

Progress of Computer-Aided Engineering of Electric Drive Vehicle Batteries (CAEBAT)

Presented at the 2013 U.S. DOE Vehicle Technologies Office
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Project ID #ES117

NREL/PR-5400-58202

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Overview

Timeline

Project Start Date: April 2010

Project End Date: September 2014

Percent Complete: 40%

Budget

Total Contractors' Project Funding:

DOE Share to Contractors: \$7 M

Contractors Share: \$7 M

NREL/ORNL Funding in FY12:

\$1.6 M

NREL/ORNL Funding for FY13:

\$1.5 M Anticipated

Barriers

- Cost and life
- Performance and safety
- Lack of validated computer-aided engineering tools for accelerating battery development cycle

Partners

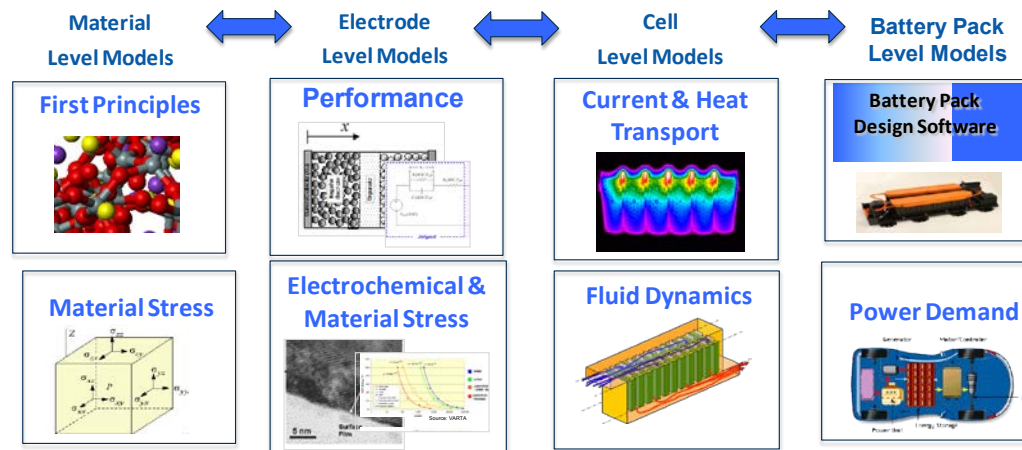
- NREL, project lead
- Oak Ridge National Laboratory (ORNL)
- **EC Power**/Penn State University/
Ford/Johnson Controls, Inc. (JCI)
- **General Motors**/ANSYS/ESim
- **CD-adapco**/Battery Design/
JCI/A123/Idaho National Laboratory

Funding provided by Dave Howell of the DOE Vehicle Technologies Office
Activity managed by Brian Cunningham of Vehicle Technologies

Computer Aided Engineering for Electric Drive Vehicle Batteries (CAEBAT)

Relevance

- 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, particularly in the automotive industry
- Realizing this, DOE's Vehicle Technologies Program initiated the CAEBAT project in April 2010 to develop a suite of software tools for designing batteries
- These CAE software tools need to be user-friendly, multi-physic, 3D, fully-integrated, and validated, and address materials, electrodes, cells, and packs for the battery community
- The CAEBAT project is bringing the capabilities and expertise of the national laboratories, car and battery industries, universities, and software vendors



Objectives

- **The overall objective of the CAEBAT project is to develop “validated” software tools by incorporating existing and new models for the battery community to design batteries faster**
- **Objectives of the past year (March 2012 to March 2013):**
 - GM: Release first version of cell and pack level tools for internal GM team evaluation
 - CD-adapco: Release first version of 3-D electrochemical-thermal code in STAR-CCM+ for the spiral cell designs to the public
 - EC Power: Release first version of the 3-D electrochemical-thermal code for all cell designs to the public
 - NREL: Oversee CAEBAT project execution and enhance NREL’s multi-scale and multi-domain framework to simulate all major cell form factors
 - ORNL: Develop “standardize inputs” and “battery states” databases to allow interface between models by CAEBAT participants

Relevance

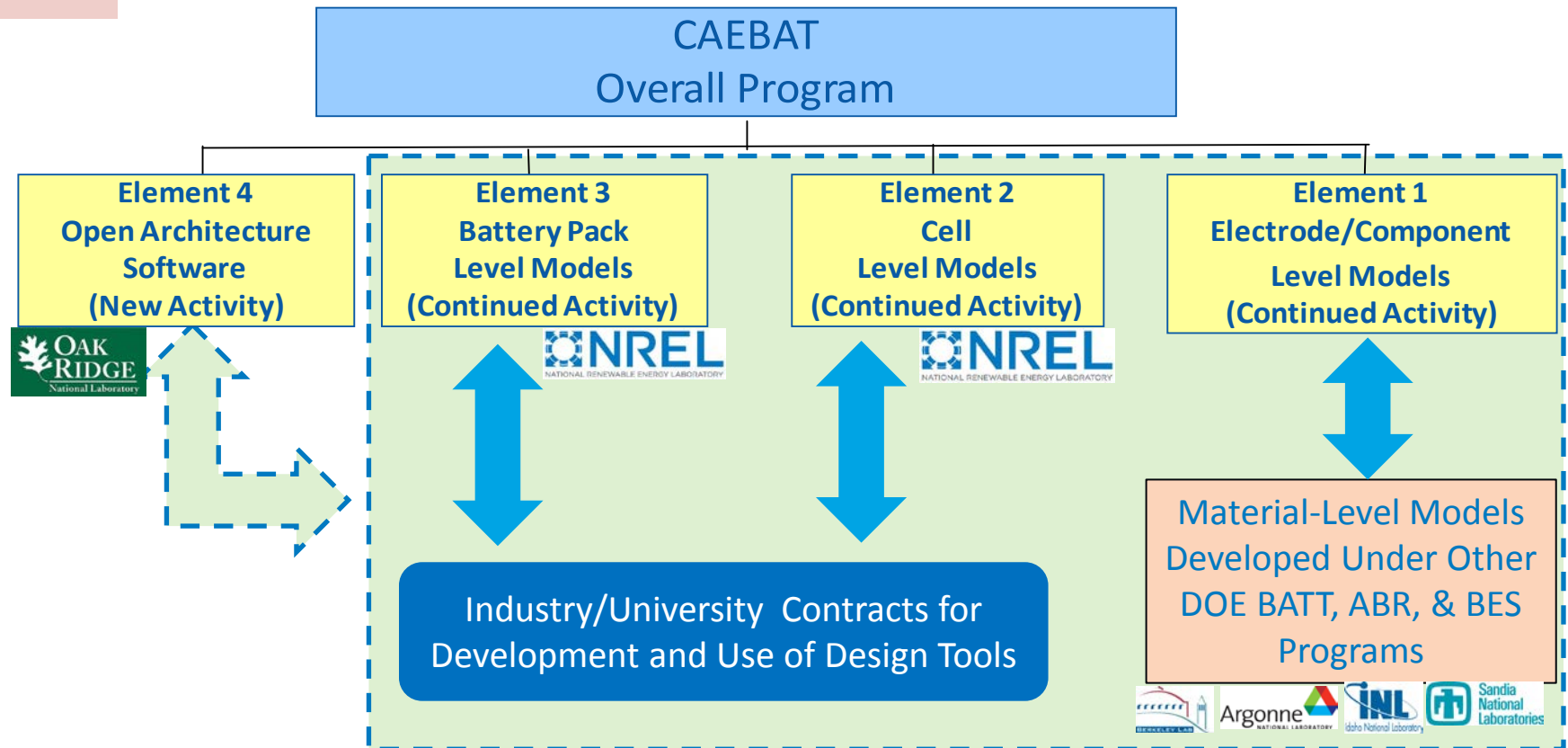
- **CAEBAT objectives are relevant to the Vehicle Technologies Program's targets of:**
 - Plug-in hybrid electric vehicle (PHEV) battery costs of \$300/kWh and life of 15 years by 2014
 - PHEV battery costs of \$270/kWh and life of 10+ years by 2017
 - Electric vehicle battery costs of \$150/kWh and life of 10 years by 2020
- **The impact of this project when CAEBAT tools are made available could be significant:**
 - Shorter design cycles and optimized batteries
 - Simultaneously address barriers of cost, performance, life, and safety of lithium-ion with quantitative tools

Milestones

Date	Milestone	Status
July 2012	Document latest NREL battery models, solution methods, and codes developed under CAEBAT (NREL)	Completed
September 2012	Technical review of the three CAEBAT subcontracts (NREL)	Completed
November 2012	Release first version of the 3D electrochemical-thermal code for all cell designs to the public (EC Power)	Completed
January 2013	Release first version of cell and pack level tools for internal GM team evaluation. (GM)	Completed
February 2013	Share first version of OAS database on Standardized Input and Battery State (ORNL)	Completed
March 2013	Release first version of 3D electrochemical-thermal code in STAR-CCM+ for the spiral cell designs to the public (CD-adapco)	Completed

Overall CAEBAT Strategy

Approach



- NREL coordinates CAEBAT project activities for DOE
- Continue development and use (existing or new) battery models at national labs
- Exchange data on fundamental materials modeling with other DOE programs
- Develop multiple commercial software tools by cost-shared contracts with industry
- Develop an interface platform for interactions among all models

CAEBAT Approach

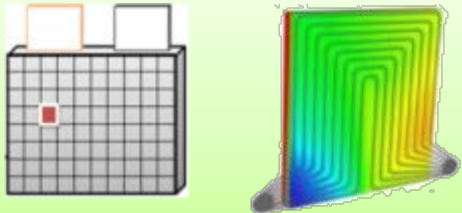
- Three industry teams, selected competitively, develop three separate validated battery design software tools with NREL as the technical monitor
- The teams hold monthly conference call and quarterly review meetings

Team	Subcontract Signed	Project Budget	NREL Subcontract Budget	NREL Technical Monitor
EC Power (with PSU, JCI, and Ford Motor Company)	May 2, 2011	\$3.0M	\$1.50	Shriram Santhanagopalan
General Motors (with ANSYS and ESim)	June 1, 2011	\$7.15M	\$3.58M	Gi-Heon Kim
CD-adapco (with Battery Design LLC, JCI and A123 Systems)	July 1, 2011	\$2.73M	\$1.37M	Kandler Smith

