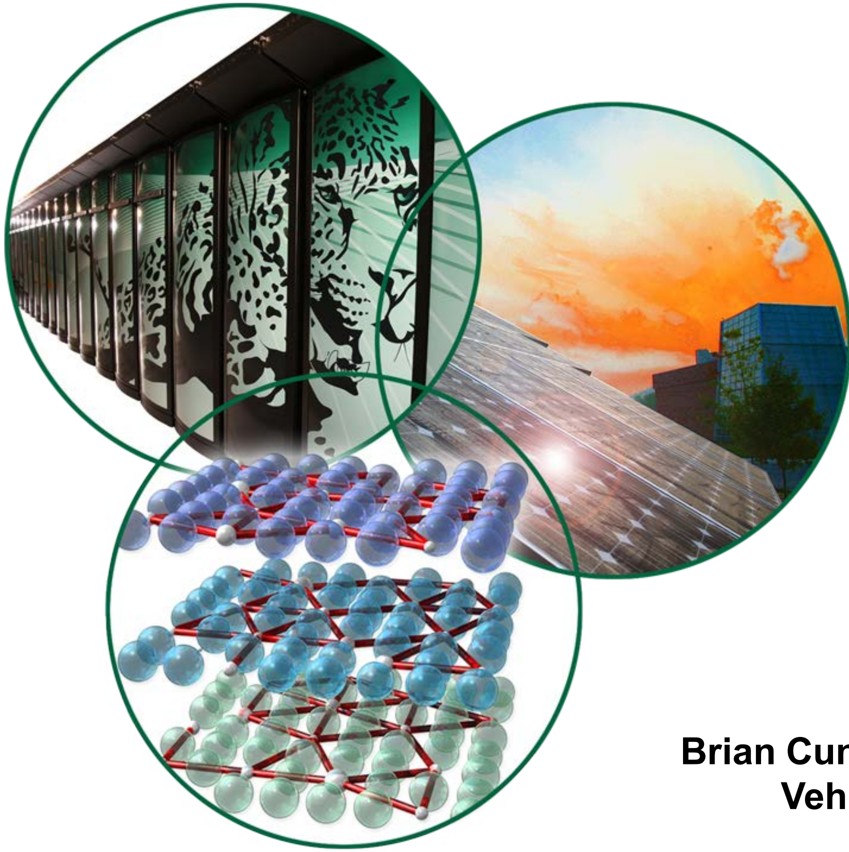
Open Architecture Software for CAEBAT

Project ID: ES121



John Turner (PI), Sreekanth Pannala, Partha Mukherjee, Srikanth Allu, Wael Elwasif, Srdjan Simunovic, and David Bernholdt

Oak Ridge National Laboratory

2012 U.S. DOE Hydrogen and Vehicle Technologies Program Annual Merit Review and Peer Evaluation

May 15, 2012

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

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U.S. DEPARTMENT OF ENERGY

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Overview

- **Timeline**
  - Start
    - June FY10
  - Finish
    - Ongoing
- **Budget**
  - FY11 Funding
    - $500K
  - FY12 Funding
    - $500K

- **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: CAEBAT will facilitate battery design by integrating battery modeling components within an *open architecture*

- **Access to commercial and non-commercial software through standardized interfaces and file formats**
  - ability to pick (and ultimately combine) the best software components available
  - standardize the design process
  - battery designer isn't limited to single vendor or software
- **Access to latest numerical methods and algorithms**
  - rapidly advance the state of the art
  - provide the best software tools to the battery designer
- **Verified and Validated**
  - ideally with quantified uncertainties as well

Relevance (2): CAEBAT Program Goals

- **Develop software tools that enable automotive battery community to design and simulate batteries:**
  - four different software suites (diversity of approaches, risk mitigation)
    - one from each of the RFP teams
      - may contain or require commercial or proprietary components
    - one based on an Open Architecture Software (OAS) infrastructure
      - we are calling this the **V**irtual **I**ntegrated **B**attery **E**nvironment (VIBE) and it will be more openly available
- **Each will (ultimately) be fully capable**
  - RFP tools focused on delivering a cell and pack modeling tool for industry
  - OAS tool integrates modules from RFP teams as well as Lab and University efforts beyond the RFP teams – community R&D platform
- **Coordination and collaboration across teams will be 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

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Milestones

FY 11 Milestones		Status
Develop test problems and extend modeling framework to include transport, thermal, and mechanical stresses	03/31/2011	Completed
Develop further capability, conduct assessment against test problems, and conduct initial validation against data available from battery packs and cell experiments.	08/31/2011	Completed
FY 12 Milestones		
Deliver pre-release version of open architecture software (integrating models of coupled multiphysics phenomena across porous 3D structures of electrodes) to partners for evaluation and comment	09/30/2012	On track

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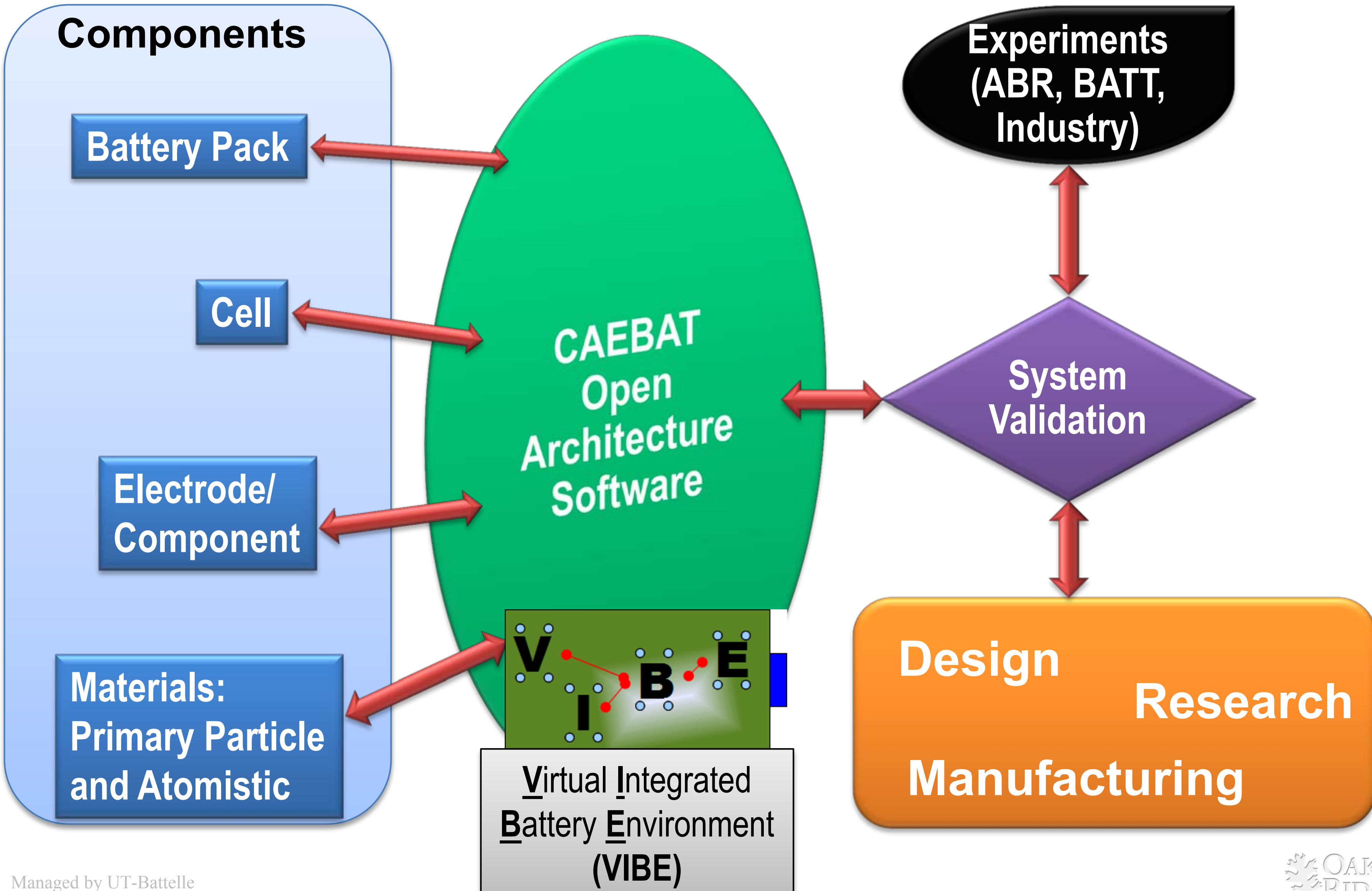
Approach (1): CAEBAT Open Architecture Software Vision



