NREL
NATIONAL RENEWABLE ENERGY LABORATORY

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

Presented at the 2013 U.S. DOE Vehicle Technologies Program
Annual Merit Review & Peer Evaluation Meeting
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**May 14, 2013**

Project ID #ES117

This presentation does not contain any proprietary, confidential, or otherwise restricted information.

# Overview

## Timeline

**Project Start Date:** April 2010
**Project End Date:** September 2014
**Percent Complete:** 40%

## Budget

**Total Contractors' Project Funding :$14M**

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

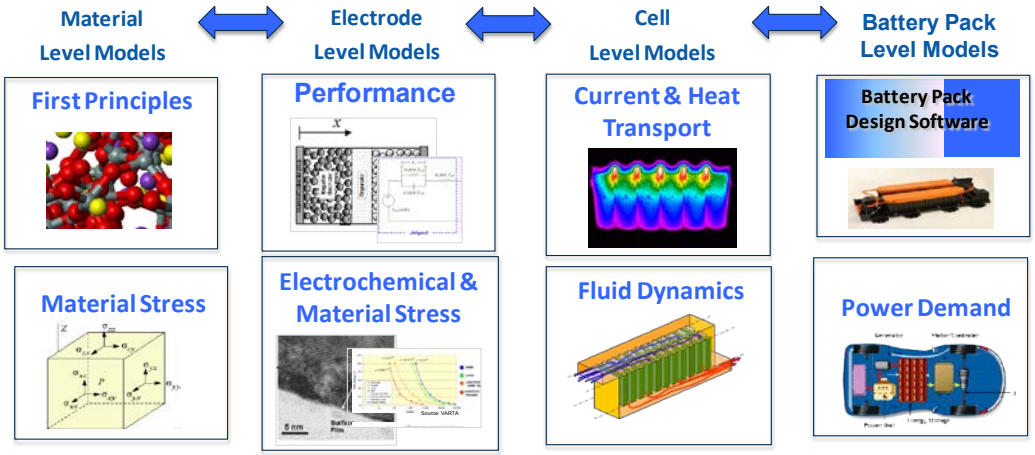
- NREL, project lead
- Oak Ridge National Laboratory (ORNL)
- **EC Power**/Penn State University/ Ford/Johnson Controls, Inc. (JCI)
- **General Motors**/ANSYS/ESim
- **CD-adapco**/Battery Design/ JCI/A123/Idaho National Laboratory

Funding provided by Dave Howell of the DOE Vehicle Technologies Program.
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, 3-D, fully integrated, 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 venders



# 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) were to:**
  - GM: Release first version of cell and pack level tools for internal GM team evaluation.
  - CD-adapco: Release 1st version of 3-D electrochemical-thermal code in STAR-CCM+ for the spiral cell designs to the public
  - EC Power: Release 1st version of the 3-D electrochemical-thermal code for all cell designs to the public
  - NREL: Oversee CAEBAT project execution and to 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

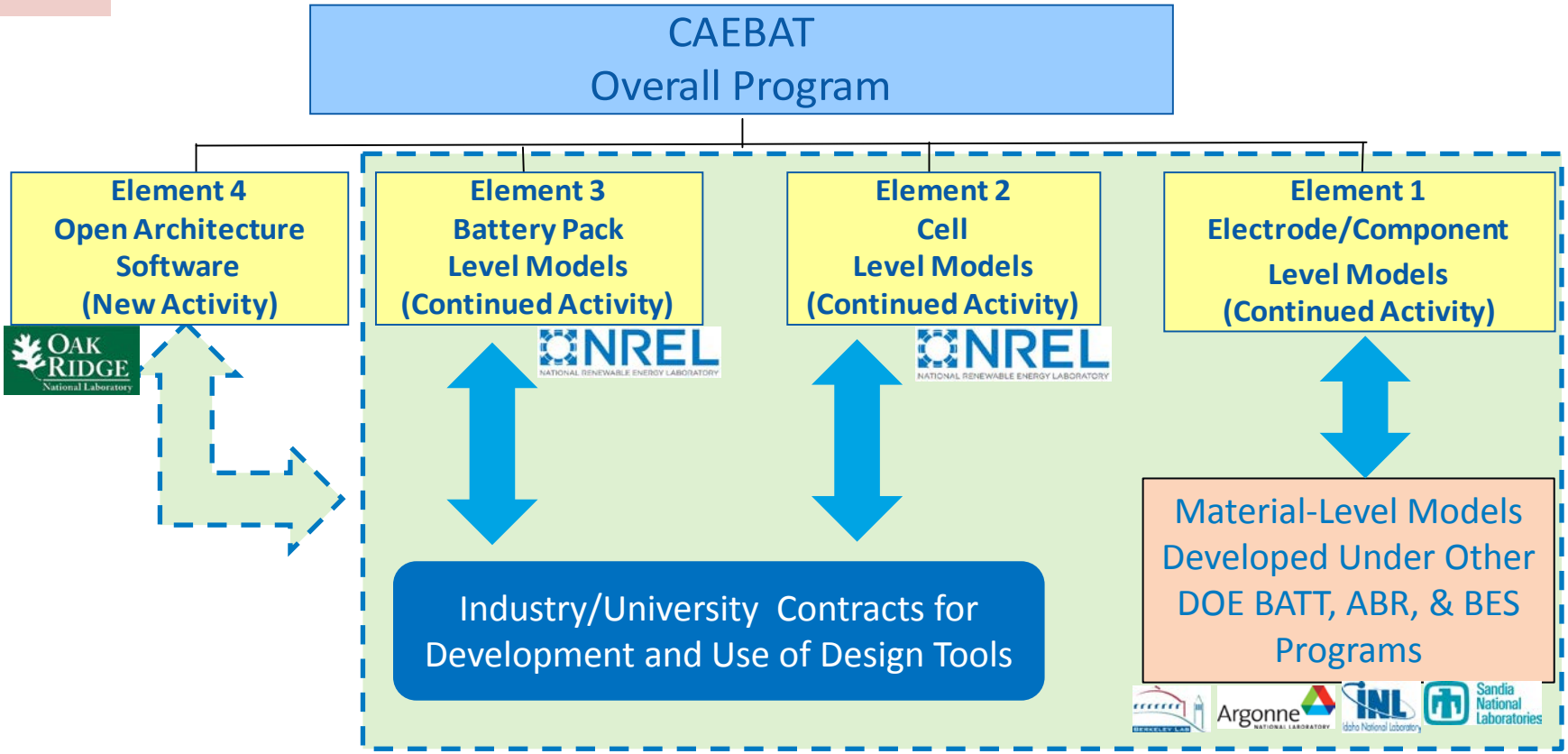
- **The impact of this project when CAEBAT tools are made available could be significant:**
  - Shorten design cycles and optimization of batteries
  - Simultaneously address the barriers of cost, performance, life, and safety of lithium-ion with quantitative tools

# Milestones

| Date | Milestone or Go/No-Go Decision | Status |
|---|---|---|
| January 2013 | Release first version of cell and pack level tools in FLUENT for internal team evaluation. (GM) | Completed |
| March 2013 | Release first version of 3D electrochemical-thermal code in STAR-CCM+ for the spiral cell designs to the public (CD-adapco) | Competed |
| November 2012 | Release first version of the 3D electrochemical-thermal code for all cell designs to the public (EC Power) | Completed |
| 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) | Competed |
| February 2013 | Share first version of OAS database on Standardized Input and Battery State (ORNL) | Competed |

# 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

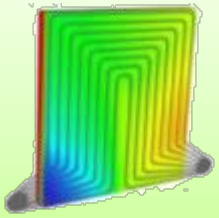
- Three Industry teams, selected competitively, develop three separate validated battery design software tools with NREL as the technical monitor
- The teams hold monthly conference call and quarterly review meetings.

| 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 sharing them with subcontract teams
- ORNL develops the elements 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

