Open Architecture Software for CAEBAT

Project ID: ES121

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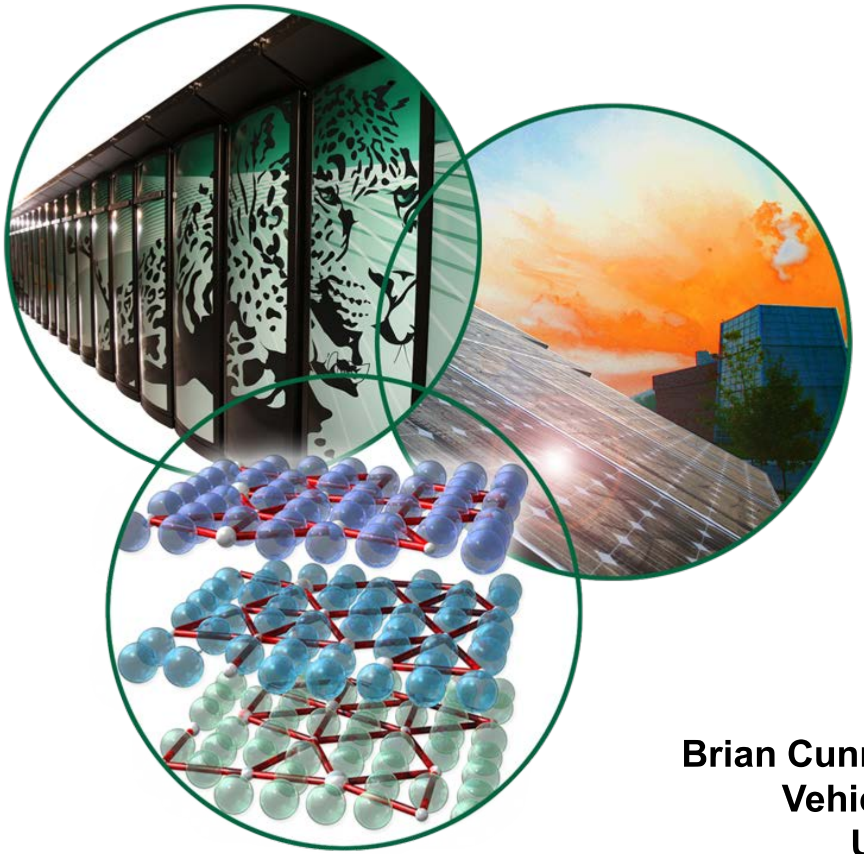


2015 U.S. DOE Hydrogen and Vehicle Technologies Program Annual Merit Review and Peer Evaluation

June 9, 2015

Brian Cunningham and Dave Howell
Vehicle Technologies Program
U.S. Department of Energy

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

Overview

- **Timeline**
  - Start
    - June FY10
  - Finish
    - Sep. 30, 2015
- **Budget**
  - FY14 Funding
    - $700K
  - FY15 Funding
    - $400K
- **Barriers**
  - Predictive battery design tools for optimizing cost, performance and life
  - No standards for battery modeling
  - No common framework for integrating battery modeling efforts
- **Collaborators**
  - NREL
  - CAEBAT Industry Partners
    - CD-adapco Team
    - ECPower Team
    - GM-ANSYS Team
  - Other labs and universities

Objective: Facilitate battery design by integrating battery models within an *open architecture*

- **Provide access to commercial and public software through standardized interfaces and file formats**
  - Enable selecting and combining different modules to solve problems
  - Improve the design process
  - Use different software and vendors
- **Implement the latest numerical methods and algorithms**
- **Verify and Validate models and methods**
  - Enable quantification of uncertainties (analogous to experimental error bars)

Relevance: CAEBAT Program Goals

- Develop software tools to design and model batteries:
  - Four software suites (diversity of approaches, risk mitigation)
    - One from each of the commercial partners (3)
      - May contain commercial or proprietary components
    - Open Architecture Software (OAS) infrastructure
      - Virtual Integrated Battery Environment (VIBE)

- Each suite is fully capable of battery simulations
  - Commercial tools focused on cell and pack models for industry
  - OAS tool integrates commercial and public domain modules for community R&D platform

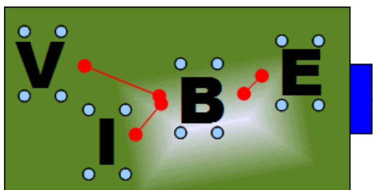
- Coordination and collaboration across teams has been critical to overall success of CAEBAT
  - Standardization of input and of “battery state” database
  - Standard test problem(s)
  - Standardized interfaces for cell, pack, etc. models

Milestones

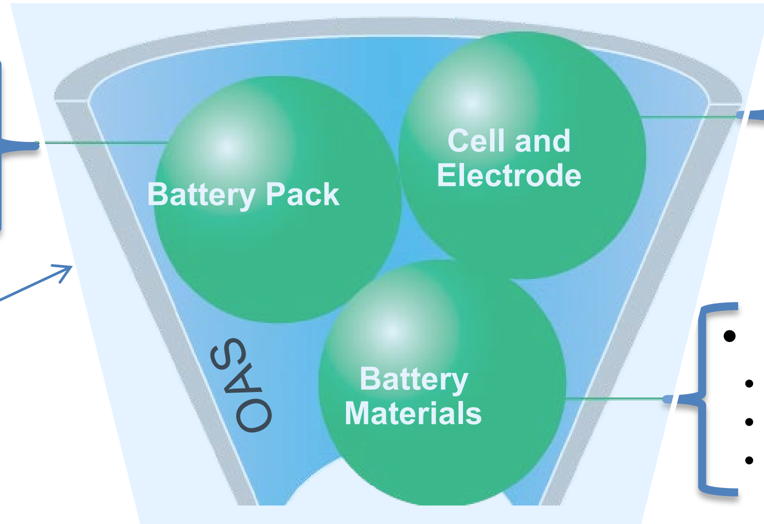
FY 14 Milestones	Due Date	Status
Pack-level thermal, electrical and electrochemical simulation	12/31/2013	Completed
Demonstrate robust integration of thermal with electrochemistry through advanced coupling algorithms	3/31/2014	Completed
Demonstrate coupling using various combinations of components from project partners	6/30/2014	Completed
User Environment V1 Software Release and Documentation	9/30/2014	Completed
FY 15 Milestones		
Documentation along with use cases of OAS, VIBE, BatML, and ICE.	12/31/2014	Completed
Install a bug tracker and clear all reported bugs.	3/31/2015	Completed
Easy-to-use website with distribution of OAS, VIBE, BatML, ICE, translators, examples, documentation, etc.	6/30/2015	Completed
Integrate components from CAEBAT-II projects into OAS.	9/30/2015	Ongoing

Approach (1): CAEBAT Open Architecture Software (OAS) Vision – A Virtual Test Bed

- **Macro**
  - **Thermal**
  - **Electrical**
  - **Mechanical**



Virtual Integrated Battery Environment (VIBE)



- **Macro-Micro**
  - **Thermal**
  - **Electrical**
  - **Mechanical**
  - **Electrochemistry**

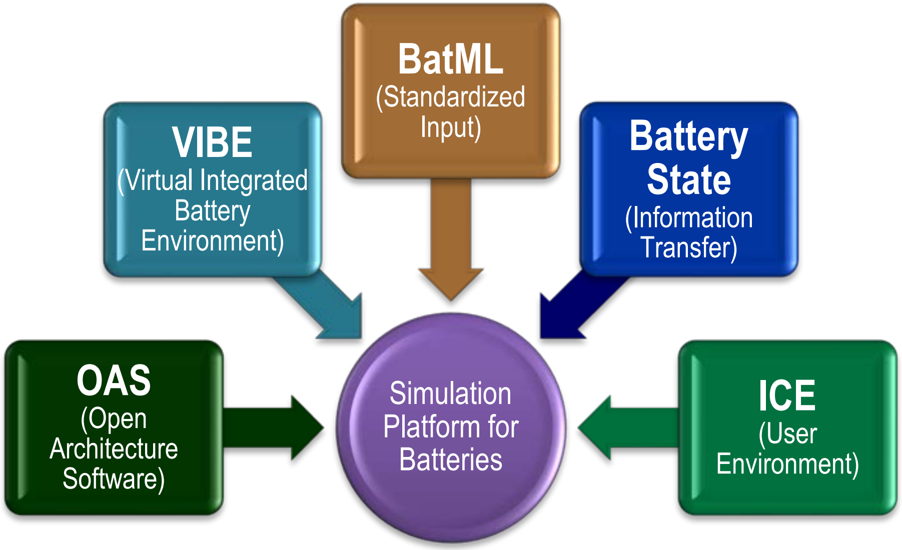
- **Atomistic-Meso**
  - **DFT/MD**
  - **Phase-field**
  - **Mean-field**

