# Adaptive Estimation and Control of Models for Battery Electrochemistry

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UCSB

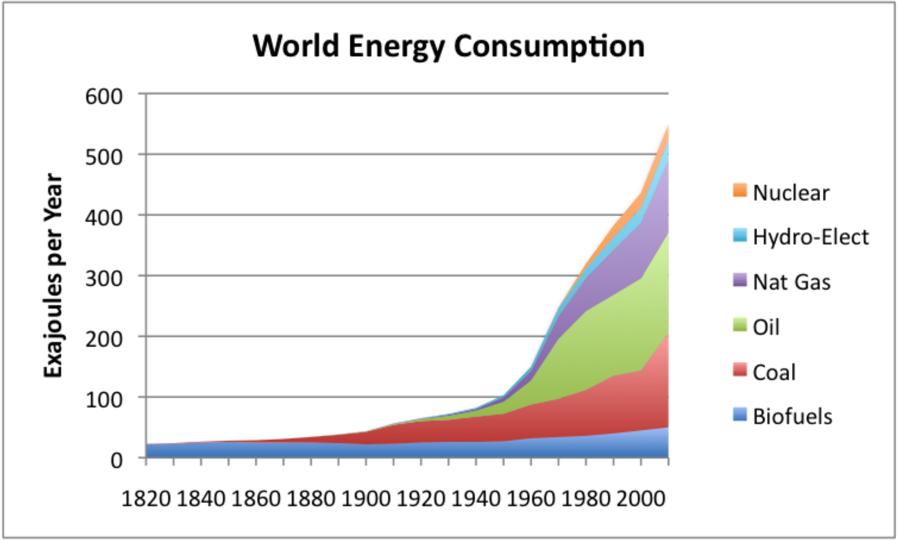
UNIVERSITY OF CALIFORNIA
SANTA BARBARA

*Core Philosophy:*

(Dynamical models of physical phenomena)

$+$ (novel control paradigms)

$=$ (transformative advancements)




Vaclav Smil Estimates from Energy Transitions

# Energy Initiatives

Denmark 50% wind penetration by 2025

China leads manufacturing of renewable tech

Brazil uses 86% renewables


EV Everywhere

SunShot

Green Button

33% renewables by 2020

Go Solar California

20% reduction of bldg. energy by 2015

# Energy Crisis Solutions

| Integrate variable renewables | Decrease energy waste |
| --- | --- |
| $\Downarrow$ | $\Downarrow$ |
| Energy storage | Intelligent energy management |
| (e.g., batteries) | (e.g., smart grids) |

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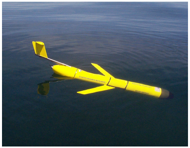
# Outline

1. Batteries
   - [Electrochemical Modeling] Incorporating Physics
   - [SOC/SOH Estimation] Looking Inside w/ Models, Meas., and Math
   - [Constrained Control] Operate at the Limits, Safely
2. Demand Response in Smart Grids
3. Future

# 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



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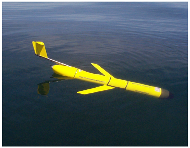
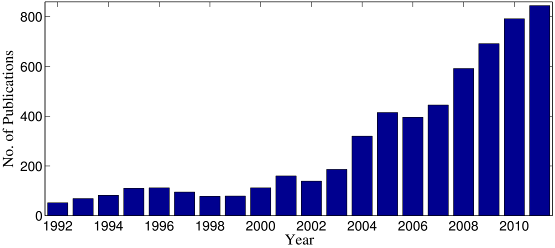


Keyword: “Battery Systems and Control”



# The Battery Problem

**Needs:** Cheap, high energy, high power, long life

**Today's reality:** Expensive, conservatively design/operated, die too quickly

### Some Motivating Facts

| | |
|---|---|
| EV Batts | \$800 / kWh now (2010)<br>\$125 / kWh for parity to IC engine<br><br>Only 75% of available capacity is used<br>Range anxiety inhibits adoption<br>Lifetime risks caused by fast charging |

### Two Solutions

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|---|---|
| Design better batteries (materials science & chemistry) | Make current batteries better (estimation and control) |

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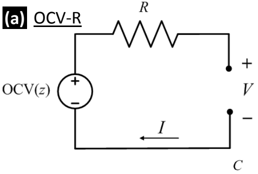
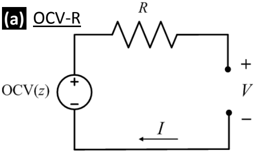
## Equivalent Circuit Model

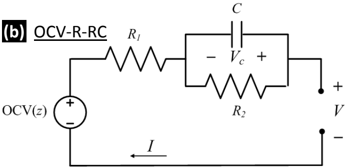


## Equivalent Circuit Model

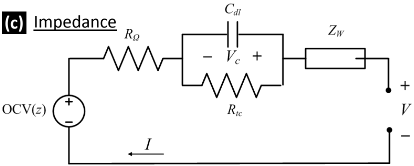
**(a)** OCV-R




**(b)** OCV-R-RC




**(c)** Impedance



# Battery Models

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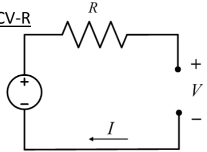


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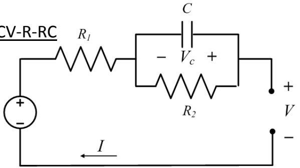


