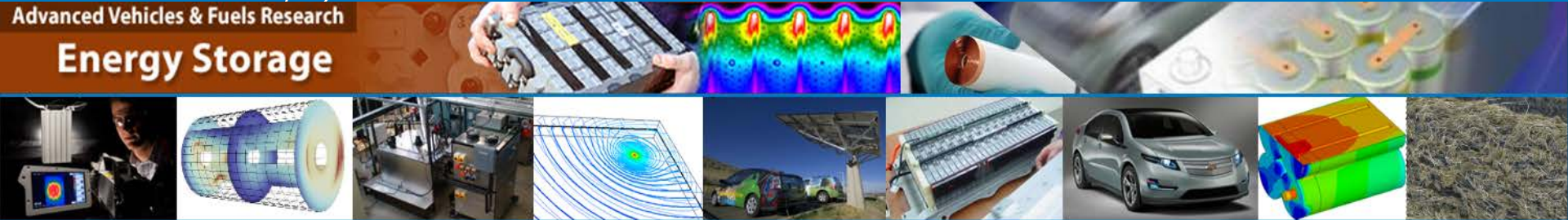![NREL - National Renewable Energy Laboratory]

Significant Enhancement of Computational Efficiency in Nonlinear Multiscale Battery Model for Computer Aided Engineering

Advanced Vehicles & Fuels Research
Energy Storage

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Jacob White: **ANSYS/MIT**

Annual Merit Review and Peer Evaluation Meeting

June 17, 2014

Washington, D.C.
PR-5400-61865

Project ID #: ES197

Overview

Timeline

- **Start Date:**   October 2013
- **End Date:**   September 2015
- **Percent Complete:** 25%

Barriers in Battery CAE

CAE accelerates product development cycle, reduce cost and improve performance

- Limited Multiphysics Integrity
- Wide-varied Time & Length Scales
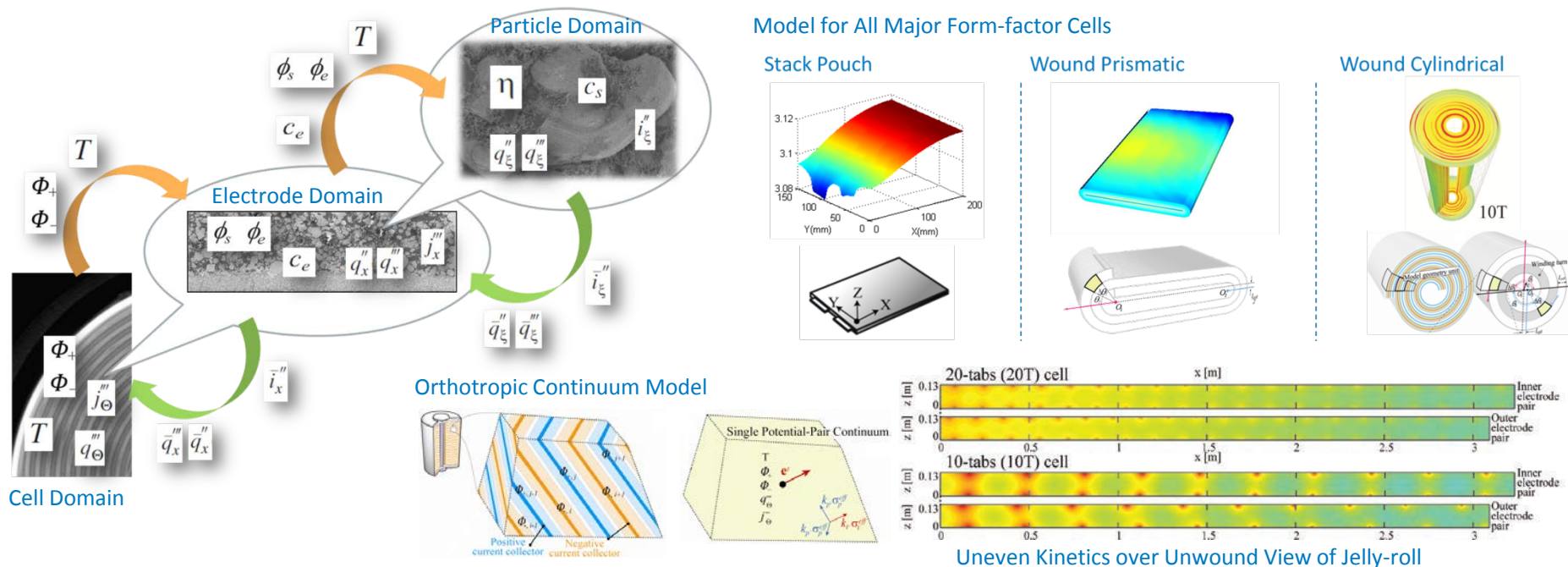- Instability Caused by Nonlinearity

Budget

- **Total Project Funding:** $1,218K
  - DOE Share : $718K
  - TARDEC Share: $500K
- **Funding Received in FY13:** $718K
- **Funding for FY14:**
  Awaiting funds from TARDEC

Partners

- **ANSYS**
  - Physics Business Unit
  - Electronics Business Unit
- **Project Lead: National Renewable Energy Laboratory (NREL)**

CAE = computer aided engineering   TARDEC = The US Army Tank Automotive Research, Development and Engineering Center

This PROJECT was awarded based on a proposal in response to FY13 DOE Vehicle Technologies Office Funding Opportunity Announcement

Modular Nonlinear Multiscale Framework "MSMD"

Particle Domain

Electrode Domain

Cell Domain

Model for All Major Form-factor Cells

Stack Pouch

Wound Prismatic

Wound Cylindrical

10T

Orthotropic Continuum Model

Single Potential-Pair Continuum

Positive current collector   Negative current collector

20-tabs (20T) cell

10-tabs (10T) cell

Inner electrode pair

Outer electrode pair

Inner electrode pair

Outer electrode pair
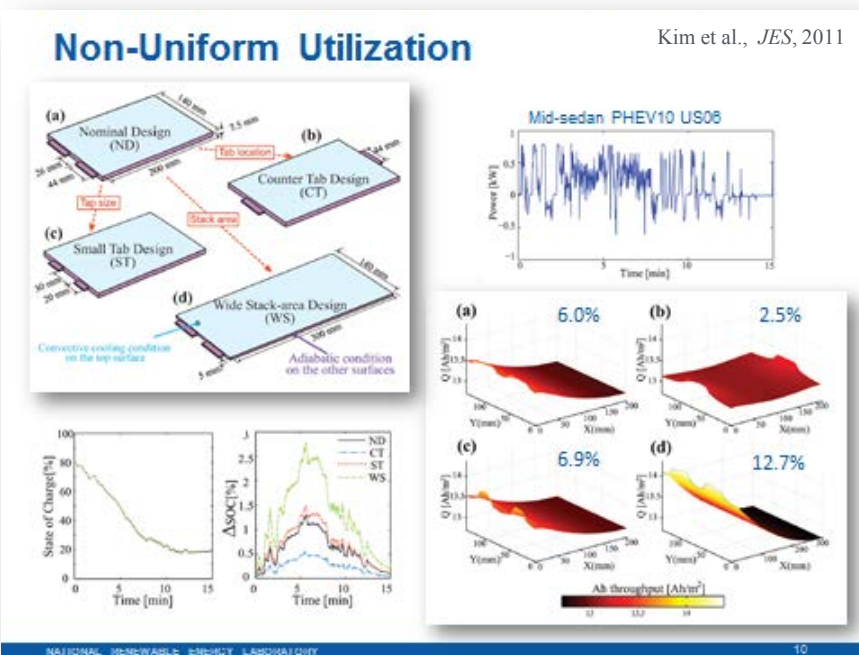
Uneven Kinetics over Unwound View of Jelly-roll

