NREL
NATIONAL RENEWABLE ENERGY LABORATORY

Computer-Aided Engineering of Automotive Batteries

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U.S. Department of Energy

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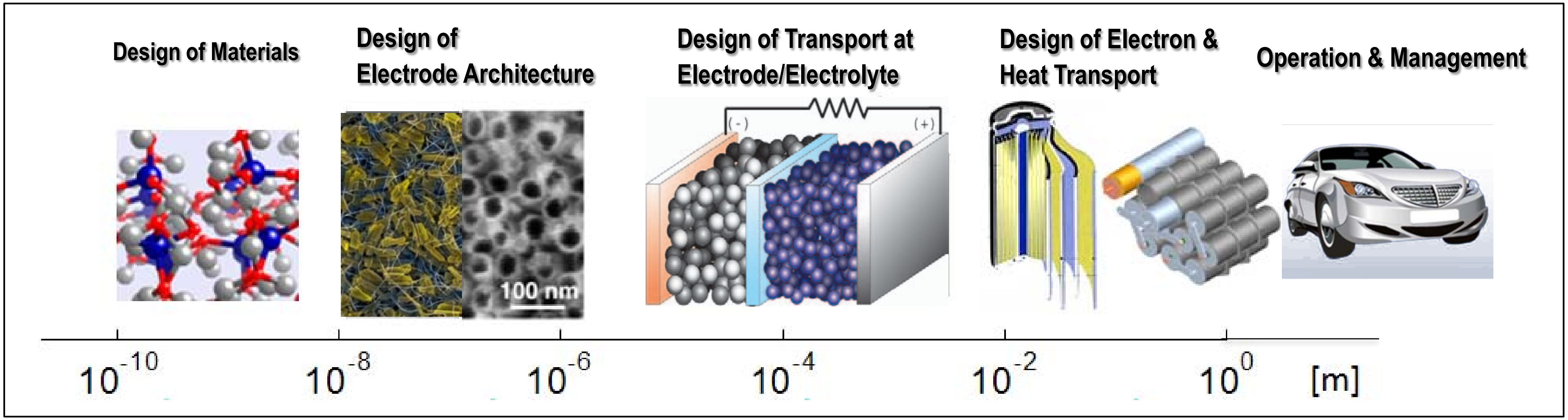
Vehicle Technologies Program U.S. Department of Energy

Introduction – Battery CAE

- Computer-aided engineering (CAE) is a proven pathway, especially in automotive industry, to
  - Improve performance by resolving relevant physics in complex systems
  - Shorten product development design cycle and thus reduce cost
  - Provide an efficient manner for evaluating parameters for robust designs
- Most battery CAE models could be enhanced
  - Academic models include relevant physics details, but neglect engineering complexities
  - Industry models include relevant macroscopic geometry and system conditions, but use too much simplification in fundamental physics
- DOE- and private-industry-funded projects have demonstrated the value of battery CAE
  - Most in-house custom model codes, however, require expert-users
- Battery CAE capabilities need to be transferred to industry
  - In time to impact the transition toward sustainable electric mobility
  - Reduce the process of design, build, test, break, redesign, rebuild, retest,…

Multi-Scale Physics in Li-Ion Battery

Various physics interact across wide range of length and time scales



Present industry needs

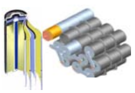
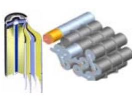
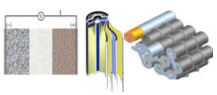
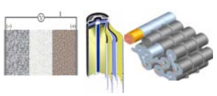
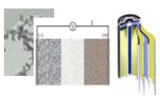
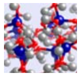
- ***Performance & Life Models:*** *Coupling electrode-level performance/life with cell/pack-level heat/current transport*
- ***Safety Models:*** *Coupling electrode-level chemical reactivity and cell/pack-level heat transport*
- *Need to include both <u>science</u> and <u>engineering</u>*

Active research areas

- ***First Principals Material Evaluation***
- ***Electrode Architecture Design***

NREL Battery Modeling Portfolio

(diverse, but not integrated)

Model	Length Scale pm --- nm --- µm --- mm ---- m	Geometry	Physics / Application
Vehicle/component (PSAT/ANL & Advisor/NREL)		Lumped	• Drivetrain power balance / Drive cycle • Battery usage & requirements • Control strategy design
Battery cost		Lumped	• Empirical • System cost ($/*kW*, $/*kWh*)
Battery life		Lumped	• Empirical • Life prediction ($t, N_{cyc}, T, \Delta DOD, SOC$)
Equivalent circuit (e.g. PNGV, FreedomCar)		Thermal/electrical network	• Electrical & thermal • Performance, design, safety evaluation
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
Molecular dynamics		3-D	• Atomic & molecular interactions • Material design

Battery CAE : What Should One Expect?

- **Multi-scale Physics Interaction**: Integrate different scale battery physics in computationally efficient manner

