Optimal dynamic operation of chemical processes: Assessment of the last 20 years and current research opportunities

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April 13, 2010
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Outline

1. The last 20 years — what tools have researchers developed
2. Industrial impact of these ideas
3. Have all the questions been answered?
   - Control of large-scale systems
   - Optimizing economics
4. Conclusions and future outlook

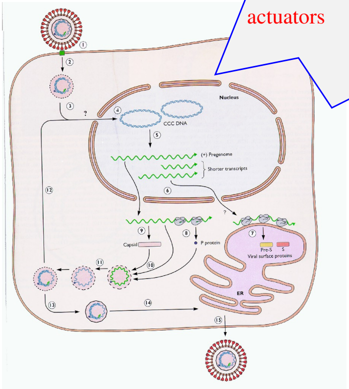
The power of abstraction

process

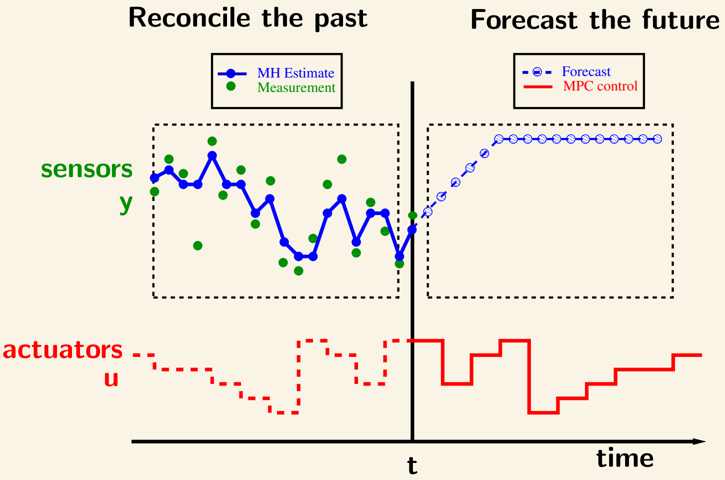
$$\frac{dx}{dt} = f(x, u)$$

$$y = g(x, u)$$

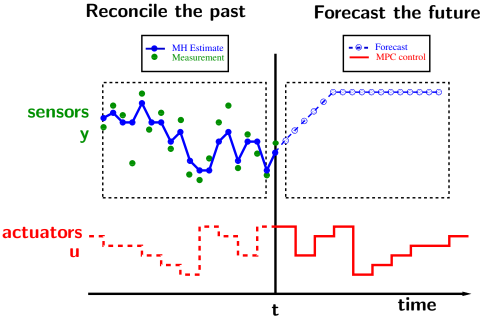
actuators   sensors



The model predictive control framework



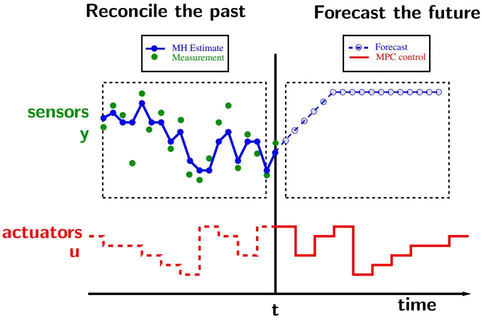
Predictive control



$$\min_{u(t)} \int_0^T |y_{sp} - g(x,u)|_Q^2 + |u_{sp} - u|_R^2 \, dt$$

$$\dot{x} = f(x,u)$$
$$x(0) = x_0 \quad \text{(given)}$$
$$y = g(x,u)$$

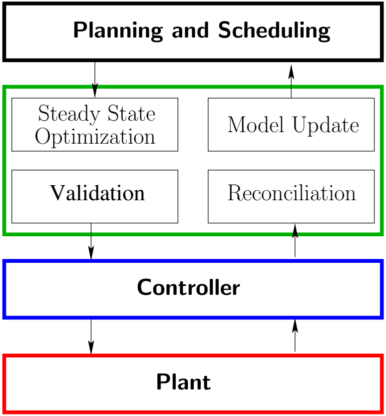
State estimation



$$\min_{x_0, w(t)} \int_{-T}^{0} |y - g(x,u)|_R^2 + |\dot{x} - f(x,u)|_Q^2 \, dt$$

$$\begin{aligned} \dot{x} &= f(x,u) + w \quad &\text{(process noise)} \\ y &= g(x,u) + v \quad &\text{(measurement noise)} \end{aligned}$$

Industrial impact of the research



Two layer structure

- Steady-state layer
  - RTO optimizes steady-state model
  - Optimal setpoints passed to dynamic layer
- Dynamic layer
  - Controller tracks the setpoints
  - Linear MPC (replaces multiloop PID)

Large industrial success story!