- Developed the Multi-Scale Multi-Domain (MSMD) model, recognized as the most comprehensive model of its kind for modular architecture, linking interdisciplinary battery physics across varied length and time scales
- Resolves the battery geometry into three coupled computational domains
- Achieves high computational efficiency
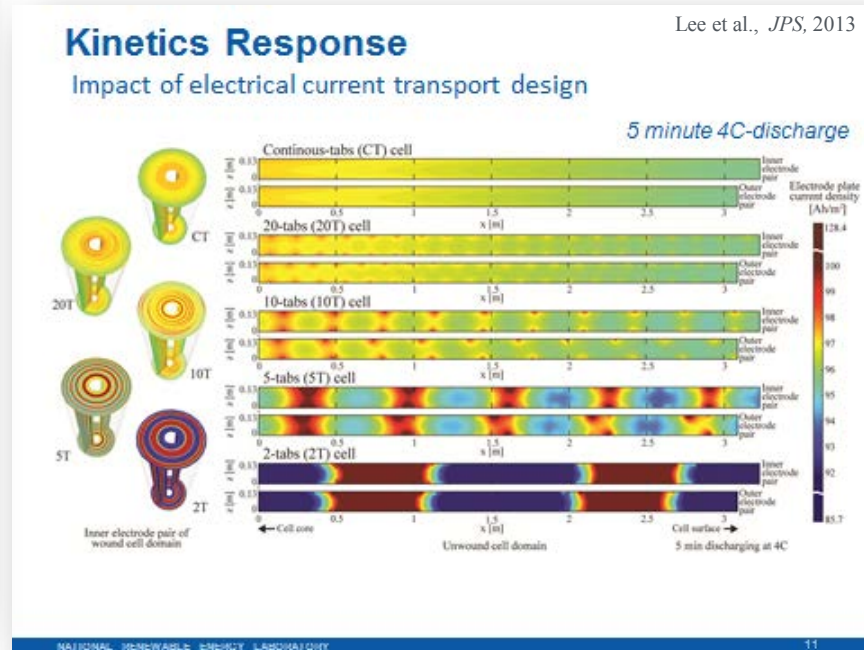- Provides flexible & expandable modularized framework

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

Relevance – Previous CAEBAT Accomplishment

Model Quantifies Non-uniform Cell Usage

Stacked Pouch Cell Model Analysis

Wound Cylindrical Cell Model Analysis

- NREL's orthotropic cell-composite model greatly reduces the computational load and resolves the complex transports and kinetics in the micron-scale strata cell geometries from various form-factor cells.
- The model captures unmeasurable internal cell quantities, revealing the impact of macroscopic design and the usage of the cells on local electrochemical processes.

Kim et al., *J. Electrochem. Soc.*, 2011, Vol. 158, No. 8, pp. A955–A969; Lee et al, *Journal of Power Sources*. Vol. 241, 1 November 2013; pp. 20-32.

Relevance – Motivation

Remaining Challenges

- **Material Engineering:** Significant efforts continue being invested to improve energy-power capability and reliability of batteries through engineering at the material level by controlling particulate morphology and size, modifying the particle surface, or redesigning thermodynamics.
- However, due to the complex nonlinear interactions across a wide range and scale of physics, computational cost becomes excessively high to quantify such improvements for the benefits in device level response even with the state-of-the-art models.

- **Pack Engineering:** The CAEBAT program has resulted in software packages providing 3-D battery pack simulation modeling capability.
- Because of the system's extreme complexity, the computational cost of simulating a battery pack response is still high: results take weeks, unless low-fidelity submodels are used to represent the battery's current/voltage response.

- **Awareness and Control:** Physics-based models are desired for use in advanced battery management to improve the performance of the battery management system and to implement sophisticated control strategies.
- However, significant reduction of model computation time and the number of states that are carried is required.
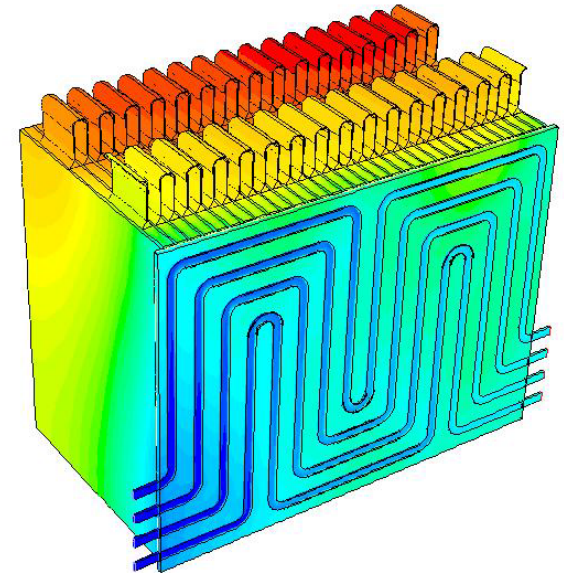
Relevance – Objectives

Speed-Up!

To develop a computational methodology for a significant enhancement in computation speed of nonlinear multiscale battery modeling while maintaining or improving the solution accuracy from the most advanced state-of-the-art models

Integrity or **Accuracy**

objectives

High Accuracy & High Speed

Convenience or **Speed**
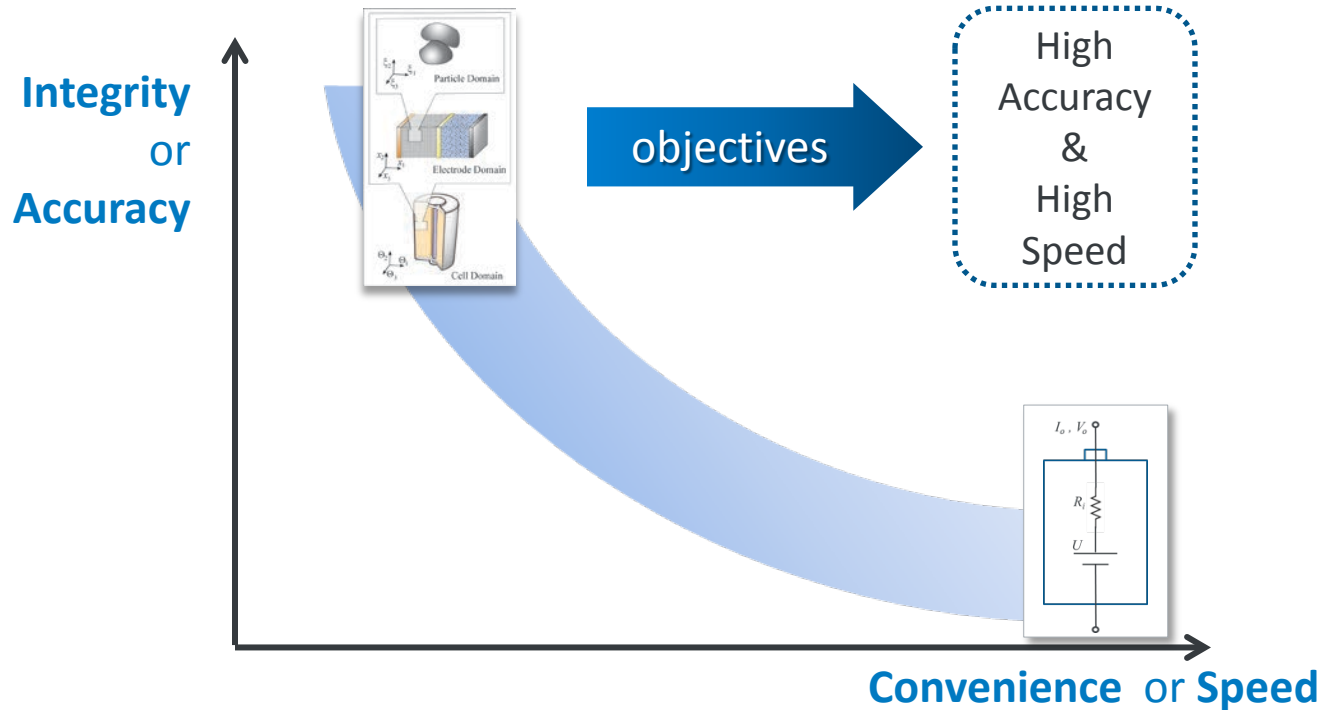
Retain or Improve Fidelity of Physics, but Run 100 times Faster

