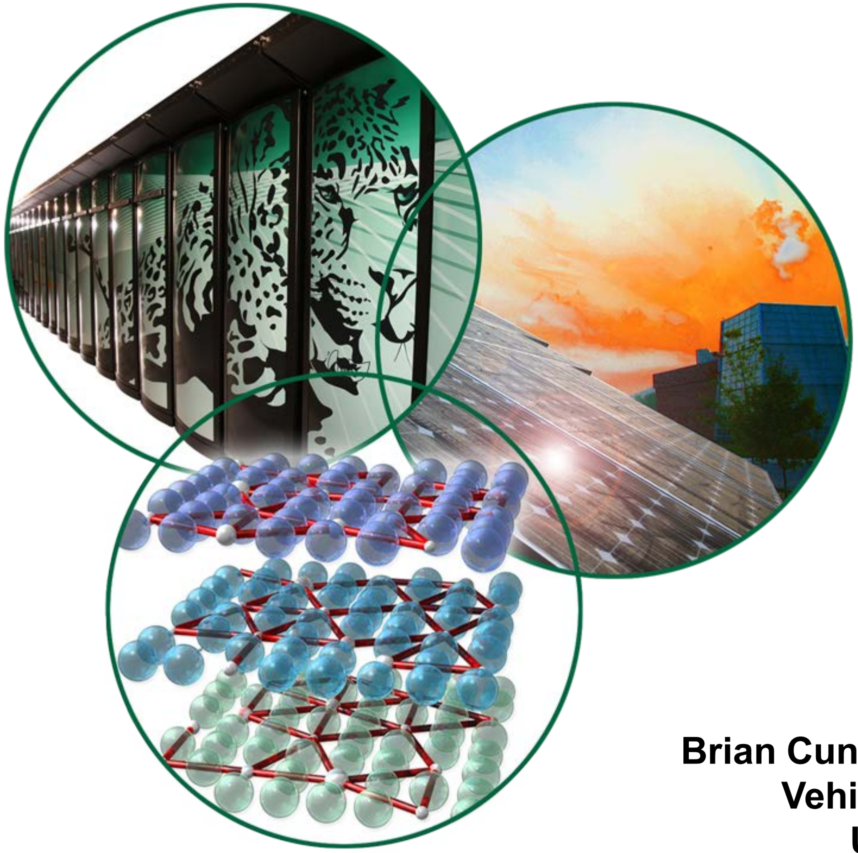
Open Architecture Software for CAEBAT

Project ID: ES121



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

Oak Ridge National Laboratory

2014 U.S. DOE Hydrogen and Vehicle Technologies Program Annual Merit Review and Peer Evaluation

June 17, 2014

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, 2014
- **Budget**
  - FY13 Funding
    - $700K
  - FY14 Funding
    - $700K
- **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

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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 the problem
  - Improve the design process
  - Use different software and vendors
- Implement the latest numerical methods and algorithms
- Verify and Validate the models and methods
  - Quantify uncertainties, as well (analogous to experimental error bars)

Relevance (2): 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

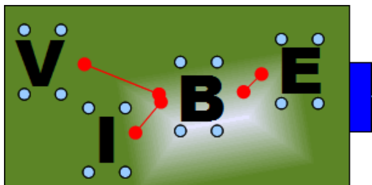
- Coordination and collaboration across teams has been critical to overall success of CAEBAT
  - Standardization of input and of “battery state” database
  - Standard test problem(s)
  - Standardized interfaces for cell, pack, etc. models

Milestones

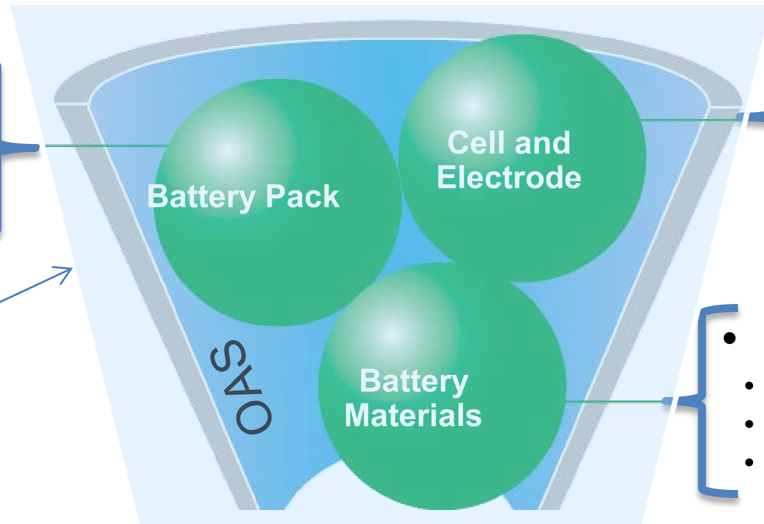
FY 13 Milestones	Due Date	Status
Input and Battery State Standard v2	12/31/2012	Completed
Link to ANL cost model and NREL MSMD model	03/31/2013	Completed
Geometric parametric sweep	06/30/2013	Completed
Initial demo of NiCE	09/30/2013	Completed
FY 14 Milestones		
Pack-level thermal, electrical and electrochemical 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	**Ongoing**
User Environment V1 Software Release and Documentation	9/30/2014	**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**

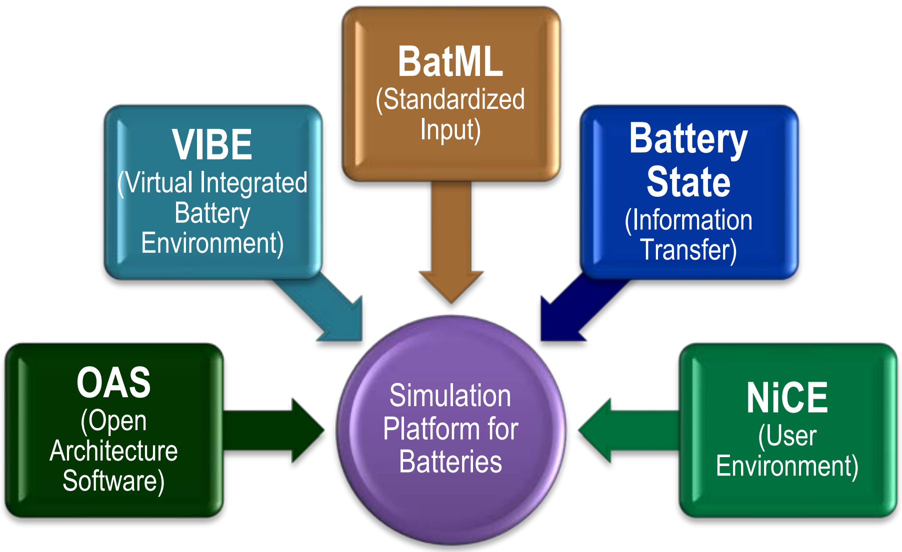
- **Atomistic-Meso**
  - **DFT/MD**
  - **Phase-field**
  - **Mean-field**

