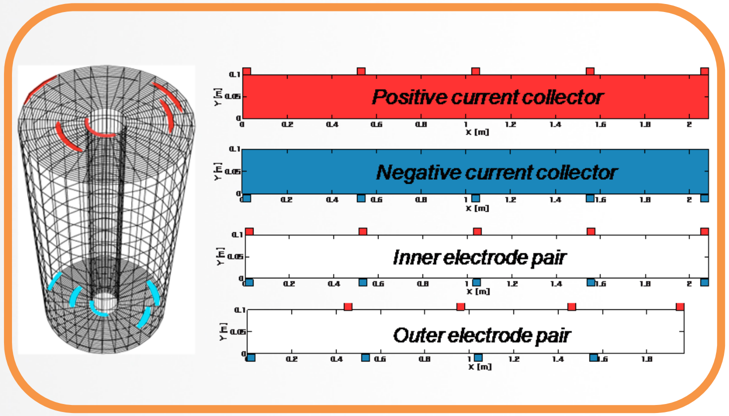
Pairing Inner electrodes

Separator
Electrode
Current collector
Electrode
Separator
Electrode
Current collector
Electrode

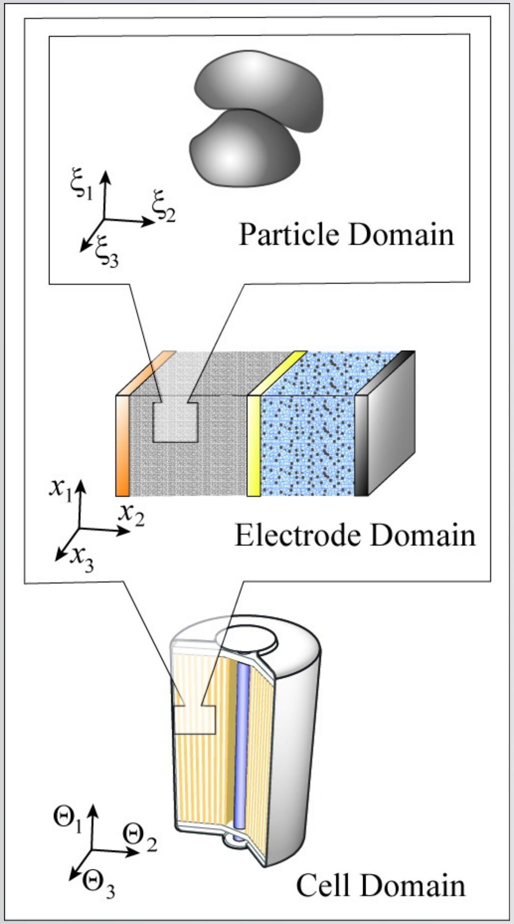
Winding : Forming the second pair between outer electrodes

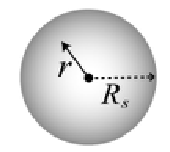
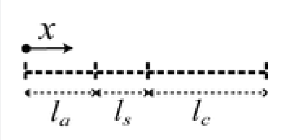


