ANSYS

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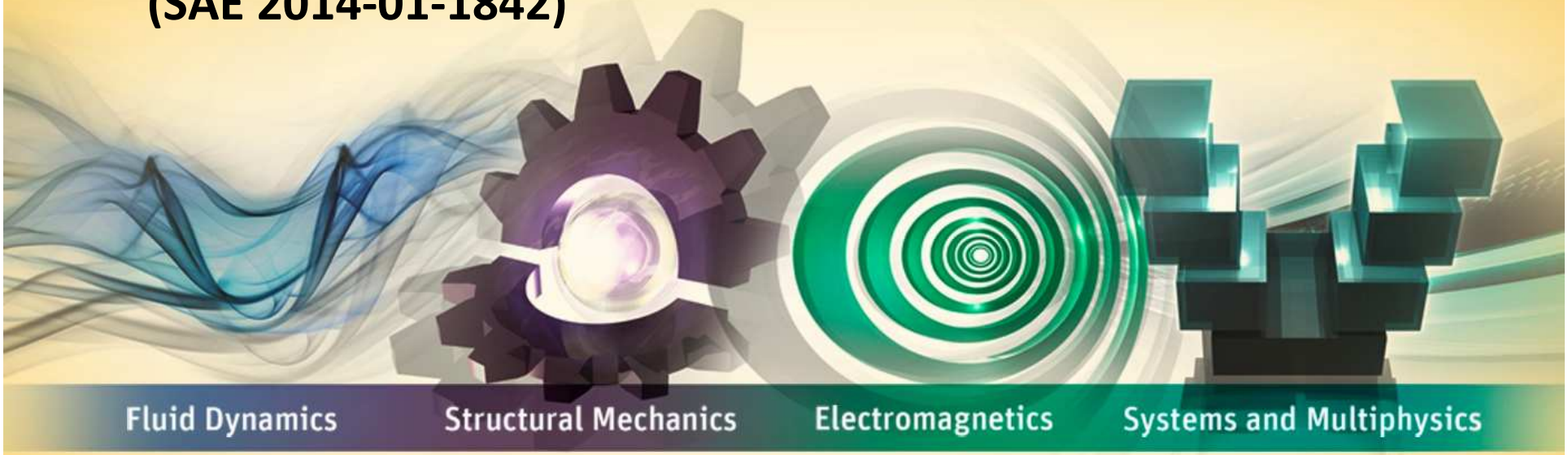
A Total Li-Ion Battery Simulation Solution

(SAE 2014-01-1842)



Xiao Hu and Scott Stanton

ANSYS Inc.

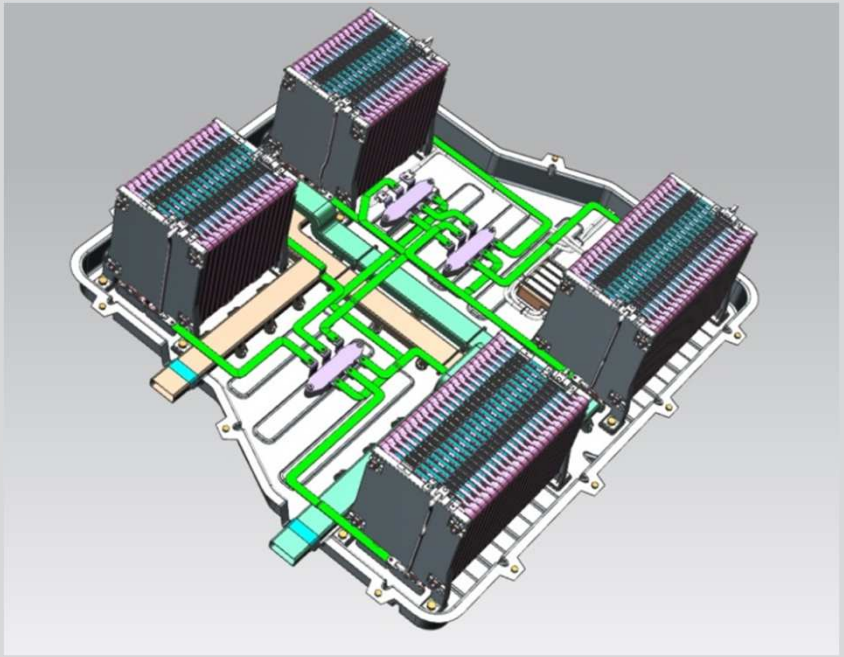
A Total Li-Ion Battery Simulation Solution

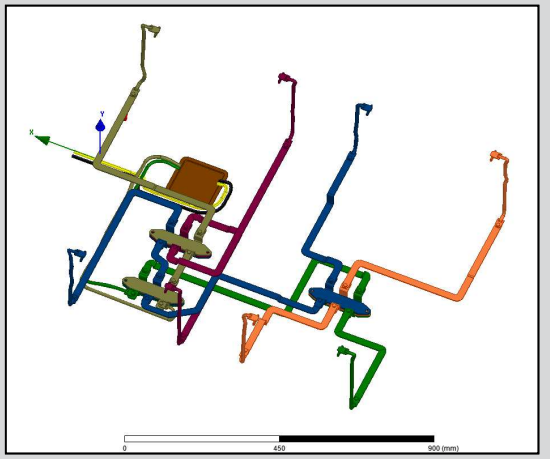
Small Scale

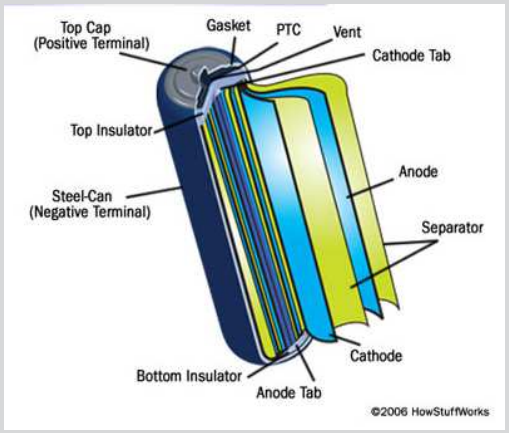
Large Scale

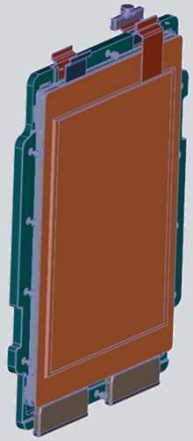
Molecular	Electrode	Cell	Module/Pack	Powertrain
Materials	Layout Process Life SEI	Charging Discharging Heating Safety	Thermal Mgt Durability NVH EMI/EMC	System Integration
	Electro-chemistry	ECM CFD FEA	ECM CFD ROM FEA	ECM ROM

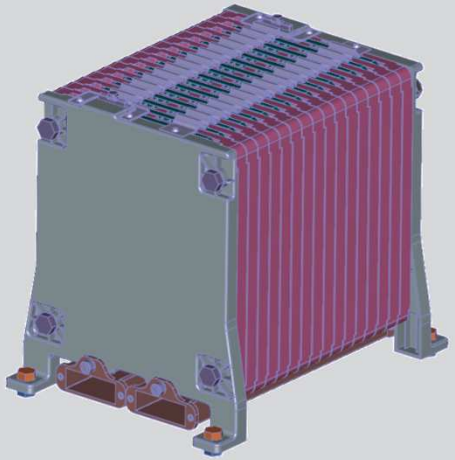
A Total Li-Ion Battery Simulation Solution



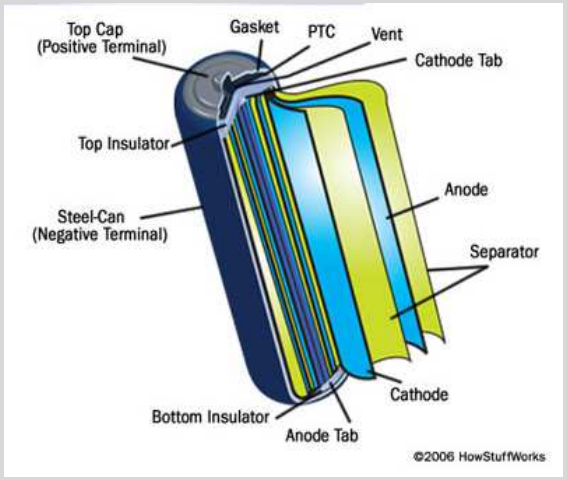


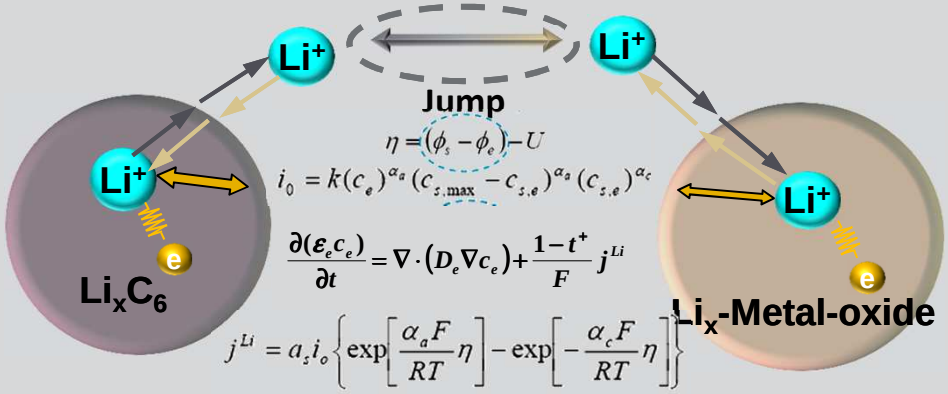




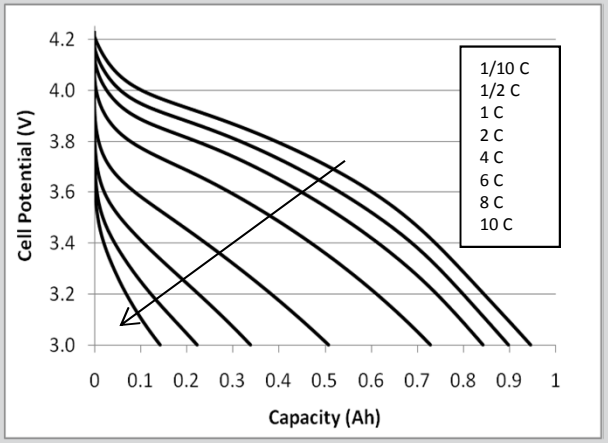


Electrode Level - Electrochemistry

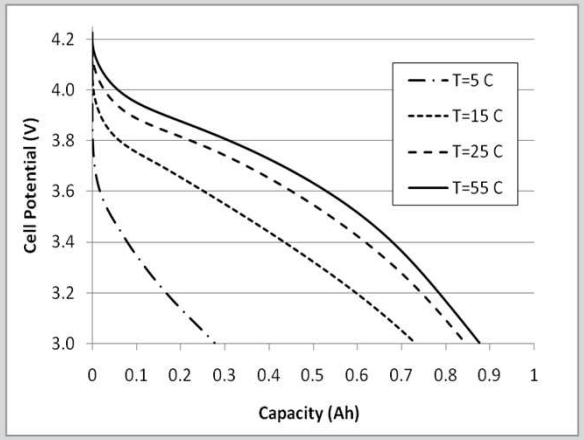




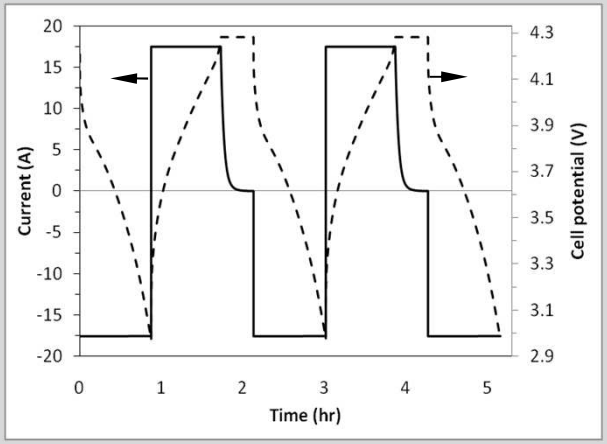
- Electrochemical Kinetics
- Solid-State Li Transport
- Electrolytic Li Transport
- Charge Conservation/Transport
- (Thermal) Energy Conservation



Impact of Discharge Rate on Capacity



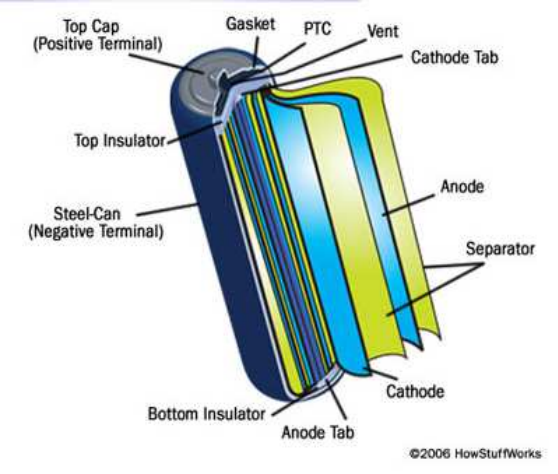
Temperature Impact on Capacity

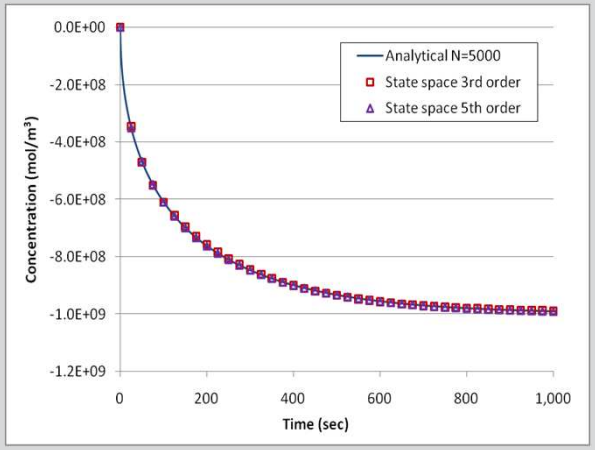


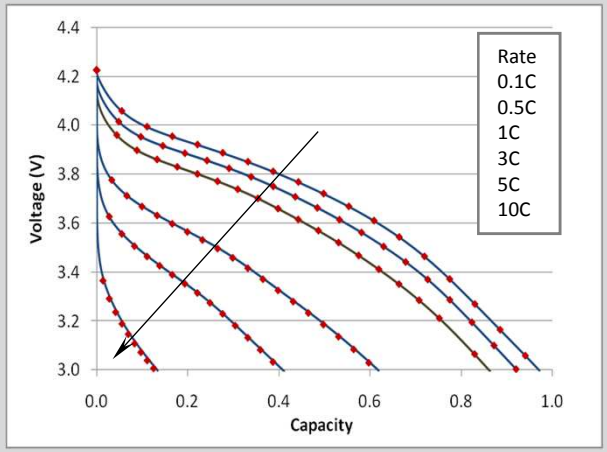
Charge Discharge Cycles

X. Hu, S. Lin, S. Stanton, SAE paper 2012-01-0665

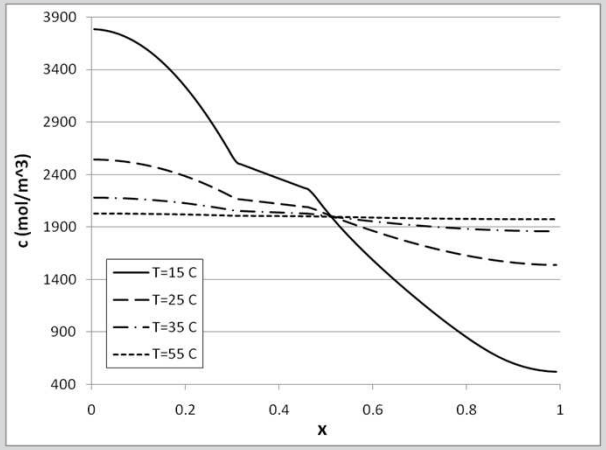
Electrode Level - Electrochemistry



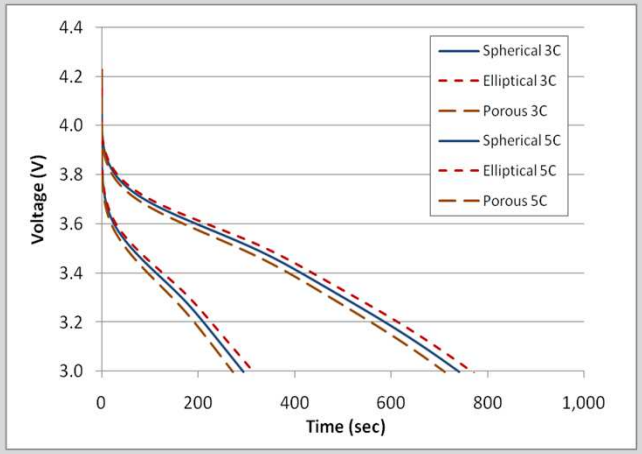




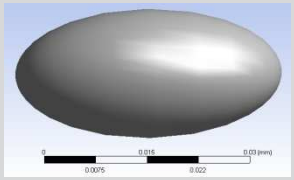
Validation of Reduced Order Electrochemistry

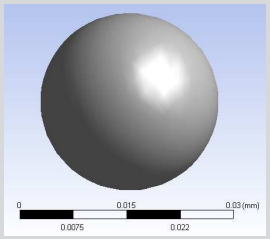


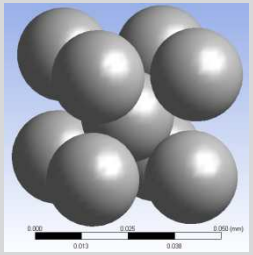
Impact of Temperature on Concentration Distribution



Impact of Particle Shape on Capacity







[1] X. Hu, S. Stanton, L. Cai, R.E. White, J. Power Sources 214, 40-50, 2012.
[2] X. Hu, S. Stanton, L. Cai, R.E. White, J. Power Sources 218, 212-220, 2012.