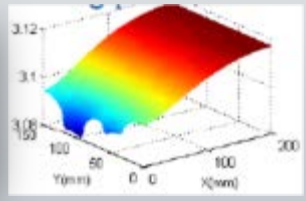
## Pack Level Model

Co-simulation

## Reduced-Order Models

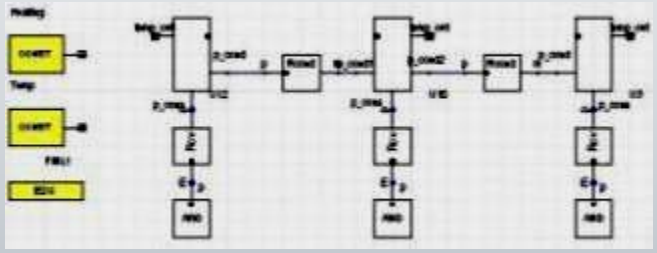
- Reduced order models for flow and thermal analysis at the pack level
- Reduced order cell models
- Ability to "expand" results

$$\dot{x} = Ax + Bu$$
$$y = Cx$$



## System Level Model

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

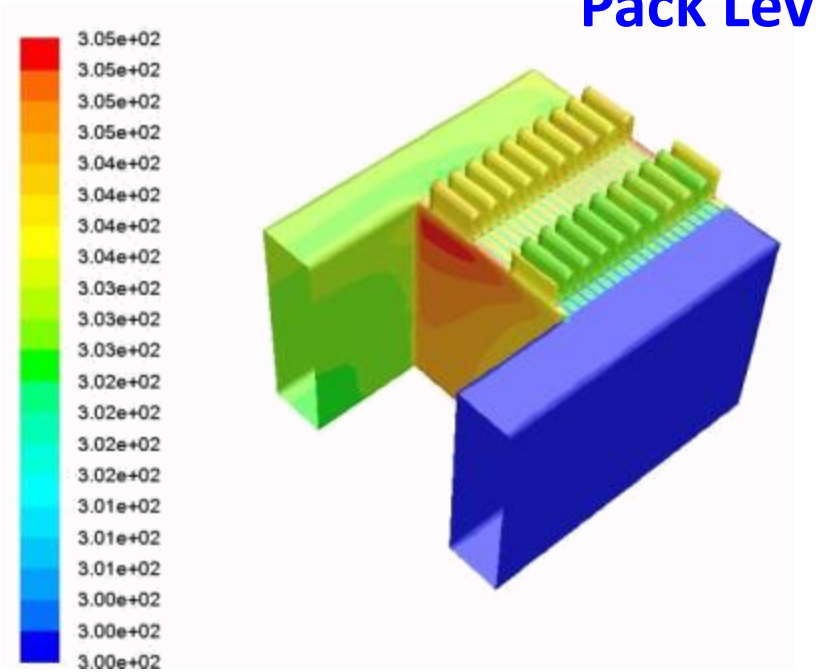


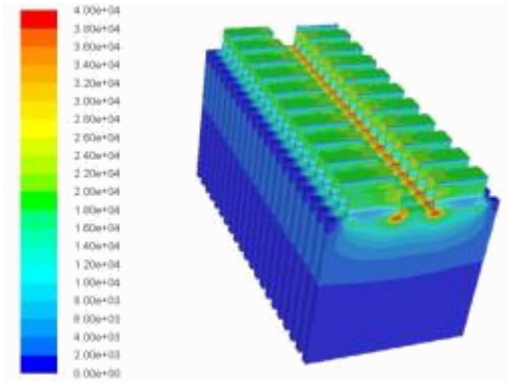
# GM Accomplishments

- **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 a 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

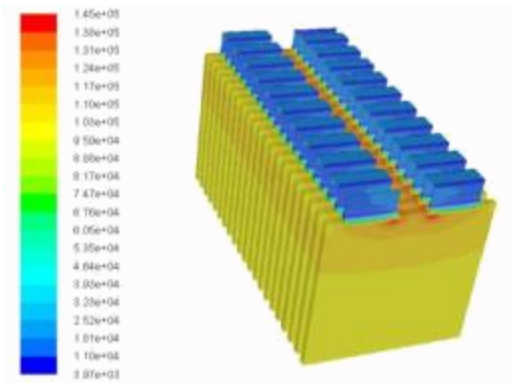
# GM Technical Accomplishments – 1

## Pack Level Field Simulation

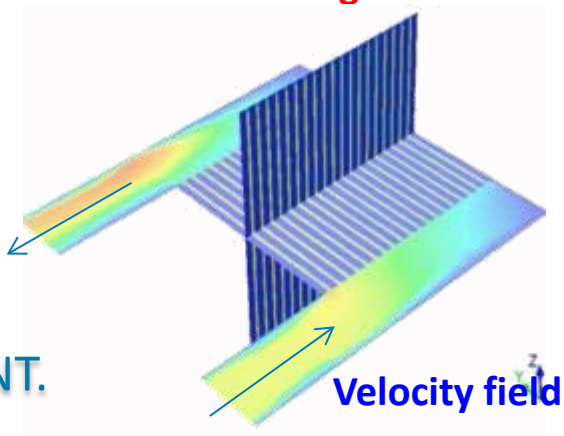


Ohmic heat generation



Total heat generation rate



Velocity field

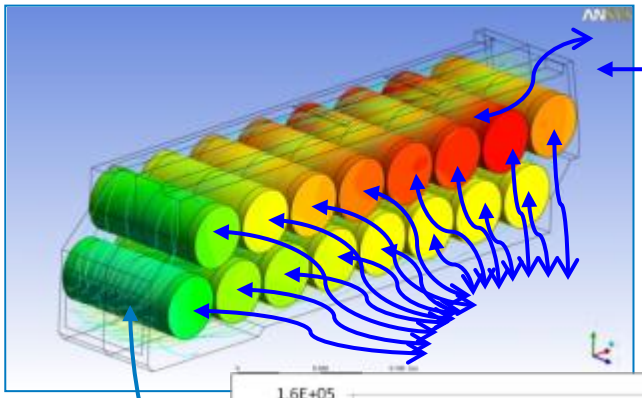
**First cell and pack level tools released to GM team**