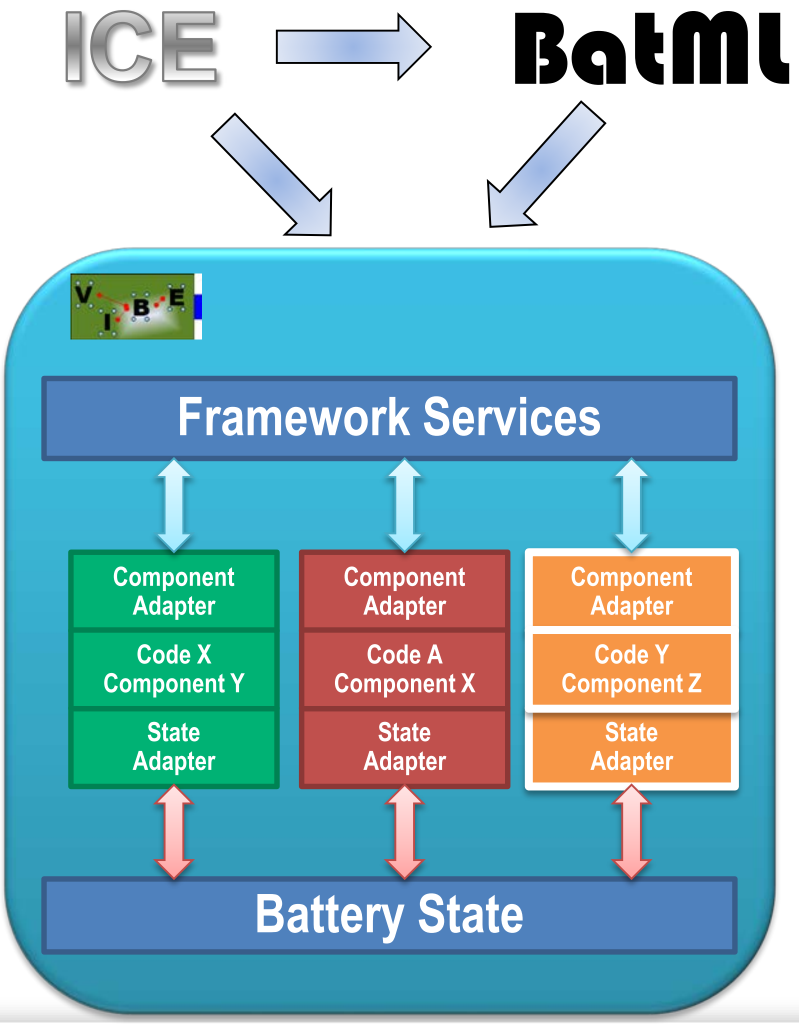
Experiments (ABR, BATT, Industry) → **Validation**

CAEBAT-I: Focus on Cell and Module and now Pack

CAEBAT-II: Focus on Cell and below (electrode, SEI, thermo-electro-chemistry)

Approach (2): Components of fully integrated simulation platform for Batteries





The CAEBAT simulation platform achieves multiple goals:

- Community software infrastructure
- Standardization to enhance leveraging
- Usability and re-use
- Scale bridging
- Scalability to many cores

Main Project Tasks

- **OAS**: Light-weight computational framework to integrate the different components
- **VIBE**: Various combinations of the components to simulate different cell and battery physics
- **BatML**: Standardize the input for cross-component compatibility and increase productivity
- **Battery State**: Standardize the transfer of information between the components
- **ICE**: A graphical workflow for BatML editing, solver setup, job launch and analysis
- Distribution, Maintenance, and support
- All the above yield a robust and user friendly CAEBAT simulation platform

Technical Accomplishments/Progress

OAS
- Capability is online
- Optimization tools
- Portable to Linux, Mac, and Windows
- Interfaces to the inputs and battery state standards
- Flexible coupling of the models using files and computer memory

VIBE
- Electrochemical, Electrical, Thermal and Mechanical
- Cell to Cell-sandwich Coupling
- Cell-sandwich to Cell to Module Coupling
- Integrated various components
- Cell-sandwich to Cell to Module Coupling to Pack Coupling
- Production Release to Users
- Maintenance and support/outreach

Standardized Input (BatML)
- Data format that is able to describe existing battery models and support new developments.
- XML database and corresponding schemas
- Issued version 2
- Translators
- Error-checking
- Units conversion

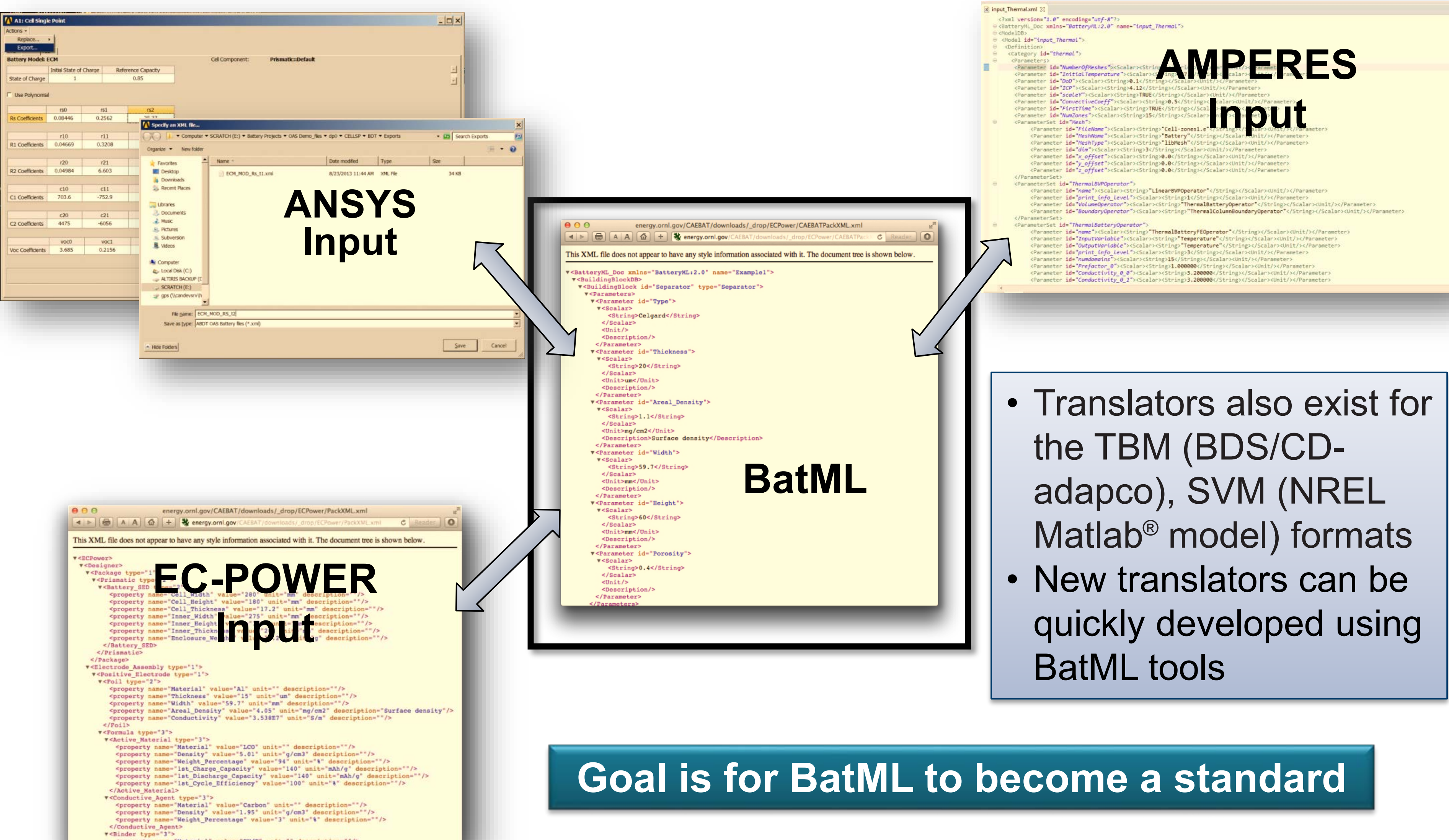
Battery State
- Defined and tested for cell to cell-sandwich coupling
- Defined and tested for cell to module coupling
- Defined and tested for module to pack coupling
- Issue version 2

ICE User Environment
- Job-launch of OAS
- Initial post-processing
- Initial edits of BatML XML files
- Graphical feedback

Green – Completed
Blue – Ongoing

Technical Accomplishments

Battery Markup Language (BatML): Model Exchange



- Translators also exist for the TBM (BDS/CD-adapco), SVM (NREL Matlab® model) formats
- New translators can be quickly developed using BatML tools

Goal is for BatML to become a standard

Battery state file

- **Serves as data conduit between components**
- **Contains the minimal set of variables required to enable components to communicate**
- **CGNS format has been selected (for all mesh-based data)**
  - http://en.wikipedia.org/wiki/CGNS

