Real-Time Optimization

Methods and Applications

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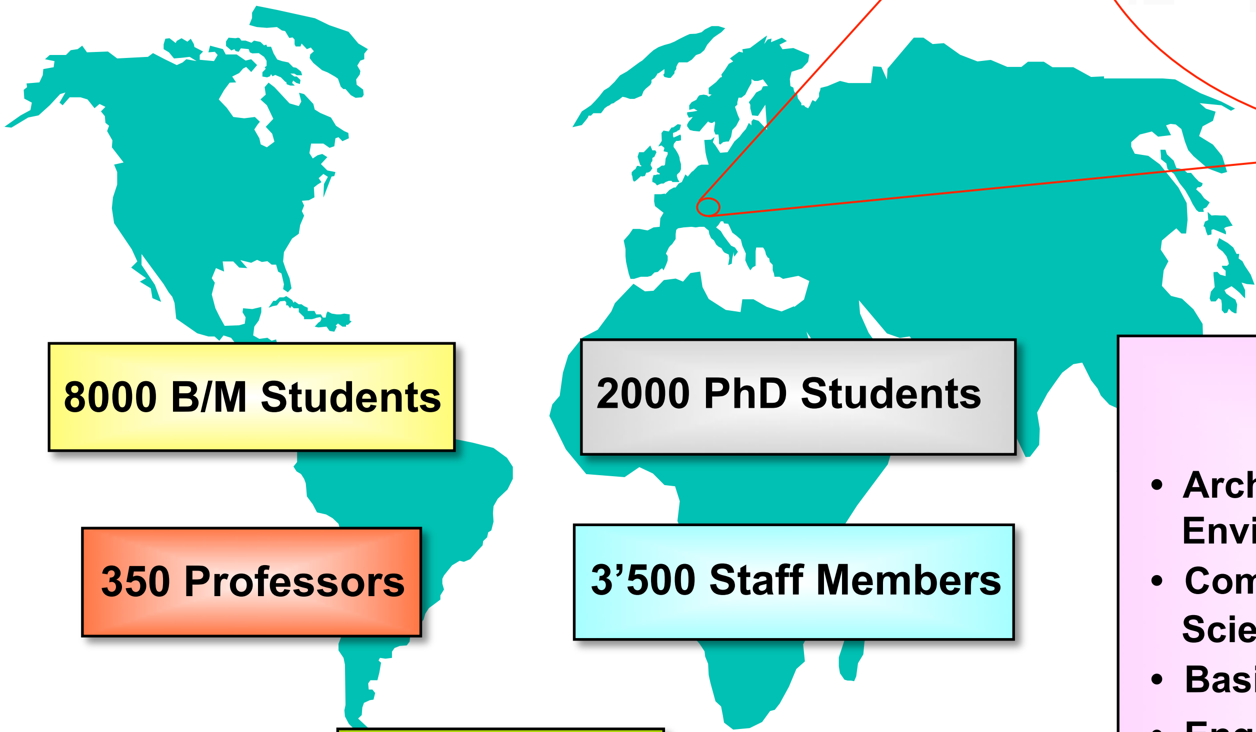


8000 B/M Students

2000 PhD Students

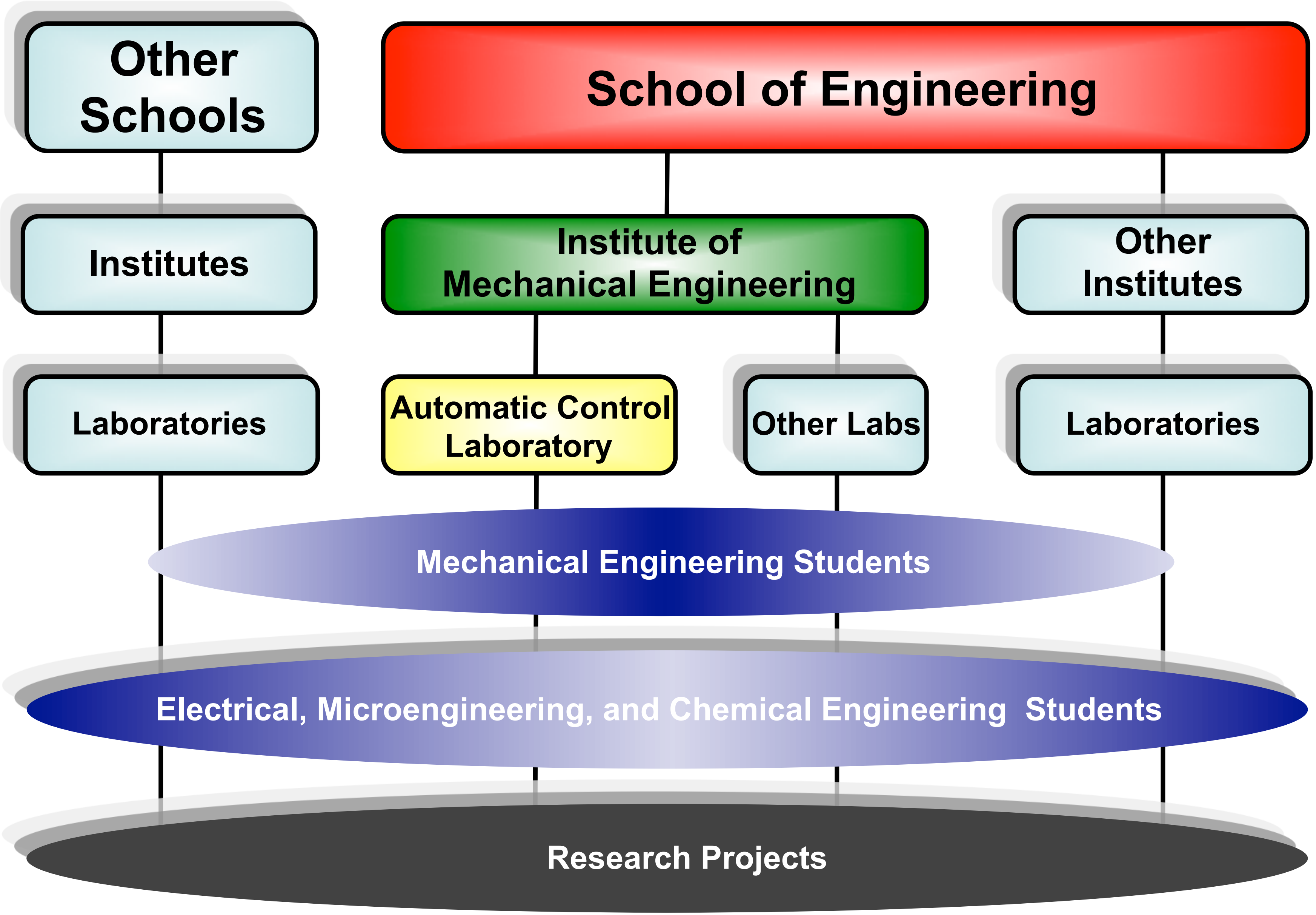
350 Professors

3'500 Staff Members

Global Budget
850 Mios CHF

5 Schools

- **Architecture, Civil & Environmental Engineering**
- **Computer & Communication Sciences**
- **Basic Sciences**
- **Engineering**
- **Life Sciences**


Other Schools
School of Engineering
Institutes
Institute of Mechanical Engineering
Other Institutes
Laboratories
Automatic Control Laboratory
Other Labs
Laboratories
Mechanical Engineering Students
Electrical, Microengineering, and Chemical Engineering Students
Research Projects

Real-Time Optimization

Methods and Applications

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Madrid, April 2016

Outline

1. Real-time optimization
   - Use of real-time measurements to improve process operation in the presence of uncertainty
   - What to measure and what to adapt?
2. Three RTO schemes
   - Update model parameters and repeat numerical optimization
   - Modify cost and constraints and repeat numerical optimization
   - Optimization via feedback control
3. Two experimental case studies
   - Solid oxide fuel cell stack
   - Batch polymerization reactor

Optimization of Process Operation

1. Features of industrial processes
   - Complexity
   - Presence of disturbances

   } → uncertainty

2. Operational objectives
   - **Feasibility**: respect operational and safety constraints
   - **Optimality**: minimize energy, maximize efficiency, maximize productivity

3. Performance improvement
   - On the basis of a model via numerical optimization
     - ✓ Difficult in practice because of model inaccuracies, disturbances
   - Use measurements → real-time optimization
     - ✓ What to measure, what to adapt?

Optimization of a Continuous Plant

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Optimize the steady-state performance of a (dynamic) process while satisfying a number of operating constraints

Plant

$$\min_{\mathbf{u}} \quad \phi_p(\mathbf{u}, \mathbf{y}_p)$$
$$\text{s.t.} \quad \mathbf{g}_p(\mathbf{u}, \mathbf{y}_p) \le \mathbf{0}$$

Inputs $\mathbf{u}$?

