Adaptive Estimation of PDE Models for Battery Electrochemistry

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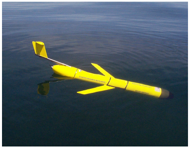
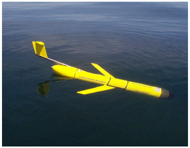
A Golden Era

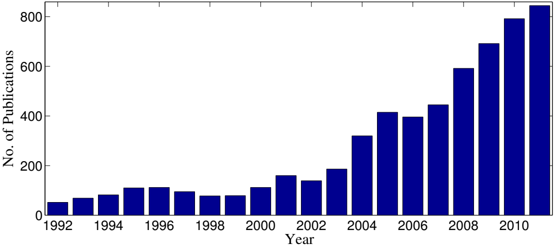

IS-1
ST. JUDE MEDICAL
Sylmar, CA USA
ACCENT SR RF
PM1210 SSR
IS-1
ST. JUDE MEDICAL
Sylmar, CA USA
ANTHEM RF
PM3212 DDDRV



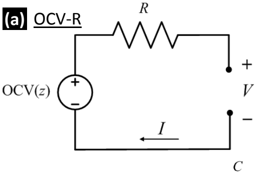
A Golden Era



Keyword: “Battery Systems and Control”

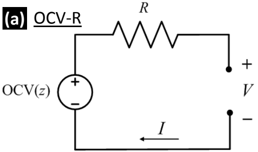


Equivalent Circuit Model

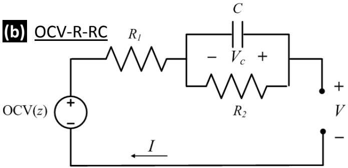


Equivalent Circuit Model

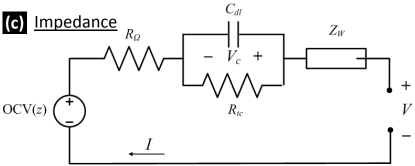
(a) OCV-R



(b) OCV-R-RC

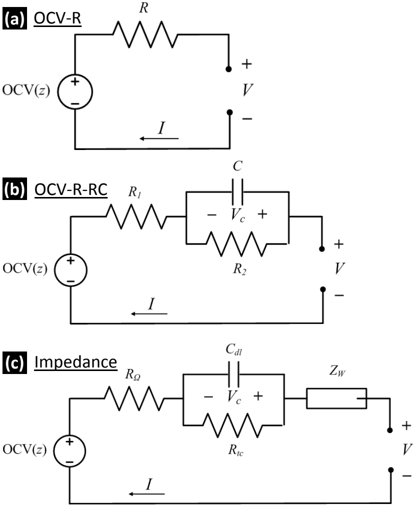


(c) Impedance

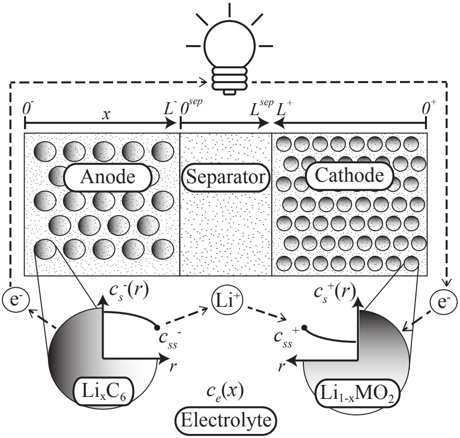


Battery Models

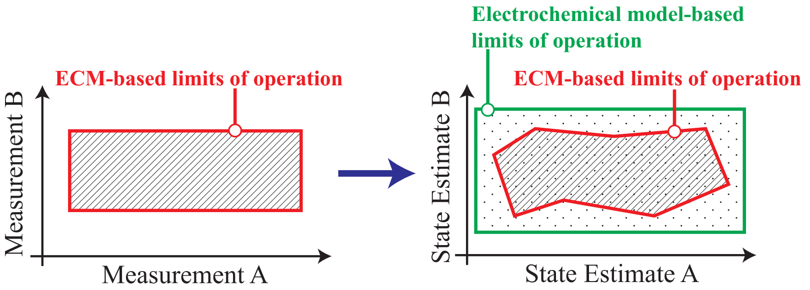
Equivalent Circuit Model



Electrochemical Model



Operate Batteries at their Physical Limits



Electrochemical Model Equations

well, some of them

Description	Equation
Solid phase Li concentration	$\frac{\partial c_s^\pm}{\partial t}(x,r,t) = \frac{1}{r^2}\frac{\partial}{\partial r}\left[D_s^\pm r^2 \frac{\partial c_s^\pm}{\partial r}(x,r,t)\right]$
Electrolyte Li concentration	$\varepsilon_e \frac{\partial c_e}{\partial t}(x,t) = \frac{\partial}{\partial x}\left[\varepsilon_e D_e \frac{\partial c_e}{\partial x}(x,t) + \frac{1-t_c^0}{F} i_e^\pm(x,t)\right]$
Solid potential	$\frac{\partial \phi_s^\pm}{\partial x}(x,t) = \frac{i_e^\pm(x,t) - I(t)}{\sigma^\pm}$
Electrolyte potential	$\frac{\partial \phi_e}{\partial x}(x,t) = -\frac{i_e^\pm(x,t)}{\kappa} + \frac{2RT}{F}(1-t_c^0)\left(1+\frac{d\ln f_{c/a}}{d\ln c_e}(x,t)\right)\frac{\partial \ln c_e}{\partial x}(x,t)$
Electrolyte ionic current	$\frac{\partial i_e^\pm}{\partial x}(x,t) = a_s F j_n^\pm(x,t)$
Molar flux btw phases	$j_n^\pm(x,t) = \frac{1}{F} i_0^\pm(x,t)\left[e^{\frac{\alpha_a F}{RT}\eta^\pm(x,t)} - e^{-\frac{\alpha_c F}{RT}\eta^\pm(x,t)}\right]$
Temperature	$\rho c_P \frac{dT}{dt}(t) = h\left[T^0(t) - T(t)\right] + I(t)V(t) - \int_{0^-}^{0^+} a_s F j_n(x,t)\Delta T(x,t)dx$

Animation of Li Ion Evolution

A Summarized History of SOC/SOH Estimation

- Equivalent Circuit Model
  - G. Plett (2004) - Extended Kalman Filter (States & Params)
  - RLS, Bias-correcting RLS, EKF on Impedance-based ECMs, LPV, Neural nets, Sliding-mode, Particle filters, and many more...

