

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

James B. Rawlings

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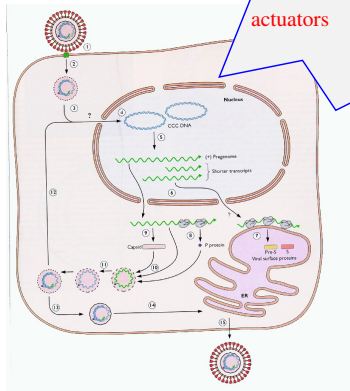
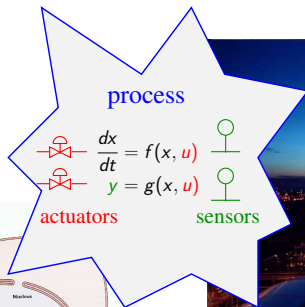


April 13, 2010

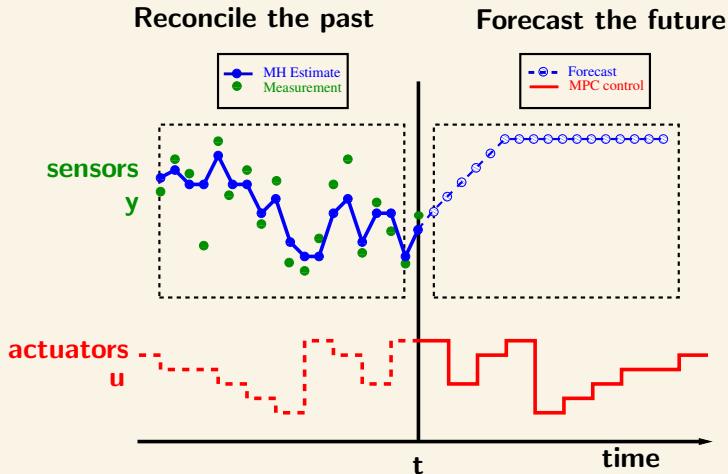
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Carnegie Mellon University

- 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

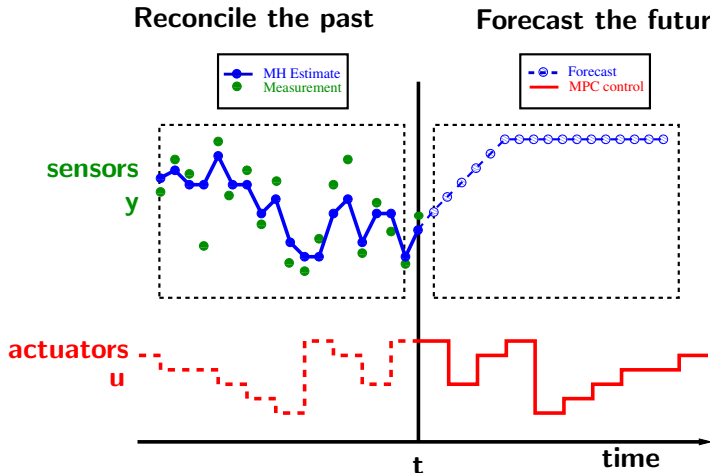


The model predictive control framework

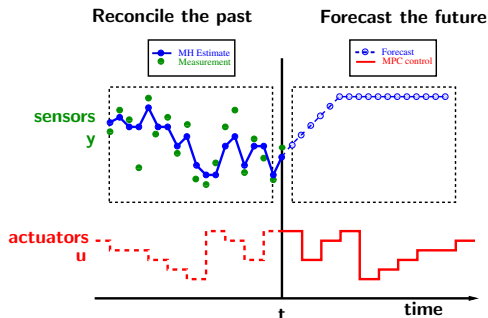


Predictive control

The future influences the present just as much as the past does.