(set points)

Plant Outputs $\mathbf{y}_\mathbf{p}$

Model-based Numerical Optimization

$$\mathbf{F}(\mathbf{u}, \mathbf{y}, \boldsymbol{\theta}) = \mathbf{0}$$
$$\min_{\mathbf{u}} \quad \Phi(\mathbf{u}, \boldsymbol{\theta}) := \phi(\mathbf{u}, \mathbf{y})$$
$$\text{s.t.} \quad \mathbf{G}(\mathbf{u}, \boldsymbol{\theta}) := \mathbf{g}(\mathbf{u}, \mathbf{y}) \le \mathbf{0}$$

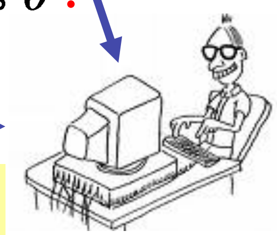
StOP

NLP

Model Parameters $\boldsymbol{\theta}$?

Inputs $\mathbf{u}$?

(set points)



Predicted Outputs $\mathbf{y}$

Optimization of a Batch Plant

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$\mathbf{u}(t)$ →  → $\mathbf{x}_p(t_f)$

Batch reactor with finite terminal time

Repetitive Dynamic Process

$$\min_{\mathbf{u}[0,t_f]} \quad \Phi := \phi\left(\mathbf{x}(t_f)\right)$$

$$\text{s. t.} \quad \dot{\mathbf{x}} = \mathbf{F}(\mathbf{x},\mathbf{u},\boldsymbol{\theta}) \quad \mathbf{x}(0) = \mathbf{x}_0$$

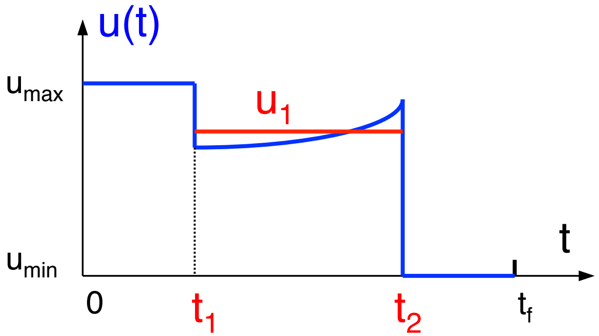
$$\mathbf{S}(\mathbf{x},\mathbf{u}) \leq \mathbf{0}$$

$$\mathbf{T}\left(\mathbf{x}(t_f)\right) \leq \mathbf{0}$$

DyOP

Input parameterization

$$\mathbf{u}[0,t_f] = \mathrm{U}(\boldsymbol{\pi})$$



$\boldsymbol{\pi}$ →  → Φ_p, $\mathbf{G}_p$

Batch reactor viewed as a static map

$$\min_{\boldsymbol{\pi}} \quad \Phi(\boldsymbol{\pi},\boldsymbol{\theta})$$

$$\text{s. t.} \quad \mathbf{G}(\boldsymbol{\pi},\boldsymbol{\theta}) \leq \mathbf{0}$$

StOP

NLP

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3. Experimental case study
   – Solid oxide fuel cell stack
   – Batch polymerization reactor

Three Approaches for Static RTO

What to measure and what to adapt?

Optimization in the presence of Uncertainty

No Measurement: Robust Optimization

Measurements: Adaptive Optimization

$$\mathbf{u}^* \in \arg\min_{\mathbf{u}} \Phi(\mathbf{u},\boldsymbol{\theta}) \quad \text{s.t.} \quad \mathbf{G}(\mathbf{u},\boldsymbol{\theta}) \leq \mathbf{0}$$

input update: $\delta\mathbf{u}$

parameter update: $\delta\boldsymbol{\theta}$

cost & constraint update: $\delta\Phi, \delta\mathbf{G}$

1. Measure Outputs and adapt Model Parameters
   - two-step approach (repeated identification and optimization)

2. Measure/Estimate KKT elements and adapt Cost & Constraints
   - bias update
   - gradient correction
   - modifier adaptation © LA

3. Measure/Estimate KKT elements and adapt Inputs
   - self-optimizing control
   - NCO tracking © LA
   - extremum-seeking control

Explicit methods (1, 2)

Implicit method (3)

1. Adaptation of Model Parameters

Two-step approach

Parameter Identification Problem

$$\boldsymbol{\theta}_k^* \in \arg\min_{\boldsymbol{\theta}} \quad J_k^{\text{id}}$$

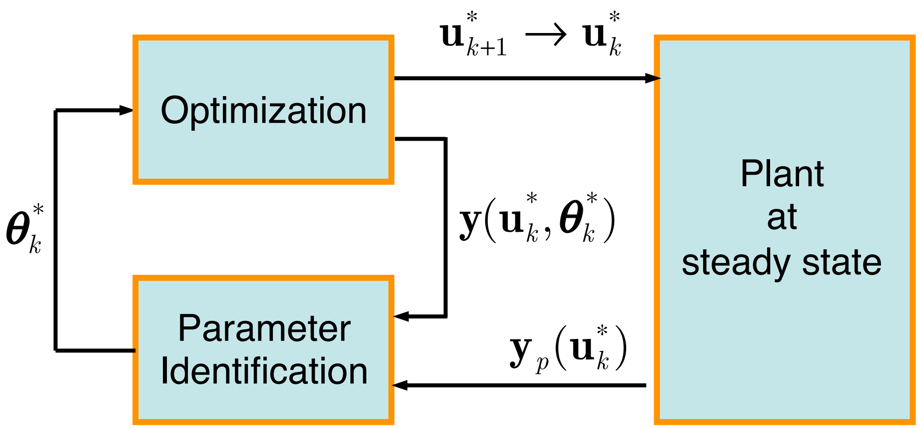
$$J_k^{\text{id}} = \left[\mathbf{y}_p(\mathbf{u}_k^*) - \mathbf{y}(\mathbf{u}_k^*, \boldsymbol{\theta})\right]^{\mathrm{T}} \mathbf{Q} \left[\mathbf{y}_p(\mathbf{u}_k^*) - \mathbf{y}(\mathbf{u}_k^*, \boldsymbol{\theta})\right]$$

Optimization Problem

$$\mathbf{u}_{k+1}^* \in \arg\min_{\mathbf{u}} \quad \phi\left(\mathbf{u}, \mathbf{y}(\mathbf{u}, \boldsymbol{\theta}_k^*)\right)$$

$$\text{s.t.} \quad \mathbf{g}\left(\mathbf{u}, \mathbf{y}(\mathbf{u}, \boldsymbol{\theta}_k^*)\right) \leq \mathbf{0}$$

$$\mathbf{u}^{\mathrm{L}} \leq \mathbf{u} \leq \mathbf{u}^{\mathrm{U}}$$

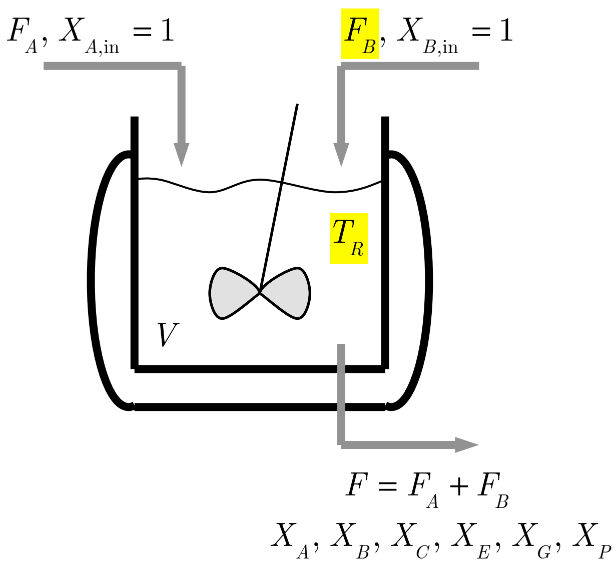


Current Industrial Practice
for tracking the changing optimum
in the presence of disturbances

T.E. Marlin, A.N. Hrymak. Real-Time Operations Optimization of Continuous Processes, *AIChE Symposium Series - CPC-V*, **93**, 156-164, 1997