Pairing Outer Electrodes



MSMD Application to Prediction of Wound Cylindrical Cell Behavior

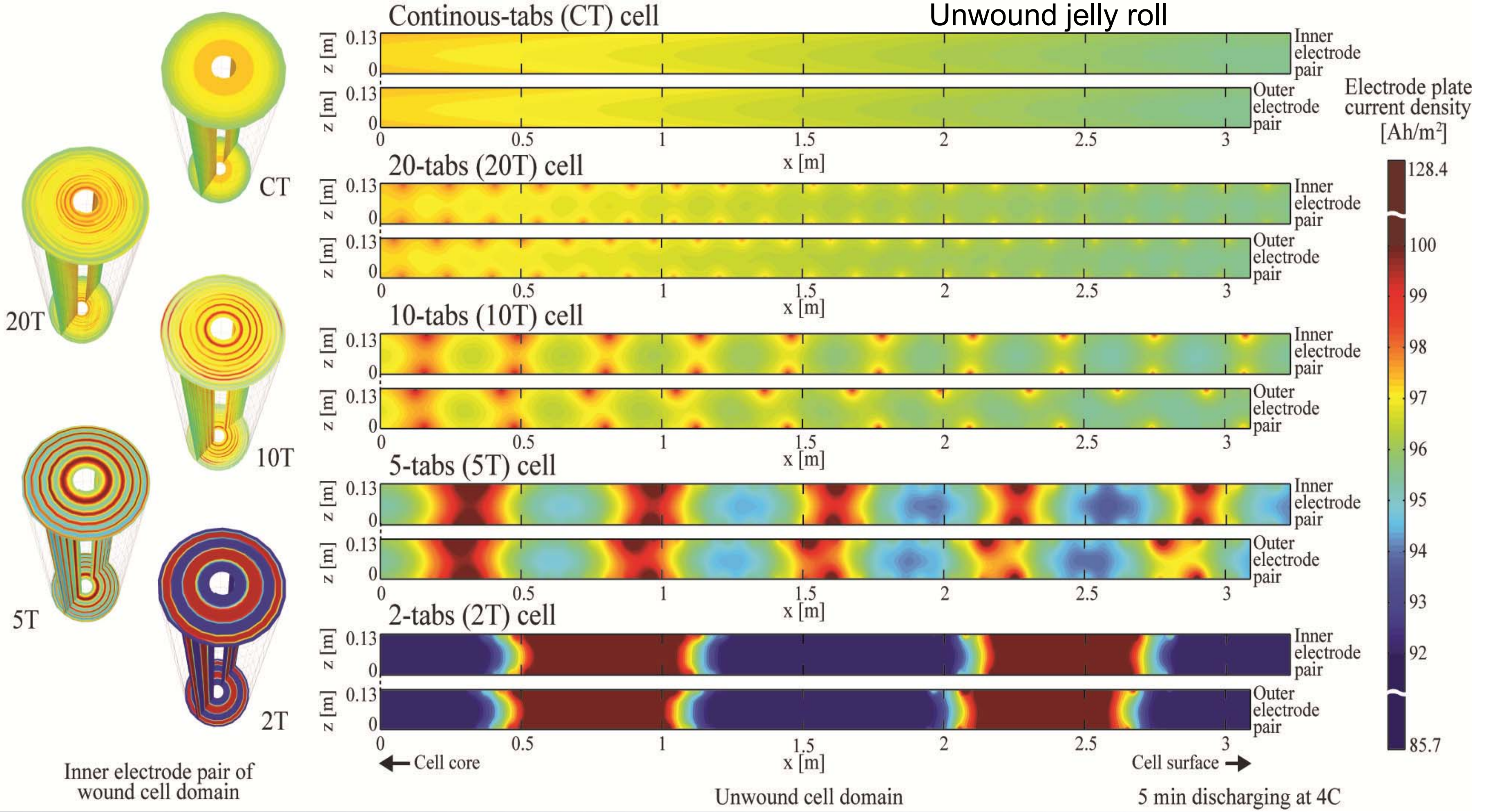


	Submodel Choice	Solution Method
Submodel in the Particle Domain		
	• *1D spherical particle model*	• *SVM (state variable method)*
Submodel in the Electrode Domain		
	• *1D porous electrode model*	• *SVM*
Submodel in the Cell Domain		
	• *3D Wound Potential-Pair Continuum Model (**WPPC**)*	• *FVM (finite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

Kinetics Response

Impact of electrical current transport design

Unwound jelly roll



Lee et al. "A Three-Dimensional Thermal-Electrochemical Coupled Model for Spirally Wound Large-Format Lithium-Ion Batteries," Space Power Workshop; Los Angeles, CA; April 18, 2011.