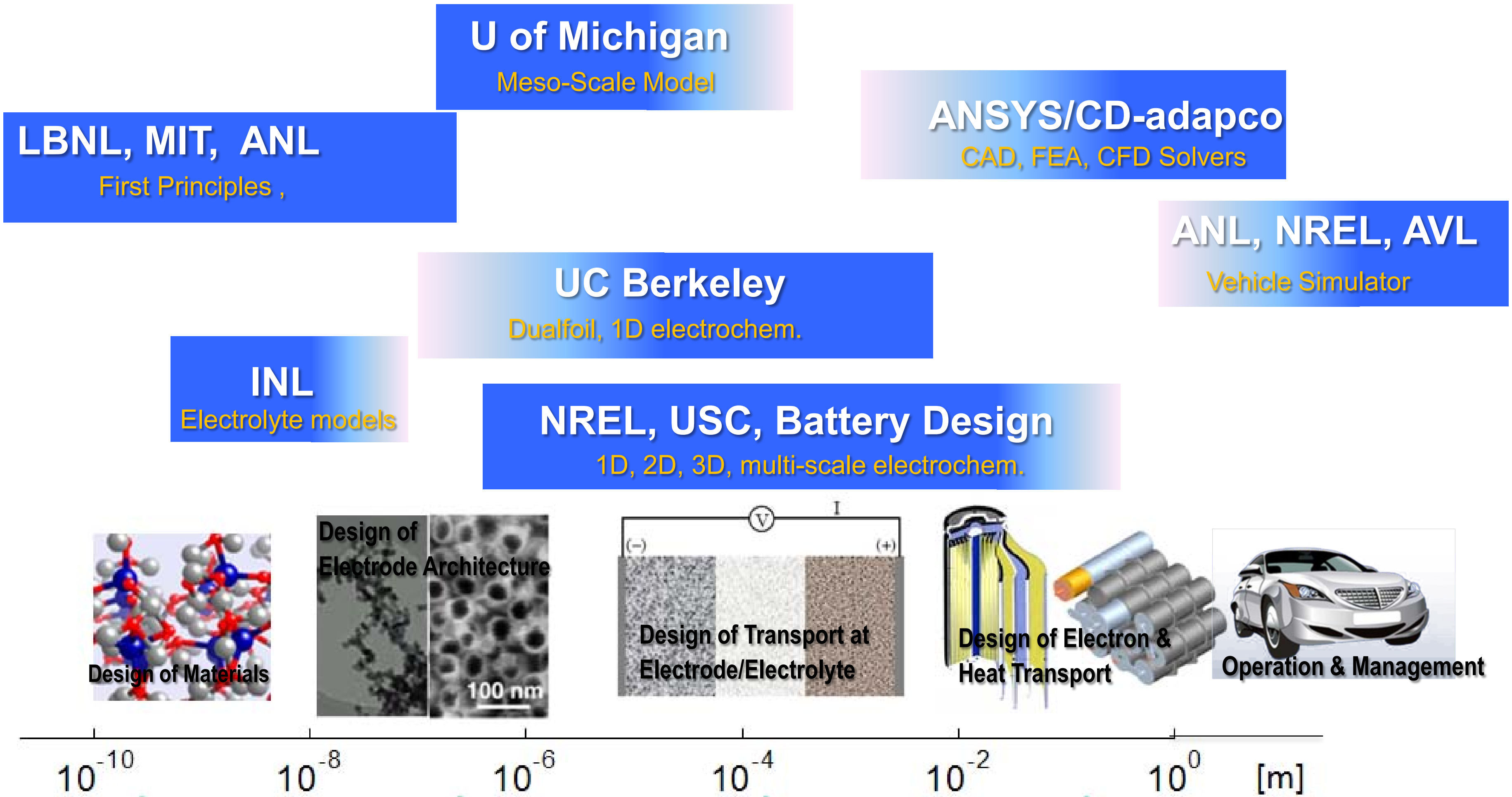
- **Flexibility**: Provide a modularized multi-physics platform – Enable user choice from multiple submodel options with various physical/computational complexity

- **Expandability**: Provide an expandable framework to “add new physics of interest” or to “drop physics of insignificance/indifference”

- **Validation and Verification:** The correct equations are solved and they are solved accurately

Length-Scale Mapping for Li-ion Battery Models

(Examples and not a complete list)