Species concentration in the electrolyte:

$$\frac{\partial(\varepsilon_e c_e)}{\partial t} - \nabla.\left(\varepsilon_e D_e^{eff}(\varepsilon_e)\nabla c_e\right) - \frac{1-t_+^0}{F} j^{Li} = 0$$

Species concentration in the solid phase:

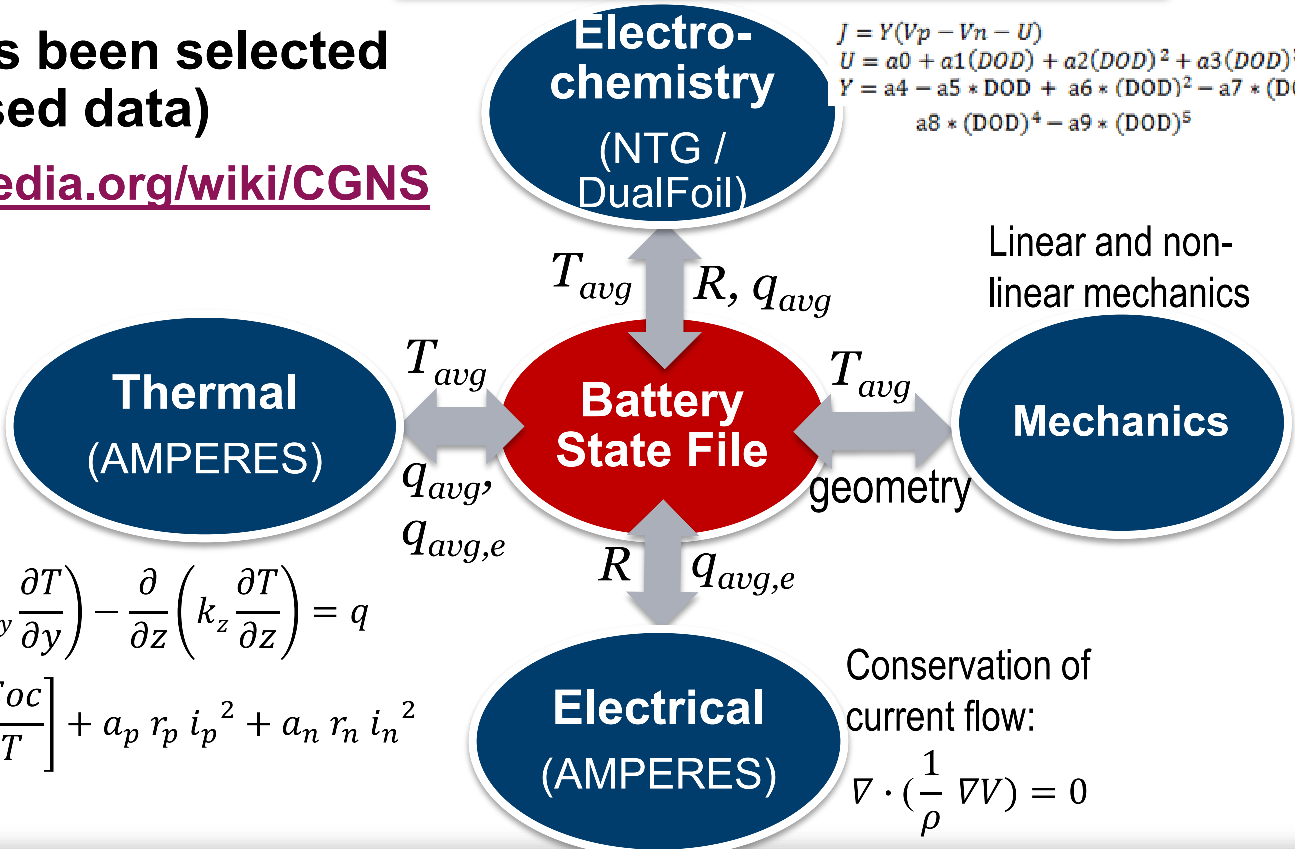
$$\frac{\partial(\varepsilon_s c_s)}{\partial t} - \nabla.\left(\varepsilon_s D_s^{eff}(\varepsilon_s)\nabla c_s\right) + \frac{j^{Li}}{F} = 0$$

Electrolyte Potential:

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

Electrode Potential:

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



$$J = Y(Vp - Vn - U)$$

$$U = a0 + a1(DOD) + a2(DOD)^2 + a3(DOD)^3$$

$$Y = a4 - a5 * DOD + a6 * (DOD)^2 - a7 * (DOD)^3 + a8 * (DOD)^4 - a9 * (DOD)^5$$

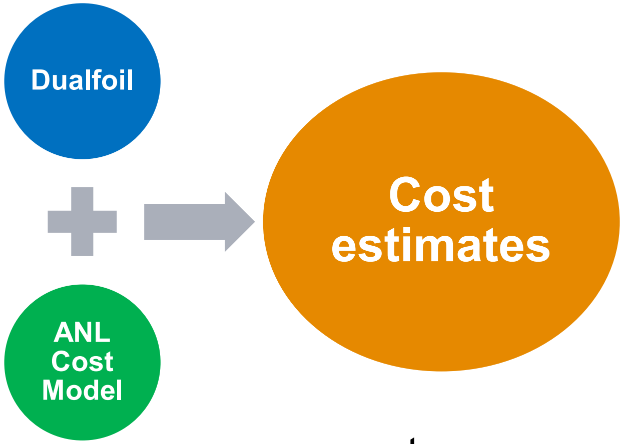
$$\nabla \cdot \left(\frac{1}{\rho}\nabla V\right) = 0$$

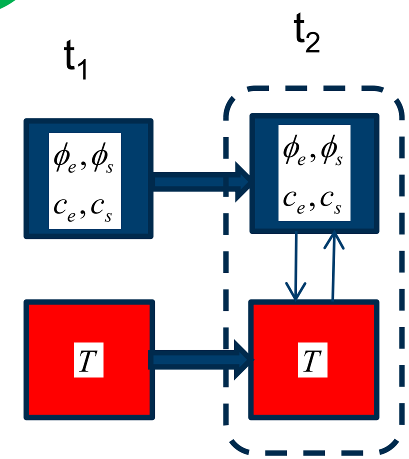
$$\rho Cp \frac{\partial T}{\partial t} - \frac{\partial}{\partial x}\left(k_x \frac{\partial T}{\partial x}\right) - \frac{\partial}{\partial y}\left(k_y \frac{\partial T}{\partial y}\right) - \frac{\partial}{\partial z}\left(k_z \frac{\partial T}{\partial z}\right) = q$$

$$\text{where} \quad q = aJ\left[E_{oc} - E - T\frac{\partial Eoc}{\partial T}\right] + a_p\, r_p\, i_p^{\,2} + a_n\, r_n\, i_n^{\,2}$$

Open Architecture Software (OAS)

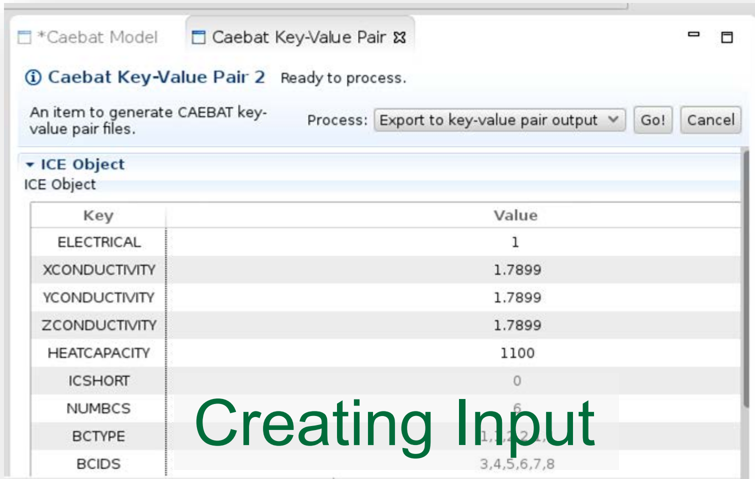
- **Porting to Windows is complete**
  - Now being merged and prepared for public release
- **Integration with ANL cost model is complete**
  - Can use simulation data to drive the cost model
- **We added computational design optimization capability**
  - Demonstrated by investigation of optimal battery tab placement (AMPERES) and optimal electrode thickness for power/energy balance (EC-Power)
  - Model generation is a part of the simulation workflow
- **Two-way tight coupling improves accuracy and ability to perform more difficult analyses**
  - Enforces consistency between thermal and electrochemical components