Linear MPC and ethylene manufacturing

- Number of MPC applications in ethylene: 800 to 1200
- Credits 500 to 800 M$/yr (2007)
- Achieved primarily by increased on-spec product, decreased energy use

Eastman Chemical experience with MPC

- First MPC implemented in 1996
- Currently 55-60 MPC applications of varying complexity
- 30-50 M$/year increased profit due to increased throughput (2008)

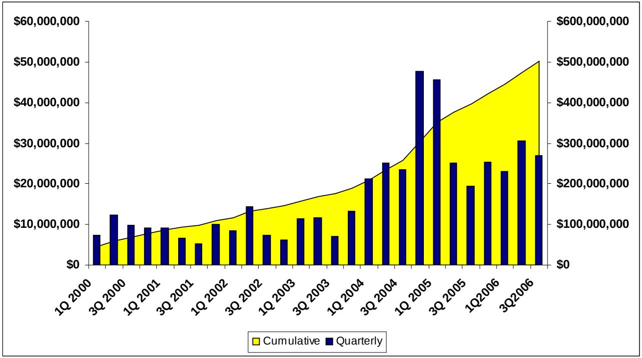
Praxair experience with MPC

- Praxair currently has more than 150 MPC installations
- 16 M$/year increased profit (2008)

Impact for 13 ethylene plants (Starks and Arrieta, 2007)

Hydrocarbons AC&O 17

We're Doing it For the Money



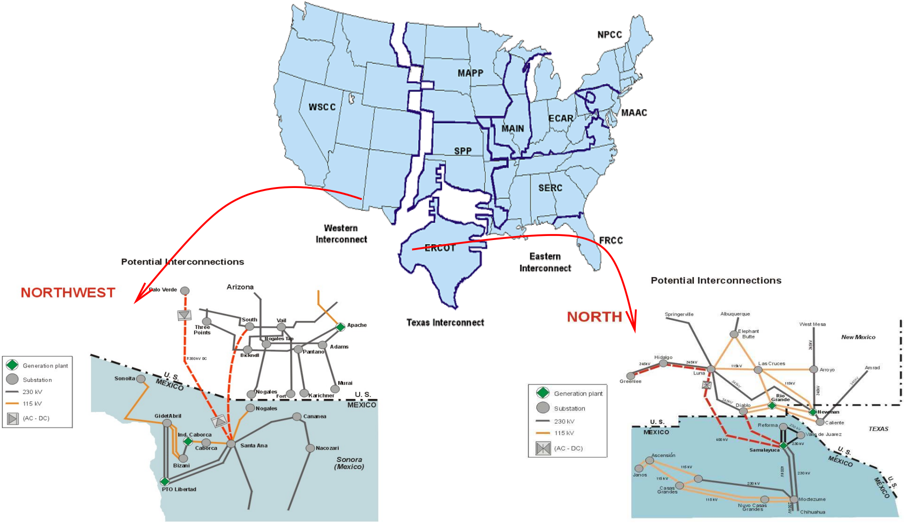
Advanced Control & Optimization

Are all the problems solved?

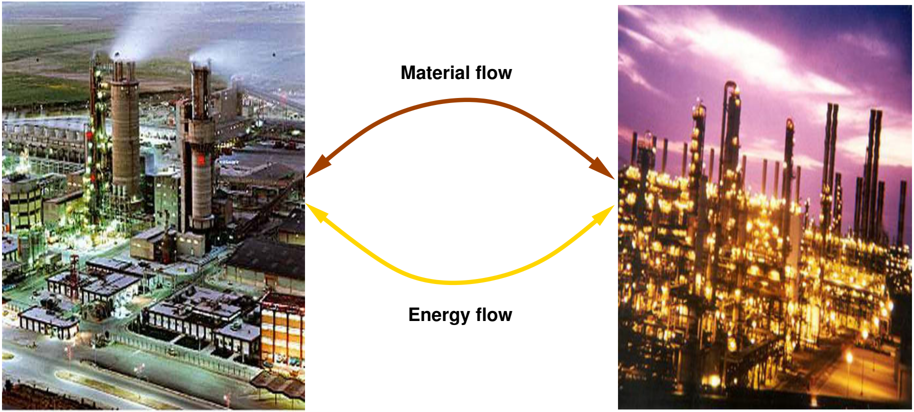
Some questions to consider

- How do we best decompose *large-scale systems* into manageable problems?
- How do we optimize dynamic *economic* operation?

