From Feedback Control to Real-Time Business Decision Making in the Process Industry

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The Business Climate

From **growing market** volume and **limited competition** to **market saturation** and **global competition** in the 21st century:

- internet and e-commerce facilitate complete market transparency,
- transportation cost continue to decrease,
- engineering and manufacturing skills are available globally.

Economic success requires to quickly **transform new ideas into marketable products:**

- product innovation to open-up new market opportunities,
- process design for best-in-class plants to maximize lifecycle profits,
- efficient and agile manufacturing to make best use of existing assets.

From **growing market** volume and **limited competition**
to **market saturation** and **global competition** in the 21st century:

- in… …litate complete market transparency,
- …e,
- …e available globally.

Systems and Control Technology

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- product innovation to ope… …up new market opportunities,
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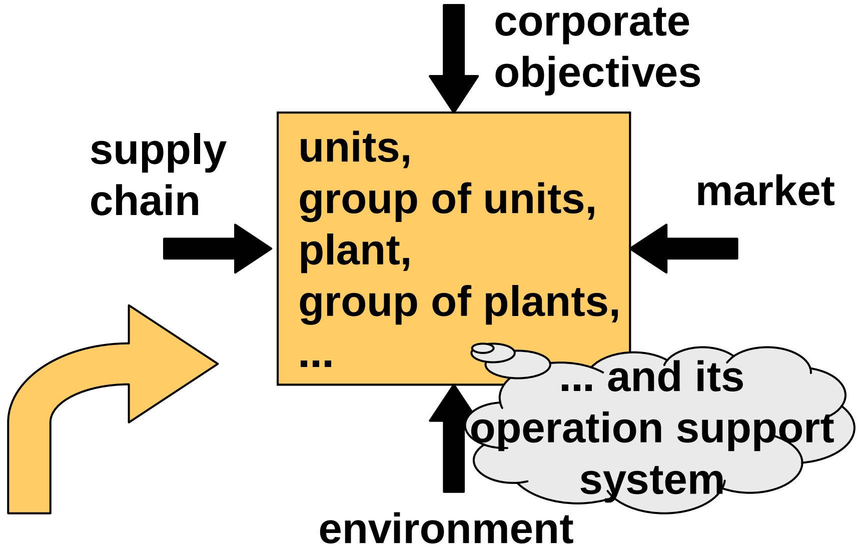
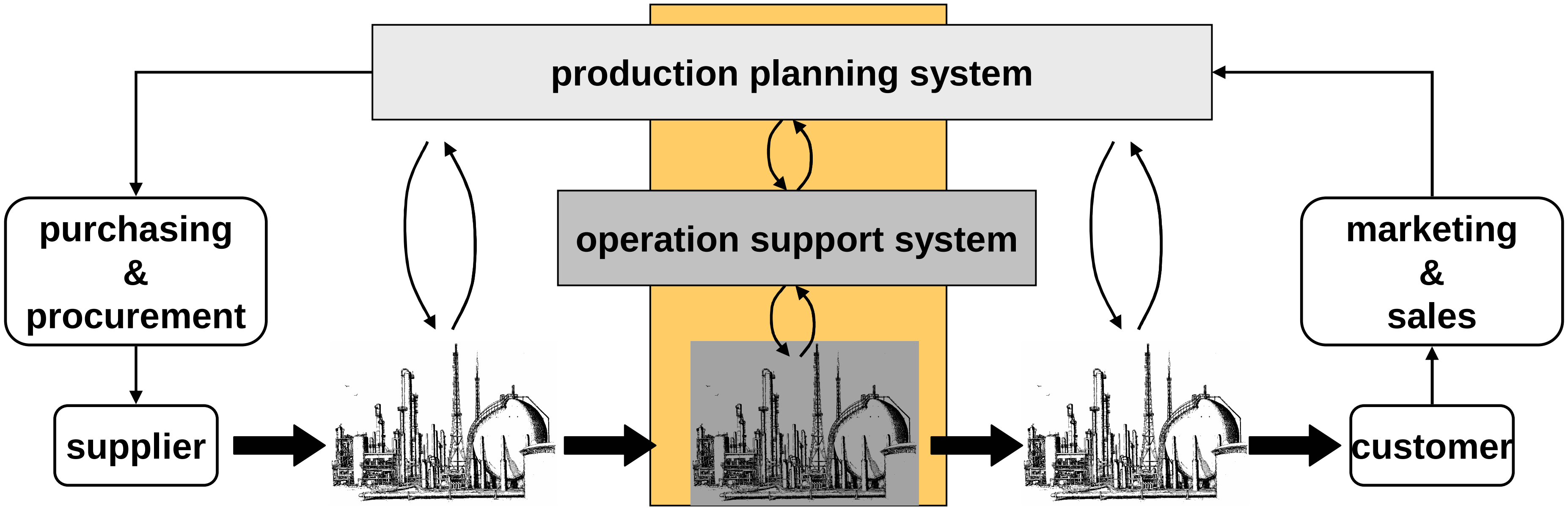
- efficient and agile manufacturing to make best use of existing assets.