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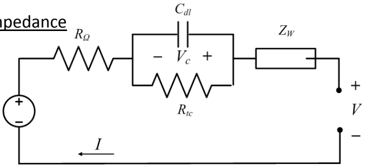
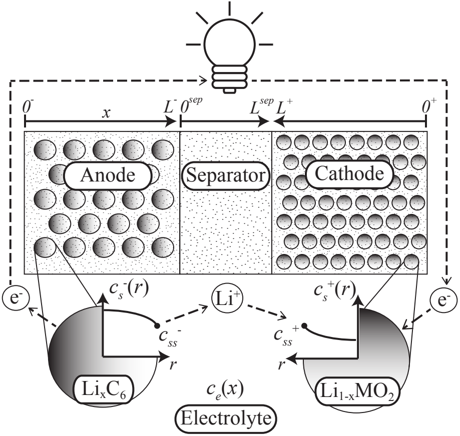
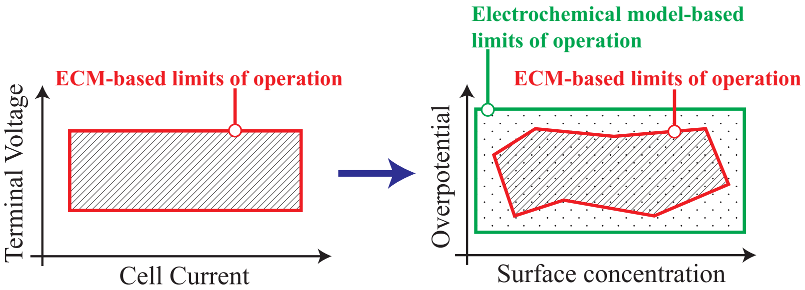



## Electrochemical Model



# Operate Batteries at their Physical Limits



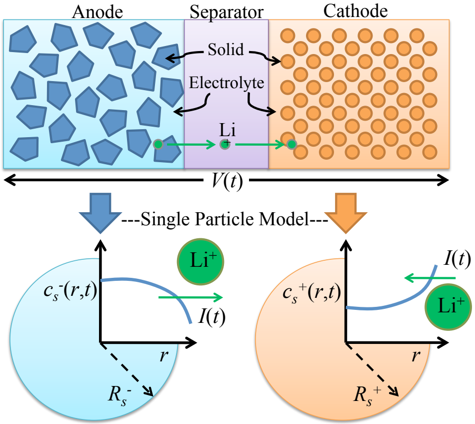
# Electrochemical Model Equations

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

# 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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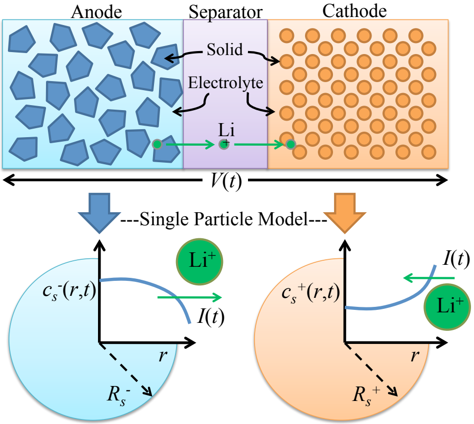

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Boundary conditions:

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

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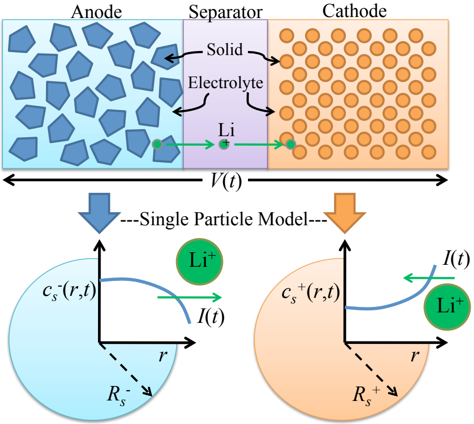

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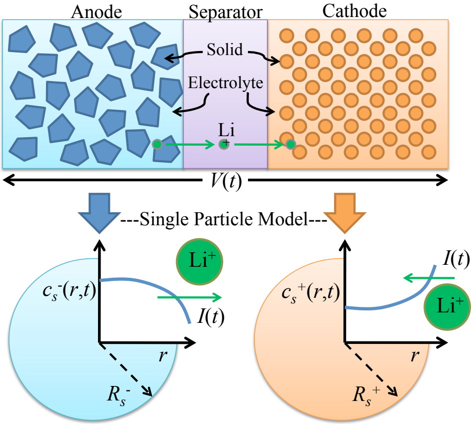
$$V(t) = h(c_{ss}^-(t), c_{ss}^+(t), I(t); \theta)$$



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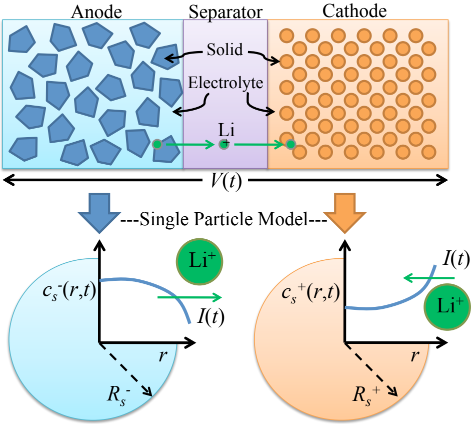


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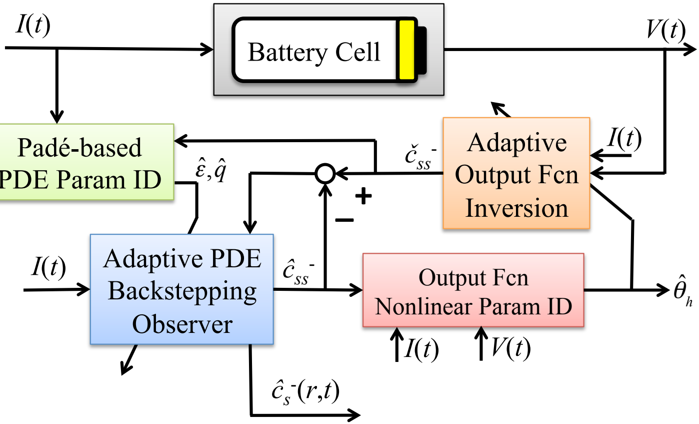
Definitions