Predictive control



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

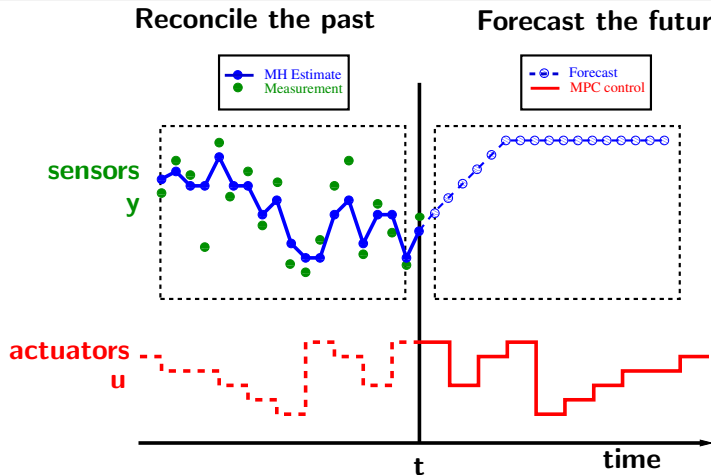
$$\dot{x} = f(x, u)$$

$$x(0) = x_0 \quad (\text{given})$$

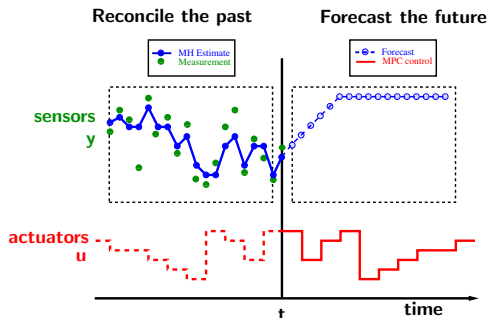
$$y = g(x, u)$$

State estimation

When I want to understand what is happening today or try to decide what will happen tomorrow, I look back.



State estimation

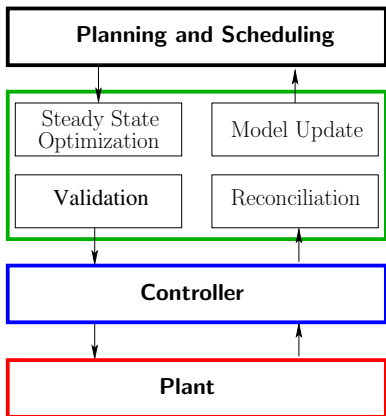


$$\min_{x_0, w(t)} \int_{-T}^0 |y - g(x, u)|_R^2 + |\dot{x} - f(x, u)|_Q^2 dt$$

$$\dot{x} = f(x, u) + w \quad (\text{process noise})$$

$$y = g(x, u) + v \quad (\text{measurement noise})$$

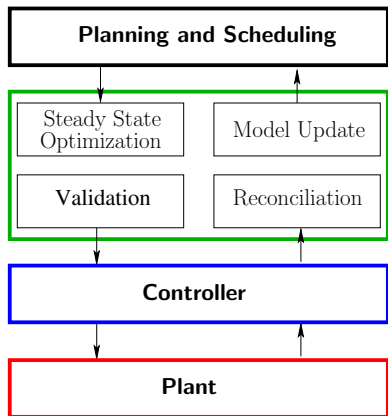
Industrial impact of the research



Two layer structure

- **Steady-state layer**
 - ▶ RTO optimizes steady-state model
 - ▶ Optimal setpoints passed to dynamic layer

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

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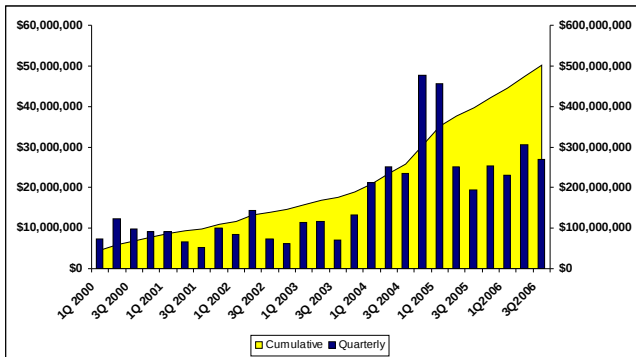
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We're Doing it For the Money



Are all the problems solved?

Some questions to consider

- How do we best decompose *large-scale systems* into manageable problems?

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

Chemical plant integration



Material flow



Energy flow



Decentralized Control

- Most large-scale systems consist of networks of interconnected/interacting subsystems
 - ▶ Chemical plants, electrical power grids, water distribution networks, . . .

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 - ▶ 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)

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	$u_1 \in \Omega_1, u_2 \in \Omega_2$

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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)	

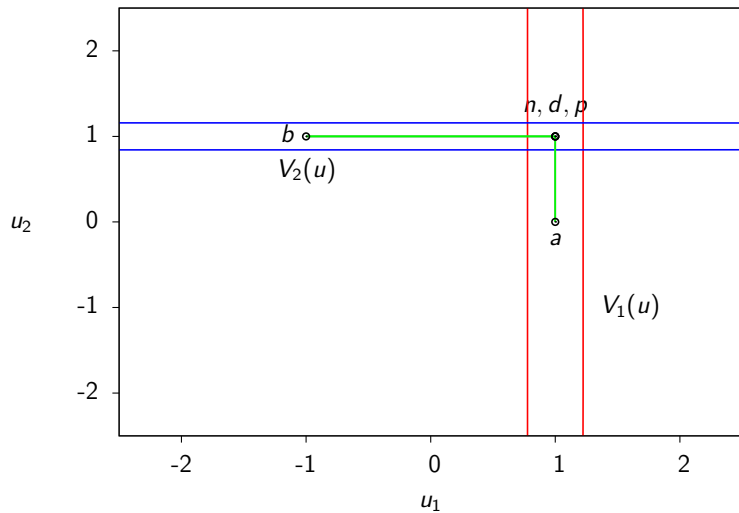
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Cooperative Control (Pareto optimal)	$\min_{u_1 \in \Omega_1} V(u_1, u_2) \quad \min_{u_2 \in \Omega_2} V(u_1, u_2)$