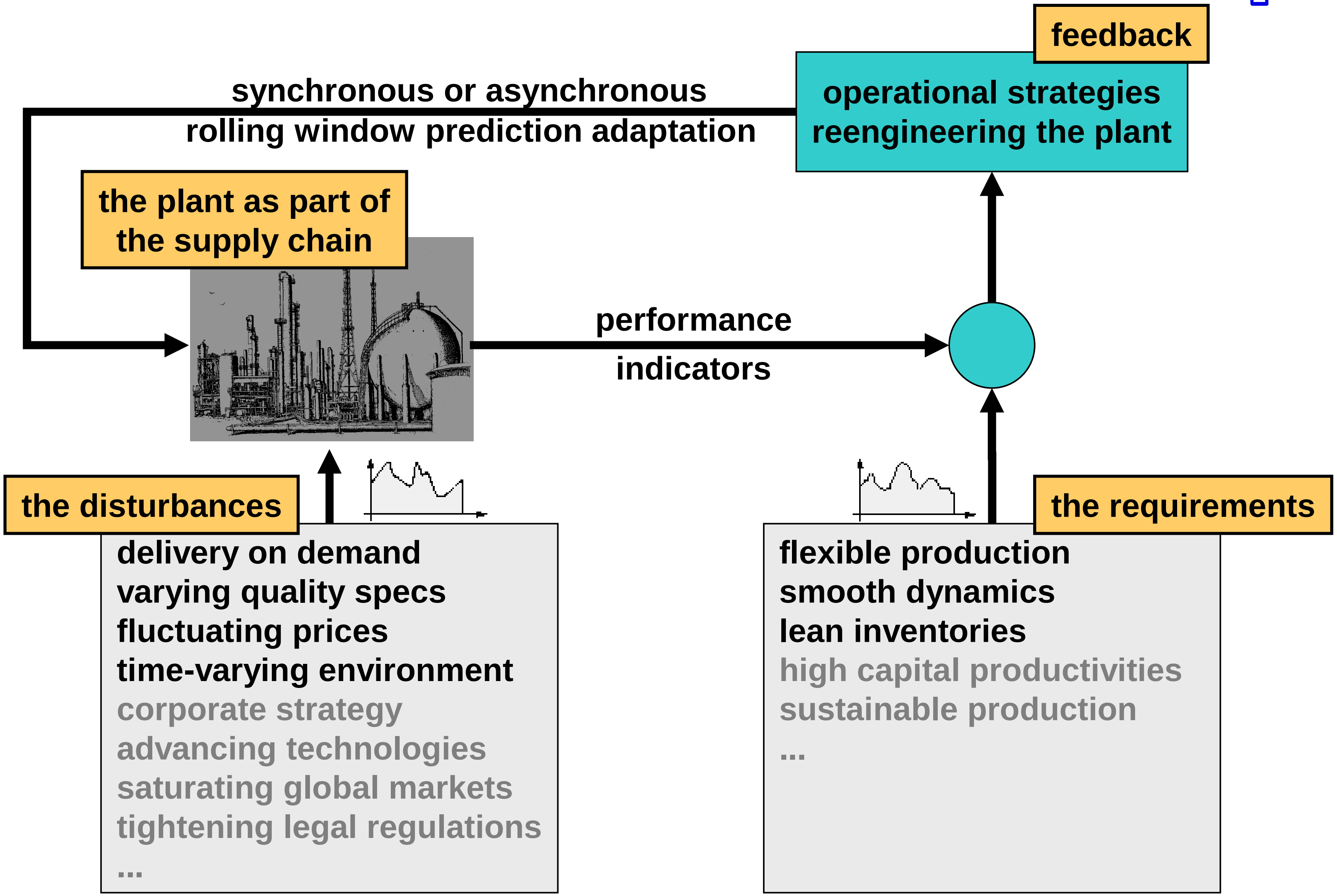
Operational Strategies – the Status

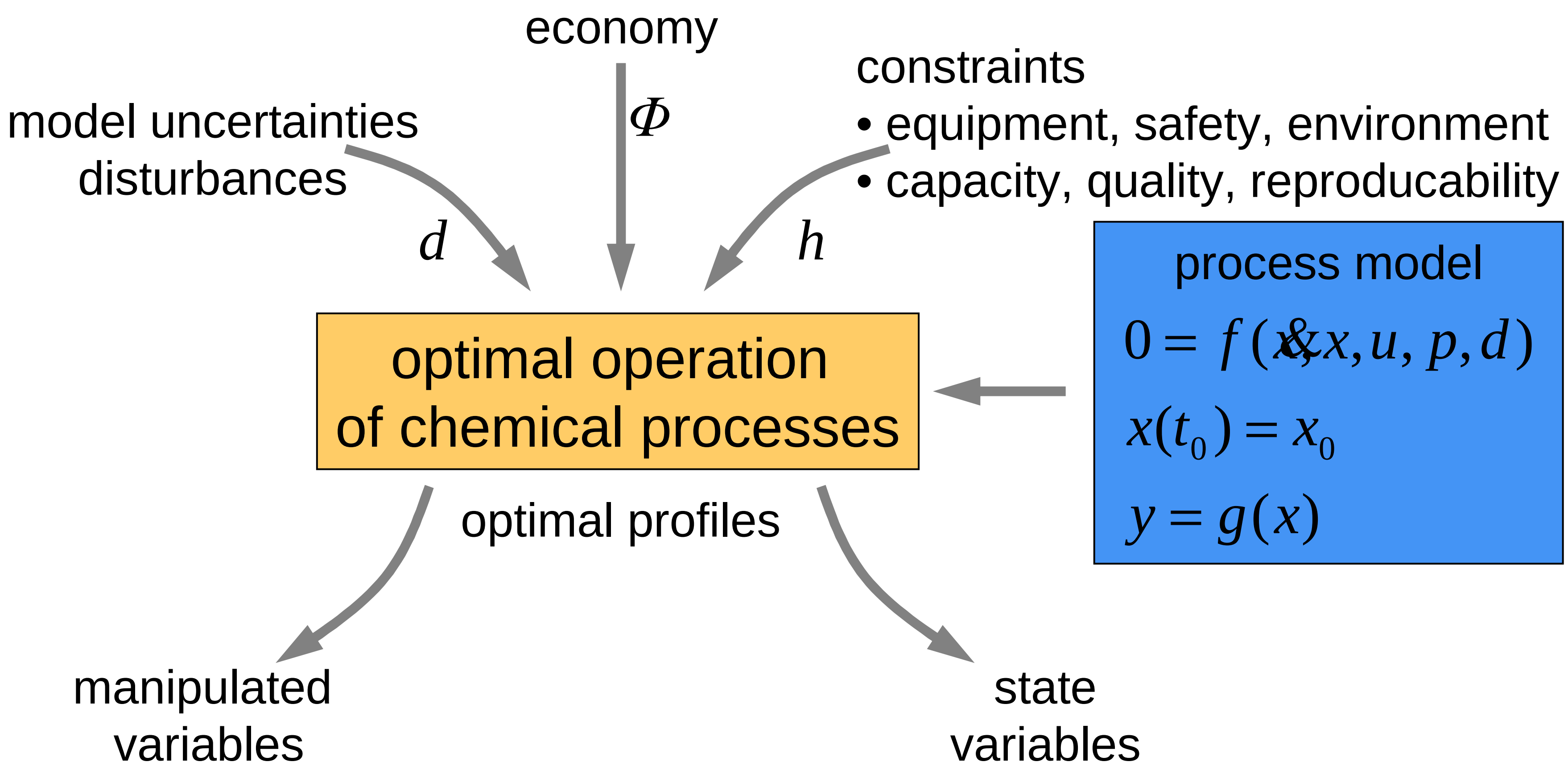
- plant in isolation
- steady-state operation
- set-point control
- disturbance rejection
- **limited flexibility**
- largely autonomous





Manufacturing in the Future





Why should they be constant over time?

Φ, h

measurements $\tilde{y}_r$ → **optimal feedback control system** → manipulated variables u_c

dynamic data reconciliation (combined estimation problem

$$\min_{x_{r,0},d_r} \Phi_r(y_r, \eta, x_{r,0}, d_r, t_c, t_f)$$

s.t.

$$0 = f(\dot{x}_r, x_r, u_r, d_r)$$
$$y_r = g(x_r)$$
$$x_r(t_r) = x_{r,0}$$
$$u_r = \mathrm{U}(u_c(\cdot))$$
$$0 \geq h_r(x_r, d_r)$$
$$t \in [t_r, t_c]$$

dynamic optimization (open/closed loop)

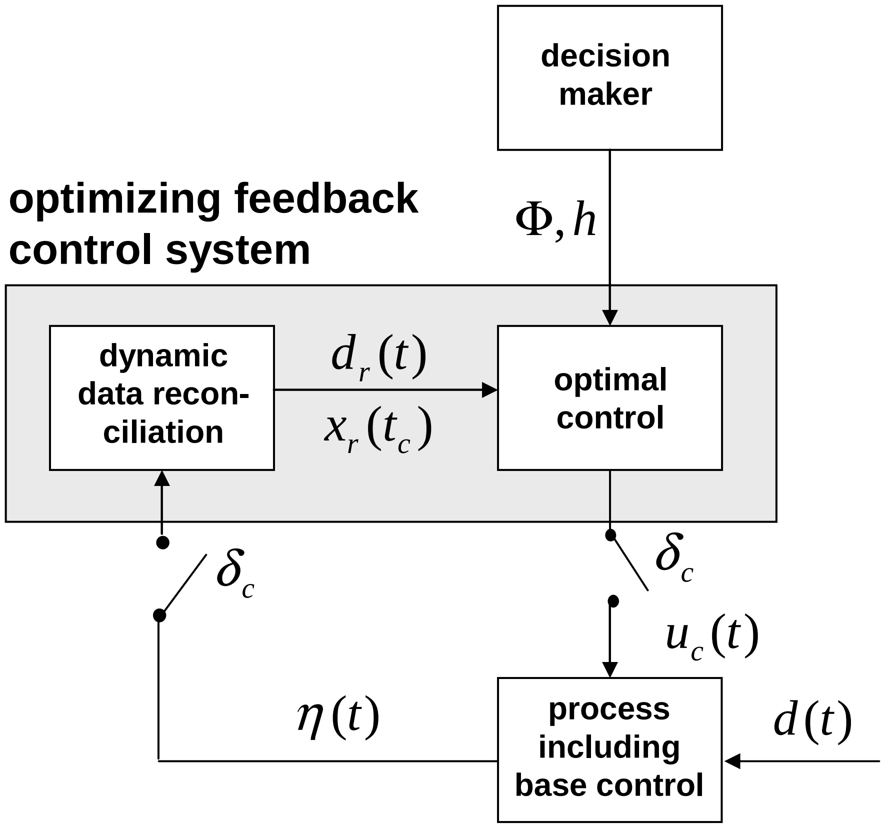
$$\min_{u_c} \Phi_c(x_c, u_c, t_c, t_f)$$

s.t.

$$0 = f(\dot{x}_c, x_c, u_c, d_c)$$
$$y_c = g(x_c)$$
$$x_c(t_c) = x_r(t_c)$$
$$d_c = \mathrm{D}(d_r(\cdot))$$
$$0 \geq h_c(x_c, u_c)$$
$$t \in [t_c, t_f]$$

2 coupled problems !