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Approach (2): CAEBAT OAS simulation platform has two aspects

Software Infrastructure

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

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**

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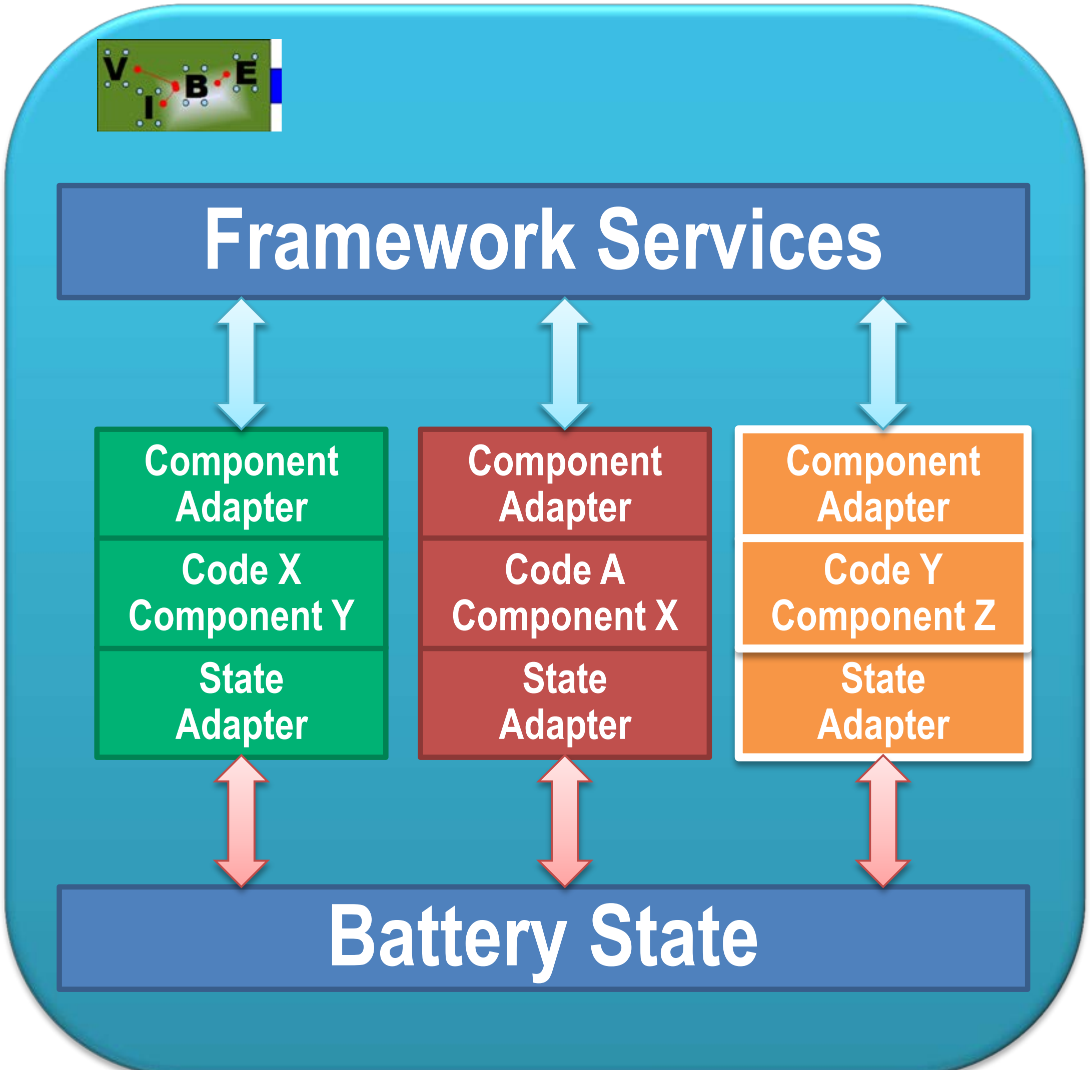
Approach (3): VIBE Software Platform for CAEBAT



- **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()

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

OAS

- Capability is online (NREL is testing it currently)
- 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

Standardized Input

- Comprehensive relational database of materials, properties, models, components, etc.
- XML database and corresponding schemas
- Issued version 1
- Translators

Battery State

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

Green – Completed
Cyan – Ongoing

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Battery state file

Technical Accomplishment

- **contains the minimal set of variables enable components to communicate**
- **CGNS format has been selected (for all mesh-based data)**
  - see also http://en.wikipedia.org/wiki/CGNS

Species Conservation

Electrolyte phase:

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

Solid phase:

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

Closures: $D_e^{eff} = D_e\varepsilon_e^{\xi}$ $D_s^{eff} = D_s\varepsilon_s^{\xi}$

Charge Conservation

Electrolyte phase:

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

Solid phase:

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

Closures: $\kappa^{eff} = \kappa\varepsilon_e^{1.5}$ $\kappa_D^{eff} = \frac{2RT\kappa^{eff}}{F}(t_+^0 - 1)\left(1 + \frac{d\ln f_\pm}{d\ln c_e}\right)$ $\sigma^{eff} = \sigma\varepsilon_s^{m}$

Electrode Kinetics

$$\bar{j} = a i_0\left[\exp\left(\frac{\alpha_a F}{RT}\eta\right) - \exp\left(-\frac{\alpha_c F}{RT}\eta\right)\right]$$