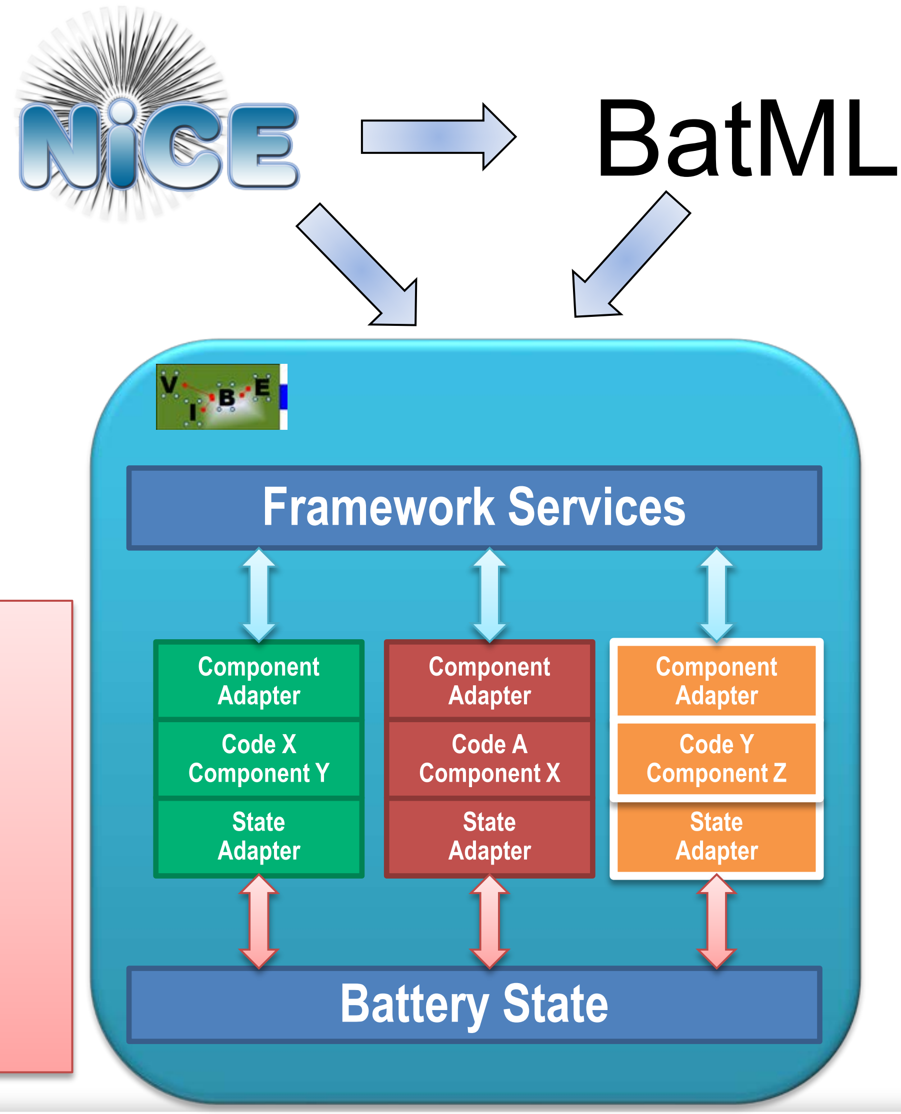
Experiments (ABR, BATT, Industry) → **Validation**

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
- **NiCE**: A graphical workflow for BatML editing, solver setup, job launch and analysis
- All the above yield a robust and user friendly CAEBAT simulation platform

Technical Accomplishments/Progress (1): On track to final release version

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

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

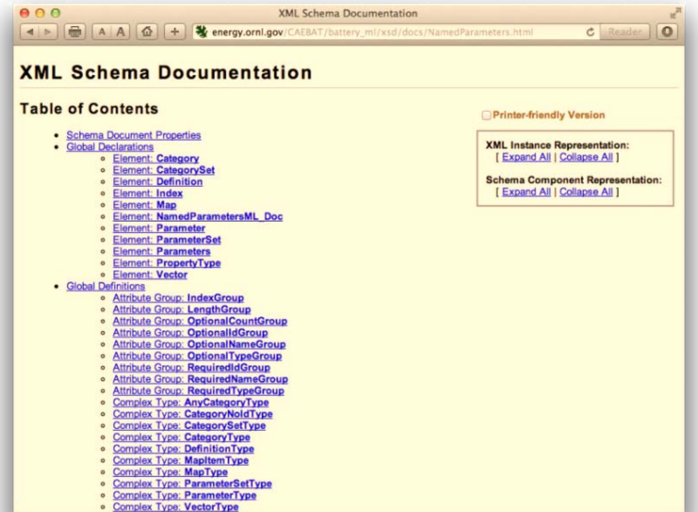
NiCE User Environment
- Job-launch of OAS
- Initial post-processing
- Initial edits of BatML XML files
- Graphical feedback
- Finalize post-processing and real-time manipulation
- BatML editing

Green – Completed
Blue – Ongoing

Battery Markup Language (BatML): Schema and Conversion

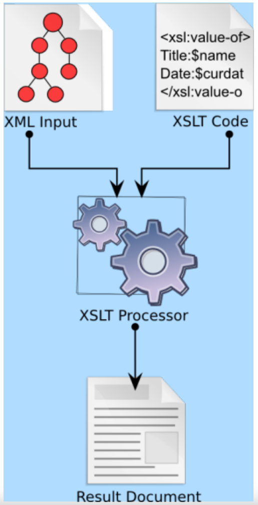
Technical Accomplishment

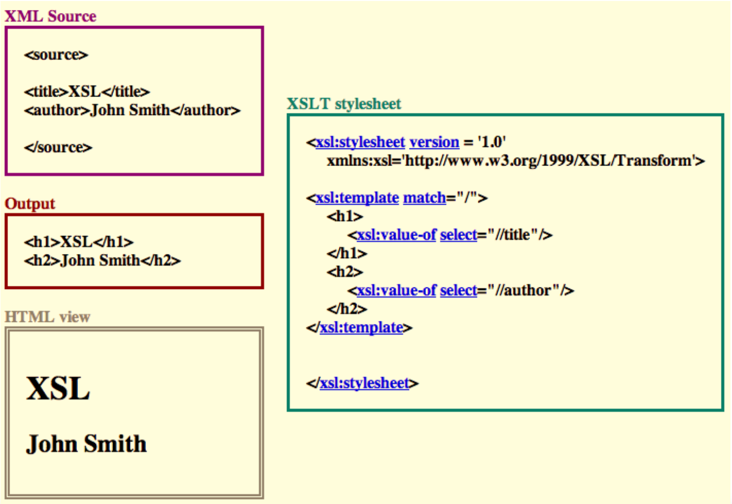
Schema



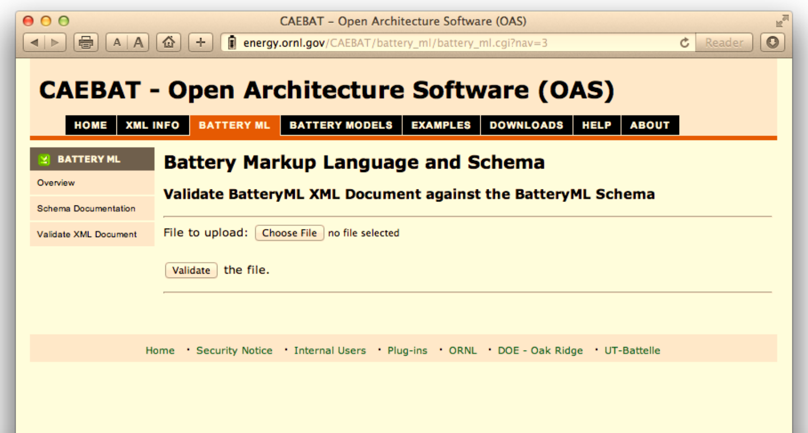
- BatML is a new XML data format for describing battery models.
- BatML is compatible with Material and Units Markup Languages used by many software vendors.
- Documentation and software tools (validation, conversion) are available at the project web site.