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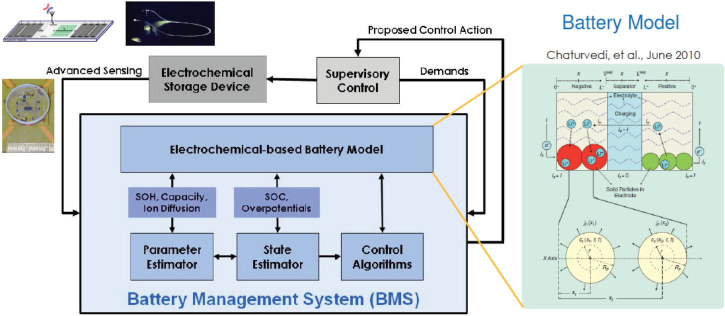

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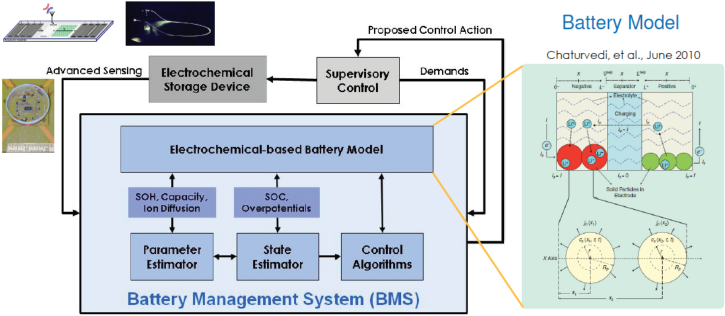

- R. White (2006) - EKF on Single Particle Model (States)
- K. Smith (2008) - KF on Reduced Freq. Domain Model (States)
- A. Stefanopoulou (2010) - EKF on Electrode Avg Model (States)
- R. Klein (2012) - Luenburger Observer on reduced PDE Model (States)

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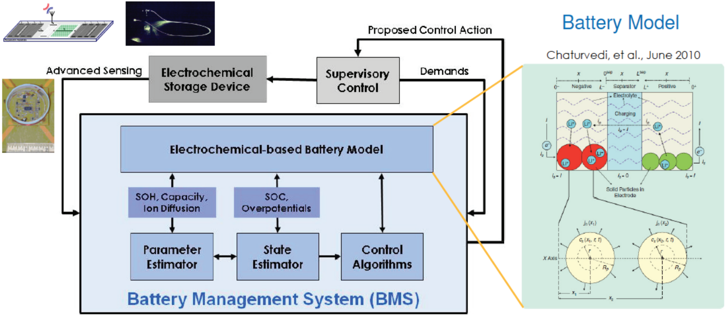

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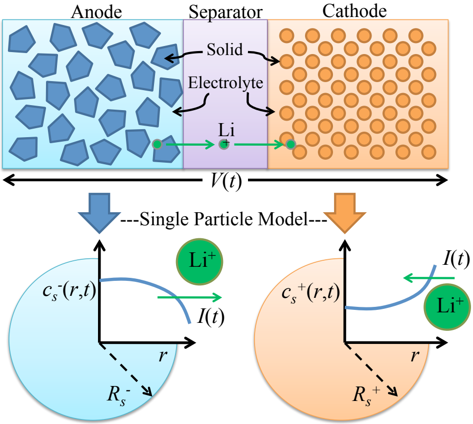
- S. Moura (2012) - Adaptive PDE Observer on SPM (States & Params)

Single Particle Model (SPM)



Single Particle Model (SPM)

Diffusion of Li in solid phase:

$$\frac{\partial c_s^-}{\partial t}(r,t) = \frac{D_s^-}{r^2}\frac{\partial}{\partial r}\left[r^2 \frac{\partial^2 c_s^-}{\partial r^2}(r,t)\right]$$

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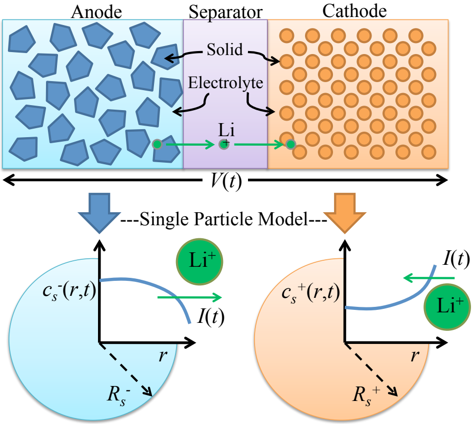