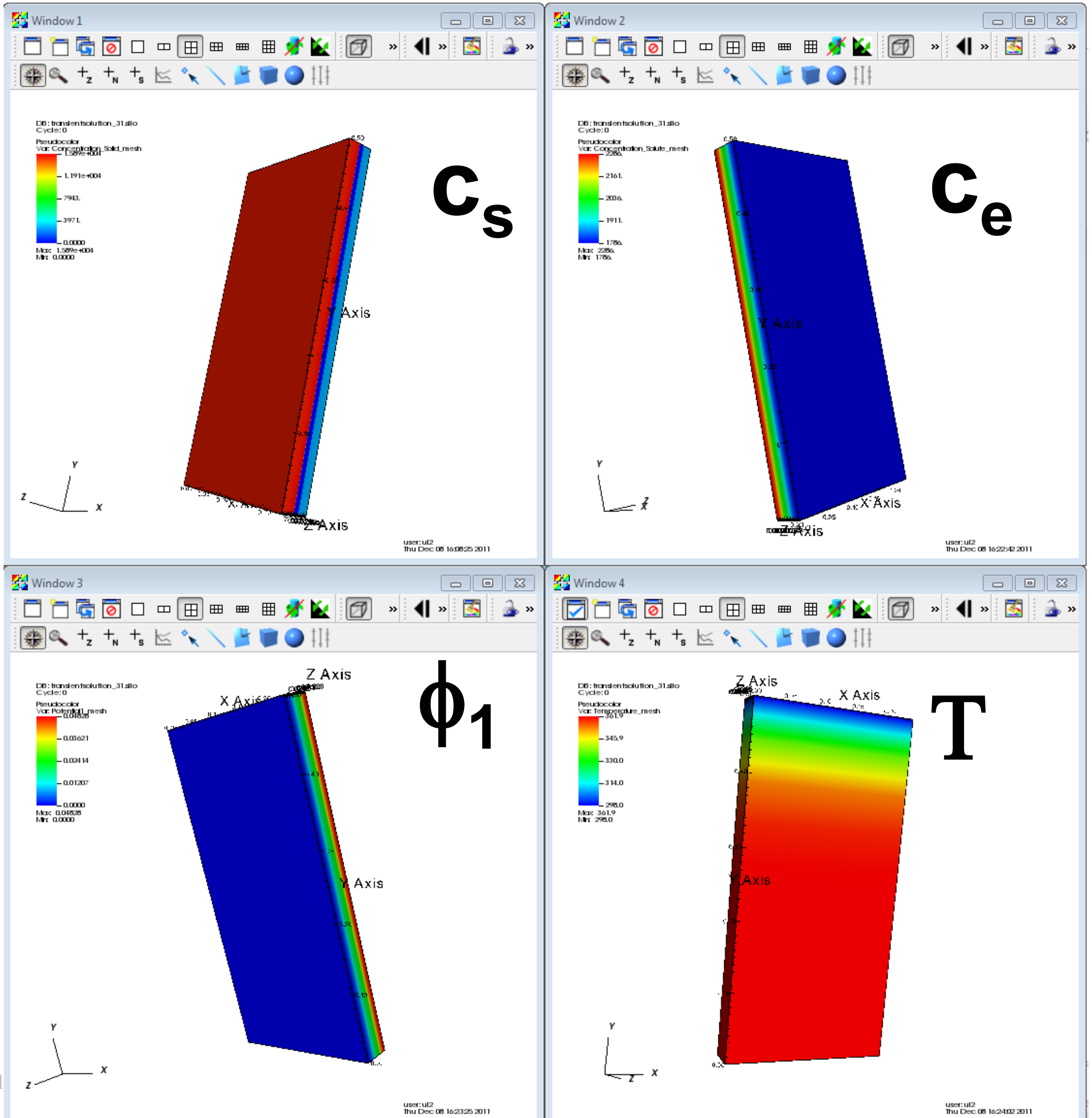
q_{avg} →

← T_{avg}

$$\frac{\partial(\rho c_p T)}{\partial t} = \nabla\cdot(\lambda\nabla T) + q$$

Sample results for demo problem 1

Technical Accomplishment



One-way coupling:
Tmax = 100 °C

Two-way loose coupling:
Tmax = 88 °C

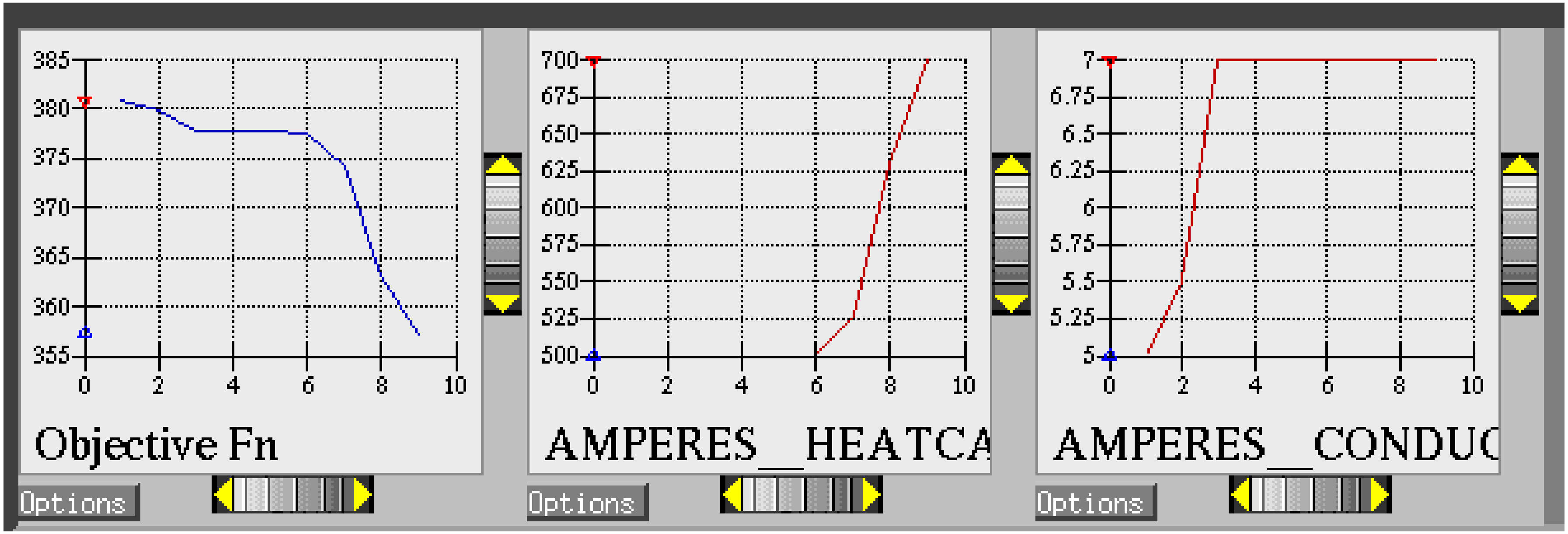
Two-way loose coupling (multi-domain):
Tmax = 89 °C (T1 = 89, T2= 89, T3 = 88, T4 = 329)

Two-way tight coupling (Srinivasan and Wang)
Tmax = 80 °C

Dakota Optimization (Simple Application)

Technical Accomplishment

Objective = Minimize T_{avg}
Cp = 300, 700 (starting 500)
λ = 3,7 (starting 5)



Critical as even small temperature changes have huge impact on safety and life

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Thermo-Electrochemical-Electrical Modeling in LIBs

Input from Sandwich calculations: Heat generation rate and resistance as a function of space and time; Stress/strain; Gas distribution