FY14 Milestones

Month/Year	Description	Status
10/2013	Project Kick-off Meeting/Report	met
02/2014	Progress Update Report: Efficient Nonlinear Multiscale Framework • *Standardize the input-output protocol and the data structure for particle domain (PD) and electrode domain (ED) models* • *Prototype the restructured PD MATLABT codes* • *Demonstrate new framework linkage between PD and ED models*	met
05/2014	Progress Update Report: Adaptive Reduced Order Model (ROM) • *Complete evaluation of possible candidate approaches* • *Begin prototype code development for electrode-level submodels*	on track
06/2014	Annual Merit Review Presentation	on track
09/2014	Annual Milestone Report	on track

Approach – Complementary Parallel Tasks

> **"The project will achieve the suggested objectives through complementary parallel efforts in the areas of framework and component efficiency and functionality improvement."**

Task 1: Project Management

Task 2: *Framework Efficiency* Improvement and Verification

To significantly improve the computational efficiency of a modular multiphysics battery model framework

> Task 2.1 Efficient Nonlinear Multiscale Framework

Task 3: *Component Model Efficiency* Improvement and Verification

To provide advanced constituent submodels to enhance overall model performance in terms of computational speed and accuracy

> Task 3.1 Adaptive Reduced Order Model
> Task 3.2 Nonlinear Reduced Order Model
> Task 3.3 Module Inventory Enhancement

**Task 4: Implementation on ANSYS Battery Simulation Platform**

To bring immediate benefits to industries, the outcome model should be numerically robust and usable in an engineering environment.

Approach – Task 2.1

T2.1 Efficient Nonlinear Multiscale Model Framework

Barrier to address:

a. *The **inevitable nested iteration**, ensuring self-consistency in the state-of-the-art MSMD, becomes a factor limiting further improvement of computation speed.*

b. *The traditional multiphysics approach, collapsing scales into a single, large, differential algebraic equation system, renders the system **impractically large and stiff, sacrificing modularity**.*

a

inevitable nested iteration

b

*impractically large and stiff,
sacrificing modularity*
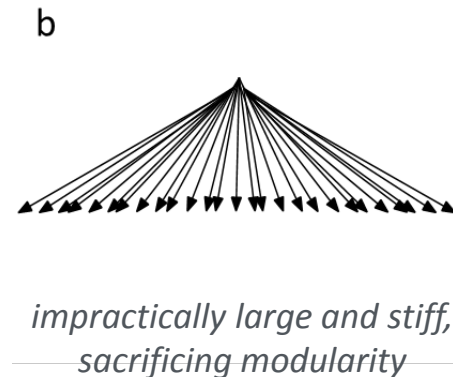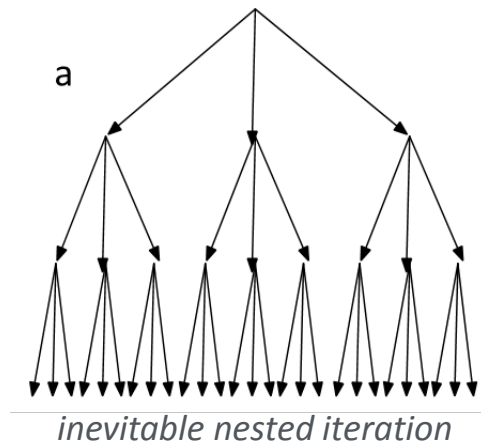
Strategy to address barriers:

› Develop an innovative multiscale coupling method using time-scale separation and variable decomposition to eliminate several layers of nested iteration, while still keeping the modular framework architecture that is critical to battery behavior simulations.

Approach – Task 2.1

Seeking for Integrity

"Battery behaviors are determined through nonlinear relations among physicochemical processes coupled across the scales."

Integrated Multiscale Model

$$I_o , V_o , P_o , R_{load}$$
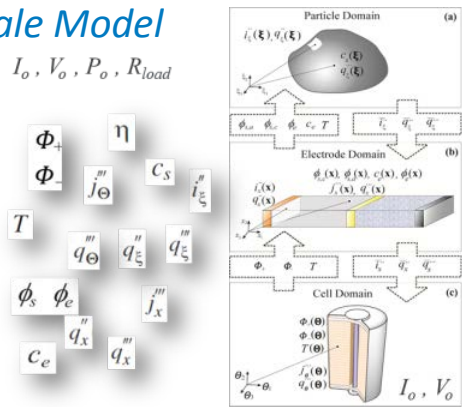
- The "states" are solved for with a nonlinear implicit system of equations.

Pursuit of "Model of Dream" – Beyond MSMD

Quasi-Explicit Physics-Based Nonlinear Multiscale Model

New Framework: GH-MSMD

- Remove nested iteration
- *Explicit* math expressions of "states"
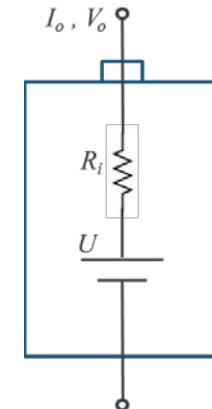- Retain modularity of framework

objectives

Integrity / **Convenience**
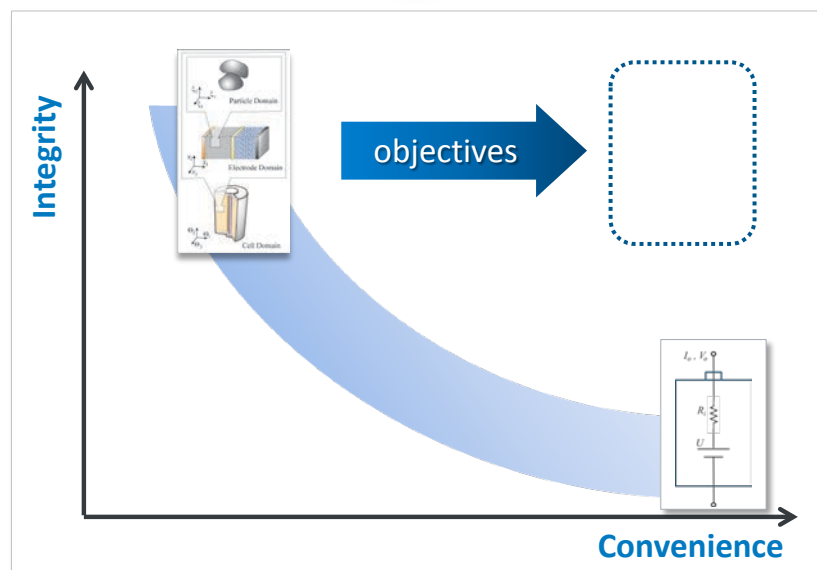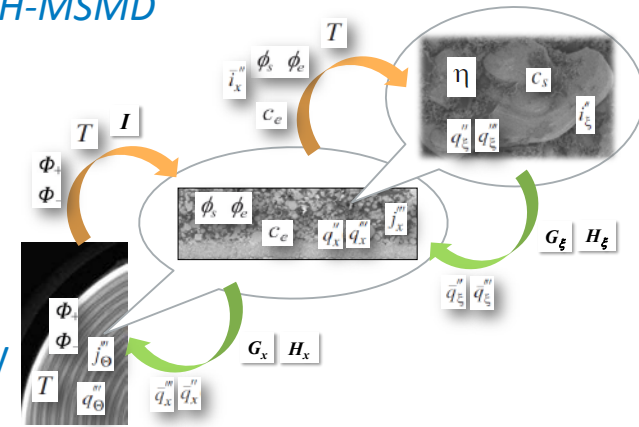
Seeking for Convenience