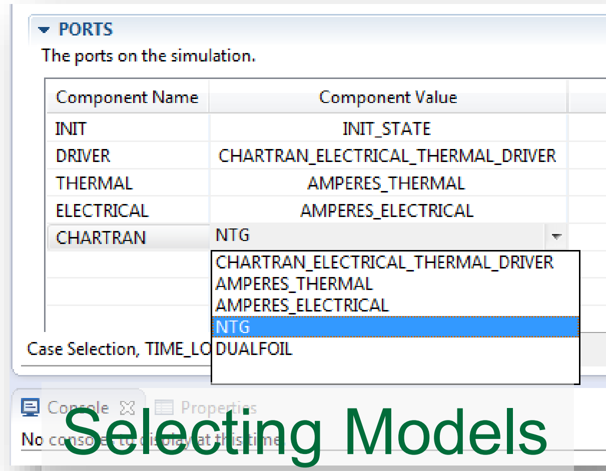




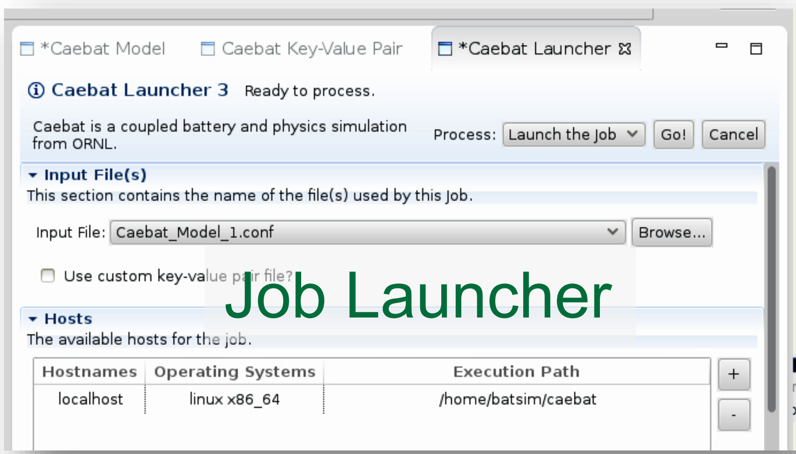
Picard Method:
self-consistent iterations to prescribed convergence criterion

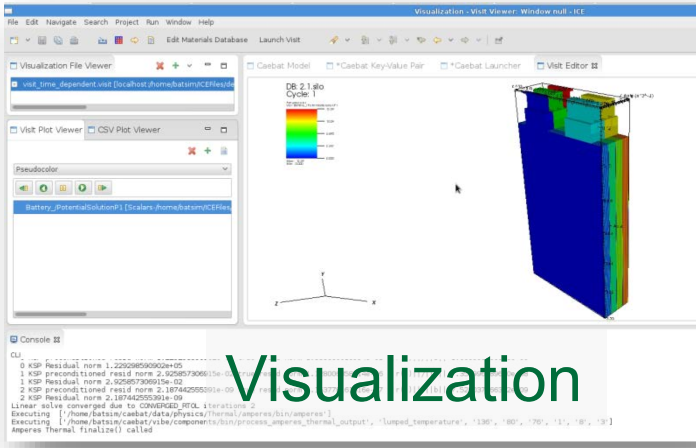
ICE – Provides user environment for battery analysis for VIBE





ICE

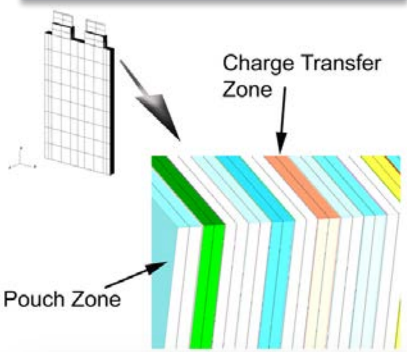


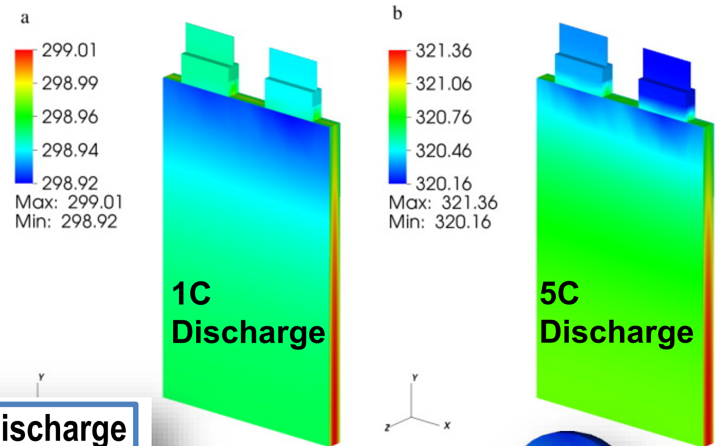


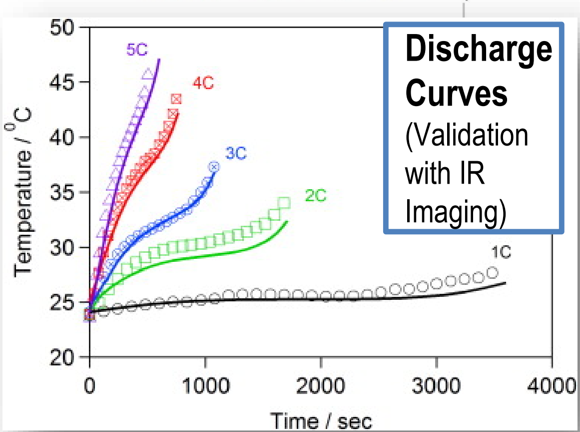
VIBE Results - Recap

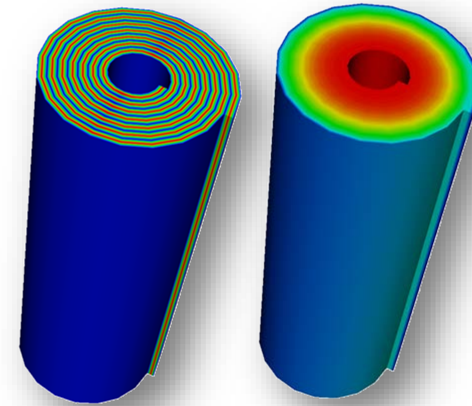
Technical Accomplishments

Detailed 3D Modeling

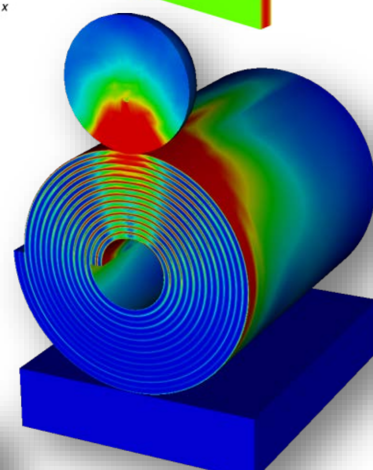




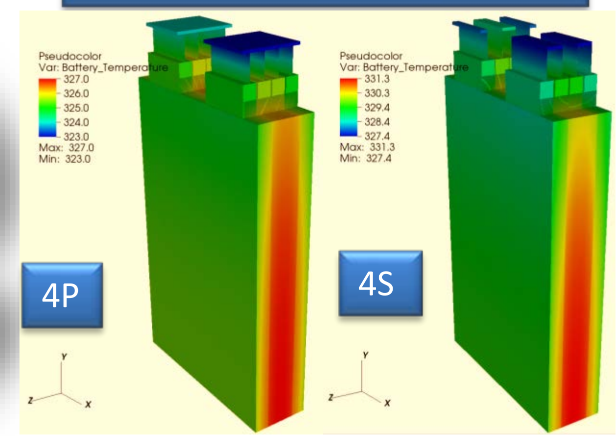




Cylindrical Cell with Current Collectors Resolved (Electrochemical – Thermal - Electrical)



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



Temperature in 4P and 4S Module with Fully Coupled Electrochemical, Electrical and Thermal Simulations in CAEBAT OAS / VIBE

ELSEVIER

Journal of Power Sources

Available online 24 August 2013

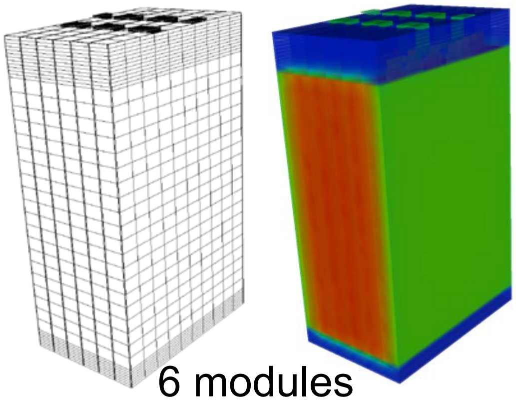
In Press, Accepted Manuscript — Note to users