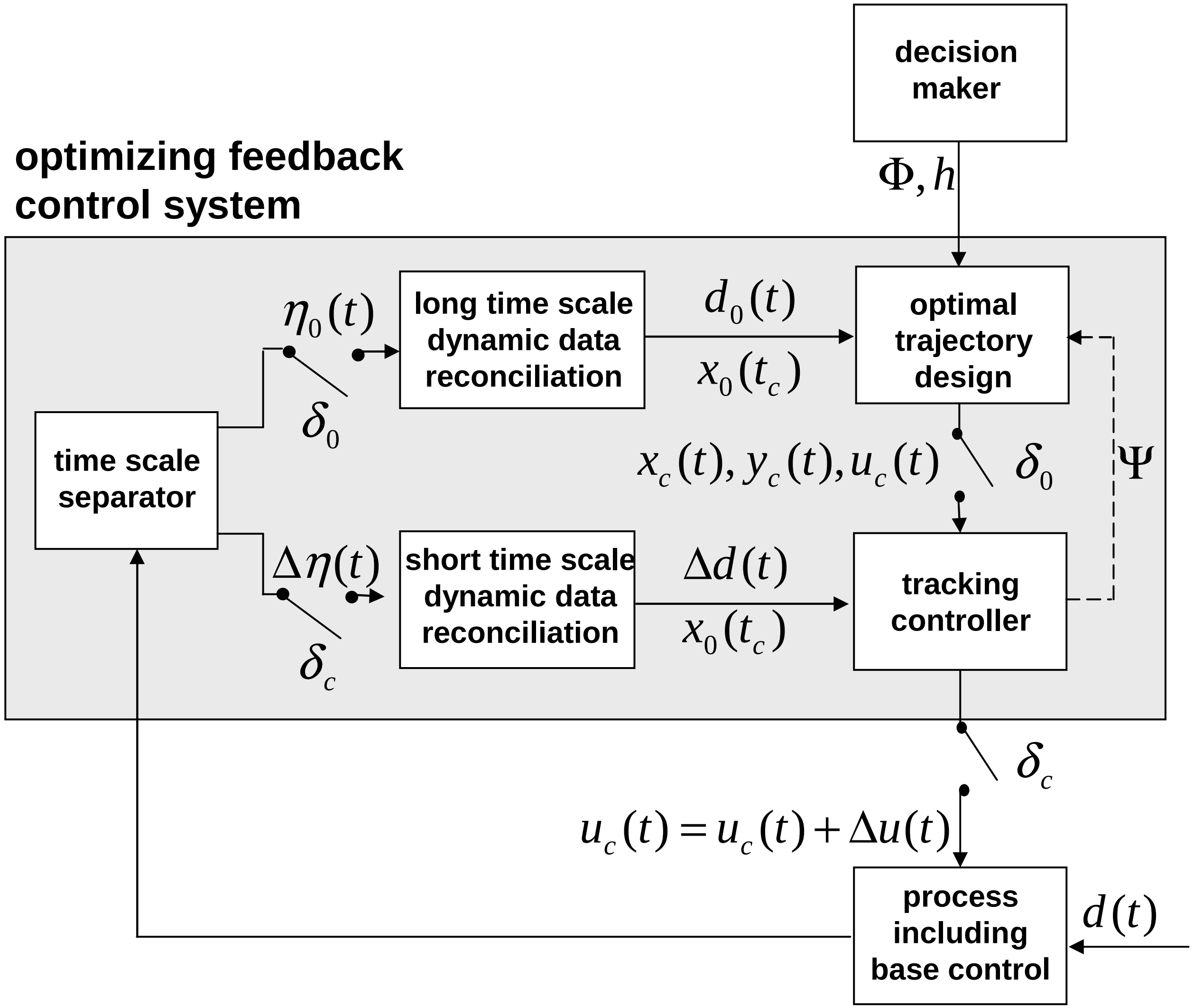
Direct Solution Approach



- solution of optimal control reconciliation problems at controller sampling frequency
- computationally demanding
- model complexity limited
  $\Rightarrow$ large models ?
- lack of transparency, redundancy and reliability

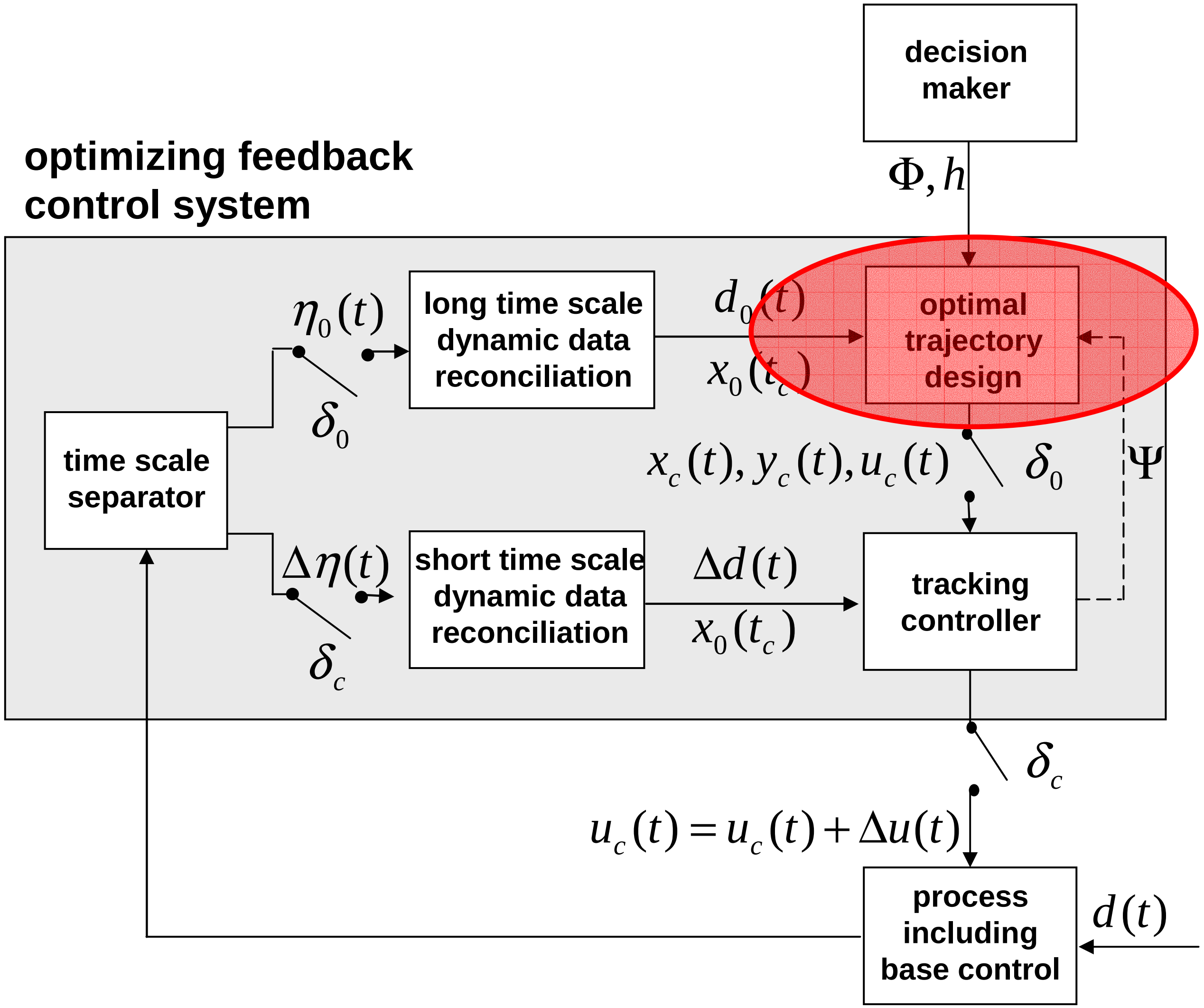
(Terwiesch et al., 1994;
Helbig et al., 1998;
Wisnewski & Doyle, 1996;
Biegler & Sentoni, 2000
Diehl et al., 2002,
van Hessem, 2004)

Vertical (Time-Scale) Decomposition



- generalizes steady-state real-time optimization and constrained predictive control
- requires (multiple) time-scale separation, e.g.
  $d(t) = d_0(t) + \Delta d(t)$
  with trend $d_0(t)$ and
  zero mean fluctuation $\Delta d(t)$

Real-time Dynamic Optimization



- dynamic optimization - a versatile means for problem formulation
- focus will be on trajectory design
- improvement of numerical methods

Mathematical problem formulation

$$\min_{u(t),p,t_f} \Phi(x(t_f))$$ objective function (e.g. cost)

s.t.

$$M\dot{x} = F(x,u,p,t), \quad t \in [t_0, t_f],$$
$$0 = x(t_0) - x_0,$$

DAE system (process model)

$$0 \geq P(x,u,p,t), \quad t \in [t_0, t_f],$$ path constraints (e.g. temp. bound)

$$0 \geq E(x(t_f))$$ endpoint constraints (e.g. prod. spec.)