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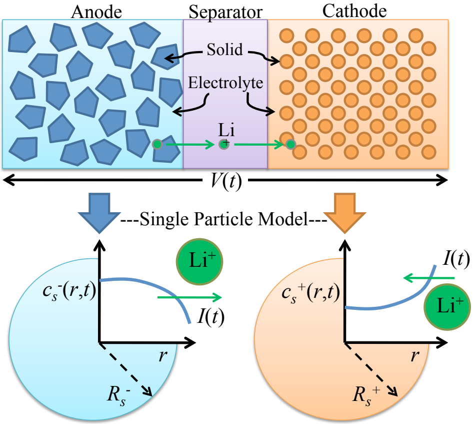
Boundary conditions:

$$\frac{\partial c_s^-}{\partial r}(R_s^-,t) = -\rho^+ I(t)$$

$$\frac{\partial c_s^+}{\partial r}(R_s^+,t) = \rho^- I(t)$$



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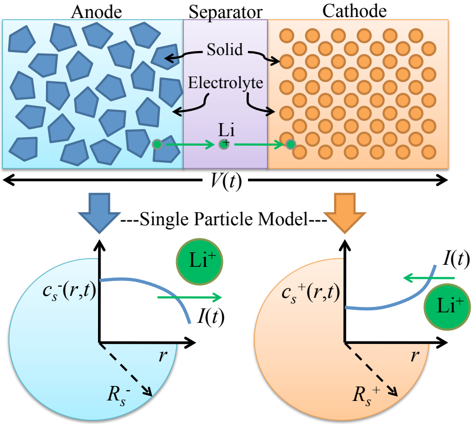
Voltage Output Function:

$$V(t) = h(c_{ss}^-(t), c_{ss}^+(t), I(t); \theta)$$



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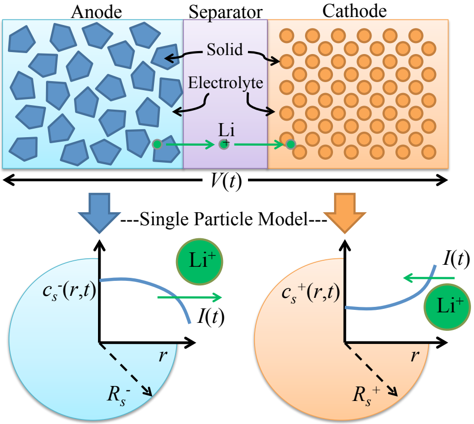
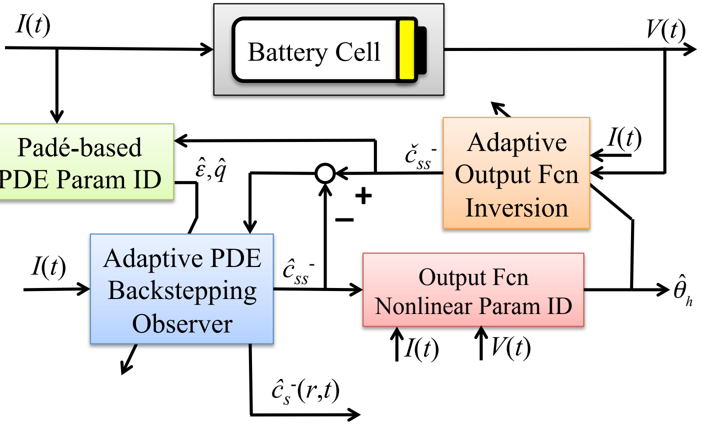


Definitions

- SOC: Bulk concentration SOC_{bulk}, Surface concentration $c_{ss}^-(t)$
- SOH: Physical parameters, e.g. ε, q, n_{Li}, R_f

Adaptive Observer

Combined State & Parameter Estimation



The SOC Estimation Problem

Problem Statement

Estimate states $c_s^-(r,t), c_s^+(r,t)$ from measurements $I(t), V(t)$ and SPM

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Simplify the Math

- Model reduction for observability
- Normalize time & space
- State transformation

Assumption: $c_{ss}^-(t)$ is measurable (to be relaxed later)

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Observer Model Equations

$$\frac{\partial c}{\partial t}(r,t) = \varepsilon \frac{\partial^2 c}{\partial r^2}(r,t) \qquad \text{Heat PDE}$$

$$c(0,t) = 0$$

$$\frac{\partial c}{\partial r}(1,t) - c(1,t) = -q\rho I(t)$$

$$\text{Measurement} = c(1,t) = c_{ss}^-(t)$$

Backstepping PDE Estimator

Estimator

$$
\begin{aligned}
\frac{\partial \hat{c}}{\partial t}(r,t) &= \varepsilon \frac{\partial^2 \hat{c}}{\partial r^2}(r,t) + p_1(r)\left[c(1,t) - \hat{c}(1,t)\right] \\
\hat{c}(0,t) &= 0 \\
\frac{\partial \hat{c}}{\partial r}(1,t) - \hat{c}(1,t) &= -q\rho I(t) + p_{10}\left[c(1,t) - \hat{c}(1,t)\right] \\
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\end{aligned}
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\end{aligned}
$$

Estimation Error Dynamics: $\tilde{c}(r,t) = c(r,t) - \hat{c}(r,t)$

$$
\begin{aligned}
\frac{\partial \tilde{c}}{\partial t}(r,t) &= \varepsilon \frac{\partial^2 \tilde{c}}{\partial r^2}(r,t) - p_1(r)\tilde{c}(1,t) \\
\tilde{c}(0,t) &= 0 \\
\frac{\partial \tilde{c}}{\partial r}(1,t) - \tilde{c}(1,t) &= -p_{10}\tilde{c}(1,t)
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\end{aligned}$$

The Concept

$$\tilde{c}(r,t) = \tilde{w}(r,t) - \int_r^1 p(r,s)\tilde{w}(s)ds$$

Backstepping Transformation

$$\frac{\partial \tilde{w}}{\partial t}(r,t) = \varepsilon \frac{\partial^2 \tilde{w}}{\partial r^2}(r,t) + \lambda \tilde{w}(r,t)$$

$$\tilde{w}(0,t) = 0$$

$$\frac{\partial \tilde{w}}{\partial r}(1,t) = \frac{1}{2}\tilde{w}(1,t)$$

Exp. Stable Target System

$$W = \frac{1}{2}\int_0^1 \tilde{w}^2(x,t)dx$$

Backstepping PDE Estimator

Estimator

$$\begin{aligned}
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\end{aligned}$$