Non-uniform Kinetics during 4C Discharge

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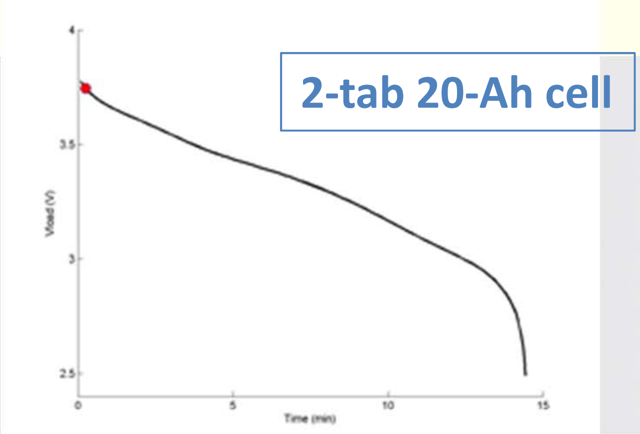
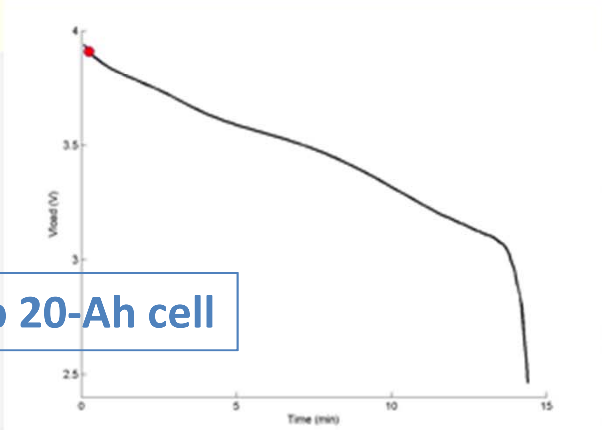
Electrode plate current density [A/m²] at inner-electrode pair