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

# GM Technical Accomplishments - 2

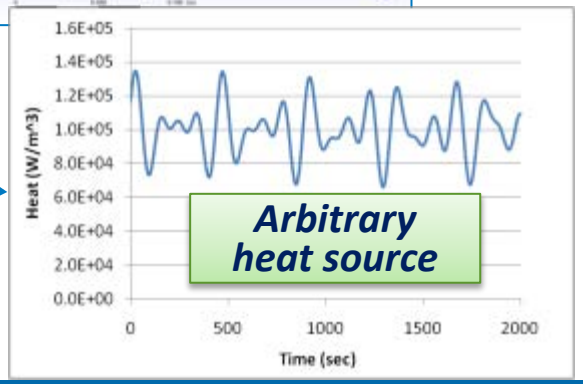
## Pack System Level Model with ROM

- 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

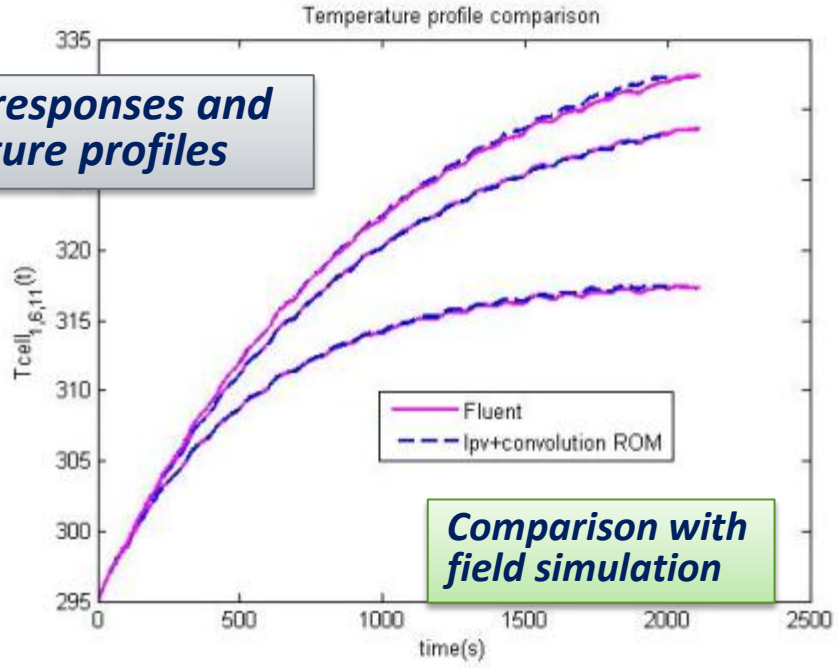


***Step response***

***Thermal responses and Temperature profiles***

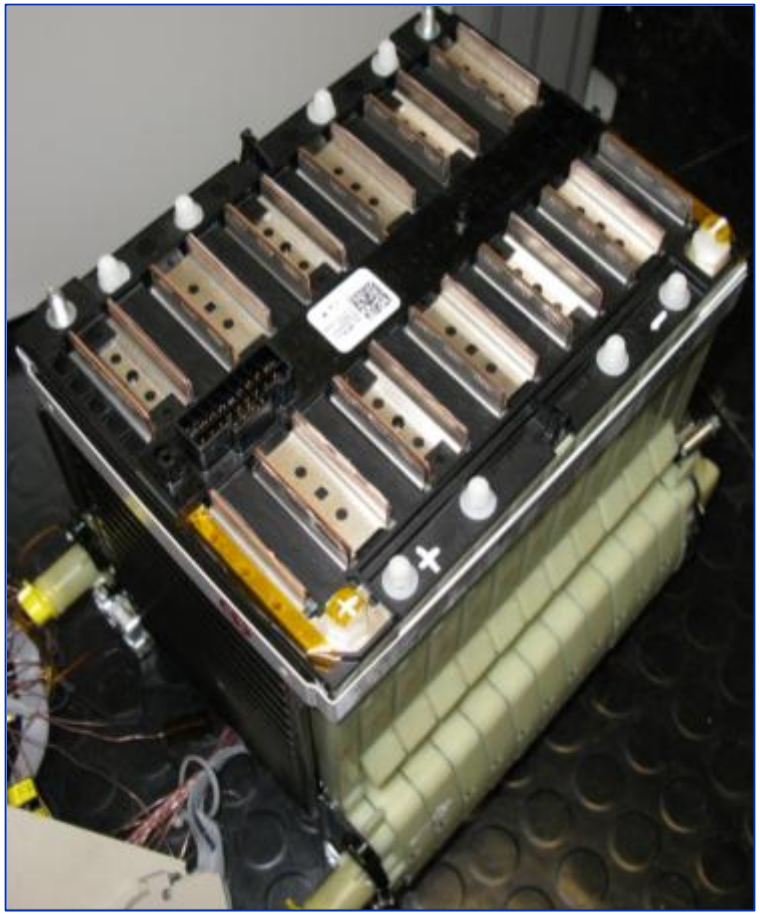



***Arbitrary heat source***

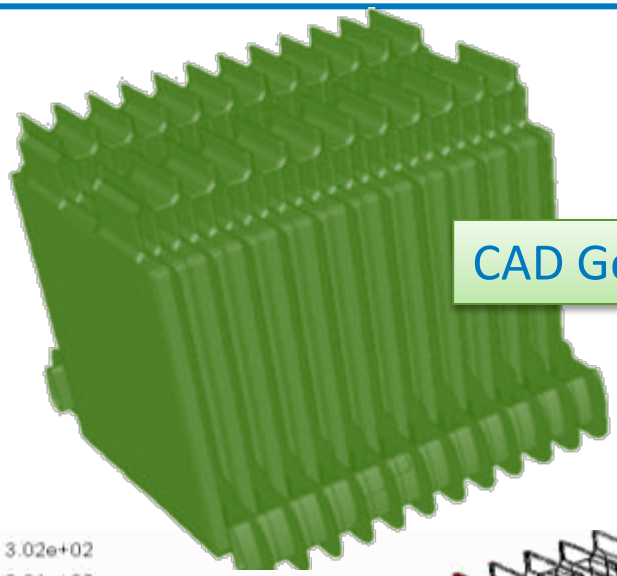



***Comparison with field simulation***

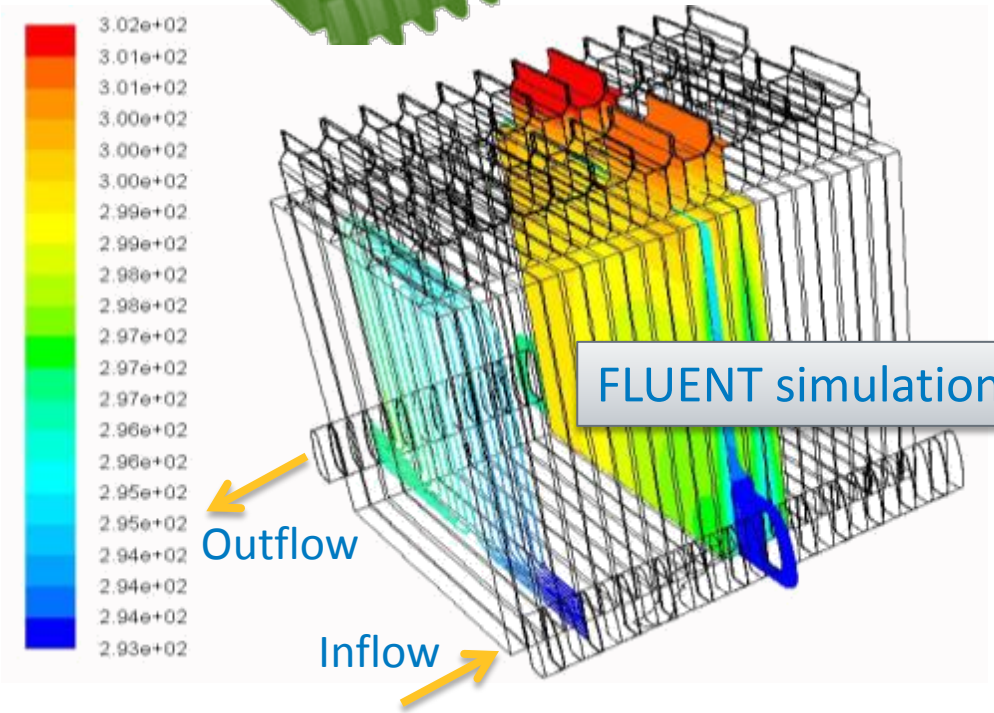
# GM Pack Level Validation in Progress



Prototype build for 24 cell module



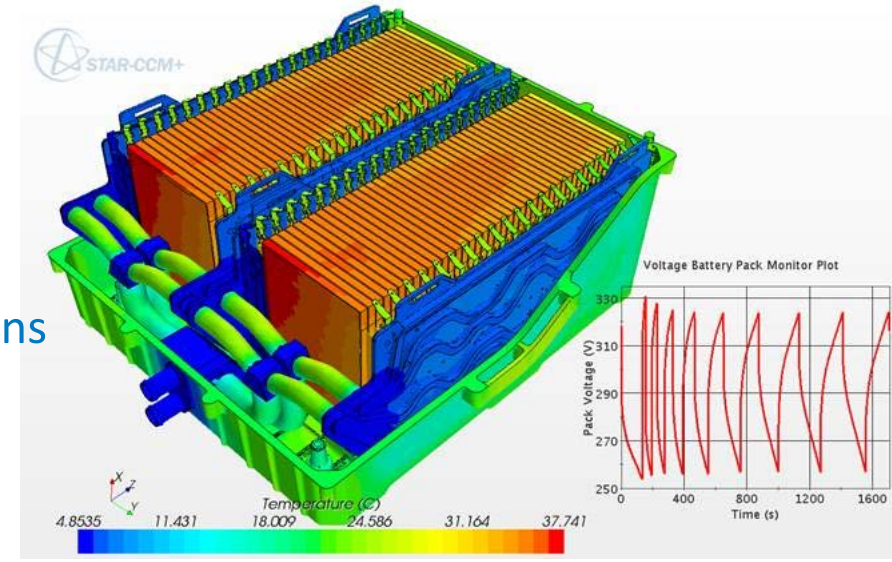
CAD Geometry model




FLUENT simulations

# 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 & electrochemical simulation – Proliferating the use of such methods
  - A staged release of code included in this wide spread CAE tool