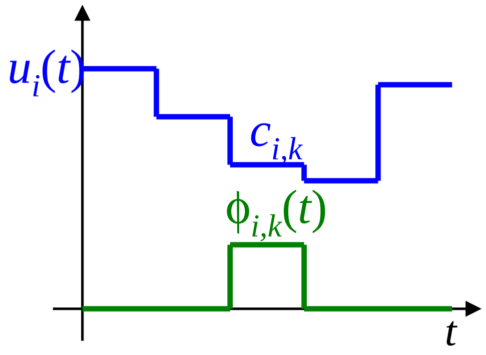
Degrees of freedom:

$u(t)$	time-variant control variables
p	time-invariant parameters
t_f	final time

Sequential Approach (Single Shooting)

Control vector parameterization

$$u_i(t) \approx \sum_{k \in \Lambda_i} c_{i,k}\, \phi_{i,k}(t)$$



$\phi_{i,k}(t)$ parameterization functions

$c_{i,k}$ parameters

Reformulation as nonlinear programming problem (NLP)

$$\min_{c,p,t_f} \Phi(x(c,p,t_f))$$

s.t. $\quad 0 \geq P(x,c,p,t_i), \quad \forall t_i \in \mathrm{T},$

$\quad 0 \geq E(x(t_f))$

DAE system solved by underlying numerical integration

Gradients for NLP solver typically obtained by integration of sensitivity systems

Improved Algorithms – Sequential Approach

Sensitivity integration is expensive

State integration is expensive

Improve efficiency of sensitivity integration

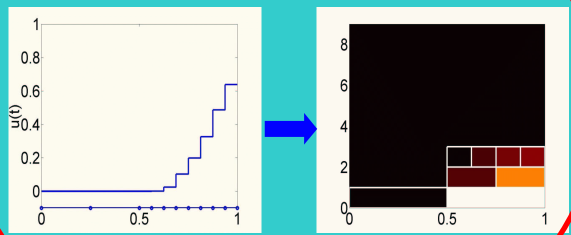
Reduce number of sensitivity parameters

Reduce model complexity

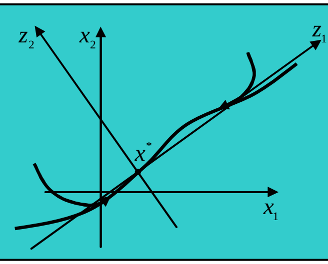
New solver for sensitivity integration

$$X_{k+1} = X_k - \begin{bmatrix} A-\frac{M}{h_j} & & \\ A_1 & A-\frac{M}{h_j} & \\ \vdots & & \ddots \\ A_{n_z} & & & A-\frac{M}{h_j} \end{bmatrix}^{-1} f(X_k, z)$$

Control grid adaptation strategy



Methods for model reduction



Multiscale Representation

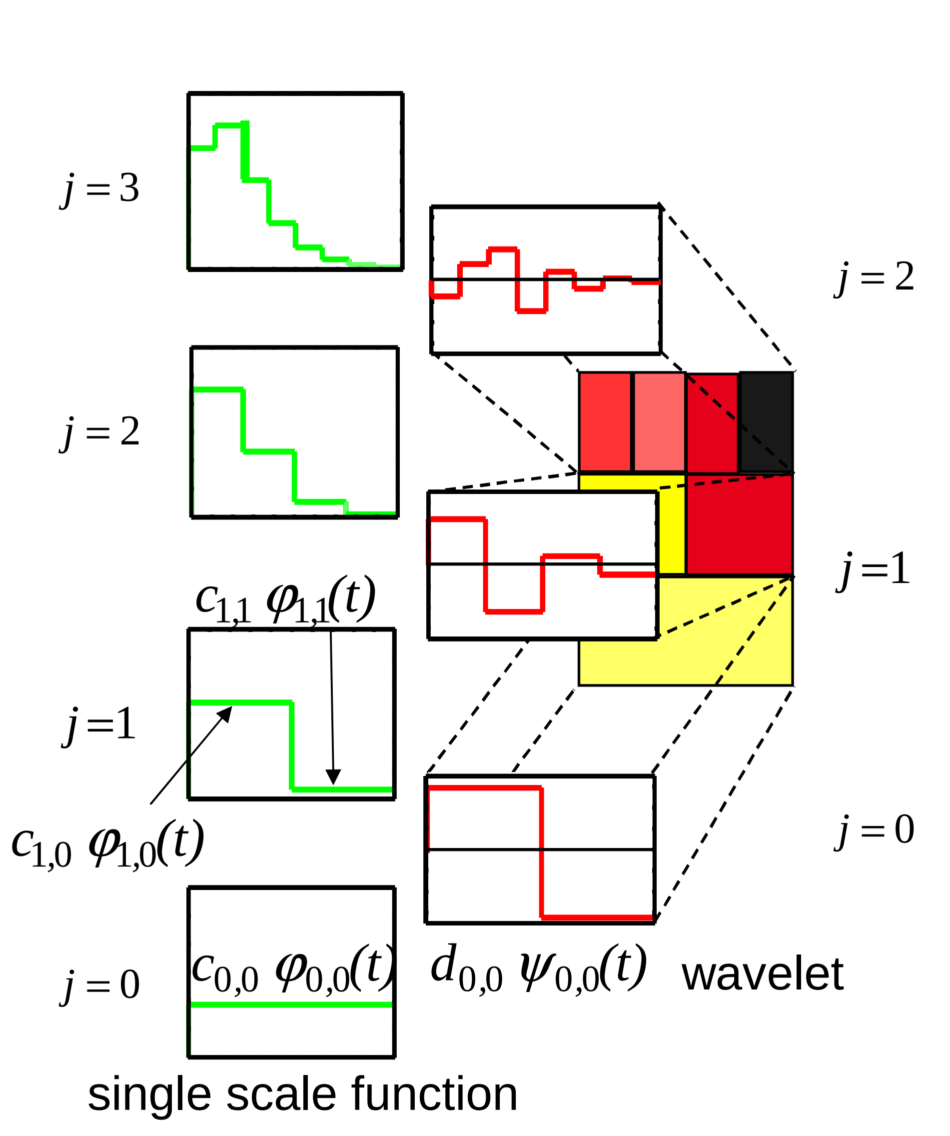
Different **representations** of the **same function …**

… for problem discretization:

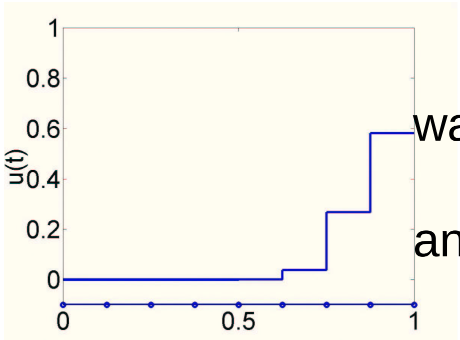
$$u = \sum_{(j,k)\in\Lambda_\varphi} c_{j,k}\varphi_{j,k}(t)$$

… for grid point elimination analysis:

$$u = c_{0,0}\varphi_{0,0}(t) + \sum_{(j,k)\in\Lambda_\psi} d_{j,k}\psi_{j,k}(t)$$

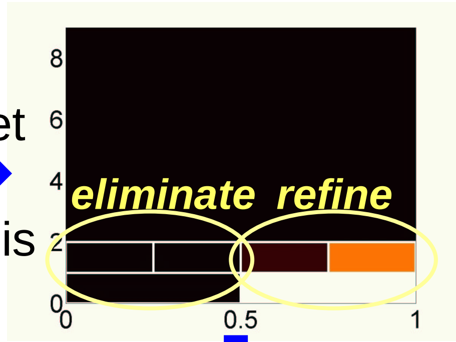


Adaptive Refinement Algorithm

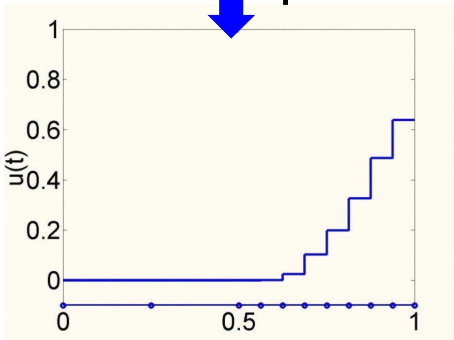


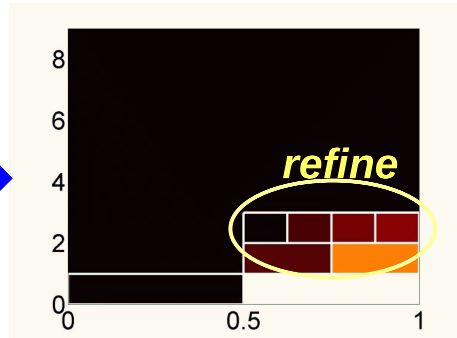
coarse initial mesh

wavelet analysis

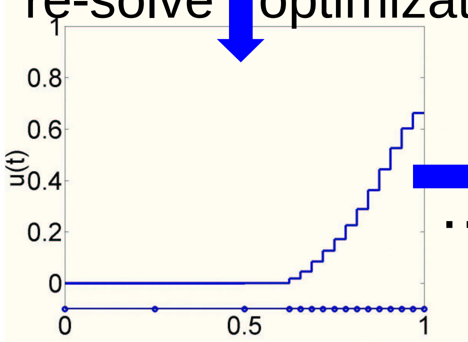


re-solve optimization





re-solve optimization



... until stopping criterion met.