- NREL extends its multi-physics battery models and shares them with subcontract teams
- ORNL develops the elements in Open Architecture Software

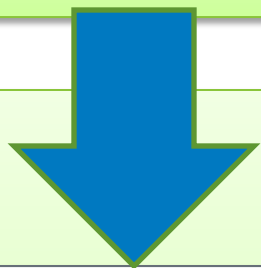
GM Approach for Cell and Pack Level Simulation

- Strategy is to offer a wide range of methods allowing analysts to trade off computational expense vs. resolution



Cell Level Model

- Reduced Order Models for electrochemistry
- Cell level performance including local cooling channels



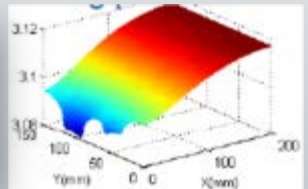
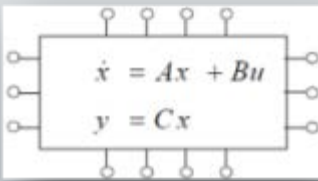
Pack Level Model

Co-Simulation



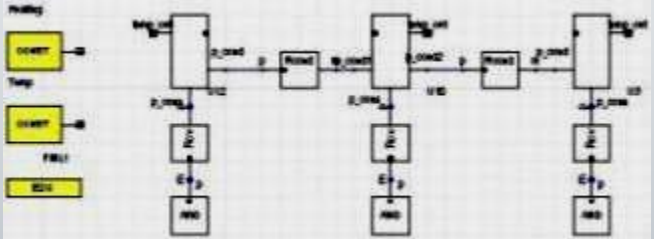
Reduced Order Models

- Reduced order models for flow and thermal analysis at the pack level
- Reduced order cell models
- Ability to “expand” results



System Level Model

- Construct a “linear” or “non-linear” system simulation model from the full pack simulation model

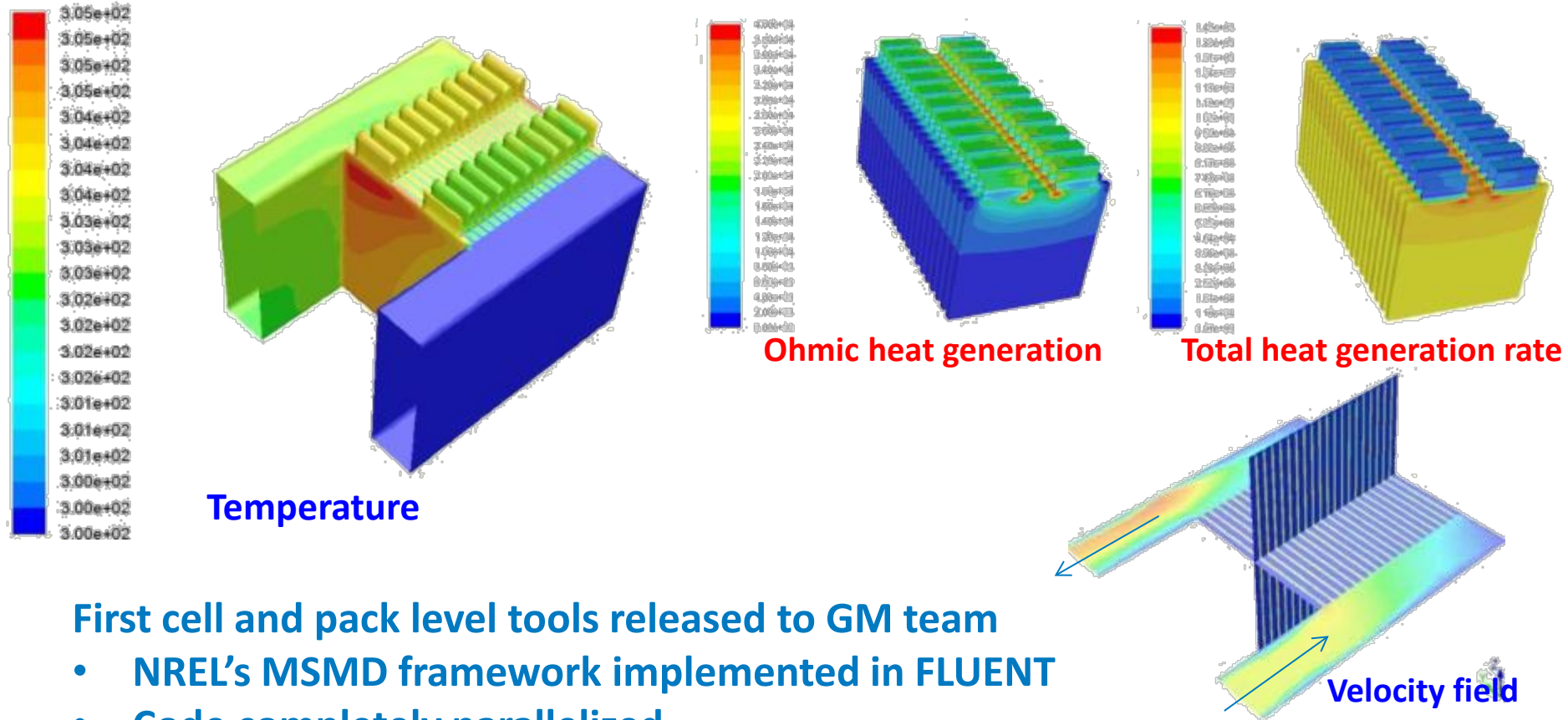


GM Accomplishments

- **First cell level tool released to GM team (Aug. 2012)**
 - NREL's MSMD framework was implemented in FLUENT; complexity of multi-scale, multi-physics interactions has been resolved with MSMD
 - All three electrochemistry sub-models were included (ECM, NTGK, P2D)
 - The model is fully parallelized
 - A detailed release note/tutorial was provided
- **First pack level tool released to GM team (Jan. 2013)**
 - Multiple cells are automatically connected from CAE model detection
 - Internal electric circuit model to speed up the potential field calculations
 - Code is completely parallelized
- **System level ROM development**
 - LTI system level model approach has demonstrated feasibilities for practical simulations of the entire pack for both air cooling and liquid cooling
 - Reduced Order Model (ROM) research has been conducted and aimed at pack level simulation with a divide-and-conquer approach
 - Simplorer-FLUENT co-simulation feature has been prototyped

GM Technical Accomplishments – 1

Pack Level Field Simulation



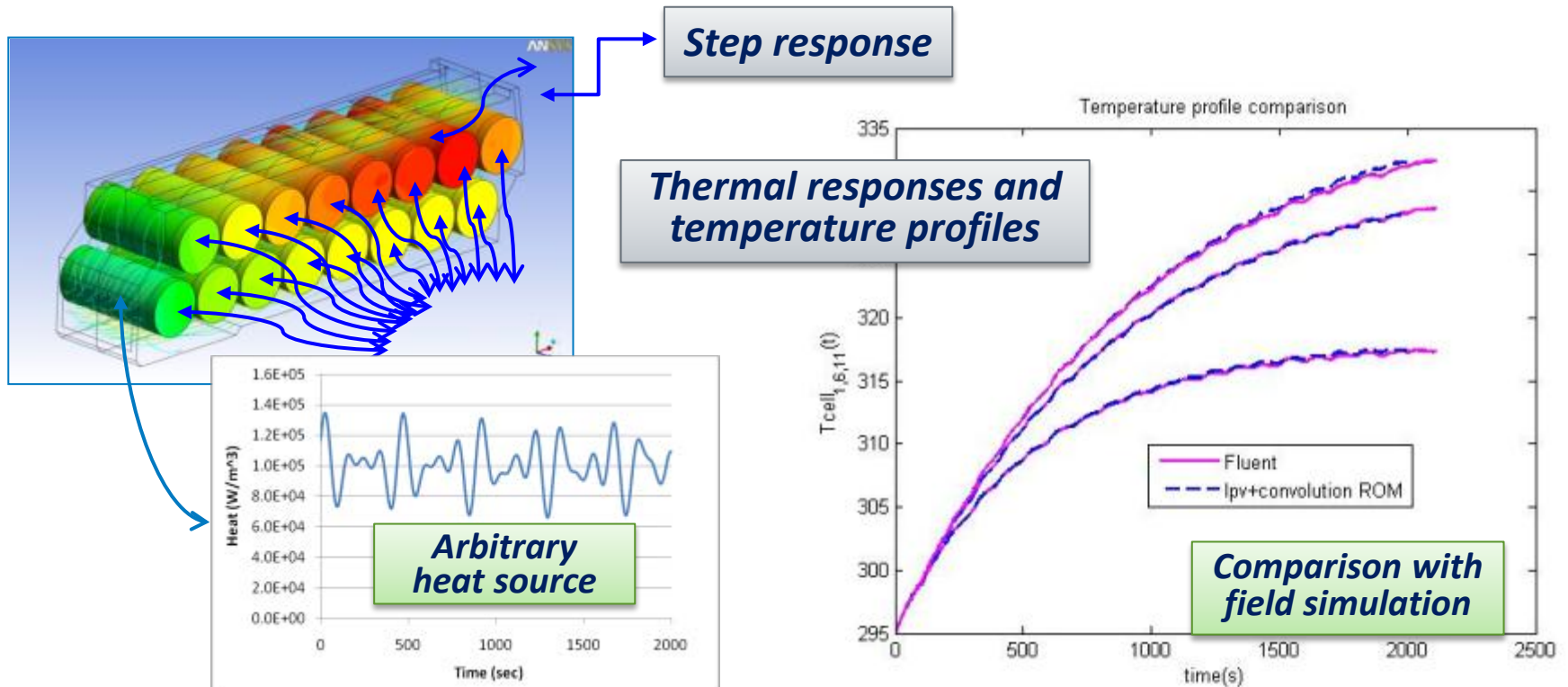
First cell and pack level tools released to GM team