"Relations between input and output ($I_o , V_o , P_o , R_{load}$) are given as explicit functions."

Empirical Polarization Model

- The explicitly given "states" (U , R_i) are induced by processing often a large amount of test data; treated as "black boxes"

$$V_o = U - I_o R_i$$

$$I_o = \frac{U - V_o}{R_i}$$

$$V_o = \frac{U + \sqrt{U - 4 P_o R_i}}{2}$$

$$I_o = \frac{U}{R_i + R_{load}}$$

Approach – Task 3.1

T3.1 Adaptive Reduced Order Model

Reduced order models (ROMs) are used in various practical applications where fast computation is needed to repeatedly solve discretized systems of differential equations.

Barrier to address:

- *As soon as the ROM basis is acquired in a reduced dimension space, physical interpretations are easily lost.*
- *The ROM basis is restricted to reuse in the system where its characteristics are evolving, such as the battery aging process.*
- *The ROM build process becomes computationally costly, especially with an increased number of parameters.*

Strategy to address barriers:

› Establish a new technique to identify low order State Variable Model (SVM) that is adaptive to system evolution, such as during aging.

- Previous SVM: Basis functions determined in the preprocessing step. Only valid for one cell design at one state of health
- Adaptive SVM *(this project)*: Analytical/numerical mapping of basis functions applicable to entire parameter space

3rd Dimension of Model Speed-up : Enhancement of Model Applicability
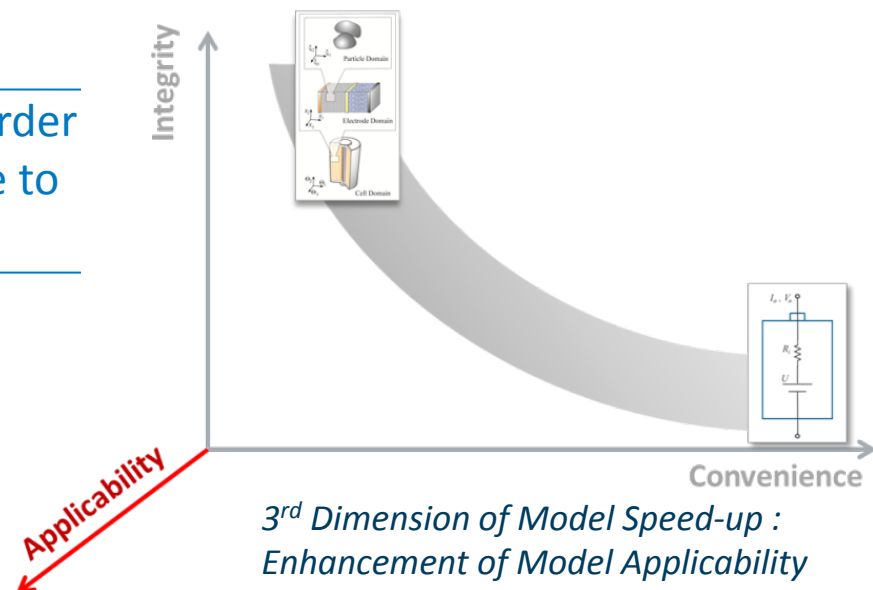
Approach – Task 3.2 & Task 3.3

T3.2 Nonlinear Reduced Order Model

Barrier to address:

- *Most state-of-the-art efficient battery models addressed coupling battery physics only within limited scales.*
- *The state-of-the-art ROMs suggested for battery models lose validity when severe nonlinearities arise.*

Strategy to address barriers

› Design a new ROM that does not fail under severe nonlinear condition and achieves speeds that are compatible with state-of-the-art ROMs for battery models.

T3.3 Module Inventory Enhancement

Barrier to address:

- *The model applicability can be limited for varied design, environment, and operation conditions.*

Strategy to address barriers

› Construct multiple options of modular component models for various subsystems.

Technical Accomplishments and Progress

Successfully implemented a newly developed "GH-MSMD" framework in linking the particle domain (PD) model into the electrode domain (ED) model

GH-MSMD Protocol
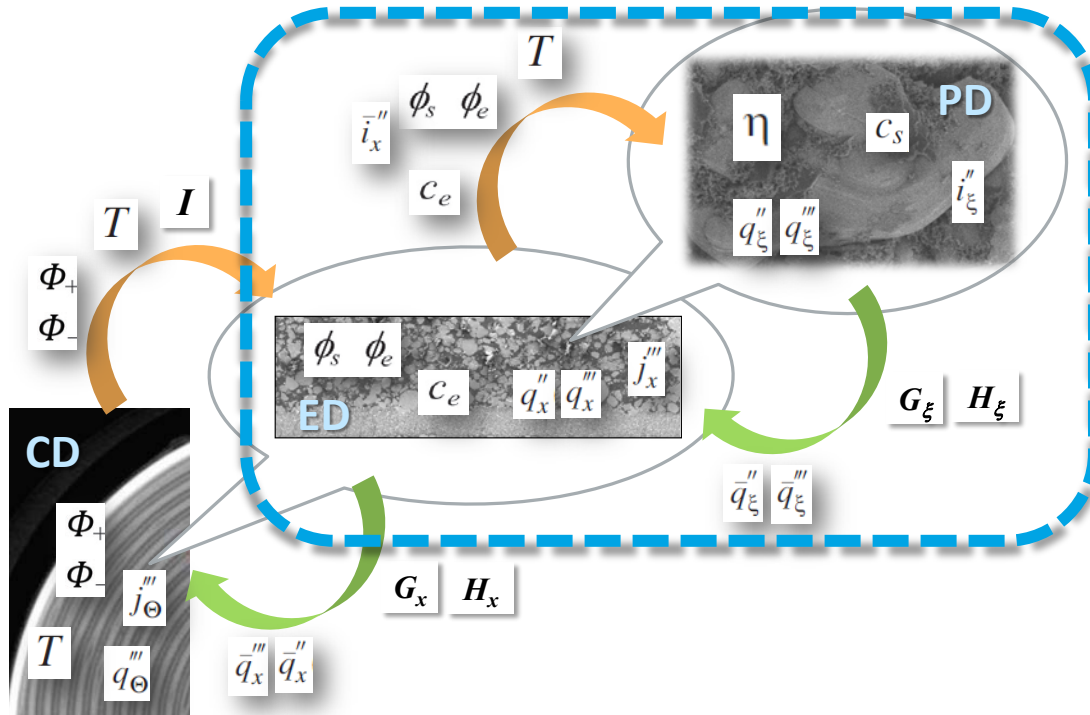
- Established a new model framework that removes nested iteration and still retains modular architecture