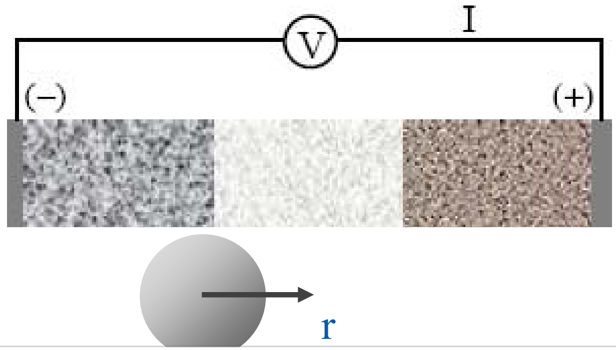


Example
Electrode-Scale Performance Model

Charge Transfer Kinetics at Reaction Sites

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

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



Species Conservation

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

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

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

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

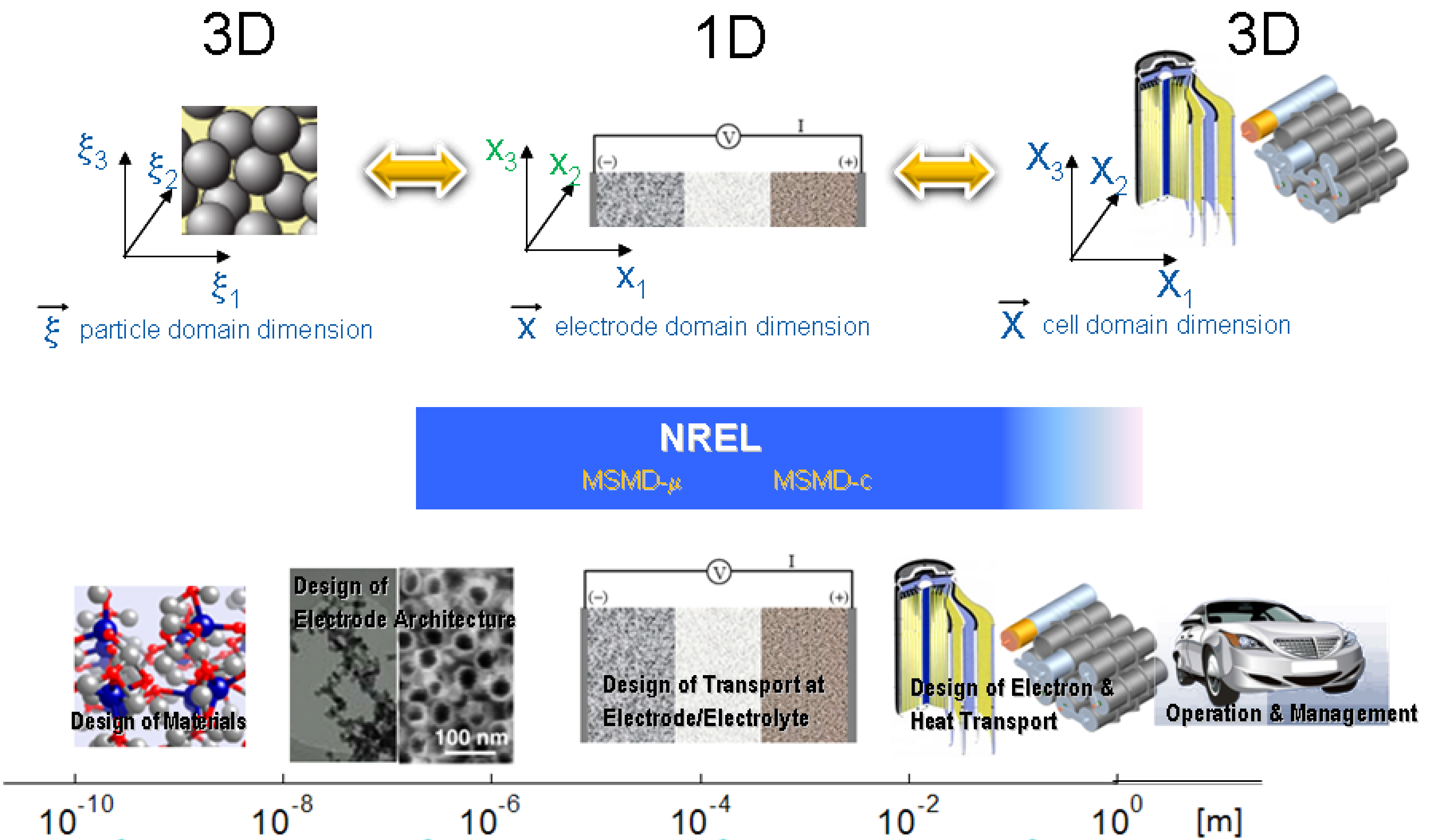
$$q''' = j^{Li} \left(\phi_s - \phi_e - U + T \frac{\partial U}{\partial T} \right) + \sigma^{eff} \nabla \phi_s \cdot \nabla \phi_s + \kappa^{eff} \nabla \phi_e \cdot \nabla \phi_e + \kappa_D^{eff} \nabla \ln c_e \cdot \nabla \phi_e$$

- Pioneered by Newman's group (*Doyle, Fuller, and Newman 1993*) – Dualfoil (cchem.berkeley.edu/jsngrp/fortran_files/Intro_Dualfoil5.pdf)
- Captures *lithium diffusion dynamics* and *charge transfer kinetics – porous media*
- Predicts *current/voltage response* of a battery
- Provides design guide for thermodynamics, kinetics, and transport across electrodes

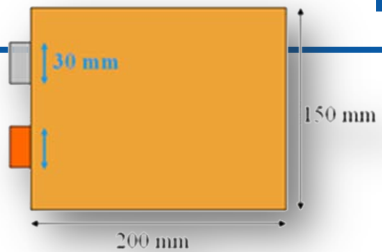
- Difficult to resolve *heat* and *electron current* transport in large cell systems

Extending Newman's model to Thermal-EChem 3D

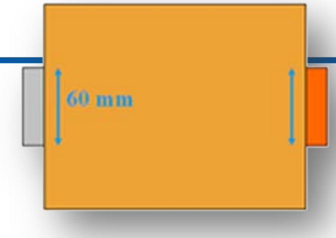
NREL's Multi-Scale Multi-Dimensional (Domain) Model Approach



Example Results of Battery Modeling Multi-Physics Interaction

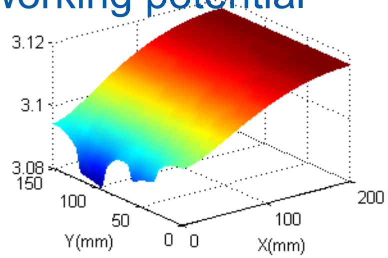


Comparison of two 40 Ah
flat cell designs
2 min 5C discharge

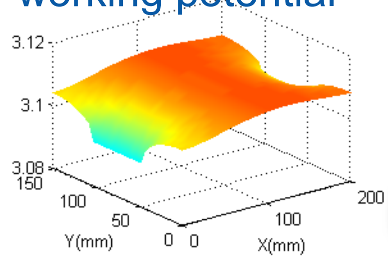


- *Larger over-potential promotes faster discharge reaction*
- *Converging current causes higher potential drop along the collectors*

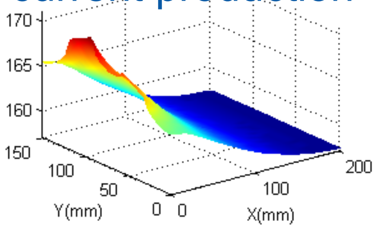
working potential



working potential



electrochemical current production



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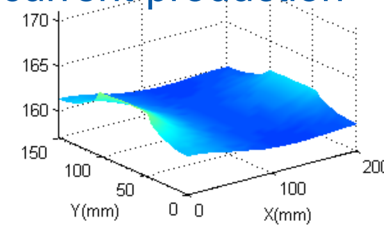

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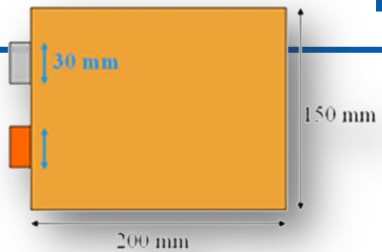