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

# Adaptive Observer

## Combined State & Parameter Estimation



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# 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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- Normalize time and space
- Scale spatial dimension

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## Model Eqns. for Observer Design

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

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

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

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

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

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

## 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

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

$$\dot{W}(t) \leq -\gamma W(t)$$

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## Kernel PDE

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

$$
p_{rr}(r,s) - p_{ss}(r,s) = \frac{\lambda}{\varepsilon} p(r,s)
$$

$$
p(0,s) = 0
$$

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

$$
p_1(r) = -p_s(r,1) - \frac{1}{2} p(r,1)
$$

$$
p_{10} = \frac{3 - \lambda/\varepsilon}{2}
$$

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## Explicit Solution to Estimator Gains

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

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

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

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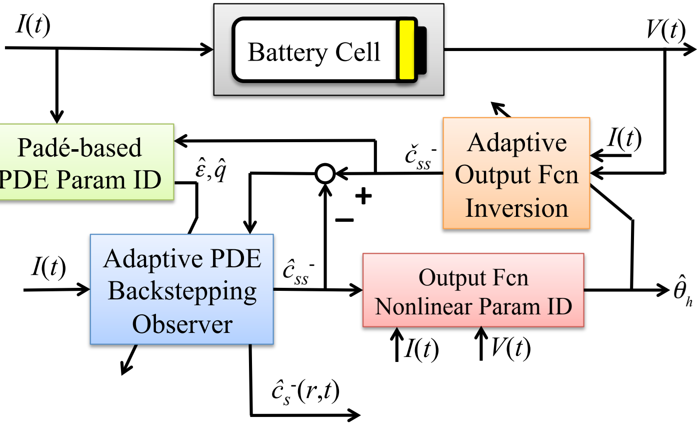
Relate uncertain parameters to SOH-related concepts

- Capacity fade
- Power fade

# Adaptive Observer

## Combined State & Parameter Estimation



# Output Function Nonlinear Parameter ID

## Nonlinearly Parameterized Output

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

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## Identifiability Analysis

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

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Apply nonlinear recursive least squares to $\theta_h$

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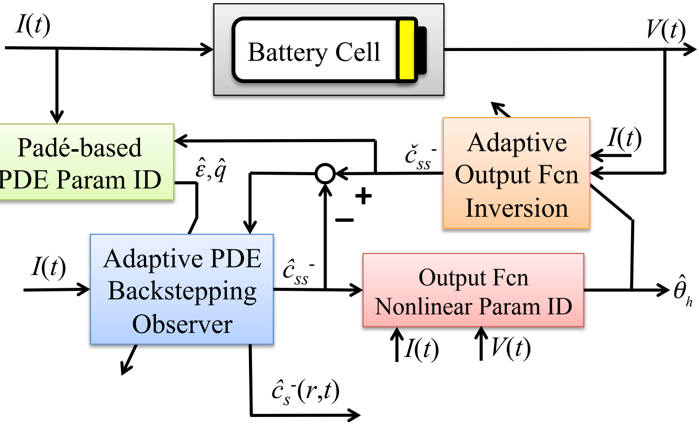

# Adaptive Output Function Inversion

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

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

# Adaptive Output Function Inversion

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

## Nonlinear Function Inversion

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

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

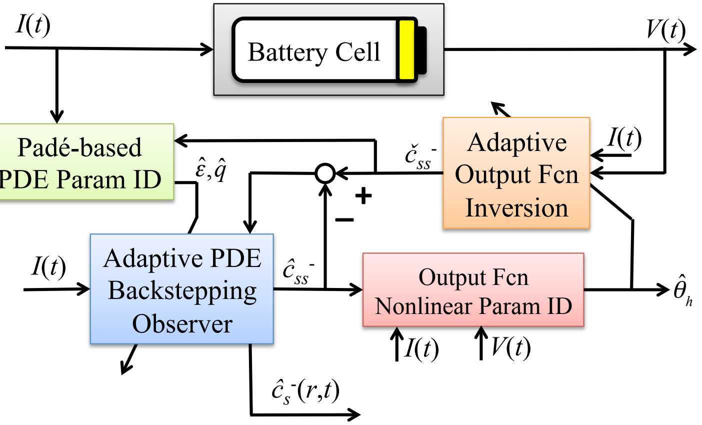
## Newton's Method

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

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

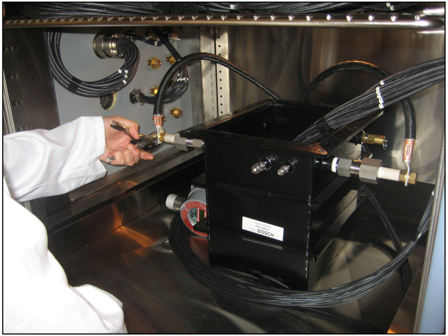
expands to a Newton's method update law:

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



$I(t)$
Battery Cell
$V(t)$
Padé-based
PDE Param ID
$\hat{\varepsilon}, \hat{q}$
$\check{c}_{ss}^{-}$
Adaptive
Output Fcn
Inversion
$I(t)$
+
−
$I(t)$
Adaptive PDE
Backstepping
Observer
$\hat{c}_{ss}^{-}$
Output Fcn
Nonlinear Param ID
$\hat{\theta}_h$
$I(t)$
$V(t)$
$\hat{c}_s^{-}(r,t)$