Kernel PDE

$$p(r,s) : \mathcal{D} \to \mathbb{R}, \qquad \mathcal{D} = \{(r,s) | 0 \le r \le s \le 1\}$$

$$p_{rr}(r,s) - p_{ss}(r,s) = \frac{\lambda}{\varepsilon} p(r,s) \qquad p_1(r) = -p_s(r,1) - \frac{1}{2} p(r,1)$$

$$p(0,s) = 0 \qquad p_{10} = \frac{3 - \lambda/\varepsilon}{2}$$

$$p(r,r) = \frac{\lambda}{2\varepsilon} r$$

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Explicit Solution to Estimator Gains

$$p_1(r) = \frac{-\lambda r}{2\varepsilon z}\left[I_1(z) - \frac{2\lambda}{\varepsilon z} I_2(z)\right] \qquad \text{where} \quad z = \sqrt{\frac{\lambda}{\varepsilon}(r^2 - 1)}$$

$$p_{10} = \frac{1}{2}\left(3 - \frac{\lambda}{\varepsilon}\right)$$

The SOH Estimation Problem

Problem Statement

Estimate physical parameters from measurements $I(t), V(t)$ and SPM

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Relate uncertain parameters to SOH-related concepts

- Capacity fade
- Power fade

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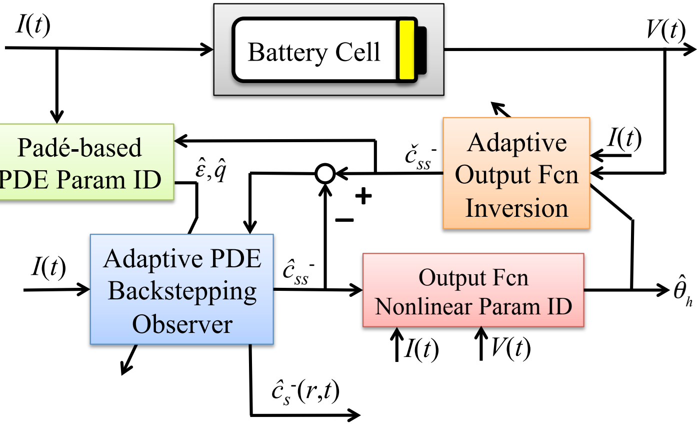

Padé-based PDE Parameter Identification

PDE Model

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Challenge:

- ε multiplies unmeasurable states

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Main Idea:

- Padé approx. of TF

$$\frac{c_{ss}(s)}{I(s)} = \frac{-q\rho \sinh\left(\sqrt{\frac{s}{\varepsilon}}\right)}{\left(\sqrt{\frac{s}{\varepsilon}}\right)\cosh\left(\sqrt{\frac{s}{\varepsilon}}\right) - \sinh\left(\sqrt{\frac{s}{\varepsilon}}\right)} \approx \frac{-3\rho q\varepsilon^2 - \frac{2}{7}\rho q\varepsilon s}{\varepsilon s + \frac{1}{35}s^2}$$

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Apply recursive least squares to $\theta_{pde} = [\varepsilon, q\varepsilon, q\varepsilon^2]^T$

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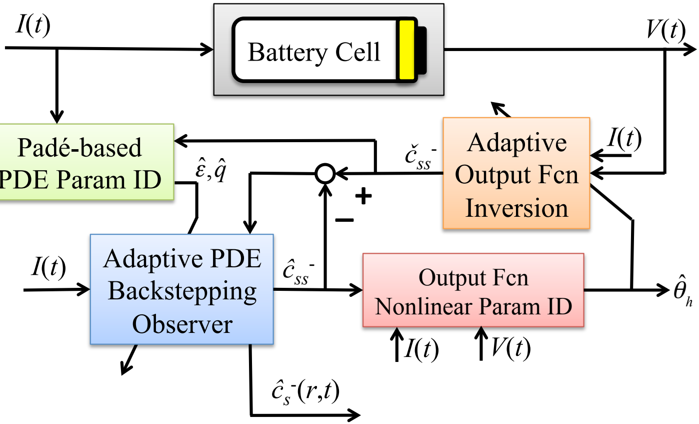

Output Function Nonlinear Parameter ID

Nonlinearly Parameterized Output

$$V(t) = h(c_{ss}^{-}(t), I(t); \theta)$$

- θ contains many parameters
- Linear dependence between parameters?

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Identifiability Analysis Result

- Linearly independent parameter subset : $\theta_h = [n_{Li}, R_f]^T$
  - n_{Li} : Total amount of cyclable Li (Capacity Fade)
  - R_f : Resistance of current collectors, electrolyte, SEI layer (Power Fade)

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Apply nonlinear recursive least squares to θ_h

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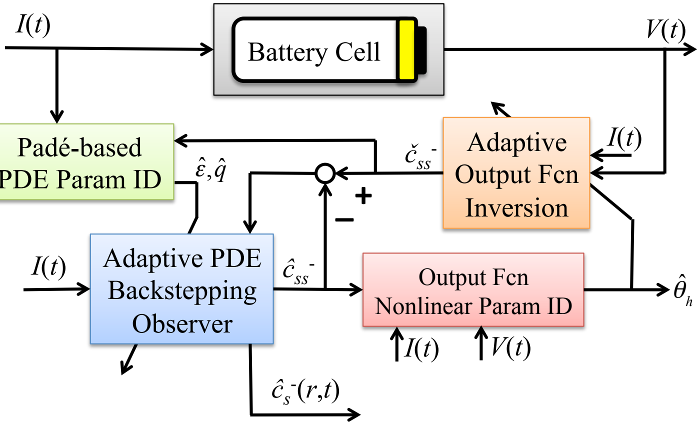