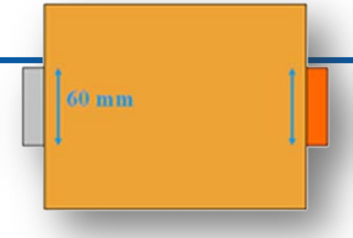

Comparison of two 40 Ah flat cell designs

2 min 5C discharge

- *Larger over-potential promotes faster discharge reaction*
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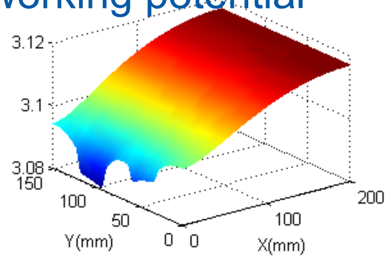
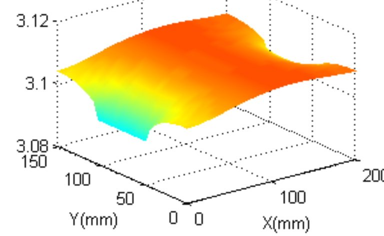
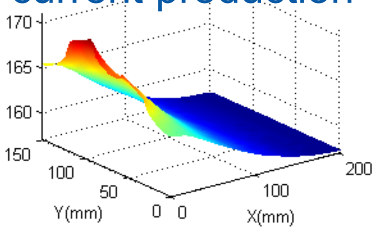
working potential



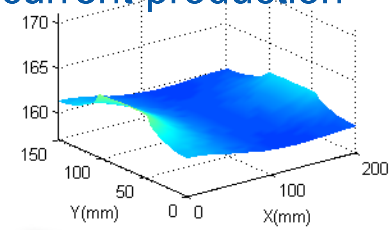
working potential



electrochemical current production

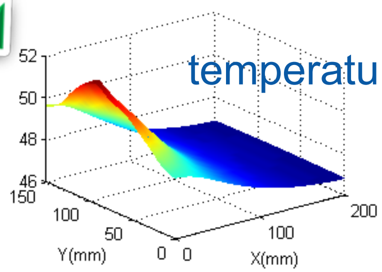


electrochemical current production

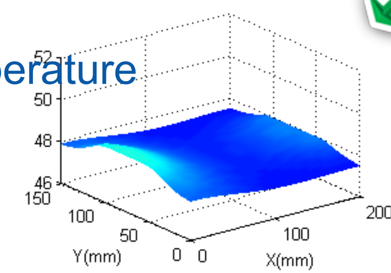


- *High temperature promotes faster electrochemical reaction*
- *Higher localized reaction causes more heat generation*

temperature



temperature



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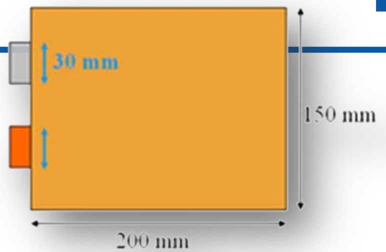

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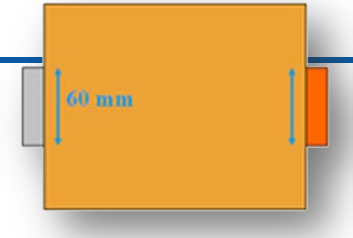

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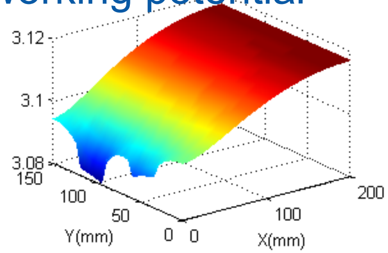
working potential



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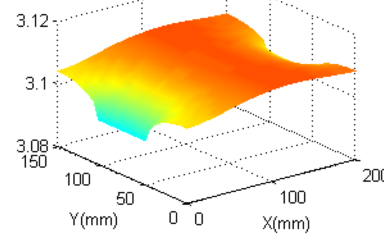

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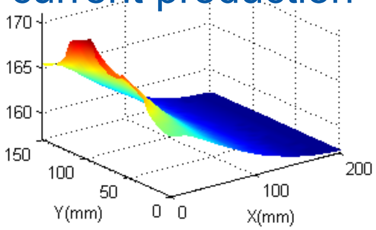

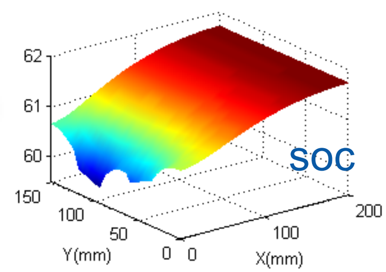

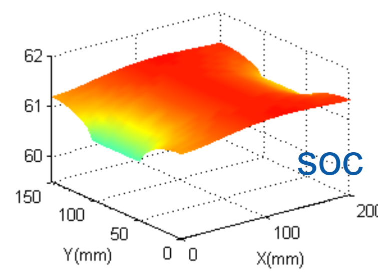

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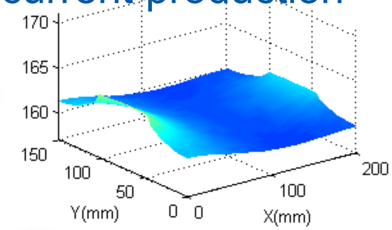