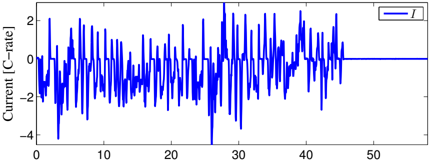
# Experimental Testing | ARPA-E AMPED Program



arpa·e BOSCH COBASYS

# Results

## UDDS Drive Cycle Input



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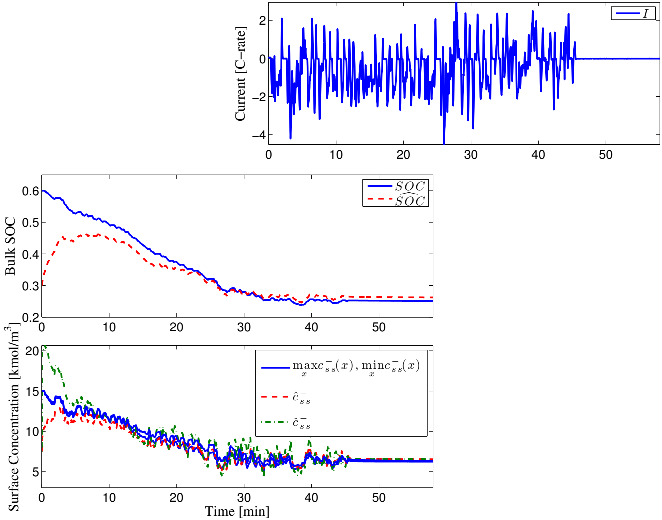

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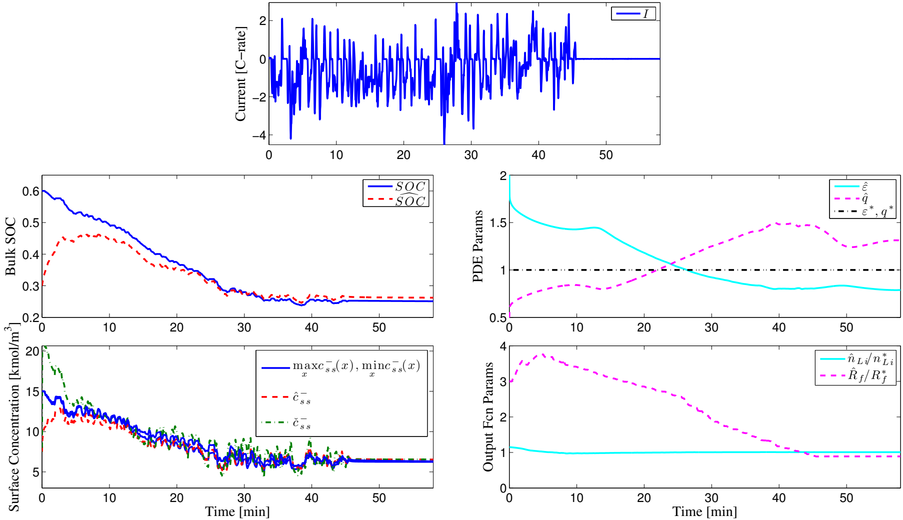
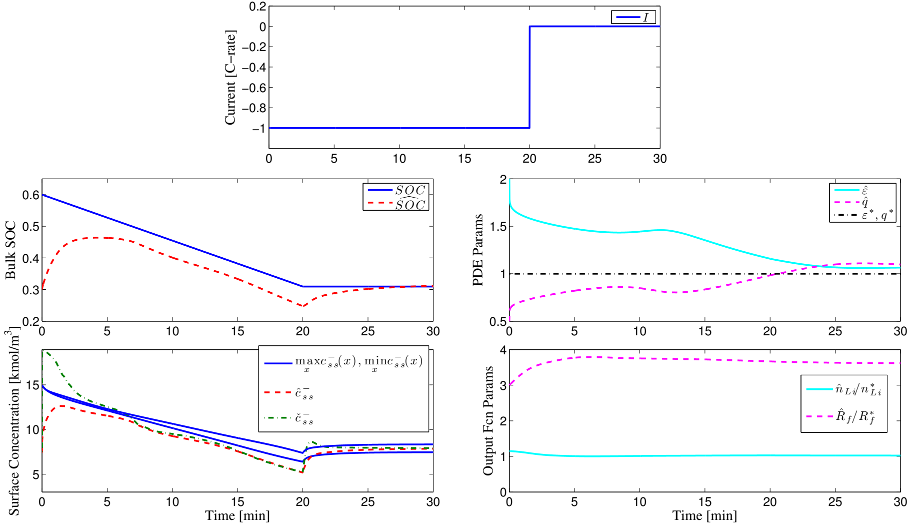


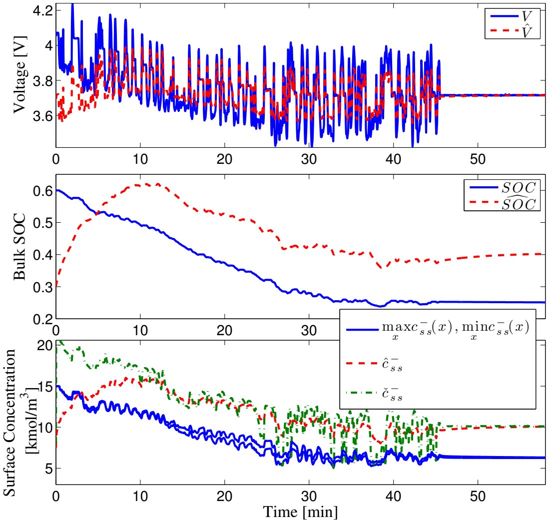
# Results

## Constant 1C Discharge



# Results

## No Parameter Adaption - Bias in State Estimates



# Outline

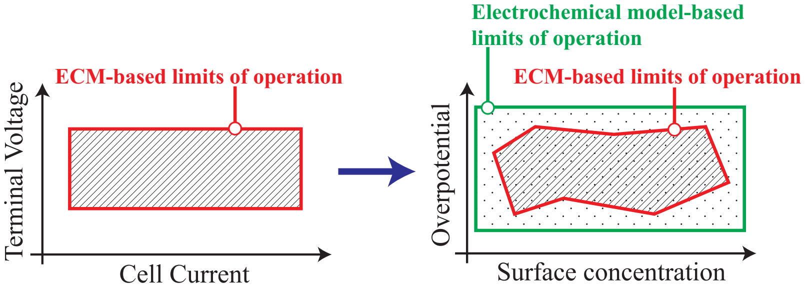
1. Batteries
   - [Electrochemical Modeling] Incorporating Physics
   - [SOC/SOH Estimation] Looking Inside w/ Models, Meas., and Math
   - [Constrained Control] Operate at the Limits, Safely
2. Demand Response in Smart Grids
3. Future