Model Translation





Model Syntax Validation



http://energy.ornl.gov/CAEBAT/battery_ml

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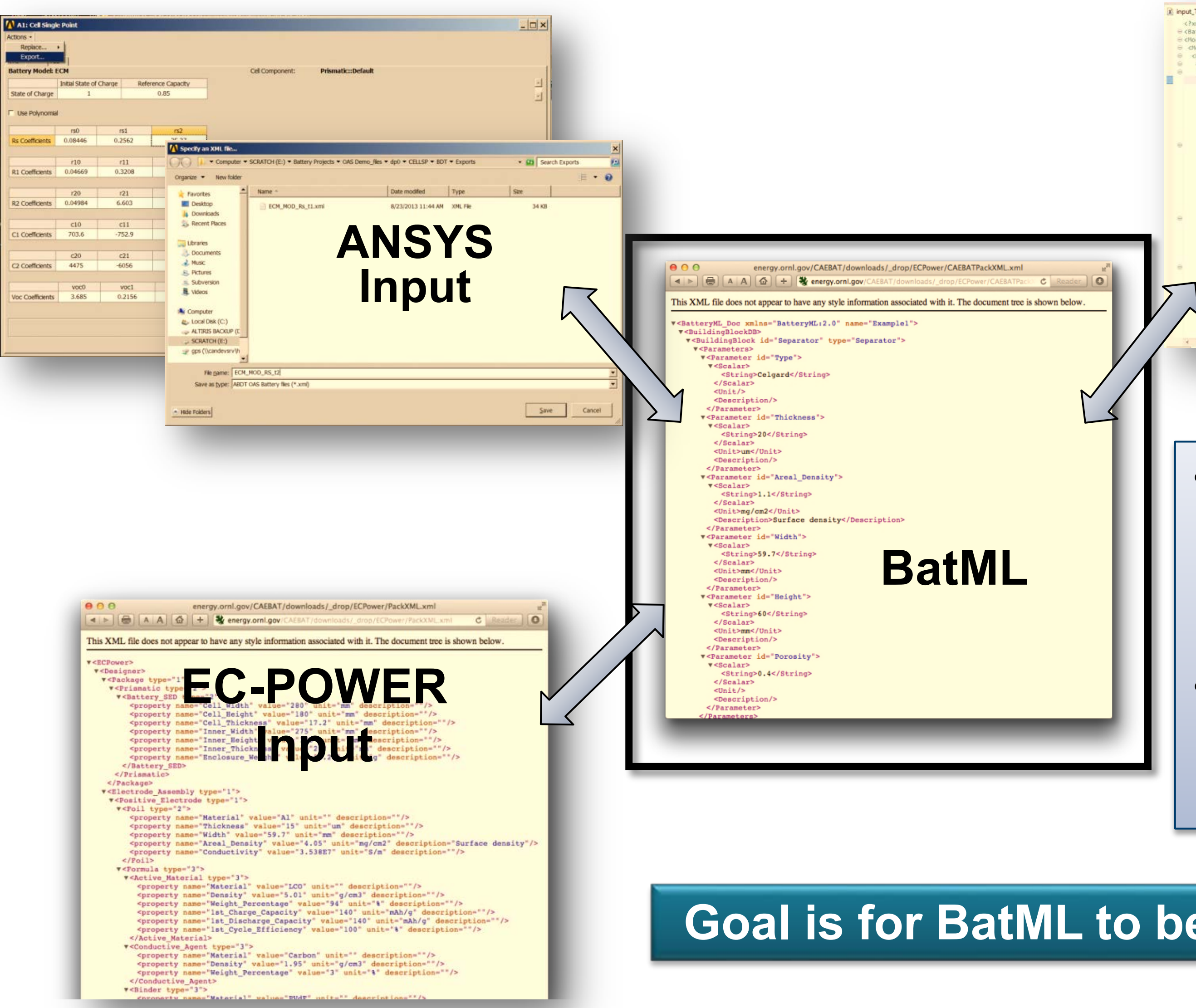
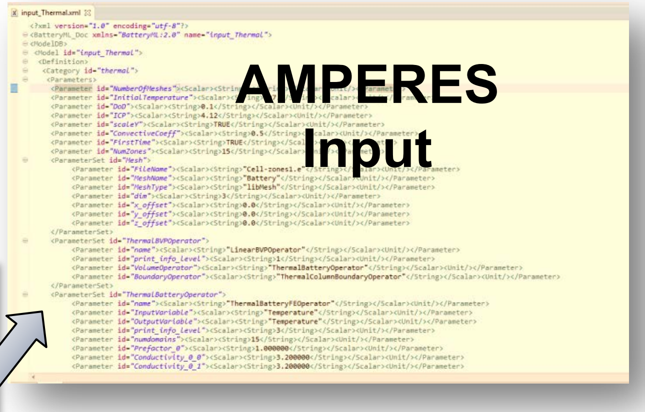
Battery Markup Language (BatML): Model Exchange

Technical Accomplishment





- 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:

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

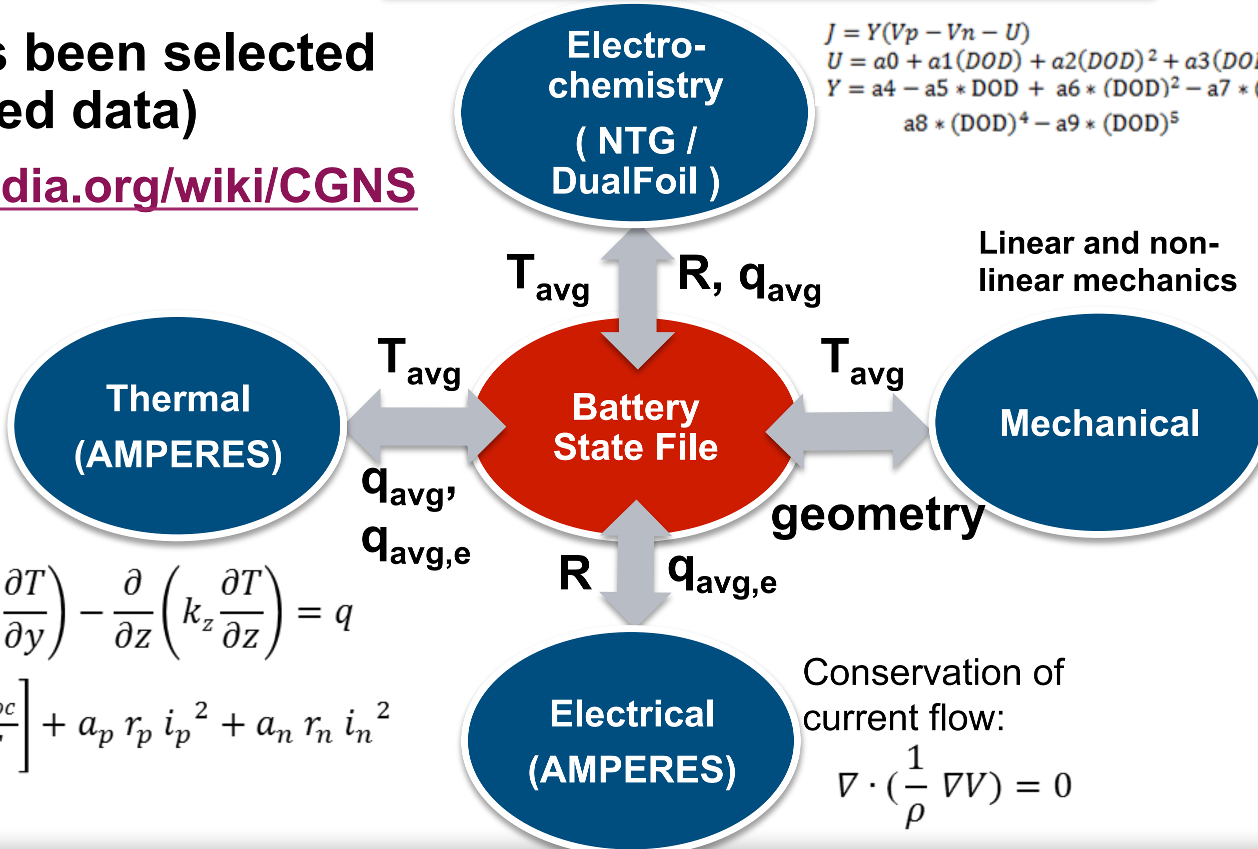
Electrolyte Potential:

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

Electrode Potential:

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

$$J = Y(Vp - Vn - U)$$
$$U = a0 + a1(DOD) + a2(DOD)^2 + a3(DOD)^3$$
$$Y = a4 - a5 * DOD + a6 * (DOD)^2 - a7 * (DOD)^3 + a8 * (DOD)^4 - a9 * (DOD)^5$$



Conservation of current flow:

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

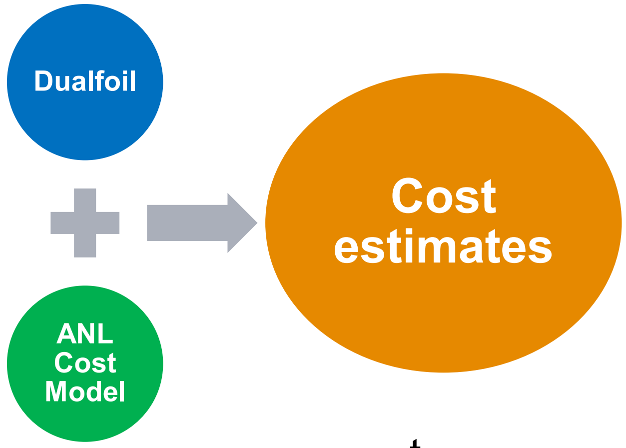
$$\rho C_p \frac{\partial T}{\partial t} - \frac{\partial}{\partial x}\left(k_x \frac{\partial T}{\partial x}\right) - \frac{\partial}{\partial y}\left(k_y \frac{\partial T}{\partial y}\right) - \frac{\partial}{\partial z}\left(k_z \frac{\partial T}{\partial z}\right) = q$$

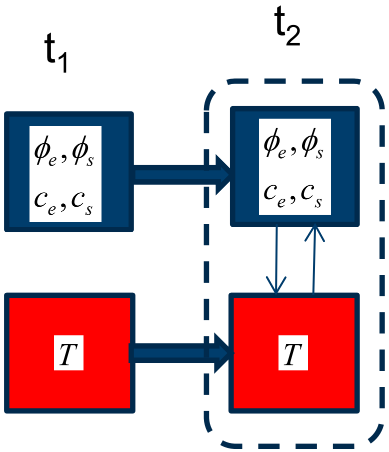
$$where \quad q = aJ\left[E_{oc} - E - T\frac{\partial E_{oc}}{\partial T}\right] + a_p\, r_p\, i_p^{\,2} + a_n\, r_n\, i_n^{\,2}$$