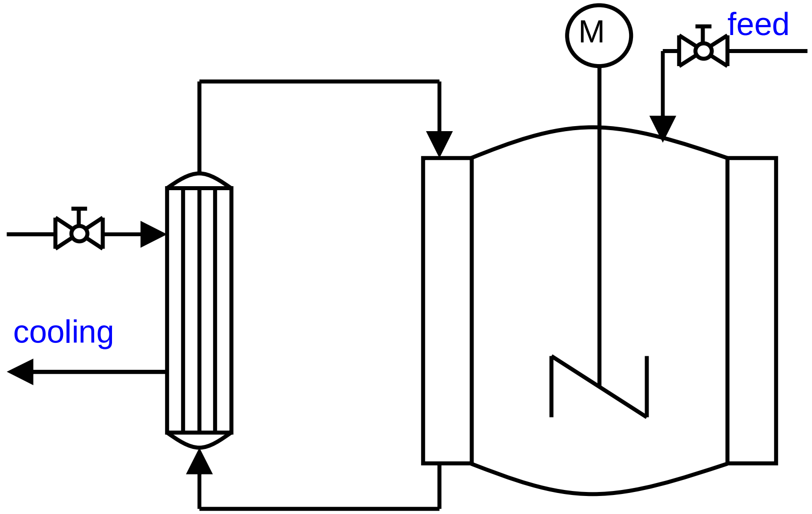
Mesh analysis

- Concepts from signal analysis
- Grid point elimination
- Grid point insertion

Repetitive procedure

- Re-optimize problem on refined mesh
- Profile from previous solution as initial guess
- Decouple optimization and adaptation

isothermal semi-batch reactor
(Srinivasan et al, 2003)

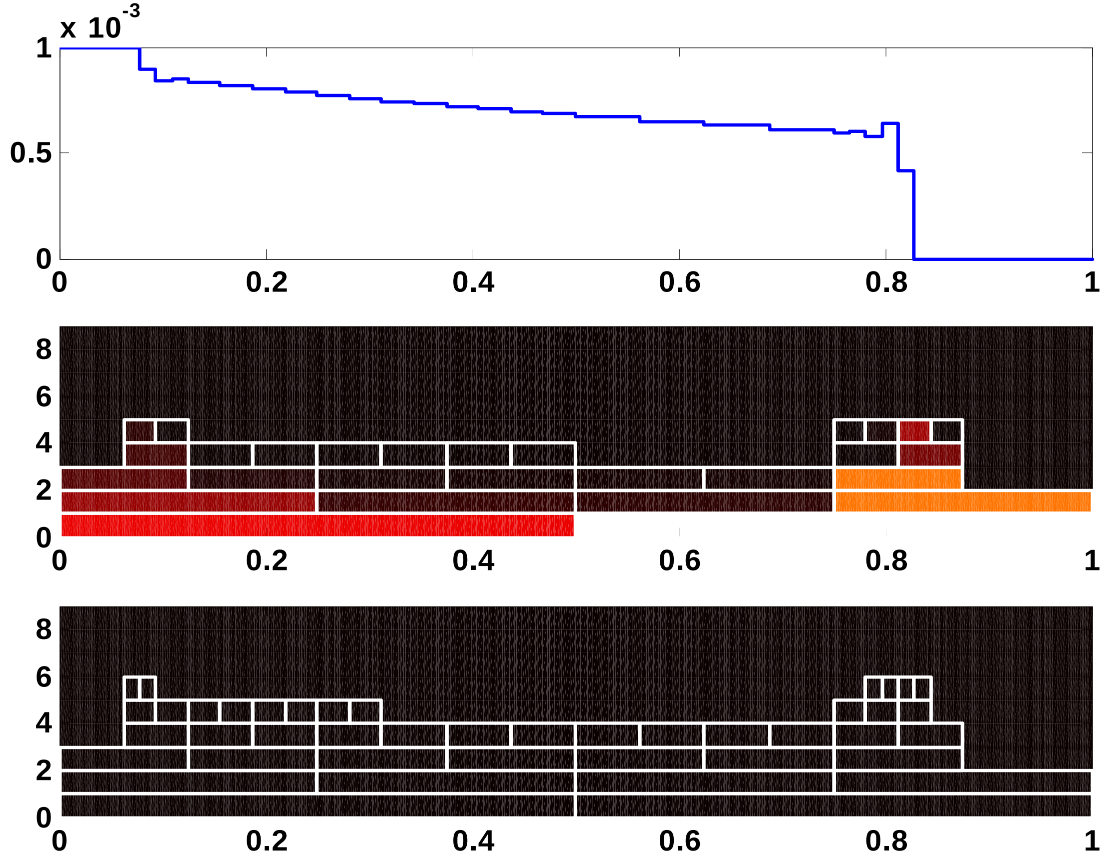


reactions: A+B→C, 2B →C
conditions: semi-batch, isothermal

objective: maximize production of C at given final time t_f
control vars.: feed rate of B
constraints: input bounds, constraints on c_B and c_C at t_f

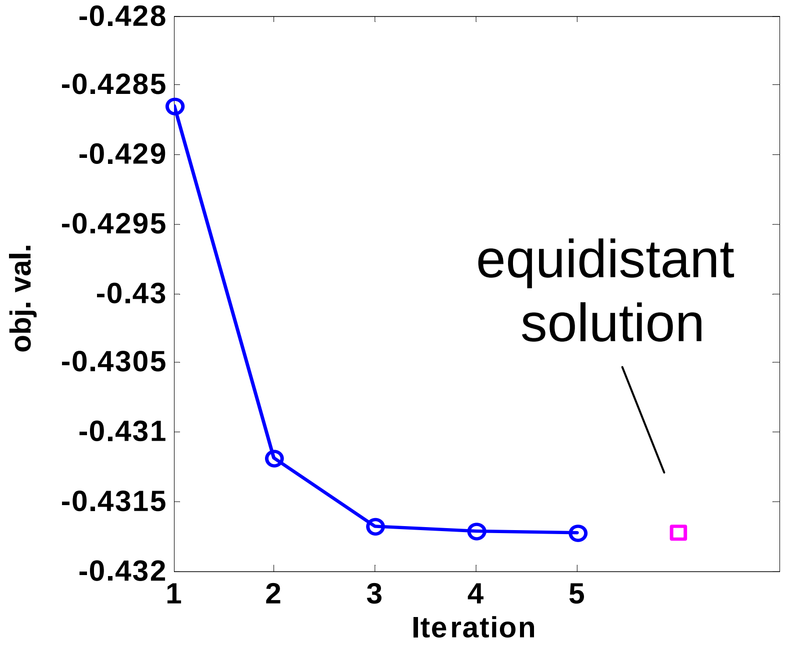
model: 3 differential and 2 algebraic equations