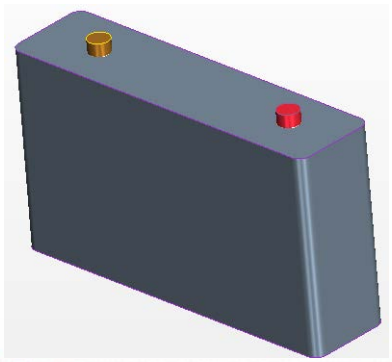


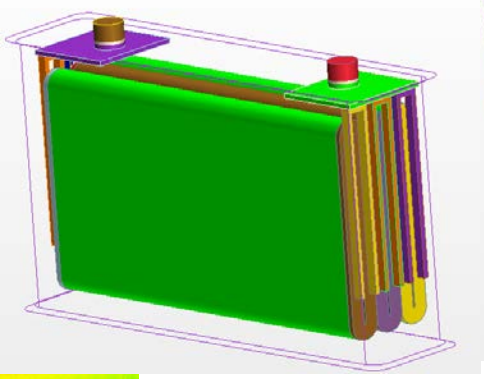

Feature Complete Public Release – March 2013

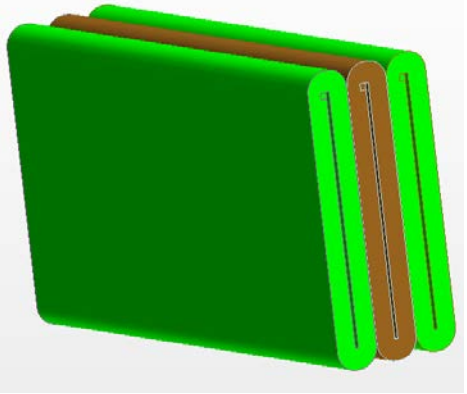
19 months in to the Project

# CD-adapco Technical Accomplishments -1

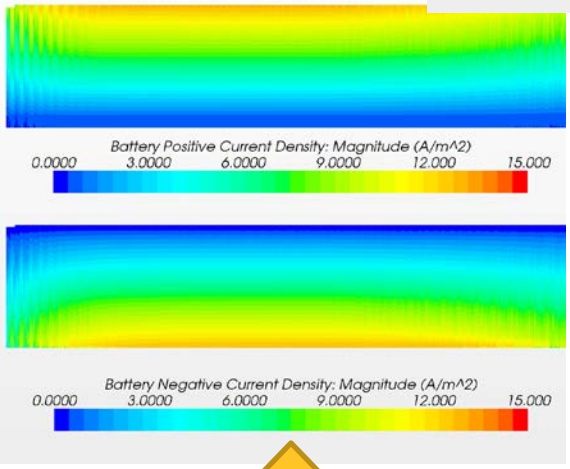
- A detailed electrochemistry model was applied to a wound cell configuration, both at the single cell level and the module level.



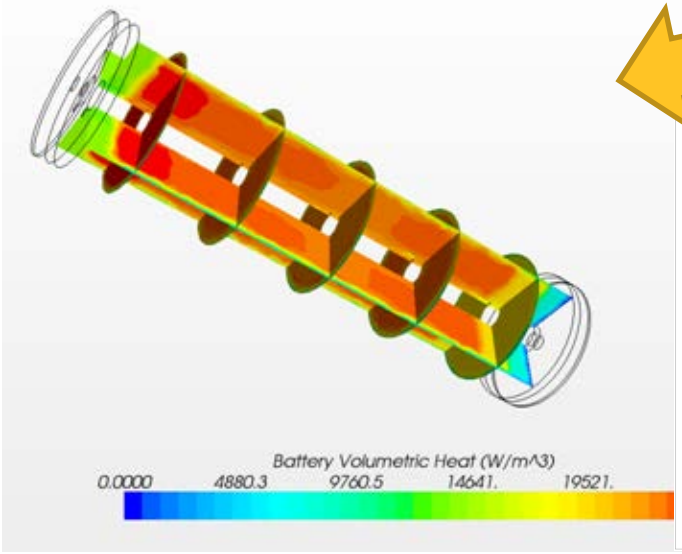




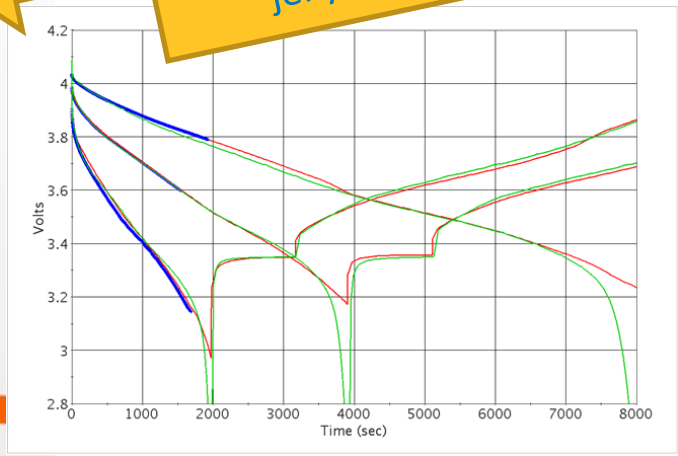
Model construction showing external can, internals and jelly rolls




Unwound prismatic electrodes showing current density

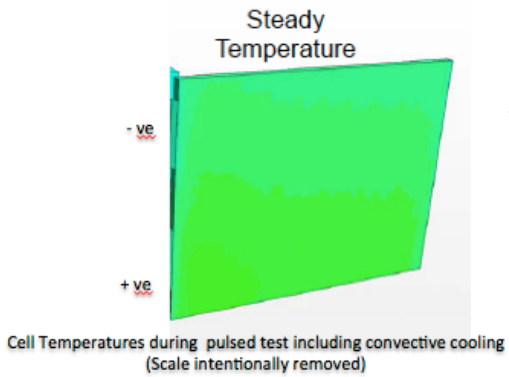



Results of simulations for wound cylindrical jelly roll



# CD-adapco Technical Accomplishments -2

- The created electrochemistry model has been applied to 4 wound cells
  - Johnson Controls inc – Cylindrical VL6P & VL41M
  - Johnson Controls inc – 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

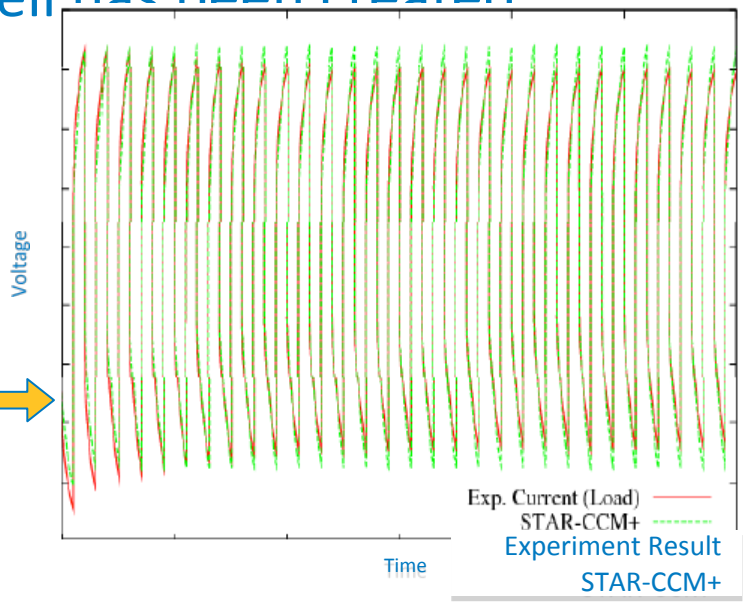


Cell Temperatures during pulsed test including convective cooling
(Scale intentionally removed)