Open Architecture Software (OAS)

Technical Accomplishment

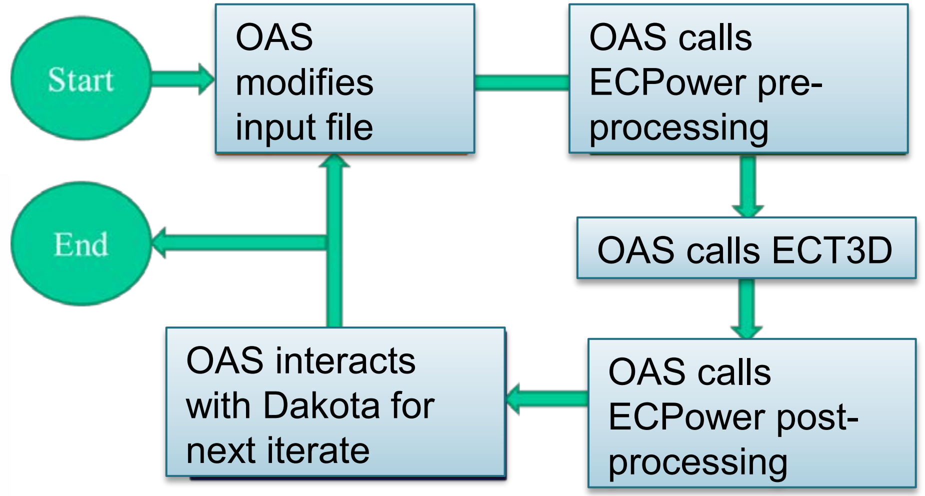
- **Porting to Windows is complete**
  – Now being merged and prepared for public release
- **Integration with ANL cost model is complete**
  – Can use simulation data to drive the cost model
- **We added computational design optimization capability**
  – Demonstrated by investigation of optimal battery 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



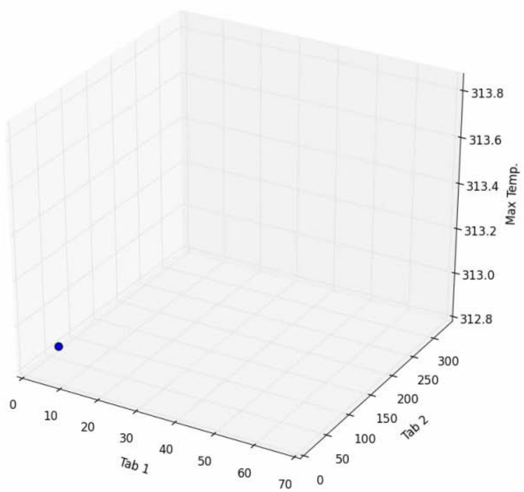


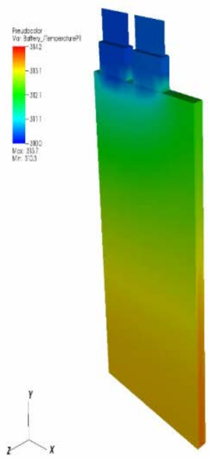
Picard Method:
self-consistent iterations to prescribed convergence criterion

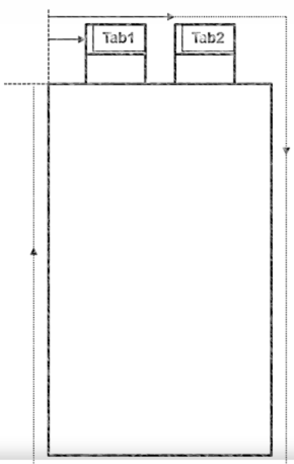
Open Architecture Software (OAS): Results



Optimal Placement of Tabs



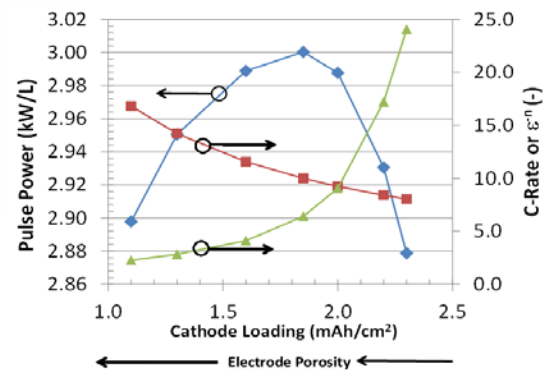




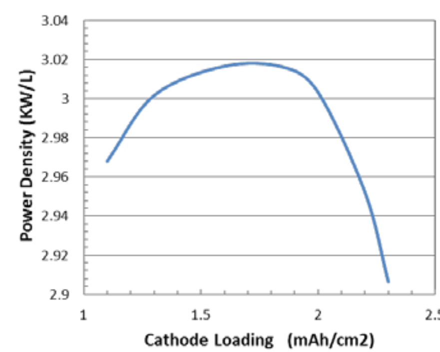
To reduce the peak cell temperature:

a) Increase the width of the tabs

b) Place them on opposite ends



Previous 1D result
(Blue curve)



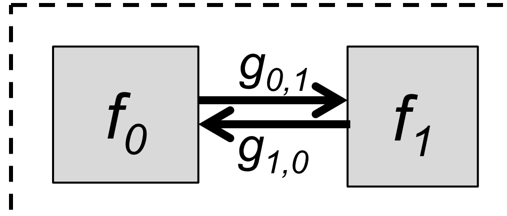
OAS/ ECT3D result

More details in ECPower's presentation

Open Architecture Software (OAS): Tight coupling

Technical Accomplishment

In general, Picard iteration to a specified convergence criteria provides tight coupling of two physics components f_0 and f_1 exchanging variables via functions *g*.



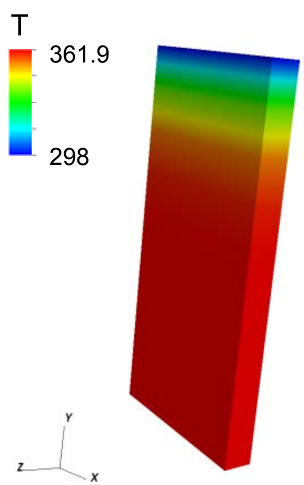
For each time step:

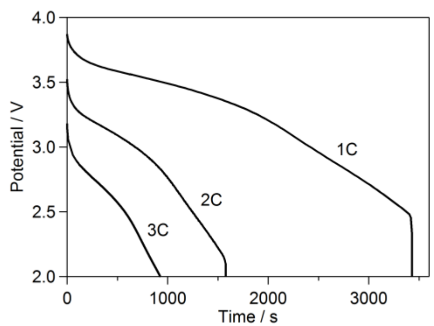
while *not converged* **do**

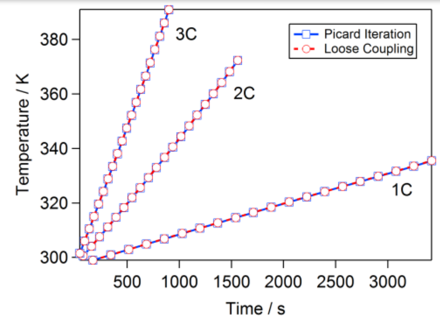
$$f_0\left(x_0^{(k)}, g_{0,1}\left(x_1^{(k-1)}\right)\right)=0$$

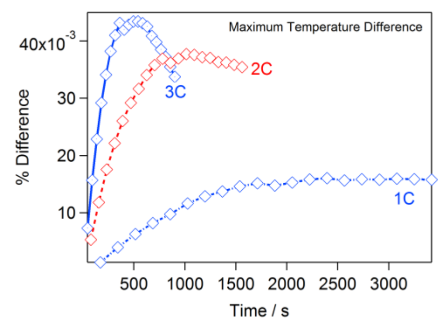
$$f_1\left(x_1^{(k)}, g_{1,0}\left(x_0^{(k)}\right)\right)=0$$