- Reformulated the model using;
  - Time-scale separation
  - Variable decomposition
  - Partial linearization

- Evaluated several options for model implementation structures

- Standardized the input-output protocol, and the data structure for PD and ED models
- Prototyped the restructured PD MATLAB codes
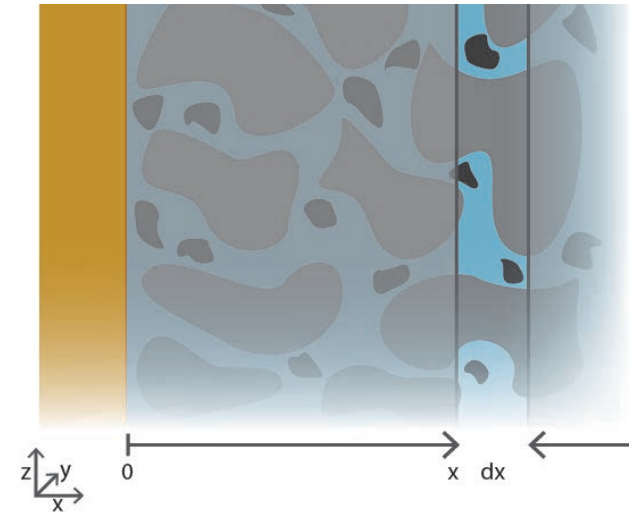- Developed the further simplified edLPD model

Technical Accomplishments and Progress

GH-MSMD enables a ED model integrated with a more sophisticated PD model to run fast enough to investigate complex dynamic response of battery systems.
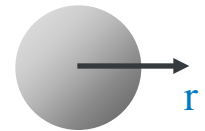
Discrete Diffusion Particle Model (DDPM)

- *The model solves solid-phase lithium diffusion dynamics and transfer kinetics in a discrete diffusion particle system.*
- *The particles are considered electronically continuous, but ionically discrete.*
- *An arbitrary number of quantized discrete particles can be given as a user input.*
- *Kinetic, transport, and thermodynamic model parameters of each discrete particle can be independently determined.*
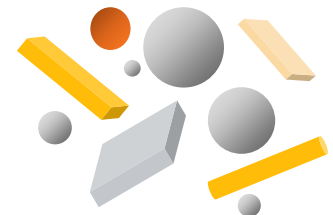
NREL has developed the **DDPM** as an advanced option for MSMD particle-domain model, addressing particulate morphology, size distribution, surface modification, contact resistances, mixture composition of active particles.
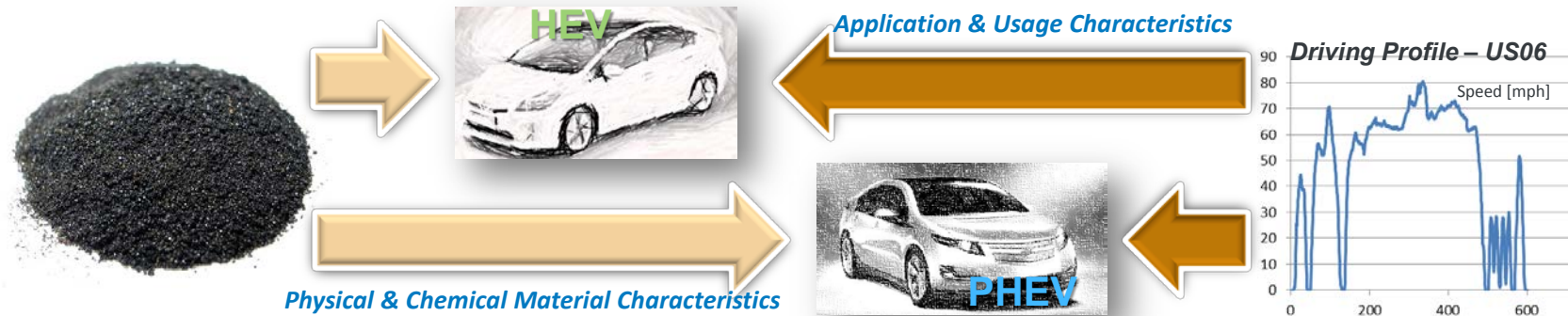
Pseudo 2D

DDPM

Technical Accomplishments and Progress

Application & Usage Characteristics

Physical & Chemical Material Characteristics

Driving Profile – US06

*A battery with NCA cathode, particles distributed in size between 0.5-5 μm (N=100)*

Model Application: Complex DDPM runs faster (x10~50) with the new framework to evaluate the impact of environmental factors on inhomogeneous use of materials with distributed particulate attributes.

- **HEV**:
  - State of charge (SOC) swing is wider in small particles than in large particles.
  - Small particles respond more sensitively to load variation.
  - Both amplitude and frequency of concentration change are larger in small particles.

- **PHEV10**:
  - Lithium concentration difference between the particles grows initially and decreases back during charge sustaining mode.
  - Change of lithium concentration is nearly monotonous in large particles, while small particle concentrations fluctuate.
  - Large particles respond mostly to energy demand and small particles to both power and energy demands.
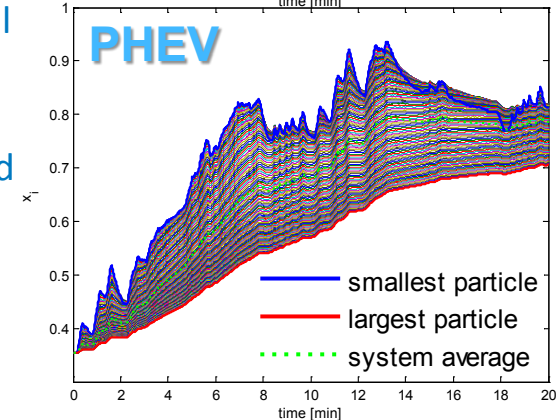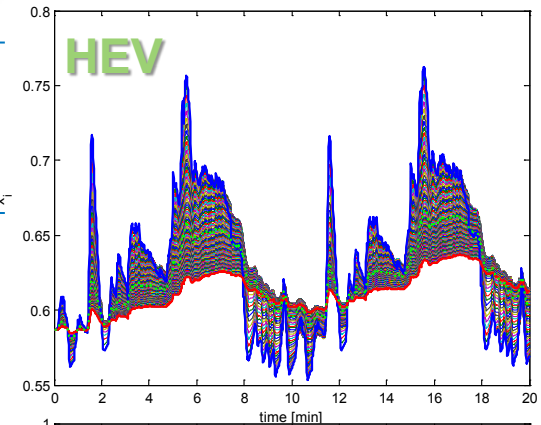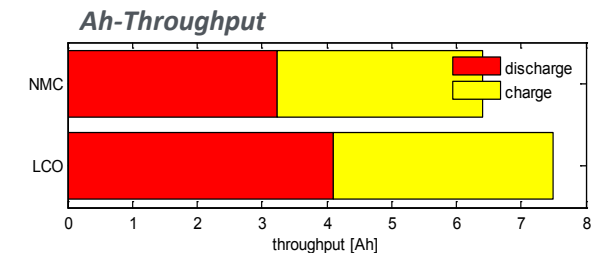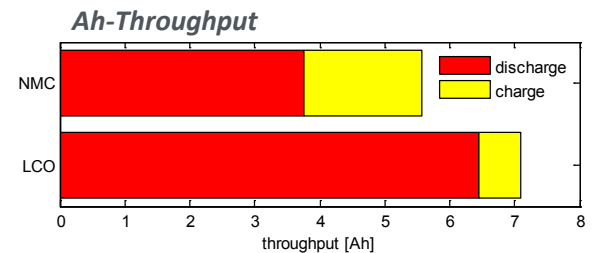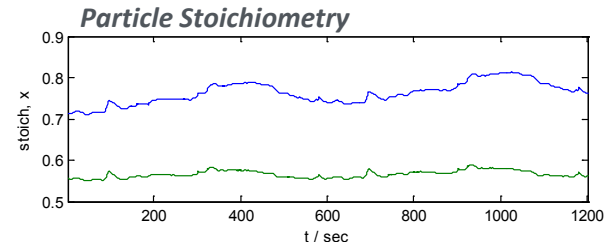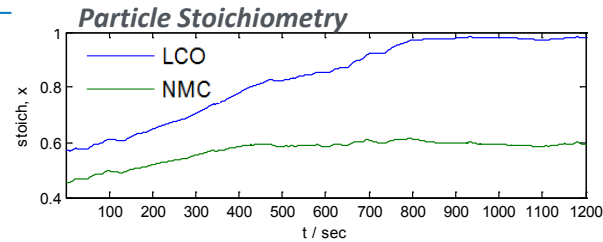
Technical Accomplishments and Progress