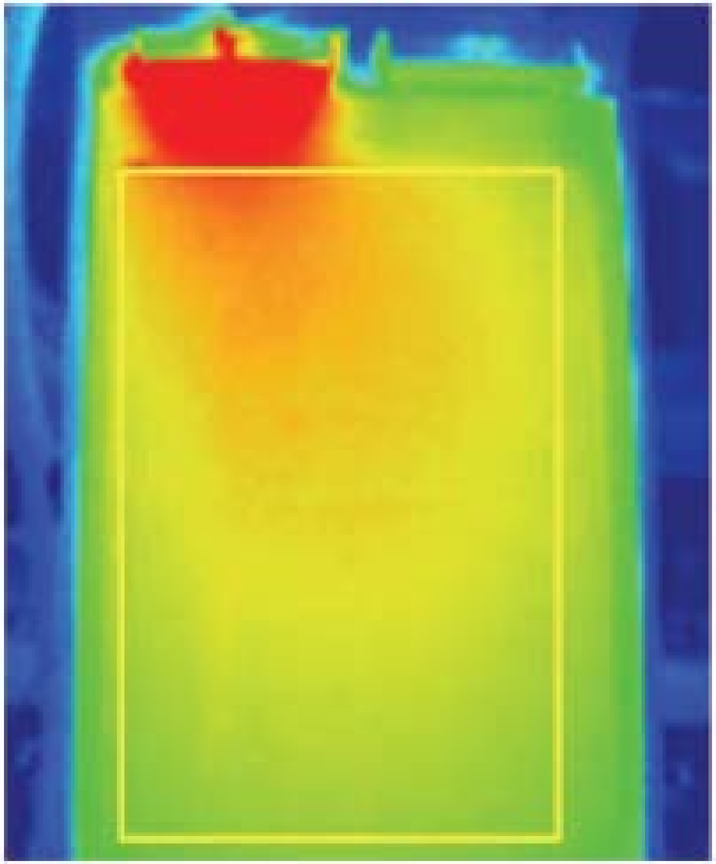
Technical Accomplishment

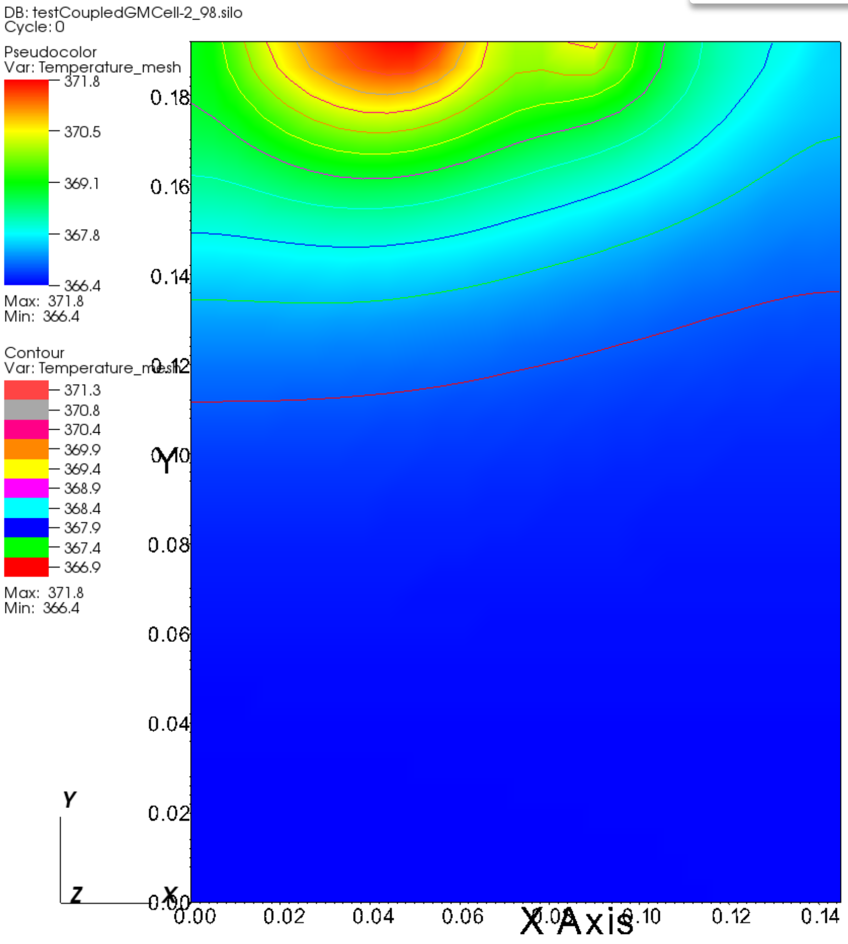
- **Typically complex geometry (prismatic or cylindrical) 3D Unstructured Grid**
  - The resolution is typically much lower than what is needed for the electrode/cell-sandwich simulations so there is upscaling of different quantities
- **Solve for temperature, ohmic resitance in the electrical connections,**
- **Variables such as Temperature, Electric potential (current collectors), Heat Sources, Stress / Strain, Gas release / composition**

Output to cell-sandwich calculations (CC voltage/current and temperature)

Comparison of Temperature distributions for LIB at 11 min with a discharge rate of 5 C – Demo Problem 2

Technical Accomplishment





Good qualitative agreement – requesting missing information from the authors to complete validation

"Modeling the Dependence of the Discharge Behavior of a Lithium-Ion Battery on the Environmental Temperature", Kim, U.S. and Yi, J. and Shin, C.B. and Han, T. and Park, S., *Journal of the Electrochemical Society*, 158, 2011

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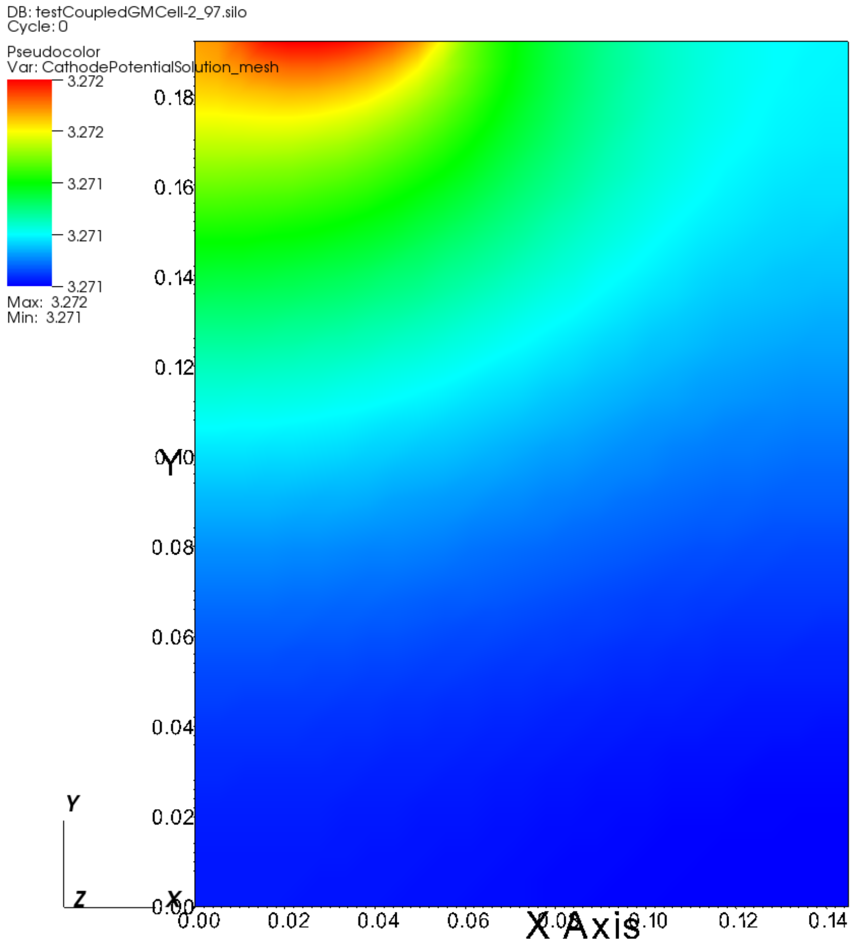
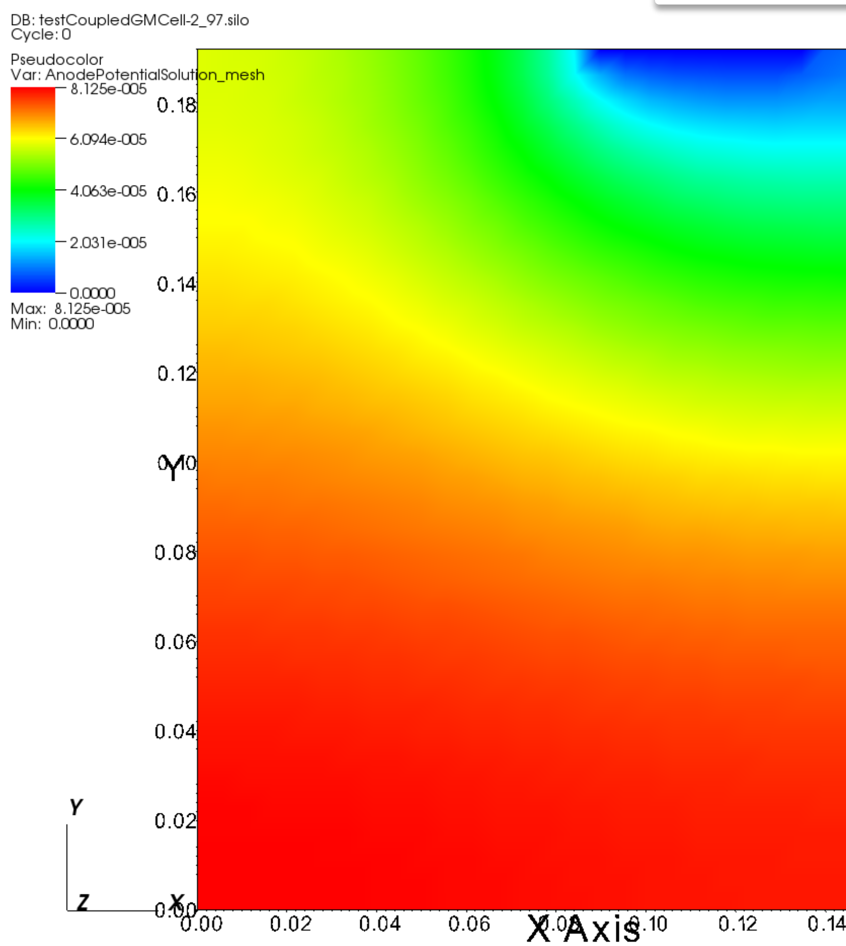
Cathode and Anode Potential distributions for LIB at 11 min with a discharge rate of 5 C