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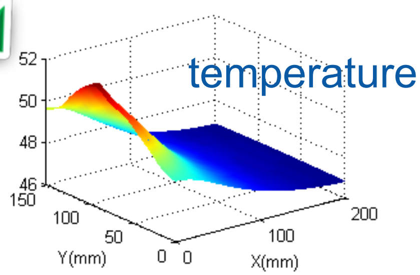
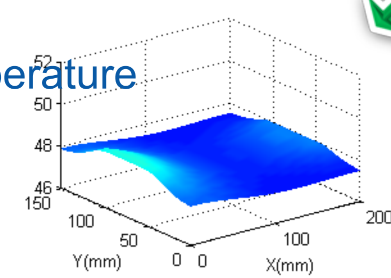
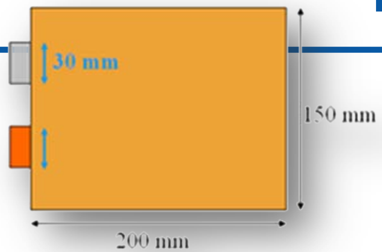


temperature



Example Results of Battery Modeling
Multi-Physics Interaction



Comparison of two 40 Ah
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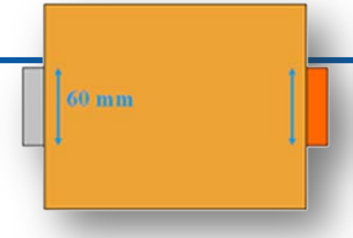

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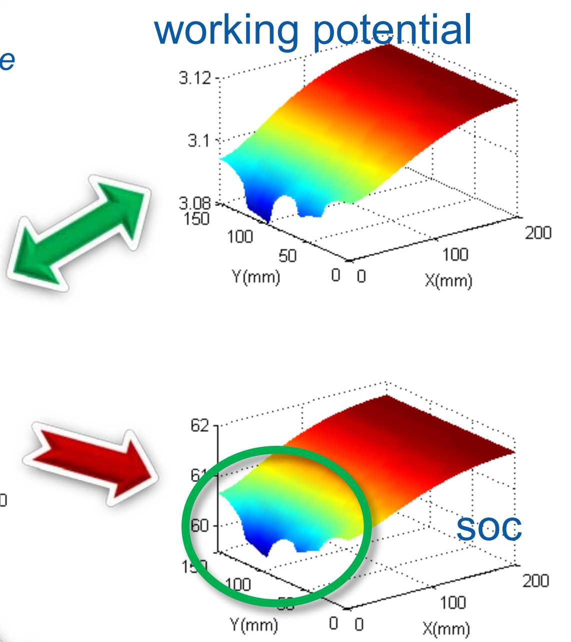
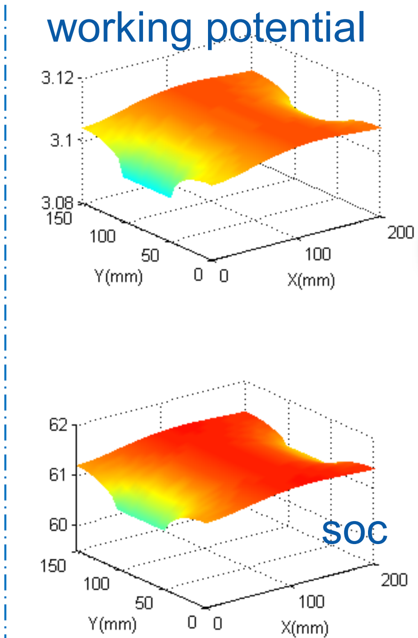
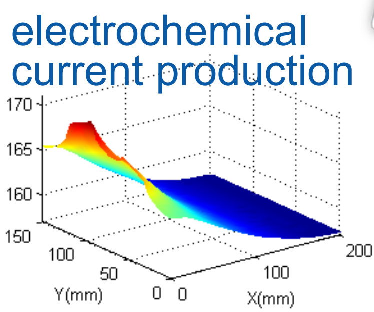
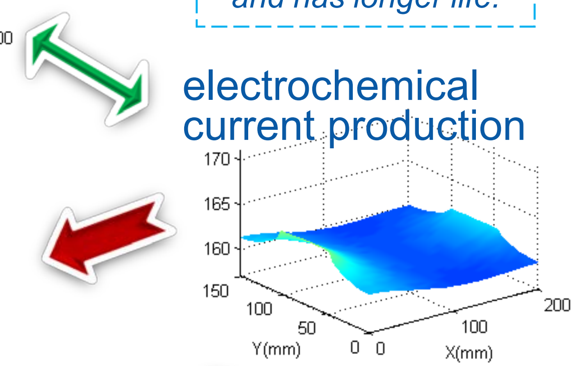




This cell is cycled more uniformly, can therefore use less active material ($) and has longer life.





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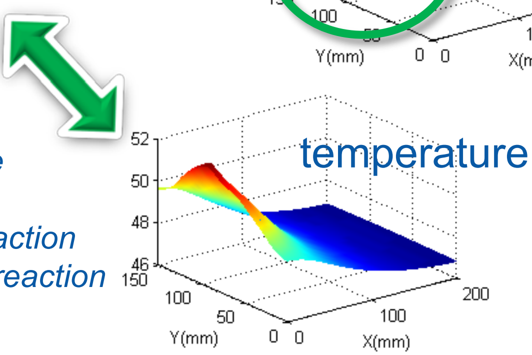
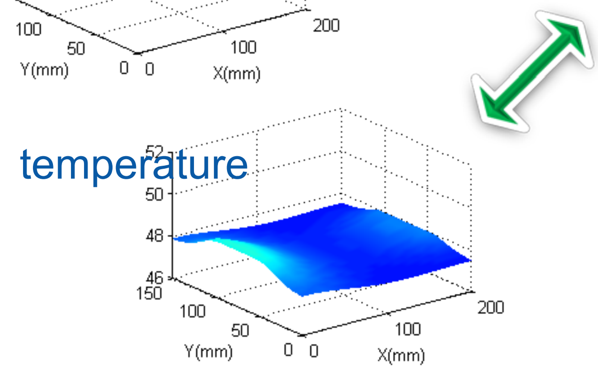