Electrical power distribution



Chemical plant integration



MPC at the large scale

Decentralized Control

- Most large-scale systems consist of networks of interconnected/interacting subsystems
  - Chemical plants, electrical power grids, water distribution networks, ...
- Traditional approach: Decentralized control
  - Wealth of literature from the early 1970's on improved decentralized control [a]
  - Well known that poor performance may result if the interconnections are not negligible

[a](Sandell Jr. et al., 1978; Šiljak, 1991; Lunze, 1992)

MPC at the large scale

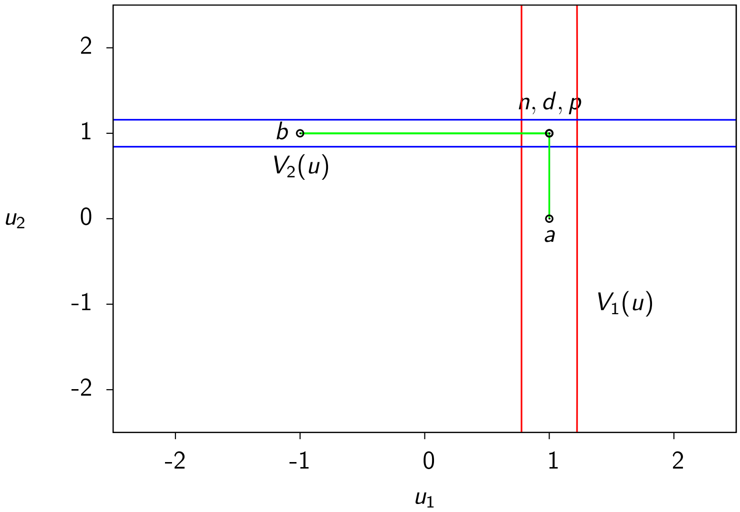
Centralized Control

- Steady increase in available computing power has provided the opportunity for centralized control
- Most practitioners view centralized control of large, networked systems as impractical and unrealistic
- A divide and conquer strategy is essential for control of large, networked systems (Ho, 2005)
- Centralized control: A benchmark for comparing and assessing distributed controllers

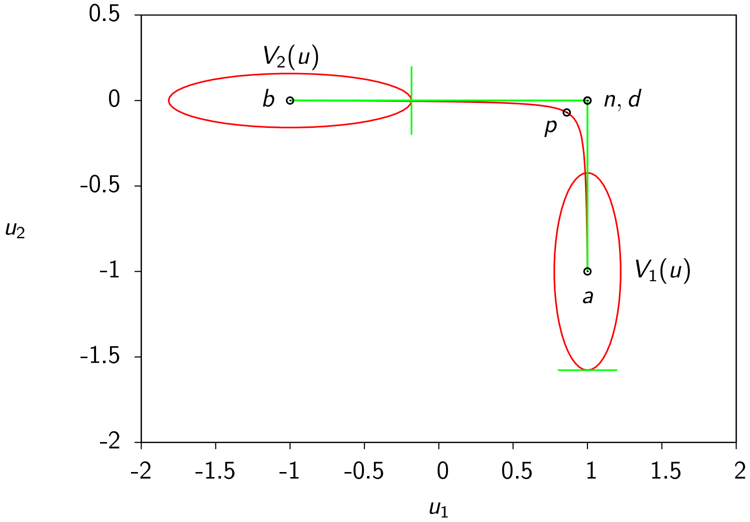
Nomenclature: consider two interacting units