Example of Plant-Model Mismatch

Williams-Otto reactor



3-reaction system

A + B → C
B + C → P + E
C + P → G

2-reaction model

$A + 2B \xrightarrow{k_1} P + E$

$A + B + P \xrightarrow{k_2} G$

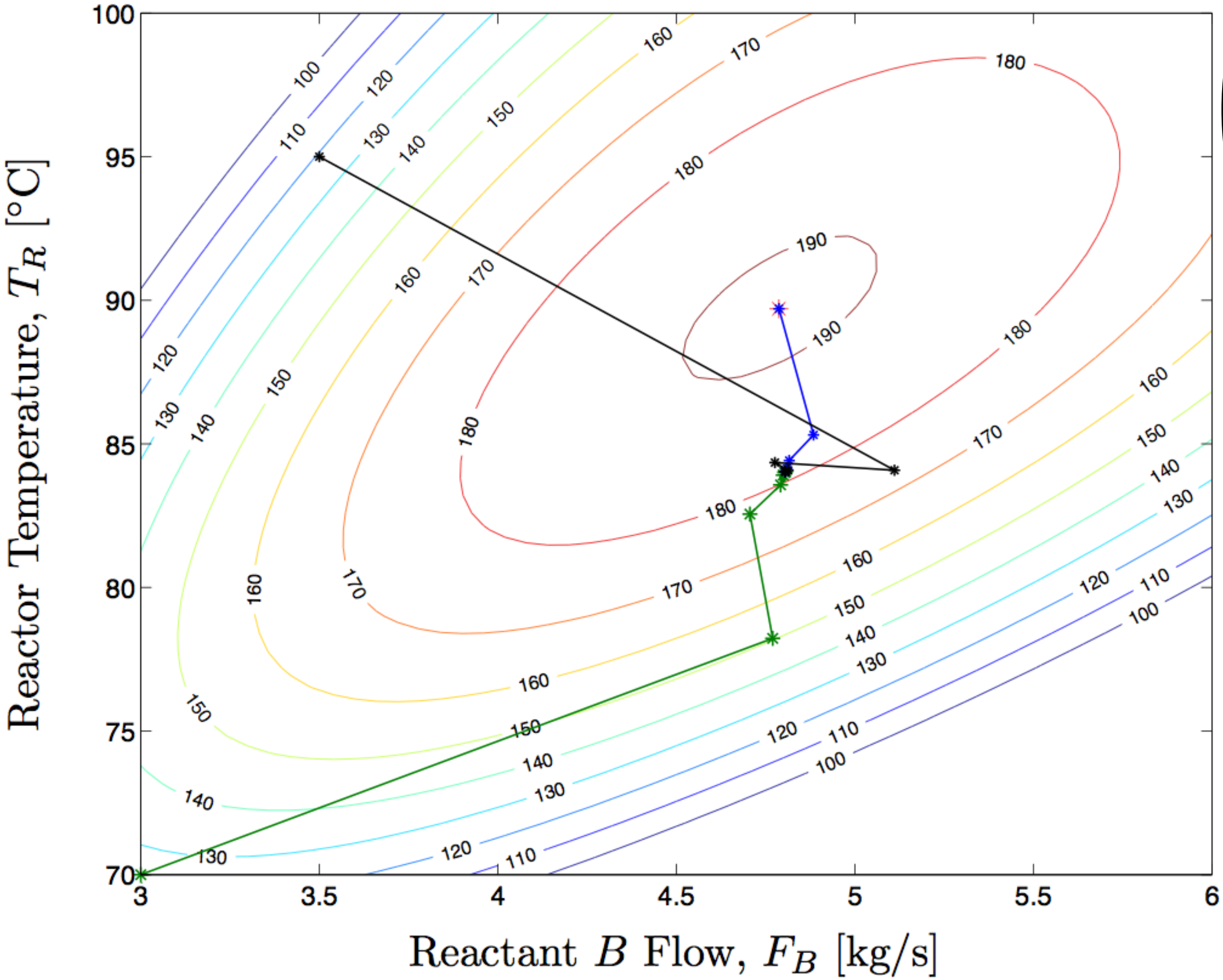
Objective: maximize productivity

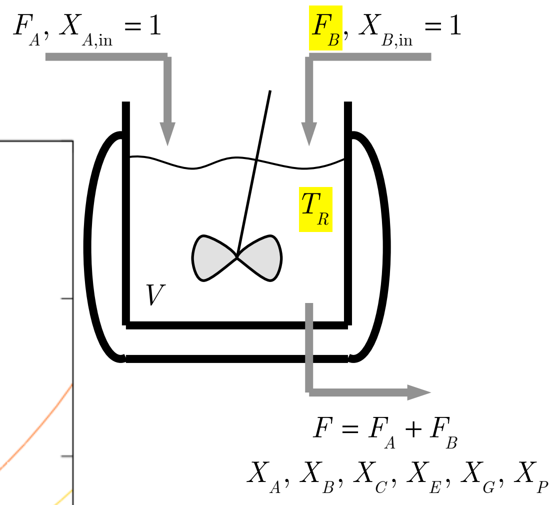
Model

- 4^{th}-order model
- 2 inputs
- 2 adjustable parameters (k_{10}, k_{20})

Two-step Approach

With structurally incorrect model





Williams-Otto Reactor

- 4th-order model
- 2 inputs
- 2 adjustable par.

Does not converge to plant optimum

2. Adaptation of Cost & Constraints

Input-affine correction to the model

Modified Optimization Problem

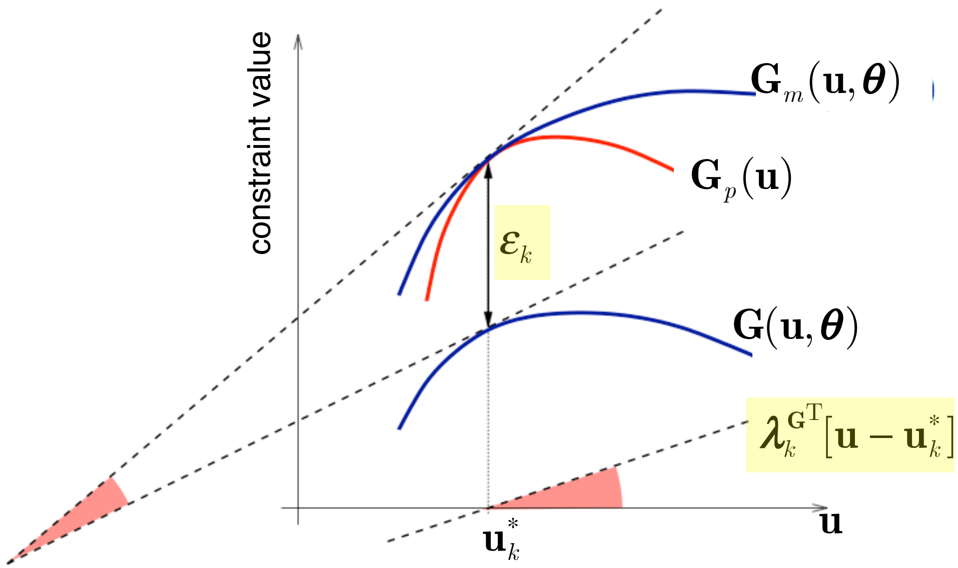
$$\mathbf{u}_{k+1}^* \in \arg\min_{\mathbf{u}} \quad \Phi_m(\mathbf{u},\boldsymbol{\theta}) := \Phi(\mathbf{u},\boldsymbol{\theta}) + \boldsymbol{\lambda}_k^{\Phi T}[\mathbf{u}-\mathbf{u}_k^*]$$

$$\text{s.t.} \quad \mathbf{G}_m(\mathbf{u},\boldsymbol{\theta}) := \mathbf{G}(\mathbf{u},\boldsymbol{\theta}) + \boldsymbol{\varepsilon}_k + \boldsymbol{\lambda}_k^{GT}[\mathbf{u}-\mathbf{u}_k^*] \leq \mathbf{0}$$

$$\mathbf{u}^L \leq \mathbf{u} \leq \mathbf{u}^U$$

Affine corrections of cost and constraint functions.

The modified problem satisfies the first-order optimality conditions of the plant



$$\boldsymbol{\lambda}_k^G = \frac{\partial \mathbf{G}_p}{\partial \mathbf{u}}(\mathbf{u}_k^*) - \frac{\partial \mathbf{G}}{\partial \mathbf{u}}(\mathbf{u}_k^*,\boldsymbol{\theta})$$