# 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.

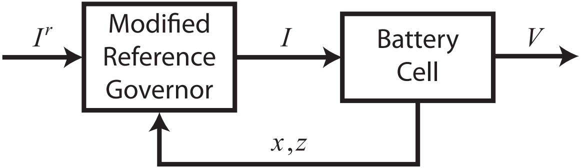


# Constraints

| Variable | Definition | Constraint |
|---|---|---|
| $I(t)$ | Current | Power electronics limits |
| $c_s^{\pm}(x,r,t)$ | Li concentration in solid | Saturation/depletion |
| $\frac{\partial c_s^{\pm}}{\partial r}(x,r,t)$ | Li concentration gradient | Diffusion-induced stress |
| $c_e(x,t)$ | Li concentration in electrolyte | Saturation/depletion |
| $T(t)$ | Temperature | High/low temps accel. aging |
| $\eta_s(x,t)$ | Side-rxn overpotential | Li plating, dendrite formation |

Each variable, $y$, must satisfy $y_{\min} \leq y \leq y_{\max}$.

# The Algorithm: Modified Reference Governor (MRG)



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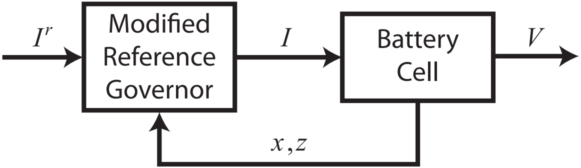


## MRG Equations

$$I[k+1] = \beta^*[k] I^r[k], \qquad \beta^* \in [0,1],$$

$$\beta^*[k] = \max \{\beta \in [0,1] : (x(t), z(t)) \in \mathcal{O}\}$$

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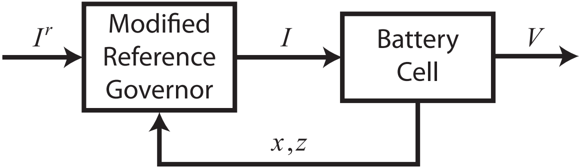


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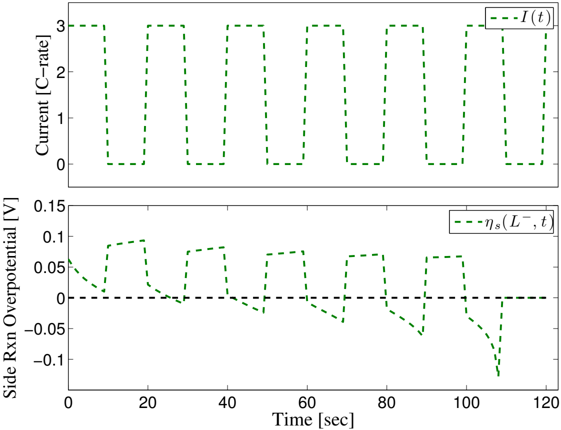
## Def'n: Admissible Set $\mathcal{O}$

$$\mathcal{O} = \{(x(t), z(t)) : y(\tau) \in \mathcal{Y}, \forall \tau \in [t, t+T_s]\}$$

$$\begin{aligned} \dot{x}(t) &= f(x(t), z(t), \beta I^r) \\ 0 &= g(x(t), z(t), \beta I^r) \\ y(t) &= C_1 x(t) + C_2 z(t) + D \cdot \beta I^r + E \end{aligned}$$

# Constrained Control of EChem States



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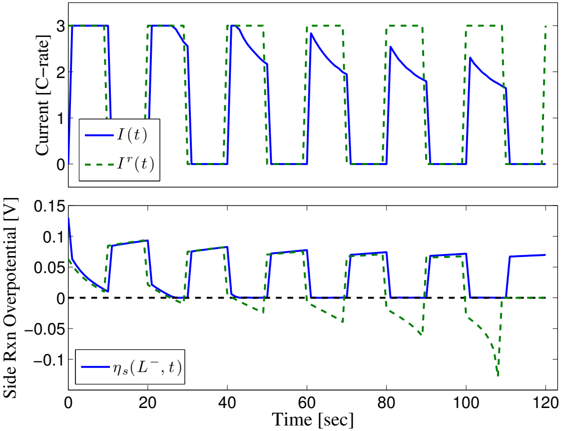
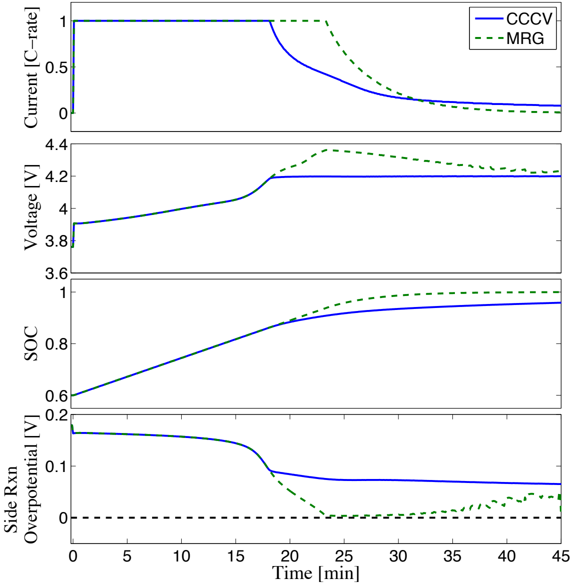