Electrochemistry for Thermal Runaway

- **Energy Equation + Heat Source**
  - **Energy Equation（Default）**

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

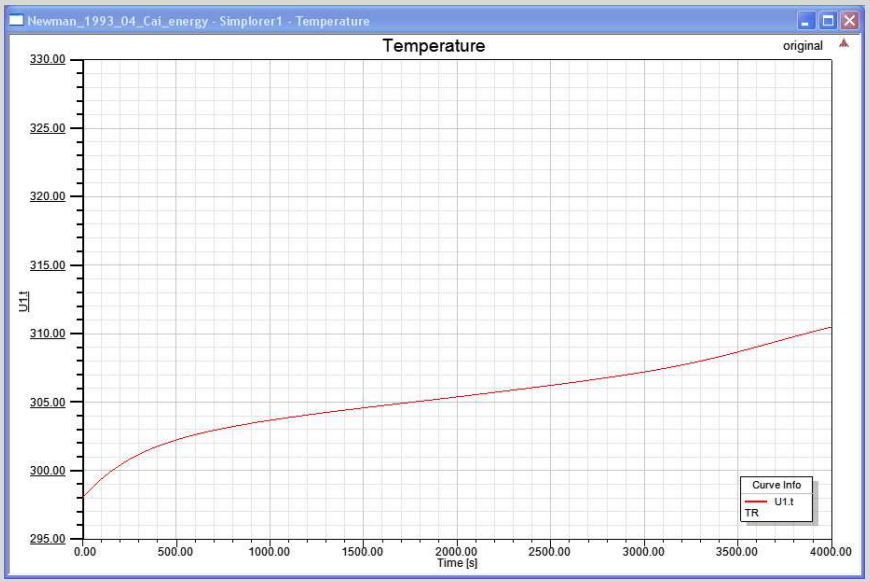
  - **Heat Source (reaction heat + Joule heating)**

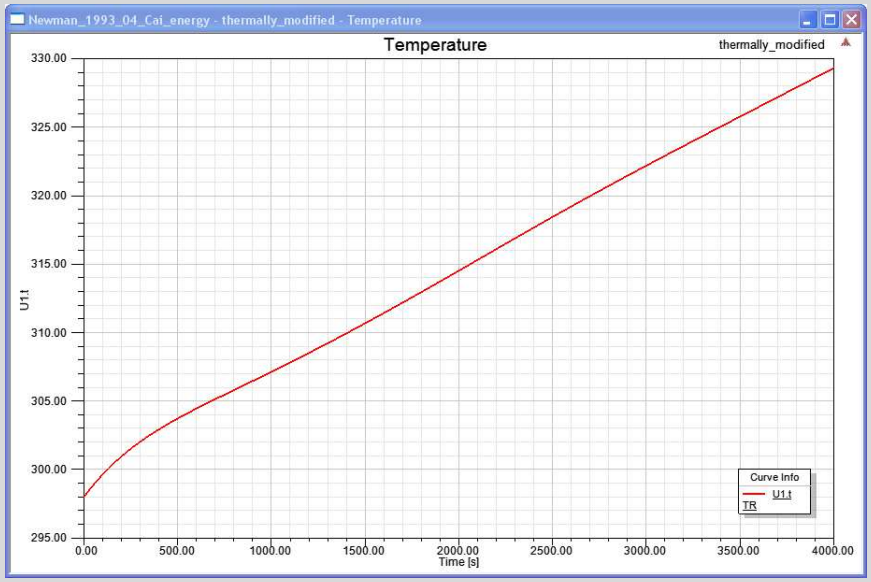
$$q = a_{sj} \bar{i}_{nj} \left(\phi_s - \phi_e - U_j + T \frac{\partial U_j}{\partial T} \right)$$

$$+ \sigma^{eff} \nabla \phi_s \cdot \nabla \phi_s + \left(\kappa^{eff} \nabla \phi_e \cdot \nabla \phi_e + \kappa_D^{eff} \nabla \ln c_e \cdot \nabla \phi_e \right)$$

W. B. Gu, C. Y. Wang, Journal of Electrochem. Soc., 147 (8), 2910-2922 (2000)

Electrochemistry for Thermal Runaway

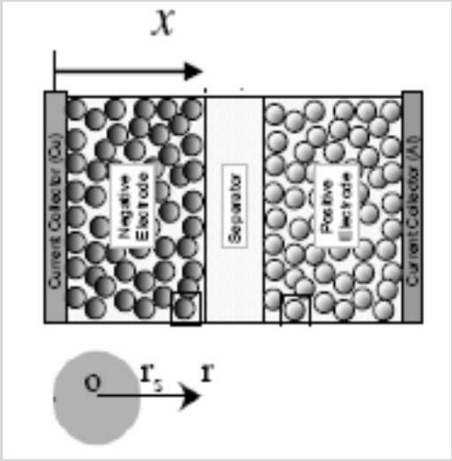




- **Shows impact of material properties on thermal behavior.**
- **Can also investigate impact of design on thermal behavior, say thickness of the separator.**

W. B. Gu, C. Y. Wang, Journal of Electrochem. Soc., 147 (8), 2910-2922 (2000)

Newman P2D Electrochemistry Model in Fluent (CAEBAT project)



Domains

- negative electrode
- separator
- positive electrode
- spherical particles

$$\nabla\cdot(\sigma\nabla\phi_s)-j^{Li}=0 \qquad \nabla\cdot(k\nabla\phi_e)+\nabla\cdot(k_D\nabla\ln c_e)+j^{Li}=0 \qquad j^{Li}=\xi_a i_0\left\{\exp\left(\frac{\alpha_a F}{RT}\eta\right)-\exp\left(-\frac{\alpha_c F}{RT}\eta\right)\right\}$$

$$\frac{\partial(\varepsilon_e c_e)}{\partial t}=\nabla\cdot(D_e\nabla c_e)+\frac{1-t^+}{F}j^{Li} \qquad \frac{\partial c_s}{\partial t}=\frac{D_s}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial c_s}{\partial r}\right)$$

A system of DAEs are solved for every CFD cells:
- Total number of equations: (n_Cs+2) *n_NE + 2n_SP+(N_Cs+2) n_PE
- Memory requirements: N_cell*{(n_Cs+1) *n_NE+ n_SP +(N_Cs+1) n_PE)}

L. Cai and R.E. White, "Reduction of Model Order Based on Proper Orthogonal Decomposition for Lithium-Ion Battery Simulations" J. of Electrochemical. Soc. 156(3) A154-A161 (2009).

Numerical Method

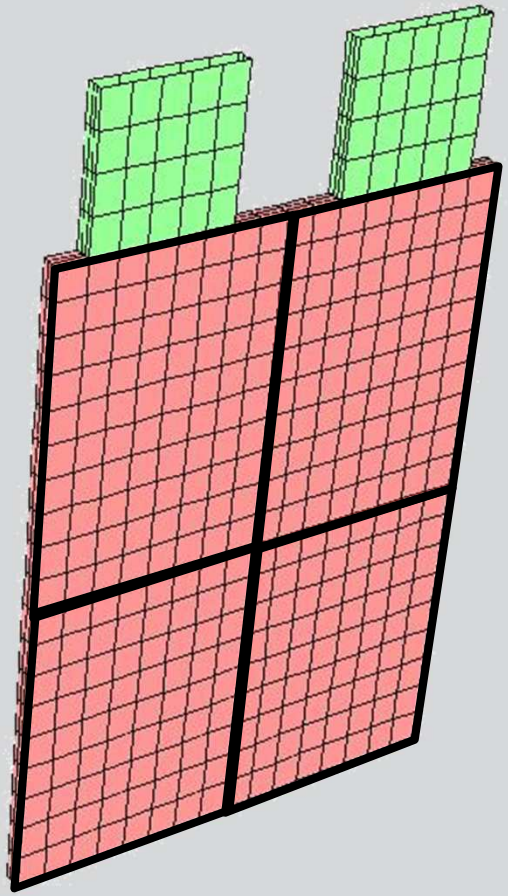
Two user defined scalars are used to solve for ϕ_+ and ϕ_- on CFD mesh

ϕ_+ and ϕ_- are loosely coupled through source term, special treatments are used to enhance the convergence for different current, voltage or power boundary condition

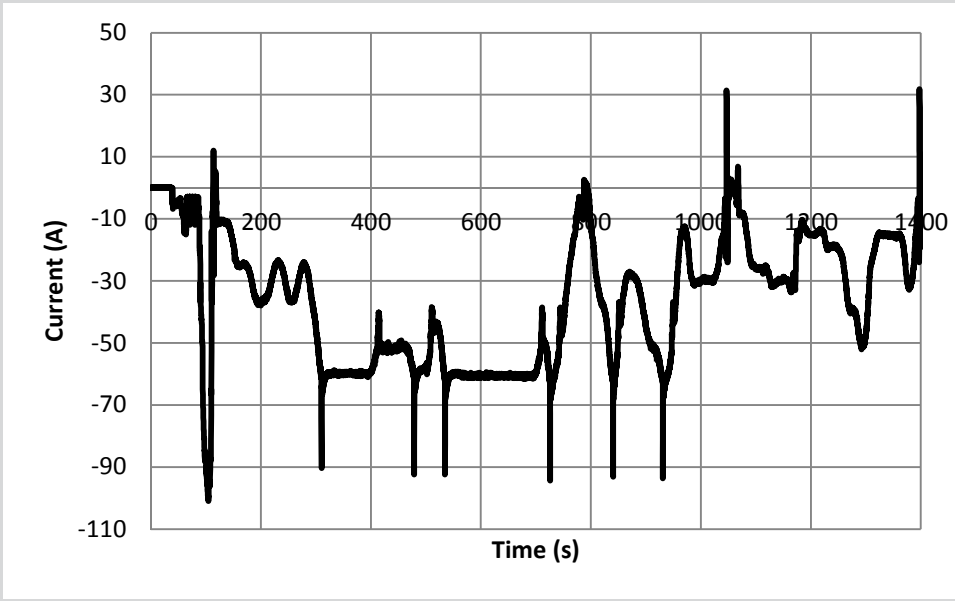
Sundials IDA solver is used to solve E-chemistry.

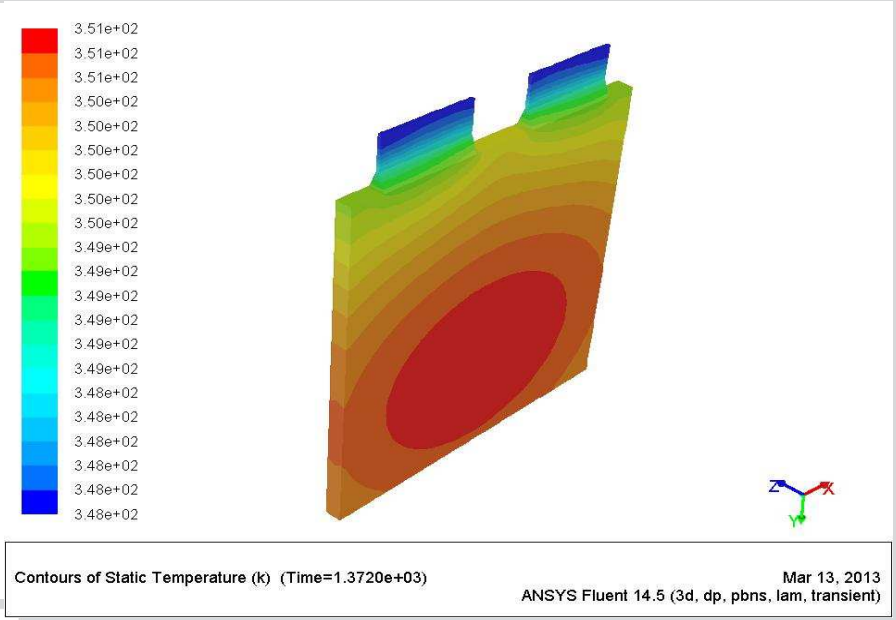
- Newman model: 300~2000 equations.

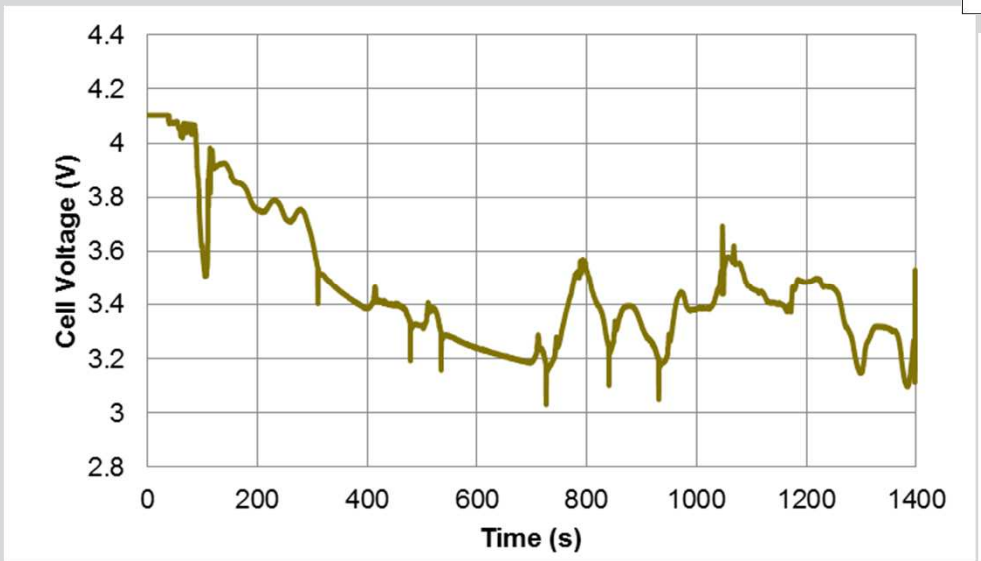
The key is try to reduce the CPU cost!