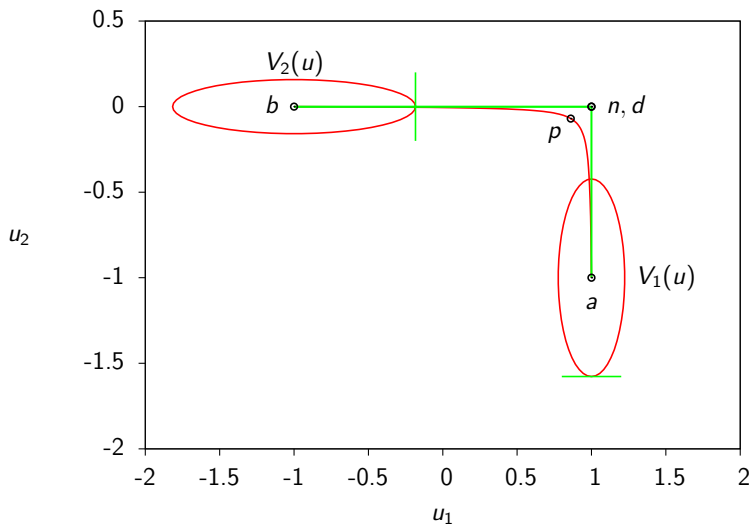
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Centralized Control (Pareto optimal)	$\min_{u_1, u_2 \in \Omega_1 \times \Omega_2} V(u_1, u_2)$