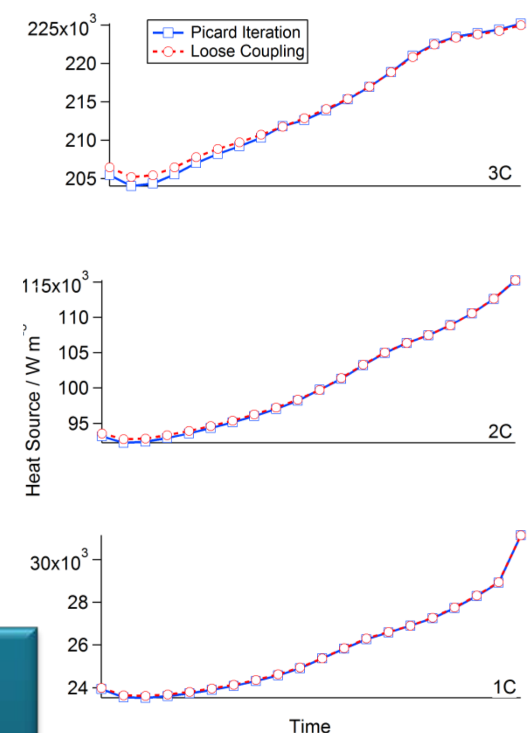
This was implemented in VIBE using OAS to couple electrochemical (*dualfoil*) and thermal components. For an unrolled Li-polymer cell:







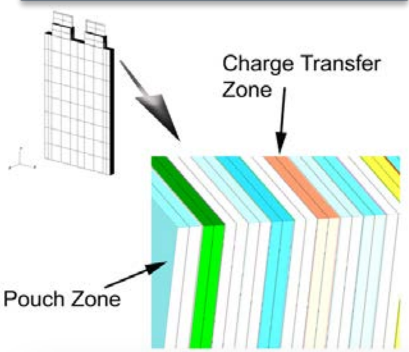


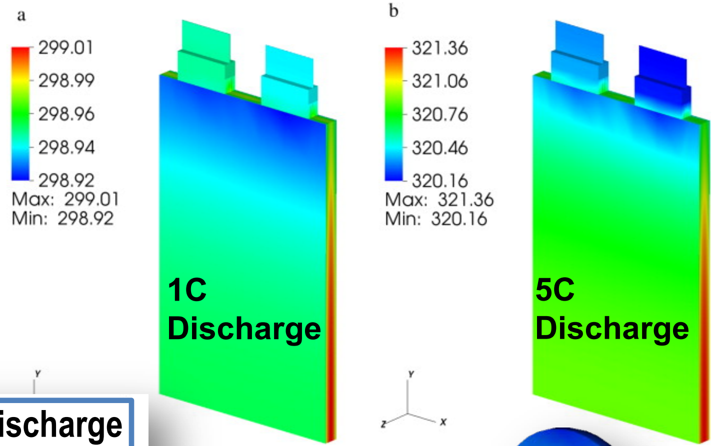


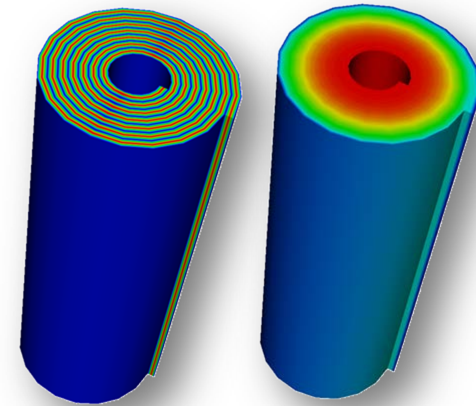
- Temperature-dependent diffusivities/BV-kinetics in *dualfoil* provide coupling with the thermal component
- Weak dependence of sources on temperature results in very fast convergence of Picard iterations (typically within 4 iterations)

VIBE Results

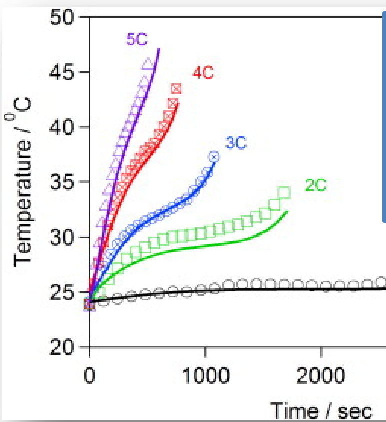
Detailed 3D Modeling







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

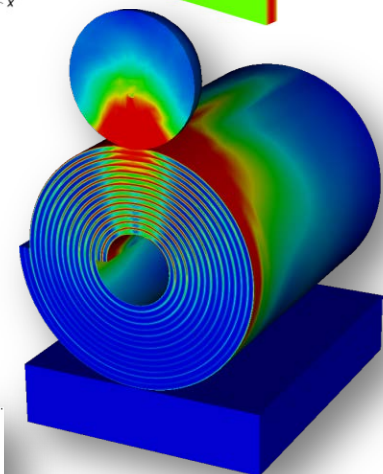


Discharge Curves (Validation with IR Imaging)

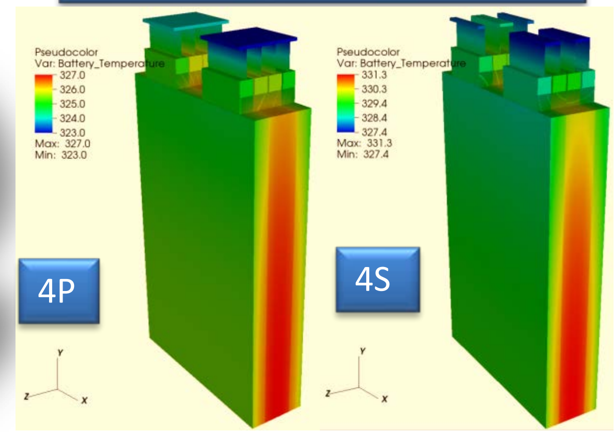
ELSEVIER
Journal of Power Sources
Available online 24 August 2013
In Press, Accepted Manuscript — Note to users

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



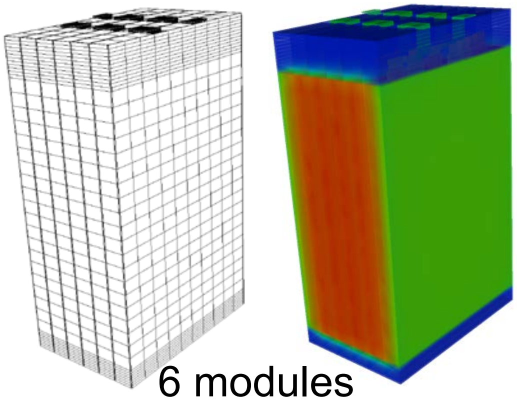
Mechanical Abuse of Cylindrical Cell with Current Collectors Resolved (Electrochemical – Thermal – Electrical – Mechanical)



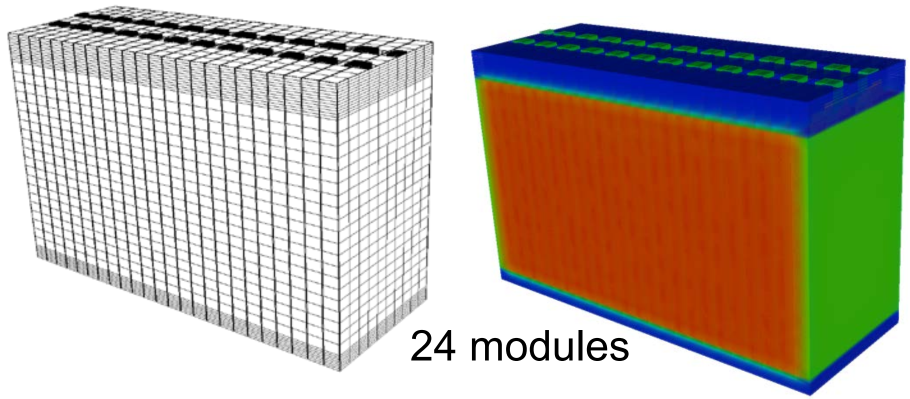
Temperature in 4P and 4S Module with Fully Coupled Electrochemical, Electrical and Thermal Simulations in CAEBAT OAS / VIBE