Technical Accomplishment





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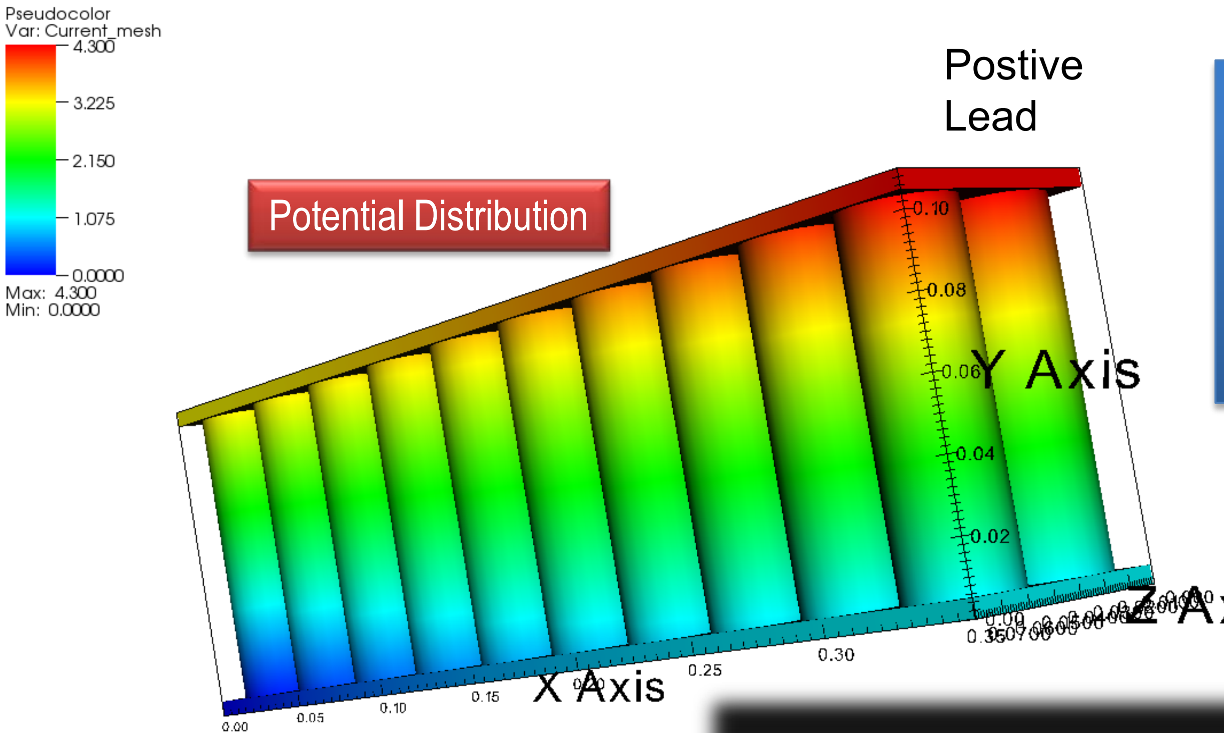
Thermo-Electrochemical-Electrical Simulation Results (Complex Module – Demo 3)

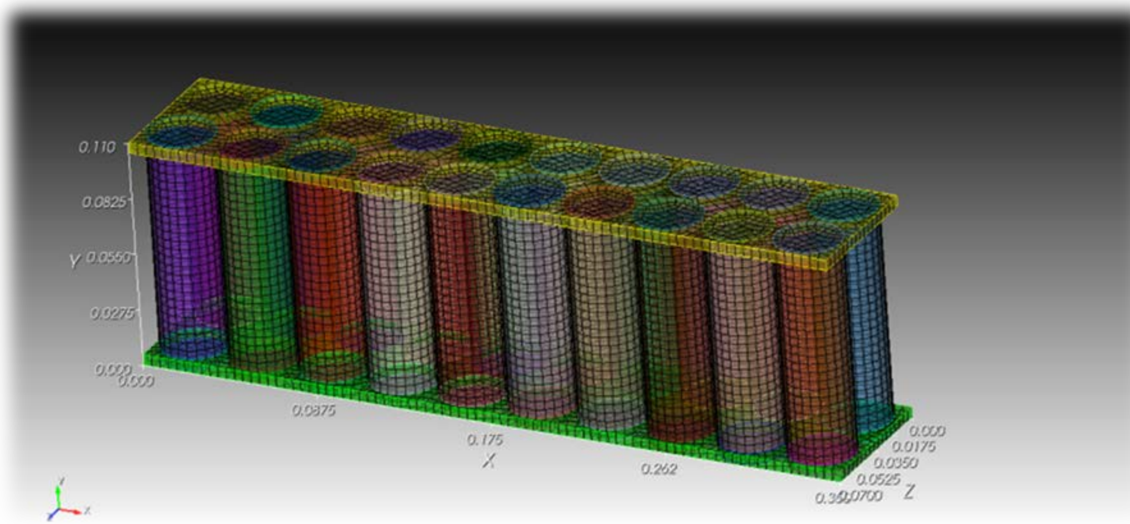
Technical Accomplishment

Postive Lead



Negative Lead

- 3D Electrical Model Coupled to DualFoil Electrochemical model
- In the process of coupling to the 3D thermal model