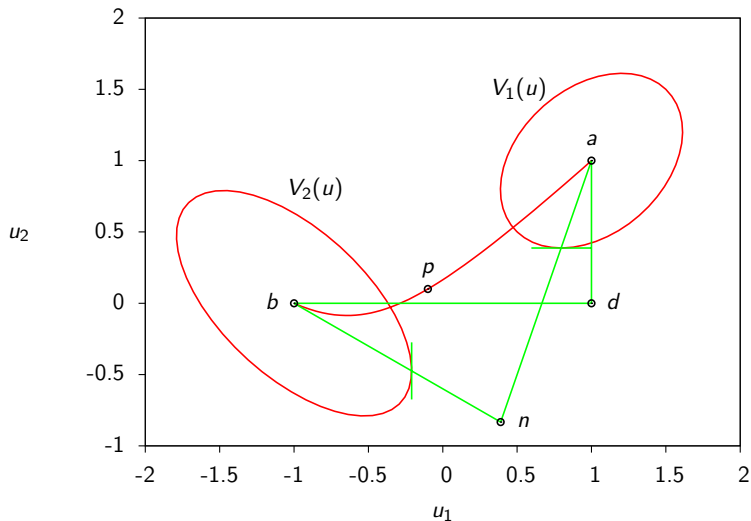
Noninteracting systems



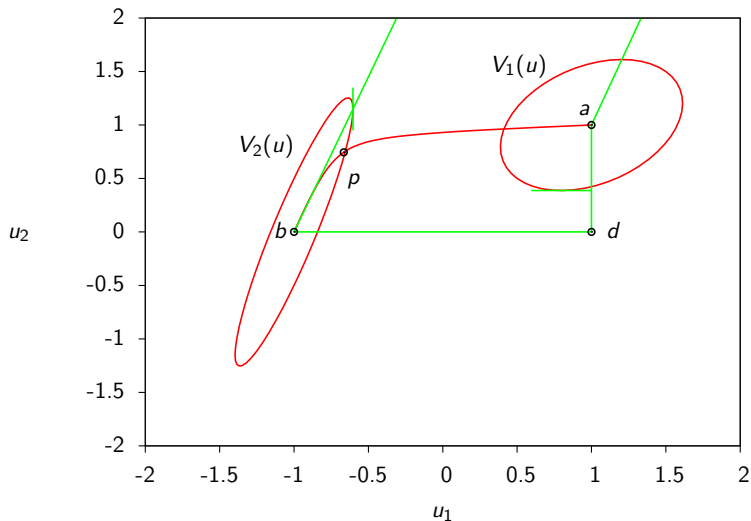
Weakly interacting systems



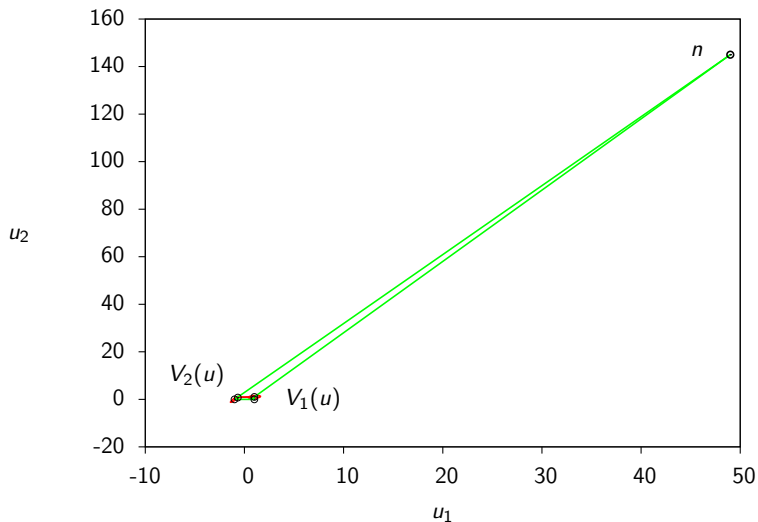
Moderately interacting systems



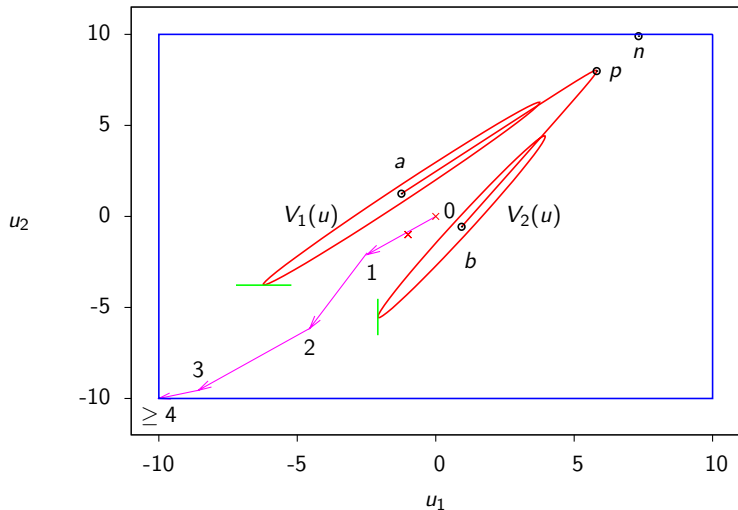
Strongly interacting (conflicting) systems



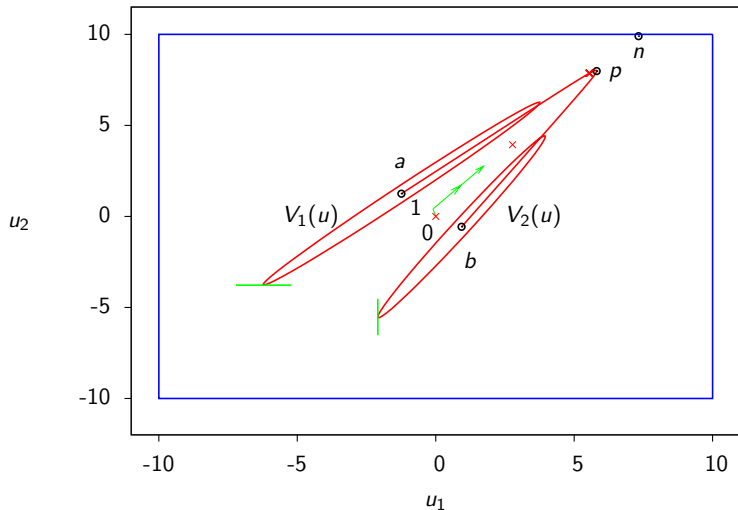
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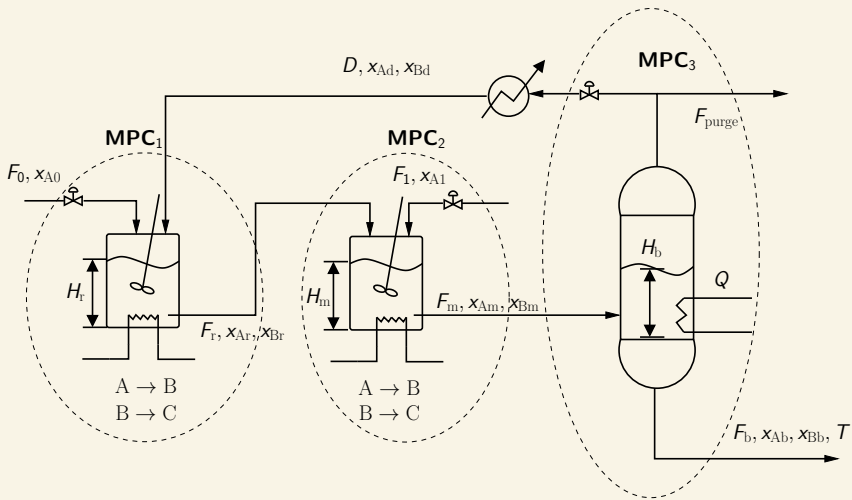
Geometry of cooperative vs. noncooperative MPC