core ← → **surface**

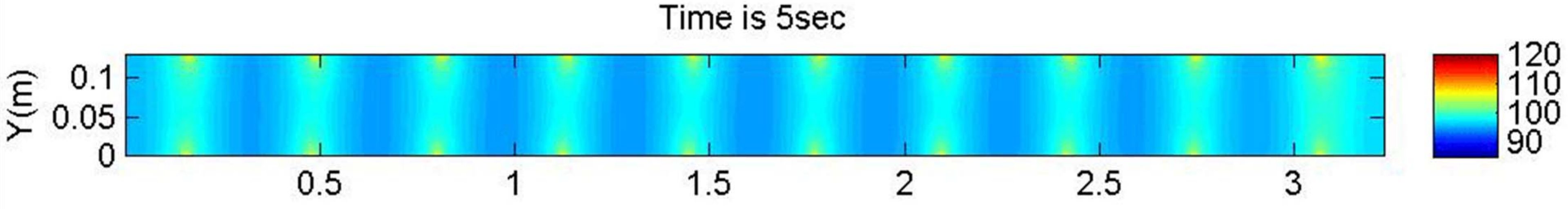
Unwound jelly roll



2-tab 20-Ah cell



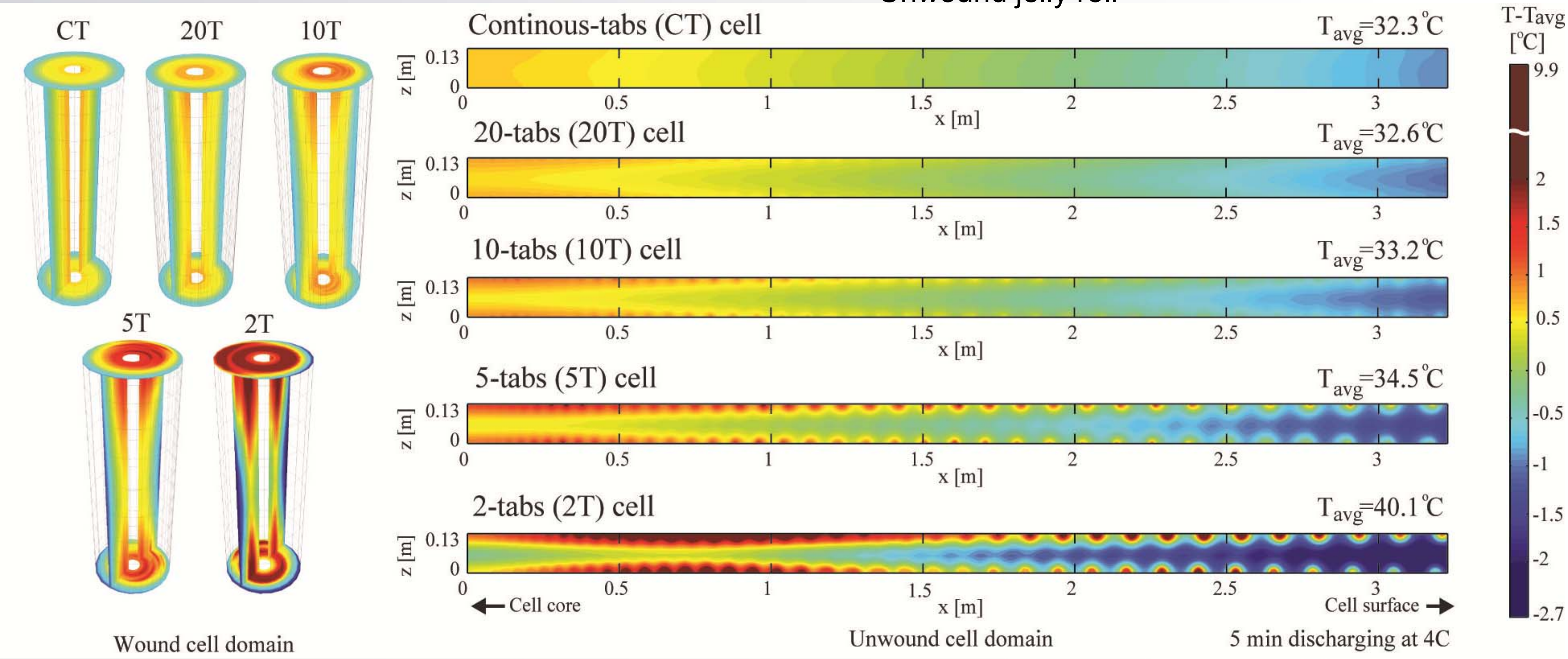
10-tab 20-Ah cell



Lee et al., Space Power Workshop; Los Angeles, CA; April 18, 2011.

Thermal Response

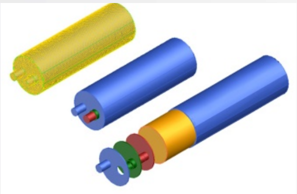
Impact of electrical current transport design


Unwound jelly roll

Temperature imbalance at 4C discharge

Lee et al. “A Three-Dimensional Thermal-Electrochemical Coupled Model for Spirally Wound Large-Format Lithium-Ion Batteries,” Space Power Workshop; Los Angeles, CA; April 18, 2011.

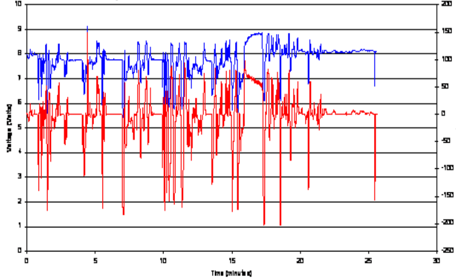
Battery Thermal Simulation/Design



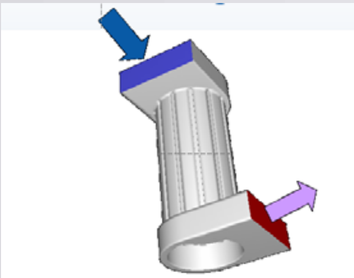
Cell Design & Characteristics Heat Source Model

