

Presented at the 2011 COMSOL Conference in Boston

Sequential Simulation in COMSOL Using Differential Equations to Perform Digital Switching

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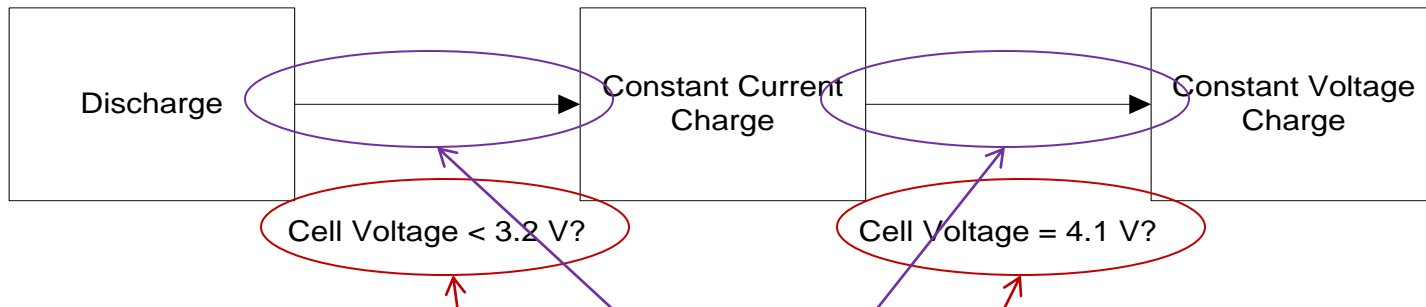
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This presentation:

A method to create a sequential and irreversible switching mechanism, such that boundary conditions can be changed dynamically based on calculated physical parameters

Our problem

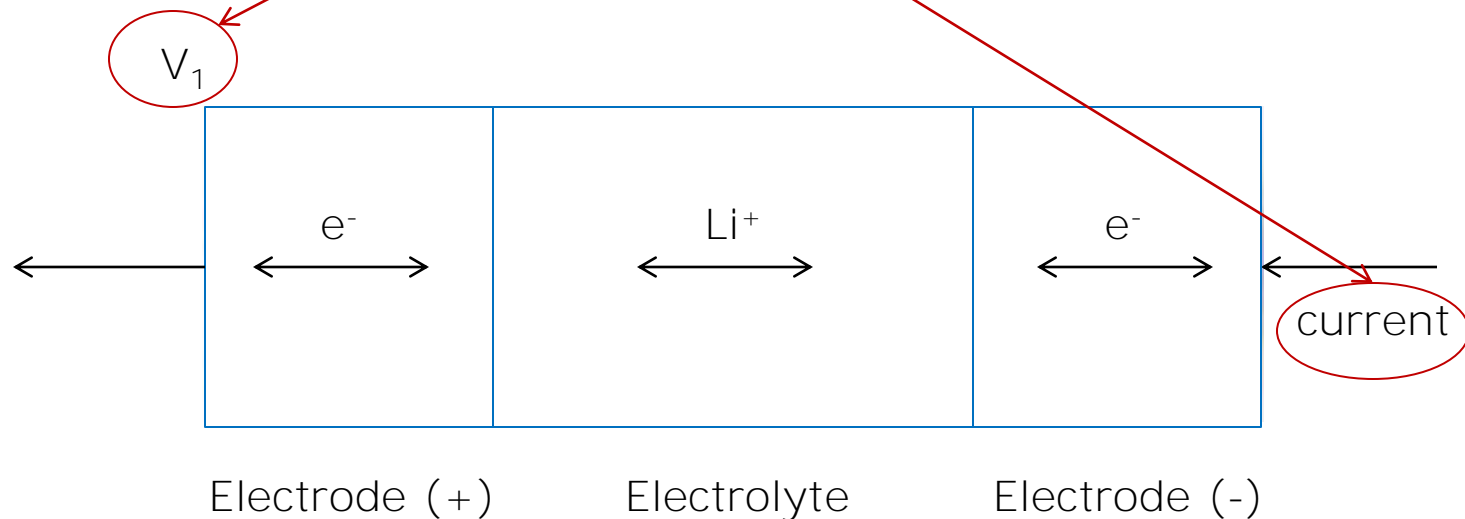
- Application level studies of lithium ion batteries based on electrochemistry



- State change
- One-way, irreversible switching
- Based on calculated parameters
- Must behave like electrical circuits

Our model (briefly)