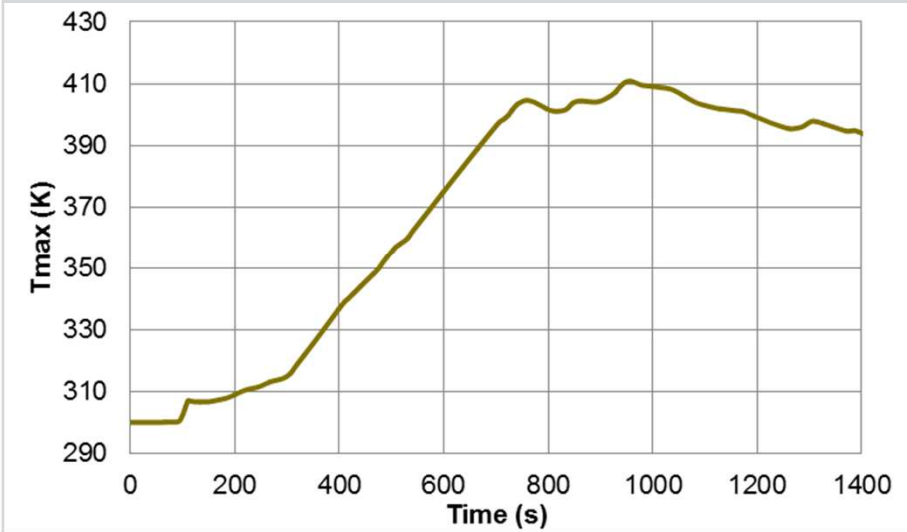


Temperature Results Based on Electrochemistry

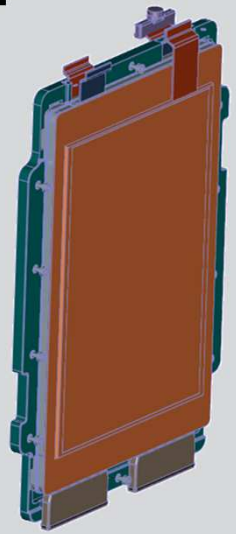


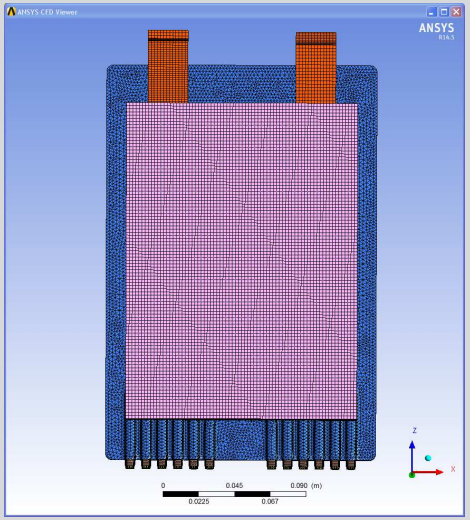


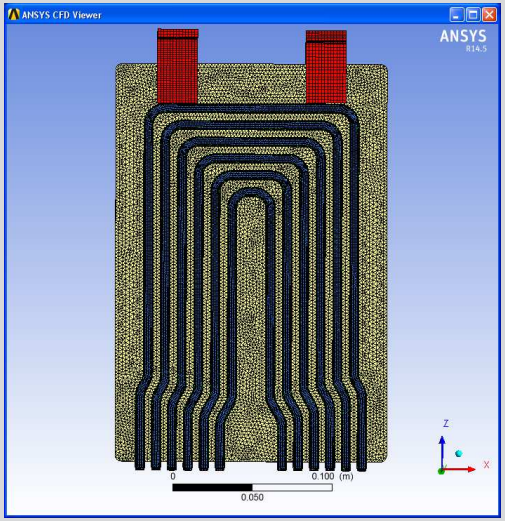


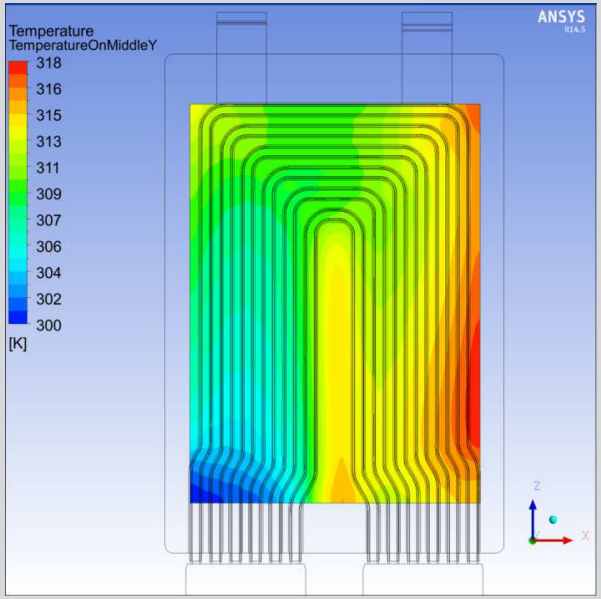


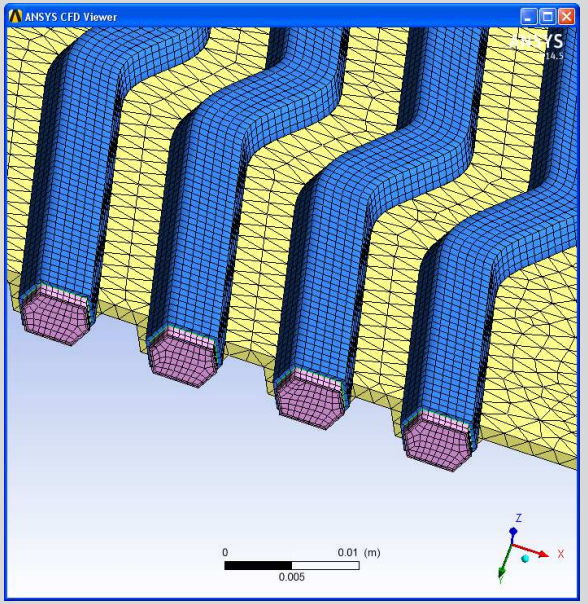
Cell Level – CFD Thermal





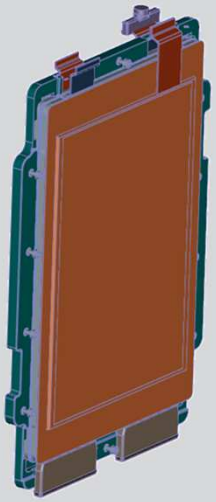






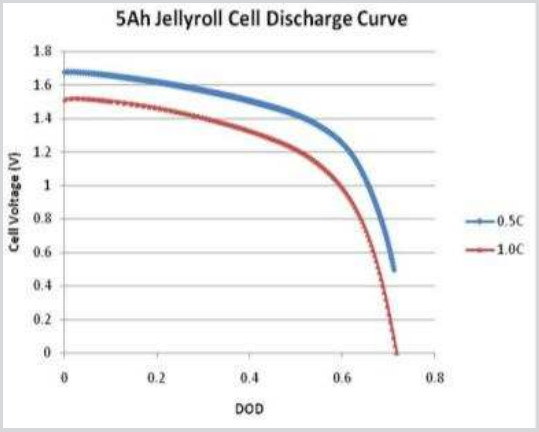
Temperature Distribution

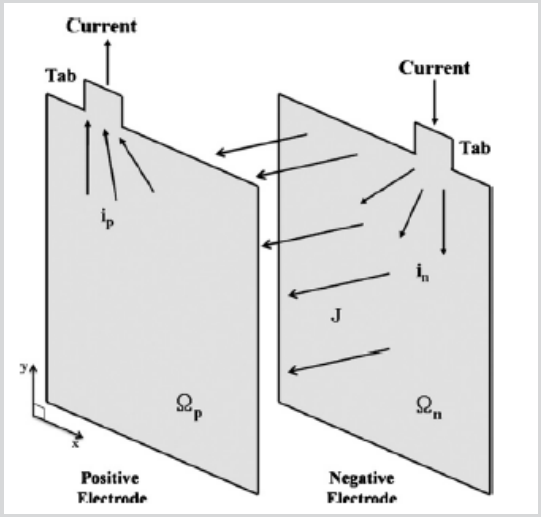
Cell Level –Electro-Thermal



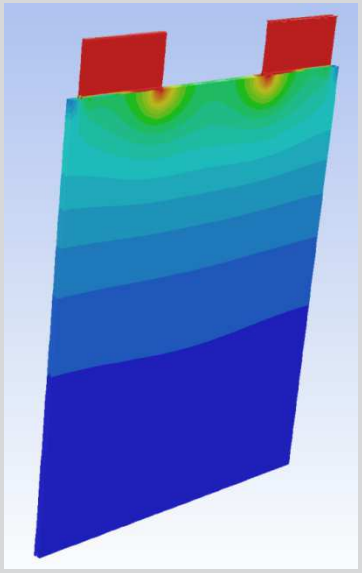
$$\nabla \cdot (\sigma \nabla \phi) = J$$

$$J = Y(\phi_c - \phi_a - U)$$

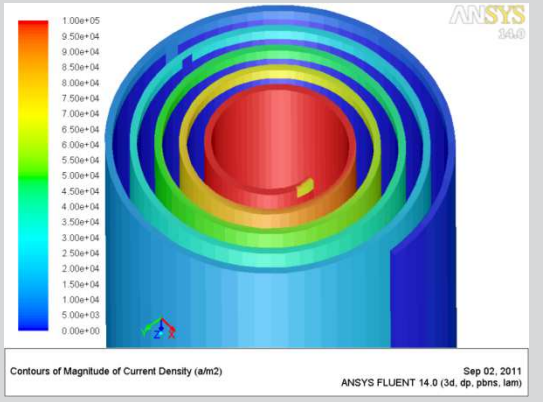




Cathode Anode

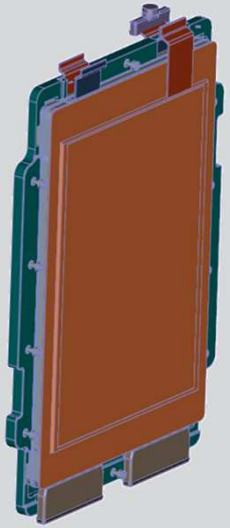


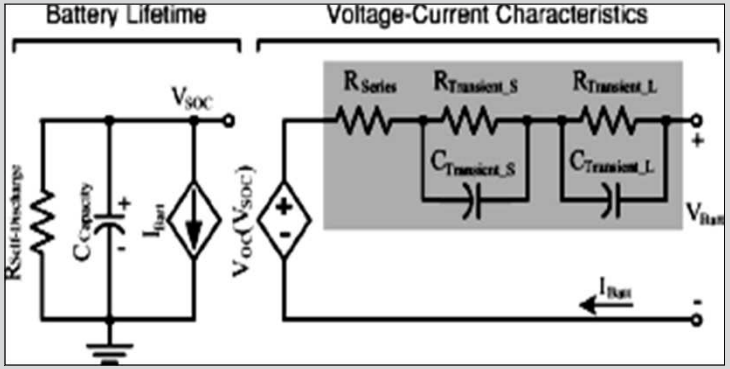
Current Density



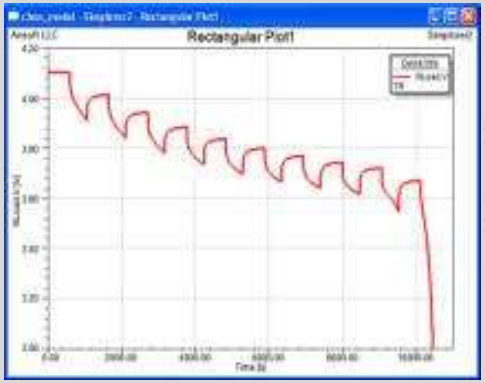
Current Density

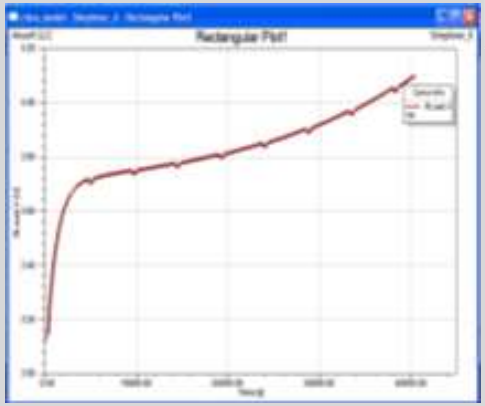
Cell Level – ECM



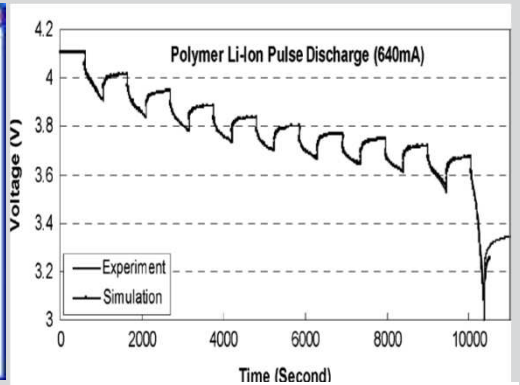


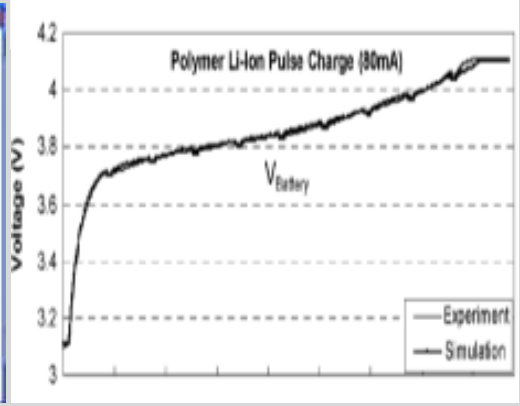
Battery Equivalent Circuit Model (ECM)





Simulation

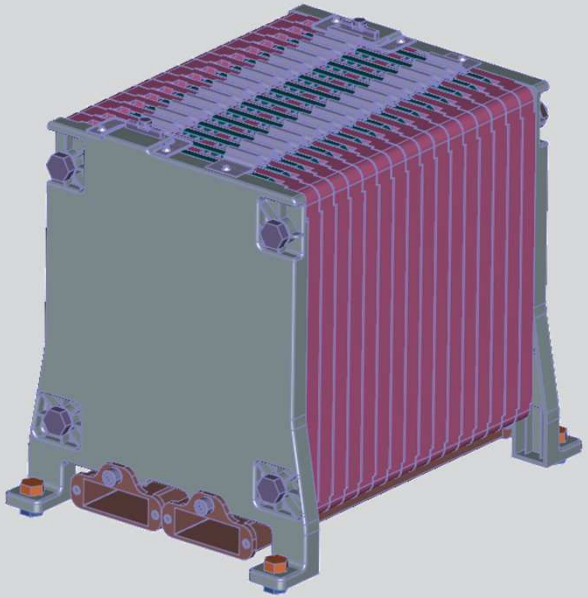




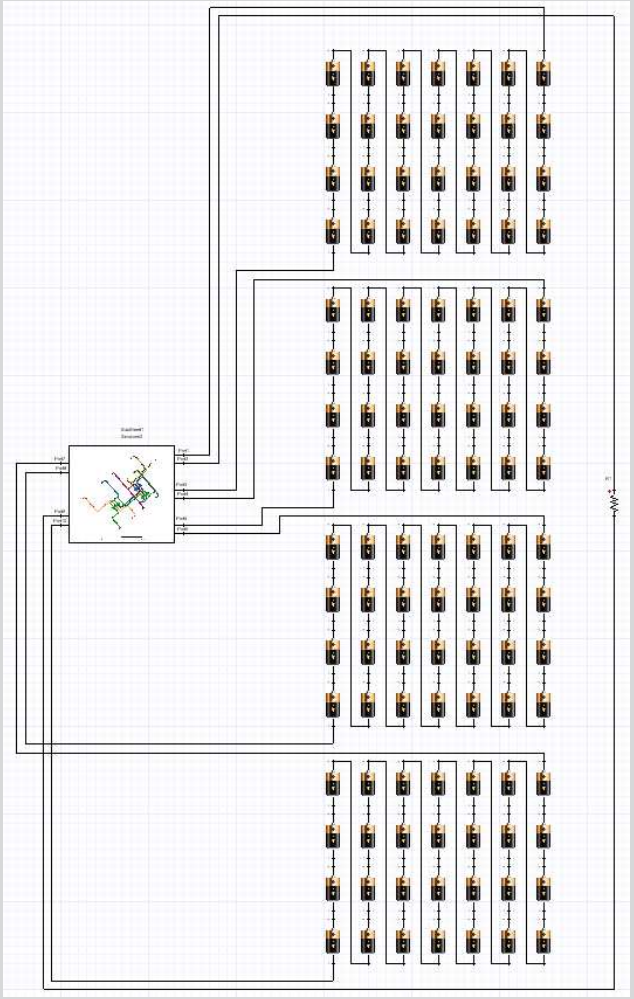
Testing

X. Hu, L. Collins, S. Stanton, S. Jiang, "A Model Parameter Identification Method for Battery Applications", SAE 2013-01-1529.