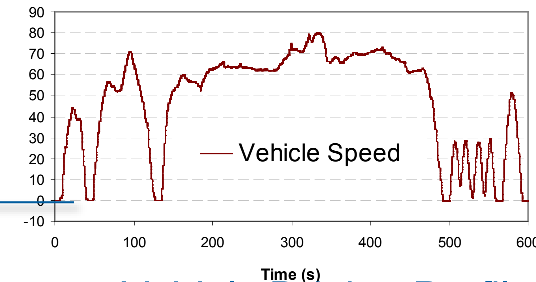
Virtual Design Evaluation
Integrated Battery – Vehicle Approach

Virtual

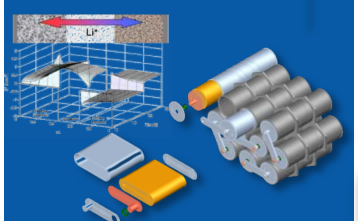
Vehicle Design

Embedded
Battery Model

Vehicle Simulator

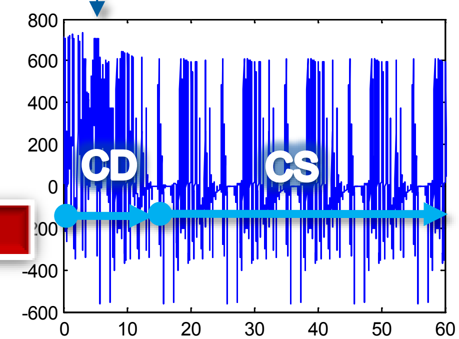


Vehicle Driving Profile



Virtual
Battery Design

Multi-Scale
Multi-Dimensional
Li-ion Battery Model



Battery Power Profile

Charge sustaining
Charge depleting
Combination
Charging

Battery Responses

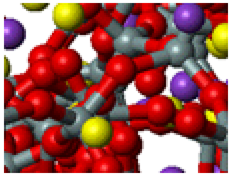
Feedback

Need to Develop Modular Plug-and-Play Modeling Design Concepts

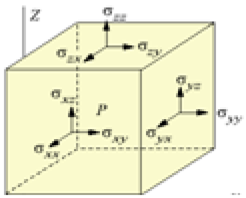
Material Level Models ⟷ **Electrode Level Models** ⟷ **Component Level Models** ⟷ **Vehicle Level Models**