Adaptive Output Function Inversion

Require $c_{ss}^{-}(t)$ for output error injection

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Nonlinear Function Inversion

Solve $g(c_{ss}^{-}, t) = 0$ for c_{ss}^{-}, where

$$g(c_{ss}^{-}, t) = h(c_{ss}^{-}(t), I(t); \hat{\theta}_h) - V(t)$$

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Newton's Method

Main Idea: Construct ODE with exp. stable equilibrium $g(c_{ss}^{-}, t) = 0$

$$\frac{d}{dt}\left[g(\check{c}_{ss}^{-}, t)\right] = -\gamma g(\check{c}_{ss}^{-}, t)$$

expands to a Newton's method update law:

$$\frac{d}{dt}\check{c}_{ss}^{-} = -\frac{\gamma g(\check{c}_{ss}^{-}, t) + \frac{\partial g}{\partial t}(\check{c}_{ss}^{-}, t)}{\frac{\partial g}{\partial c_{ss}^{-}}(\check{c}_{ss}^{-}, t)}$$

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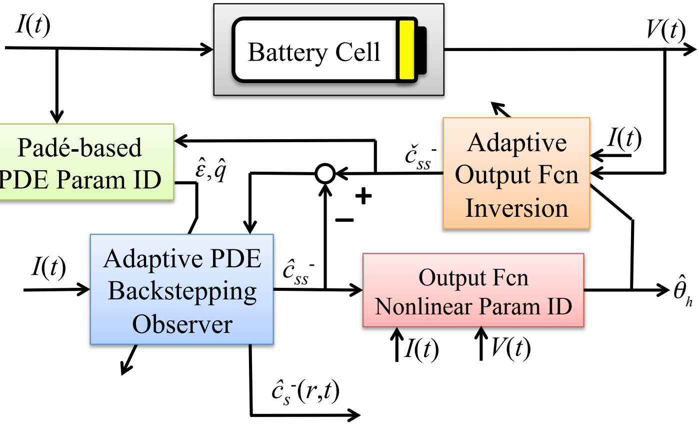
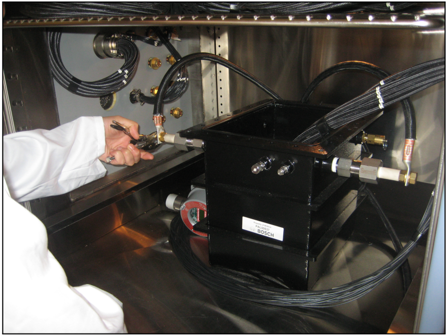
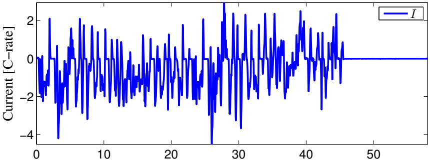