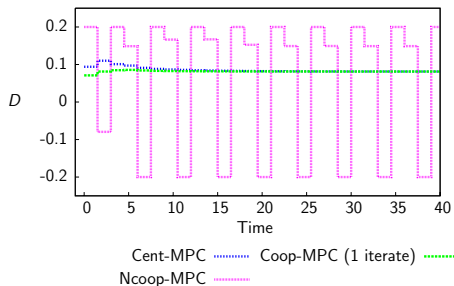
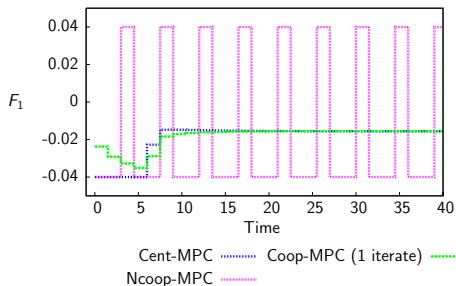
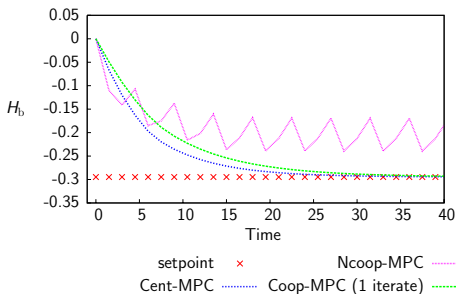
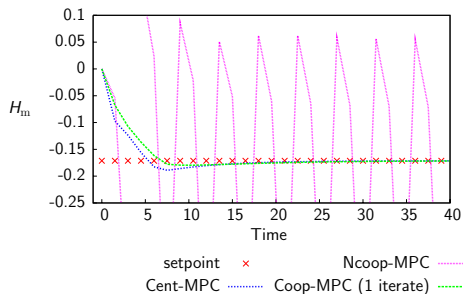
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Two reactors with separation and recycle



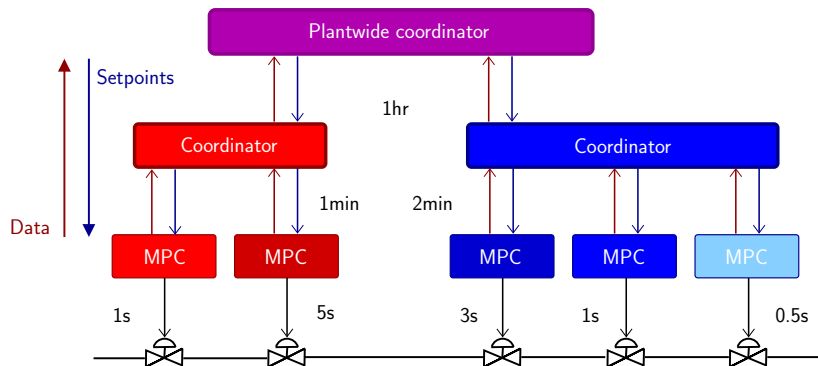
Two reactors with separation and recycle