- NREL's MSMD framework implemented in FLUENT
- Code completely parallelized
- Electric circuit created automatically for the pack level by detecting the cell connections to speed up the potential field calculations
- All three electrochemistry sub-models included (ECM, NTGK, P2D)

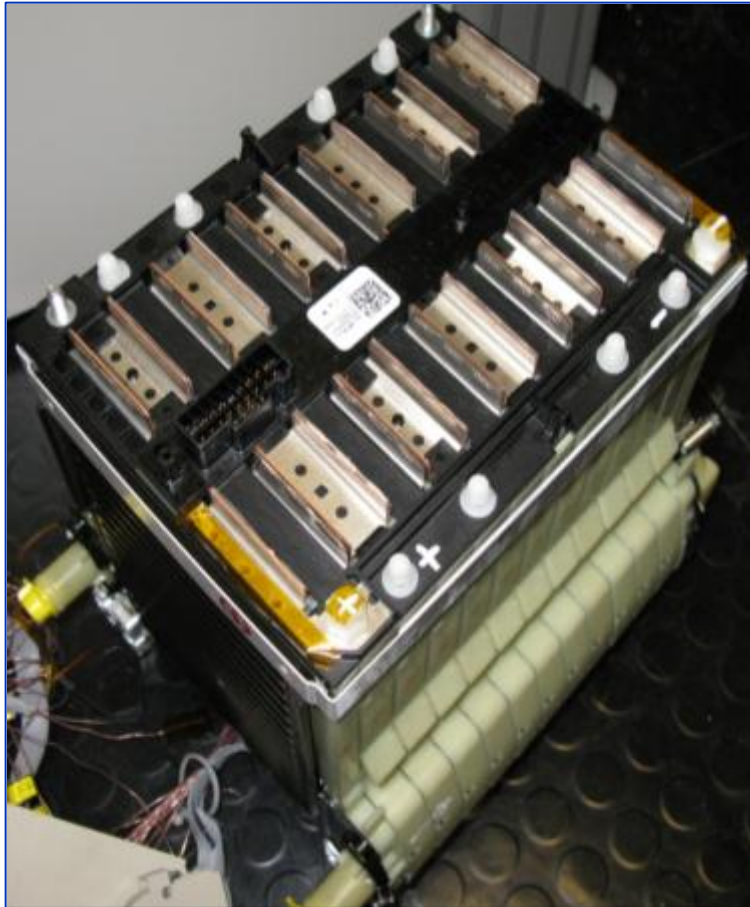
GM Technical Accomplishments - 2

Pack System Level Model with ROM

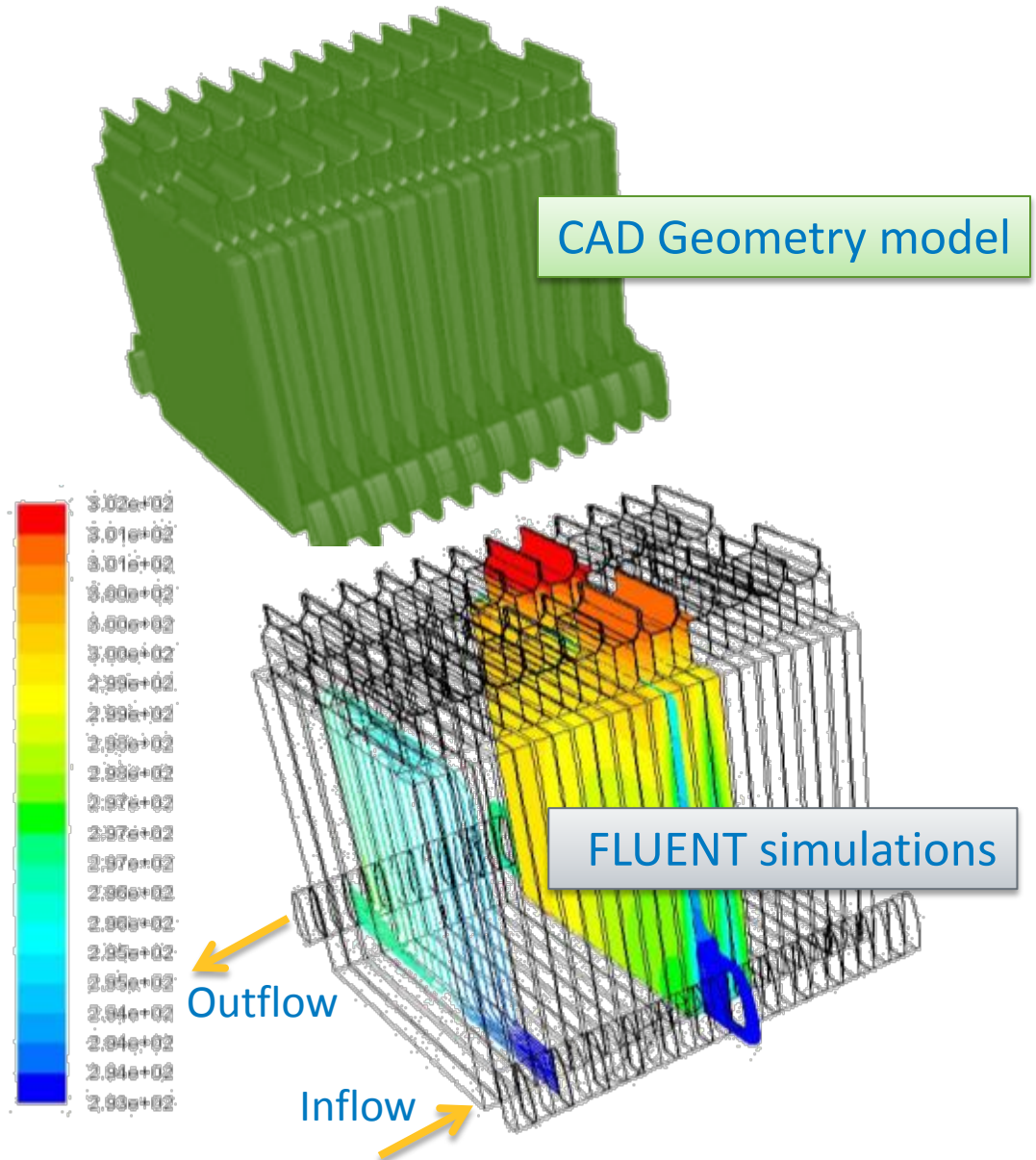
- Linear Parameter Varying(LPV) was implemented with a Linear-Time-Invariant (LTI) system theory to build a system level model with ROM to handle both variable flow rates and arbitrary heat generations
- Proper-Orthogonal-Decomposition (POD) is planned to decompose the temperature field into separable functions of time and space
- LPV demonstrated on GM 1x16 cylindrical air-cooled pack, with good results



GM Pack Level Validation in Progress



Prototype build for 24-cell module



CAD Geometry model

FLUENT simulations

Outflow

Inflow

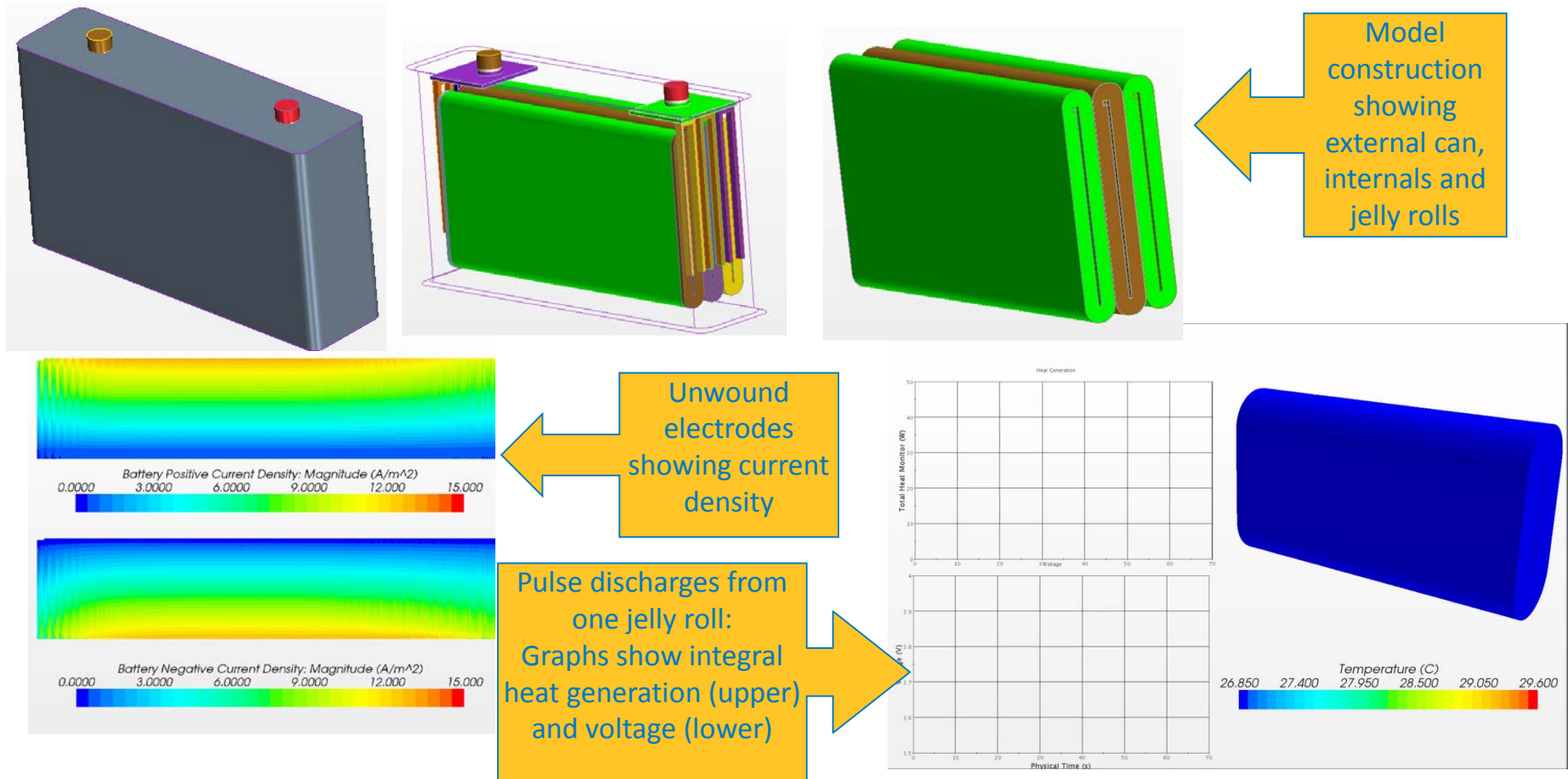
CD-adapco Approach & Strategy

- **Produce electrical and thermal simulation tools applicable for spirally wound lithium-ion cell designs, both cylindrical and prismatic**
 - Covering both complex electrochemistry and equivalent circuit approaches
 - Add contemporary electrolyte formulations for use in the electrochemistry model
- **Validate such models at the cell and module level with test work**
 - Both cell and module/pack level analysis will be carried out
- **Include the created simulation models into the readily available 3D multi-physics code STAR-CCM+, for combined flow, thermal and electrochemical simulation – proliferating the use of such methods**
 - A staged release of code included in this widespread CAE tool