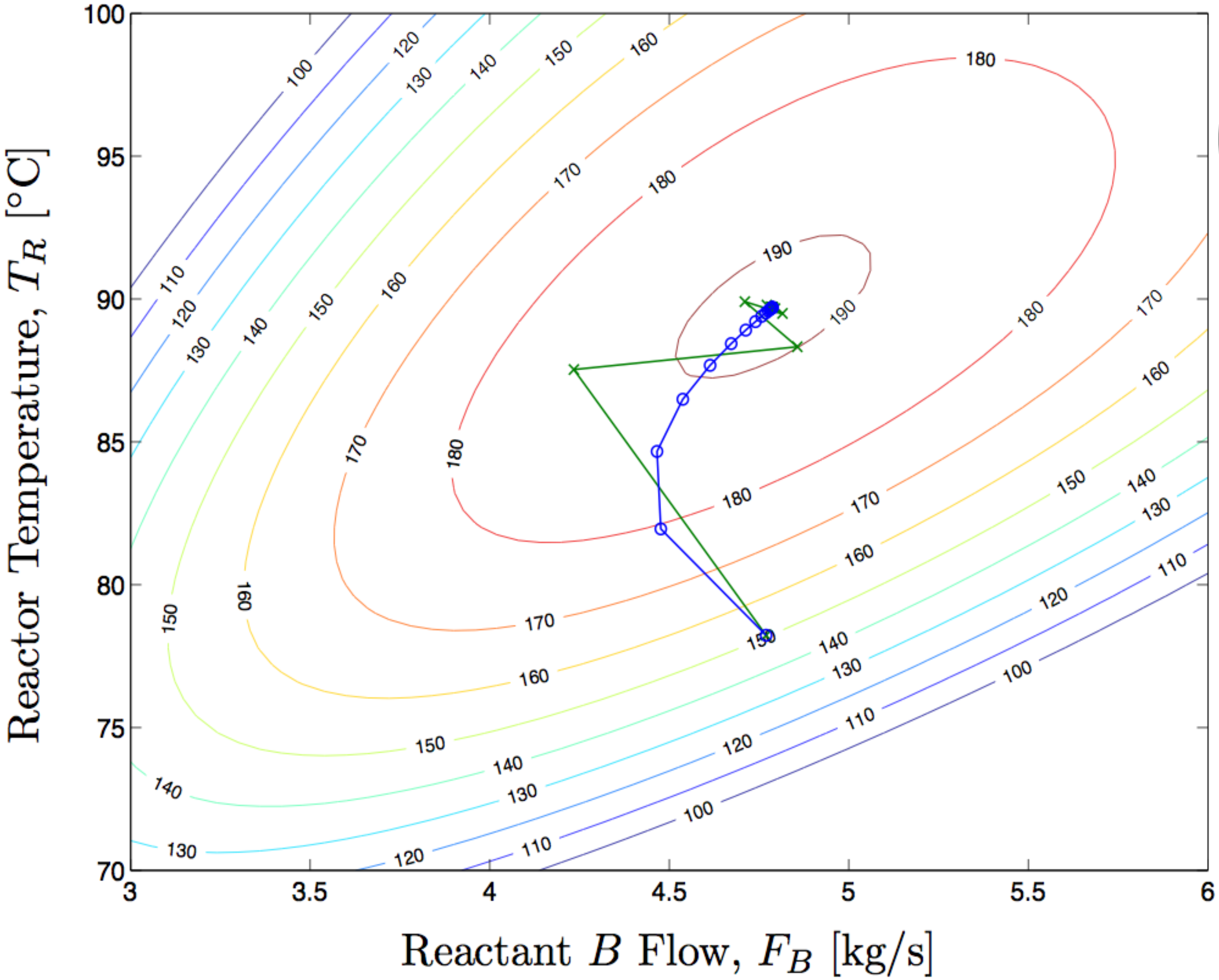
plant gradients

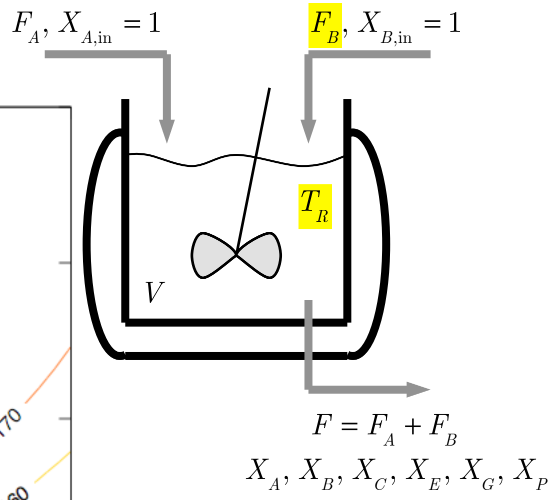
P.D. Roberts, On an Algorithm for Combined System Optimization and Parameter Estimation, *Automatica,* **17**, 199–209, 1981

A. Marchetti, Modifier-Adaptation Methodology for Real-Time Optimization, *I&EC Research*, **48**, 6022-6033, 2009

Example Revisited

Modifier adaptation





Williams-Otto Reactor

- 4^{th}-order model
- 2 inputs
- 2 adjustable par.

Converges to plant optimum

Requires estimation of experimental gradient

A. Marchetti, PhD thesis EPFL, Modifier-Adaptation Methodology for Real-Time Optimization, 2009

3. Direct Adaptation of Inputs

NCO tracking © LA

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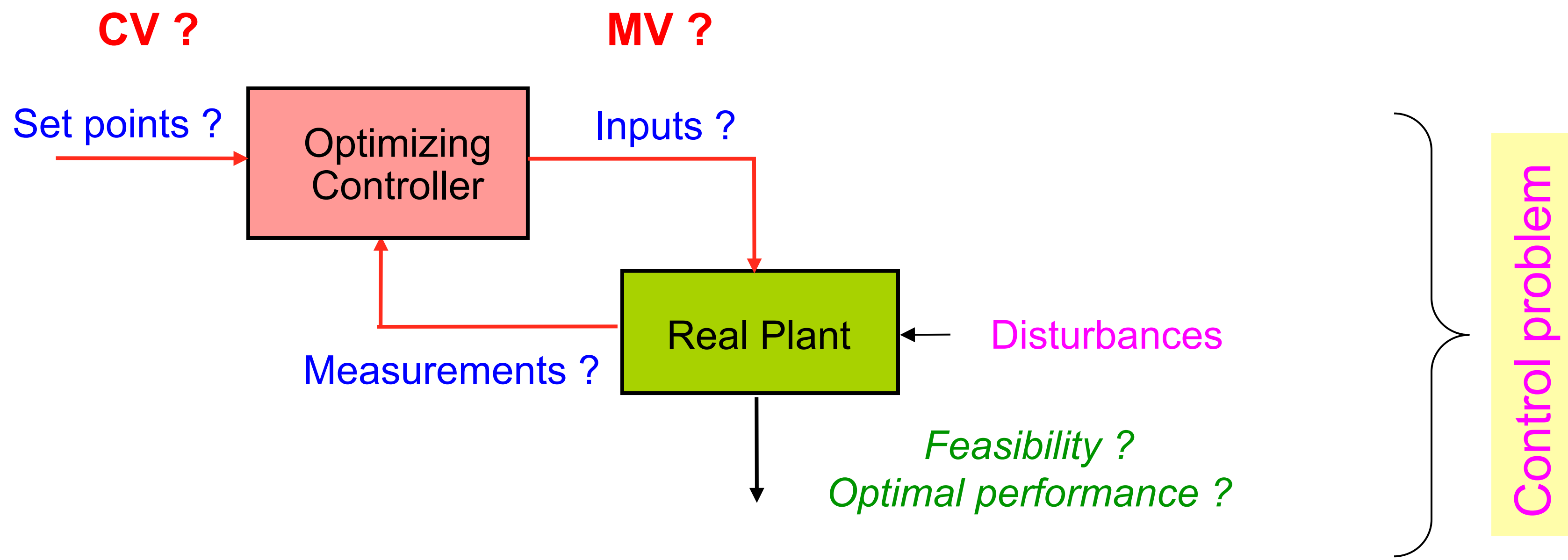
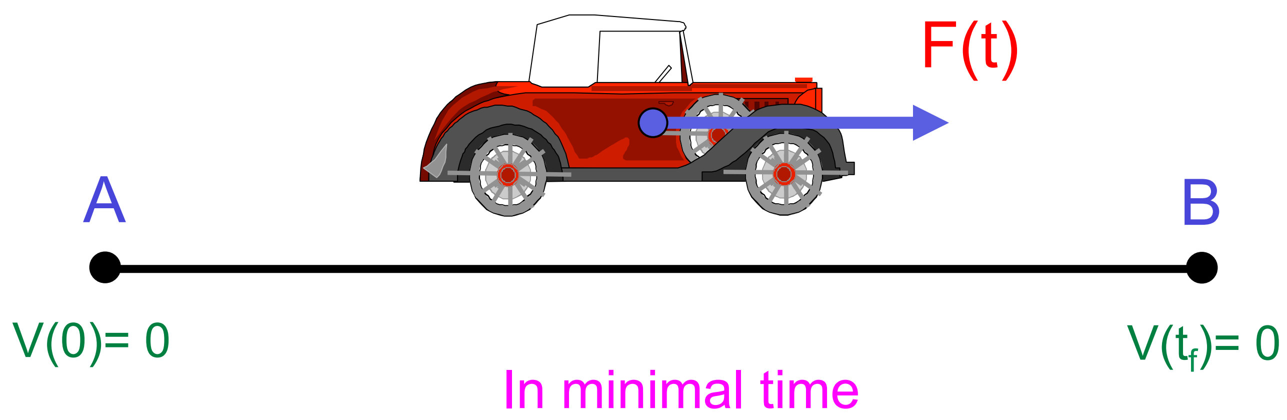
- Transform the optimization problem into a control problem
- Which setpoints to track for optimality?
  - The optimality conditions (active constraints, gradients)
  - Requires appropriate measurements



B. Srinivasan and D. Bonvin, Real-Time Optimization of Batch Processes by Tracking the Necessary Conditions of Optimality, *I&EC Research*, 46, 492-504 2007.