Objective functions	$V_1(u_1, u_2), \; V_2(u_1, u_2)$
and	$V(u_1, u_2) = w_1 V_1(u_1, u_2) + w_2 V_2(u_1, u_2)$
decision variables for units	$u_1 \in \Omega_1, \quad u_2 \in \Omega_2$
Decentralized Control	$\min_{u_1 \in \Omega_1} \widetilde{V}_1(u_1) \quad \min_{u_2 \in \Omega_2} \widetilde{V}_2(u_2)$
Noncooperative Control	$\min_{u_1 \in \Omega_1} V_1(u_1, u_2) \quad \min_{u_2 \in \Omega_2} V_2(u_1, u_2)$
(Nash equilibrium)	
Cooperative Control	$\min_{u_1 \in \Omega_1} V(u_1, u_2) \quad \min_{u_2 \in \Omega_2} V(u_1, u_2)$
(Pareto optimal)	
Centralized Control	$\min_{u_1, u_2 \in \Omega_1 \times \Omega_2} V(u_1, u_2)$
(Pareto optimal)	

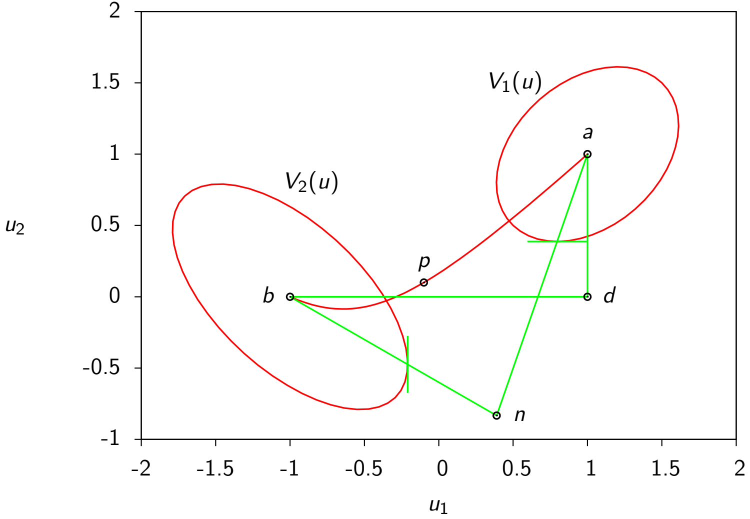
Noninteracting systems



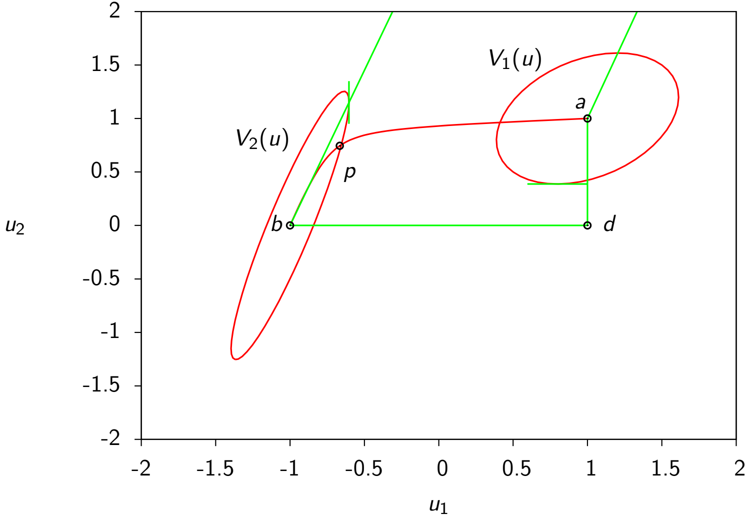
Weakly interacting systems



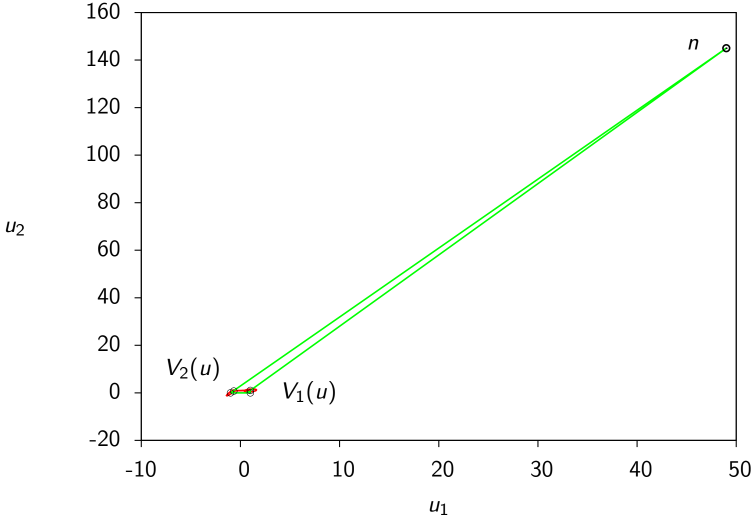
Moderately interacting systems



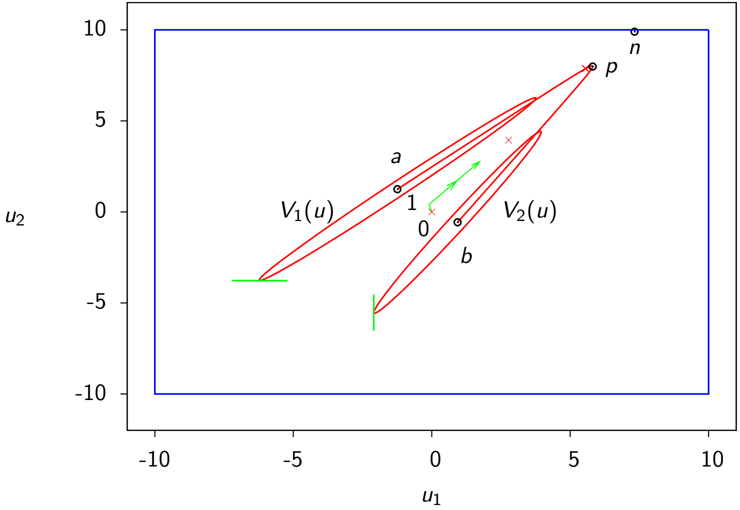
Strongly interacting (conflicting) systems



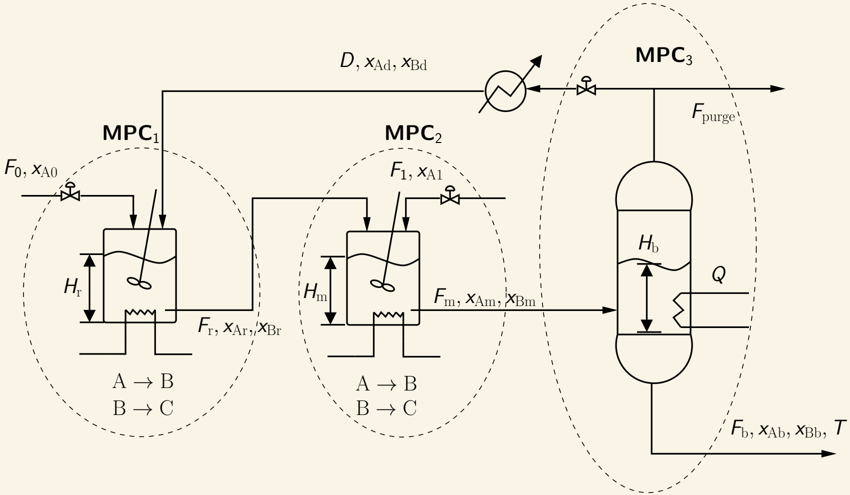
Strongly interacting (conflicting) systems



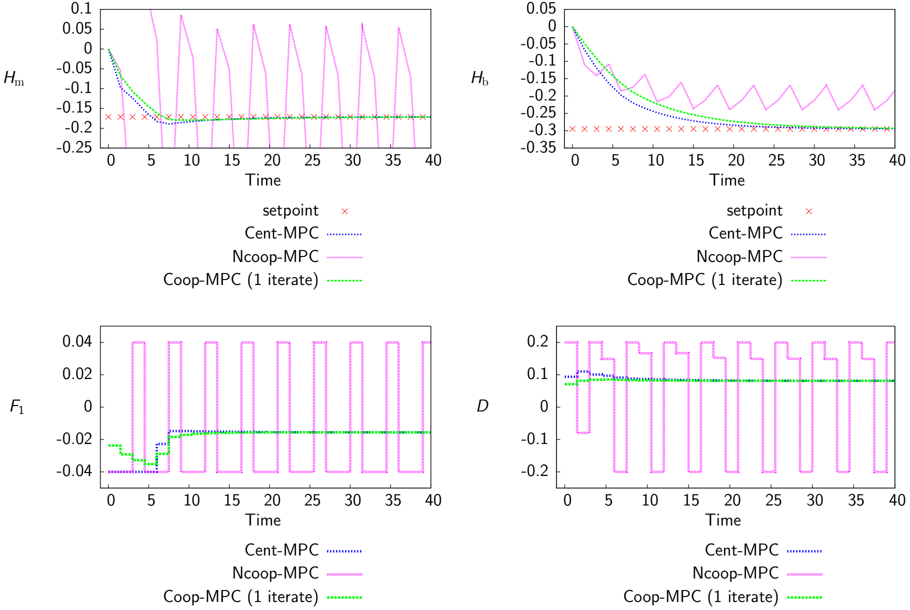
Geometry of cooperative vs. noncooperative MPC