Material Level Models

First Principles

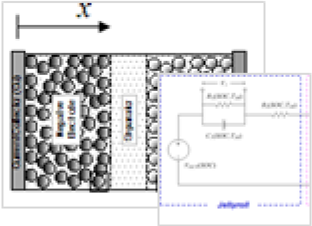


Material Stress

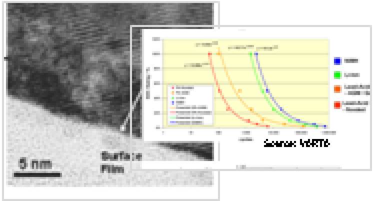


Electrode Level Models

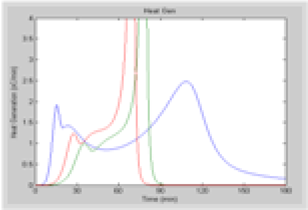
Performance



Electrochemical & Material Stress

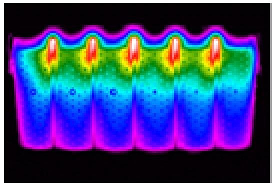


Abuse

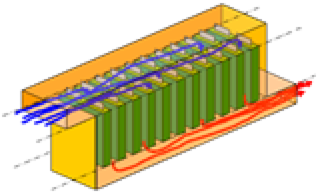


Component Level Models

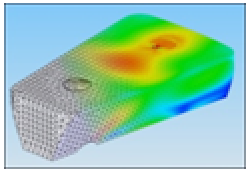
Current & Heat Transport



Fluid Dynamics

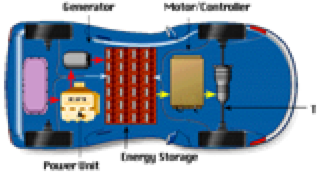


Stress & Vibration



Vehicle Level Models

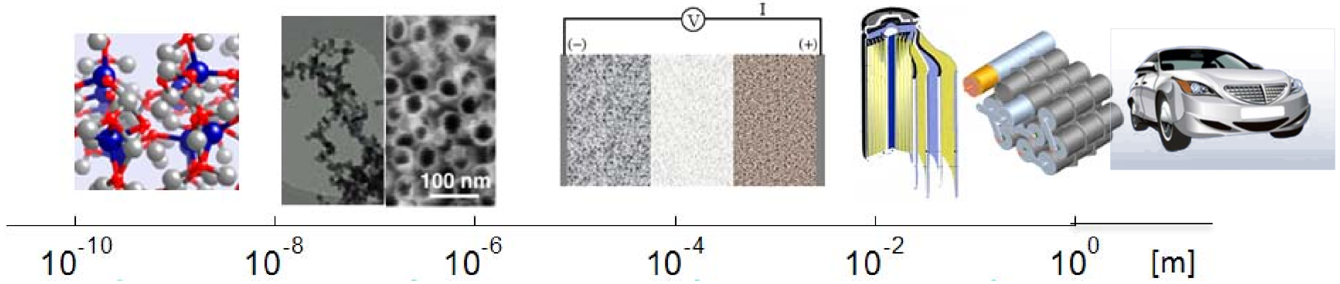
Power Demand



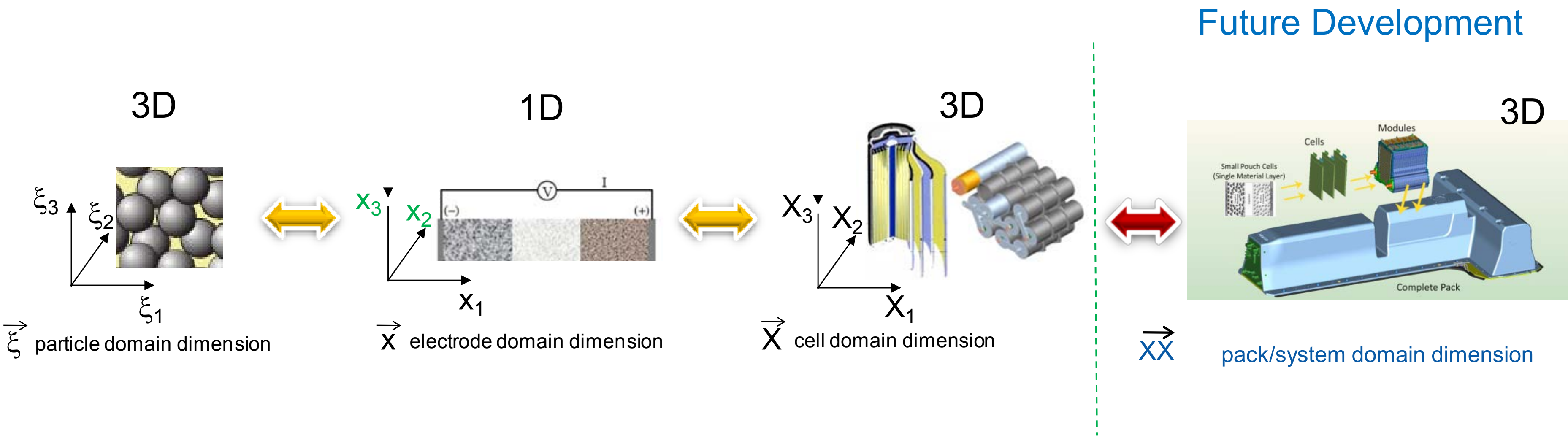
External Thermal Load

Future Plans – Battery CAE

- Integrating various models in one single platform for industry to use
- Bottom-up model validation and demonstration study
- Enhancing physics models