Cell temperatures

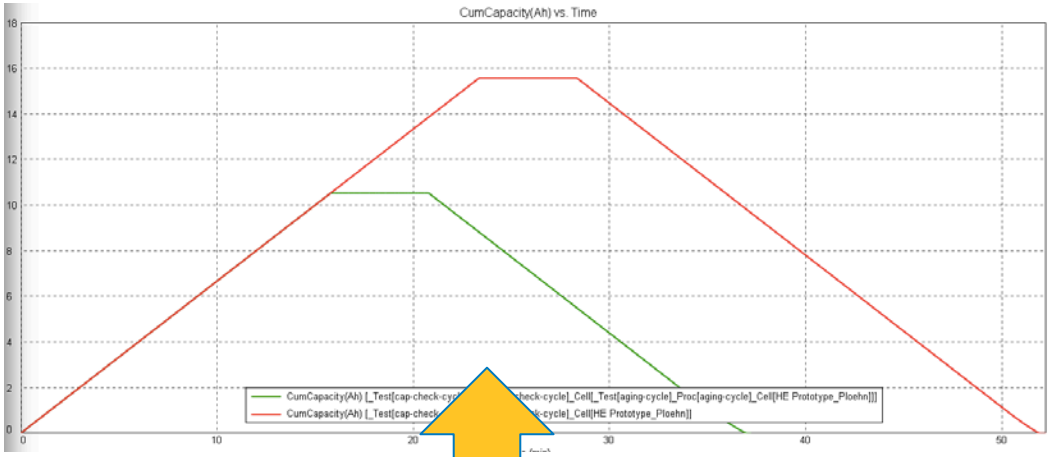
Electrical validation

Pouch experimental work courtesy of A123 Systems



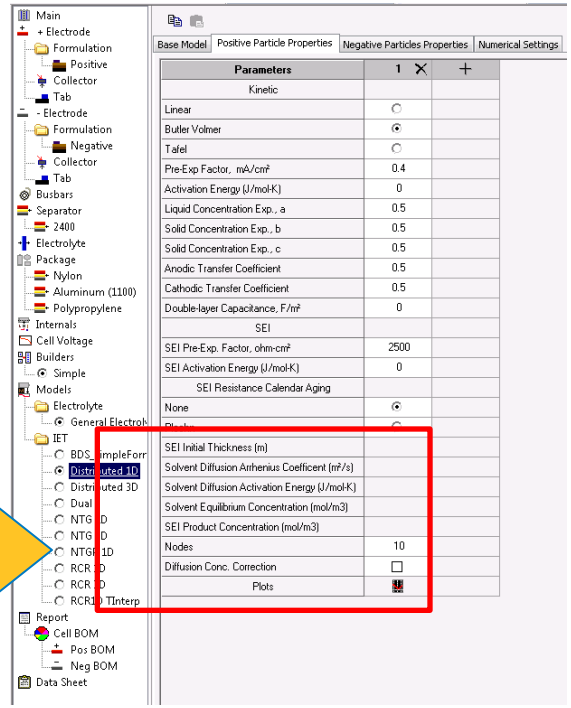
# CD-adapco Technical Accomplishments -3

- A set of electrolyte properties for contemporary electrolytes from INL 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

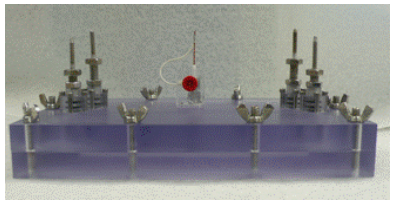


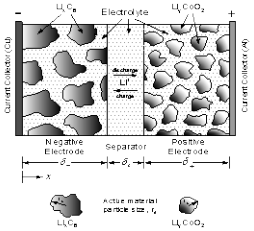

Example of capacity change due to model
Virginal vs 60 weeks @ elevated temp

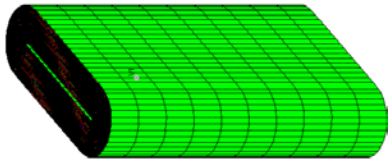
Ageing parameter inputs to model

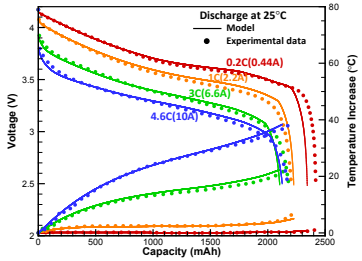


# EC Power Team Project Approach








**Task 1: Materials Characterization** — PENNSTATE

**Task 2: Physico-chemical Models** — EC POWER

**Task 3: Advanced Algorithms** — EC POWER

**Task 4: Experimental Validation** — EC POWER, PENNSTATE

## EC Power Software: **ECT3D**

***Feedback***

Ford · NREL NATIONAL RENEWABLE ENERGY LABORATORY · Johnson Controls

***Suggestions***

- Performance
- Cycle Life
- Safety

# EC Power Technical Accomplishments - 1

- ECT3D v2 delivered to Ford and JCI for cell & pack simulations with following features:
  - 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)