Feature Complete Public Release – March 2013
19 Months into the Project

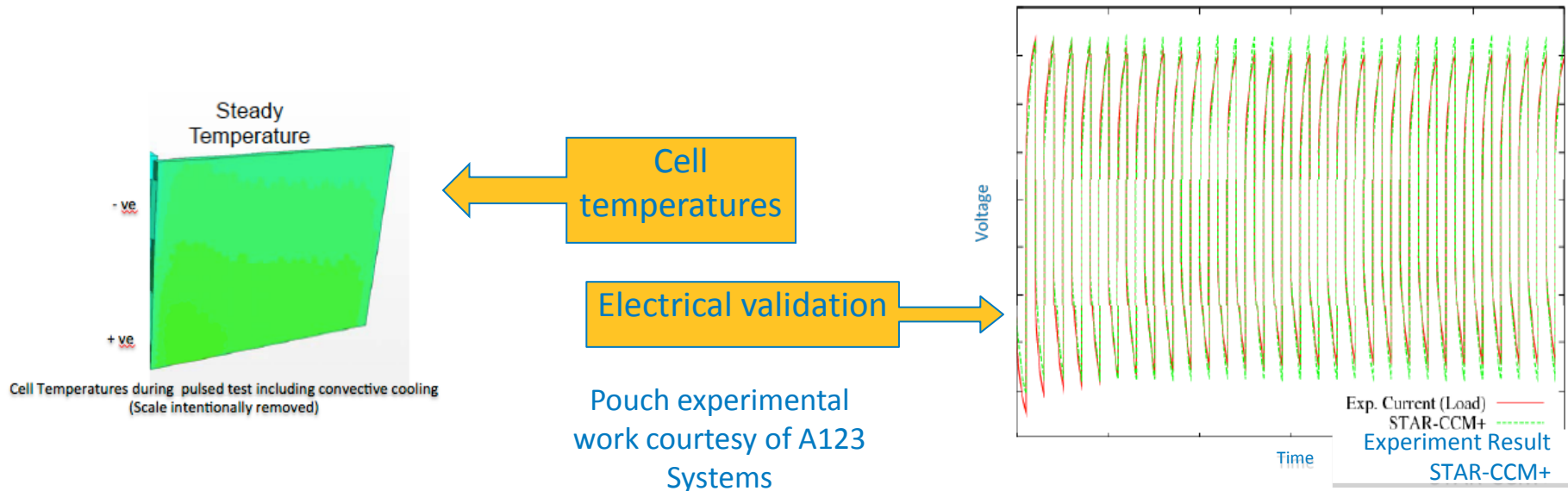
CD-adapco Technical Accomplishments – 1

A detailed electrochemistry model was applied to a wound cell configuration, both at the single cell level and the module level



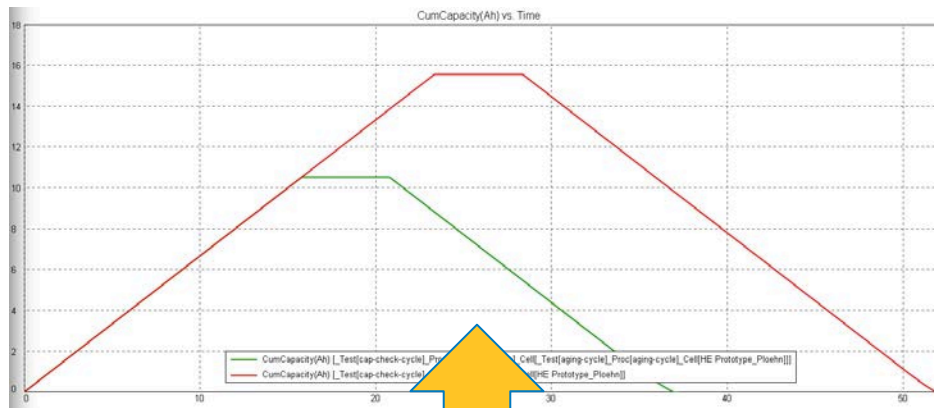
CD-adapco Technical Accomplishments – 2

- The created electrochemistry model has been applied to 4 wound cells
 - JCI – Cylindrical VL6P & VL41M
 - JCI – Prismatic PL27M & PL6P
- Single cell tests have been carried out to parameterise a model
- Drive cycle tests have been carried out to validate the model
 - Results remain confidential
- An equivalent circuit model of a pouch cell has been created
 - A123 Systems – Pouch 20 Ahr



CD-adapco Technical Accomplishments – 3

- A set of electrolyte properties for contemporary electrolytes has been added to the electrochemistry model
 - Available in July 2013
- A first release of a calendar ageing model has been added to the electrochemistry model and is also available from March 2013
 - Capturing SEI increase based on temperature and time



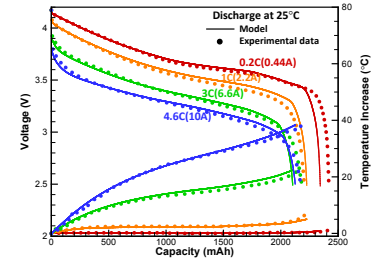
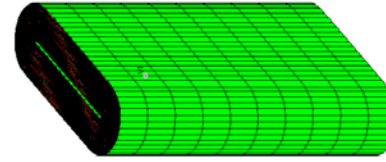
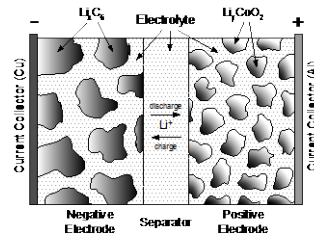
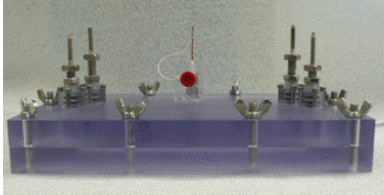
Example of capacity change due to model
Virginal vs. 60 weeks @ elevated temp

Ageing parameter inputs to model

The screenshot shows the software interface with a tree view on the left and a parameter table on the right. The tree view includes 'Main', 'Electrode', 'Formulation', 'Collector', 'Tab', 'Separator', 'Electrolyte', 'Package', 'Internals', 'Cell Voltage', 'Builders', 'Models', 'Electrolyte', 'IET', 'Nodes', 'Report', 'Cell BOM', 'Pos BOM', 'Neg BOM', and 'Data Sheet'. The parameter table is titled 'Parameters' and has columns for the parameter name, a '1' column, and a '+' column. The table includes parameters for Kinetic, Butler Volmer, Tafel, Pre-Exp Factor, Activation Energy, Liquid Concentration Exp., Solid Concentration Exp., Anodic Transfer Coefficient, Cathodic Transfer Coefficient, Double-layer Capacitance, SEI, SEI Pre-Exp. Factor, SEI Activation Energy, SEI Resistance Calendar Aging, SEI Initial Thickness, Solvent Diffusion Athernius Coefficient, Solvent Diffusion Activation Energy, Solvent Equilibrium Concentration, SEI Product Concentration, Nodes, Diffusion Conc. Correction, and Plots.

Parameters	1	+
Kinetic		
Linear	<input type="radio"/>	
Butler Volmer	<input checked="" type="radio"/>	
Tafel	<input type="radio"/>	
Pre-Exp Factor, mA/cm ²	0.4	
Activation Energy (J/molK)	0	
Liquid Concentration Exp. a	0.5	
Solid Concentration Exp. b	0.5	
Solid Concentration Exp. c	0.5	
Anodic Transfer Coefficient	0.5	
Cathodic Transfer Coefficient	0.5	
Double-layer Capacitance, F/m ²	0	
SEI		
SEI Pre-Exp. Factor, ohm-cm ²	2500	
SEI Activation Energy (J/molK)	0	
SEI Resistance Calendar Aging		
None	<input checked="" type="radio"/>	
SEI Initial Thickness (m)		
Solvent Diffusion Athernius Coefficient (m ² /s)		
Solvent Diffusion Activation Energy (J/molK)		
Solvent Equilibrium Concentration (mol/m ³)		
SEI Product Concentration (mol/m ³)		
Nodes	10	
Diffusion Conc. Correction	<input type="checkbox"/>	
Plots	<input checked="" type="checkbox"/>	

EC Power Team Project Approach



Task 1: Materials Characterization



Task 2: Physio-chemical Models



Task 3: Advanced Algorithms



Task 4: Experimental Validation



EC Power Software: **ECT3D**

Feedback



Suggestions

Performance

Cycle Life

Safety

EC Power Technical Accomplishments - 1

- **ECT3D v2 delivered to Ford and JCI for cell and pack simulations with:**
 - Pack thermal management design and optimization
 - Pack-level electrochemical-thermal coupling: simultaneous electrochemical and thermal output (Fig. 1)
 - Proof-of-concept nail penetration simulations for stacked electrode cells in pack (Fig. 2)
- **AutoLion-3D™ (commercial version of ECT3D software) released Nov. 2012**
- **In-Situ current density measurements for large format cells– currently being used for model validation (Fig. 3)**