Performance comparison

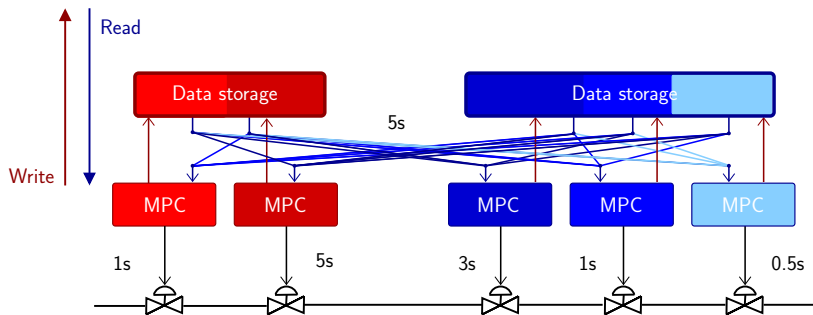
	Cost ($\times 10^{-2}$)	Performance loss
Centralized MPC	1.75	0
Decentralized MPC	∞	∞
Noncooperative MPC	∞	∞
Cooperative MPC (1 iterate)	2.2	25.7%
Cooperative MPC (10 iterates)	1.84	5%

Traditional hierarchical MPC



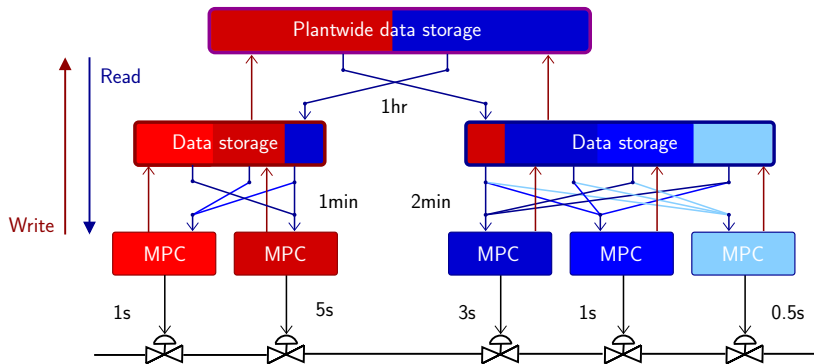
- Multiple dynamical time scales in plant
- Data and setpoints are exchanged on slower time scale
- Optimization performed at each layer

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

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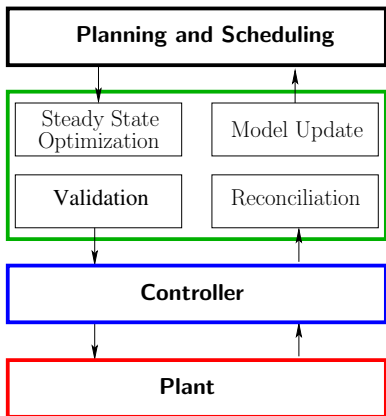
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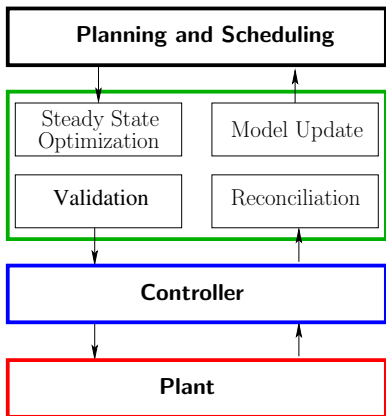
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— Morari, Arkun, and Stephanopoulos (1980) ... (–30 years)*

Optimizing economics: Current industrial practice



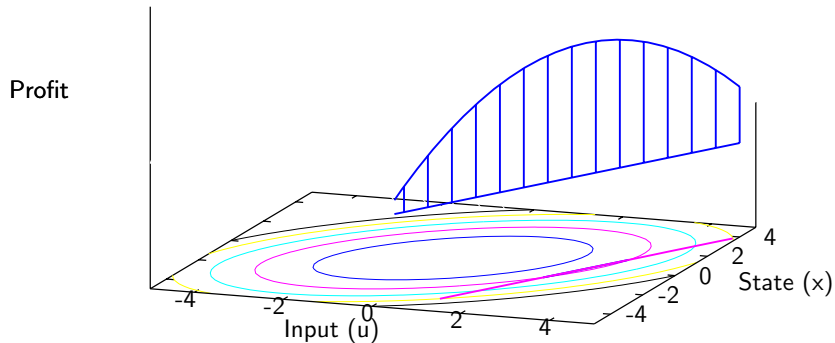
- Two layer structure
- Drawbacks

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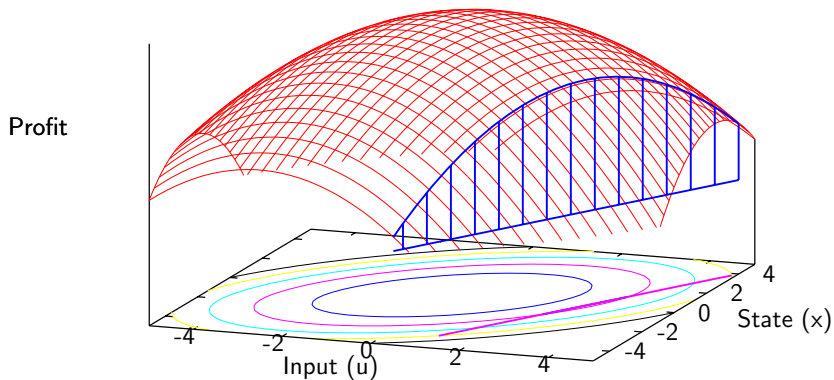