- Enhancing solver capability & solution schemes



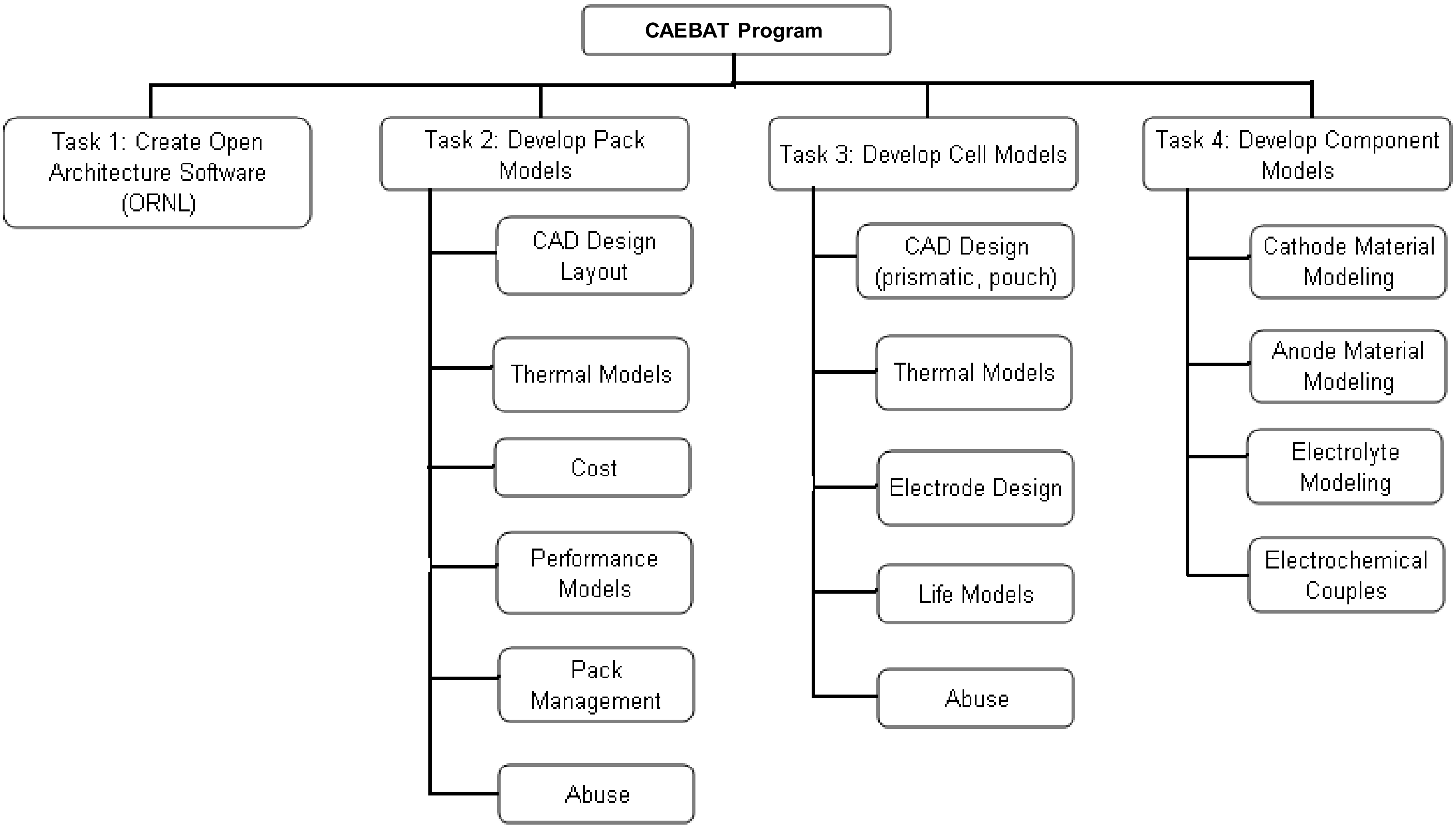
A New Activity – CAE for Batteries

- In the last several years, DOE's Vehicle Energy Storage Program has been funding battery modeling as part of its
  - Exploratory Battery Activity (BATT)
  - Applied Battery Research Activity (ABR)
  - Battery Development Activity
- DOE has been evaluating approaches to integrate these battery modeling activities and make them more accessible as design tools for industry
- In April 2010, DOE initiated implementing the Computer-Aided Engineering for Electric Drive Vehicle Batteries (CAEBAT) activity
  - Objective is to incorporate existing and new models into software battery modeling suites/tools
  - Goal is to shorten design cycle and optimize batteries (cells and packs) for improved thermal uniformity, safety, long life, low cost

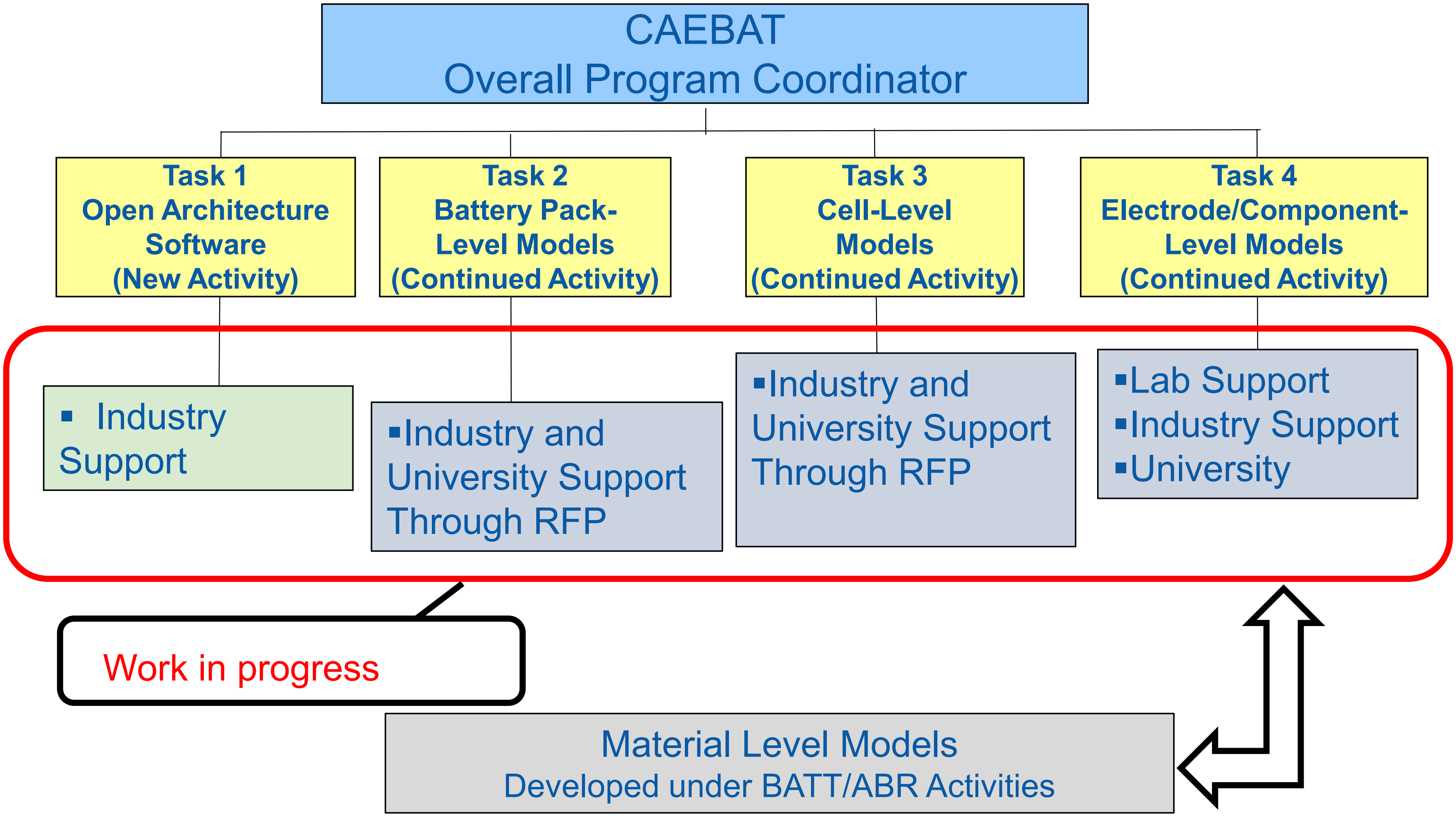
CAEBAT Operating Structure and Plans

- Operate similarly to BATT and ABR activities
- Include several National Laboratories
- One Lab coordinating the activities for DOE (NREL for CAEBAT)
- Include competitive collaborations with universities and industry (cell developers, pack integrators, vehicle makers, and software venders)
- Include structured tasks and subtasks dealing with materials/components, cells, packs, and open software architecture
- Seek collaboration with federal, state, and private organizations for leveraging resources
- Conduct annual planning, progress, and review meetings

Elements of CAEBAT Structure



CAEBAT Program



Planned Activities – CAEBAT Program

- Interact with other, National Labs, industry, and universities
- Develop detailed description of tasks and overall program plan
- Conduct model development and integration in National Labs and later by industry and universities
- Issue Request for Proposals (RFP) in July, receive proposals, review them, and select awardees by end of September
  - Multi-year, multi-partner projects
- More to come……………….