Two reactors with separation and recycle



Two reactors with separation and recycle

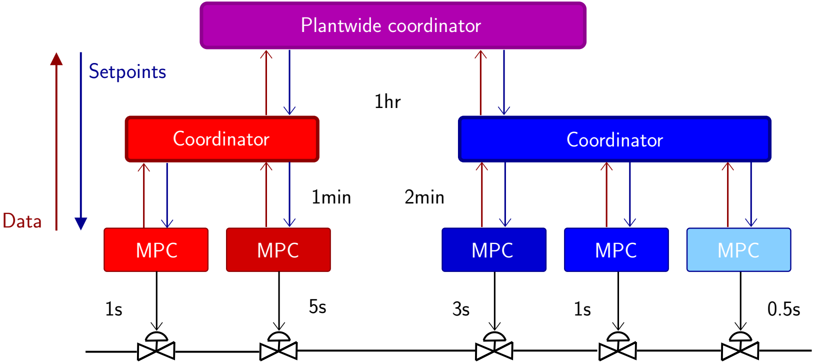


Two reactors with separation and recycle

Performance comparison

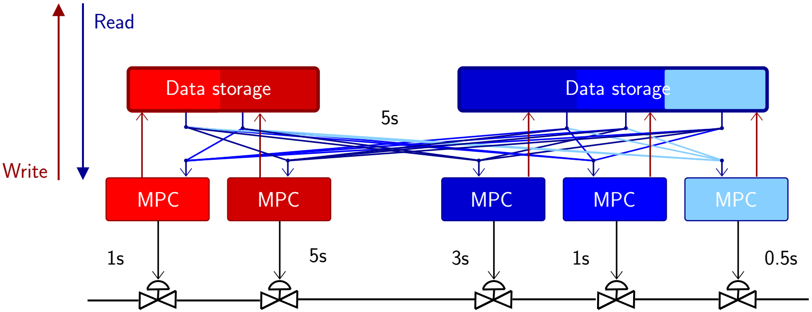
	Cost ($\times 10^{-2}$)	Performance loss
Centralized MPC	1.75	0
Decentralized MPC	∞	∞
Noncooperative MPC	∞	∞
Cooperative MPC (1 iterate)	2.2	25.7%
Cooperative MPC (10 iterates)	1.84	5%

Traditional hierarchical MPC



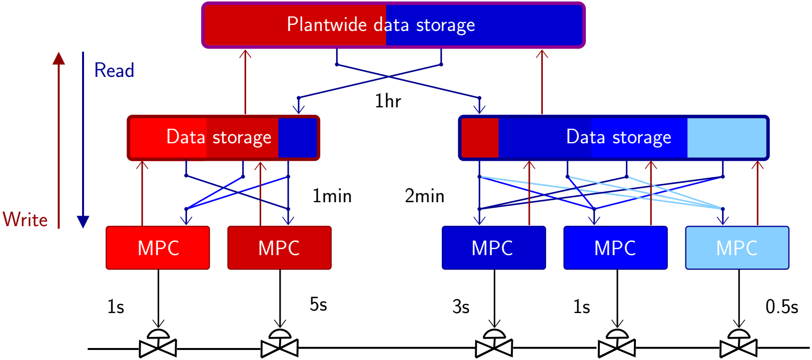
- Multiple dynamical time scales in plant
- Data and setpoints are exchanged on slower time scale
- Optimization performed at each layer

Cooperative MPC data exchange



- All data exchanged plantwide
- Slowest MPC defines rate of data exchange

Cooperative hierarchical MPC



- Optimization at MPC layer only
- Only subset of data exchanged plantwide
- Data exchanged at slower time scale

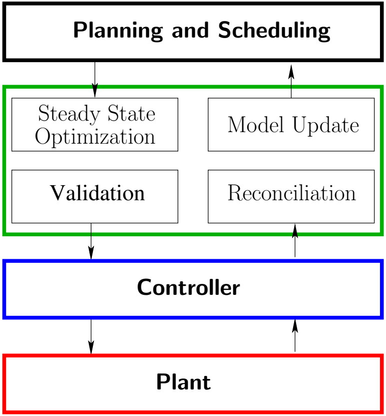
The big(ger) picture — What is the goal?