Mixed Cathodes

20-minutes Drive of Midsize Sedan on US06 Driving Profile

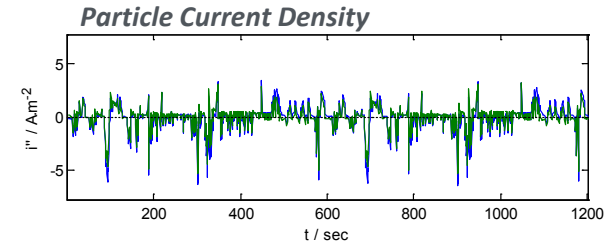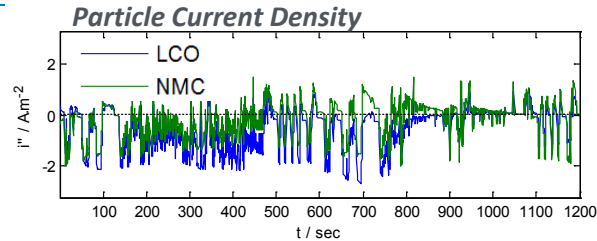PHEV10   HEV

Model Application: The model captures the impact of application characteristics on inhomogeneous use of materials for a mixed chemistry battery.
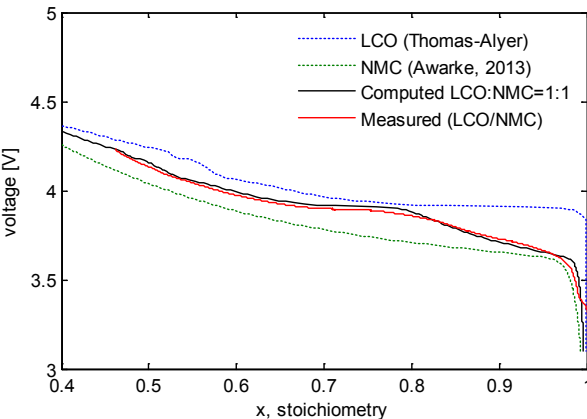
- **PHEV10**: Since the battery is operated over a wide range of SOC in charge depleting mode, thermodynamic balance between the mixture components substantially varies, so is the usage of the materials. Stoichiometry difference between LCO and NMC grows during the drive. In charge sustaining mode (after ~ 800 sec), the battery is cycled with LCO nearly saturated. Discharge throughput is much larger for LCO particles, but NMC takes more current in charging events.
- **HEV**: While discharge and charge throughputs are balanced for the both components, LCO is used more .

Technical Accomplishments and Progress

Connectivity to Existing CAEBAT Platform: Prototyped ANSYS/Fluent API for NREL's edLPD
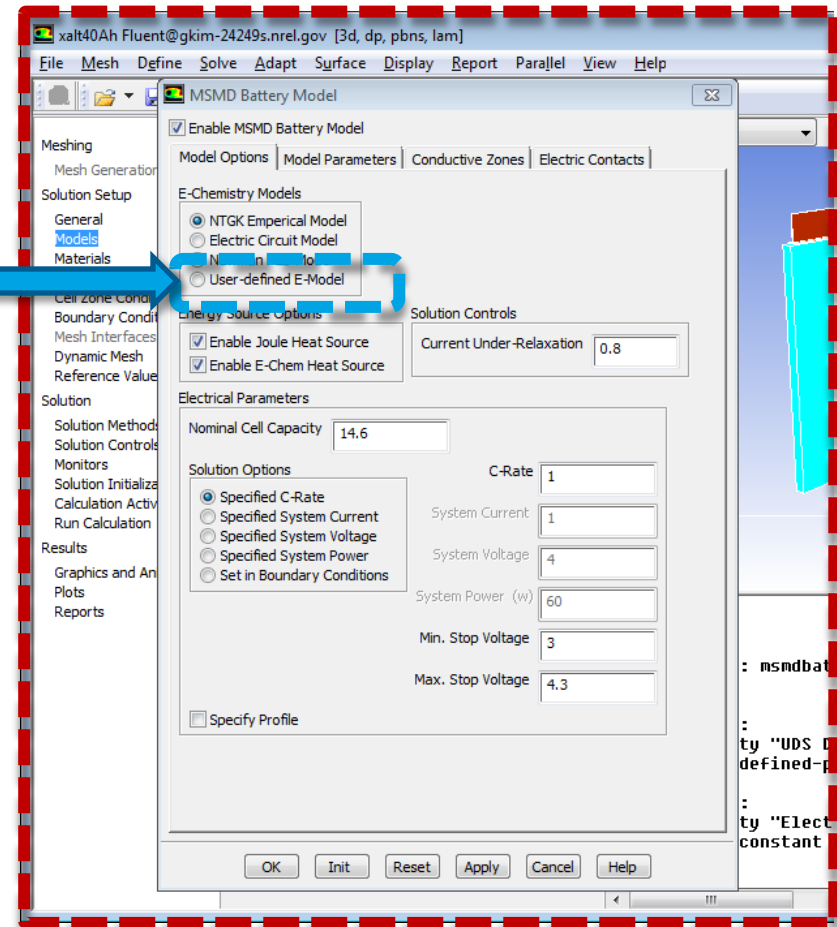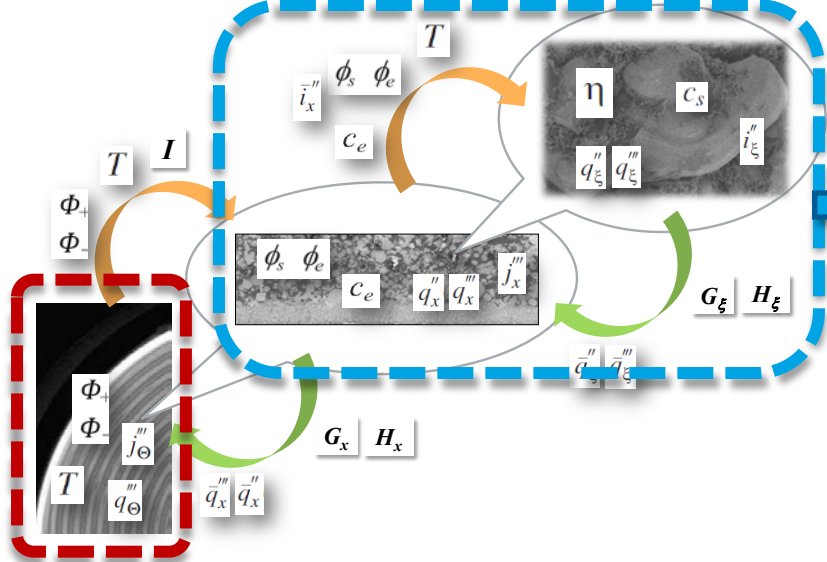
- Significant enhancement of computation speed ($\sim 10^2$) was demonstrated with ANSYS's "MSMD Battery Model," when it runs integrated with NREL's edLPD model for a physics-based submodel option.