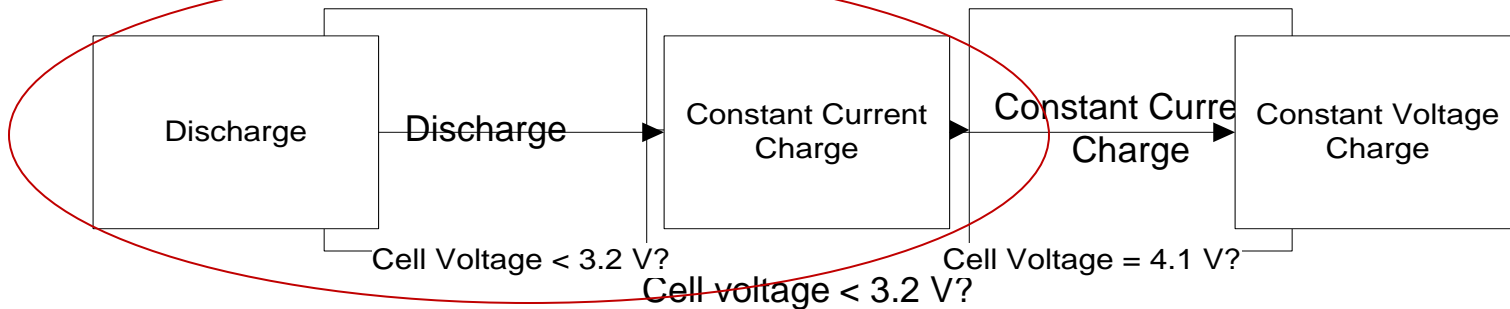
- Based on Newman¹
- **Boundary condition:** current (i)
- **Physics:** cell potential, transport, internal concentration distribution, degradation etc.



¹ R. Darling and J. Newman, "Modeling Side Reactions in Composite $Li_yMn_2O_4$ Electrodes", *J. Electrochem. Soc.*, **vol.** 145, pp. 990 (1998)

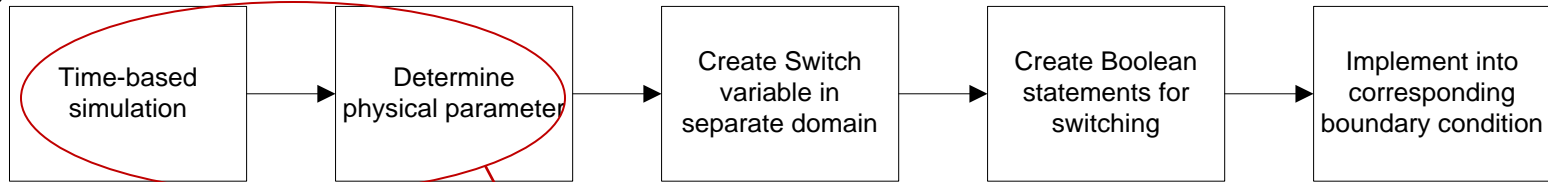
For demo - simplifying

- Simplified switching

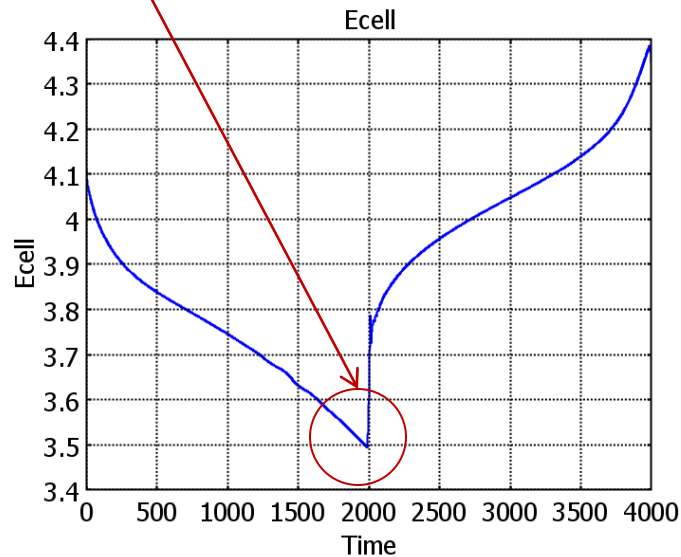


- 2-state, 1-bit
- Easily extending to multiple states
- li_battery as base for demo (Chem. Eng. Module)
- Developed in 3.5, usable in 4.2