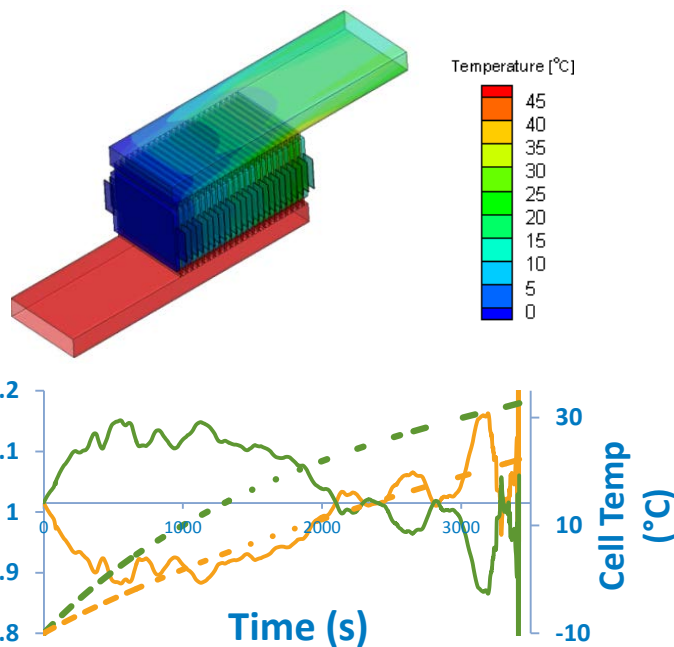


Fig. 1 Thermally driven current imbalance within pack during discharge

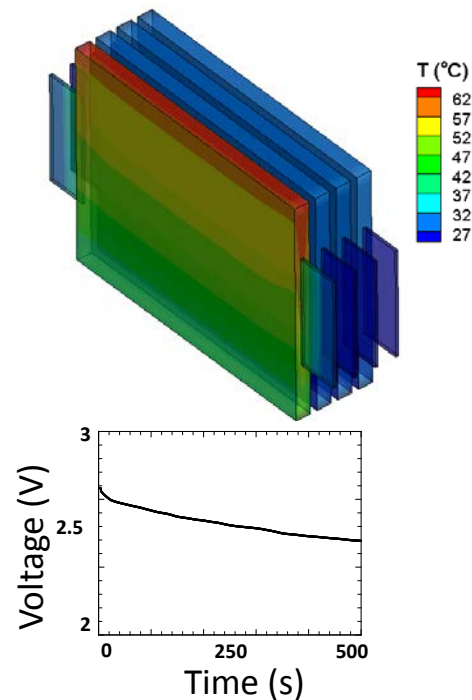


Fig. 2 Preliminary pack safety simulations

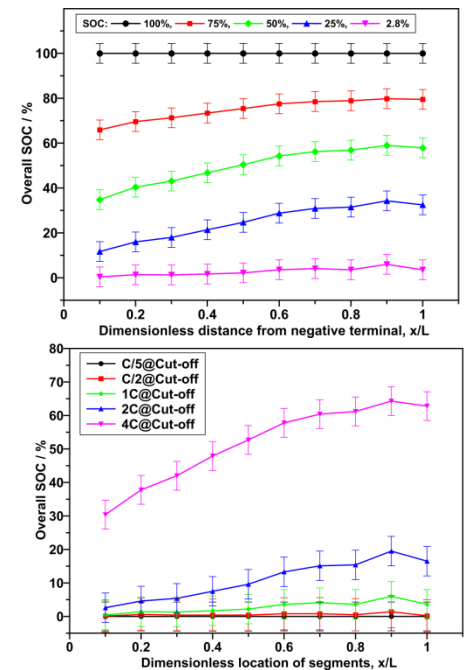


Fig. 3 In-Situ data showing non-uniform SOC during discharge

EC Power Technical Accomplishments - 2

Tested Temperature Range for Materials

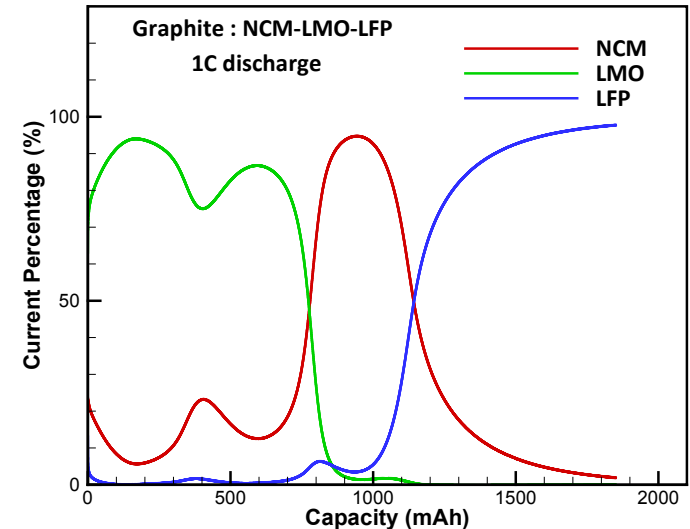
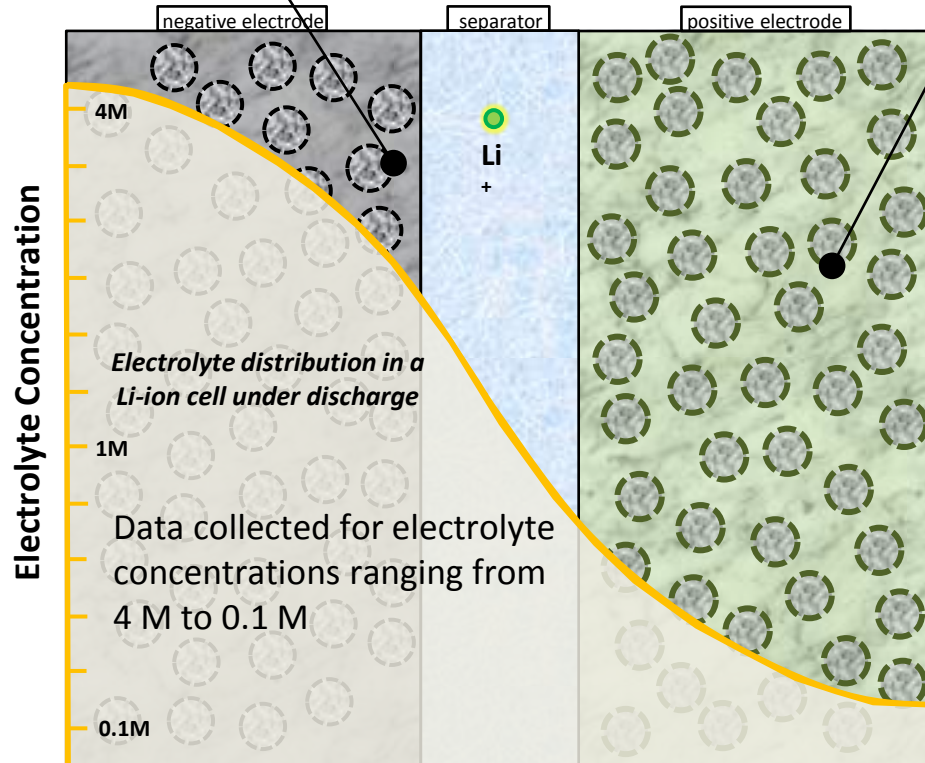


Anode Materials

- Graphite (blended natural/synthetic)
- LTO
- others

Cathode materials

- NCM
- LFP
- LMO
- others



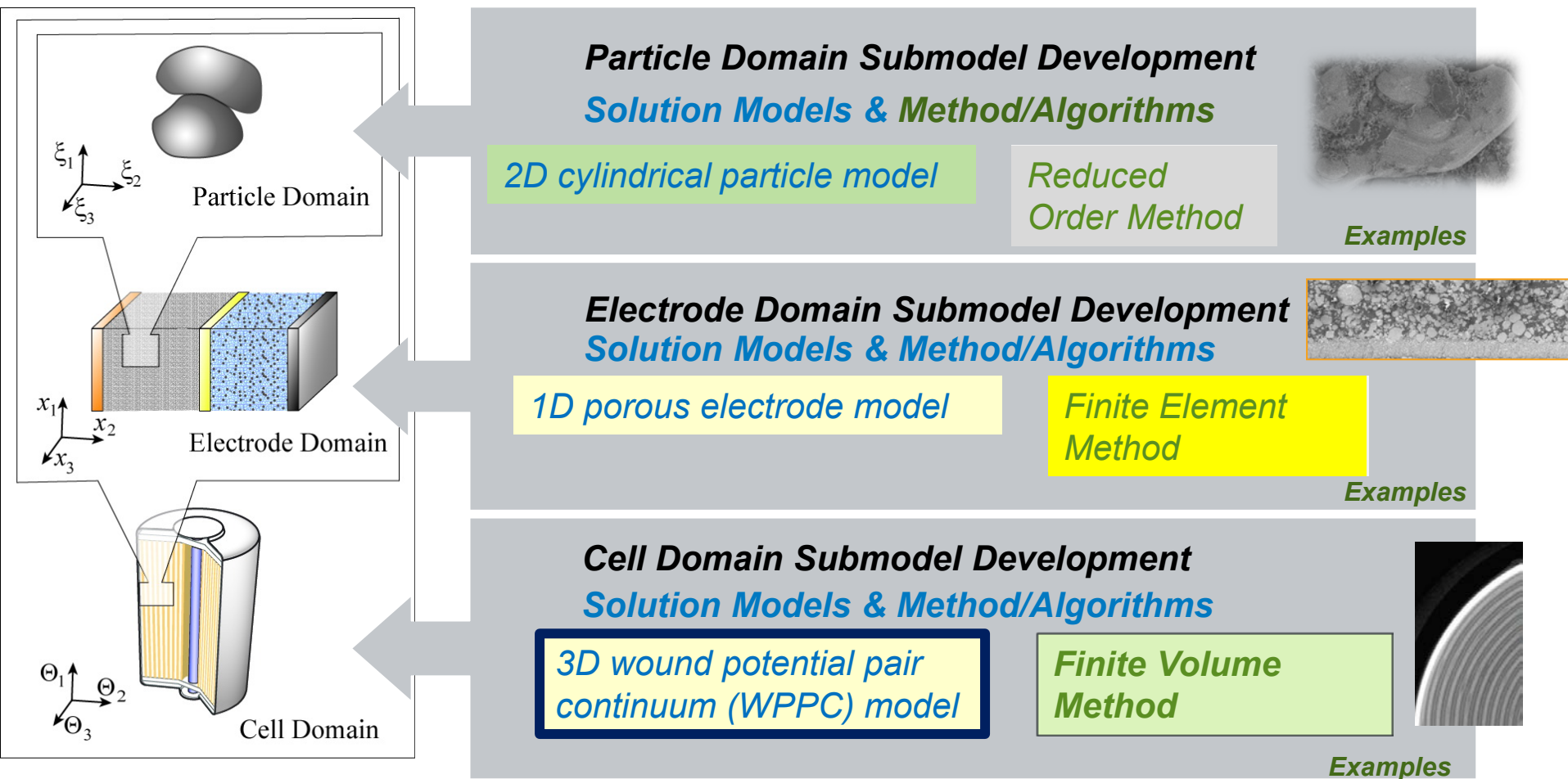
Preliminary Results for Blended Active Material Simulations