VIBE – Facilitates Hierarchical Process to Construct Battery Packs

Technical Accomplishment



6 modules



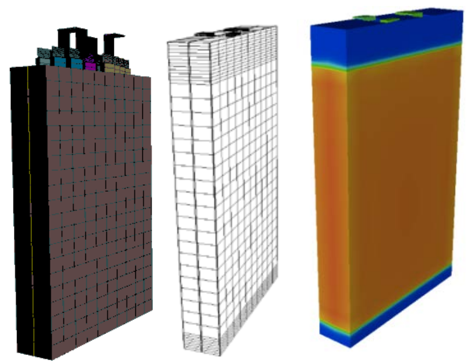
24 modules

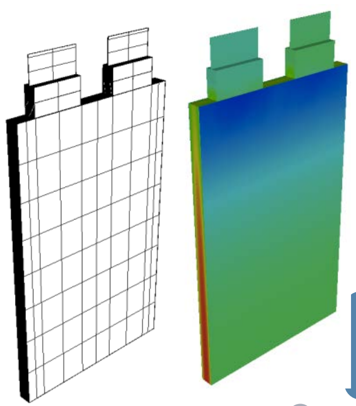
Pack

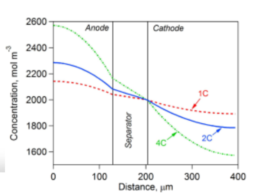
Module

Cell

Cell Sandwich







- 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

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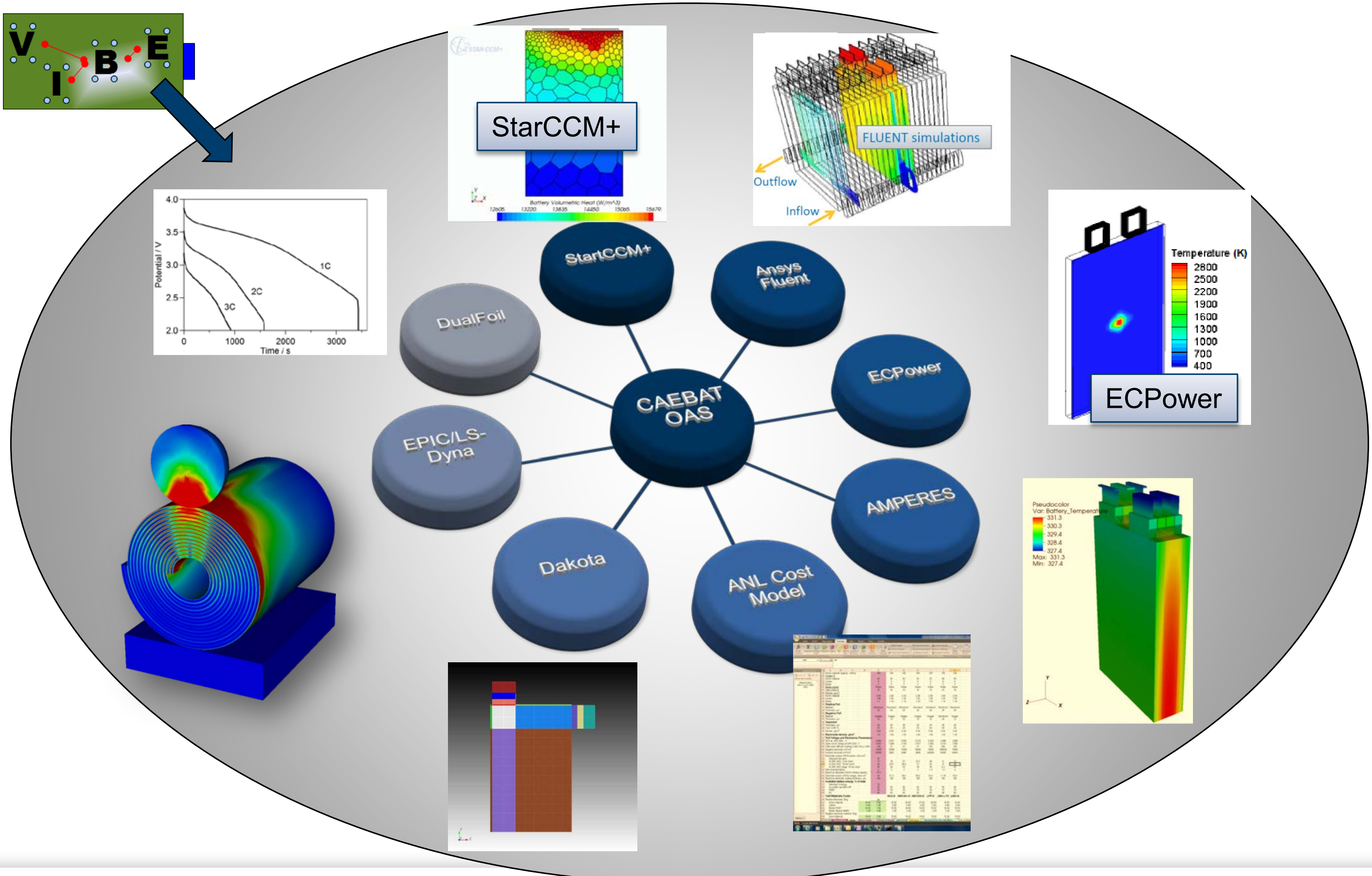
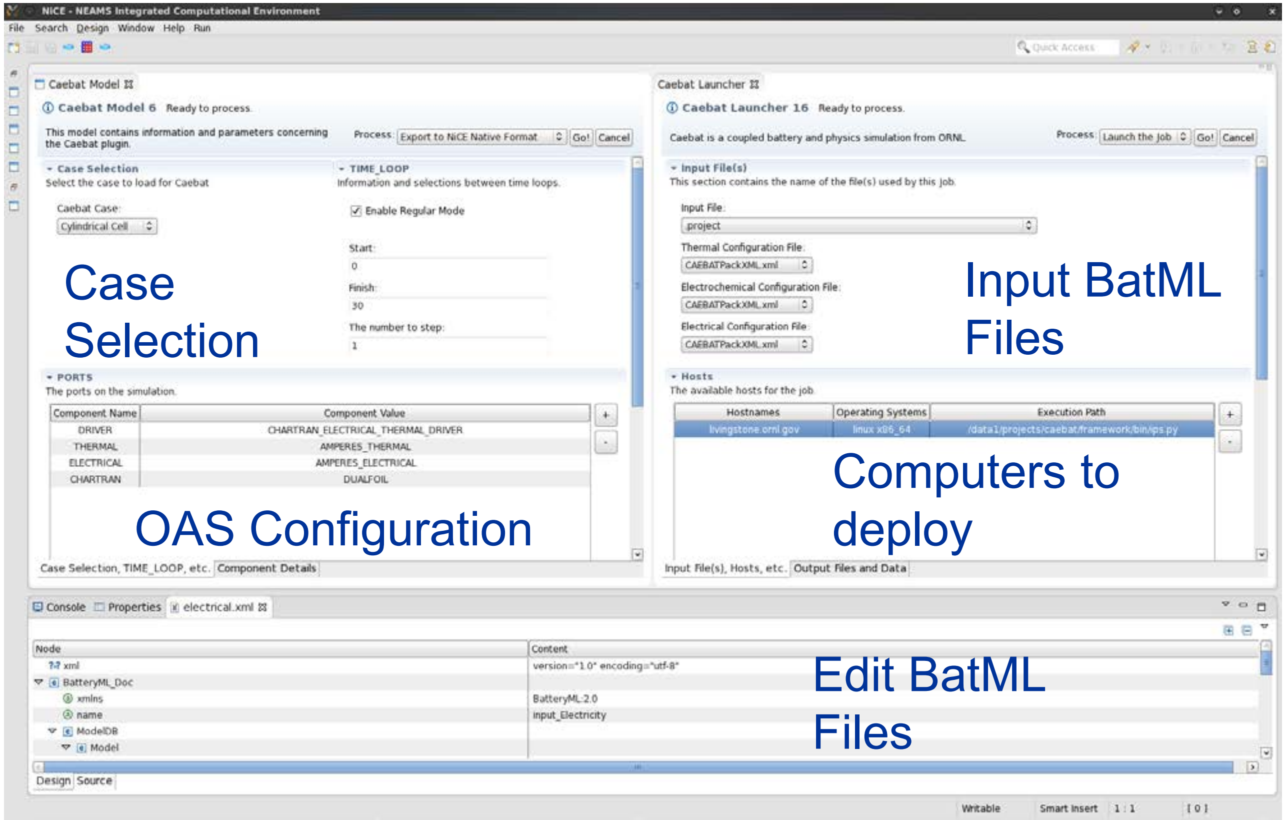
VIBE Computational Ecosystem: Coupling open and proprietary components