- Two layer structure
- Drawbacks
 - ▶ Inconsistent models
 - ▶ Re-identify linear model as setpoint changes
 - ▶ Time scale separation may not hold
 - ▶ Economics unavailable in dynamic layer

Motivating the idea



Motivating the idea



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

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- Target tracking (standard)

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

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- Target tracking (standard)

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- 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

$$\min_{x,u} L(x, u)$$

$$f(x, u) = 0$$

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

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

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

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

- 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., 2009)

Example

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

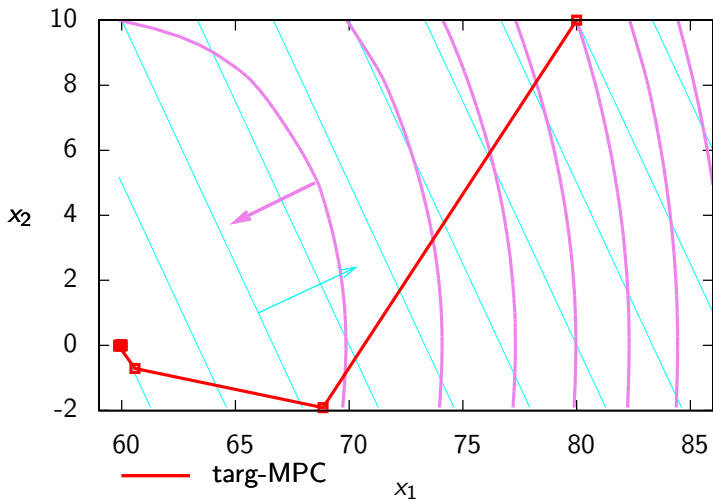
Input constraint: $-1 \leq u \leq 1$

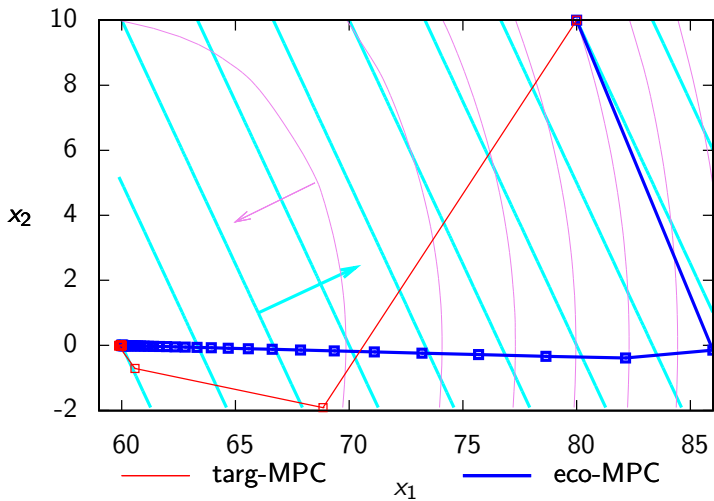
Economics

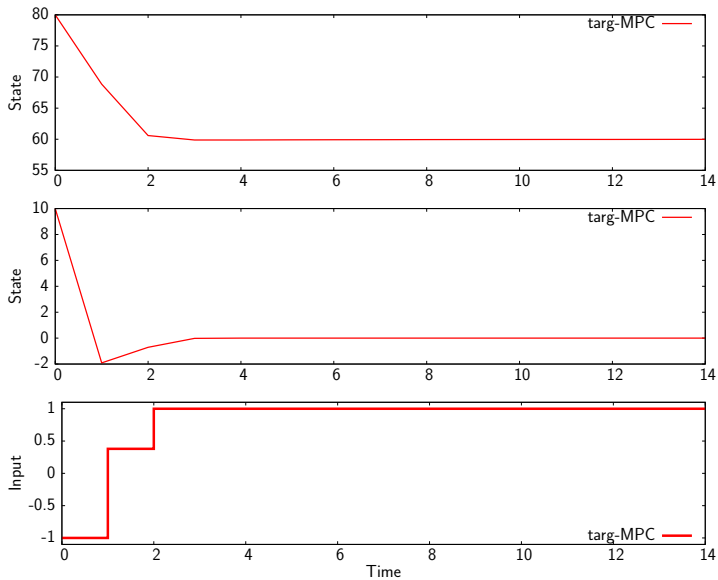
- $L_{eco} = \alpha'x + \beta'u$
- $\alpha = [-3 \quad -2]'$ $\beta = -2$