Collaboration and Coordination with Other Institutions

To bring immediate benefits to industries, the outcome model should be numerically robust and usable in an engineering environment

To leverage what has been accomplished through the previous efforts in the program

Partner: ANSYS

- *The project team will integrate the outcome models on ANSYS's battery simulation platform. ANSYS developers will support NREL researchers with required software engineering.*

- *With the ANSYS battery simulation software as a platform for the MSMD research, appropriate source code access, prototype versions of ANSYS tools, developer-level technical support, and advisory consultation on NREL's use will be provided.*

- *Professor **Jacob White**, the Associate Director of the Research Laboratory of Electronics at MIT and an ANSYS Director of Research, brings his leading expertise in numerical methods focusing on simulation and optimization algorithms and software.*

- *From the previous collaboration, ANSYS developers participating in the project have established a profound understanding of the MSMD architecture.*

Proposed Future Work

- Extend GH-MSMD nonlinear multiscale framework to the linkage between Cell-Domain (CD) models and the subscale domain models.
- Look into opportunities to further reduce balanced reduction, while desiring explicit method to achieve reduction.
- Implement the Discrete Empirical Interpolation Method (DEIM) for a representation of the nonlinear functions needed to retain the ROM in the low-dimensional reduced space.

GH-MSMD Framework

- Link the outcomes from each task to the MSMD infrastructure, providing synergistically integrated battery simulation capability.
- Develop and suggest an appropriate metric to evaluate the advancement of model computation speed.
- Incorporate into ANSYS CAEBAT framework and Oak Ridge National Laboratory's Open Architecture Software
- Validate and verify the model codes against the baseline full-order models.
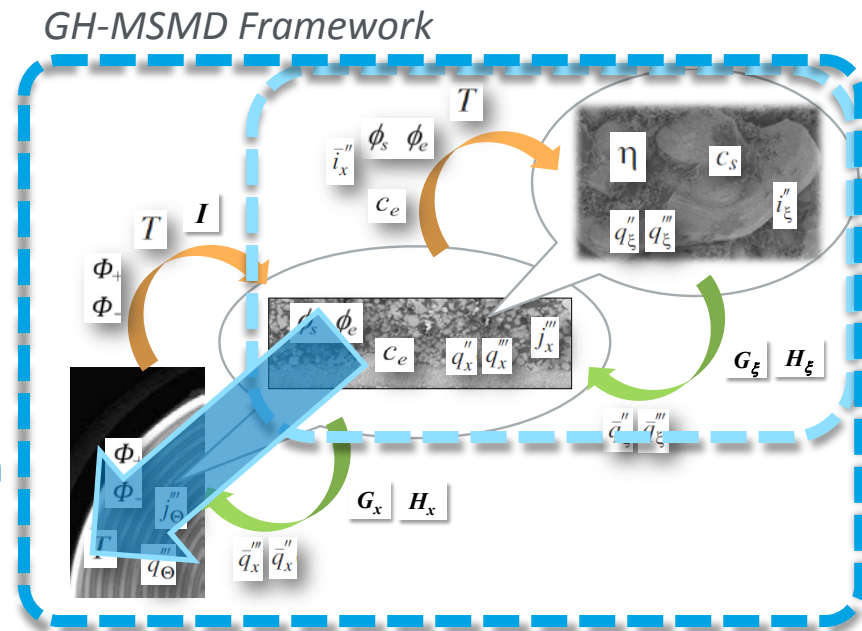
Summary

- The objective of the project is to develop a computational methodology for a significant enhancement in computation speed of nonlinear multiscale battery modeling while maintaining or improving the solution accuracy from the most advanced state-of-the-art models.
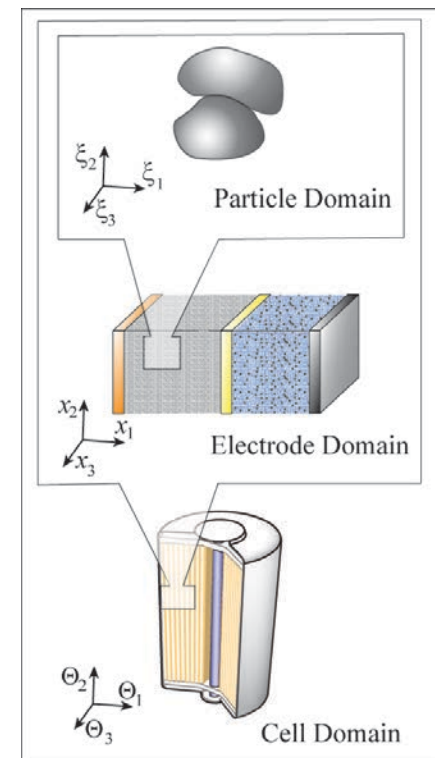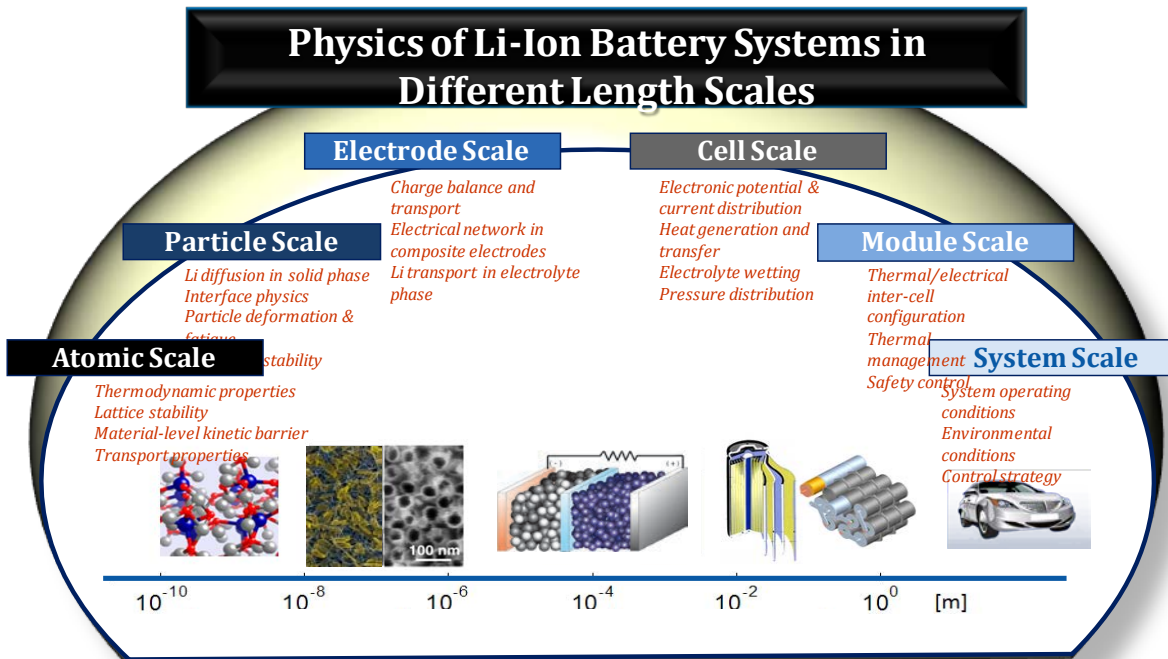
- This will be achieved through complementary parallel efforts in the areas of framework and component efficiency and functionality improvement.