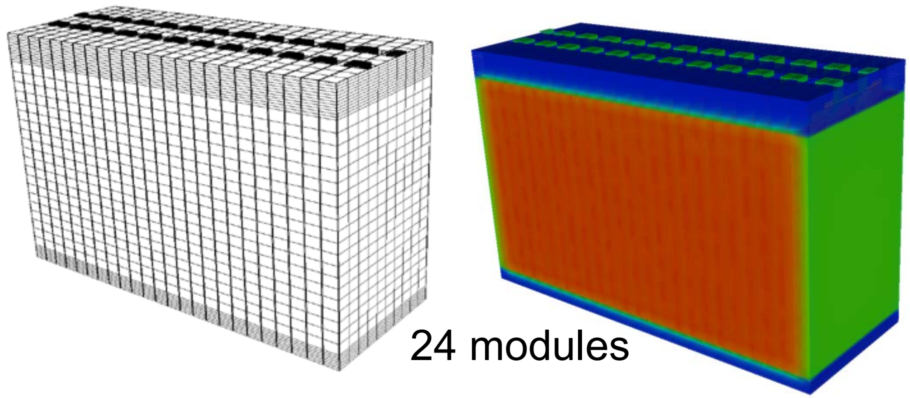
A new open computational framework for highly-resolved coupled 3D multiphysics simulations of Li-Ion Cells ☆

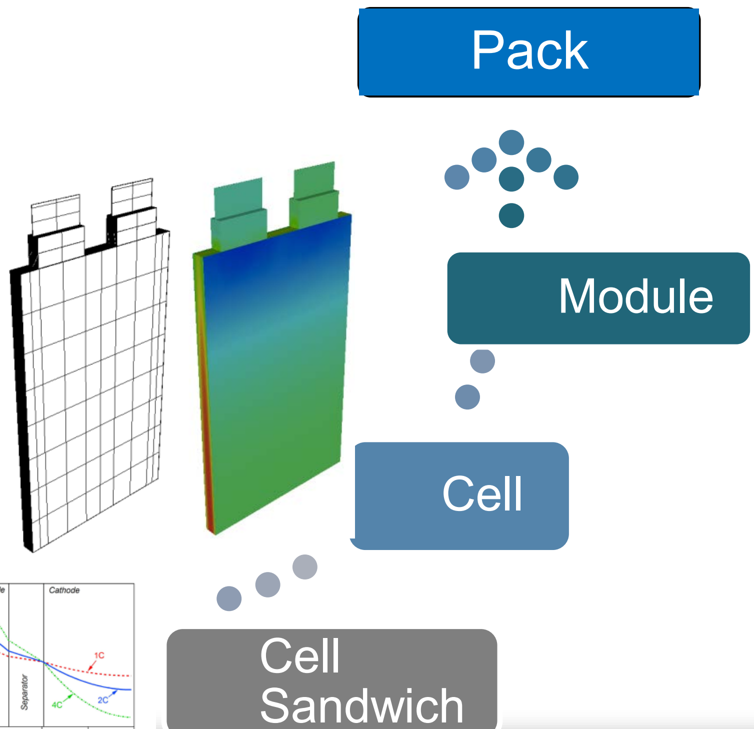
Srikanth Allu, Sergiy Kalnaus, Wael Elwasif, Srdjan Simunovic, John Turner, Sreekanth Pannala

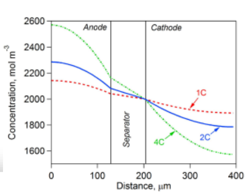
Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, TN-37831

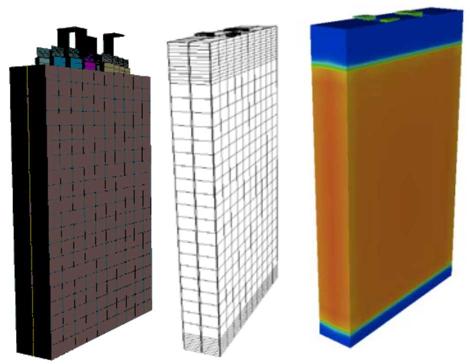
VIBE – Facilitates Hierarchical Process to Construct Battery Packs









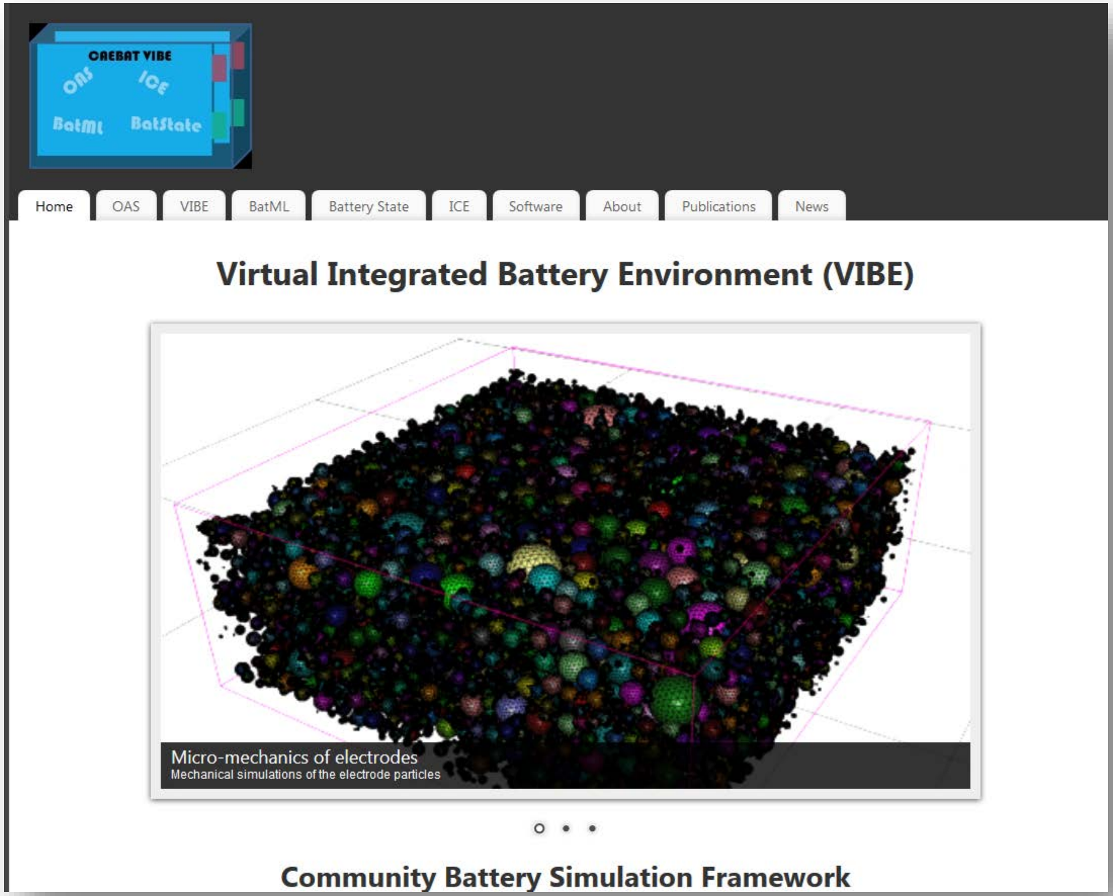


- Current module has 2 cells in series and 2 cells in parallel (similar to Nissan-Leaf)
- Each Cell has 17 cathode layers with 33 Ah capacity
- Dimensions ≈ 290mm × 210mm × 6mm
- Coarsest mesh for each module has ½ million degrees of freedom

Advantages

- Test models sequentially
- Ability to stack cells and modules in series and parallel
- Both module and pack simulations can be performed
- Simulations can be distributed across multiple processors

VIBE Release – Via Website (http://batterysim.org/)



- OAS/VIBE has been deployed and is available from http://batterysim.org/
- Can be downloaded in a Virtual Machine as an ova file (no installation required)
- Separate binaries can be downloaded and installed as well
- Users mailing list has been created for updates and support
- Release document can be downloaded from the same website

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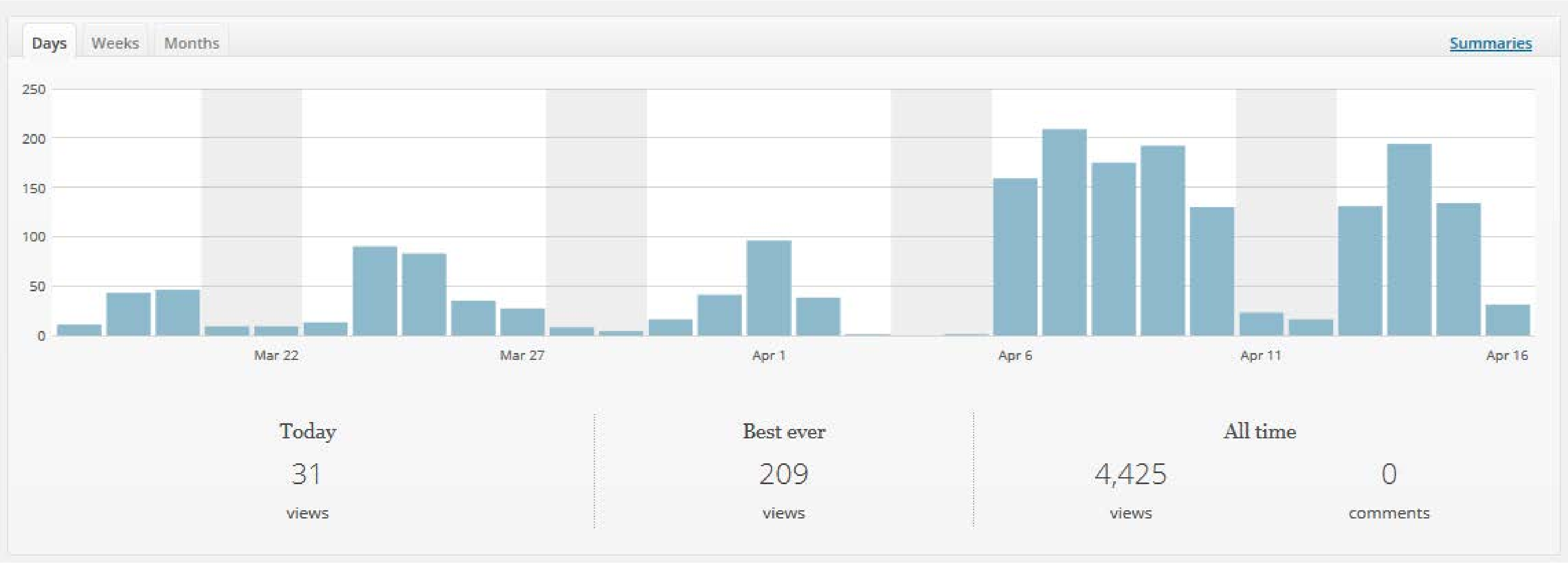
VIBE – Website Statistics