Adaptation Strategy

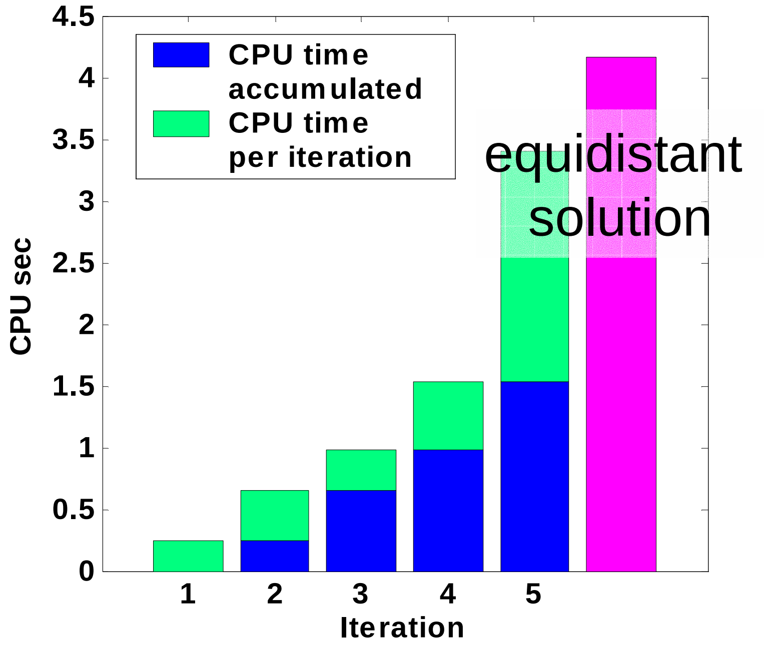


Performance Comparison

objective function value



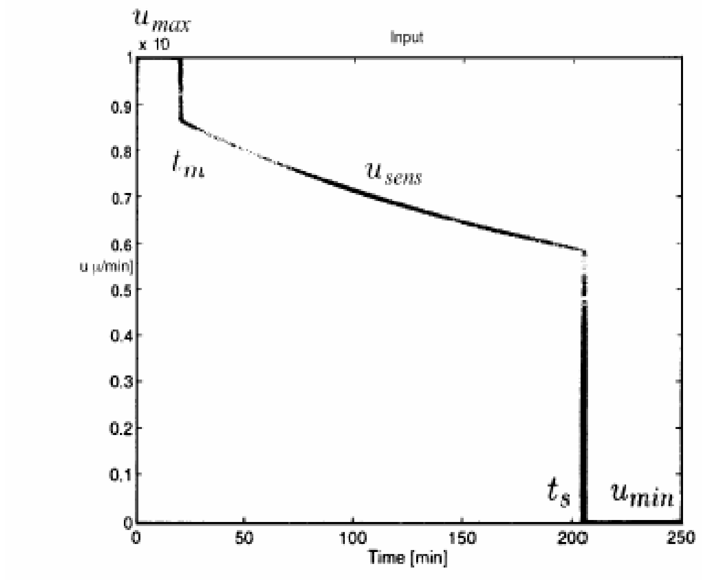
computation time



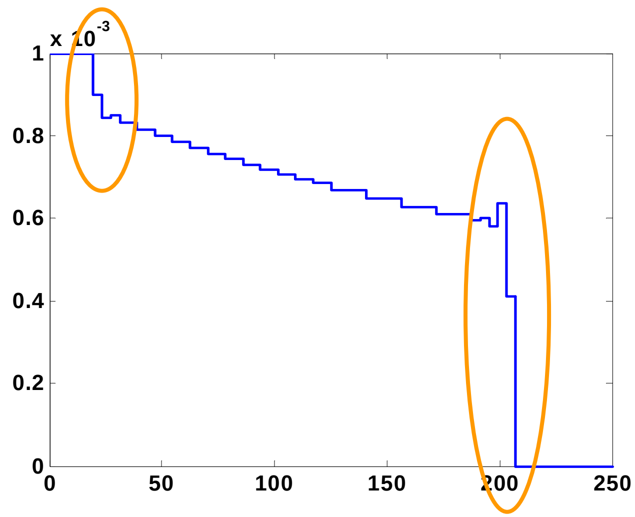
- error-controlled computations
- intermediate results available after short computation times
- favorable for on-line applications

Integration of NCO in Numerical Algorithm

Theoretical Analysis

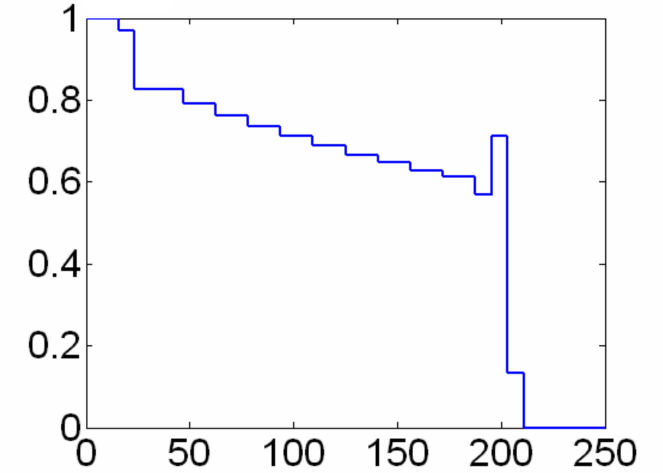


- true solution contains different arcs
- sequence and structure of arcs is determined by necessary conditions of optimality (NCO)
- NCO hard to assess for large nonlinear problems (theory complicated, partly even lacking)

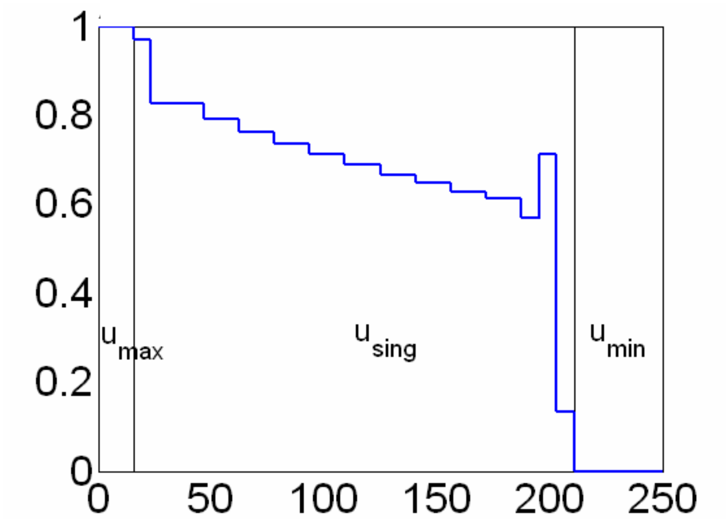


Is there a way to
detect and exploit switching structure
during numerical solution?

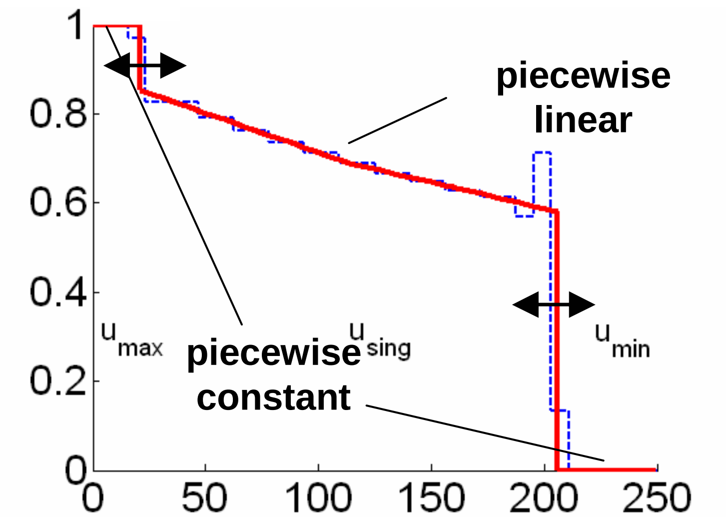
Detection and Exploitation of Solution Structure



1. Solve problem to obtain a (possibly adaptive) *single-stage* solution

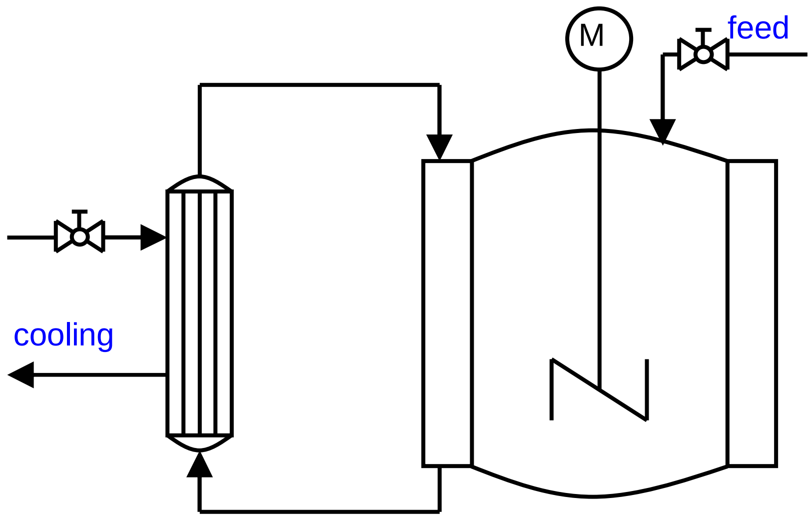


2. Analyze the results of the NLP to determine the different arcs in the solution structure



3. Reformulate as a *multi-stage* problem according to switching structure, resolve the problem with lengths of arc intervals as additional degrees of freedom with adapative algorithm

non-isothermal semi-batch reactor
(Srinivasan et al, 2003)