Example

Minimum-time Problem

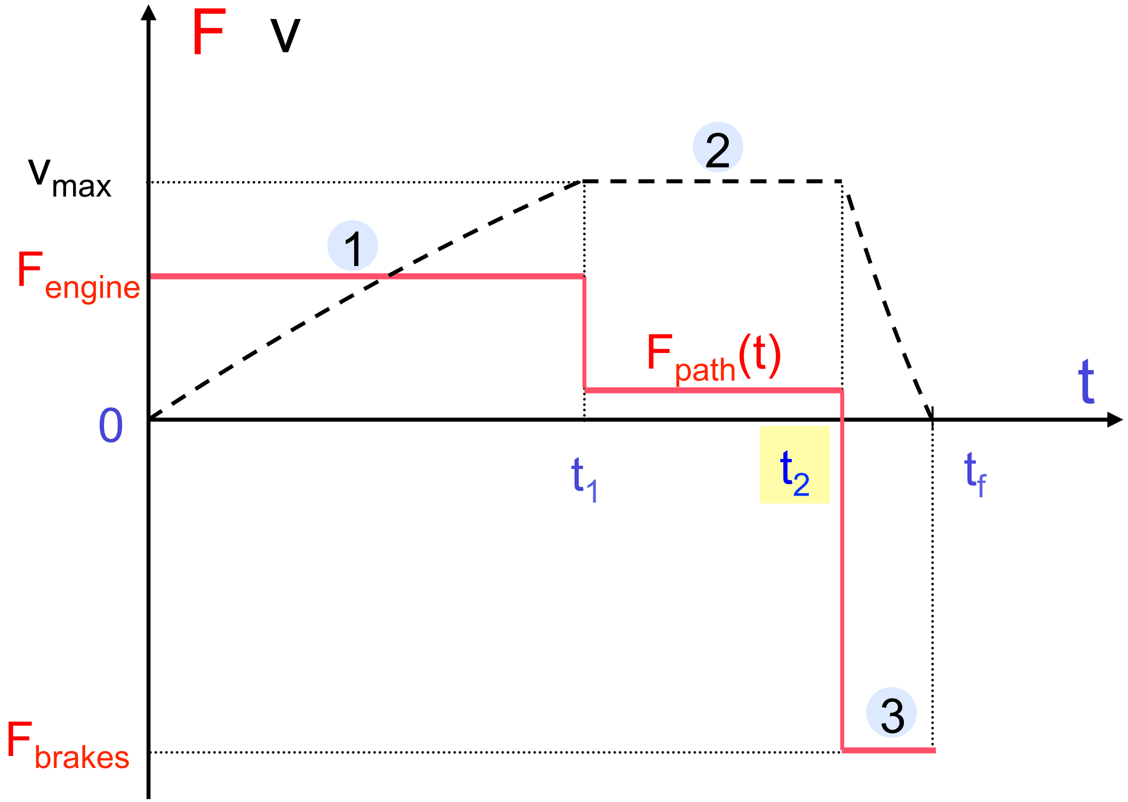


Path constraints: $F_{brakes} \leq F(t) \leq F_{engine}$ $v(t) \leq v_{max}$

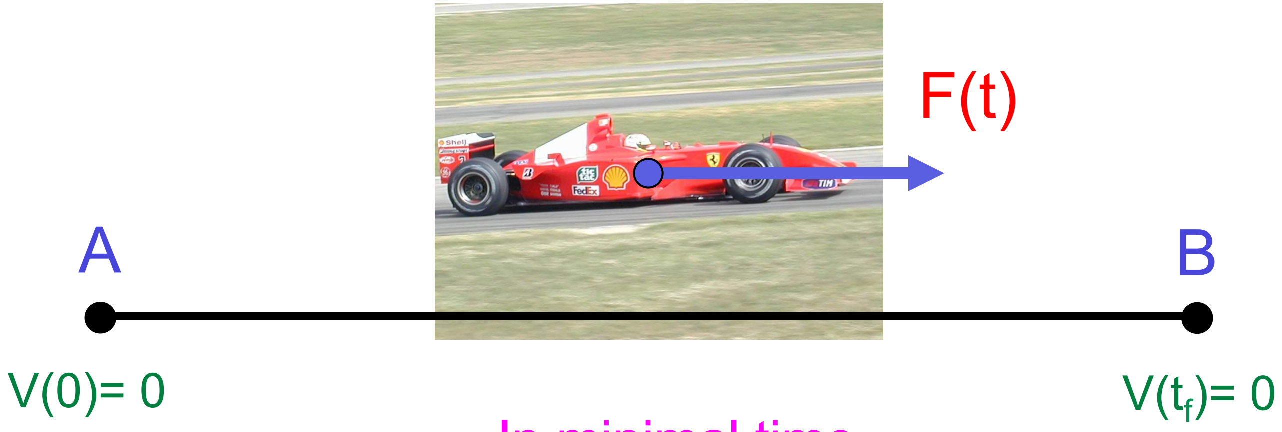
Terminal constraints: $v(t_f) = 0$ $x(t_f) \geq x_{des}$

Problem: Find the force $F(t)$ that minimizes t_f

Optimal Trajectories



Faster Car



In minimal time

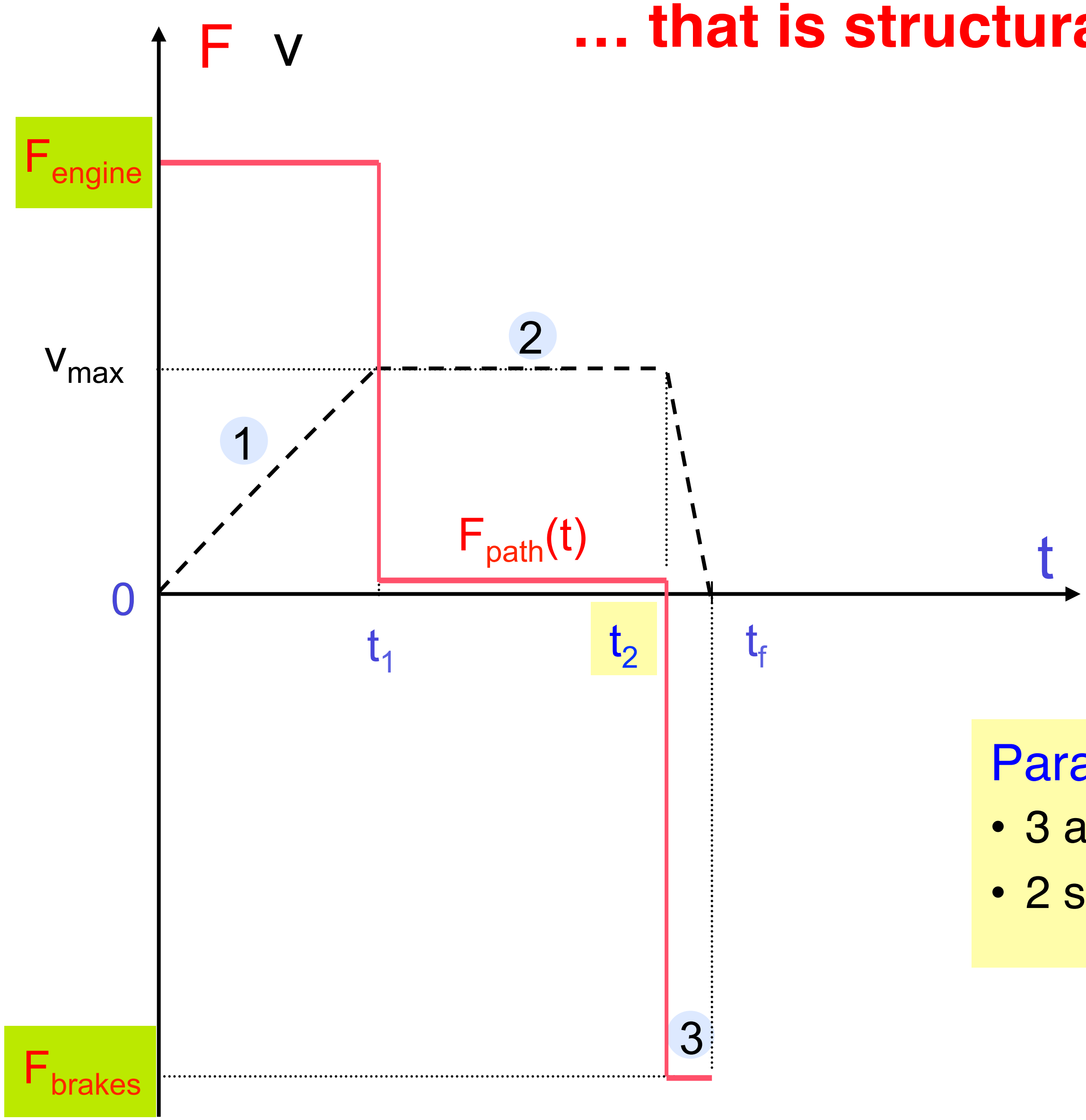
Path constraints: $F_{brakes} \leq F(t) \leq F_{engine}$ $v(t) \leq v_{max}$