The goal of optimal process operations is to maximize profit.
— Helbig, Abel, and Marquardt (1998) . . . (−10 *years)*

Thus with more powerful capabilities, the determination of steady-state setpoints may simply become an unnecessary intermediate calculation. Instead nonlinear, dynamic reference models could be used directly to optimize a profit objective.
— Biegler and Rawlings (1991) . . . (−20 *years)*

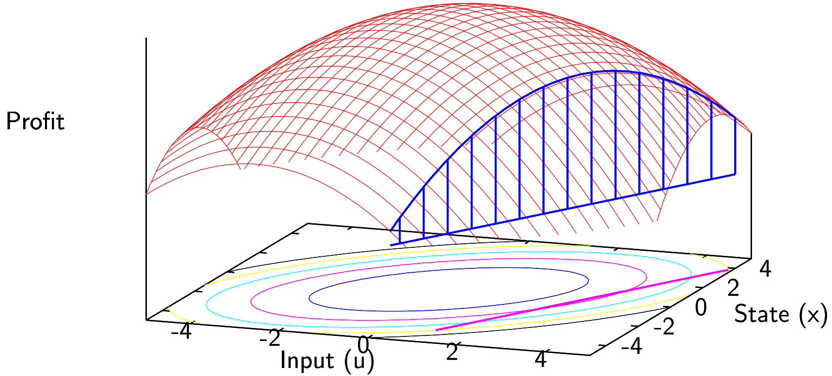
In attempting to synthesize a feedback optimizing control structure, our main objective is to translate the economic objective into process control objectives.
— Morari, Arkun, and Stephanopoulos (1980) . . . (−30 *years)*

Optimizing economics: Current industrial practice



- Two layer structure
- Drawbacks
  - Inconsistent models
  - Re-identify linear model as setpoint changes
  - Time scale separation may not hold
  - Economics unavailable in dynamic layer

Motivating the idea



Economics controller

$$\min_{u(t)} \int_0^T L(x,u)dt \qquad \text{subject to:} \qquad \begin{aligned} \dot{x} &= f(x,u) \\ y &= g(x,u) \end{aligned}$$

- Target tracking (standard)

$$L(x,u) = |y_{sp} - g(x,u)|_Q^2 + |u_{sp} - u|_R^2$$

- Economic optimization (new)
  L is the negative of economic profit function

$$L(x,u) = -P(x,u)$$

Strong duality and asymptotic stability

Strong Duality

If there exists a λ such that the the following problems have the same solution

$$\min_{x,u} L(x,u) \qquad\qquad \min_{x,u} L(x,u) - \lambda(f(x,u))$$

$$f(x,u) = 0 \qquad\qquad h(x,u) \leq 0$$

$$h(x,u) \leq 0$$

- Asymptotic stability of the closed-loop economics controller with a strictly convex cost and linear dynamics (Rawlings et al., 2008)
- Asymptotic stability of the closed-loop economics controller with strong duality in the steady-state problem (Diehl et al., 2010)

Example

$$x_{k+1} = \begin{bmatrix} 0.857 & 0.884 \\ -0.0147 & -0.0151 \end{bmatrix} x_k + \begin{bmatrix} 8.565 \\ 0.88418 \end{bmatrix} u_k$$