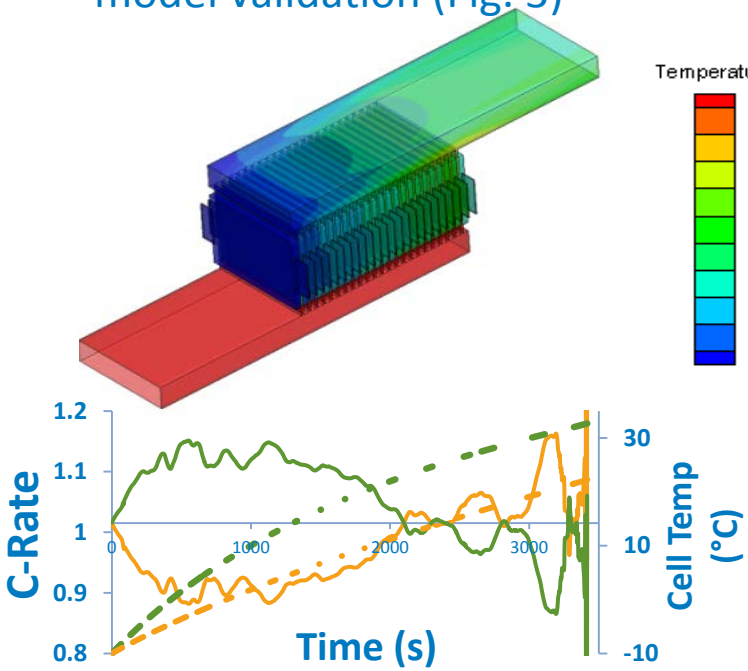



Fig. 1 Thermally driven current imbalance within pack during discharge

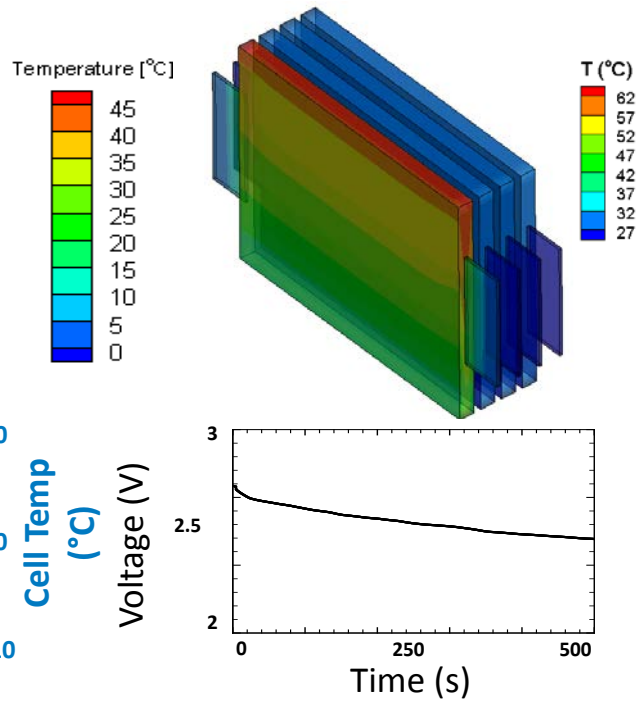



Fig. 2 Preliminary pack safety simulations

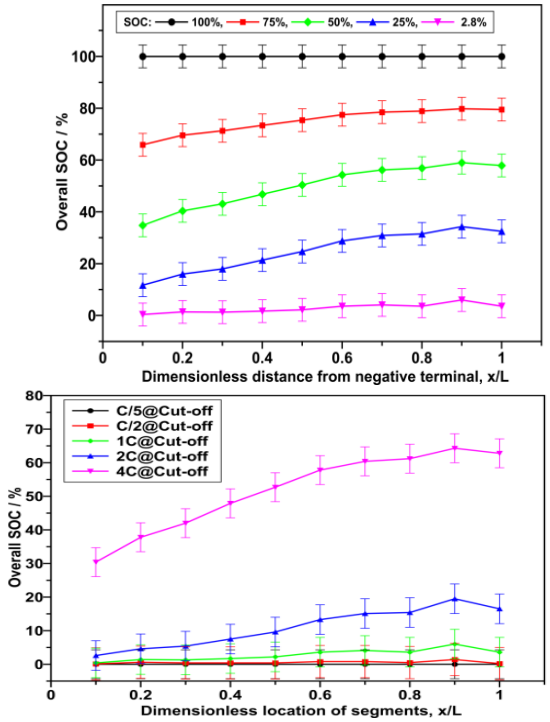



Fig. 3 In-situ data showing non-uniform SOC during discharge

# EC Power Technical Accomplishments - 2

## Tested temperature range for materials

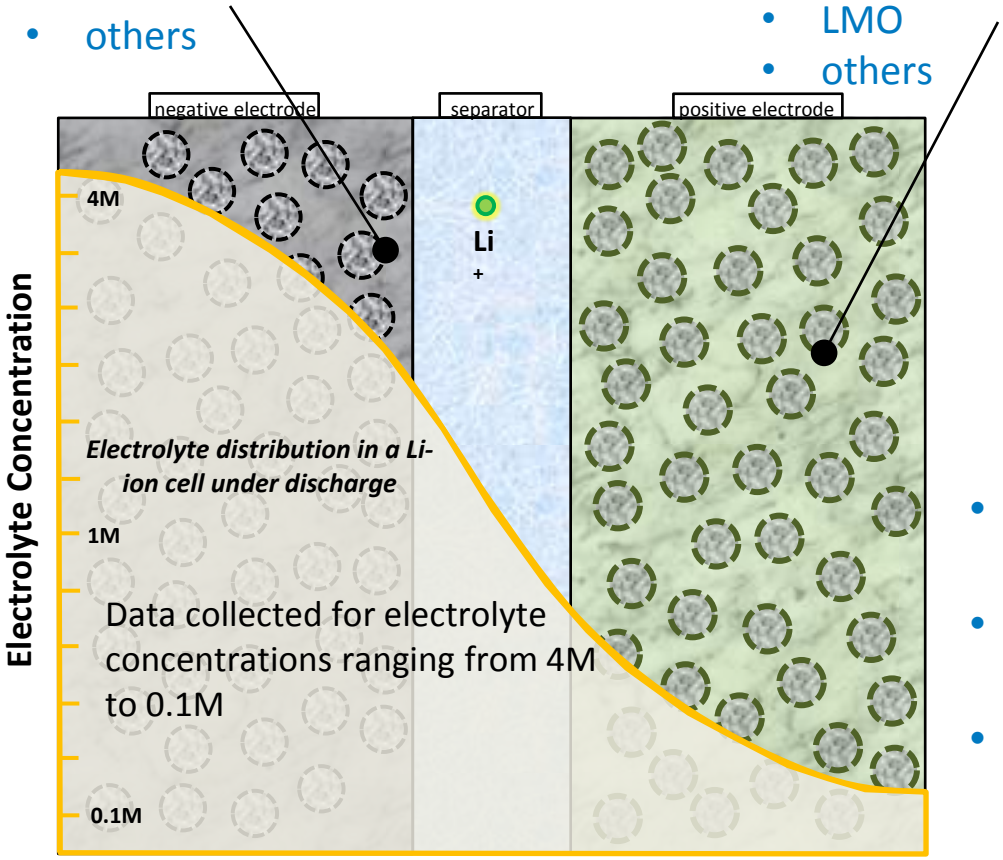
-30°C 100°C

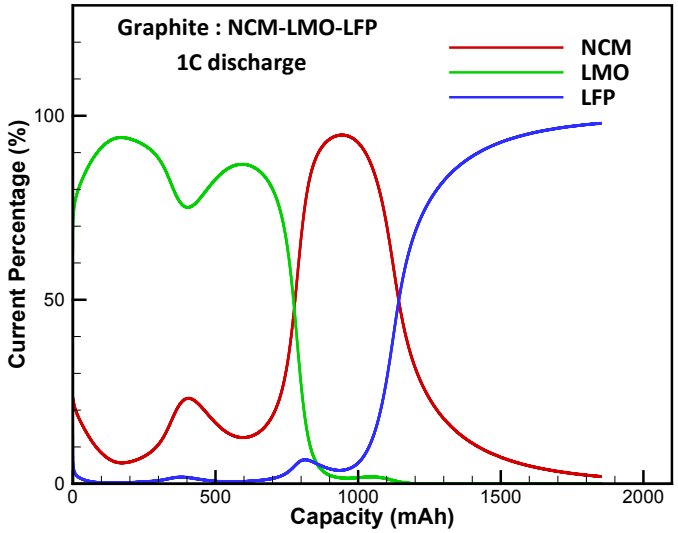
**Anode Materials:**

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

**Cathode materials:**

- NCM
- LFP
- LMO
- others




**Preliminary results for blended active material simulations**

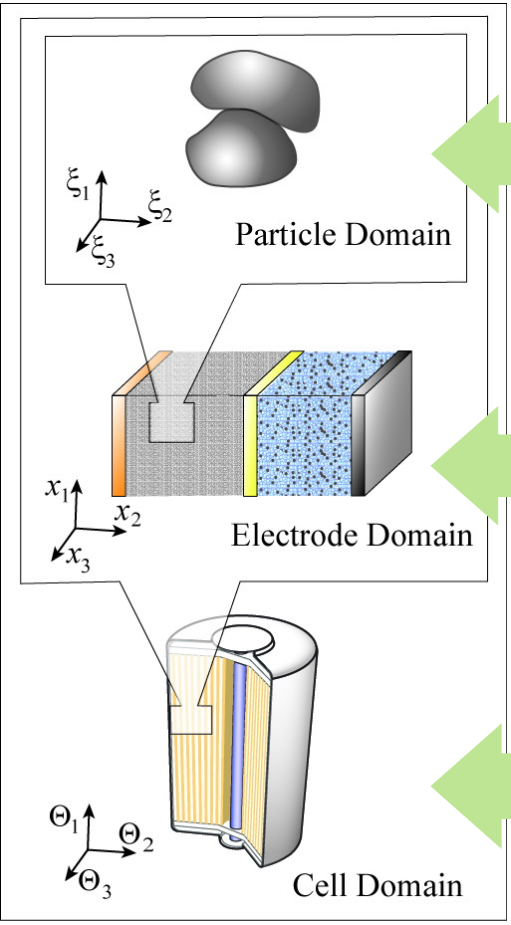
# 100,000+

## 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*

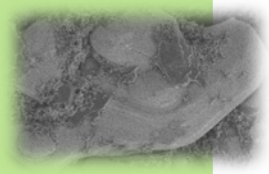



**Particle Domain Submodel Development**

**Solution Models & Method/Algorithms**

*2D cylindrical particle model*

*Reduced Order Method*



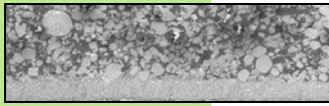
***Examples***

**Electrode Domain Submodel Development**

**Solution Models & Method/Algorithms**

*1D porous electrode model*

*Finite Element Method*



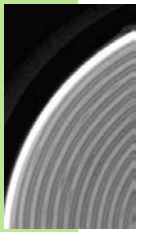
***Examples***

**Cell Domain Submodel Development**

**Solution Models & Method/Algorithms**

*3D wound potential pair continuum (WPPC) model*

***Finite Volume Method***



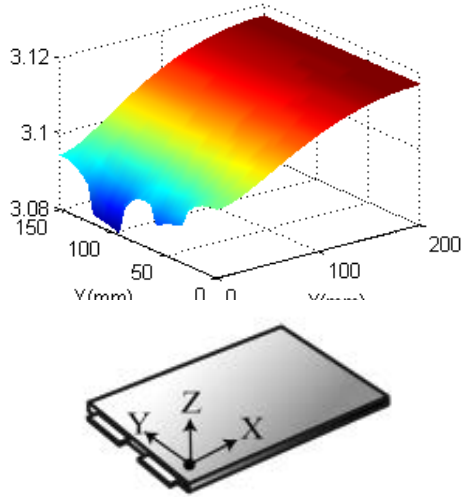
***Examples***

*The modularized framework facilitates collaboration with experts across organizations.*