# Application to Charging



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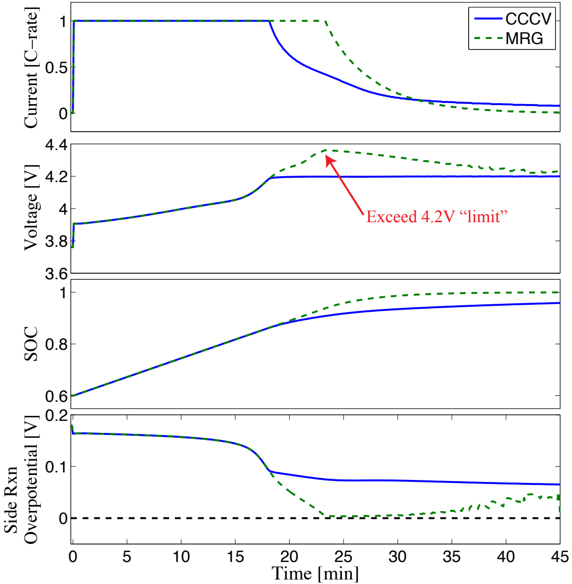
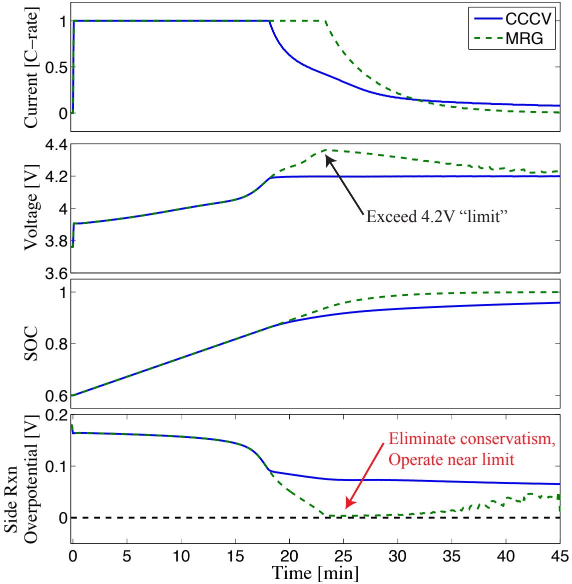
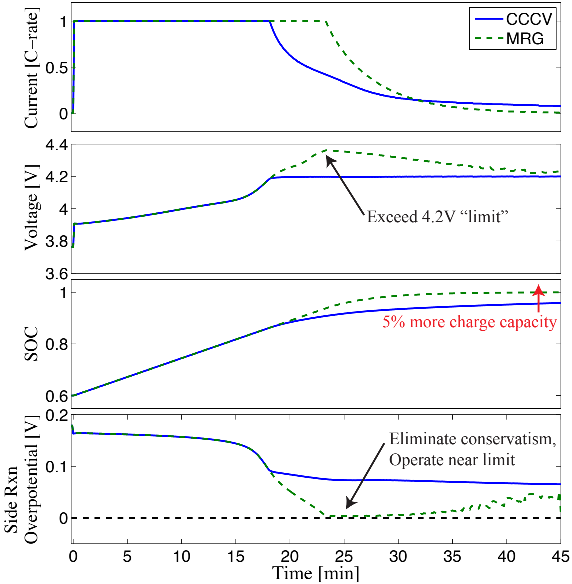
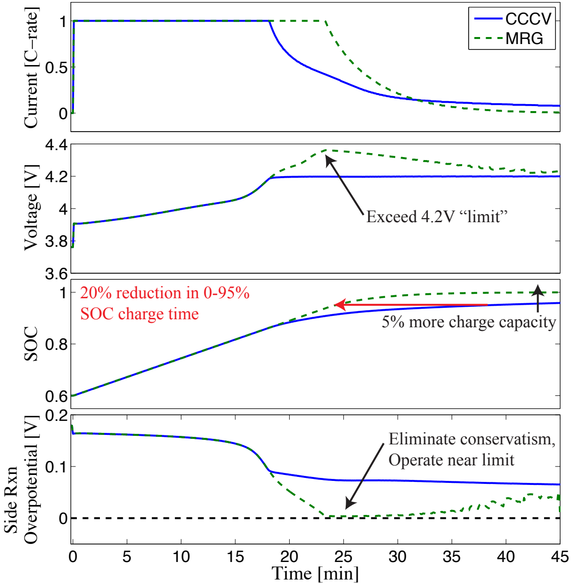


# Application to Charging




CCCV
MRG
Current [C−rate]
1
0.5
0
Voltage [V]
4.4
4.2
4
3.8
3.6
Exceed 4.2V "limit"
SOC
1
0.8
0.6
5% more charge capacity
Side Rxn
Overpotential [V]
0.2
0.1
0
Eliminate conservatism,
Operate near limit
0
5
10
15
20
25
30
35
40
45
Time [min]

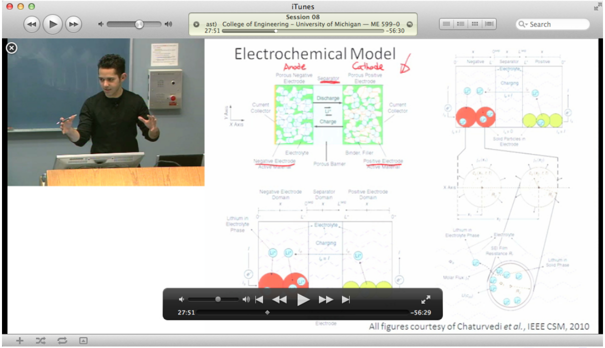
# Application to Charging



## 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 of Contributions

Simultaneous SOC/SOH estimation
of physically meaningful variables via electrochemical models,
PDE estimation theory, and adaptive control.

Constrained control of batteries
via an electrochemical model
and reference governors.

Impact through education.