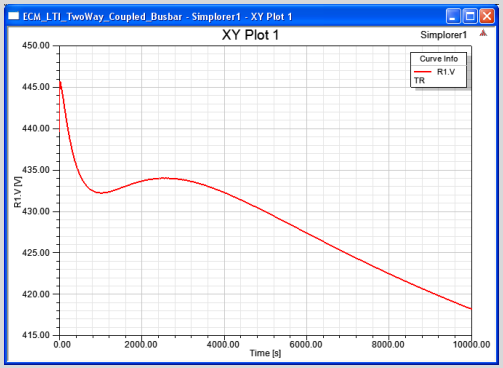
Module/Pack Level – ECM

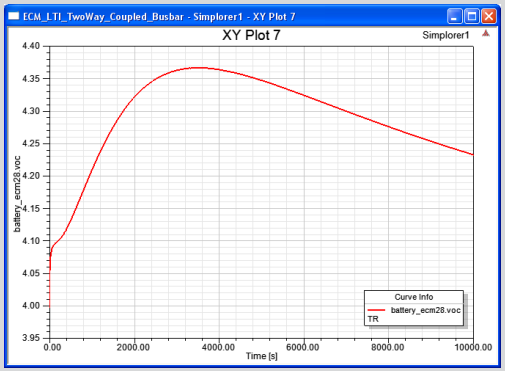


- **28 cells are connected in a module**
- **4 modules are connected to the final configuration**



Battery Pack ECM

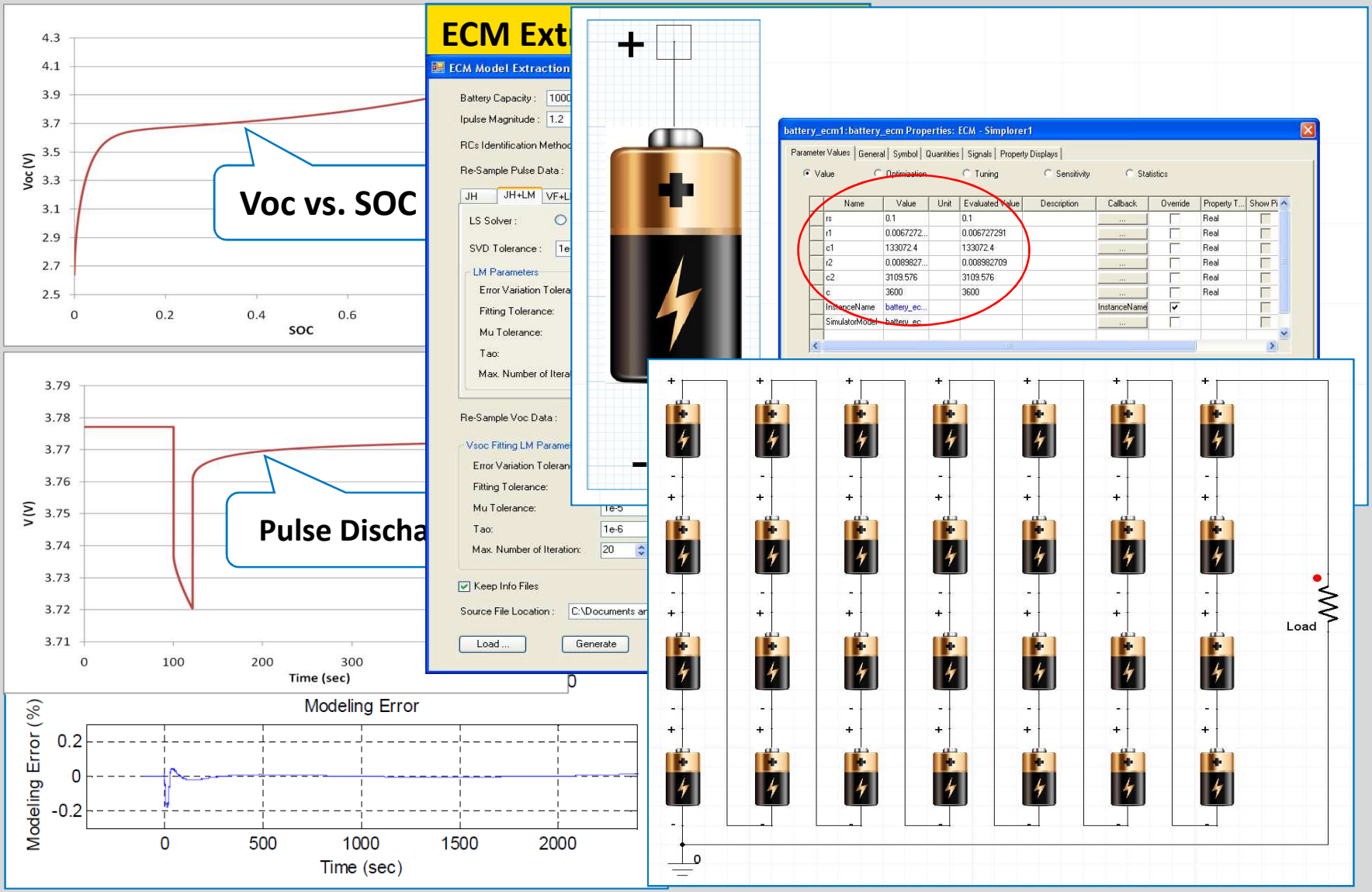




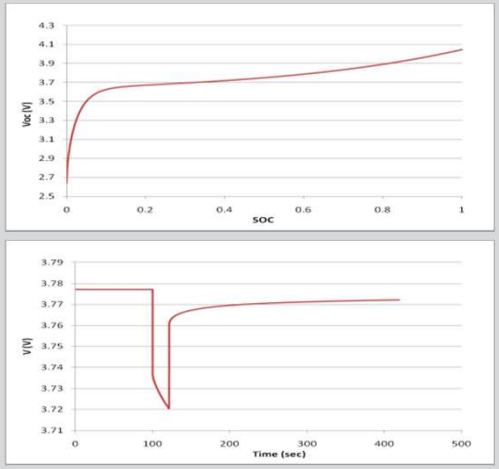
Simulation Results

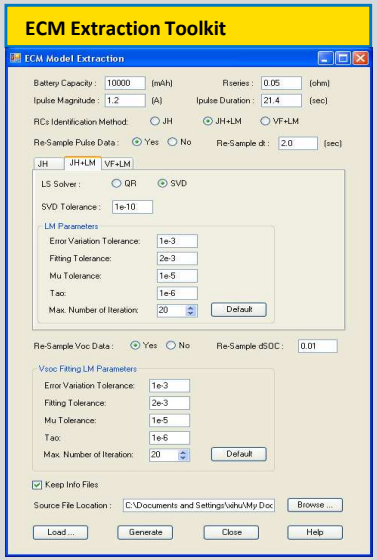
X. Hu, L. Collins, S. Stanton, S. Jiang, "A Model Parameter Identification Method for Battery Applications", SAE 2013-01-1529.

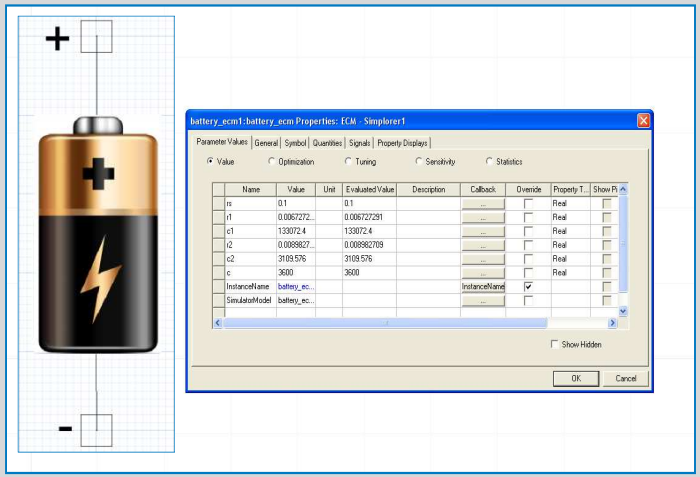
Cell Level – ECM Extraction Tool



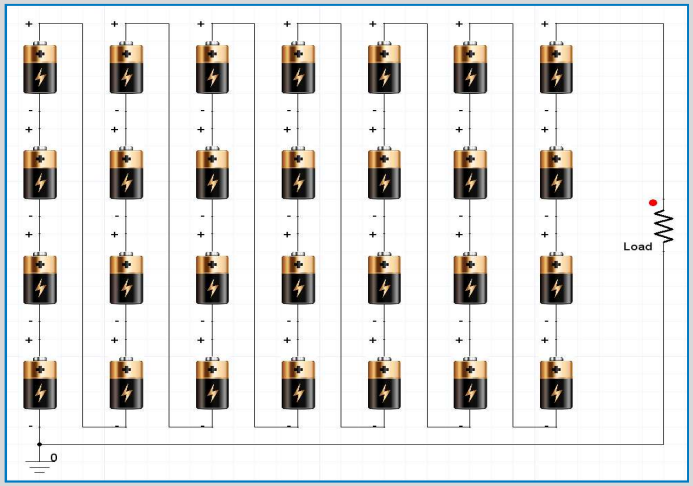
Cell Level – ECM Extraction Tool

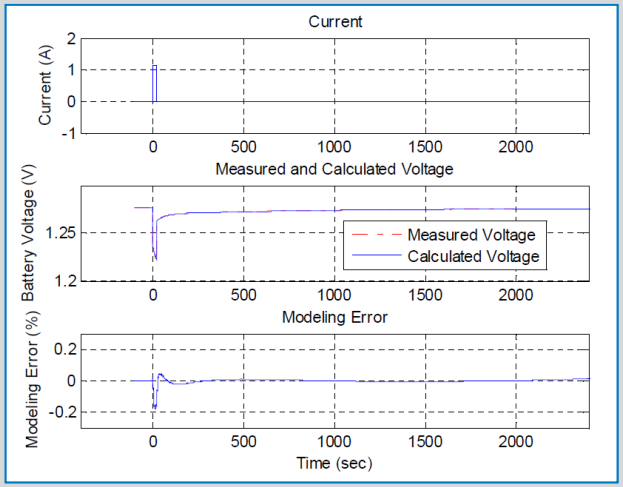






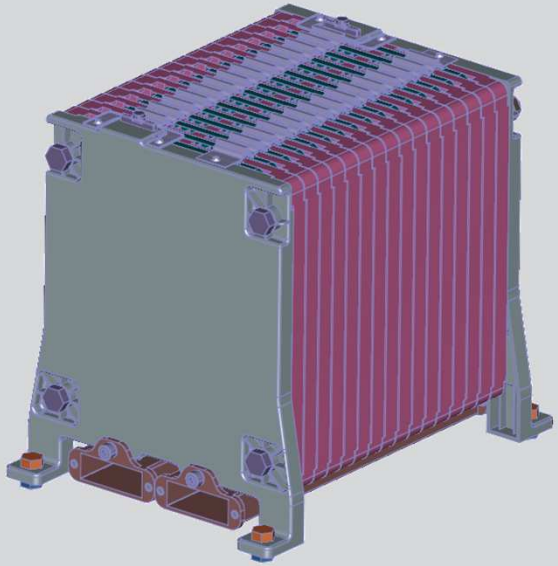
ECM Model Workflow

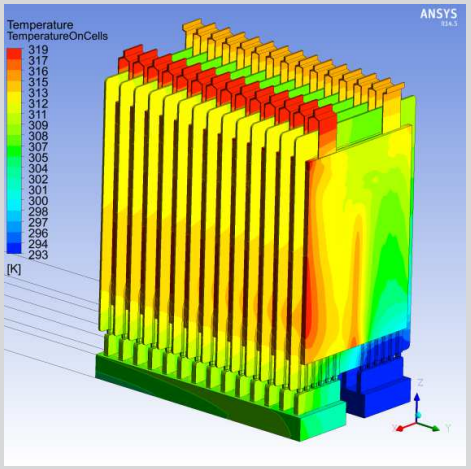




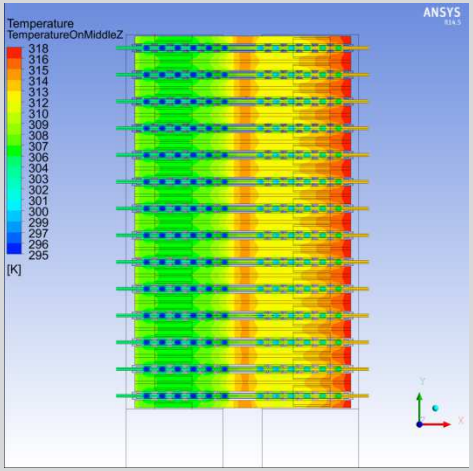
X. Hu, L. Collins, S. Stanton, S. Jiang, "A Model Parameter Identification Method for Battery Applications", SAE 2013-01-1529.

Module Level – CFD Thermal

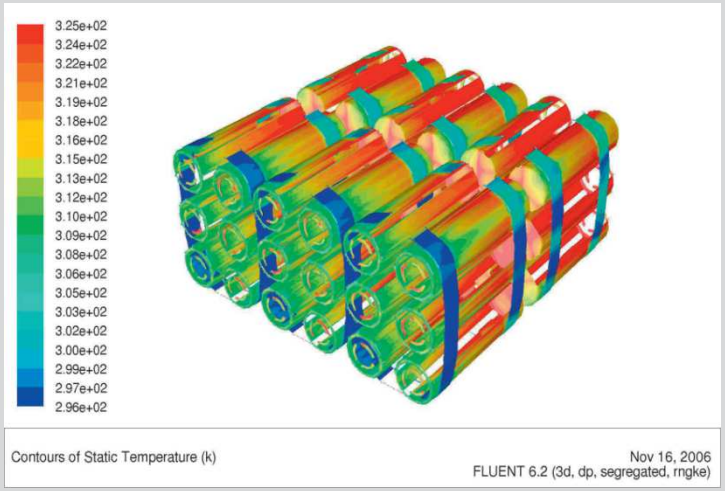




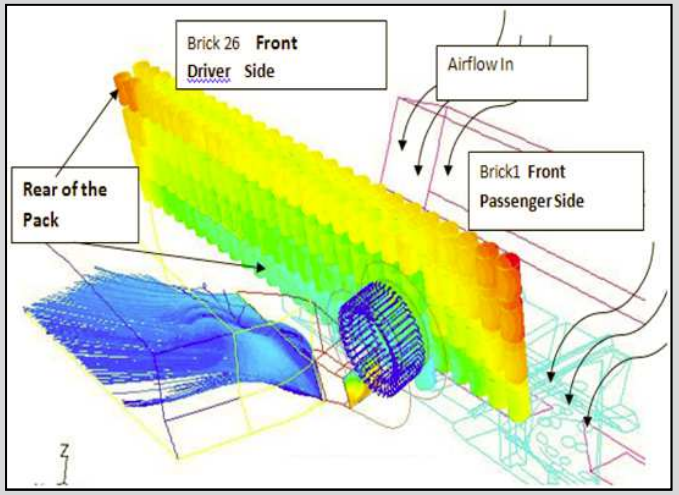
Temperature Distribution



Temperature Distribution



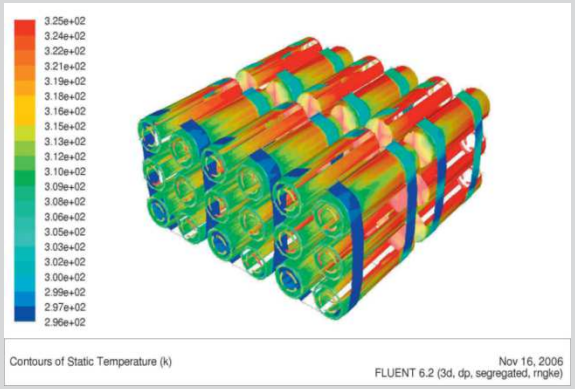
Temperature Distribution

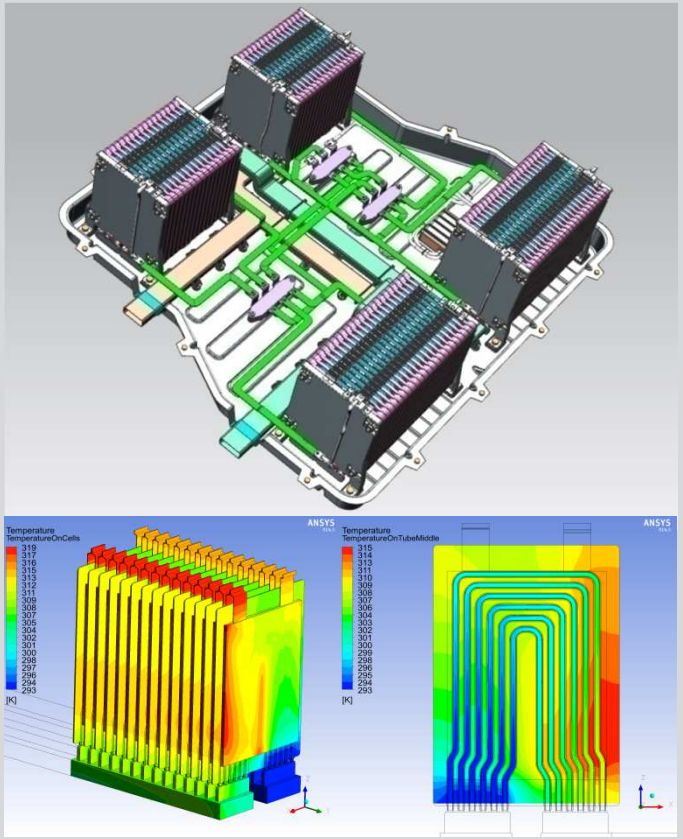


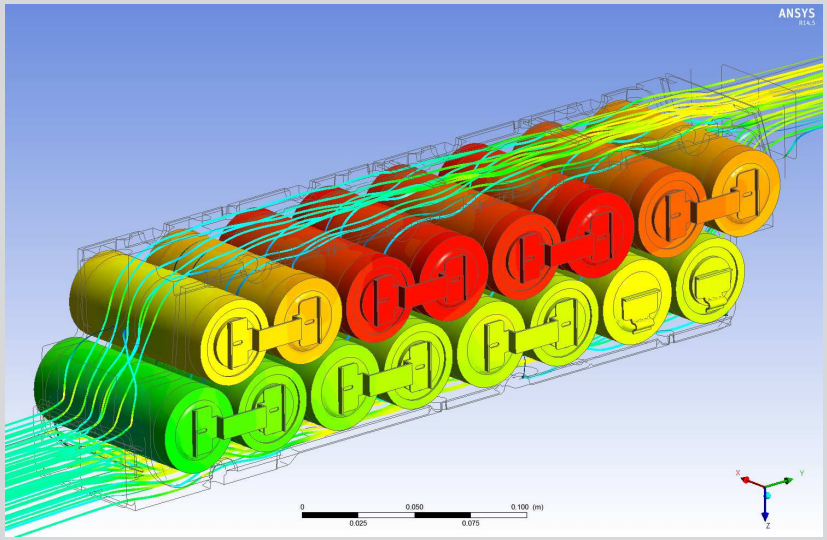
Temperature and Pathlines

Motivation of Reduced Order Model(ROM)

- **CFD as a general thermal analysis tool is accurate.**
  - Can be computationally expensive for system level analysis
- **ROM can significantly reduce the model size and simulation time.**
- **ROM is an import tool for system level simulation.**