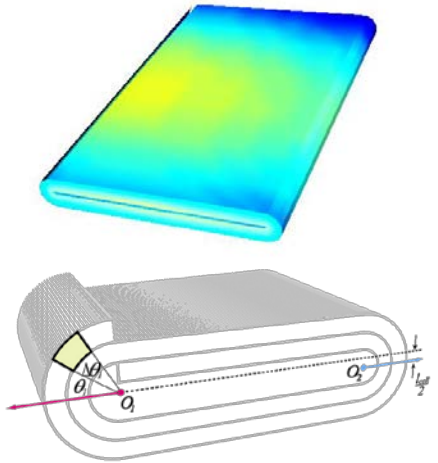
# NREL Technical Accomplishments – 1

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

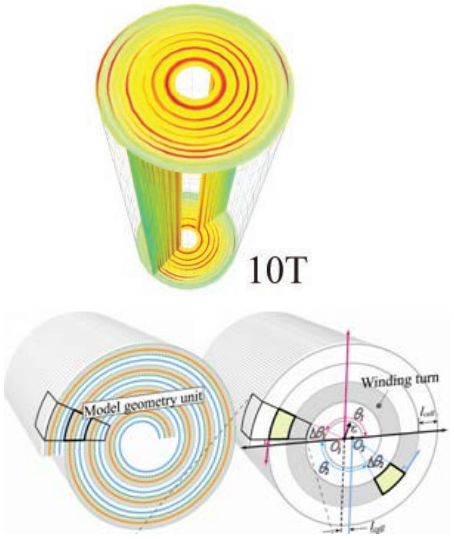
## Stack Pouch



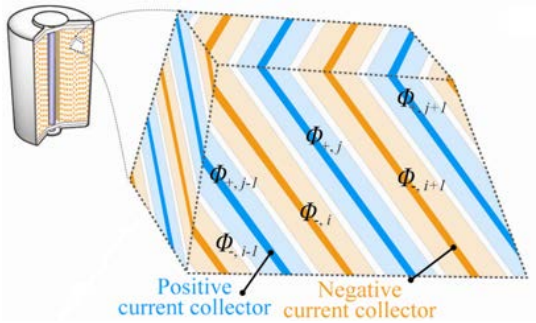

## Wound Prismatic (FY12 Focus)



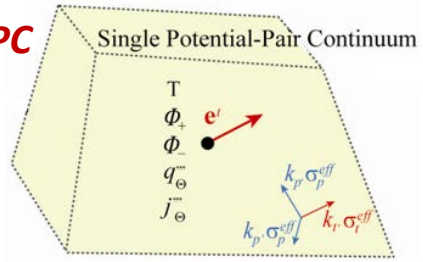
## Wound Cylindrical



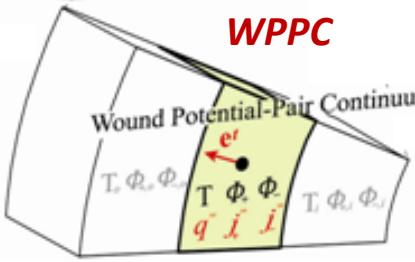

## Orthotropic Continuum Models for Cell Composites




**SPPC**

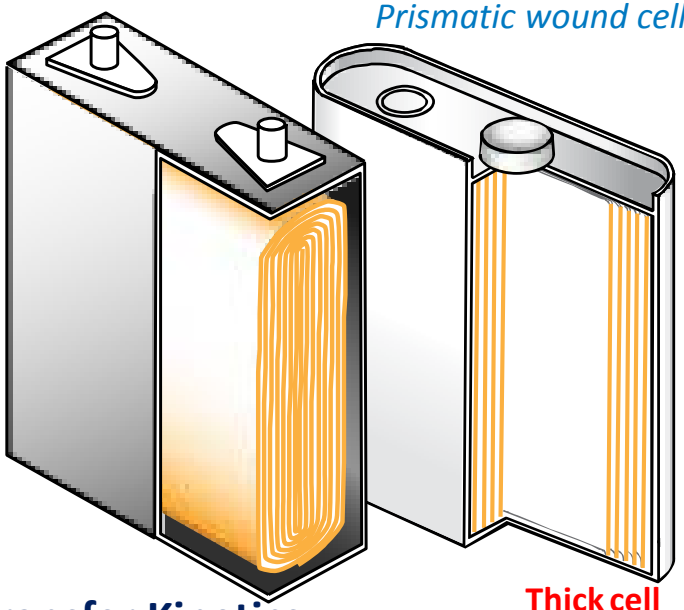


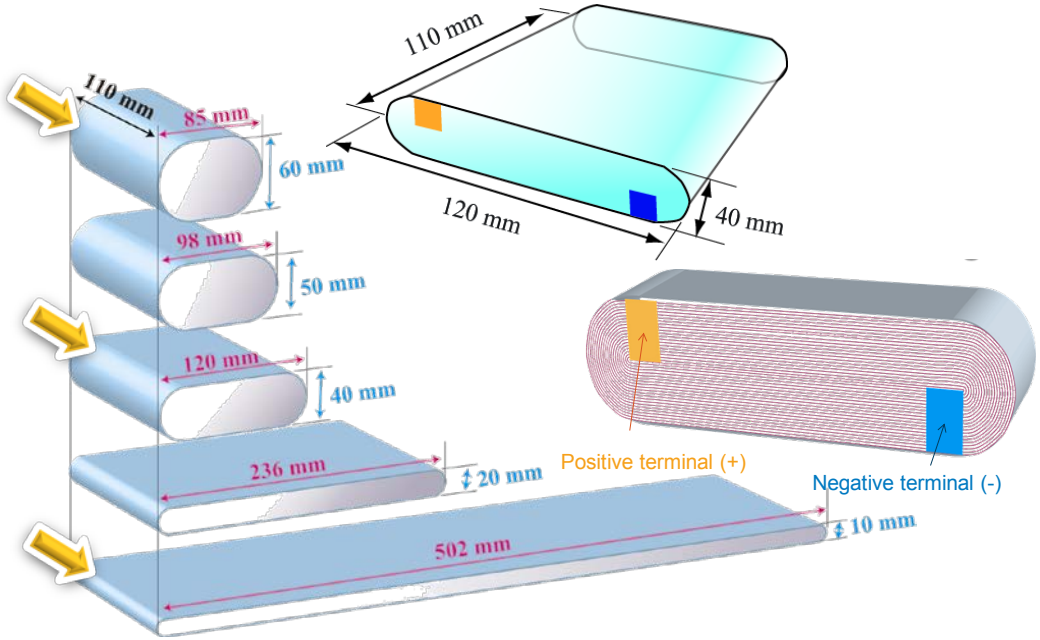

**WPPC**



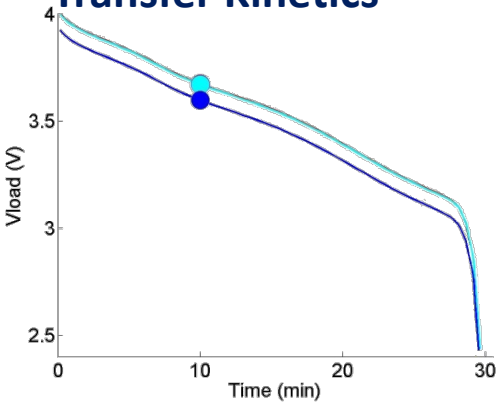
# NREL Technical Accomplishments – 2

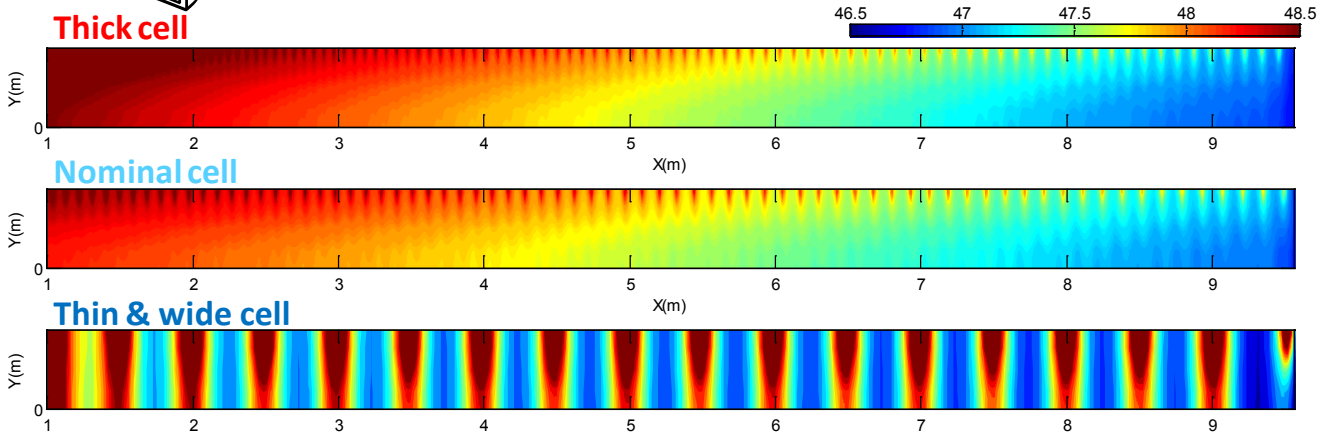
## Developed MSMD Wound Prismatic Cell Model