# Energy Crisis Solutions

| Integrate variable renewables | Decrease energy waste |
| --- | --- |
| $\Downarrow$ | $\Downarrow$ |
| Energy storage | Intelligent energy management |
| (e.g., batteries) | (e.g., smart grids) |

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# Outline

# The Renewable Integration Problem

**Needs:** 33% renewables in CA by 2020

**Obstacle:** Must install 4 GW reserve capacity to support variability

**Some Interesting Facts**

| | |
|---|---|
| Thermostatically Controlled Loads (TCLs) | 50% of U.S. energy consumption is TCLs<br>Only 11% of thermostats are programmed |

**The Punchline**

Flexible loads (e.g. TCLs) can absorb variability in renewable generation

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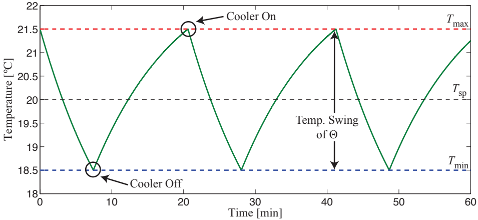
# Modeling Aggregations of TCLs

**Individual** TCL models

$\Downarrow$

(Tens of) Thousands of hybrid ODEs



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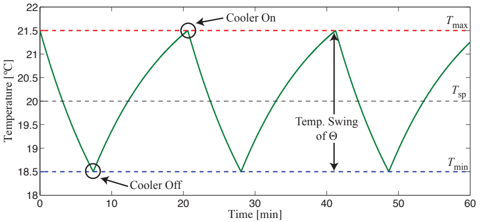
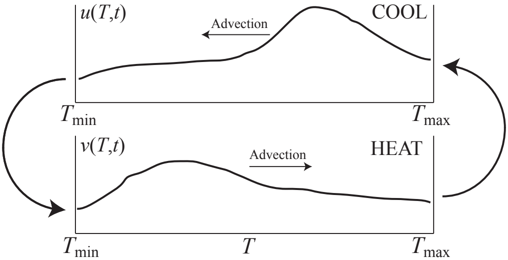



Model **aggregations** of TCLs

$\Downarrow$

Two coupled linear PDEs




| | |
|---|---|
| $u(T,t)$ | # TCLs/°C, in COOL state, @ temp $T$, time $t$ |
| $v(T,t)$ | # TCLs/°C, in HEAT state, @ temp $T$, time $t$ |

# On-campus Wireless Sensor Network for Demand Response

**Goal:**
Match demand to renewable generation

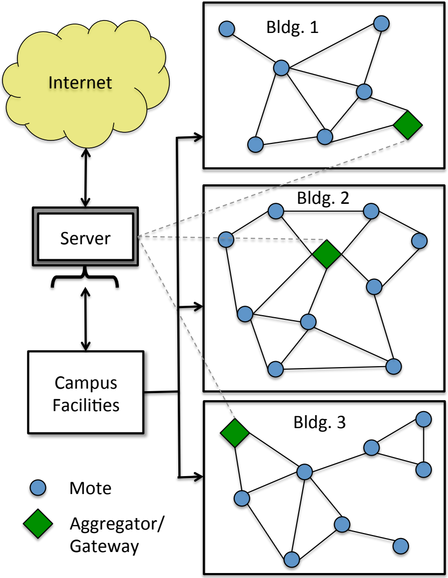
Measure:

- Temperature
- Humidity
- Luminosity
- Presence (PIR)

Actuate:

- Thermostat set-point

Libelium Waspmotes and Meshlium Gateway



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3. Future

# Future

| Battery Systems and Control | |
|---|---|
| | Estimator + Ref. Governor |
| | Observability for full model |
| | Electrochemical-Thermal Dynamics |
| | Experimental Testing |
| | Materials Science $\Leftrightarrow$ Dynamics Systems & Control |

| Demand Response for Renewable Integration | |
|---|---|
| | Campus implementation |
| | Predictive control via forecasting |
| | Vehicle-to-grid |
| | Price-based control |

*Core Philosophy:*

(Dynamical models of physical phenomena)

$+$ (novel control paradigms)

$=$ (transformative advancements)

Publications available at http://flyingv.ucsd.edu/smoura/

# Managing Overparameterization

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

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

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

# Managing Overparameterization

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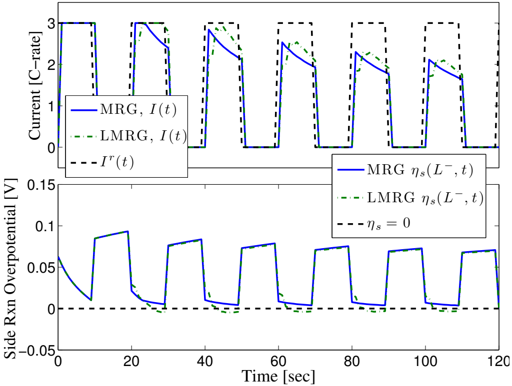
Remark: $A_{\varepsilon q}^{+} = \left(A_{\varepsilon q}^T A_{\varepsilon q}\right)^{-1} A_{\varepsilon q}^T$ is the Moore-Penrose psuedoinverse of $A_{\varepsilon q}$

# Linear Reference Governor

Modified Reference Governor (MRG) : Simulations
Linearized MRG (LMRG) : Explicit function evaluation



# PHEV Power Management

## Problem Statement

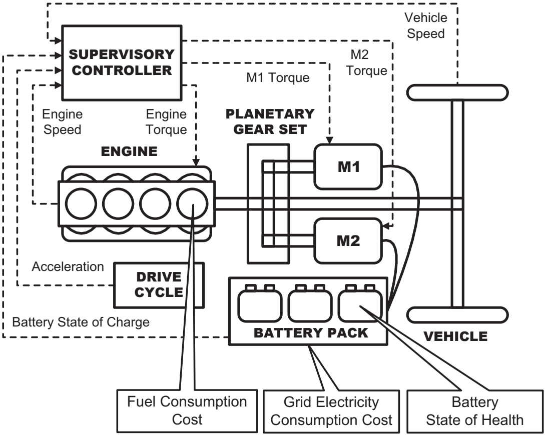
Design a supervisory control algorithm for plug-in hybrid electric vehicles (PHEVs) that splits engine and battery power in some optimal sense.