Terminal constraints: $v(t_f) = 0$ $x(t_f) \geq x_{des}$

Problem: Find the force $F(t)$ that minimizes t_f

Different Solution

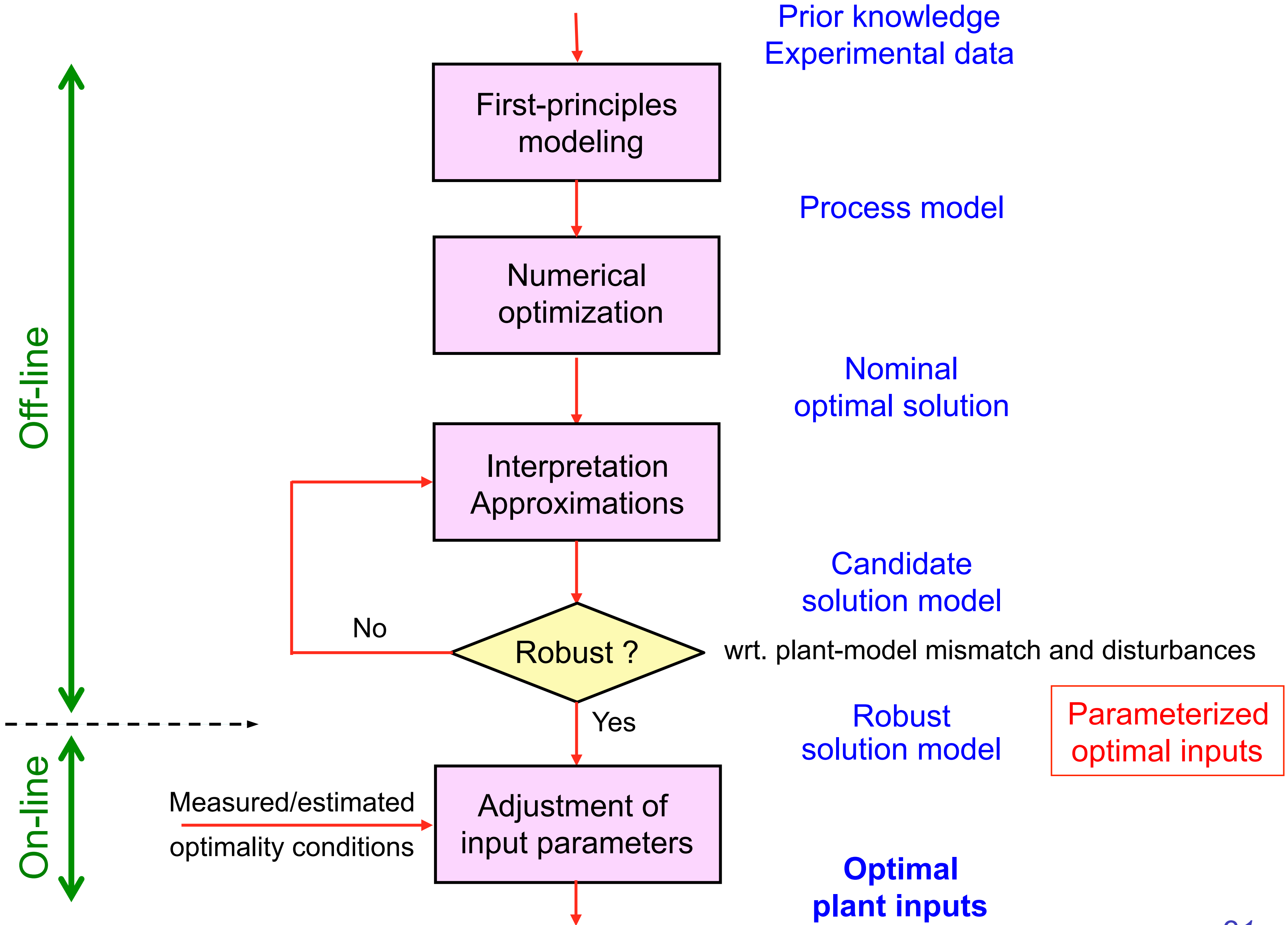
… that is structurally identical !



Parameterized optimal input

- 3 arcs: F_{engine}, v_{max} and F_{brakes}
- 2 switching times: t_1 and t_2

Generation of a Solution Model



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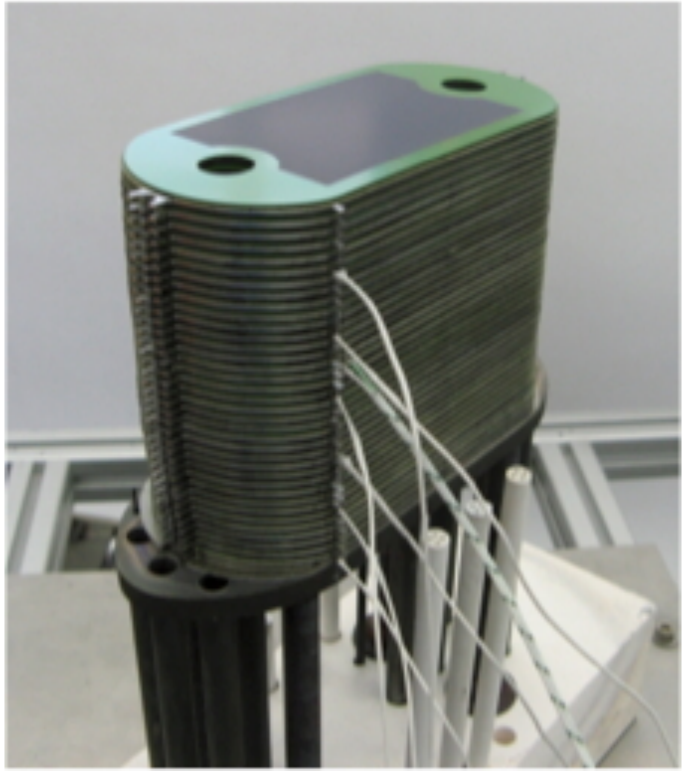
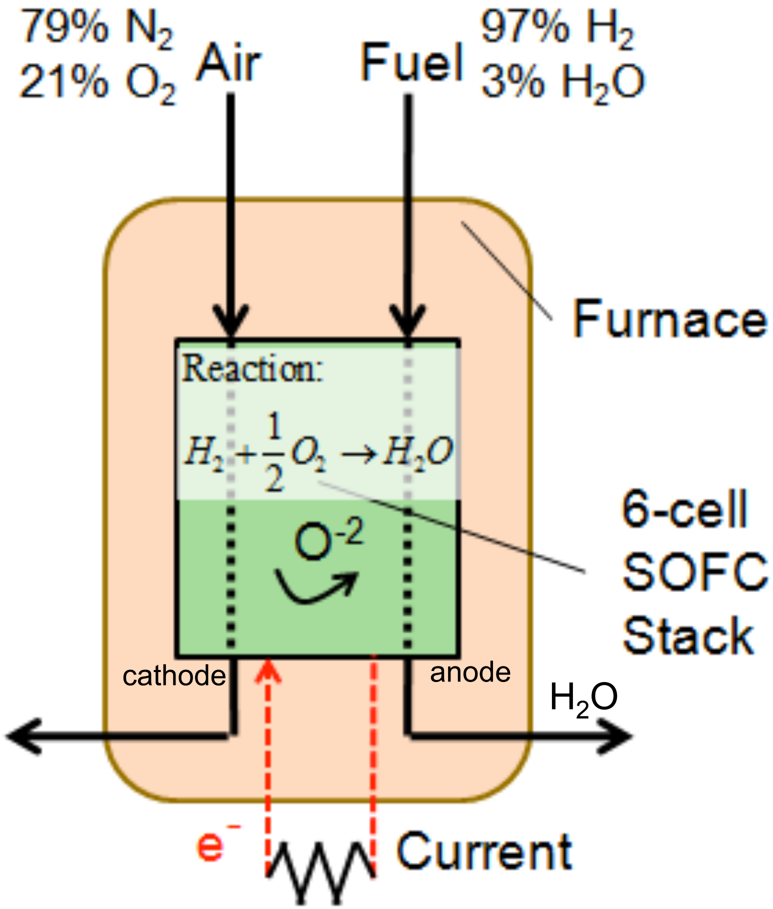
   - Batch polymerization reactor (NCO tracking)

1. Solid Oxide Fuel Cell Stack

RTO via Modifier Adaptation © LA





- Stack of 6 cells, active area of 50 cm^2, metallic interconnector
- Anodes : standard nickel/yttrium stabilized-zirconia (Ni-YSZ)
- Electrolyte : dense YSZ.
- Cathodes: screen-printed (La, Sr)(Co, Fe)O_3
- Operation temperatures between 650 and 850°C.