Experimental Testing at Bosch RTC



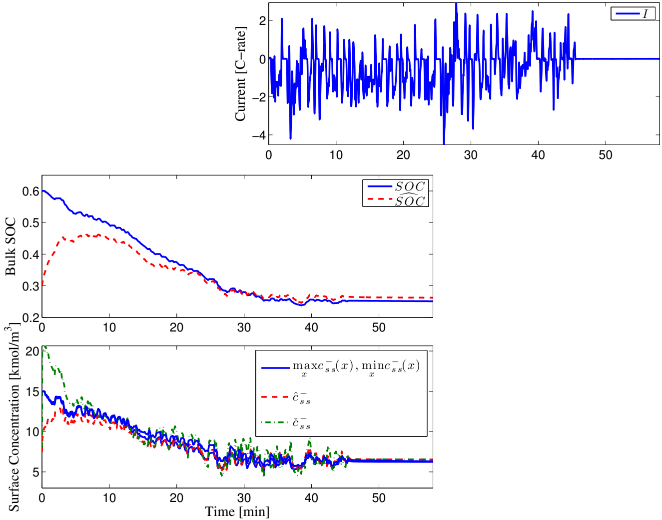
Results

UDDS Drive Cycle Input



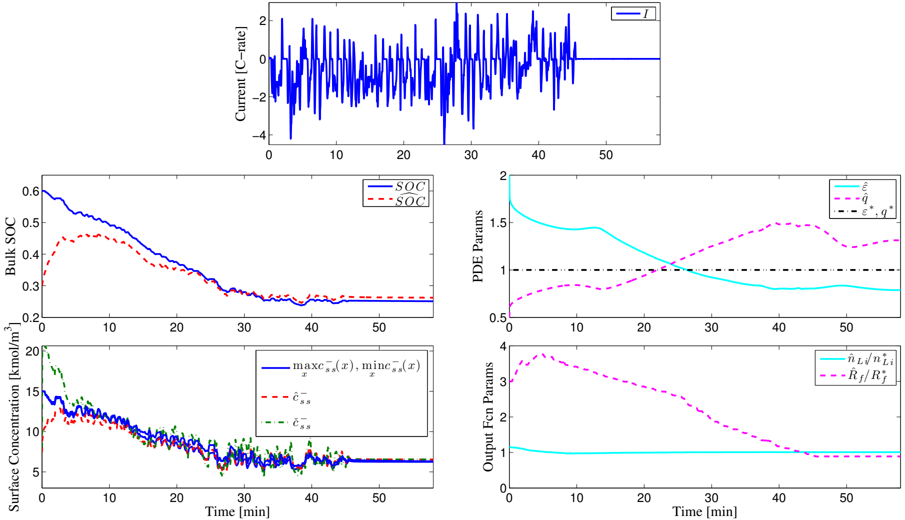
Results

UDDS Drive Cycle Input



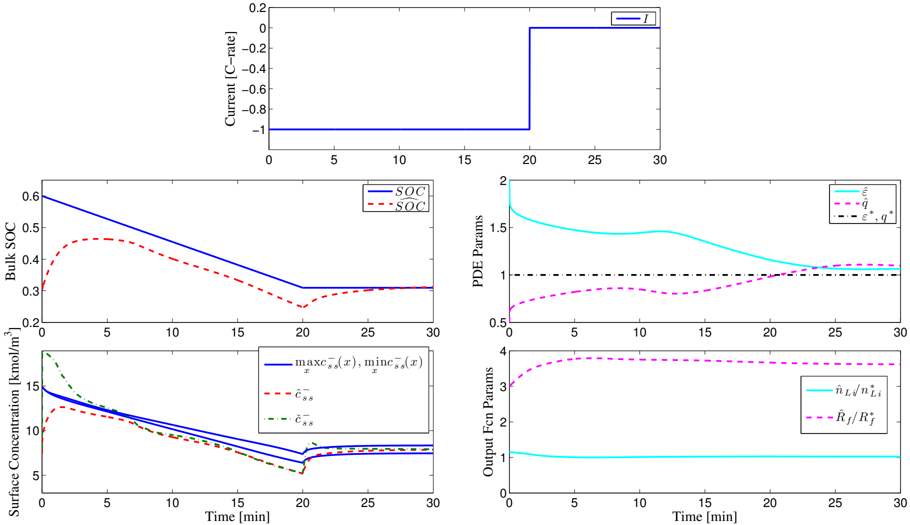
Results

UDDS Drive Cycle Input



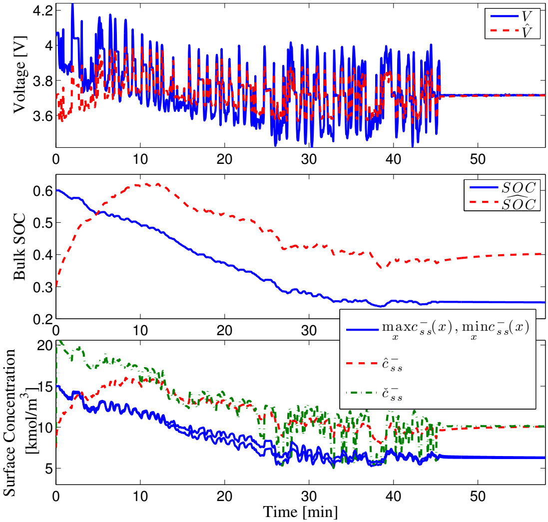
Results

Constant 1C Discharge



Results

No Parameter Adaption - Bias in State Estimates

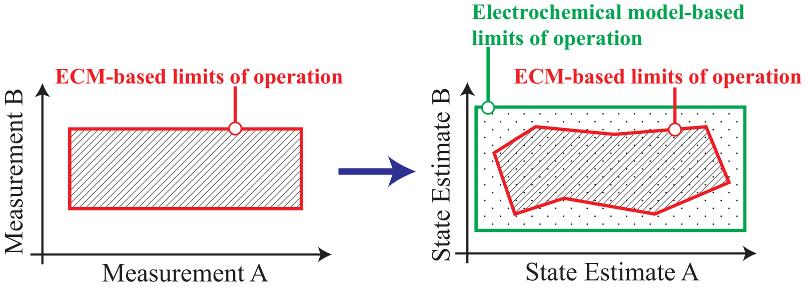


Operate Batteries at their Physical Limits

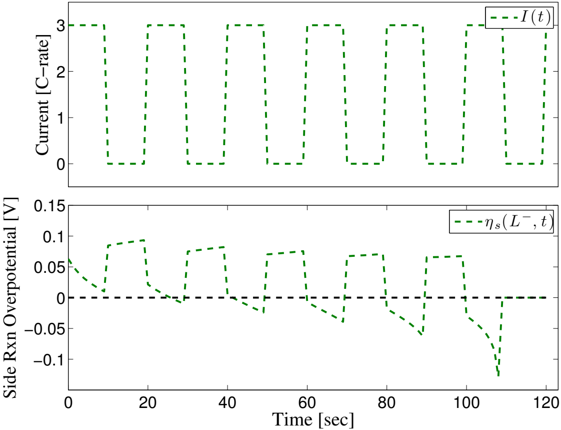
Operate Batteries at their Physical Limits

Problem Statement

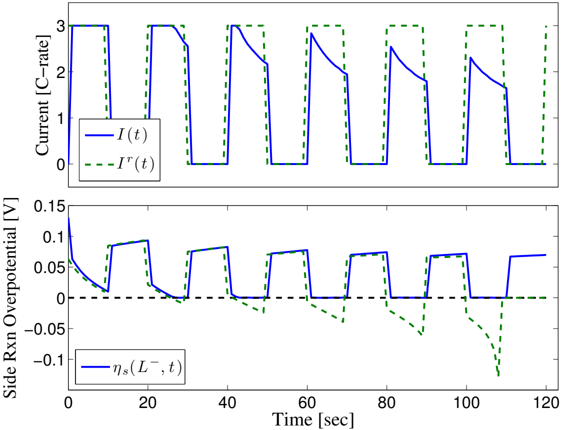
Given accurate state estimates, govern the electric current such that safe operating constraints are satisfied.