J. Voelcker, "Plugging Away in a Prius," *IEEE Spectrum*, vol. 45, pp. 30-48, 2008.

# Power-Split PHEV Model

Ex: Toyota Prius, Ford Escape Hybrid

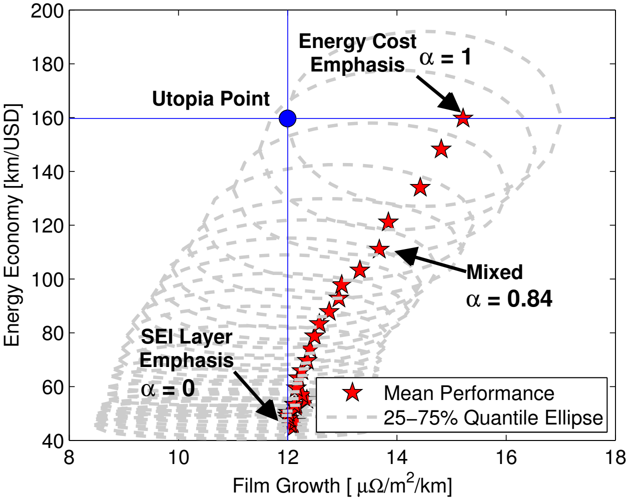
- Control Inputs
  - Engine Torque
  - M1 Torque
- State Variables
  - Engine speed
  - Vehicle speed
  - Battery SOC
  - Vehicle acceleration (Markov Chain)




Control Optimization: Minimize energy consumption cost AND battery aging

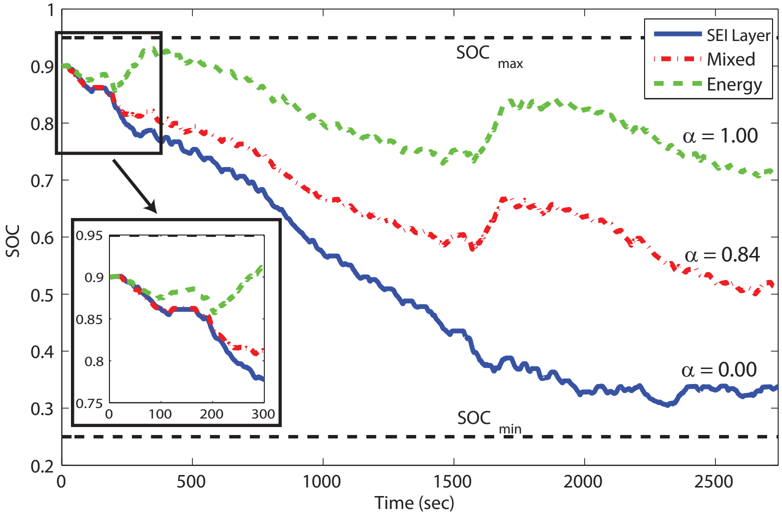
# Pareto Set of Optimal Solutions

## Anode-side SEI Layer Growth



# SOC Trajectories

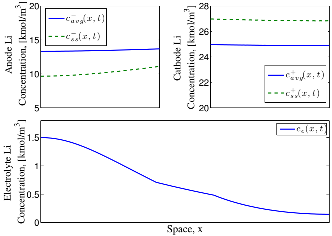
## Anode-side SEI Layer Growth | UDDSx2



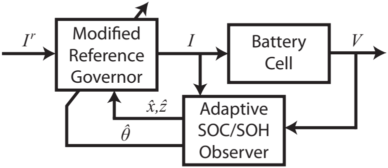
# Advanced Battery Management Systems

ARPA-E

## State Estimation w/ Electrolyte




## Estimator + Reference Governor




## Optimal charge/discharge

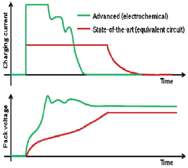



**Figure 2**: Charging phase of each duty cycle for BMS validation

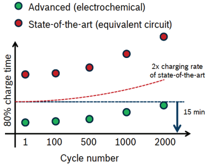
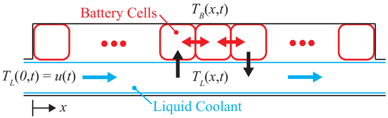



**Figure 3:** Comparison of charging time on a cycle to cycle basis for conventional BMS and advanced BMS

## Thermal Management



# Optimal Control of Distributed Parameter Systems

**Models**

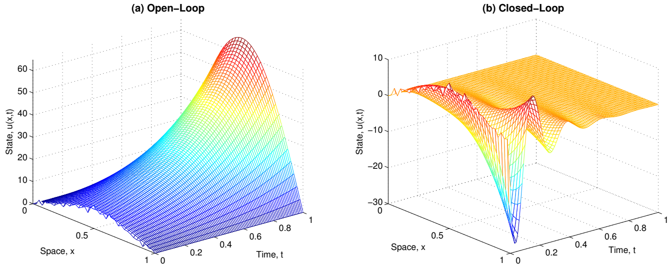
- Diffusion-Reaction-Advection
- Transport, Delays
- Waves, Beams, Nonlinear
- ...

**Apps**

- Fluid Dynamics
- Contaminant transport
- Solar Forecasting
- Heat Transfer
- ...

**Control Results**

- LQR
- Reference tracking
- Estimation
- Acutator/Sensor placement
- ...



# Demand Response of Aggregated Storage

Joint Work with Jan Bendsten, Aalborg University, Denmark