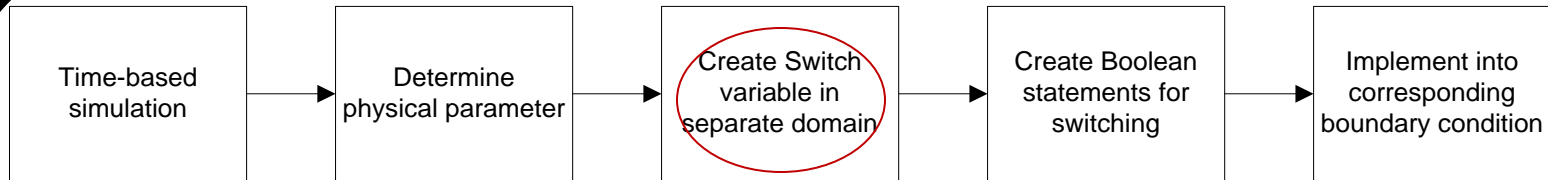
The solution – 4-step process



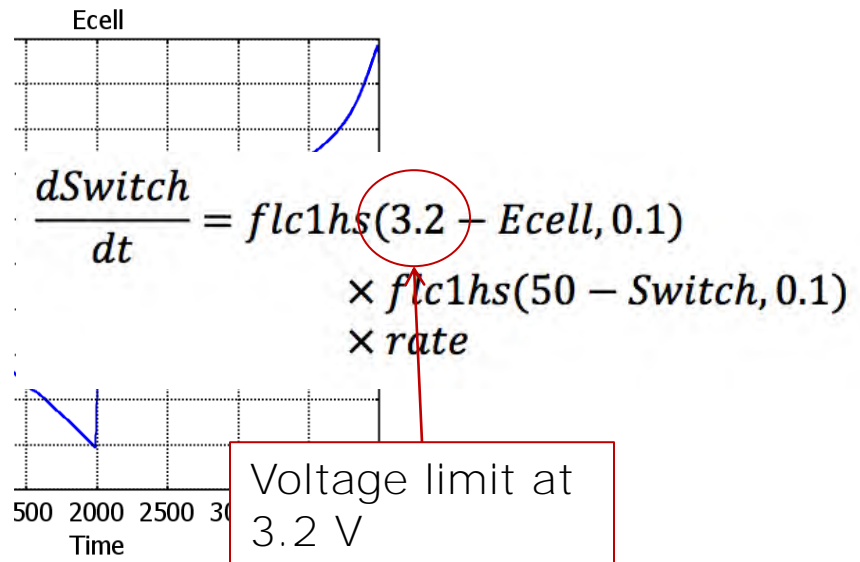
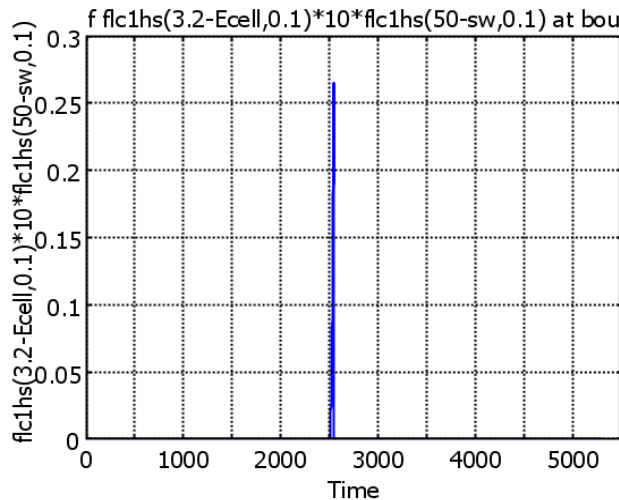
- Making use of COMSOL's strength



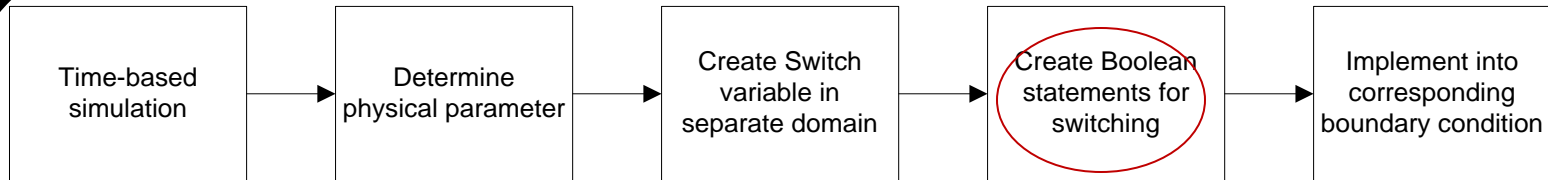
The solution – 4-step process



- Create a pulse based on the calculated solution (Ecell) with conditional statement