100,000+ coin cells

- Materials Database: 100,000+ coin cells built and tested
- Massive undertaking spanning length of project
- High-quality material properties lead to validated results for large format cells and packs

NREL Approach: Expand Multi-Physics Multi-Scale Multi-Dimensional (MSMD) Framework

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

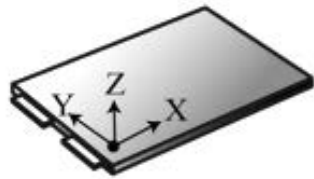
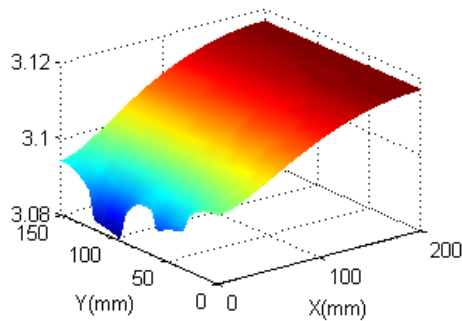


The modularized framework facilitates collaboration with experts across organizations

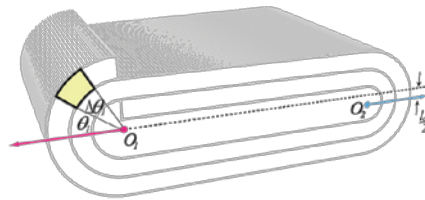
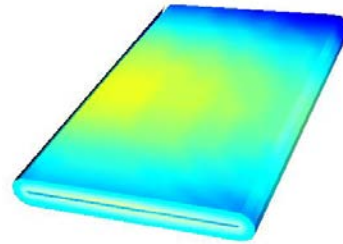
NREL Technical Accomplishments – 1

NREL enhanced framework functionality of *cell domain models/solution methods*, providing complete tool sets for simulating *all major cell form-factors*; stack pouch, wound cylindrical, and wound prismatic cells

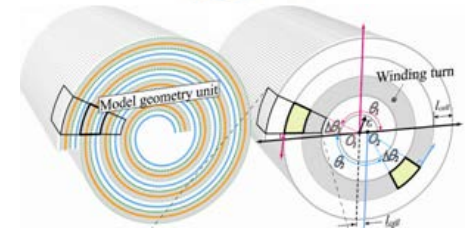
Stack Pouch



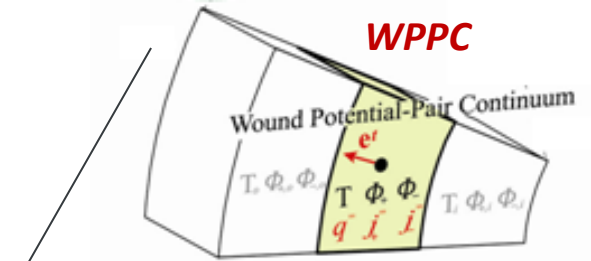
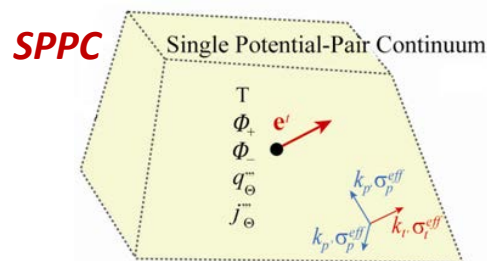
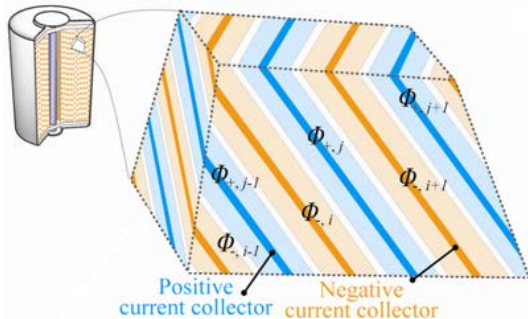
Wound Prismatic (FY12 Focus)



Wound Cylindrical

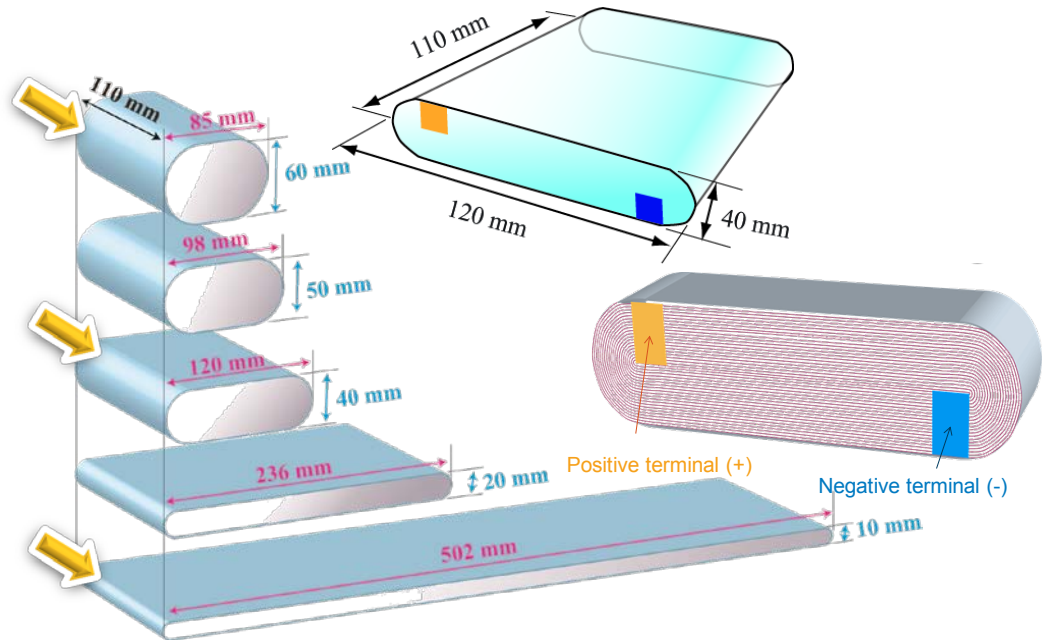
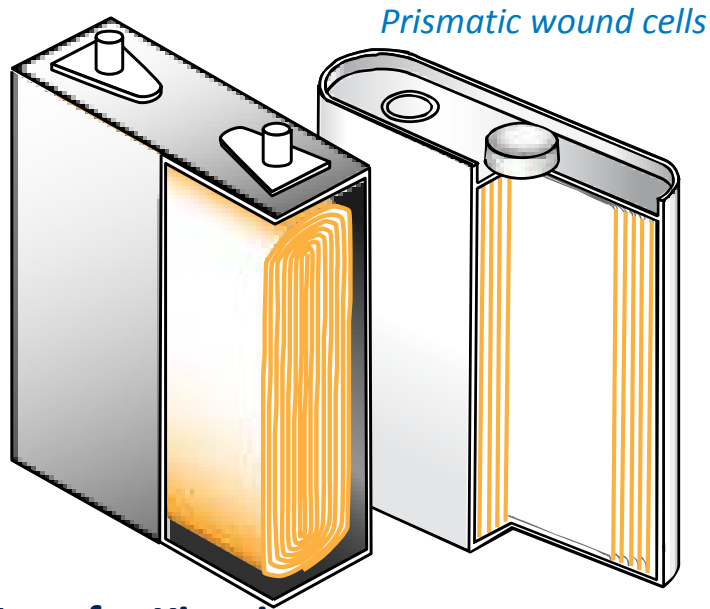