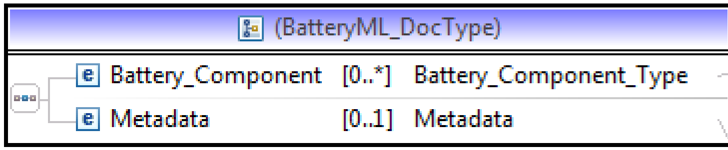
Standardized Input

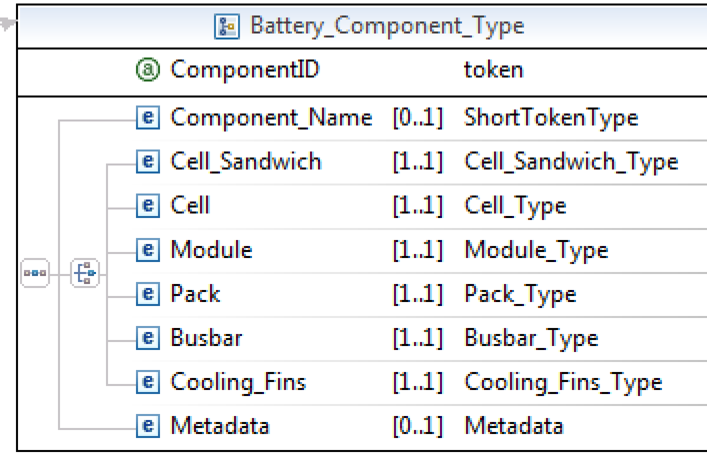
Technical Accomplishment

- Exploit the hierarchical nature of batteries
- Consensus on XML as the standard for the input specification
  - Leverage many third-party tools
  - Facilitates interactive web-based input capability (GUI)
- Translators enable generation of CFD mesh from standard CAD packages
- Common set of tools to process, visualize, and analyze the input data

Inputs (XML Schema and XML data)

Technical Accomplishment





XML Schema exploits the hierarchical structure and provides good design and error checking

```xml
<?xml version="1.0" encoding="UTF-8"?>
<BatteryML_Doc xmlns="Battery:ML"
    xmlns:ns0="Battery:Cell_Sandwich:ML"
    xmlns:ns1="CommonDataTypes:ML:0.1"
    xmlns:ns2="urn:oasis:names:tc:unitsml:schema:xsd:UnitsMLSchema-1.0"
    xmlns:w0="http://www.matml.org" xmlns:x0="http://www.w3.org/2001/XMLSchema">
    <Battery_Component ComponentID="cs1">
        <Cell_Sandwich>
            <ns0:Dual_Foil_Model Dual_FoilID="doyle_1996">
    </Cell_Sandwich>
    </Battery_Component>

    <Battery_Component ComponentID="NREL-RC">
        <Cell_Sandwich>
            <ns0:RC_Model RCID="rc1">
        </Cell_Sandwich>
    </Battery_Component>

    <Battery_Component ComponentID="cs3">
        <Cell_Sandwich>
            <ns0:NTG_Model NTGID="ntg11">
        </Cell_Sandwich>
    </Battery_Component>
</BatteryML_Doc>
```

XML file as standard input – easy to re-use elements and component inputs

Collaboration and Coordination

- Monthly telecon/web-meeting with DOE and NREL
- Visit to NREL in Dec. 2010
- Participated in the three kick-off meetings
- We had a joint meeting at ORNL with ORNL, NREL, CAEBAT Partners and DOE
- Several telecons/web-meetings to present and discuss the Battery State and Input Standards with all the CAEBAT partners
- US Drive Energy Storage meeting
- Interactions with ANL on the cost model

Future Work - Planned Activities

- **Near term**
  - Improve workflow as well as portability to Windows
  - Interfaces to the inputs and battery state standards
  - Integrate additional components (NREL models and ANL cost model)
  - Demonstrate for complex geometries with new interfaces
  - Integrate additional components (NREL models and ANL cost model)
  - Demonstrate for complex geometries with new interfaces
- **Longer term**
  - Component interfaces and in-memory transfer
  - Integrate the components from the three project commercial partners
  - Integrate the components from other national labs and universities
  - Thorough verification and validation
  - Extensively populate the input state

Summary

- We have a very good version of the open architecture software for file-based transfer between different components for electrochemistry, transport, electrical and mechanical stresses
- We have an initial standard for the battery state
- We have an initial XML schema and standard for the inputs
- We have integrated 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
  - Integrate models from NREL
  - Integrate the ANL cost model
- We are on track for the year-end release of the beta version of OAS + VIBE (with few examples) along with input XML schema and battery state definition

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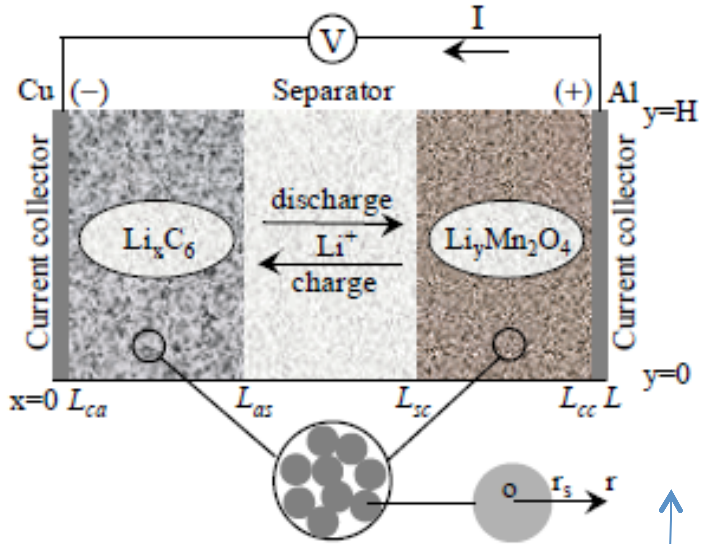
Technical Backup Slides