  - *To develop an innovative nonlinear multiscale model framework*
  - *To provide advanced ROMs with enhanced model applicability*
  - *To connect to previously developed CAEBAT development platforms*

- Newly developed "GH-MSMD" framework has been successfully implemented to link Particle-Domain (PD) models into a Electrode-Domain (ED) model.

- GH-MSMD enables a ED model integrated with a more sophisticated PD model to run fast enough to investigate complex dynamic responses of battery systems.

- Significant enhancement of computation speed (~10^2) was demonstrated with ANSYS's "MSMD" battery simulation module, when it runs integrated with NREL's edLPD model for a physics based electrochemistry submodel option.

- **Future Implication**: *The success of the project would shift the paradigm to using a model for battery system design and evaluation, with significant potential to change the standard development process while advancing battery system management and control.*
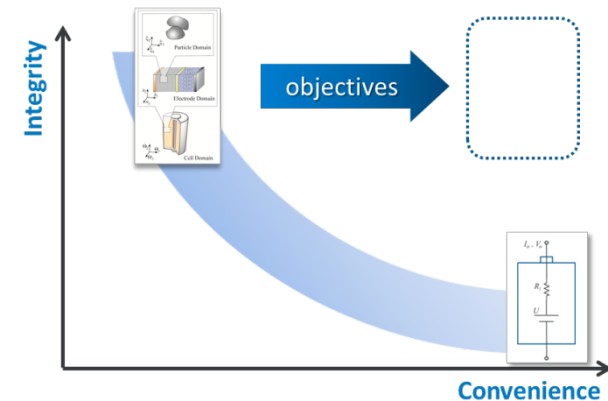
Technical Back-Up Slides

Relevance – Background

Multiphysics Coupled across Scales

Physics of Li-Ion Battery Systems in Different Length Scales

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

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

Module Scale
- Thermal/electrical inter-cell configuration
- Thermal management
- Safety control

Atomic Scale
- Thermodynamic properties
- Lattice stability
- Material-level kinetic barrier
- Transport properties

System Scale
- System operating conditions
- Environmental conditions
- Control strategy

10^{-10} 10^{-8} 10^{-6} 10^{-4} 10^{-2} 10^{0} [m]

Particle Domain

Electrode Domain

Cell Domain

- Physicochemical processes in lithium batteries occur in intricate geometries over a wide range of time and length scales.
- Without better knowledge of the interplay among the multiphysics occurring across the varied scales, it is costly to design long-lasting, high-performing, safe, large battery systems.
- The electric-drive vehicle (EDV) industry recognizes that the lack of a battery model that can predict thermal, electrical, electrochemical, and mechanical responses in various operating conditions is an urgent barrier to overcome.
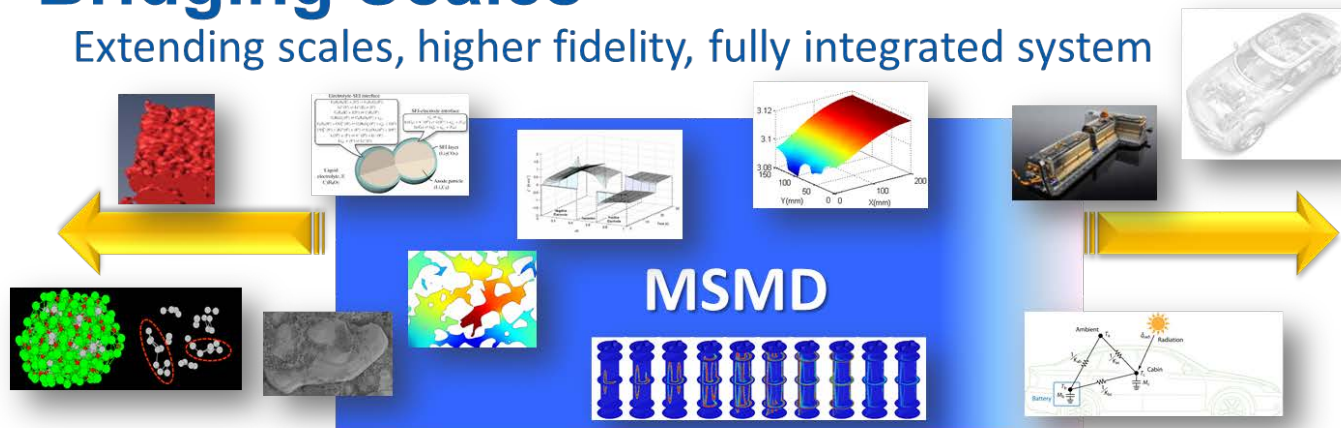
Relevance – Background

Computer Aided Engineering of Batteries (CAEBAT) Program

DOE initiated the CAEBAT program *to help industry shorten the time and cost to design and develop EDV battery systems* through development of models and tools that can:
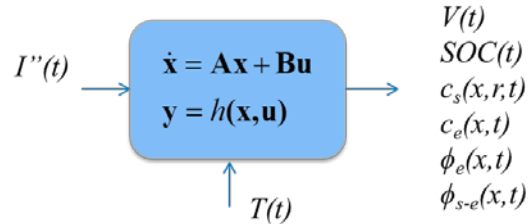
1. Integrate battery physics on a widely varied scale in a computationally efficient manner.
2. Provide a modularized multiphysics platform so the user can choose from multiple submodel options with various physical/computational complexities.
3. Provide an expandable framework to add new physics of interest or to drop physics of low significance or of indifference.

Bridging Scales
Extending scales, higher fidelity, fully integrated system

MSMD

Technical Accomplishments and Progress

$$\dot{x} = \mathbf{A}x + \mathbf{B}u$$
$$y = h(\mathbf{x}, \mathbf{u})$$

$I''(t)$

$V(t)$
$SOC(t)$
$c_s(x,r,t)$
$c_e(x,t)$
$\phi_e(x,t)$
$\phi_{s\text{-}e}(x,t)$

$T(t)$

1) Nonlinear Governing Equations
- *Partial differential equations*
- *Constitutive relations*

Linearize, Laplace Transform, analytical/numerical solution

(This project seeks a direct mapping)

2) Linear Impedance Model
- *Infinite dimensional transfer functions*
- *High order transfer matrices*

Model order reduction

3) Linear Reduced Order Impedance Model
- *Rational, low order transfer matrices*

Inverse Laplace transform

4) Linear State Variable Model
- *Valid for small perturbations*

Approximate nonlinearities on a lumped basis

5) Nonlinear State Variable Model
- *Valid throughout operating range*

*Two different approaches are examined and pursued for an **adaptive SVM** to be flexible for design space searches, model parameter identification and coupling with aging models.*

Analytical:
- Developed interconnection-of-systems approach for assembling state-space matrices of ROM.
- Analytical approach results in ~60th order state-space model.
- This can be further reduced to ~15th order using numerical "balanced realization" technique from control theory.

Numerical:
- Developed prototype code for fitting model transfer functions in low-order pole/residue form using vector fitting.
- Method results in ~15th order models.
- Drawback is large look-up tables necessary to represent parameter space.