Orthotropic Continuum Models for Cell Composites

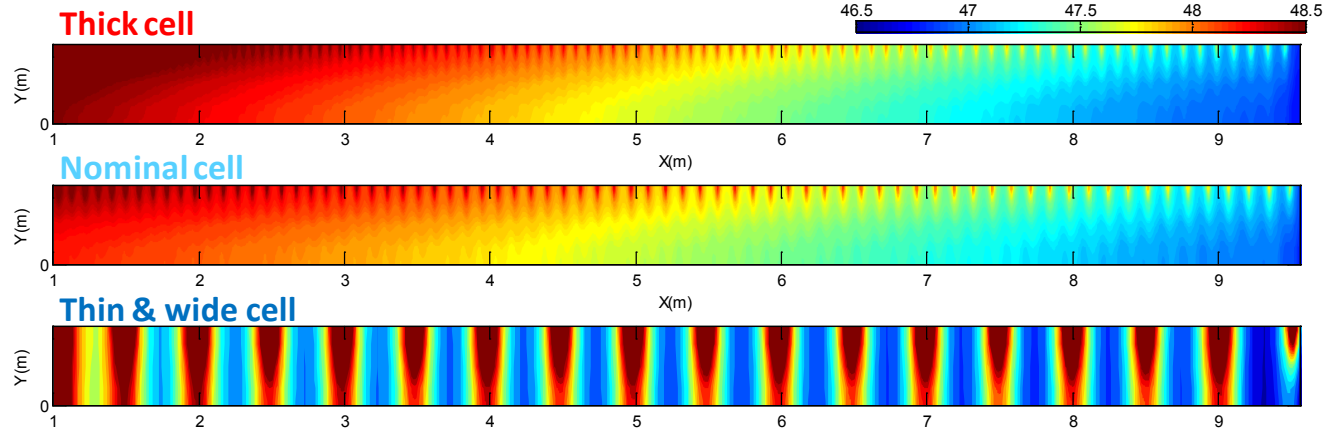
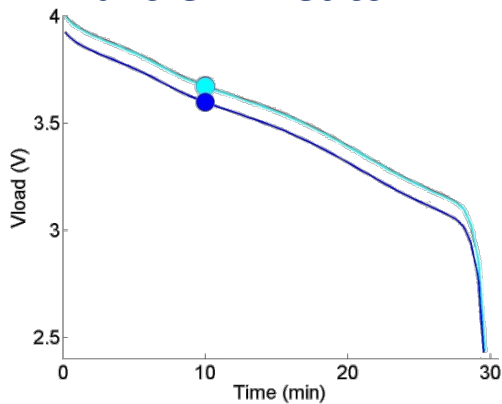


NREL Technical Accomplishments – 2

Developed MSMD Wound Prismatic Cell Model

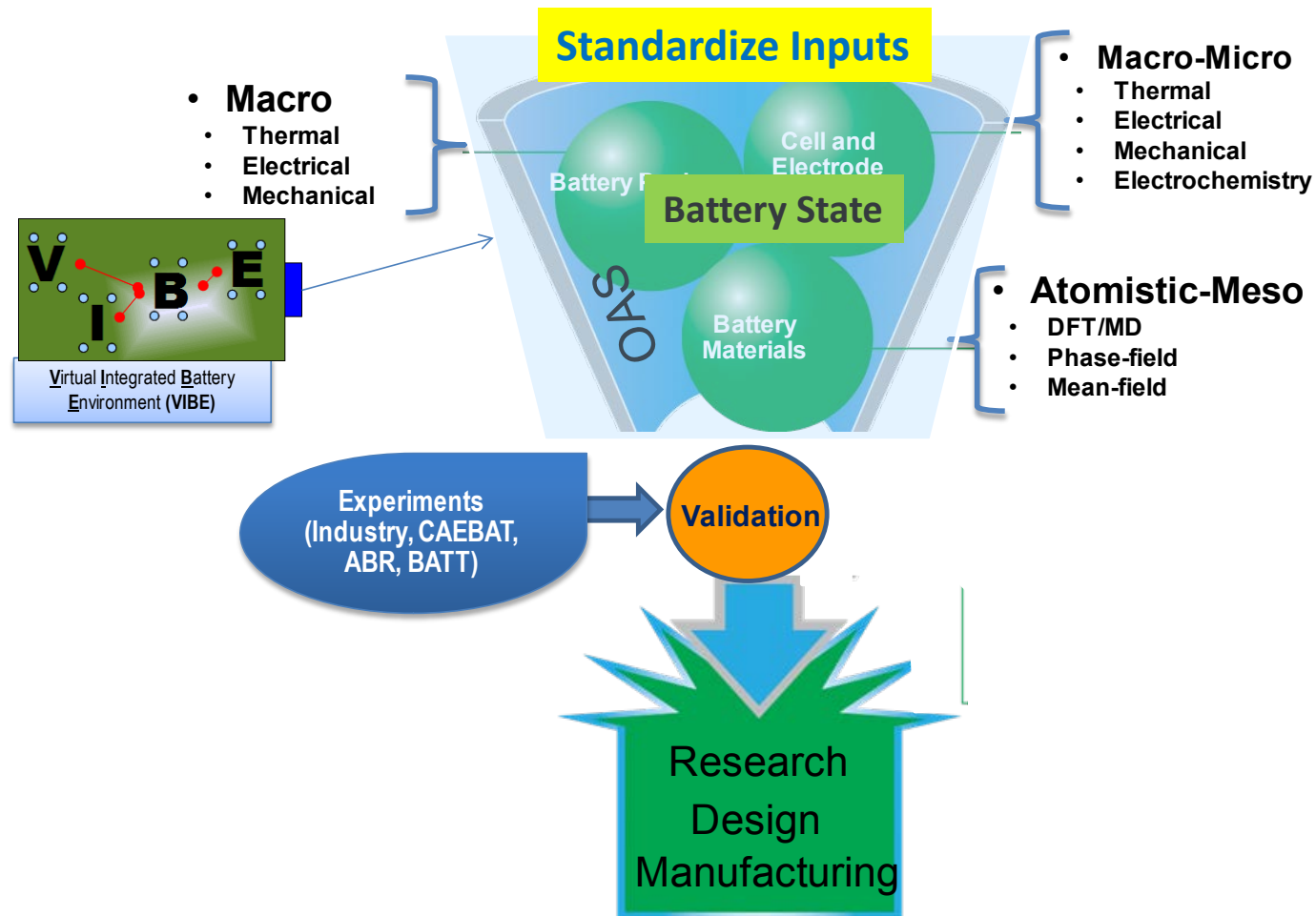


Transfer Kinetics



The model quantifies the impacts of the electrical/thermal pathway design on uneven charge-discharge kinetics in large format wound prismatic cells

ORNL Approach for Open Architecture Software



Develop interface platforms for successful collaboration across CAEBAT teams

- “Standardization of input” and of “Battery state” database
- Standard test problem(s)
- Standardized interfaces for cell, pack, etc. models

ORNL Technical Accomplishments – 1

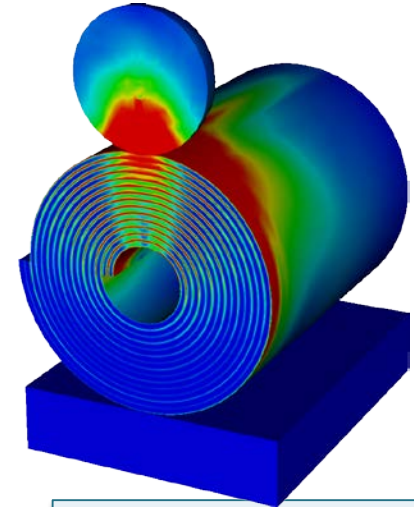
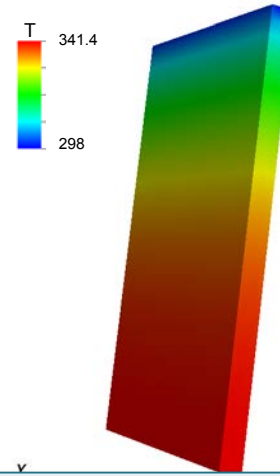
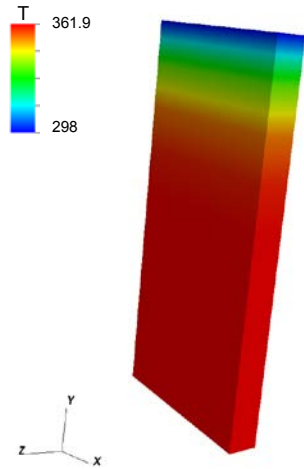
On Track to Release New Version

OAS	VIBE	Standardized Input	Battery State
<ul style="list-style-type: none"> • Capability is online (and available to partners) • Integrated with Dakota optimization • Improve workflow as well as portability to Windows • Interfaces to the inputs and battery state standards 	<ul style="list-style-type: none"> • Electrochemical-thermal coupling • Electrochemical-thermal-electrical coupling • Integrate additional components (NREL models and ANL cost model) • Demonstrate for complex geometries with new interfaces • Mechanical 	<ul style="list-style-type: none"> • Comprehensive relational database of materials, properties, models, components, etc. • XML database and corresponding schemas • Version 11. ANSYS/GM adopted this standard and translator for EC-power • Translators for CD-Adapco) 	<ul style="list-style-type: none"> • Define for cell to cell-sandwich coupling • Define for cell to pack coupling • Issued version 1

Green – Completed
Blue – Ongoing

ORNL Technical Accomplishments – 2

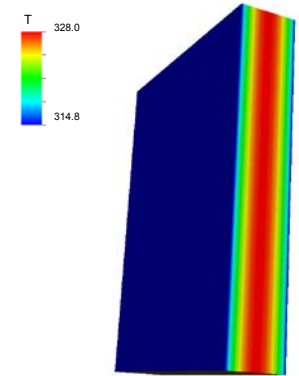
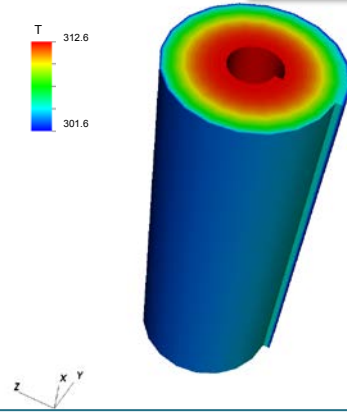
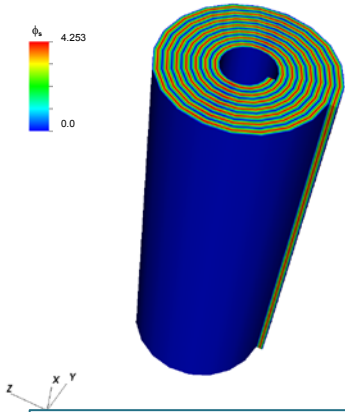
Coupling Various Physics at Cell Level



Unrolled Cell (Electrochemical - Thermal)

Unrolled Cell (Electrochemical – Thermal - Electrical)