Technical Accomplishment



Typical weekday web traffic between 50-200

VIBE – Download Statistics

Technical Accomplishment

- ~ 100 downloads since December
- Downloads from all over the world from labs, academia, and industry. Some of the institutions are listed below:

Lockheed Martin	Stanley Black & Decker	Georgia Tech
Ford Motor Company	BASF Corporation	Iowa State University
Bosch, LLC	Saft America	University of Maryland
Honda R&D Co, Ltd	EMF1v	University of Michigan
Samsung Electronics	Pan Asia Technical Automotive Center	Purdue University
Virtual Vehicle Research Center	CEA – Commissariat Energie Atomique	North Carolina State University
Zee Aero	Northeastern University	University of Dayton
IK4-CIDETEC	Washington University	University of Nevada, Las Vegas
Institute for Energy and Environmental Research, Heidelberg, GmbH	TU Muenchen	SAIT Polytechnic

VIBE in the News – part of the outreach

Green Car Congress

Energy, technologies, issues and policies for sustainable mobility

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Print this post

ORNL VIBE open-architecture framework for improved EV battery design

6 April 2015

As part of the US Department of Energy's (DOE) CAEBAT (Computer Aided Engineering for Batteries) activities (earlier post), scientists at Oak Ridge National Laboratory (ORNL) have developed a flexible, robust, and computationally scalable open-architecture framework that integrates multi-physics and multi-scale battery models.

VIBE provides an open architecture framework for pre-experimental design simulation as part of the CAEBAT program. Click to enlarge.

The Virtual Integrated Battery Environment (VIBE) allows researchers to test lithium-ion batteries under different simulated scenarios before the batteries are built and used in electric vehicles. The physics phenomena of

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News

Battery boost

Wed, 03/25/2015 - 8:14am

by Christopher R. Samoray, Oak Ridge National Laboratory

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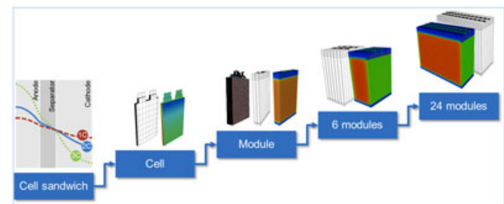

The VIBE simulation tool provides great flexibility in designing batteries all the way from cell components to full battery pack.

Rechargeable lithium-ion batteries are commonly found in portable electronics such as cell phones and notebook PCs. They're also gaining popularity in electric vehicles, where their compact, lightweight build and high-energy storage potential offers a more efficient and environmentally safe alternative to nickel metal hydride and lead-acid batteries traditionally used in vehicles.

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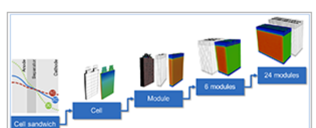
BATTERY BOOST

ORNL computing software aims to help electric vehicle industry better design high-performing and safe lithium-ion batteries through simulation

Rechargeable lithium-ion batteries are commonly found in portable electronics such as cell phones and notebook PCs. They're also gaining popularity in electric vehicles, where their compact, lightweight build and high-energy storage potential offers a more efficient and environmentally safe alternative to nickel metal hydride and lead-acid batteries traditionally used in vehicles.

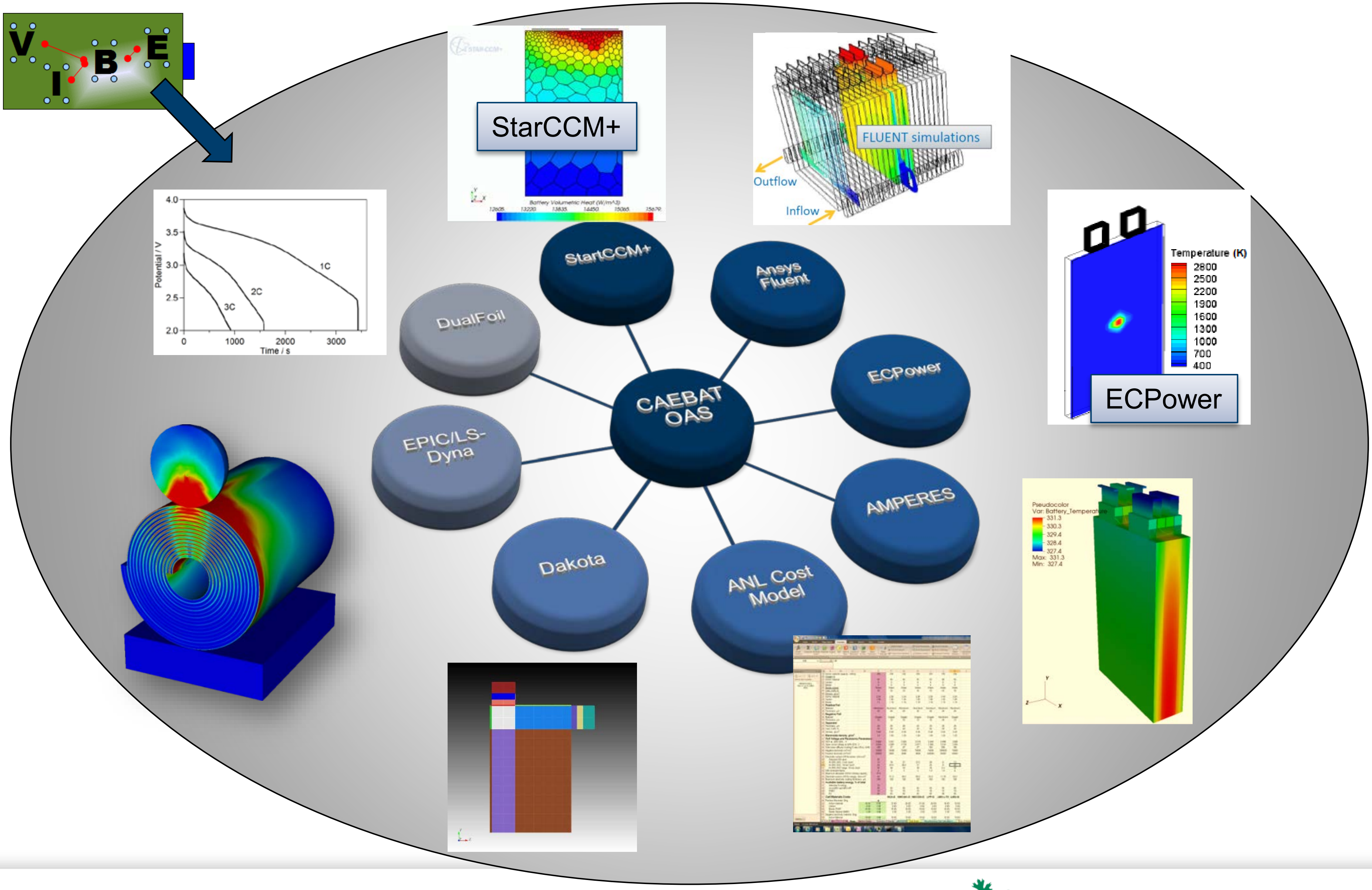


The VIBE simulation tool provides great flexibility in designing batteries all the way from cell components to full battery pack. (hi-res image)

Scientists at the Department of Energy's Oak Ridge National Laboratory have developed modeling software to help other researchers and battery manufacturers improve the design of lithium-ion batteries for electric vehicles. The modeling tool, known as the Virtual Integrated Battery Environment, or VIBE, will allow researchers to test lithium-ion batteries under different simulated scenarios before the batteries are built and used in electric vehicles.