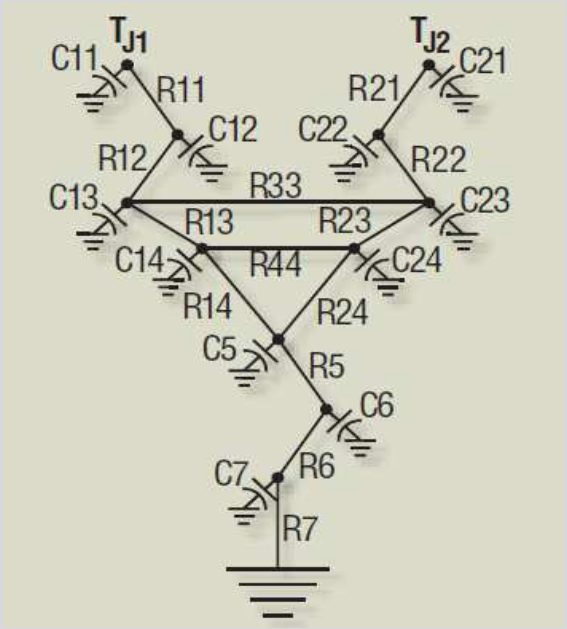


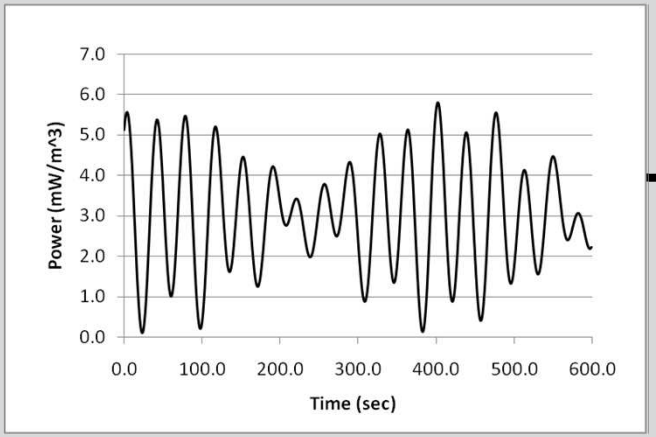


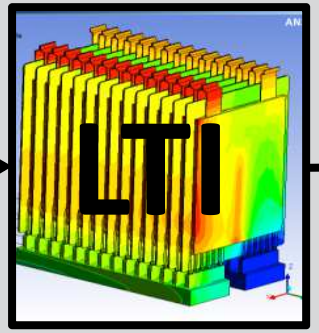


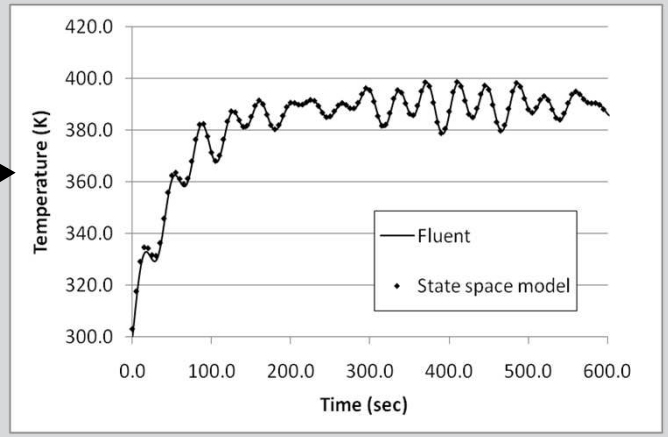
Battery Thermal Behavior via ROM

- **Type 1: Thermal Network**
  - Careful calculation and calibration needed
  - Accuracy compromises
- **Type 2: LTI – state space**
  - Can be as accurate as CFD
  - No calibration





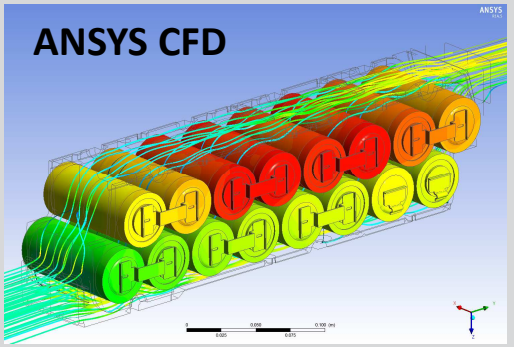




LTI ROM for Battery Cooling

1. **Create the CFD model**
2. **Generate step responses**
   - Icepak has specialized tools
   - Other CFD codes are fine
3. **Extract LTI ROM**
   - Use Simplorer
4. **Simulate inside Simplorer**

1



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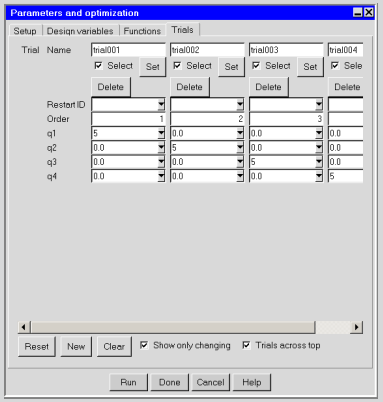

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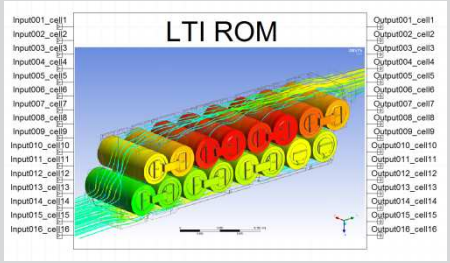

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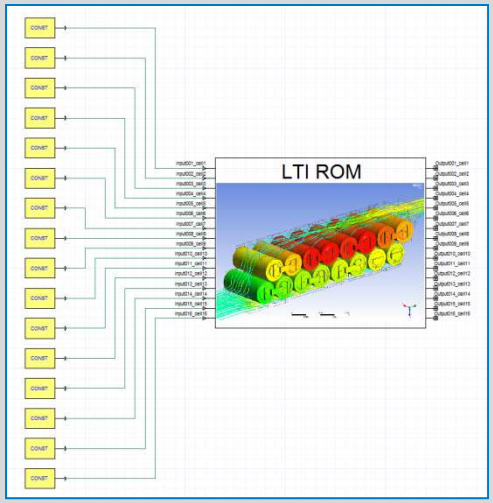
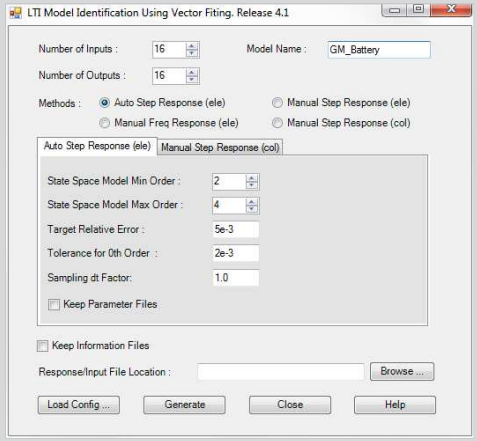
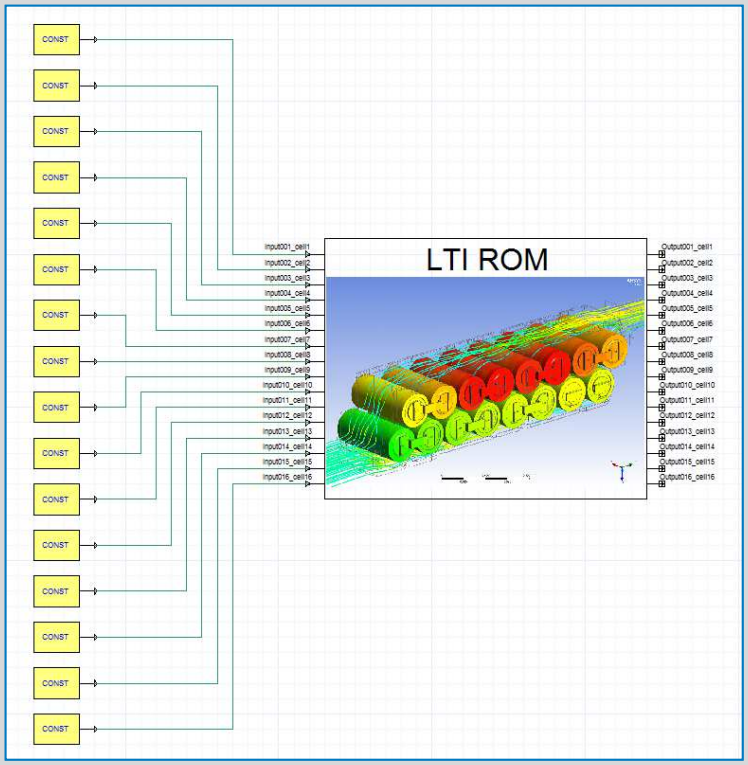
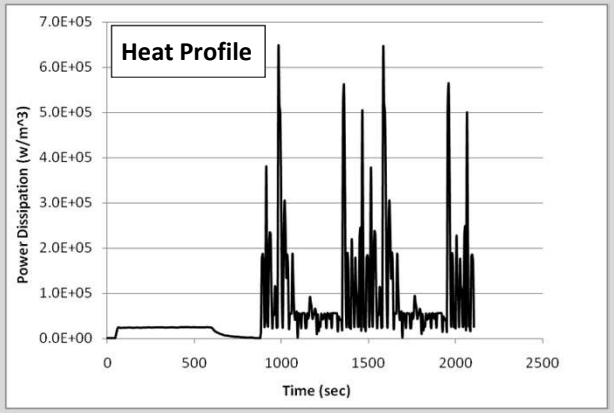
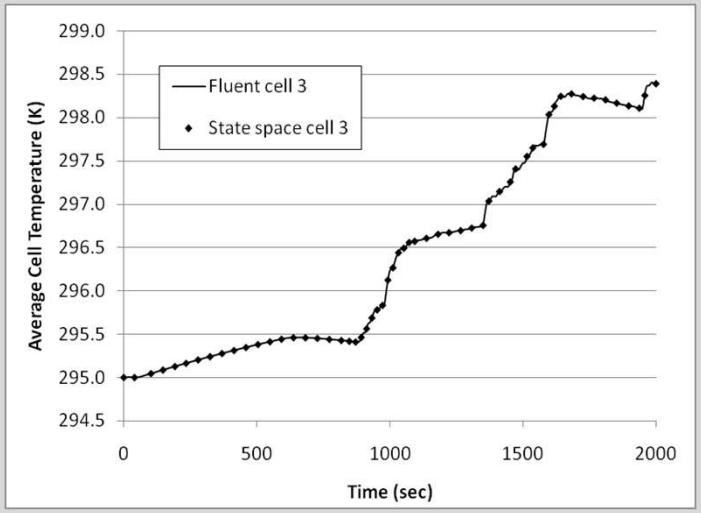




LTI ROM for GM Battery Module



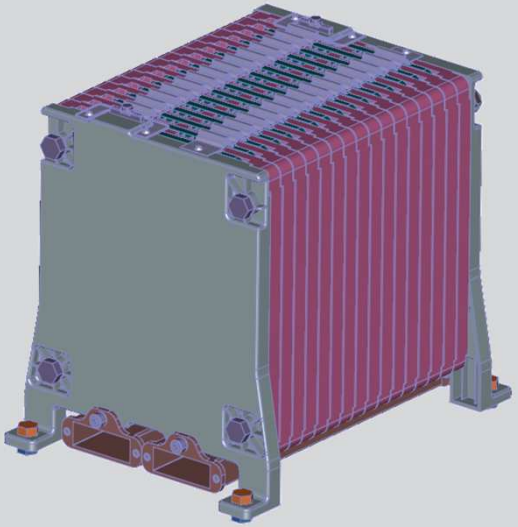


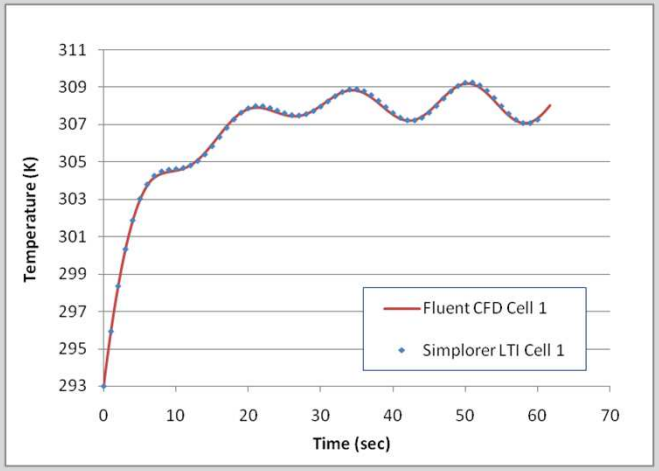


LTI ROM gives the same results as CFD. LTI ROM runs in less than 2 seconds while the CFD runs 2 hours on one single CPU.

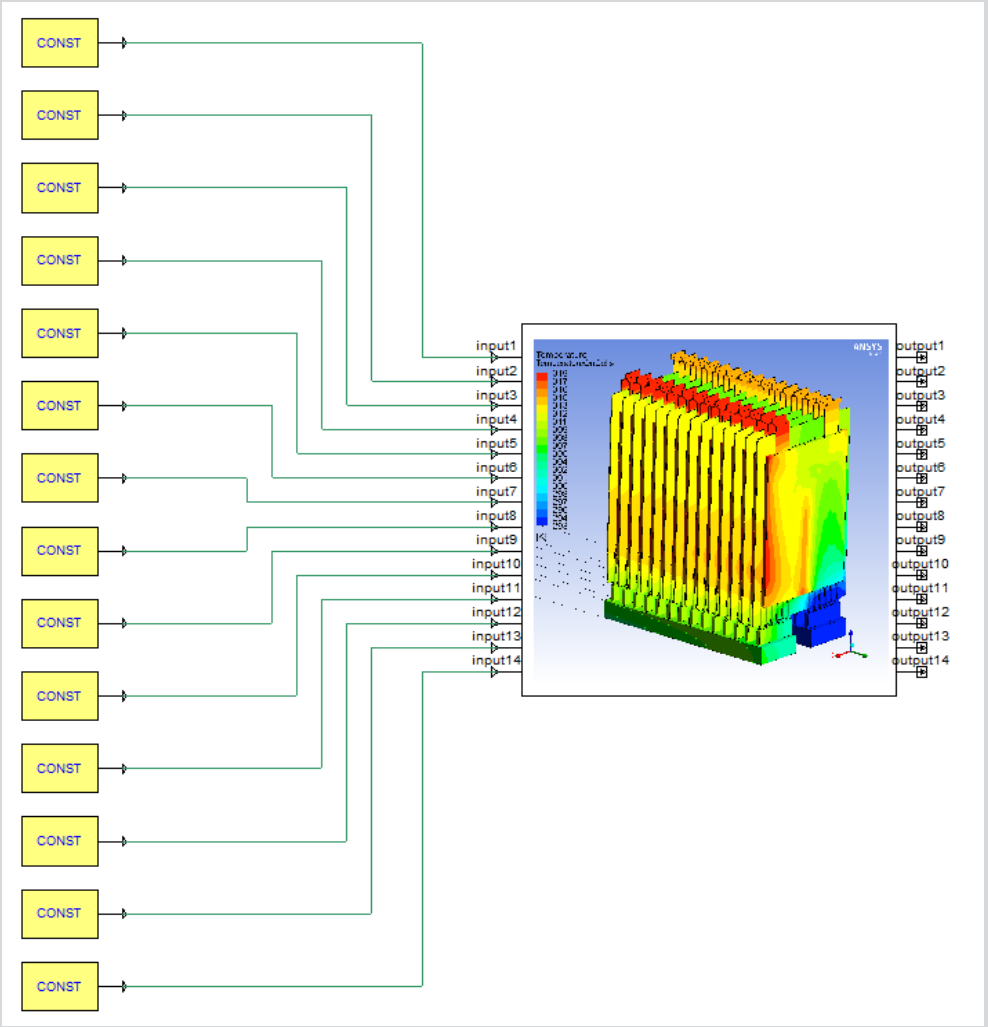
X. Hu, S. Lin, S. Stanton, W. Lian, “A Foster Network Thermal Model for HEV/EV Battery Modeling,” IEEE TRANSACTIONS ON INDUSTRY APPLICATIONS, VOL. 47, NO. 4, JULY/AUGUST 2011
X. Hu, S. Lin, S. Stanton, W. Lian, “A State Space Thermal Model for HEV/EV Battery Modeling", SAE 2011-01-1364