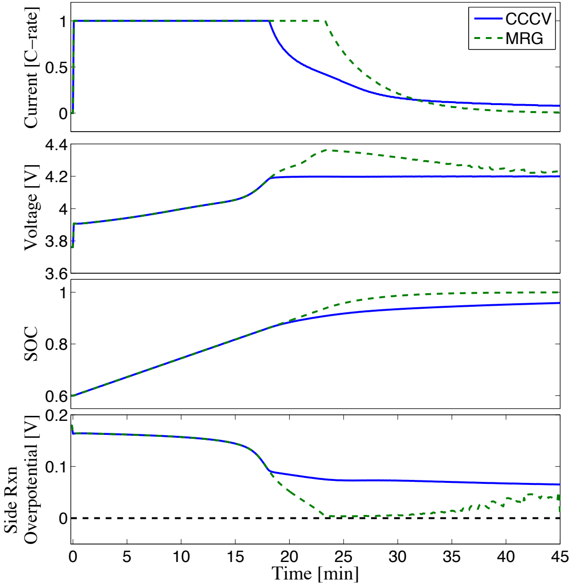
Constrained Control of EChem States



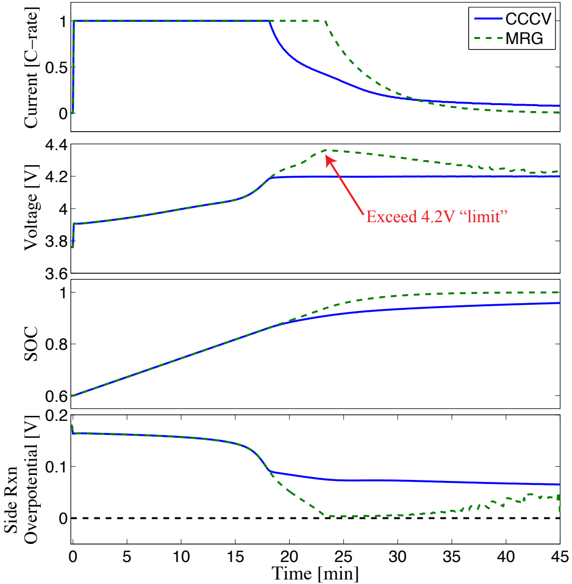
Constrained Control of EChem States



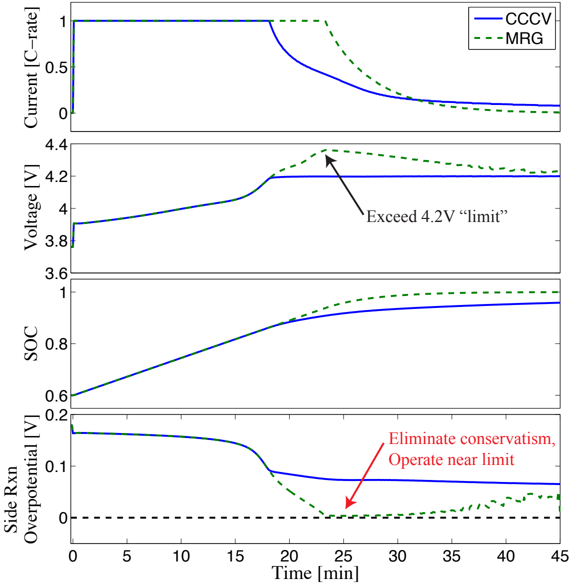
Application to Charging



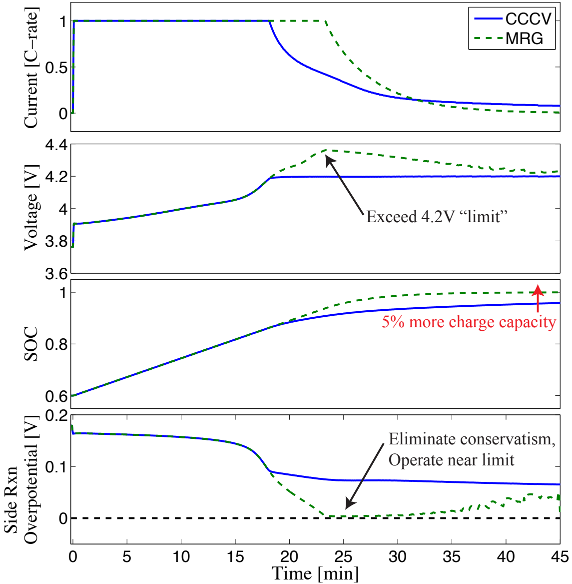
Application to Charging



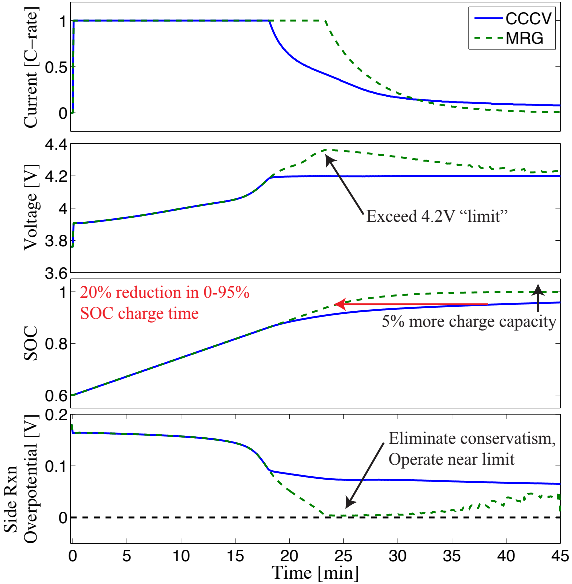
Application to Charging



Application to Charging

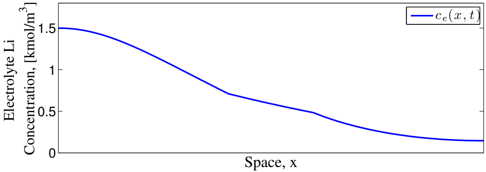


Application to Charging



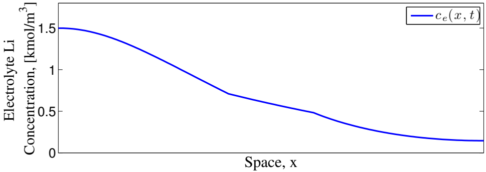
Future

Incorporate electrolyte dynamics

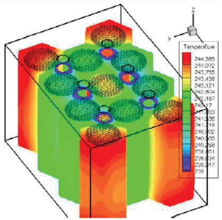


Future

Incorporate electrolyte dynamics



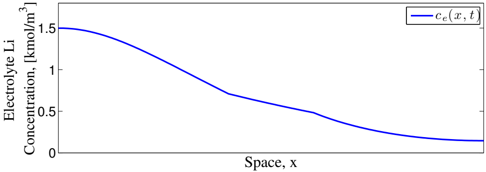
Thermal management of large battery packs



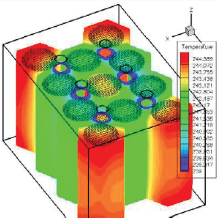
CFD simulation

Future

Incorporate electrolyte dynamics

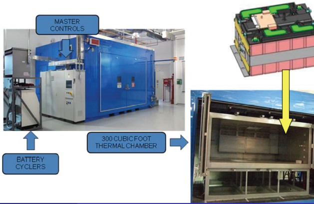


Thermal management of large battery packs



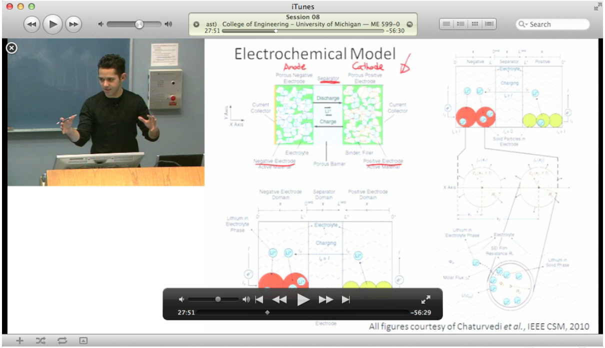
CFD simulation

Experimental validation - continued collaboration w/ Bosch RTC, Cobasys, and ARPA-E



Enrollment

- Winter 2010: 59 + 5 distance
- Winter 2011: 50 + 26 distance
- ME, EE, ChemE, CS, Energy Systems, MatSci, Physics, Math
- Undergraduates
- Graduate students
- Professionals
  - Tesla Motors, General Motors, Roush, US Army



Summary

Rich playground for DSC researchers

High-fidelity models + Adv. estimation/control = Enhanced performance

Battery Systems and Control:
Critically important & Fundamentally rich

Questions?

Scott Moura, Ph.D.
http://flyingv.ucsd.edu/smoura/

Managing Overparameterization

$$\hat{\theta}_{pde} = \begin{bmatrix} \widehat{q\varepsilon^2} \\ \widehat{q\varepsilon} \\ \hat{\varepsilon} \end{bmatrix} \longrightarrow \begin{bmatrix} \hat{\varepsilon} \\ \hat{q} \end{bmatrix} = \hat{\theta}_{\varepsilon q}$$