Experimental Features

- Objective: maximize electrical efficiency
- Meet power demand that changes unexpectedly
- Inputs: flowrates of H_2 and O_2, current
- Outputs: power density, cell potential
- Time-scale separation
  - *slow temperature dynamics, treated as process drift !*
  - *static model (for the rest)*
- Inaccurate model in the operating region (power, cell)

G.A. Bunin, Experimental Real-Time Optimization of a Solid Oxide Fuel Cell Stack via Constraint Adaptation, *Energy,* 39(1), 54-62, 2012

Strategy for Online Optimization

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Repeated Numerical Optimization

- Solve a static optimization problem every 10 sec
- Apply the optimal inputs to the stack
- Measure the resulting constraint values
- Adapt the modifiers ε to match the active constraints

$$\max_{\boldsymbol{u}_k} \quad \eta\left(\mathbf{u}_k, \boldsymbol{\theta}\right)$$

$$\text{s.t.} \quad \boldsymbol{p}_{\text{el}}\left(\mathbf{u}_k, \boldsymbol{\theta}\right) + \varepsilon_{k-1}^{p_{\text{el}}} = \boldsymbol{p}_{el}^{S}$$

$$\boldsymbol{U}_{\text{cell}}\left(\mathbf{u}_k, \boldsymbol{\theta}\right) + \varepsilon_{k-1}^{U_{\text{cell}}} \geq 0.75\,\boldsymbol{V}$$ to avoid cell degradation

$$\nu\left(\mathbf{u}_k\right) \leq 0.75$$ to avoid local fuel starvation

$$4 \leq \lambda_{air}\left(\mathbf{u}_k\right) \leq 7$$ to avoid steep thermal gardients

$$\boldsymbol{u}_{1,k} \geq 3.14\,\text{mL}/(\text{min cm}^2)$$

$$\boldsymbol{u}_{3,k} \leq 30\text{A}$$

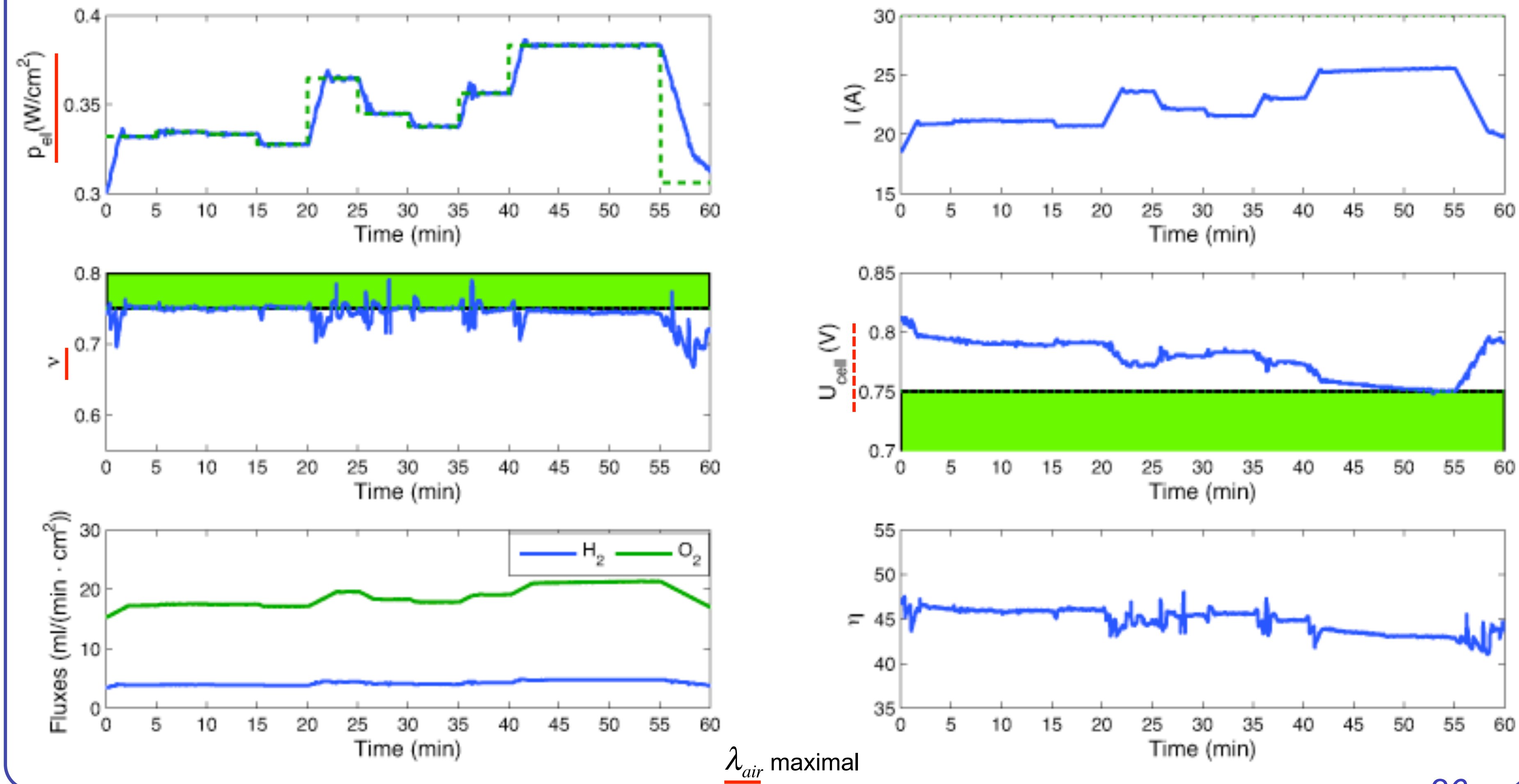
$$\mathbf{u}_k = \begin{bmatrix} u_{1,k} = \dot{n}_{H_2,k} \\ u_{2,k} = \dot{n}_{O_2,k} \\ u_{3,k} = I_k \end{bmatrix}$$

$$\varepsilon_k^{p_{\text{el}}} = \left(1\text{-}K_{p_{\text{el}}}\right)\varepsilon_{k\text{-}1}^{p_{\text{el}}} + K_{p_{\text{el}}}\left[p_{\text{el,p,k}} - p_{\text{el}}\left(\mathbf{u}_k, \boldsymbol{\theta}\right)\right]$$

$$\varepsilon_k^{U_{\text{cell}}} = \left(1\text{-}K_{U_{\text{cell}}}\right)\varepsilon_{k\text{-}1}^{U_{\text{cell}}} + K_{U_{\text{cell}}}\left[U_{\text{cell,p,k}} - U_{\text{cell}}\left(\mathbf{u}_k, \boldsymbol{\theta}\right)\right]$$

Experimental Results

- Random power changes every 5 min
- RTO every 10 s, matches the active constraints at steady state



2. Optimization of Polymerization Reactor

NCO tracking © LA

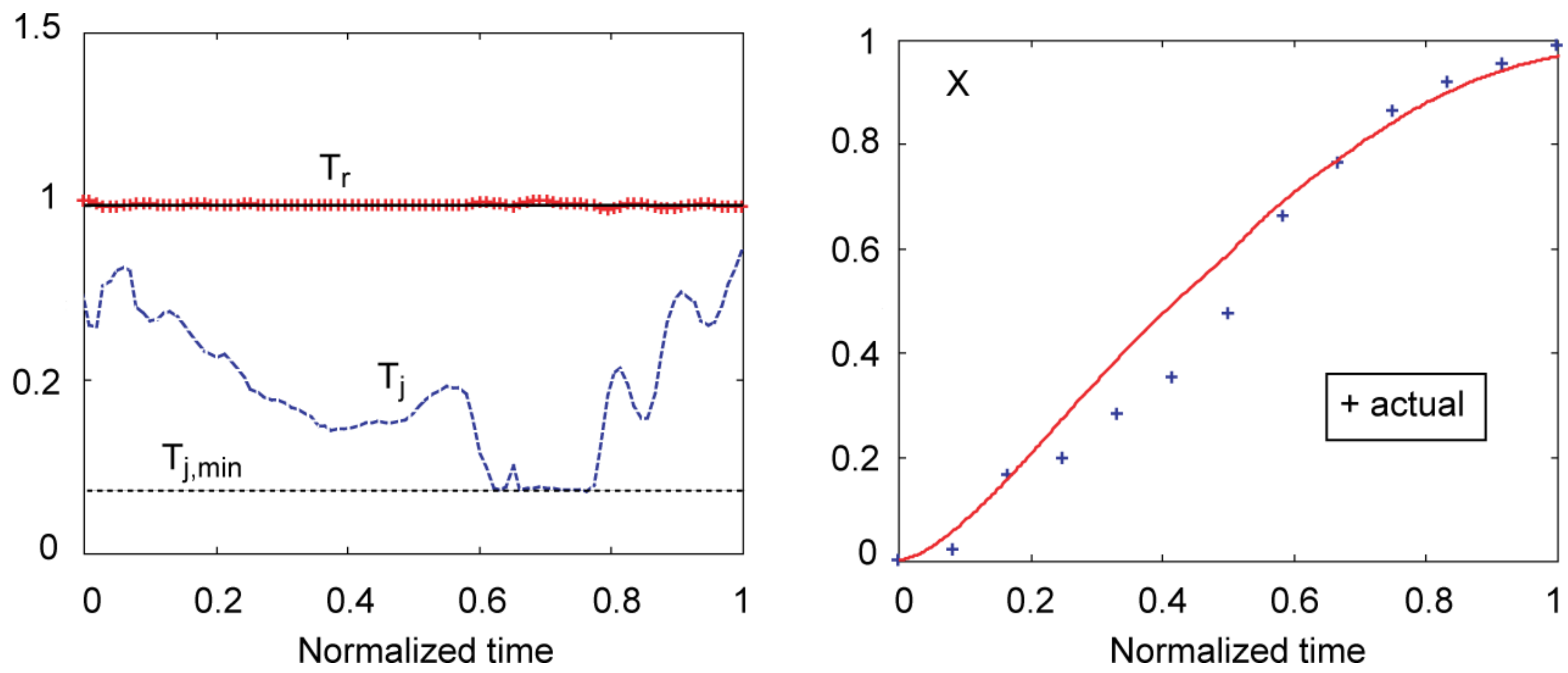
- Industrial features
  - 1-ton reactor, risk of runaway
  - Initiator efficiency can vary considerably
  - Several recipes
    - *different initial conditions*
    - *different initiator feeding policies*
    - *use of chain transfer agent*
    - *use of reticulant*