Module Level – ROM for Thermal

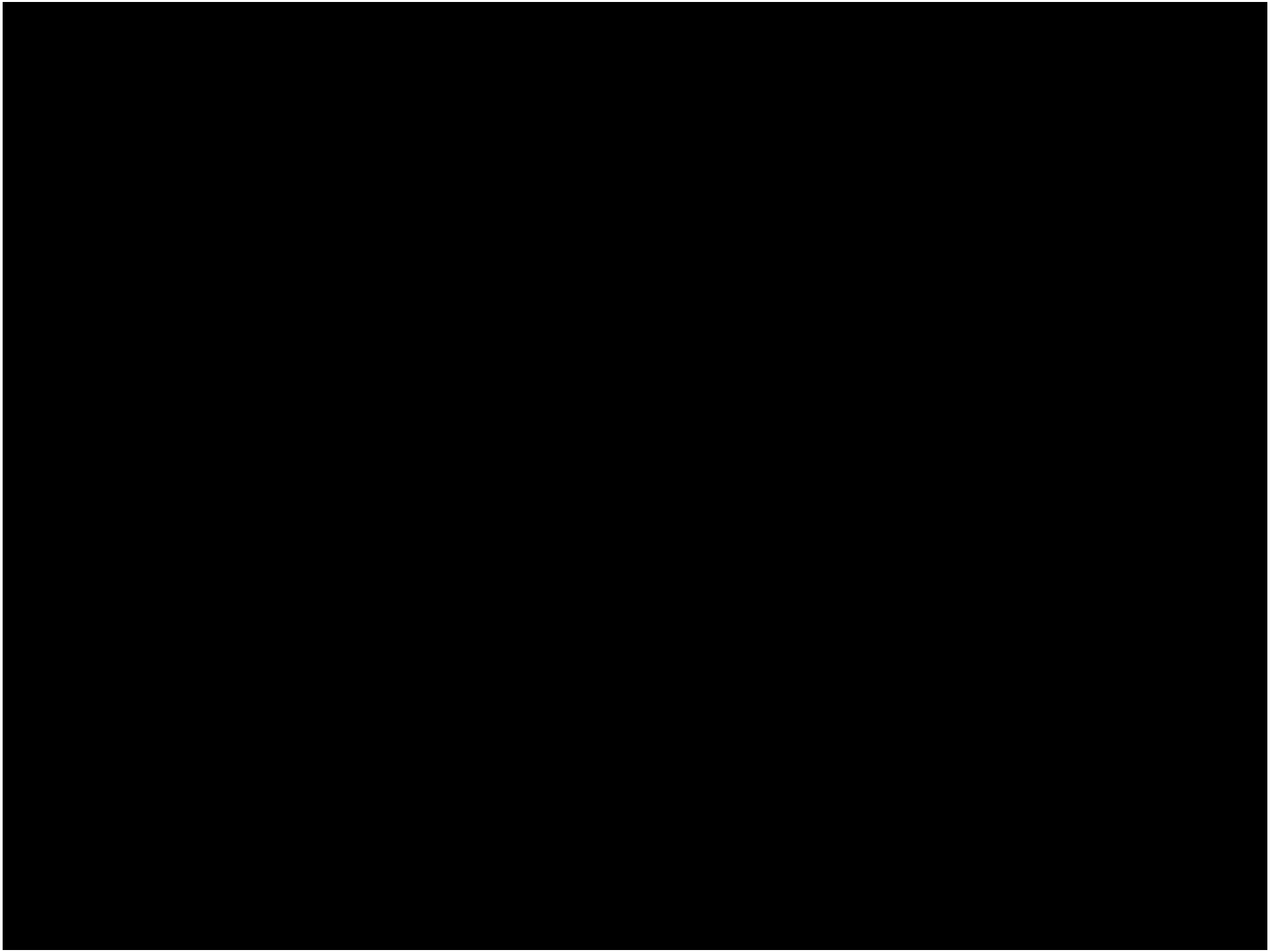




ROM vs CFD

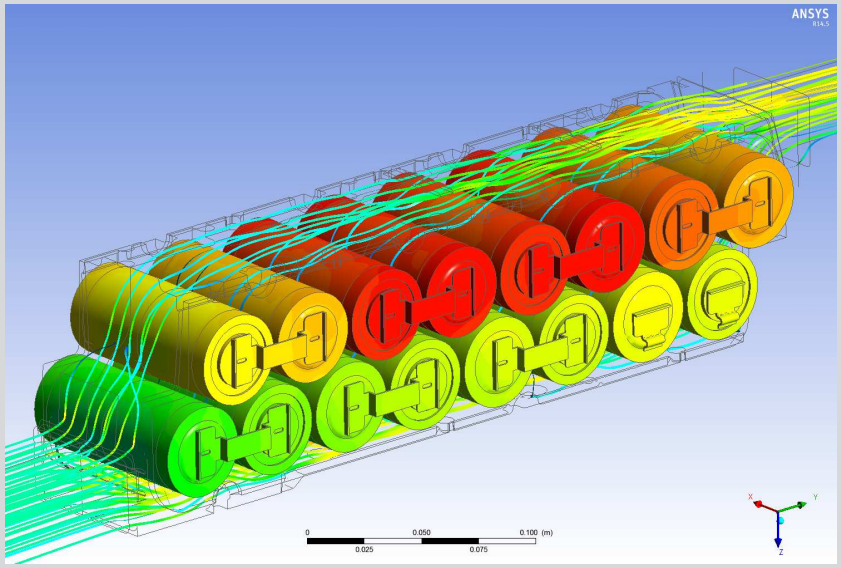


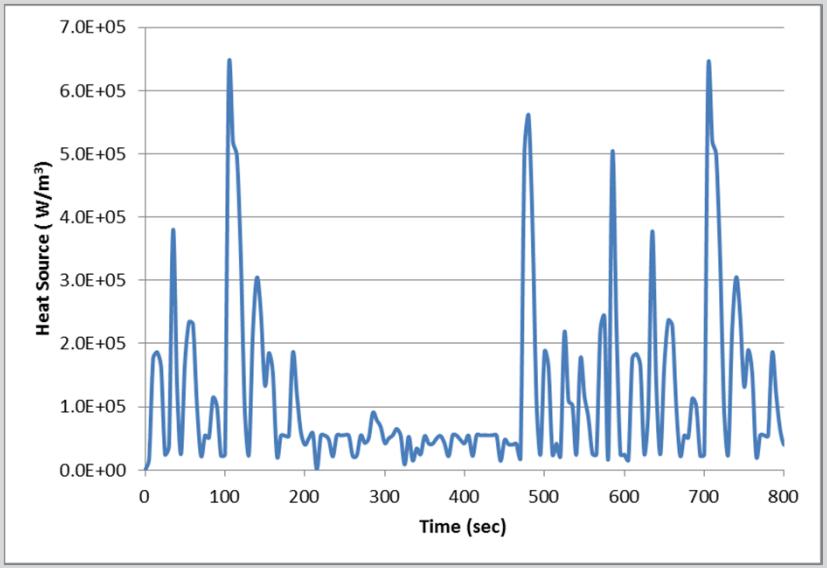
ROM for the Battery Module



SVD ROM : GM 16 Cell Test Case

- **SVD ROM technology allows for quick temperature distribution calculation in addition to average temperature calculation.**
- **Using a heat source from GM, SVD ROM is applied to the GM 16 cell case.**





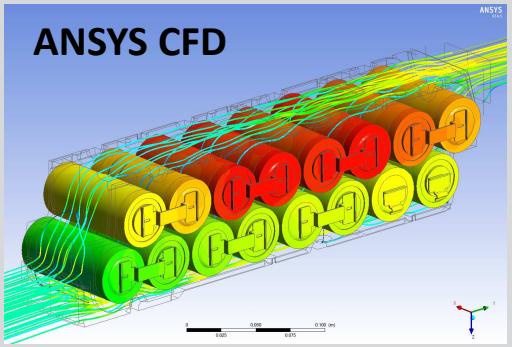
Heat source used

S. Asgari, X. Hu, M. Tsuk, S. Kaushik, "Application of POD plus LTI ROM to Battery Thermal Modeling: SISO Case," SAE 2014.-01-1843
X. Hu, S. Asgari, I. Yavuz, S. Stanton, C-C Hsu, Z. Shi, B. Wang, H-K Chu, "A Transient Reduced Order Model for Battery Thermal Management Based on Singular Value Decomposition,"IEEE Energy Conversion Congress and Expo, 2014

SVD ROM for Battery Cooling

1. **Create the CFD model**
2. **Generate step responses**
   - Cannot use Icepak
   - Can only use FLUENT
3. **Extract SVD ROM**
   - Use Simplorer
4. **Simulate inside Simplorer**

1



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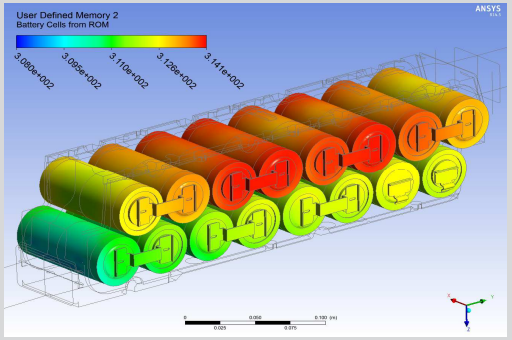

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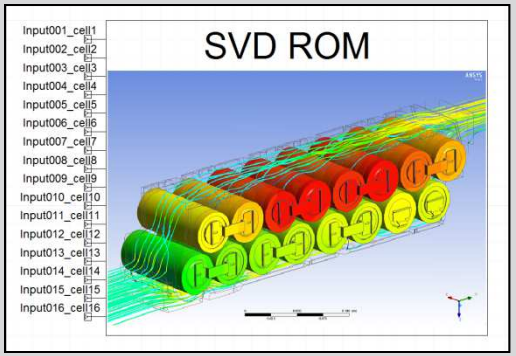

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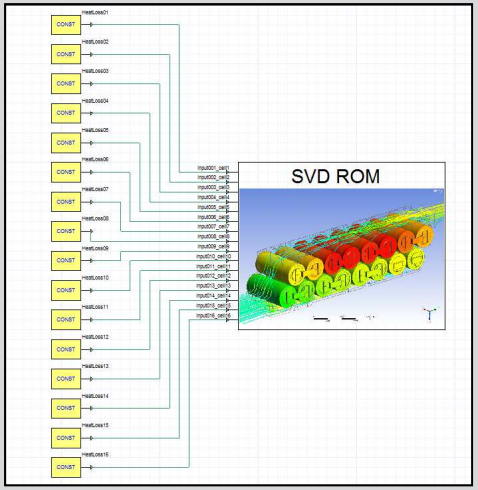
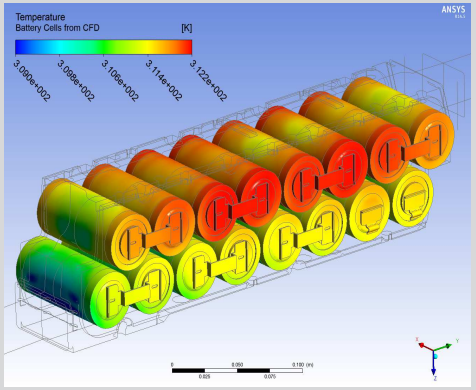
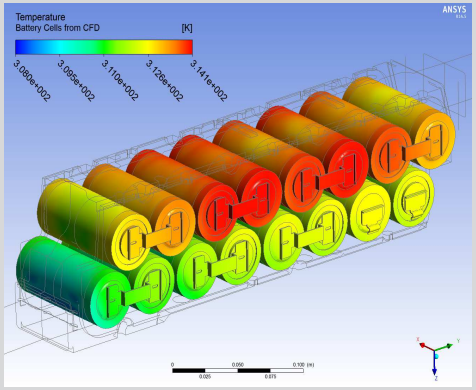


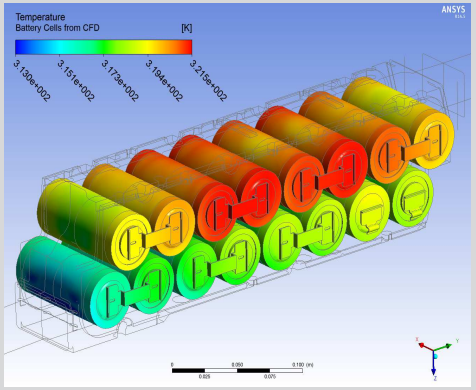
SVD ROM Validation: GM 16 Cell Test Case



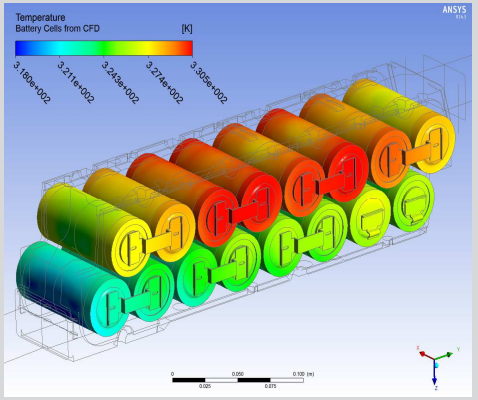
CFD (200 sec)



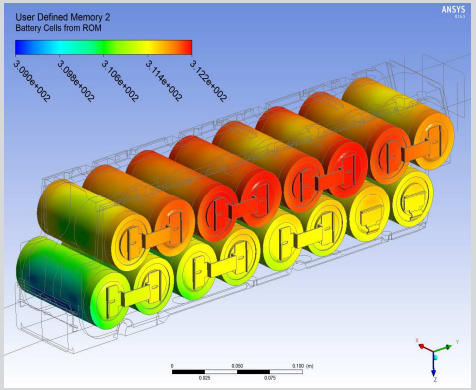
CFD (400 sec)



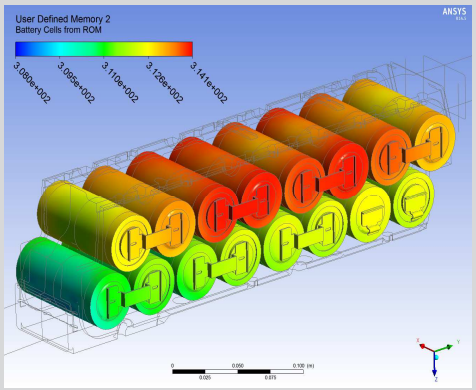
CFD (600 sec)



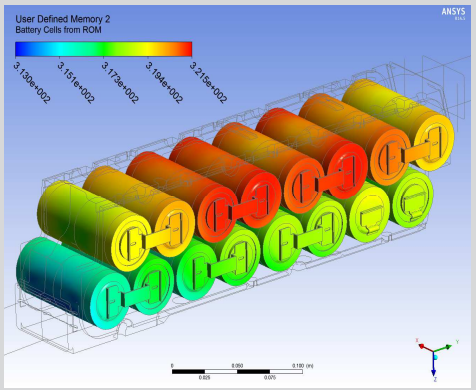
CFD (800 sec)



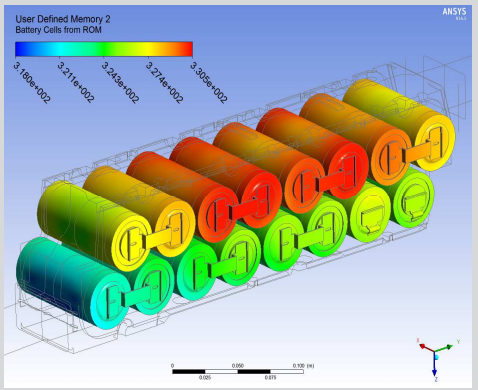
SVD ROM (200 sec)



SVD ROM (400 sec)



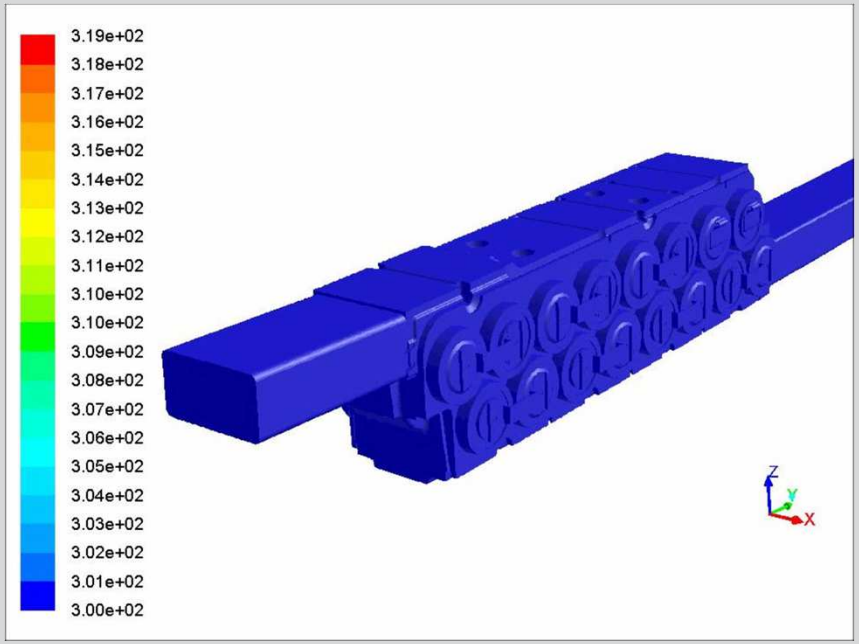
SVD ROM (600 sec)



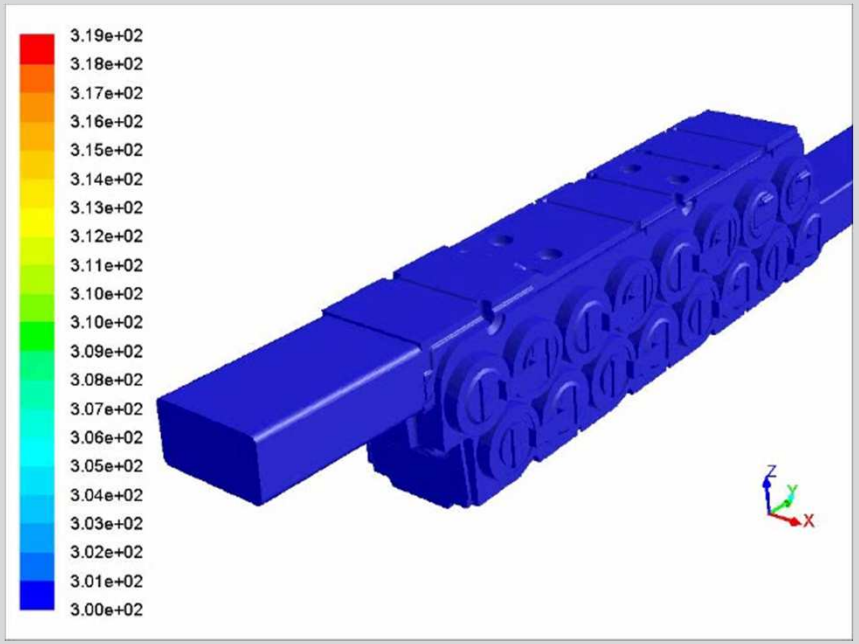
SVD ROM (800 sec)

X. Hu, S. Asgari, I. Yavuz, S. Stanton, C-C Hsu, Z. Shi, B. Wang, H-K Chu, “A Transient Reduced Order Model for Battery Thermal Management Based on Singular Value Decomposition,” Submitted to ECCE 2014.