http://insideevs.com/vibe-allows-researchers-test-electric-car-batteries-simulated-scenarios/

VIBE Computational Ecosystem: Coupling open and proprietary components

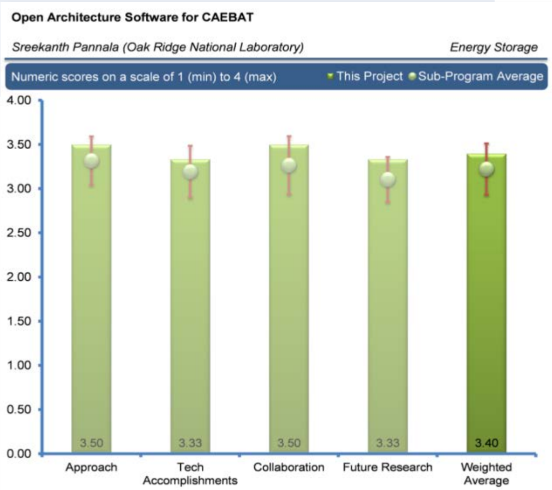


Collaboration and Coordination

- Monthly telecon/web-meeting with DOE and NREL
- Interactions with SNL to bring in their modeling capabilities into VIBE/OAS (CAEBAT-II)
- Interactions with U. Michigan to bring in their modeling capabilities into VIBE/OAS
- Graduate students from U. Michigan, Texas A&M, UC Davis, and Colorado School of Mines (CAEBAT-II)
- Reaching out to OEMs (Ford) and Battery Manufacturer (through an ARPA-E grant)
- Interaction with NHTSA on safety simulations
- Made links to several Office of Science (Applied Math) and ARPA-E efforts

Response to previous review comments

AMR 2014 Review Comments	Response
“to this reviewer it is not clear why there was a need to integrate different battery models”.	Integration of battery models and codes from different partners was an essential part of this project in order to provide user with flexibility in choice suitable for particular device or system.
“It was not clear how difficult this [software] will be for users to learn and operate” “… few written documents had been produced to demonstrate the capabilities …”	Extended release manual was supplied with the recent release. Positive feedback from users indicates that they are able to install and use the product. Users group email list was created to respond to requests.



Response to previous review comments

AMR 2014 Review Comments	Response
"… no solid accomplishment examples on integration of models"	ORNL was tasked to provide the infrastructure for integration and only now we are working towards different use cases and validation. The NHTSA project on mechanical abuse and ARPA AMPED project are good examples of applying the integrated models to practical scenarios
"reviewer pointed out that $700,000 per year seemed excessive for integration effort. Some of the resources should be used to benchmark various battery models"	The effort included integration of models as well as development of AMPERES 3D code for electrochemical solution. Different coupling strategies were implemented and a set of defined problems (pouch, cylindrical cell geometries, modules and packs) was generated. Cell level simulations (prismatic cell) were validated by experiment..

Future Work - Planned Activities

- Near term (FY15)
  - OAS
    - Compatible with at least some components of all CAEBAT partner products
  - VIBE
    - Revisions based on community feedback
  - BatML
    - Revisions based on community feedback
    - Additional translators as necessary
  - Battery State
    - Revisions based on community feedback
  - ICE
    - Revisions based on community feedback
    - Refined BatML editing with focus on usability
- Longer term
  - Community adoption
  - Support and maintenance
  - Adding new features

Summary

- We have developed an open architecture software for file-based coupling of electrochemistry, transport, electrical and mechanical stress model.
- We developed method and data model for defining the battery state in battery models
- We have developed a data format for describing battery models and tools for input data exchange between models.
- We have implemented and demonstrated various components in VIBE
- Software production release has been made in October 2014 with update followed in March 2015
- Project website has been created with software users mailing list for support and collecting feedback

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http://batterysim.org

Technical Backup Slides

CAEBAT OAS simulation platform has two aspects

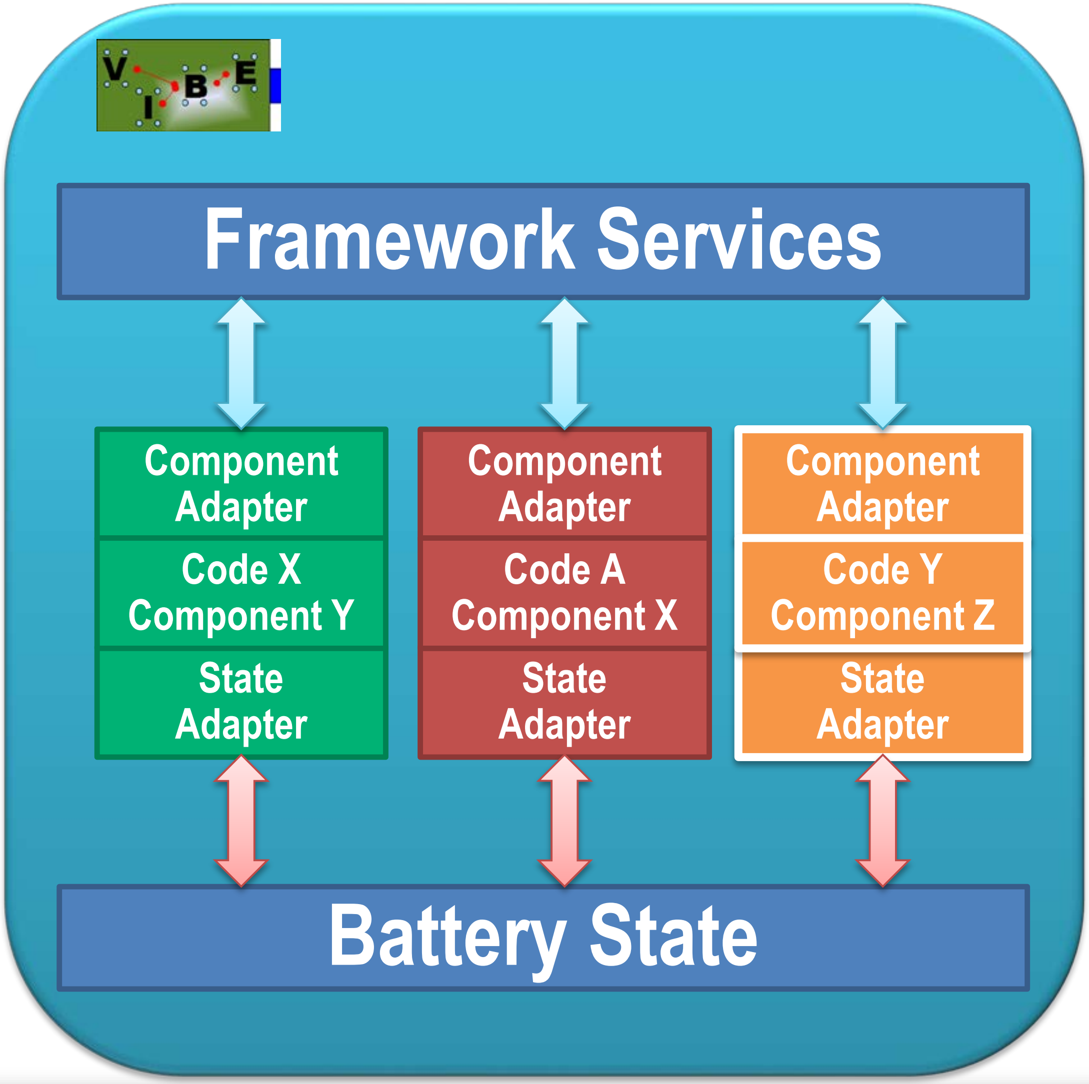
Software Infrastructure

- **flexible**
  - multiple modeling approaches
  - combine appropriate component models for problem at hand
  - support integrated sensitivity analysis and uncertainty quantification
  - programming language-agnostic
- **extensible**
  - ability to add and combine proprietary component models
- **scalable from desktop to HPC platforms**