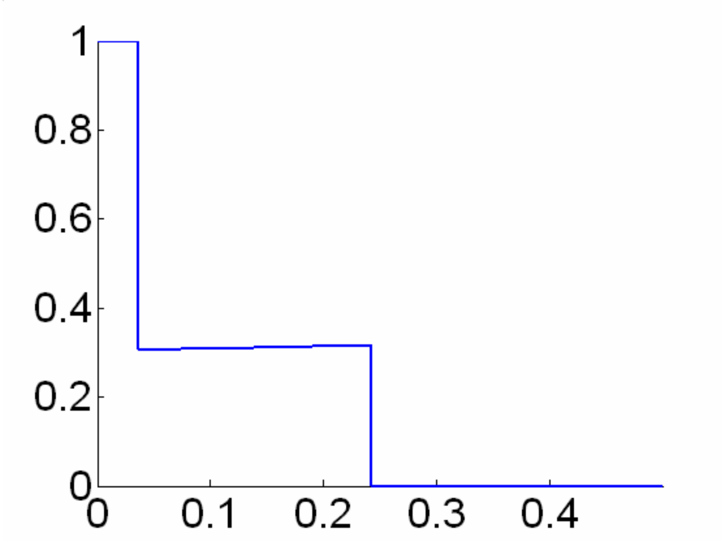
reactions: $A+B \rightarrow C$, $2B \rightarrow C$
conditions: semi-batch, non-isothermal exothermic reaction

objective: maximize production of C at given final time t_f
control vars.: feed rate of B and reactor temperature
constraints: input bounds, constraints on c_B and c_C at t_f

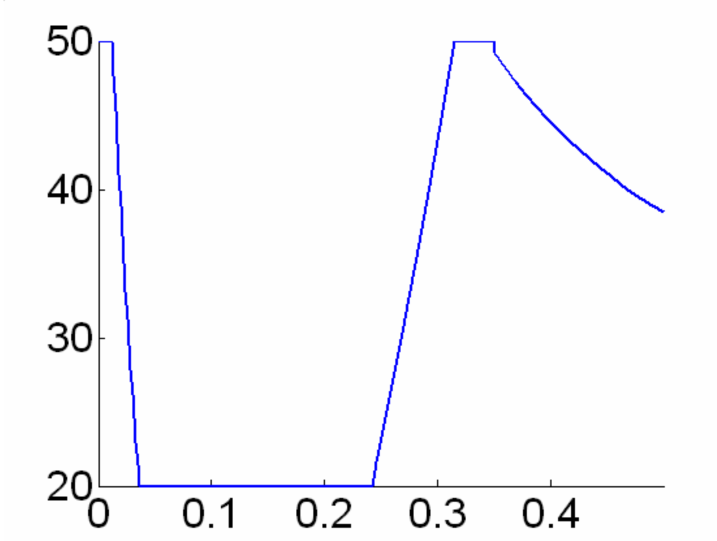
model: 4 differential and 4 algebraic equations