Temperature Distribution - Animation

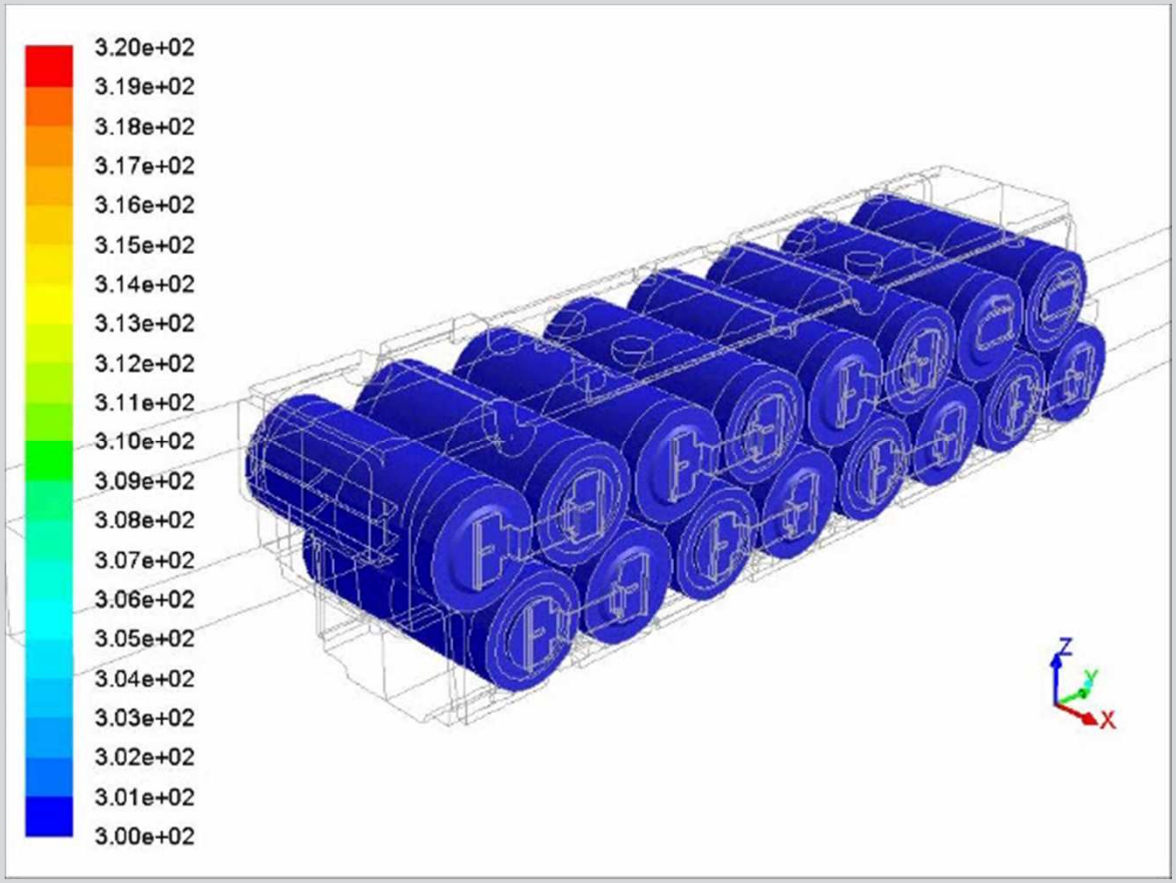


Temperature calculated from CFD.
7 hr simulation time with 6 CPUs.



Temperature calculated from SVD ROM.
0.5 hr simulation time with 1 CPU.

Temperature Distribution - Animation

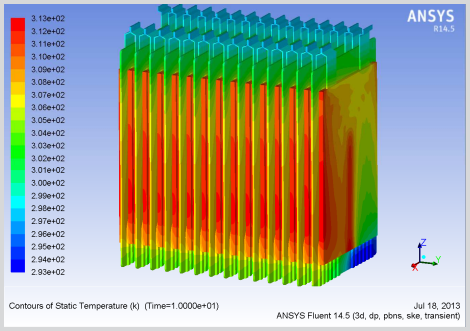


Temperature calculated from SVD ROM.
0.5 hr simulation time with 1 CPU.

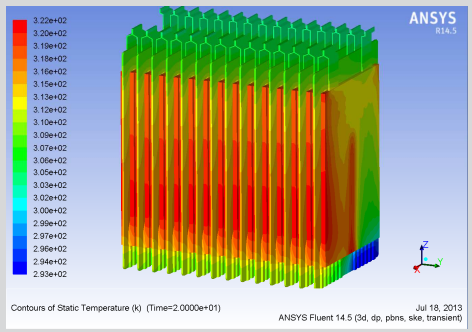
SVD ROM Statistics for GM 16 Cell Test Case

CFD mesh size	**3,025,067**
Number of steps in step response run	180
Size of matrix ***A***	3,025,067×180
Number of snap shots used for SVD calculation	180
SVD calculation time	5 minutes
SVD calculation memory usage	8.1 G
SVD ROM extraction time	5 minutes
CFD validation simulation time on single CPU	**5 hours**
SVD ROM simulation time on the same single CPU	**a few seconds**
Using SVD ROM results for an animation on one CPU	**10 to 30 minutes**

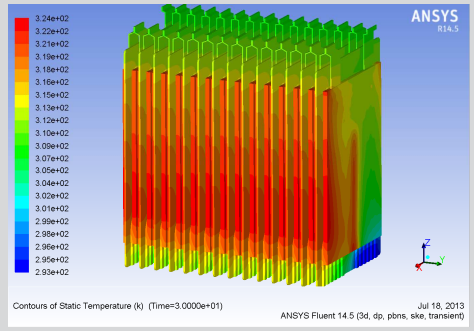
SVD ROM Validation



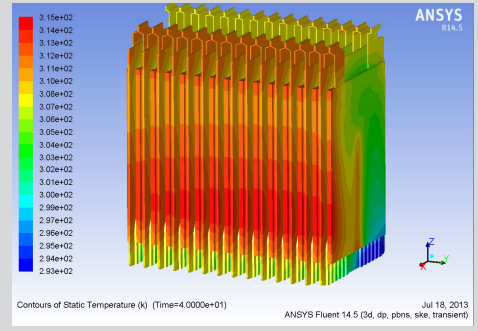
CFD (10 sec)



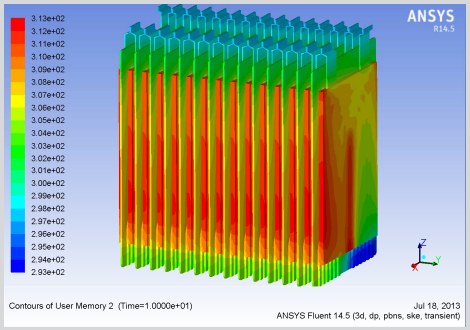
CFD (20 sec)



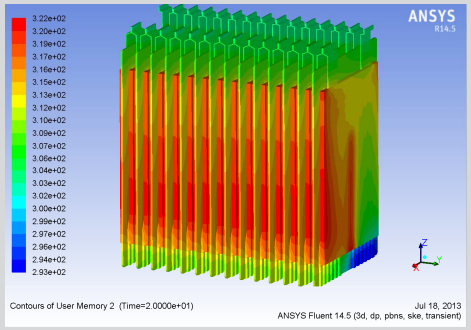
CFD (30 sec)



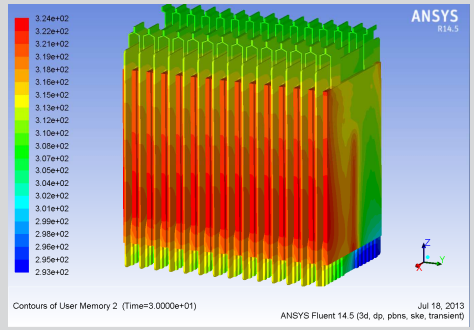
CFD (40 sec)



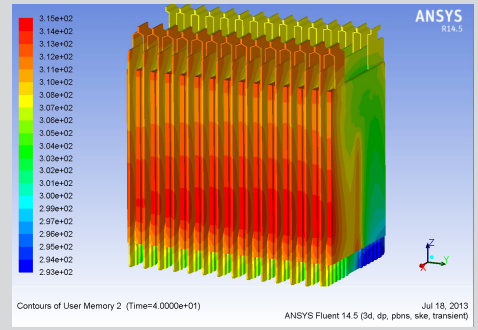
SVD ROM (10 sec)



SVD ROM (20 sec)



SVD ROM (30 sec)



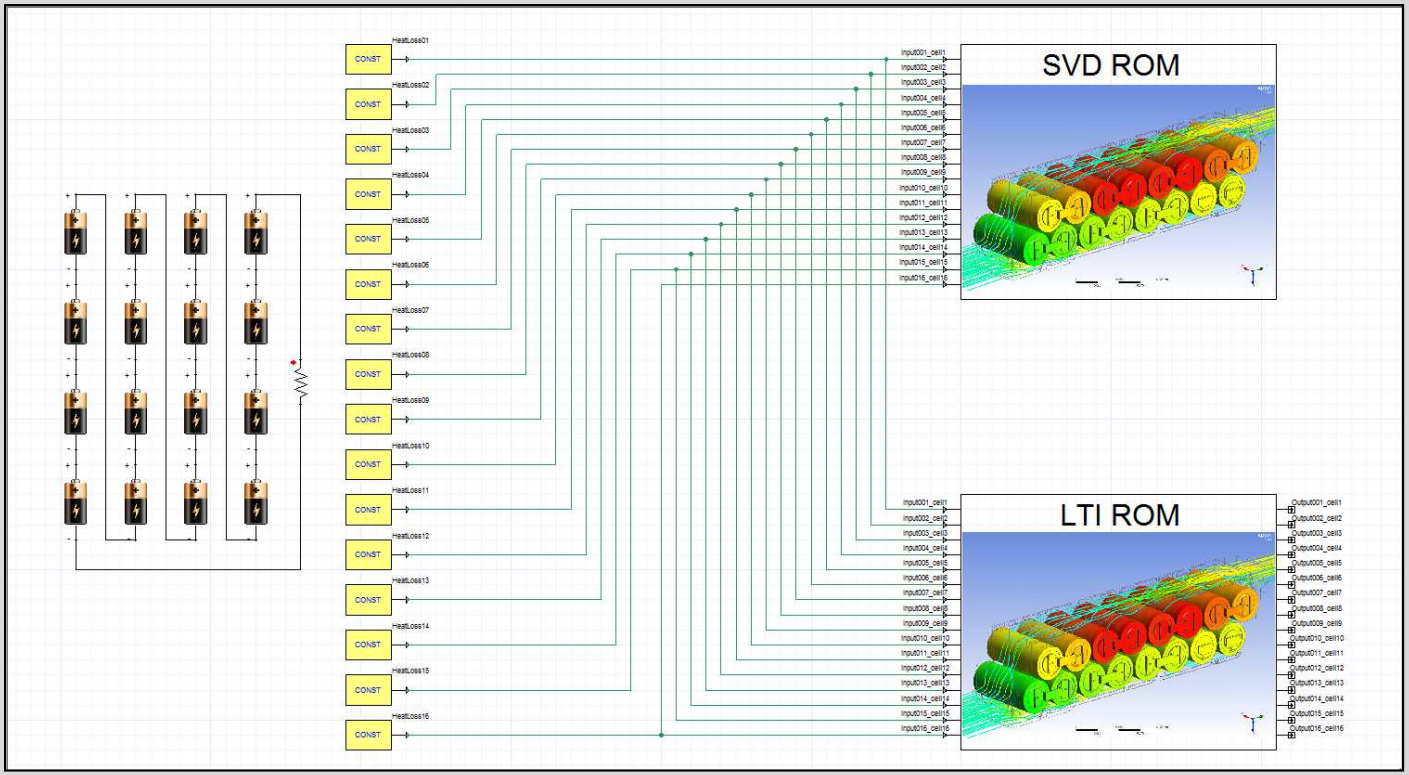
SVD ROM (40 sec)

SVD ROM Statistics for the Test Case

CFD mesh size	**12,209,486**
Number of steps in step response run	120
Size of matrix ***A***	12,209,486×120
Number of snap shots used for SVD calculation	60
SVD calculation time	3 minutes
SVD calculation memory usage	18 G
SVD ROM extraction time	5 minutes
CFD validation simulation time on six CPUs	**20 hours**
SVD ROM simulation time on the same single CPU	**a few seconds**
Using SVD ROM results for an animation on one CPU	**20 to 40 minutes**

GM Battery Module – ECM Coupled with ROMs

- ECM calculates heat source and sends it to the two ROMs.
- LTI ROM calculates average temperature and sends it to ECM.
- SVD ROM *calculates* temperature distribution.



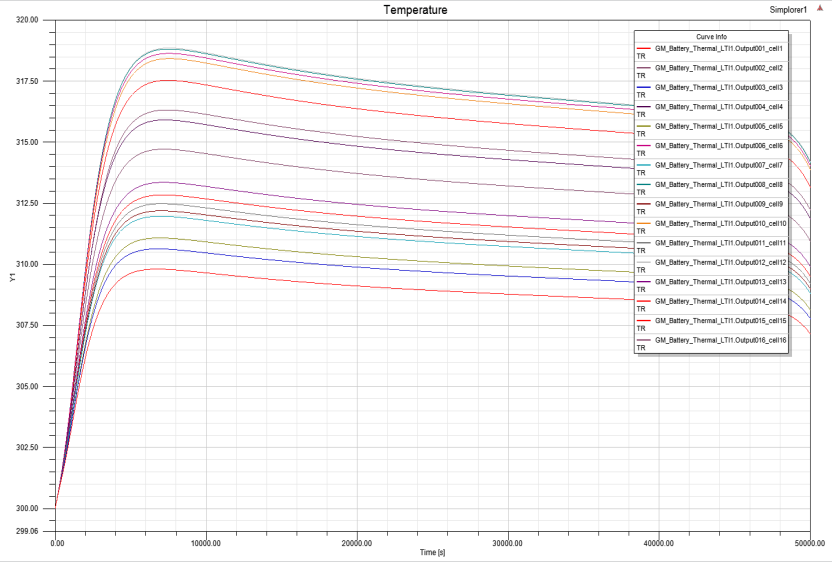
ROMs/ECM Coupled Results

LTI ROM calculates average temperature.

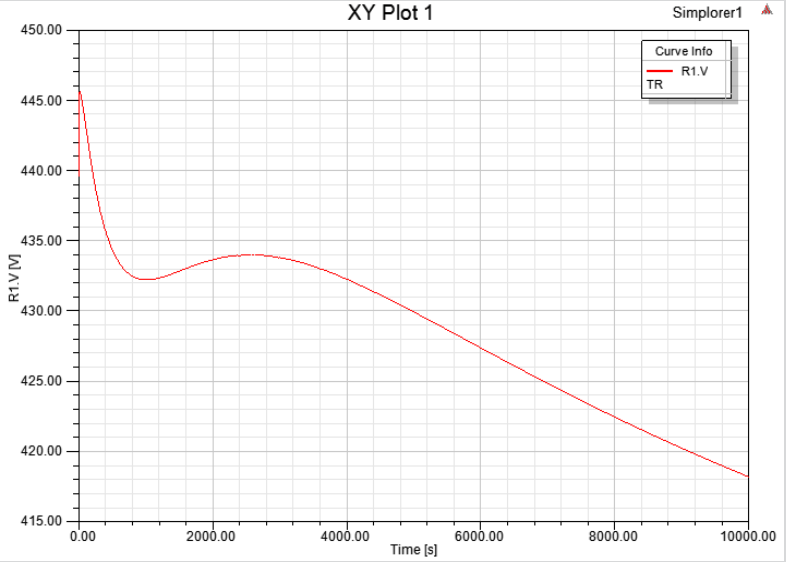
SVD ROM calculates temperature field.