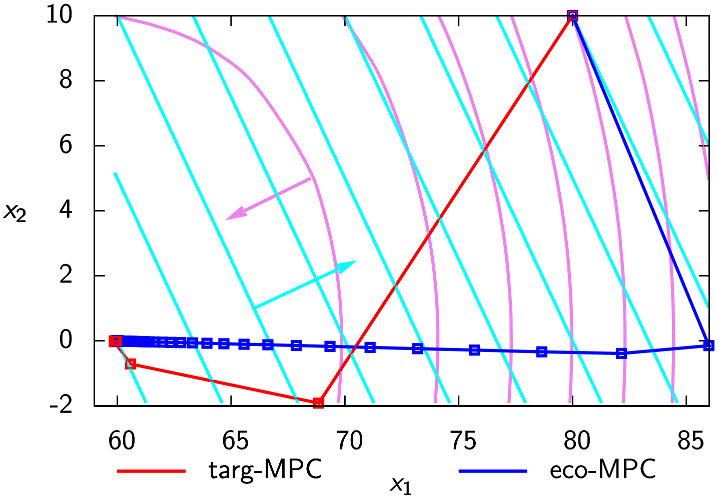
Input constraint: $-1 \leq u \leq 1$

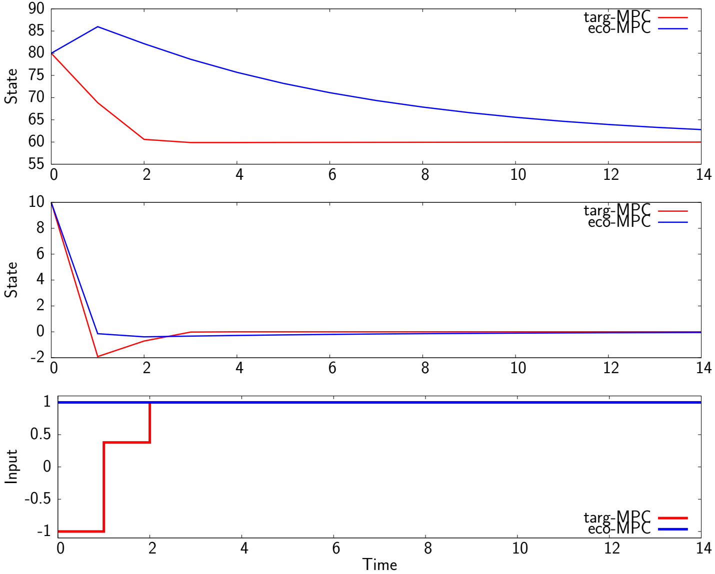
Economics

- $L_{eco} = \alpha' x + \beta' u$
- $\alpha = \begin{bmatrix} -3 & -2 \end{bmatrix}' \qquad \beta = -2$

Tracking

- $L_{targ} = |x - x^*|_Q^2 + |u - u^*|_R^2$
- $Q = 2I_2 \qquad R = 2$
- $x^* = \begin{bmatrix} 60 & 0 \end{bmatrix}' \qquad u^* = 1$


10
8
6
4
2
0
-2
x_2
60
65
70
75
80
85
x_1
targ-MPC
eco-MPC



90
85
80
75
70
65
60
55
State
targ-MPC
eco-MPC
0
2
4
6
8
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12
14
10
8
6
4
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0
-2
State
targ-MPC
eco-MPC
0
2
4
6
8
10
12
14
1
0.5
0
-0.5
-1
Input
targ-MPC
eco-MPC
0
2
4
6
8
10
12
14
Time

Conclusions

- Optimal dynamic operation of chemical processes has undergone a total transformation in the last 20 years. Both in theory and in practice.
- The currently available theory splits the problem into state estimation and regulation. Both are posed and solved as online optimization problems. Basic properties have been established. Lyapunov functions are the dominant theoretical tool for analysis and design.
- Industrial implementations and vendor software are basically keeping pace with the best available theory and algorithms. That is a surprising and noteworthy outcome!

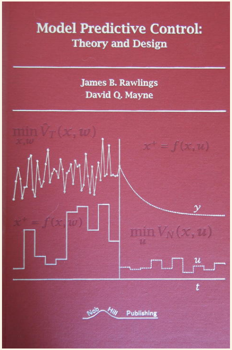
Critiquing the research enterprise

- The abstraction level is high and barrier to entry is significant.
- But the barrier is no higher than any other mathematically intensive research field in chemical engineering. Fluid mechanics, statistical mechanics, molecular dynamics, ...
- Researchers in this community have *not* done a good job communicating the significant advances in this field to their colleagues outside the field.

Future directions — Current research in MPC

- Distributed versions of MPC
  - Controlling large-scale systems composed of many small-scale MPCs
  - How to structure the small-scale MPCs so they cooperate on plantwide objectives
- Optimizing economics with MPC
  - The optimal economic point is not necessarily a steady state
  - Allows removal of the steady-state economic optimization layer
  - Dynamic economic optimization subject to settling at the optimal steady state

New MPC graduate textbook



- 576 page text
- 214 exercises
- 335 page solution manual
- 3 appendices on web (133 pages)
- www.nobhillpublishing.com

Further reading I

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Further reading II

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