The solution – 4-step process



- Result of “Switch” (irreversible)
- Boolean statements

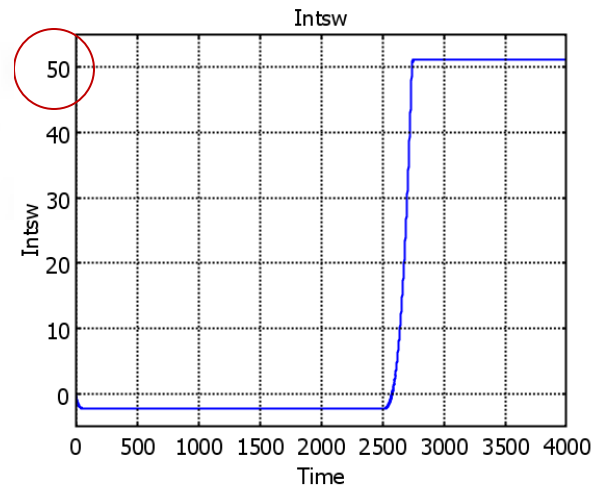
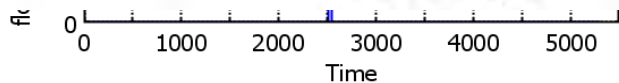
f flc1hs(3.2-Ecell.0.1)*10*flc1hs(50-sw.0.1) at bou

$$Discharge = flc1hs(25 - IntSwitch, 0.05)$$

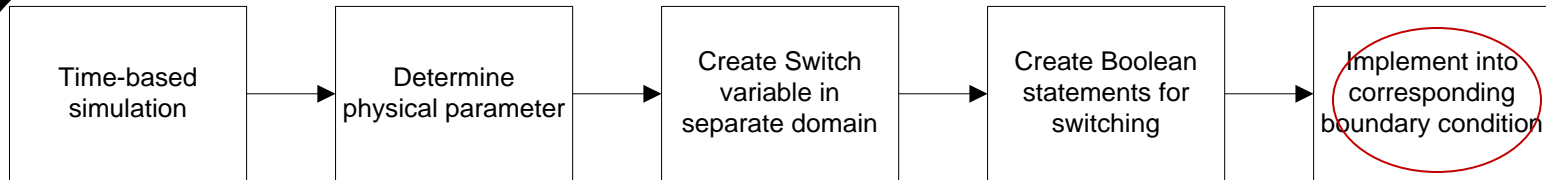
$$Charge = flc1hs(IntSwitch - 25, 0.1)$$



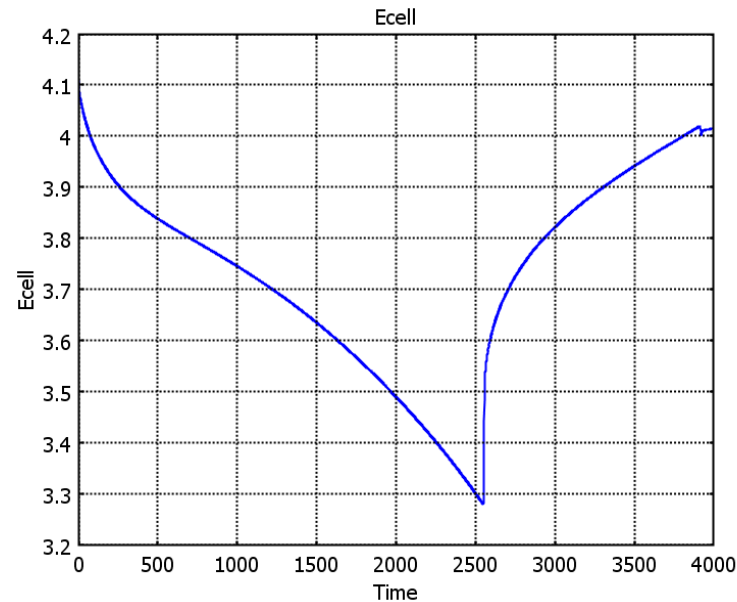
$$i_{app} = i_{discharge} \times Discharge + i_{charge} \times Charge$$



The solution – 4-step process



- Note: Boolean values will change
- Iteration needed
- Final result:



Acknowledgement:

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- Dr. Líney Árnadóttir (Chemical Engineering, Oregon State University)
- Prof. Ralph E. White (Chemical Engineering, University of South Carolina)
- COMSOL

Summary:

- A 4-step process that enables COMSOL users to perform sequential simulation with dynamic switching based on calculated parameters.
- **Thank you**