- **Needs to be post-processed back in FLUENT.**

ECM calculates electrical performance.

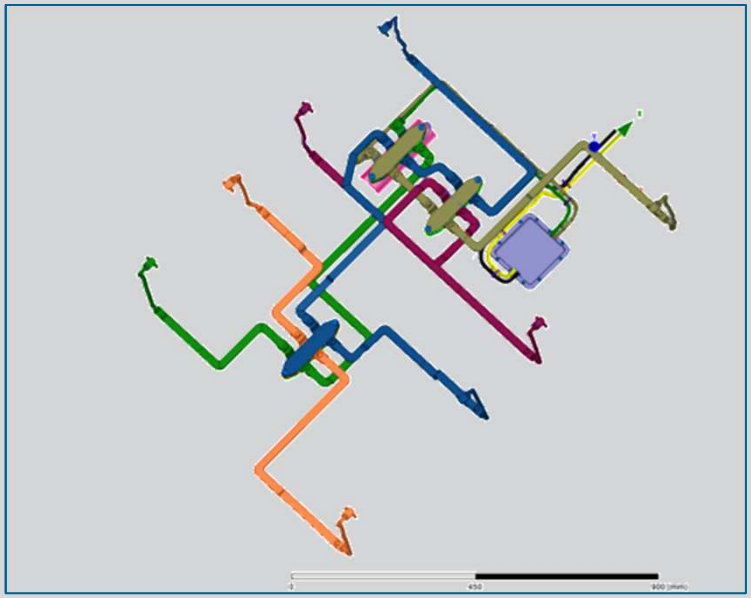


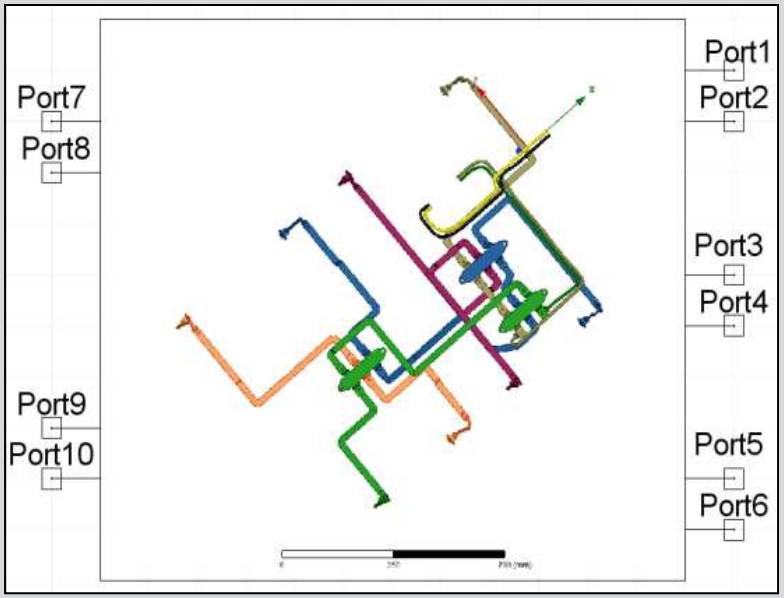
Average Cell Temperature



Battery Voltage as a Function of Time

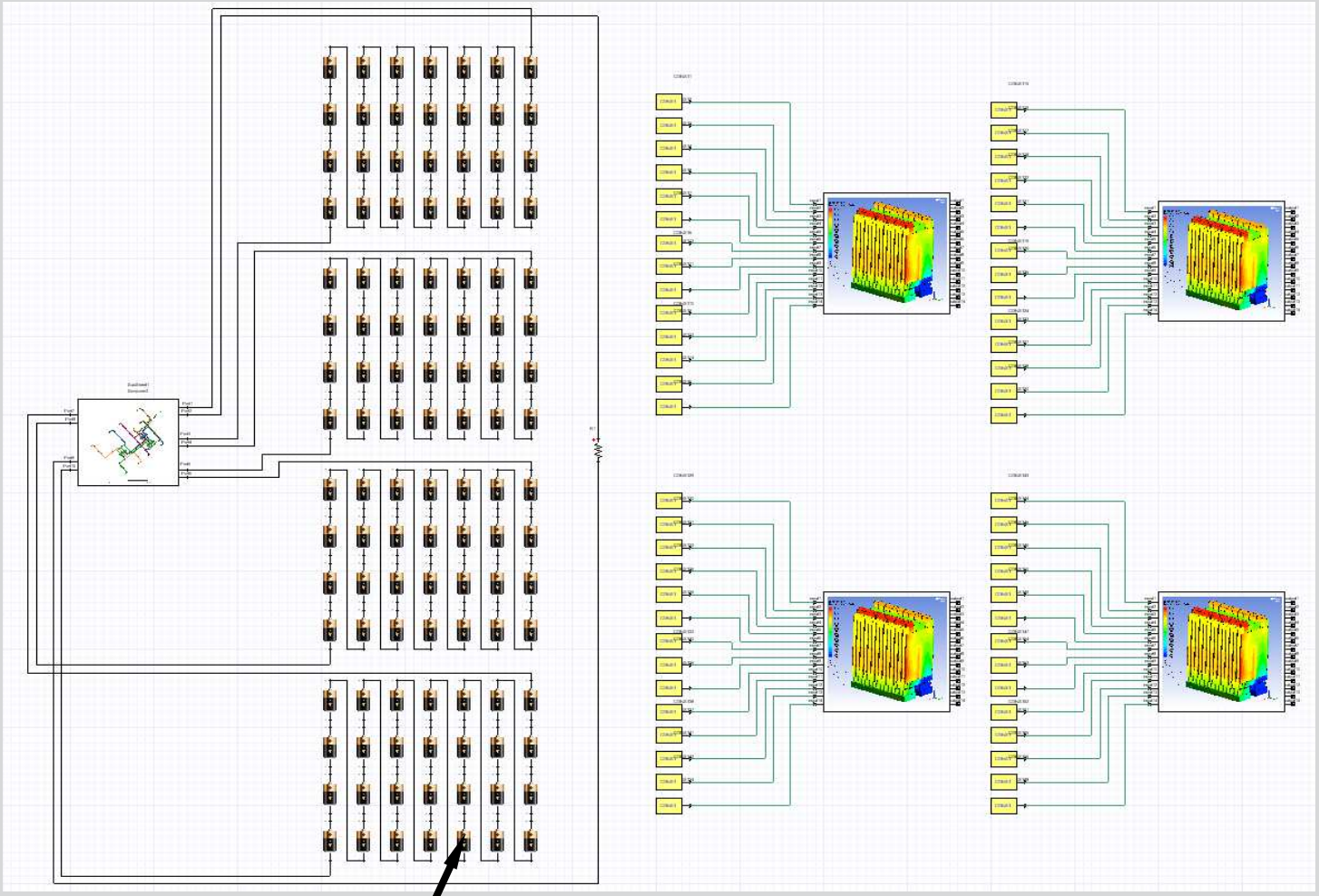
Module/Pack Level – Bus Bar Model





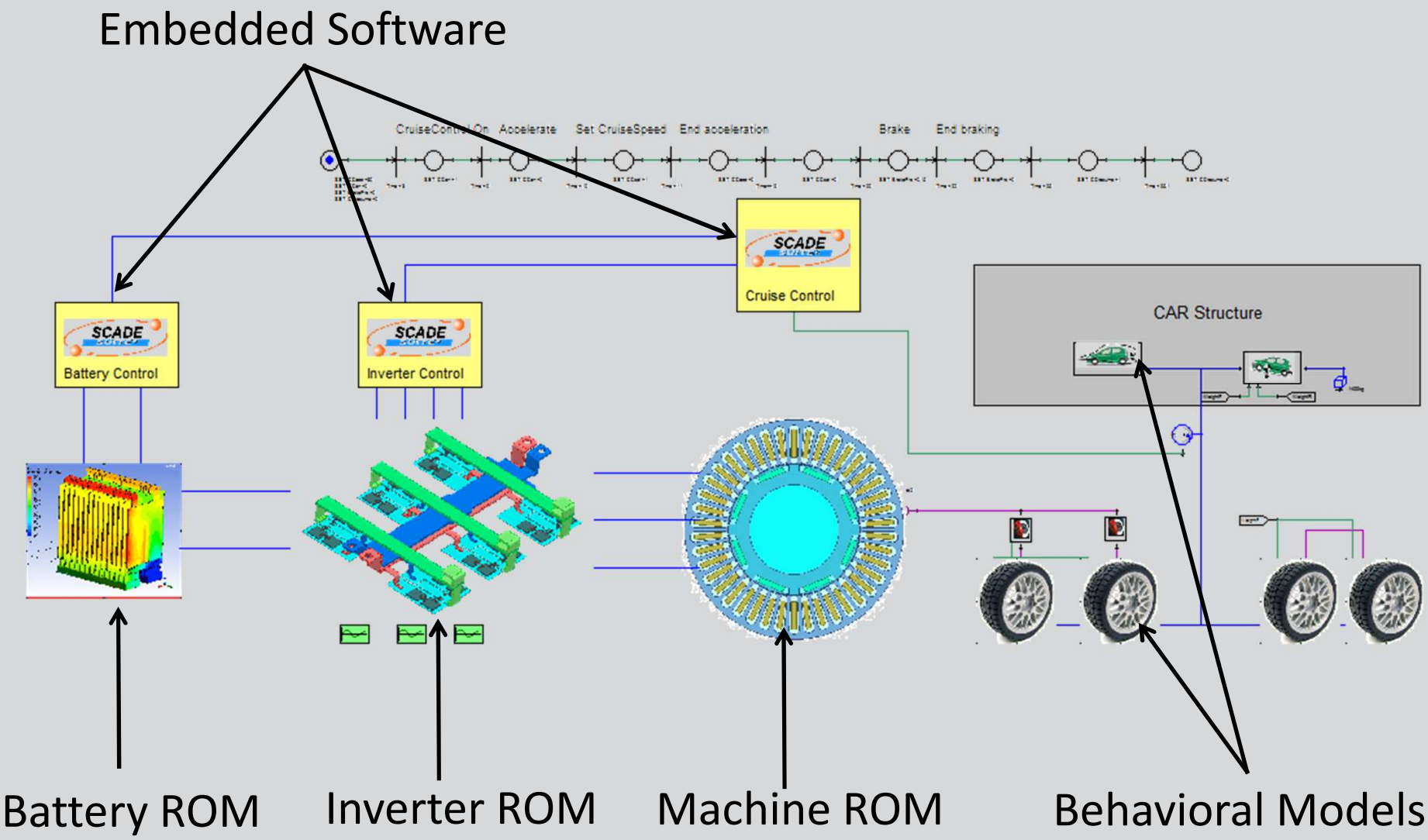
Electromagnetic FEA Analysis for Busbar RLC Network Extraction

Full Battery Simulation



Voc = -1.031*exp(-35*(abs(IBatt.V/Vinit))) + 3.685 + 0.2156*(abs(IBatt.V/Vinit)) - 0.1178*(abs(IBatt.V/Vinit))^2 + 0.3201*(abs(IBatt.V/Vinit))^3 + 0.3/30.0*(U1.Temp_block_1-273)

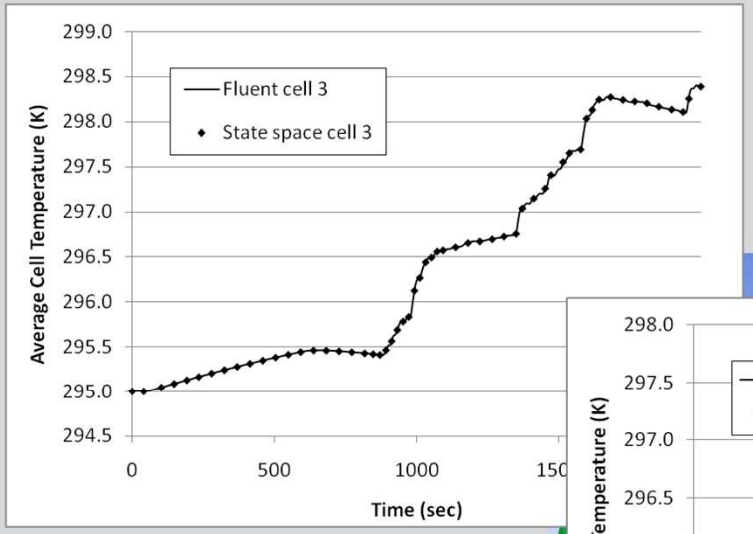
System Assembly

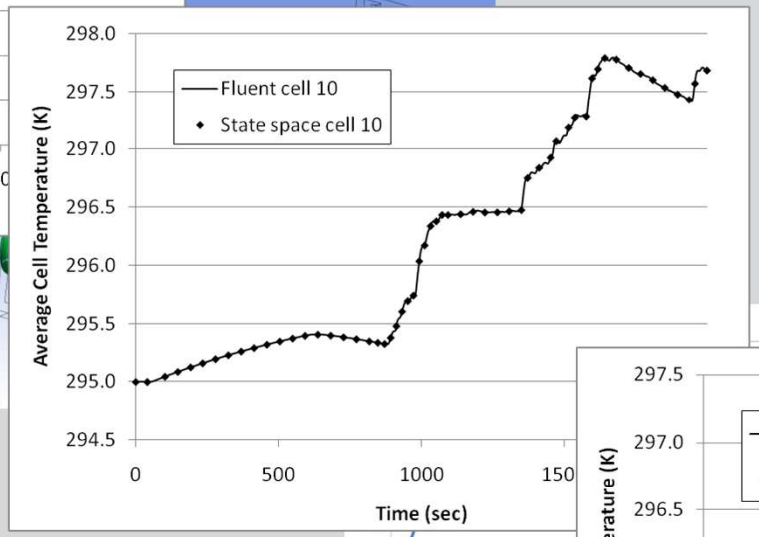


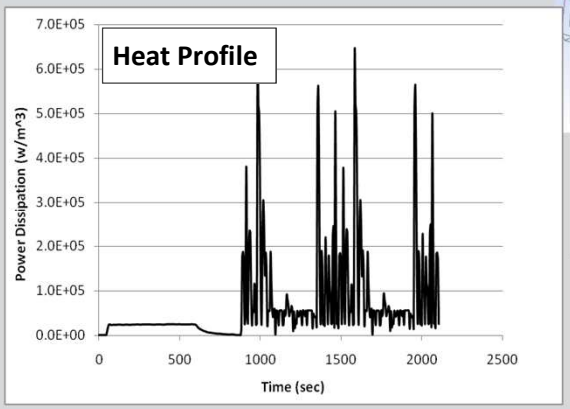
Conclusions

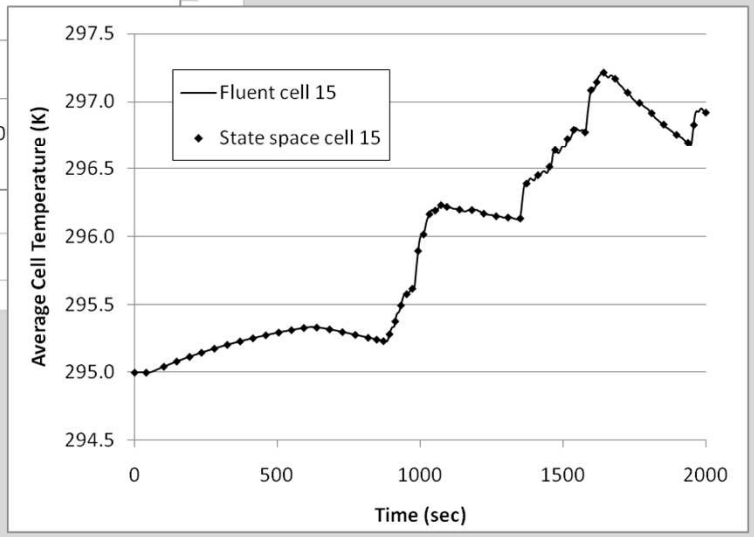
- **Battery is a multi-scale multi-physics application.**
- **ANSYS provides tools for all aspects of battery simulation.**
- **Furthermore, ANSYS integrates different models into battery system level simulation through model order reduction.**

Module Level – ROM for Thermal









ROM gives the same results as CFD. ROM runs in less than 5 seconds while the CFD runs 2 hours on one single CPU.

X. Hu, S. Lin, S. Stanton, W. Lian, "A Foster Network Thermal Model for HEV/EV Battery Modeling," IEEE TRANSACTIONS ON INDUSTRY APPLICATIONS, VOL. 47, NO. 4, JULY/AUGUST 2011
X. Hu, S. Lin, S. Stanton, W. Lian, "A State Space Thermal Model for HEV/EV Battery Modeling", SAE 2011-01-1364