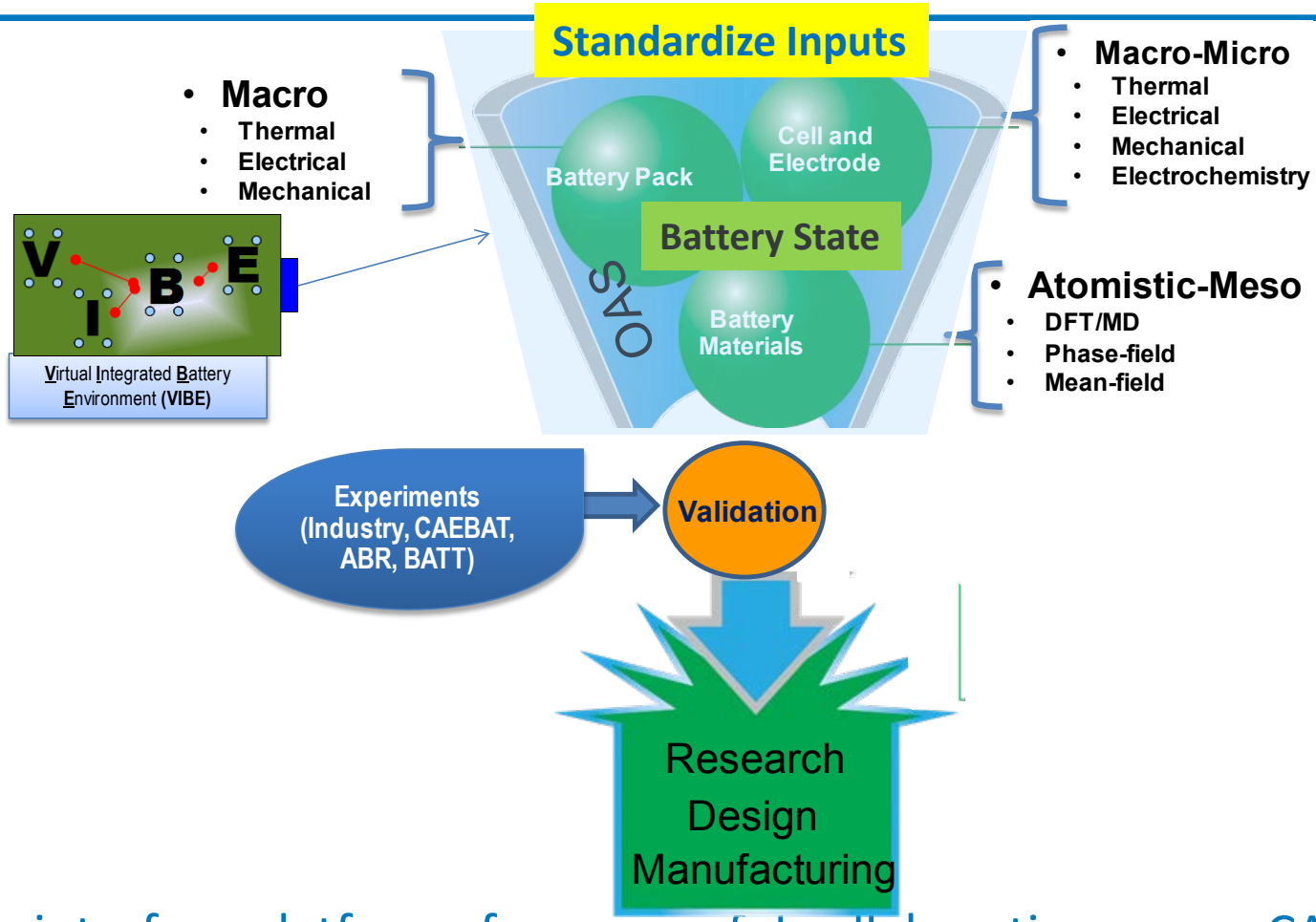

**Transfer Kinetics**




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 of a new version

### OAS

- 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

### VIBE

- Electrochemical-thermal coupling
- Electrochemical-thermal-electrical coupling
- Integrate additional components (NREL models and ANL cost model)
- Demonstrate for complex geometries with new interfaces
- Mechanical

### Standardized Input

- 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)

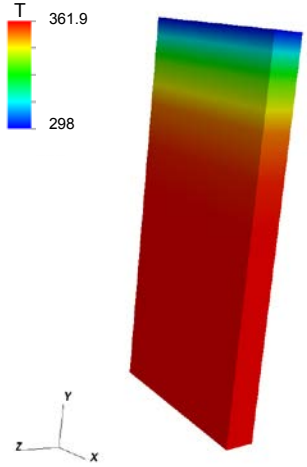
### Battery State

- Define for cell to cell-sandwich coupling
- Define for cell to pack coupling
- Issued version 1

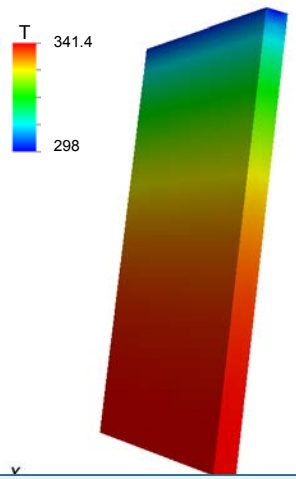
Green – Completed
Blue – Ongoing

# ORNL Technical Accomplishments - 2

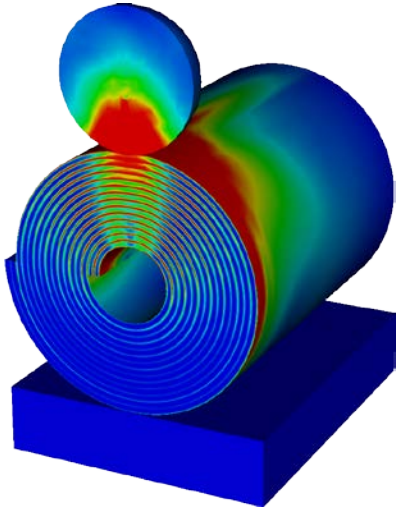
## Coupling various physics at cell level



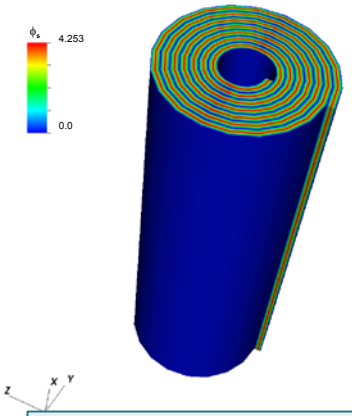

Unrolled Cell (Electrochemical - Thermal)

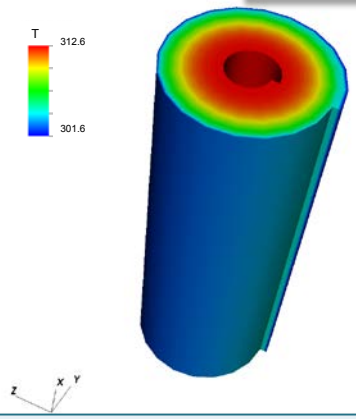



Unrolled Cell (Electrochemical – Thermal - Electrical)

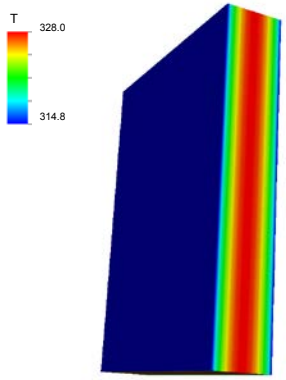


Mechanical Abuse of Cylindrical Cell with Current Collectors Resolved (Electrochemical – Thermal – Electrical – Mechanical)




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

# Summary

- CAEBAT activities consist of three parallel paths:
  - Develop 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 batter models
  - EC Power has released AutoLion™, a comercial version of ECT3D
  - CD-adapco has released its tools for wound spirally 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