→ • Modeling difficulties
• Uncertainty

- Challenge: Implement (near) optimal operation for various recipes

G. François *et al.*, Run-to-run adaptation of a semi-adiabatic policy for the optimization of an industrial batch polymerization process, *I&ECResearch*, *43*, 7238-7242 (2004)

Industrial Practice



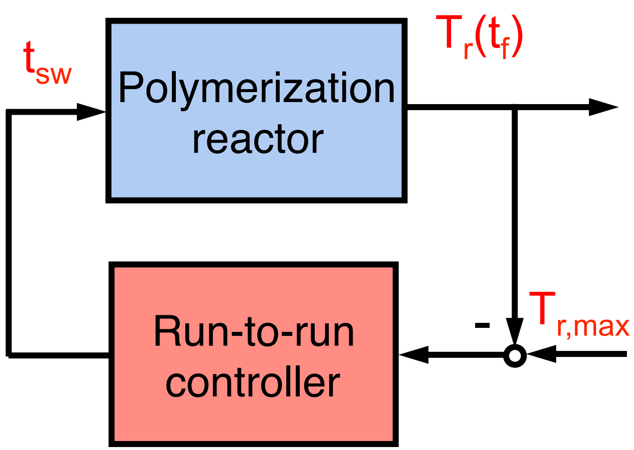
$T_r(t)$ to minimize the batch time ?

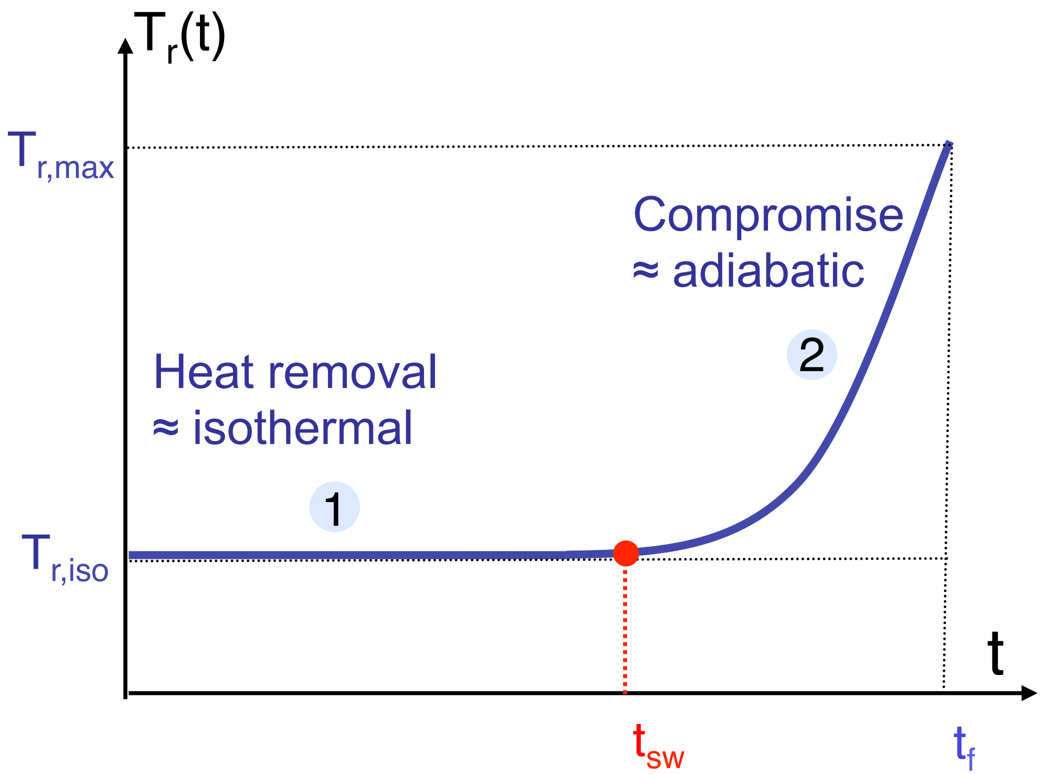
Strategy for Run-run Optimization

Tendency model

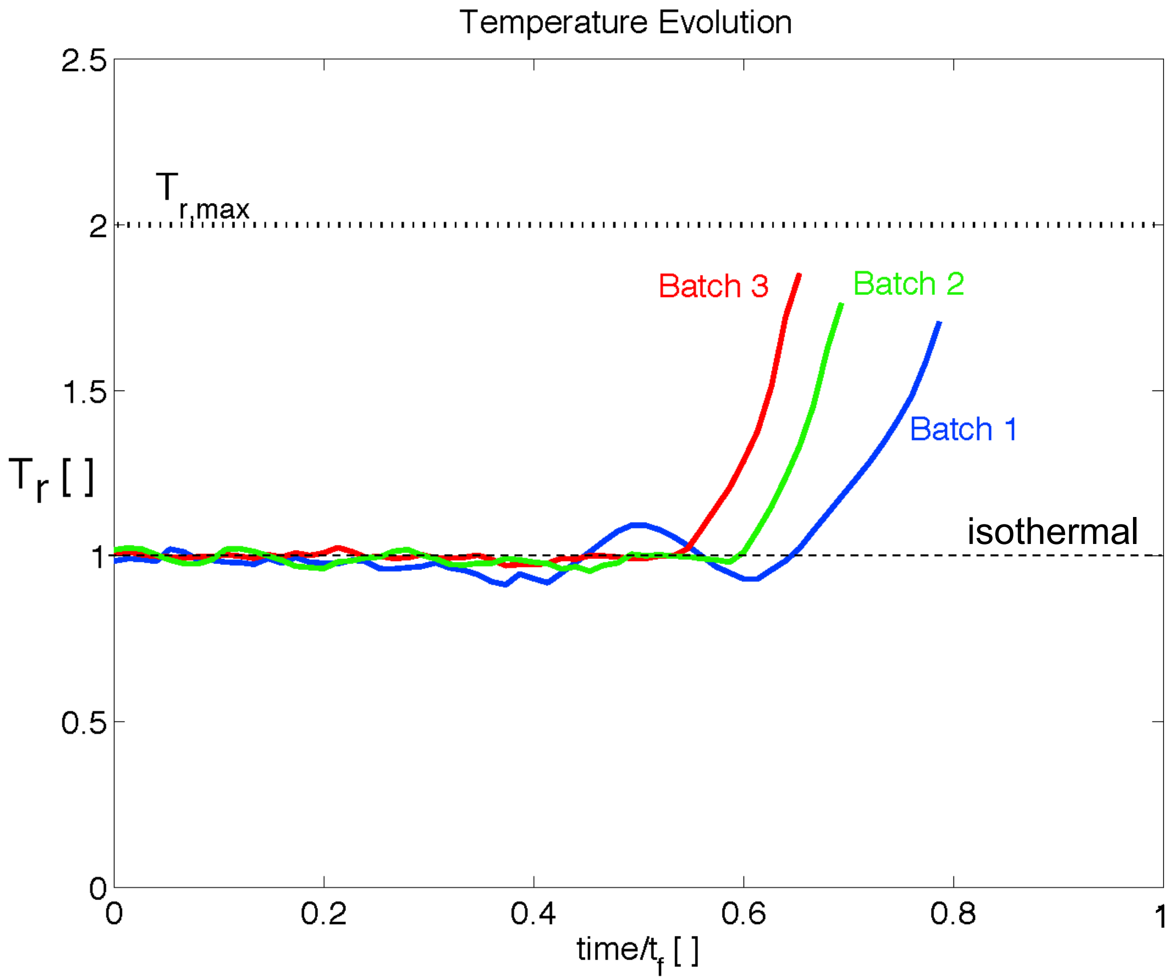
Optimality is linked with meeting the most restrictive constraint $T_r(t_f) = T_{r,max}$

Strategy: Manipulate t_{sw} on a run-to-run basis to force $T_r(t_f)$ at $T_{r,max}$





Industrial Results



Final time

- Isothermal: 1.00
- Batch 1: 0.78
- Batch 2: 0.72
- Batch 3: 0.65

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Conclusions

- Process models are often inadequate for optimization

→ use real-time measurements for appropriate adaptation

- Which measurements to use? How to best exploit them?
  - Outputs: easily available, not necessarily appropriate → KKT elements
  - KKT modifiers allow meeting KKT conditions
    - modifier adaptation© *LA* (explicit optimization)
    - NCO tracking© *LA* (implicit optimization)

- Key challenge is estimation of plant gradient
  - Use of successive operational points → BFGS-type of scheme
  - Dual RTO

Thank you for your attention !