Thermo-Electrochemical Modeling – Demo problem 1

Technical Accomplishment



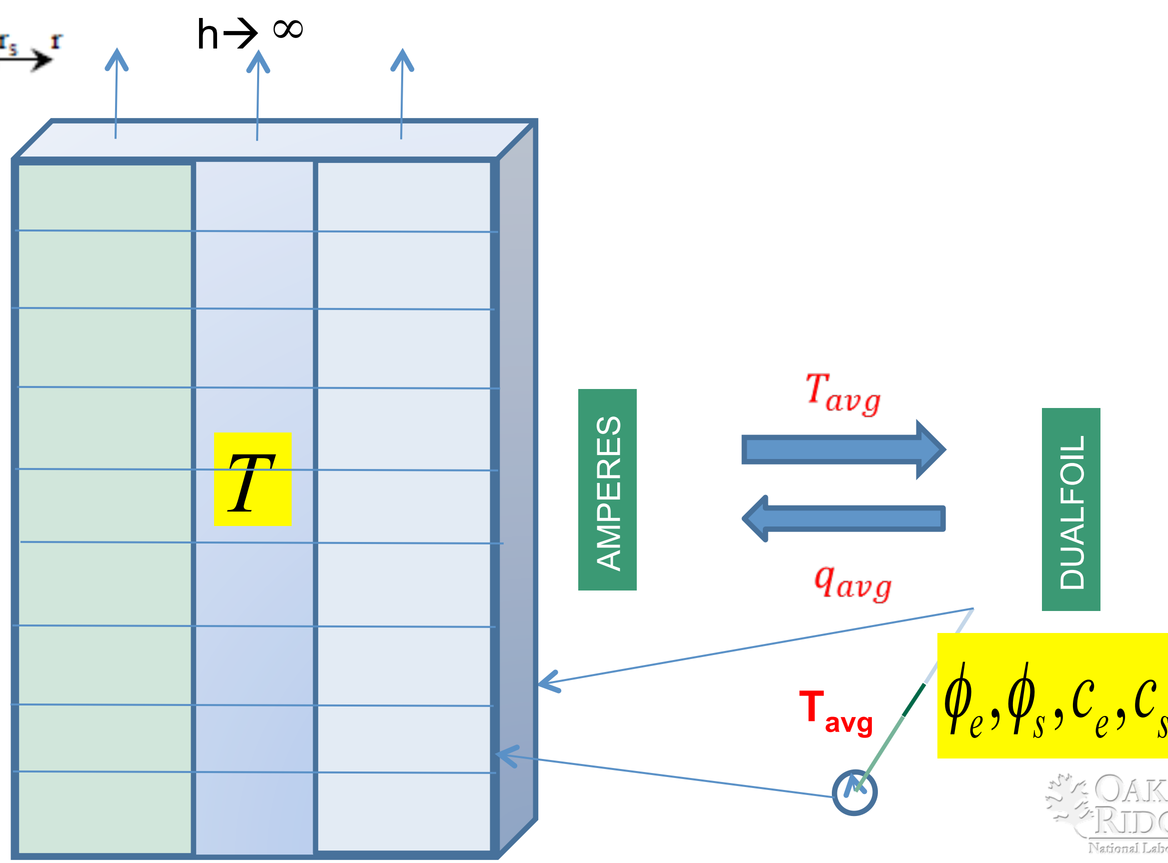
Composite positive electrode

$$Li_{y-x}Mn_2O_4 + xLi^+ + xe^- \underset{\text{charge}}{\overset{\text{discharge}}{\rightleftharpoons}} Li_yMn_2O_4$$

Composite negative electrode

$$Li_xC_6 \underset{\text{charge}}{\overset{\text{discharge}}{\rightleftharpoons}} Li_0C_6 + xLi^+ + xe^-$$

Solution Methodology



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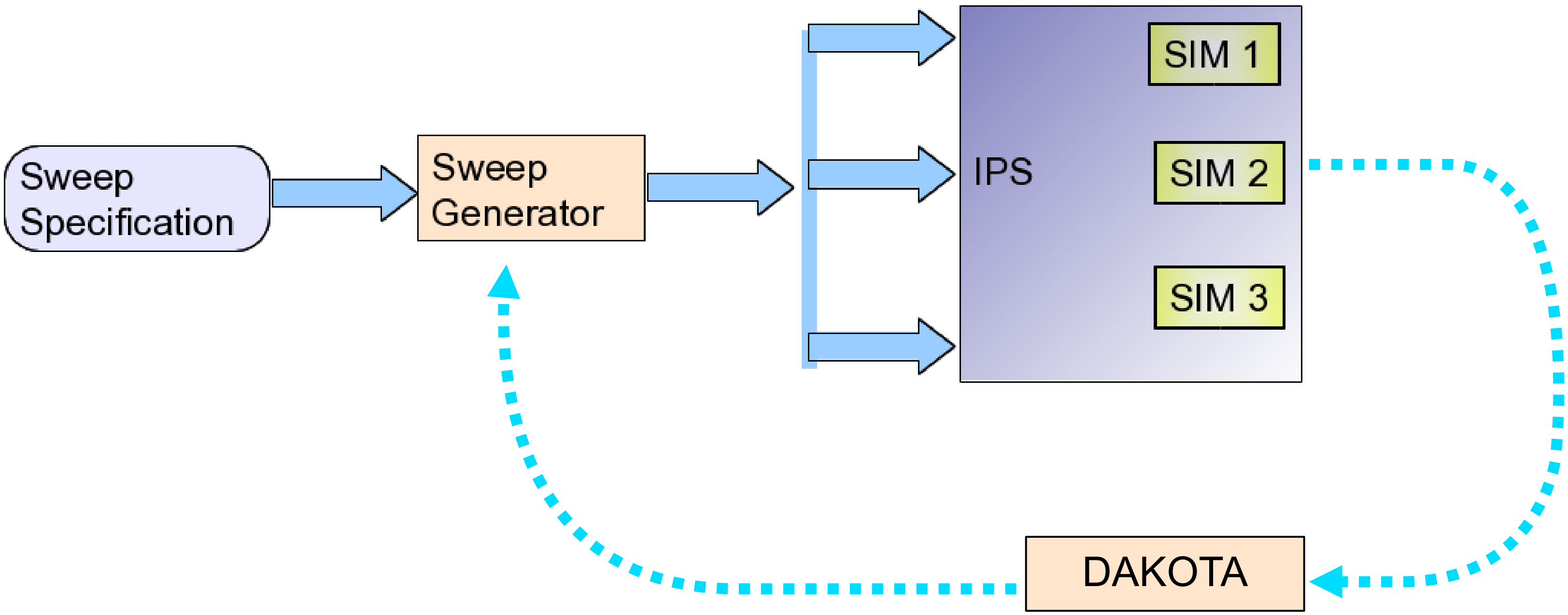
Parameter Sweep using the IPS (Phase 1)

Technical Accomplishment



- **Dynamic parameter generation for design optimization using the DAKOTA tool kit (From Sandia National Lab)**

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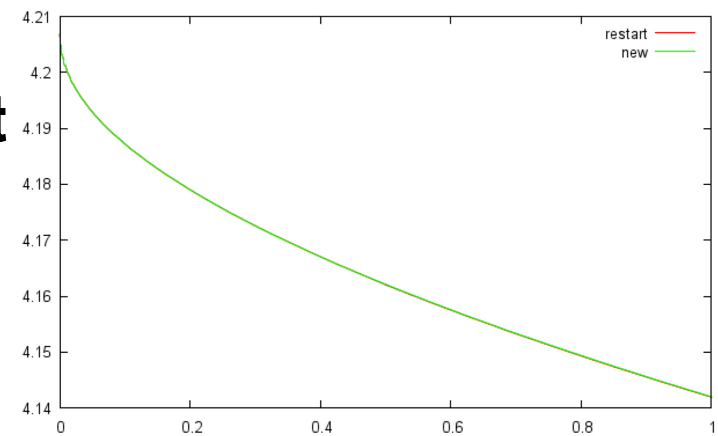
Modifications to software components for initial demonstration

Technical Accomplishment

- **Changes to DualFoil**
  - very minimal changes for one way coupled
  - minor modifications to write the information needed for battery state as a function of time and space
  - **additional modifications to allow restart**
- **Changes to Amperes**
  - very minimal changes
  - minor modifications to read the input files generated by the prepare input wrapper
  - additional arguments for conducting the parametric sweeps through the IPS-VIBE framework