Mechanical Abuse of Cylindrical Cell with Current Collectors Resolved (Electrochemical – Thermal – Electrical – Mechanical)



Cylindrical Cell with Current Collectors Resolved (Electrochemical – Thermal - Electrical)

Pouch Cell with Current Collectors Resolved (Electrochemical – Thermal - Electrical)

More details: <http://thyme.ornl.gov/CAEBAT/home/home.cgi>

Collaborations and Coordination

- NREL interactions with all team members

- General Motors, ANSYS, ESim
- CD-adapco, Battery Design, A123 Systems, JCI, and INL
- EC Power, Penn. State University, JCI, and Ford
- ORNL



- ORNL interactions with CAEBAT team leads

- General Motors, ANSYS
- CD-adapco, Battery Design
- EC Power
- University of Michigan and Sandia National Laboratory



- CAEBAT subcontractor collaborations with team members

- General Motors, ANSYS, ESim
- CD-adapco, Battery Design, A123 Systems, and JCI
- EC Power, Penn State University, JCI, and Ford



Proposed Future Work

- Perform cell level verification and validation
- Develop model order reduction methods for the pack level
- Extend cell-level models for aging and abuse
- Perform pack level verification, validation, and demonstration
- Complete electrochemical model validation
- Complete build of each cells respective module
- Run remaining module tests
- Compare and validate module level work
- Validate large format, multi-dimensional models against In-Situ SOC, current density, and temperature data
- Further develop materials database with full mixed electrode capabilities
- Develop an advanced particle domain model for better representation of complex kinetic/dynamic behavior of mixture composition of active particles
- Extend the MSMD paradigm to pack-level simulation to capture non-uniform electrochemical, electrical, thermal response over a pack
- Define battery state for cell-to-pack coupling and demonstrate the same
- Perform initial demonstration of the graphical user interface for setting up OAS, example cases, and launch simulations

GMGMCD-adapcoE3 POWERNREL
NATIONAL RENEWABLE ENERGY LABORATORYOAK RIDGE
National Laboratory

Summary

- CAEBAT activities consist of three parallel paths:
 - Developing CAEBAT tools through cost-shared contracts with industry (GM, CD-adapco, EC Power)
 - Enhancing and developing NREL in-house electrochemical battery model
 - Developing an open architecture software at ORNL to link the CAEBAT battery models
- Each developer has made significant progress toward releasing beta version of their battery models
 - EC Power has released AutoLion™, a commercial version of ECT3D
 - CD-adapco has released its tools for wound spiral cells in STAR-CCM+
 - ANSYS (GM) is planning to release its version this summer
- NREL has hierarchal electrochemical-thermal models for all cell types and is extending them to modules
- ORNL has developed and distributed the first generation of the Open Architecture Software for linking various battery models.
- CAEBAT project is on track to deliver advanced battery design software tools

Reviewer-Only Slides

Responses to Previous Year's Reviewers' Comments – NREL

- **The reviewers gave an average score of 3.71 out of 4.00. We appreciate it.**
- **On Question 1, does this project support the overall DOE objectives?**
 - The Reviewers provided positive feedback that this project support the DOE objectives
- **On Question 2, one reviewer raised concern about but the success of these indicated that previous TLVT was not used by battery developers**
 - We appreciate concern and that is why each CAEBAT team has one or two end-users to make sure the final product is useful and to be innovative, elegant, tractable and as user-friendly as the researchers could be so that the project could bring real benefit to the users.
- **On Question 3, one reviewer inquired whether there was any modeling work on tab locations (prismatic) on the long side**
 - Although there are no designs out there which considered such locations especially for EVs, we feel that based on testing of other cells, temperature data match well with those in real cells.
- **On Question 4, The second reviewer expressed real concern for the collaborations as programs with many participants have lost momentum**
 - We appreciate the concern by this reviewer. Although there is a large number of participants in this program, there is three major smaller teams that each responsible to deliver a competitive products. So we feel the overall risk is less as the software vendors in each team are working competitively and we believe, at least, one would be successful.
- **On Question 5, The third reviewer asked how the final judgments would be made among the “three horses”, what criteria would be used to determine the success , and who would market the software.**
 - ANSYS, CD-adapco and EC Power will market and sell their software. They will not be open source, but the open architecture software will be made available for free by ORNL. The cost modeling will got incorporated in the program; There are plans to develop abuse-tolerance models and they are underway by EC Power & GM.

Responses to Previous Year's Reviewers' Comments – ORNL

- **Question 2, Reviewer 1:** “The first reviewer observed there were solid thoughts behind the approaches. Of course, the goals were rather grand and it would be interesting to see how the three programs were incorporated into this architecture.”
 - We realize the goals are rather grand and thus we are using a very methodical way of building cell-level models with good definition of input/output before moving to cell-module and cell-pack coupling
- **Question 2, Reviewer 2:** This was such a complex area that if the program could discover or put together a model that could simplify and explain certain battery issues -to battery people with limited theoretical knowledge- could end up being very useful.
 - This is a very useful suggestion and after we finish developing the user interface, we will incorporate an “expert system” that interprets some common issues
- **Question 3, Reviewer 1:** The reviewer was curious how customizable the package would be.
 - This is very customizable (for e.g., various different cathode chemistries can be evaluated at once – this should address Reviewer 2’s question)
- **Question 4, Reviewer 2:** This reviewer highlighted the hope that at some point industrial battery companies would decide to engage a little more in this area of research and development.
 - We have started interacting with battery manufacturers
- **Question 4, Reviewer 3:** This reviewer encouraged monthly meetings with each and every one of the modeling teams/PIs feeding into this program, not just NREL.
 - We are having regular meetings with NREL/DOE and when needed talking to all the teams.
- **Question 5:** The first reviewer questioned how ORNL planned to incorporate proprietary information into its model architecture. The second reviewer indicated that increased portability to Windows could be of great value. Similarly, the incorporation of a cost model could have important practical implications.
 - We have already made links to proprietary models and the users need to have access to the proprietary modules before they can use them in conjunction with OAS. We have already added increased portability to Windows and also linked to ANL cost model.
- **Question 6:** The second reviewer supported this effort, but found \$500,000/year to be a bit excessive for this activity. The overall work is important, but this reviewer did not believe it to be that hard or to require so much in the way of resources. It seemed to be mostly a coordination and computer/modeler interface design development and study.
 - This project has 5 different activities (OAS, VIBE, Input Standardization, Battery State and User Interface) and covers a very broad set of requirements in terms of supporting various models and various computing platforms such as Windows, Linux, Clusters, etc. and thus the need for allotted funding.

Publications and Presentations - 1

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- Taeyoung Han, Gi-Heon Kim, Lewis Collins, “Development of Computer-Aided Design Tools for Automotive Batteries-CAEBAT,” *Automotive Simulation World Congress (ASWC)*, Detroit, October 2012.
- Xiao Hu, Scott Stanton, Long Cai, Ralph E. White, “A linear time-invariant model for solid-phase diffusion in physics-based lithium ion cell models.,” *Journal of Power Sources 214 (2012) 40-50*.
- Xiao Hu, Scott Stanton, Long Cai, Ralph E. White, “Model order reduction for solid-phase diffusion in physics-based lithium ion cell models,” *Journal of Power Sources 218 (2012) 212-220*.
- Meng Guo, Ralph E. White, “A distributed thermal model for a Li-ion electrode plate pair,” *Journal of Power Sources 221 (2013) 334-344*.
- Kyu-Jin Lee et al., “Three Dimensional Thermal-, Electrical-, and Electrochemical-Coupled Model for Cylindrical Wound Large Format Lithium-ion Batteries”, *J. of Power Sources*, 2013, *accepted*
- Gi-Heon Kim et al., “Integrated multiscale lithium battery model”, *245th ACS National Meeting , April 7-11, 2013, New Orleans, Louisiana*
- Ahmad Pesaran, et. al. “Accelerating Development of EV Batteries Through Computer-Aided Engineering,” *Automotive Simulation World Congress*, Detroit, MI, Oct 30-31, 2012

Publications and Presentations - 2

- Gaetan Damblanc, “Multi-Scale Electrochemistry Modeling within CAE Software,” Advanced Automotive Battery Conference, Pasadena, CA, February 4-8, 2013
- Zhang, G., Shaffer, C. E., Wang, C. Y., & Rahn, C. D. (2013). In-situ measurement of current distribution in a li-ion cell. *Journal of the Electrochemical Society*, 160(4), A610-A615.
- Ji, Y., Zhang, Y., and Wang, C.Y. (2013). Li-Ion operation at low temperatures. *Journal of the Electrochemical Society*, 160(4), A636-A649.
- Yan Ji and C.Y. Wang (2013). Heating Strategies for Li-ion Batteries Operated from Subzero Temperatures. *Electrochimica Acta* (accepted for publication).
- Featured in textbook: Rahn, C. D., & Wang, C. Y. (2013). *Battery Systems Engineering*. (1 ed.). John Wiley & Sons.
- “CAEBAT OAS BETA RELEASE V1,” S. Pannala, S. Allu, W. Elwasif, S. Simunovic, D. Bernholdt, and J. Turner, Internal report to CAEBAT partners
- “Parameter Sweep and Optimization of Loosely Coupled Simulations Using the DAKOTA Toolkit,” Elwasif, W. R., D. E. Bernholdt, et al., IEEE 15th International Conference on Computational Science and Engineering (CSE), 2012.
- “Computational Framework for Modeling Multi-Physics Phenomenon of Li-Ion Batteries across Various Hierarchies”, S. Allu, S. Pannala, W. Elwasif, S. Simunovic, J.T. Turner, Electrochemical Society (ECS) PRiME Meeting, Honolulu, 2012.

Critical Assumptions and Issues

- Industry teams are able to resolve technical challenges by solving complex sets of equations in various scales so software tools are faster and can be run on typical consumer computers
- Models developed by labs and CAEBAT subcontractors are open and accessible for exchange of information
- Cell and pack models are adequately validated with relevant data
- Open Architecture Software can link the major models across different platforms
- Software tools developed by CAEBAT are adopted widely by the battery community as whole