Technical Accomplishment



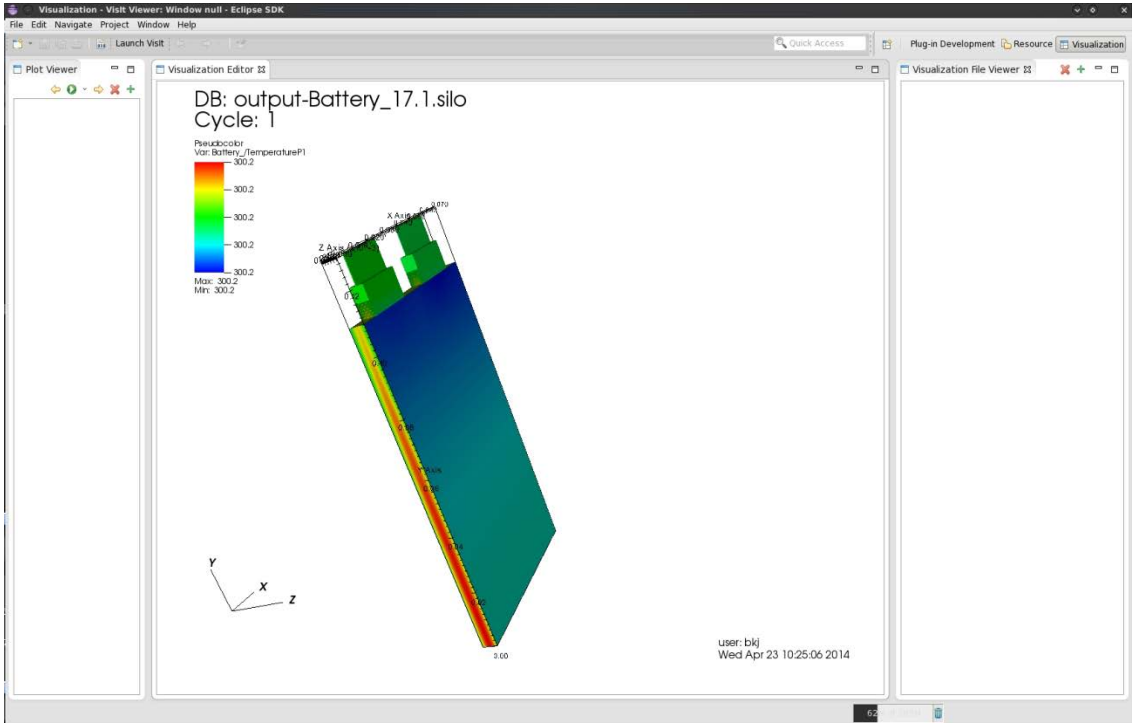
NiCE – A battery user environment!



User environment includes BatML editing, solver setup, job launch and analysis

- **Users can switch components easily and choose from preconfigured inputs**
- **Editing BatML is possible through a standard XML editor**

NiCE with ideal BatML editing support



New visualization capability under development

But editing batteries should be interactive…

- **Show the physical battery and facilitate interaction**
- **Map quantities of interest to the battery in useful ways before AND after the simulation**

Collaboration and Coordination

- Monthly telecon/web-meeting with DOE and NREL
- Several telecons/web-meetings with CAEBAT partners to coordinate the development of BatML translations and OAS integration
- 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
- Recent publications
  - JPS
  - Battery Safety Conference
  - Several ECS Conference presentations

Response to reviewer's comments

- **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 ambitious, so we are using a very methodical way of building cell-level models with formal 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 are actively 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 have regular meetings with NREL/DOE and additional meetings with RFP teams on an as-needed basis.*
- **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 by porting to Windows and have also linked to the 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. In addition, this project is actively developing software for deployment – well beyond simple coordination and design/study.*

Future Work - Planned Activities

- Near term (FY14)
  - OAS
    - Compatible with at least some components of all CAEBAT partner products
  - VIBE
    - Electrochemical, Electrical, Thermal and Mechanical (complete)
    - Cell-sandwich to Cell to Module Coupling to Pack Coupling
  - BatML
    - Revisions based on community feedback
    - Additional translators as necessary
  - Battery State
    - Standard for electrochemical, electrical, thermal and mechanical coupling
    - Release another version of the standard and associated tools
  - NiCE
    - Graphical feedback of input configuration
    - Finalize post-processing and real-time manipulation
    - Refined BatML editing with focus on usability
- Longer term
  - Community adoption
  - Support and maintenance

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
  - Electrochemistry (dualfoil) with thermal (AMPERES) for a cell
  - Electrochemistry (NTG) with thermal (AMPERES) and electrical (AMPERES) for a cell
  - Electrochemistry (dualfoil) with thermal (AMPERES) and electrical (AMPERES) for a cell module
  - Integrated models from NREL
  - Integrated the ANL cost model (initial)
- We are on track for the year-end release of a new version of OAS + VIBE + NiCE (with several examples) along with input XML schema and battery state definition