Verification of the restart capability



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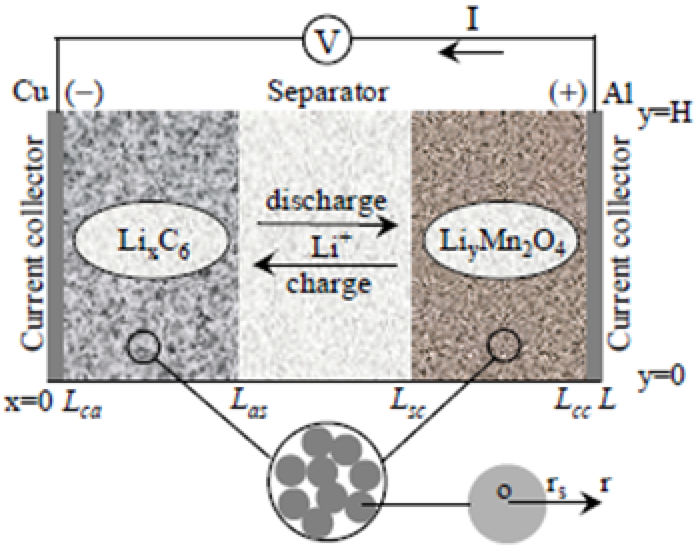
Thermo-Electrochemical-Electrical Modeling – Demo Problem 2

Technical Accomplishment



Composite positive electrode

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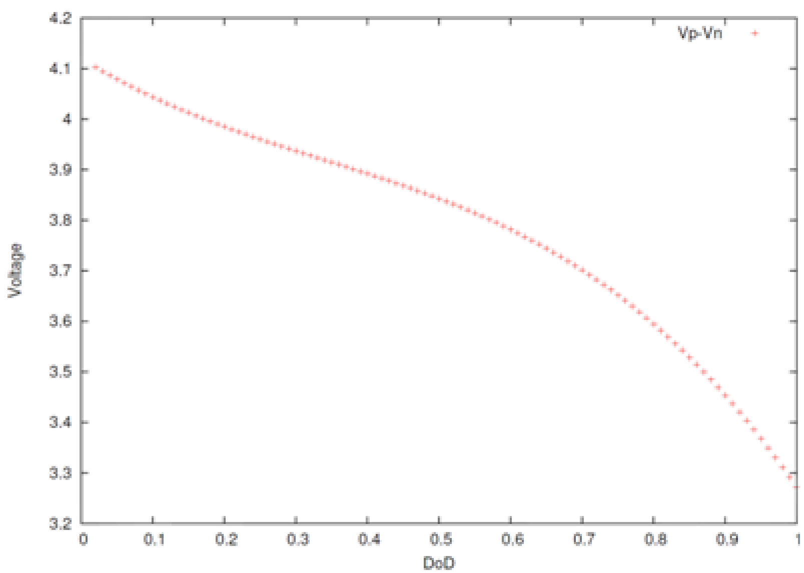
Composite negative electrode

$$Li_xC_6 \underset{\text{charge}}{\overset{\text{discharge}}{\rightleftharpoons}} Li_0C_6 + xLi^+ + xe^-$$

Discharge curve at rate of 5 C



Conservation of current flow is given by:

$$\nabla \cdot i = J$$

$$where \quad i_p = -\frac{1}{r_p}\nabla V_p \text{ in } \Omega p \quad \text{and} \quad i_n = -\frac{1}{r_n}\nabla V_n \text{ in } \Box n$$

Conservation of energy is given by:

$$\rho Cp\frac{\partial T}{\partial t} - \frac{\partial}{\partial x}\left(kx\frac{\partial T}{\partial x}\right) - \frac{\partial}{\partial y}\left(ky\frac{\partial T}{\partial y}\right) - \frac{\partial}{\partial z}\left(kz\frac{\partial T}{\partial z}\right) = q - qconv$$

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

"Modeling the Dependence of the Discharge Behavior of a Lithium-Ion Battery on the Environmental Temperature", Kim, U.S. and Yi, J. and Shin, C.B. and Han, T. and Park, S., *Journal of the Electrochemical Society*, 158, 2011

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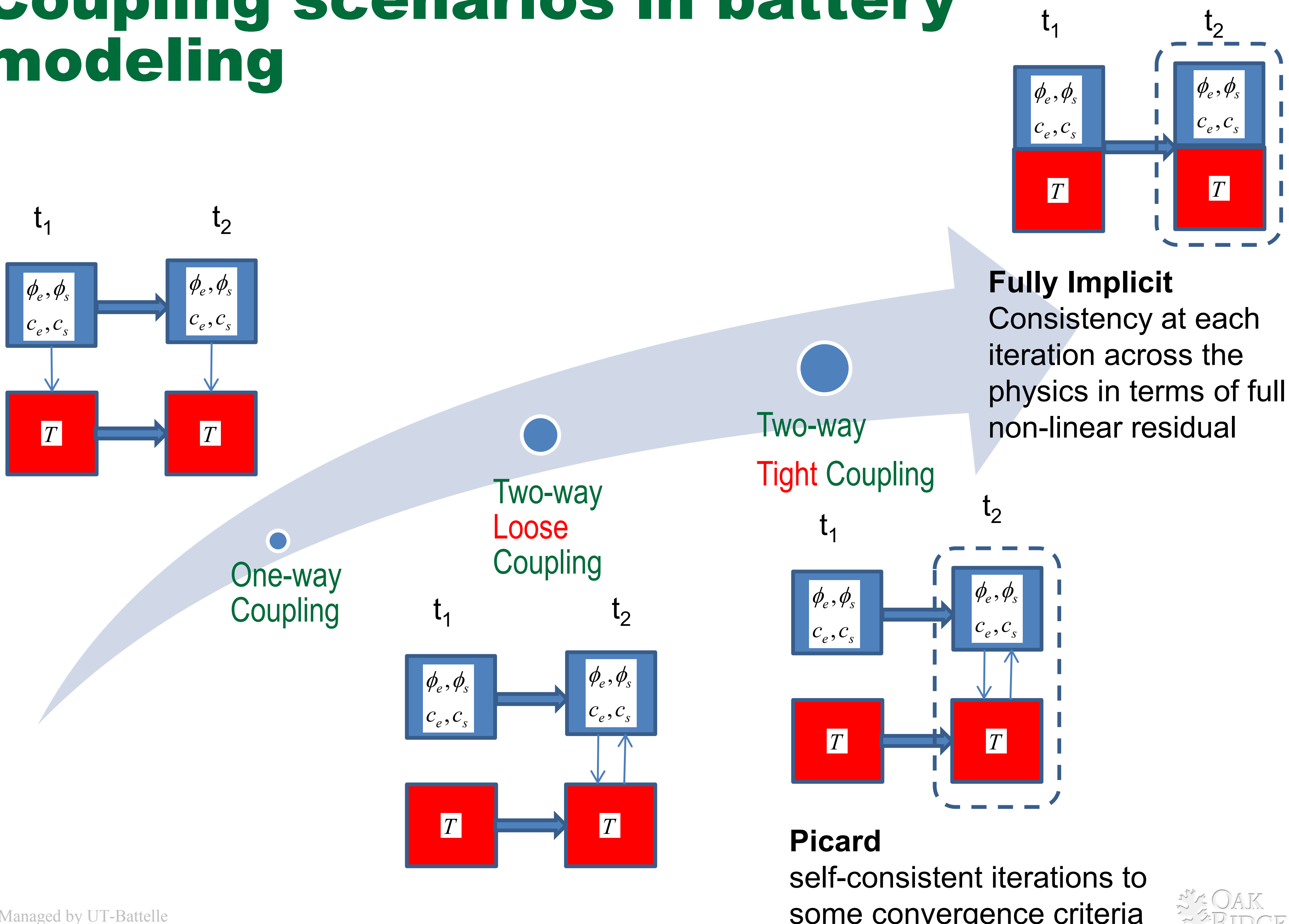
Coupling scenarios in battery modeling



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