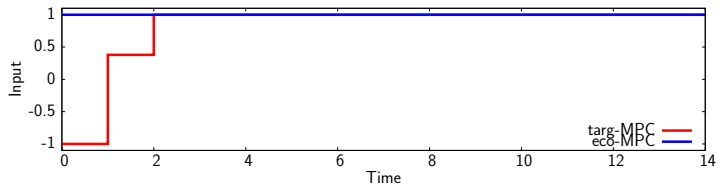
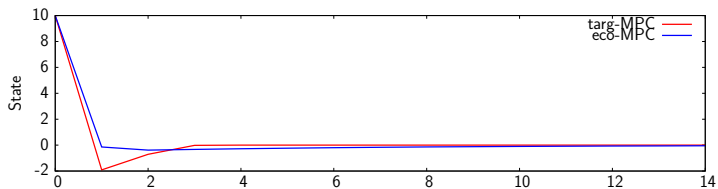
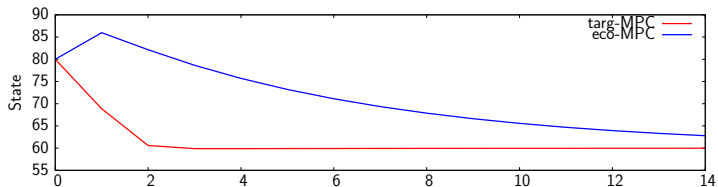
Tracking

- $L_{targ} = |x - x^*|_Q^2 + |u - u^*|_R^2$
- $Q = 2I_2$ $R = 2$
- $x^* = [60 \quad 0]'$ $u^* = 1$









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Conclusions

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- Industrial implementations and vendor software are basically keeping pace with the best available theory and algorithms. That is a surprising and noteworthy outcome!

- The abstraction level is high and barrier to entry is significant.

Critiquing the research enterprise

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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.

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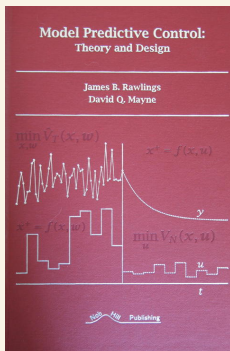
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 - ▶ Dynamic economic optimization subject to settling at the optimal steady state

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

- L. T. Biegler and J. B. Rawlings. Optimization approaches to nonlinear model predictive control. In Y. Arkun and W. H. Ray, editors, *Chemical Process Control–CPCIV*, pages 543–571. CACHE, 1991.
- M. Diehl, R. Amrit, and J. B. Rawlings. A Lyapunov function for economic optimizing model predictive control. *IEEE Trans. Auto. Cont.*, 2009. Submitted for publication.
- A. Helbig, O. Abel, and W. Marquardt. Structural concepts for optimization based control of transient processes. In *International Symposium on Nonlinear Model Predictive Control, Ascona, Switzerland*, 1998.
- Y.-C. Ho. On Centralized Optimal Control. *IEEE Trans. Auto. Cont.*, 50(4):537–538, 2005.
- J. Lunze. *Feedback Control of Large Scale Systems*. Prentice-Hall, London, U.K., 1992.
- M. Morari, Y. Arkun, and G. Stephanopoulos. Studies in the synthesis of control structures for chemical processes. Part I: Formulation of the problem. Process decomposition and the classification of the control tasks. Analysis of the optimizing control structures. *AIChE J.*, 26(2):220–232, 1980.
- S. J. Qin and T. A. Badgwell. A survey of industrial model predictive control technology. *Control Eng. Prac.*, 11(7):733–764, 2003.

Further reading II

- J. B. Rawlings, D. Bonné, J. B. Jørgensen, A. N. Venkat, and S. B. Jørgensen. Unreachable setpoints in model predictive control. *IEEE Trans. Auto. Cont.*, 53(9): 2209–2215, October 2008.
- N. R. Sandell Jr., P. Varaiya, M. Athans, and M. Safonov. Survey of decentralized control methods for larger scale systems. *IEEE Trans. Auto. Cont.*, 23(2):108–128, 1978.
- D. D. Šiljak. *Decentralized Control of Complex Systems*. Academic Press, London, 1991. ISBN 0-12-643430-1.
- D. M. Starks and E. Arrieta. Maintaining AC&O applications, sustaining the gain. In *Proceedings of National AIChE Spring Meeting*, Houston, Texas, April 2007.