Vehicle Simulator

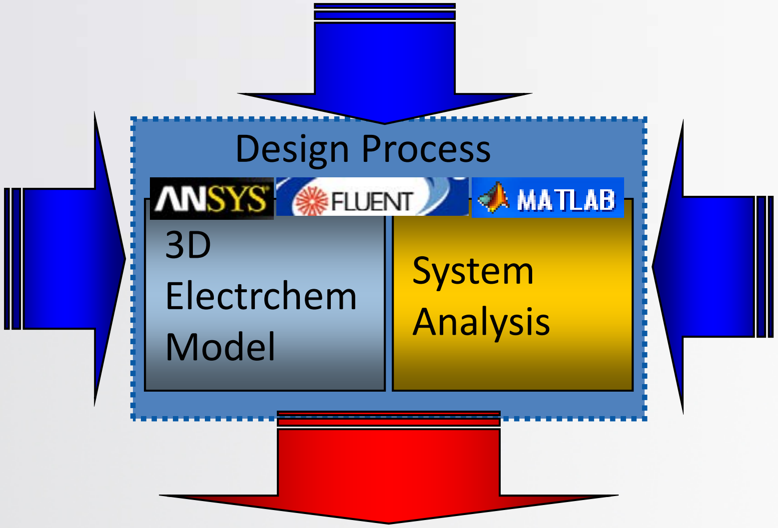
Speed and Power



Load and Operating Conditions



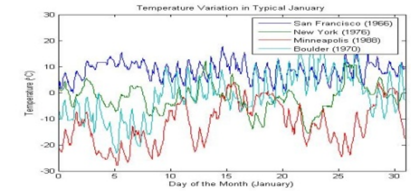
Cooling Strategy and Design



Design Process

3D Electrchem Model

System Analysis

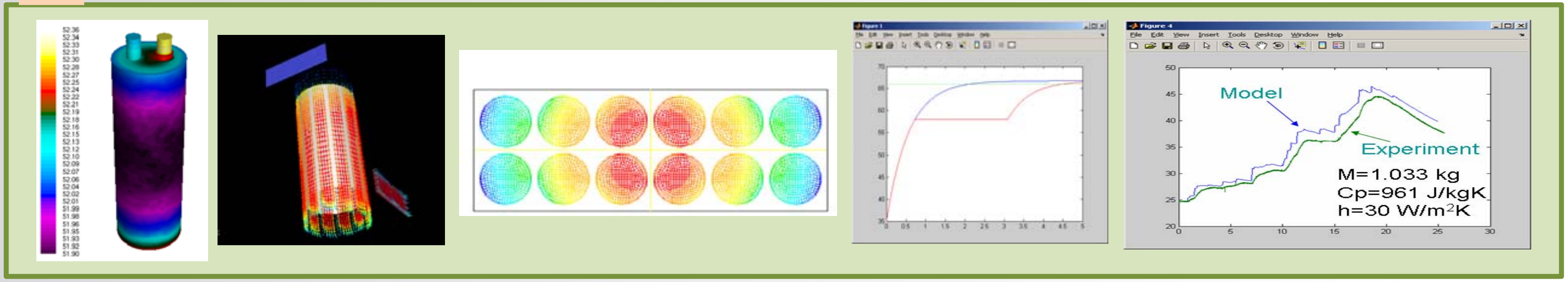


Ambient Temperatures

Feed-back

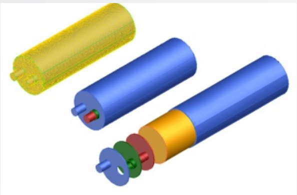
Impact on life, performance

Battery Thermal Responses



Simulating Other Physics

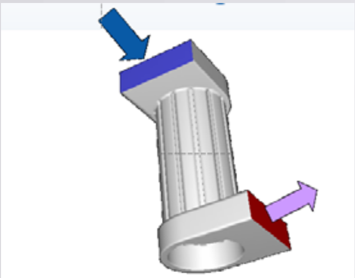
Electrical
Structural (Stress, Fracture)
Mechanical (Shock and Vibration)