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Technical Backup Slides

CAEBAT OAS simulation platform has two aspects

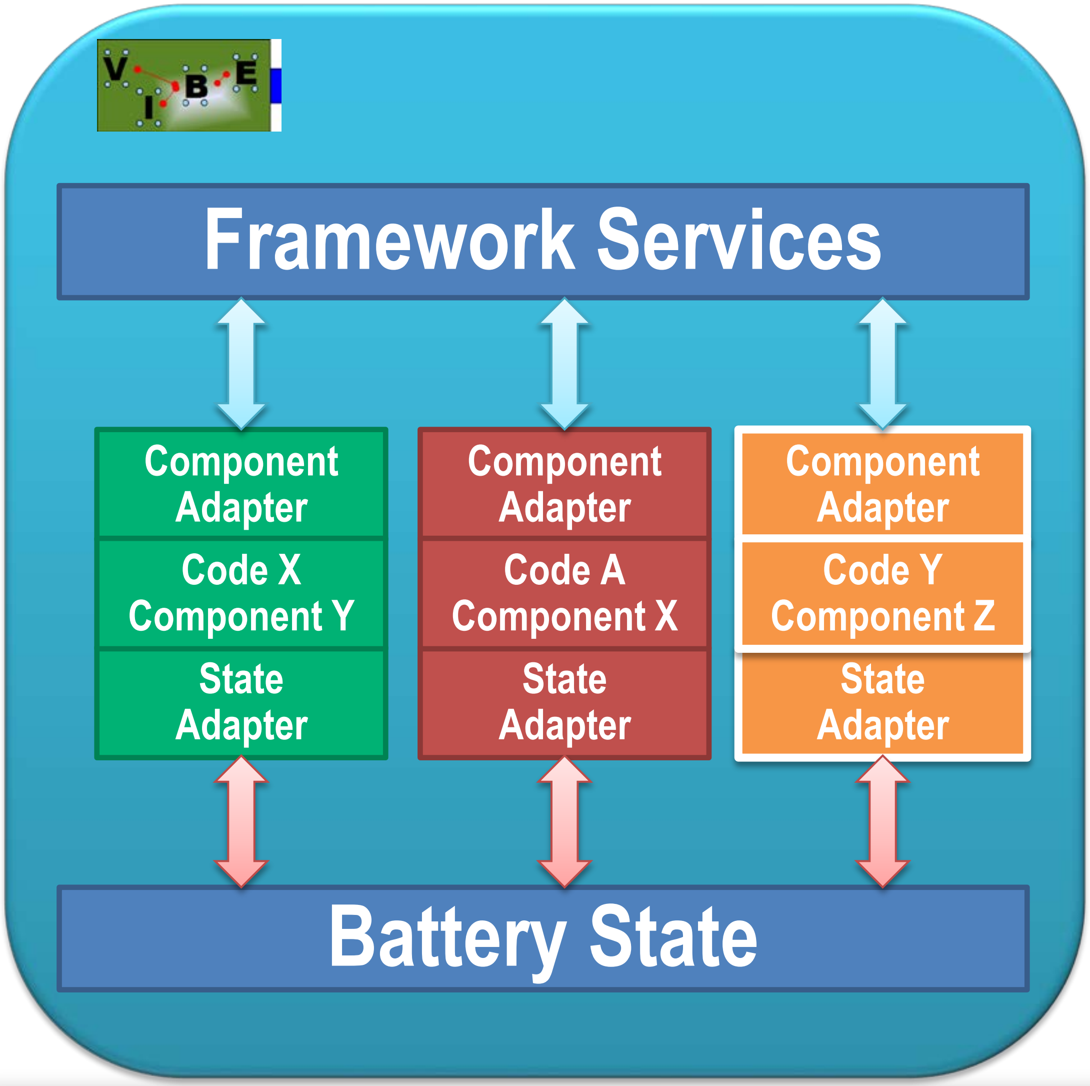
Software Infrastructure

- **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

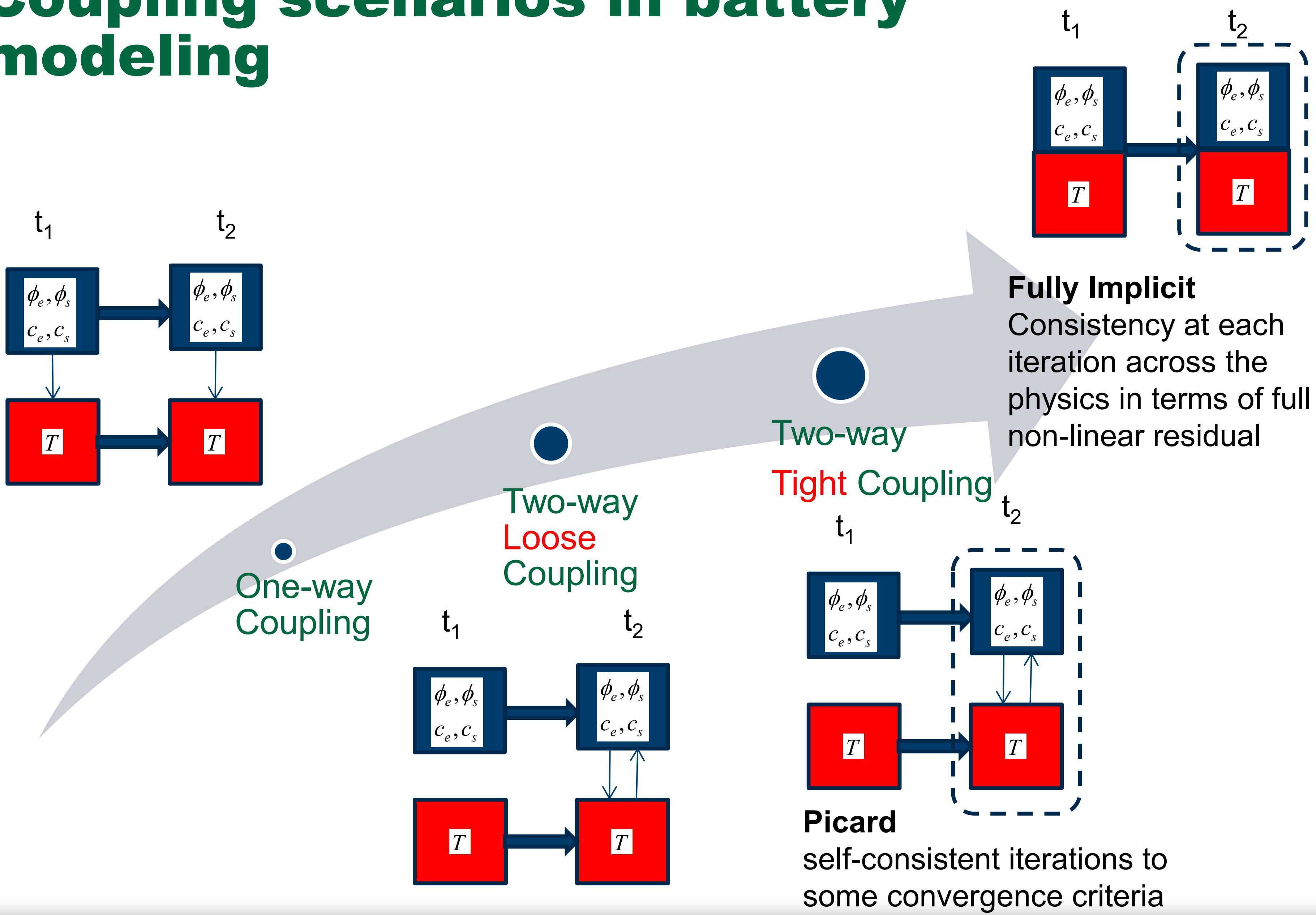
- **flexible coupling strategy**
  - one-way
  - two-way loose
  - two-way tight
  - fully implicit
- **ability to transfer information across different models in a mathematically / physically consistent fashion**
- **similarly for bridging time-scales**

VIBE Software Platform for CAEBAT

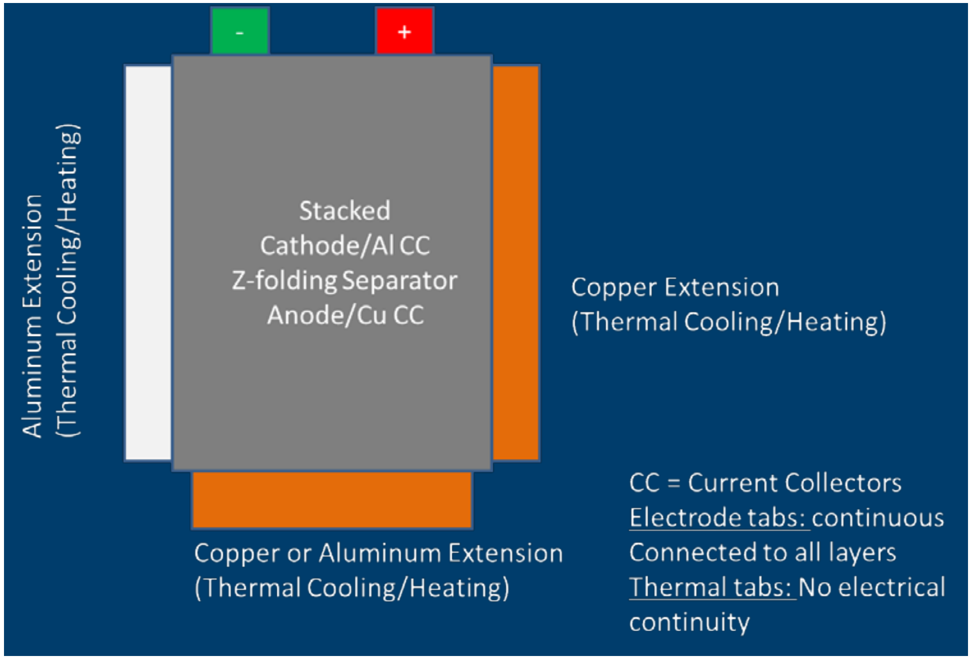


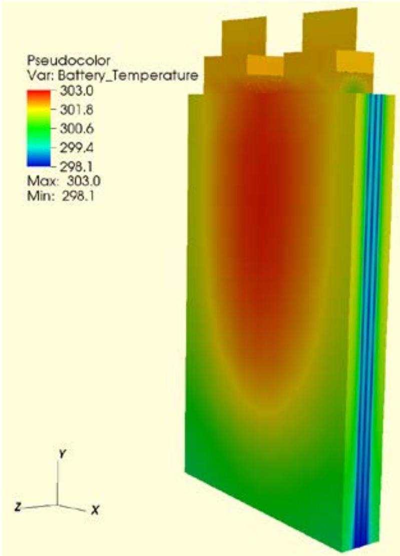
- **Component-based approach**
  - *extensibility*, V&V, independent development
- **Common solution (battery) state layer**
  - data repository
  - conduit for inter-component data exchange
- **File-Based data exchange**
  - no change to underlying codes
  - simplify *"unit testing"*
- **Scripting Based 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

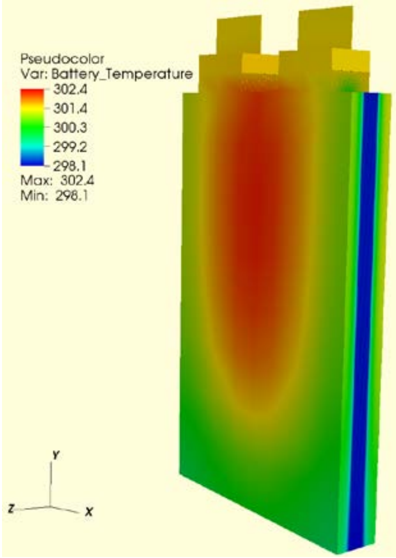


Novel Thermal Management (ARPA-E project)



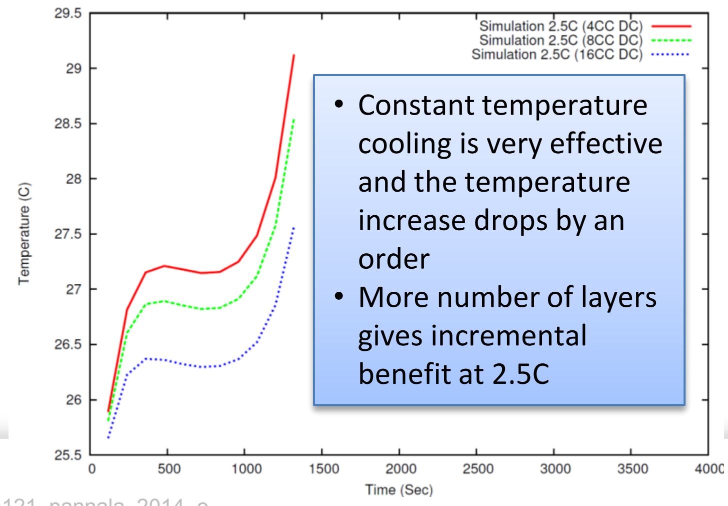


4 Anode CCs +
4 Cathode CCs



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