Managing Overparameterization

$$\hat{\theta}_{pde} = \begin{bmatrix} \widehat{q\varepsilon^2} \\ \widehat{q\varepsilon} \\ \hat{\varepsilon} \end{bmatrix} \longrightarrow \begin{bmatrix} \hat{\varepsilon} \\ \hat{q} \end{bmatrix} = \hat{\theta}_{\varepsilon q}$$

$$\begin{bmatrix} 2 & 1 \\ 1 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \log \hat{\varepsilon} \\ \log \hat{q} \end{bmatrix} = \begin{bmatrix} \log \left(q\hat{\varepsilon}^2 \right) \\ \log \left(\hat{q\varepsilon} \right) \\ \log \left(\hat{\varepsilon} \right) \end{bmatrix}$$

$$\begin{aligned} A_{\varepsilon q} \log(\hat{\theta}_{\varepsilon q}) &= \log(\hat{\theta}_{pde}) \\ \log(\hat{\theta}_{\varepsilon q}) &= A_{\varepsilon q}^{+} \log(\hat{\theta}_{pde}) \end{aligned}$$

Managing Overparameterization

$$\hat{\theta}_{pde} = \begin{bmatrix} \widehat{q\varepsilon^2} \\ \widehat{q\varepsilon} \\ \hat{\varepsilon} \end{bmatrix} \longrightarrow \begin{bmatrix} \hat{\varepsilon} \\ \hat{q} \end{bmatrix} = \hat{\theta}_{\varepsilon q}$$

$$\begin{bmatrix} 2 & 1 \\ 1 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \log \hat{\varepsilon} \\ \log \hat{q} \end{bmatrix} = \begin{bmatrix} \log\left(\widehat{q\varepsilon^2}\right) \\ \log\left(\widehat{q\varepsilon}\right) \\ \log\left(\hat{\varepsilon}\right) \end{bmatrix}$$

$$\begin{aligned} A_{\varepsilon q} \log(\hat{\theta}_{\varepsilon q}) &= \log(\hat{\theta}_{pde}) \\ \log(\hat{\theta}_{\varepsilon q}) &= A_{\varepsilon q}^{+} \log(\hat{\theta}_{pde}) \end{aligned}$$

Remark: $A_{\varepsilon q}^{+} = \left(A_{\varepsilon q}^{T} A_{\varepsilon q}\right)^{-1} A_{\varepsilon q}^{T}$ is the Moore-Penrose psuedoinverse of $A_{\varepsilon q}$