Numerical coupling and Scale-bridging approaches

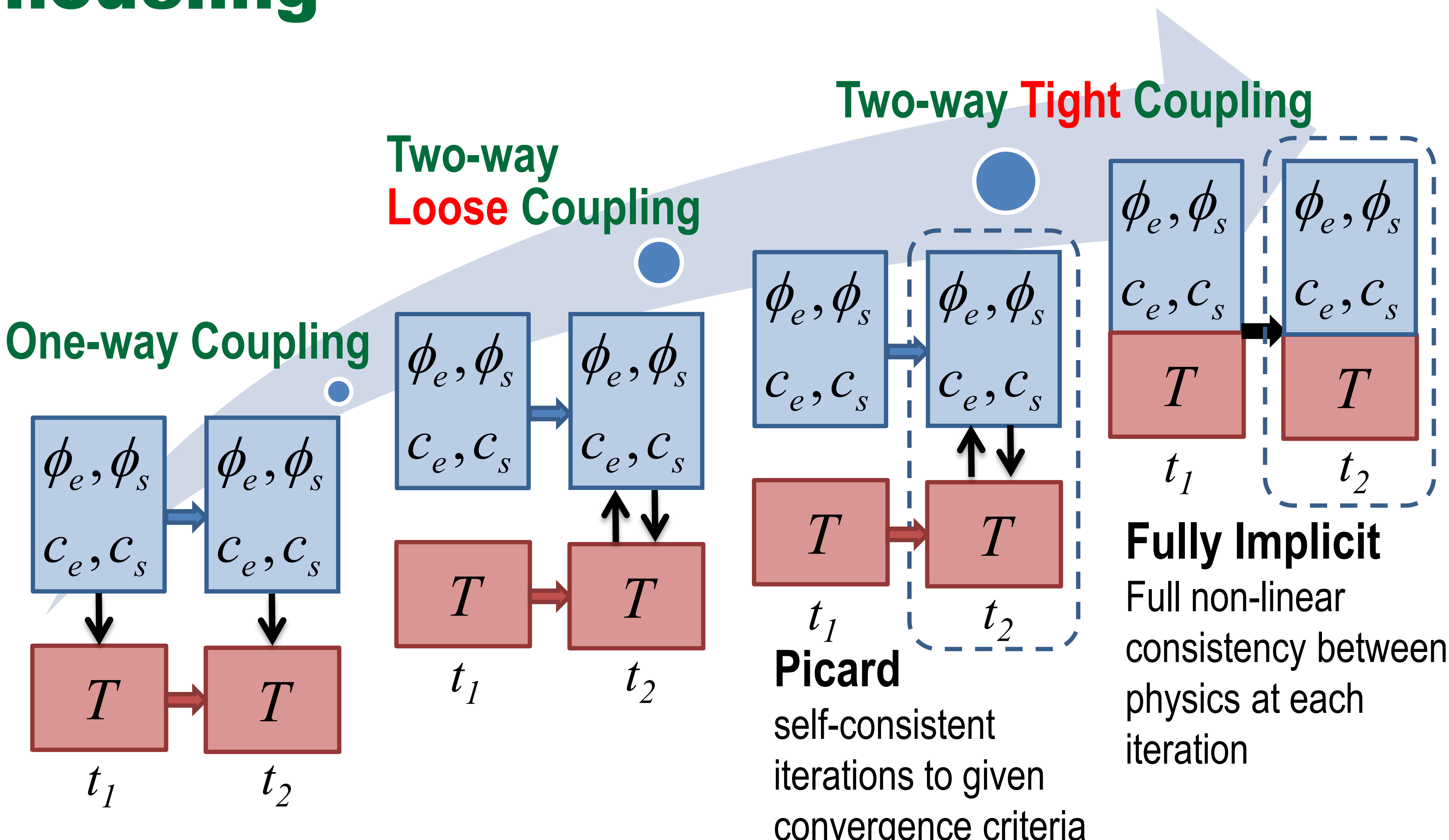
- **flexible coupling strategy**
  - one-way
  - two-way loose
  - two-way tight
  - fully implicit
- **ability to transfer information across different models in a mathematically / physically consistent fashion**
- **similarly for bridging time-scales**

VIBE Software Platform for CAEBAT

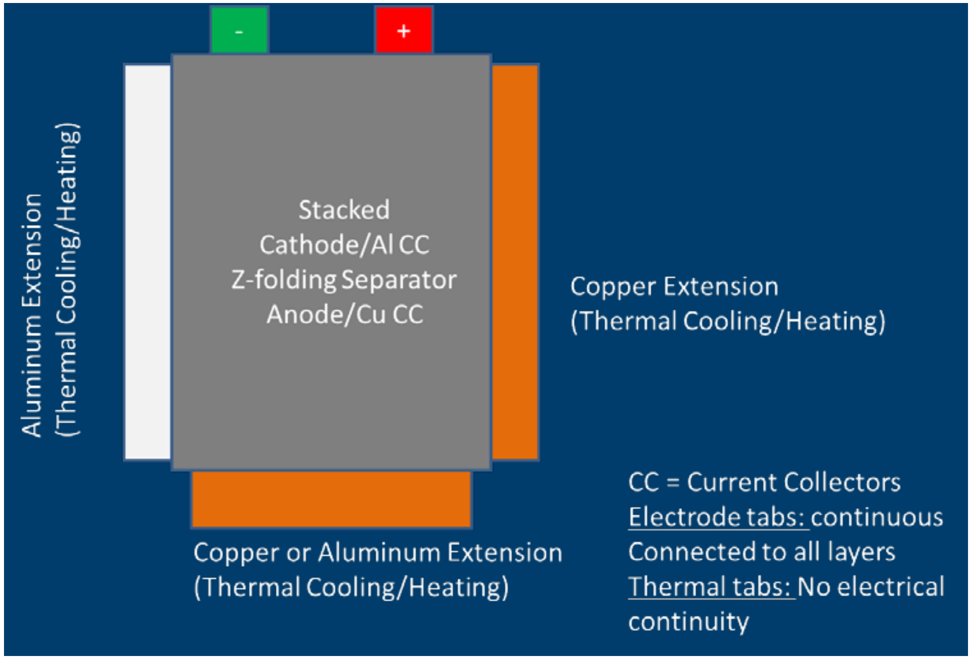


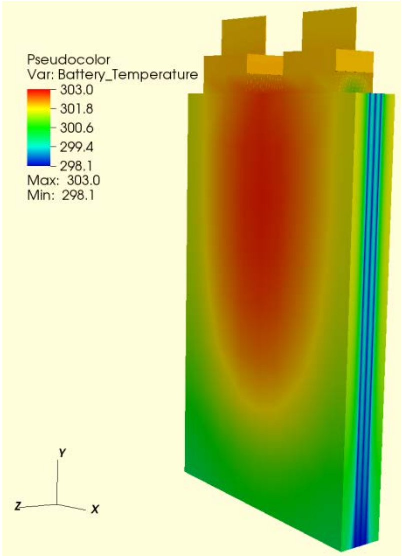
- **Component-based approach**
  - *extensibility*, V&V, independent development
- **Common solution (battery) state layer**
  - data repository
  - conduit for inter-component data exchange
- **File-Based data exchange**
  - no change to underlying codes
  - simplify *"unit testing"*
- **Scripting Based Framework (Python)**
  - Rapid Application Development (RAD)
  - adaptability, changeability, and flexibility
- **Simple component connectivity pattern**
  - driver/workers topology
- **Codes as components:**
  - focus on code-coupling vs physics-coupling as first step
- **Simple unified component interface**
  - init(), step(), finalize()

Coupling scenarios in battery modeling

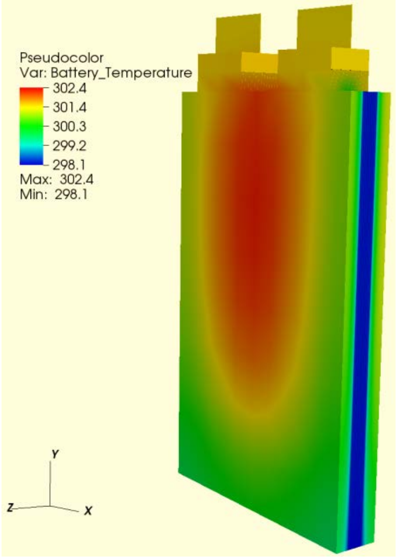


Novel Thermal Management (ARPA-E project)



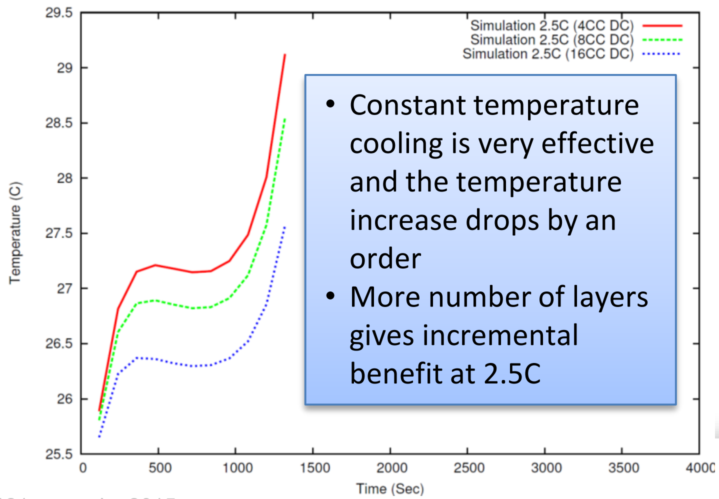


4 Anode CCs +
4 Cathode CCs



8 Anode CCs +
8 Cathode CCs

- Side cooling reduces the peak temperature dramatically
- The cooling is further improved for larger L/W formats



- Constant temperature cooling is very effective and the temperature increase drops by an order
- More number of layers gives incremental benefit at 2.5C

Modeling is used to evaluate different design scenarios so that only the most optimal configurations are built and tested – validation of the CAEBAT philosophy