Cell Design & Characteristics

Vehicle Simulator

Speed and Power



Operating Strategy and Design

Design Process

ANSYS FLUENT MATLAB

3D Component Analysis

System Analysis

Load and Operating Conditions

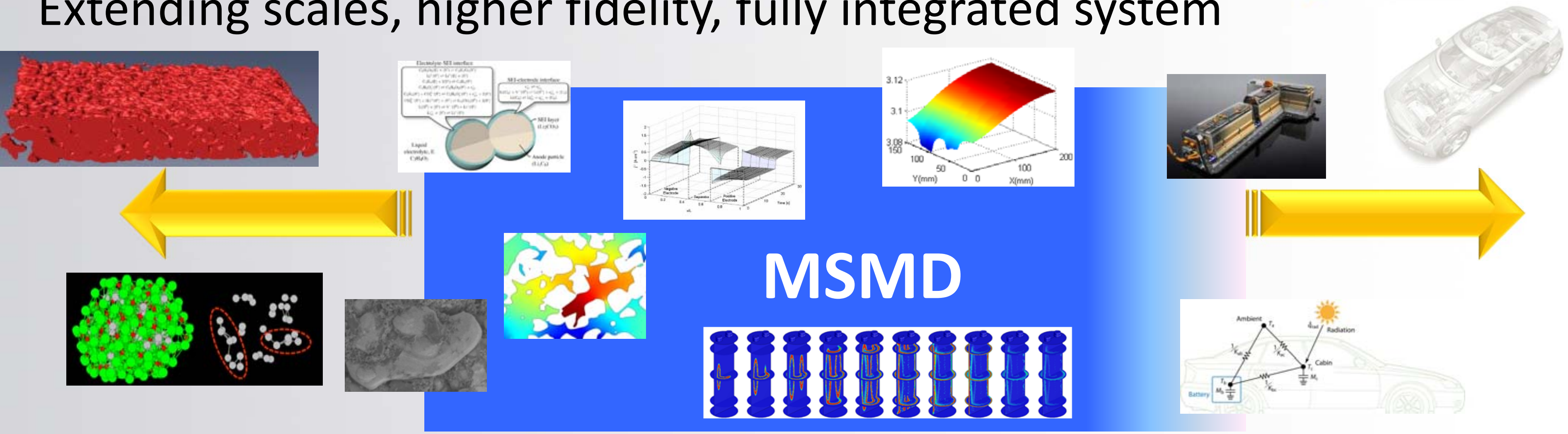
Feed-back

Impact on life, performance, safety

Components and System Response

The Road Ahead:

Extending scales, higher fidelity, fully integrated system



MSMD

Meso-Scale Electrode Model

First Principles

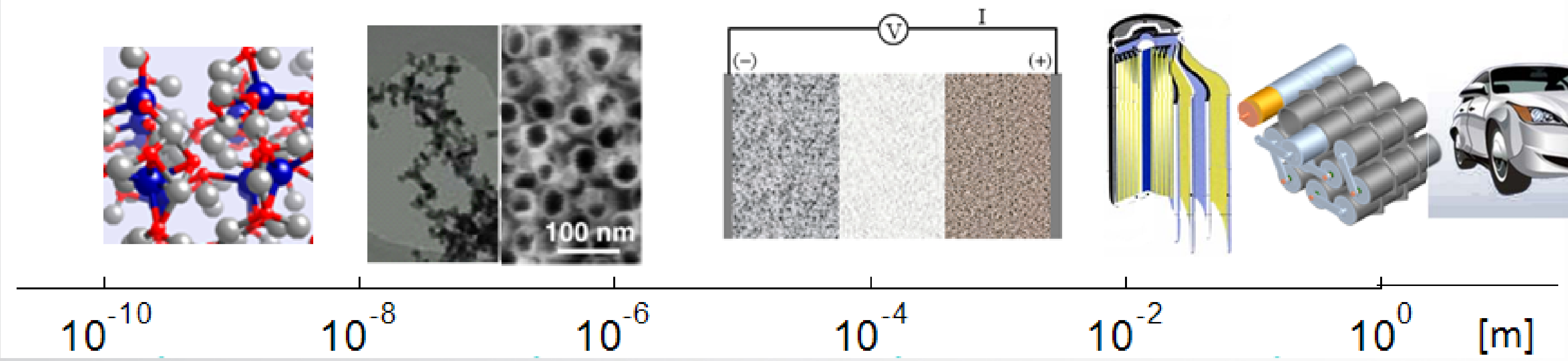
Particle Fracture

Porous Electrode Model

Safety Degradation

CFD Structural

Vehicle Simulation



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  - Dave Howell, Hybrid and Electric Systems Team Lead
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- Feedback from CAEBAT Subcontract Technical Leads
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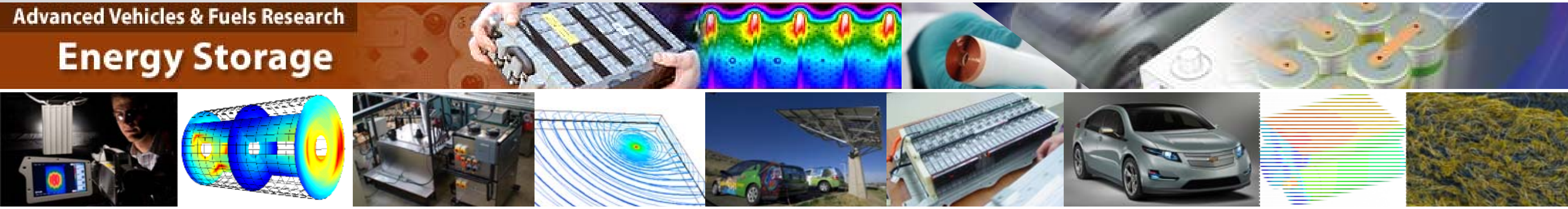
  - Christian Shaffer (EC Power)



nrel.gov/vehiclesandfuels/energystorage/