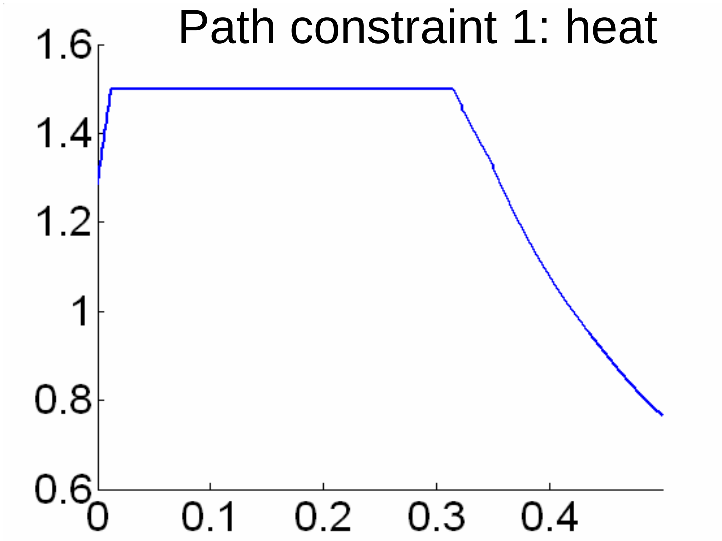
Results

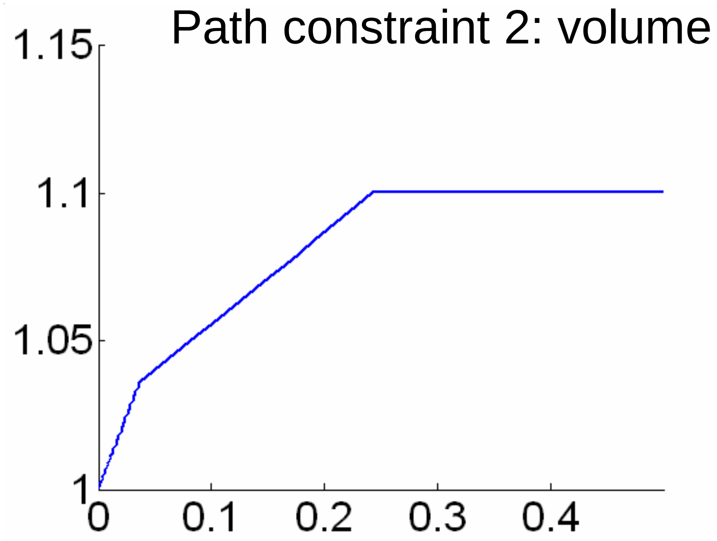
MV 1: Feed rate



MV 2: Temperature







Results

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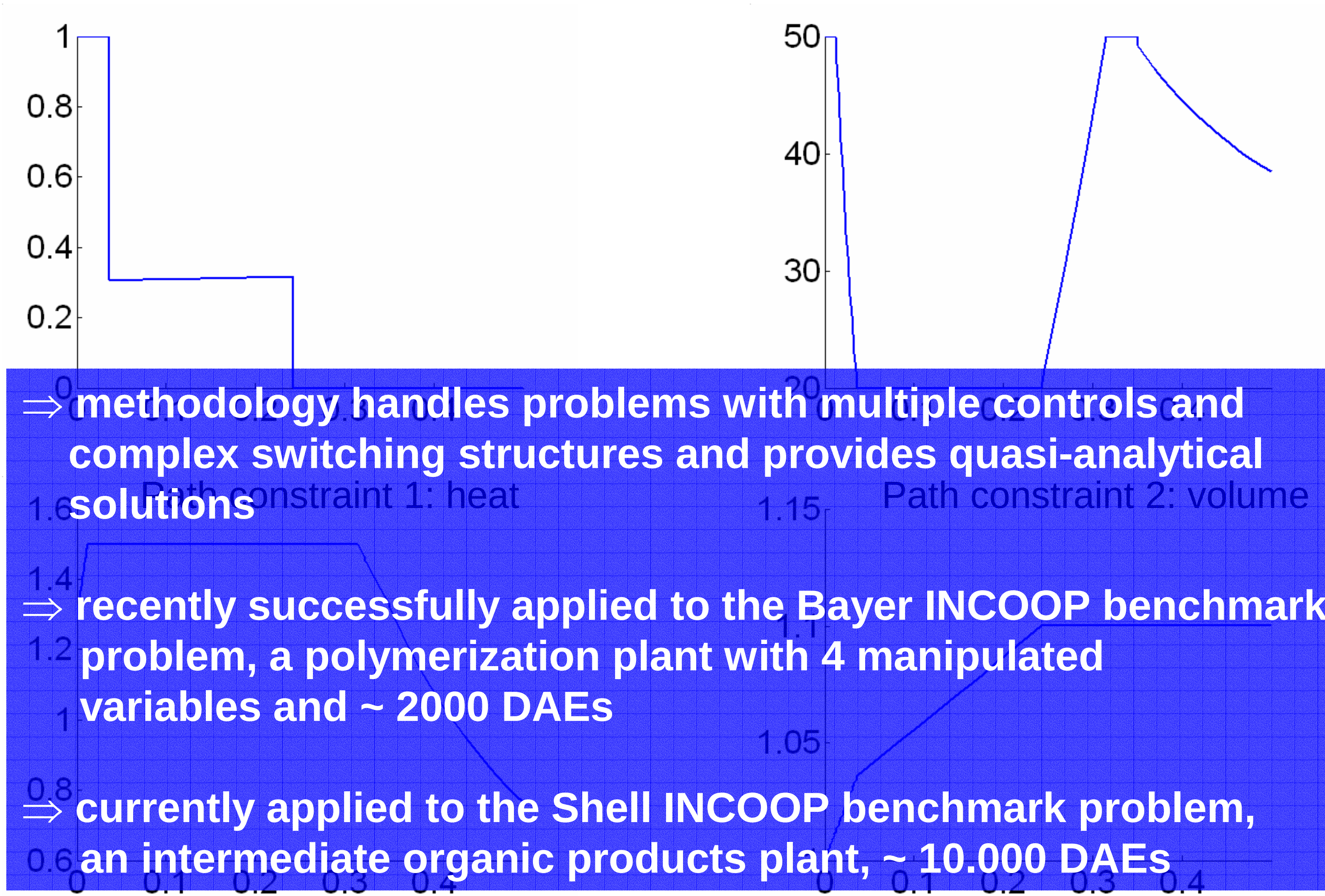
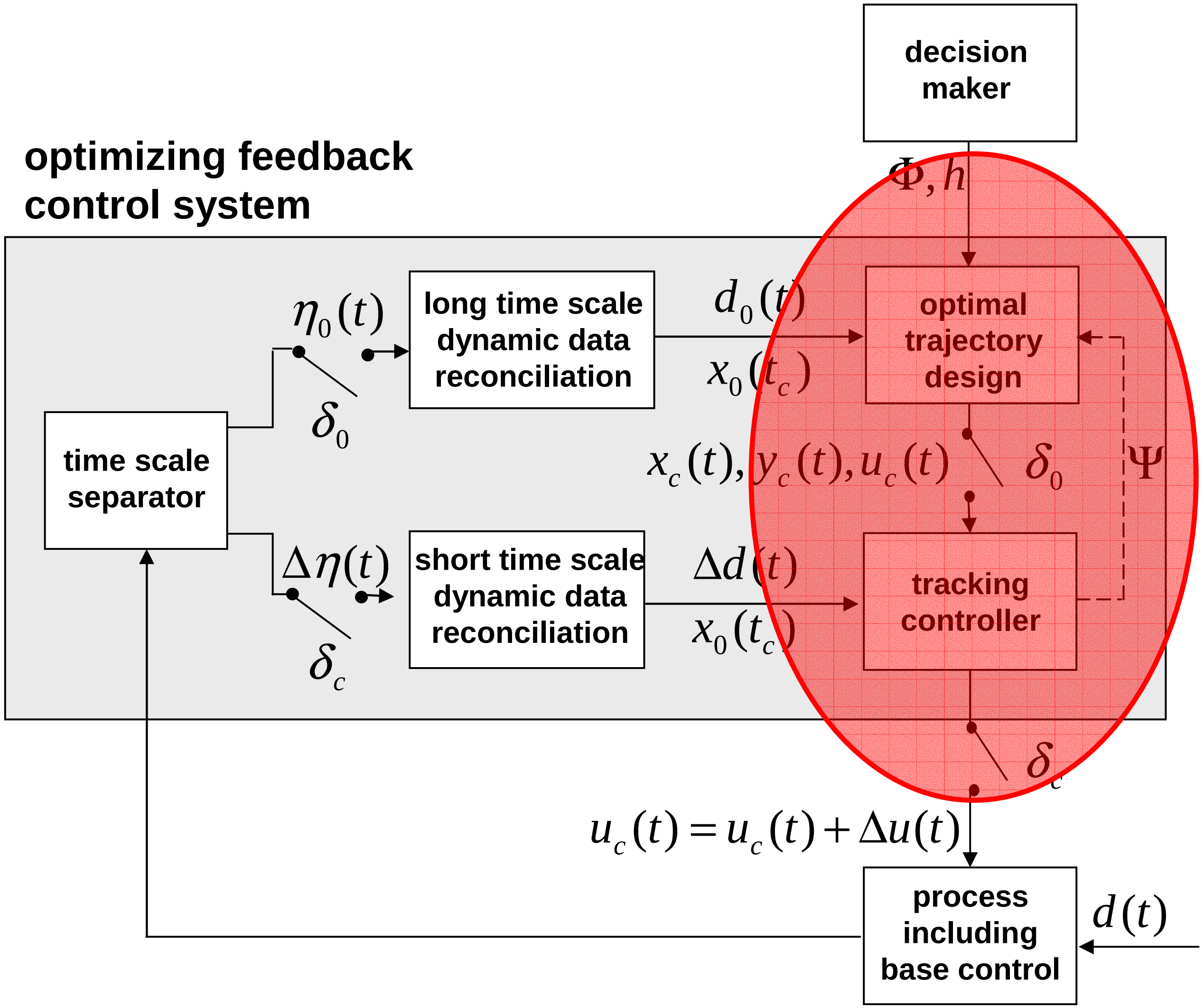


⇒ methodology handles problems with multiple controls and complex switching structures and provides quasi-analytical solutions

⇒ recently successfully applied to the Bayer INCOOP benchmark problem, a polymerization plant with 4 manipulated variables and ~ 2000 DAEs

⇒ currently applied to the Shell INCOOP benchmark problem, an intermediate organic products plant, ~ 10.000 DAEs

Real-time Dynamic Optimization



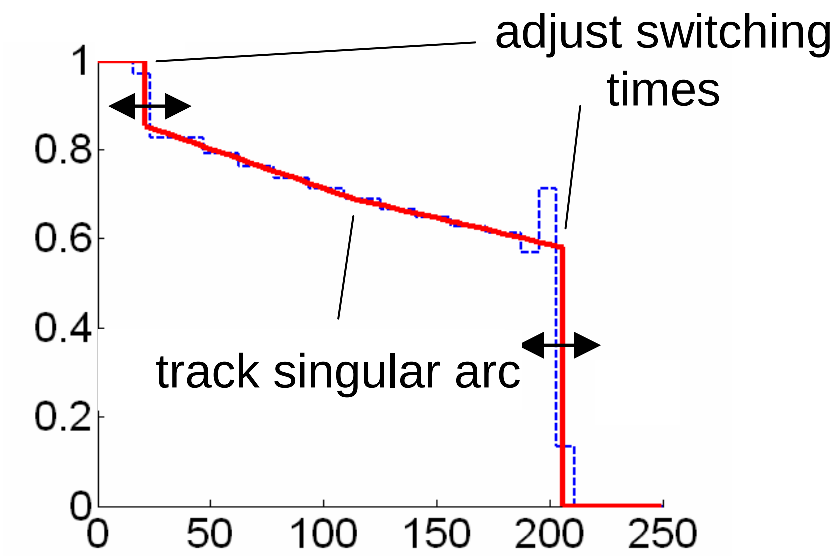
integration of dynamic optimization and model predictive control

- models, formulations, algorithms, ...
- when to trigger an update of trajectory?
- how to account for control performance on optimization level ?
- ...

Alternative 1: NCO Tracking

Bonvin, Srinivasan et al., 2003

- minimal parameterization of the nominal optimal solution: sequence / type of arcs
- assume non-changing switching structure due to uncertainty
- implement a linear multi-variable (decentralized, switching) control system to track the NCO



- supervisory control on dynamic optimization level
  - check potential changes of switching structure
  - quantitatively assess optimality loss
  - trigger dynamic optimization and new switching structure detection

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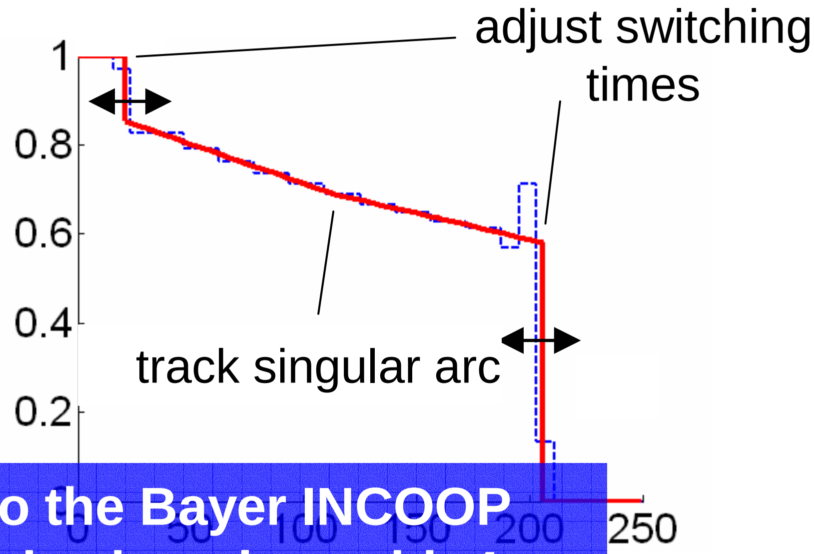

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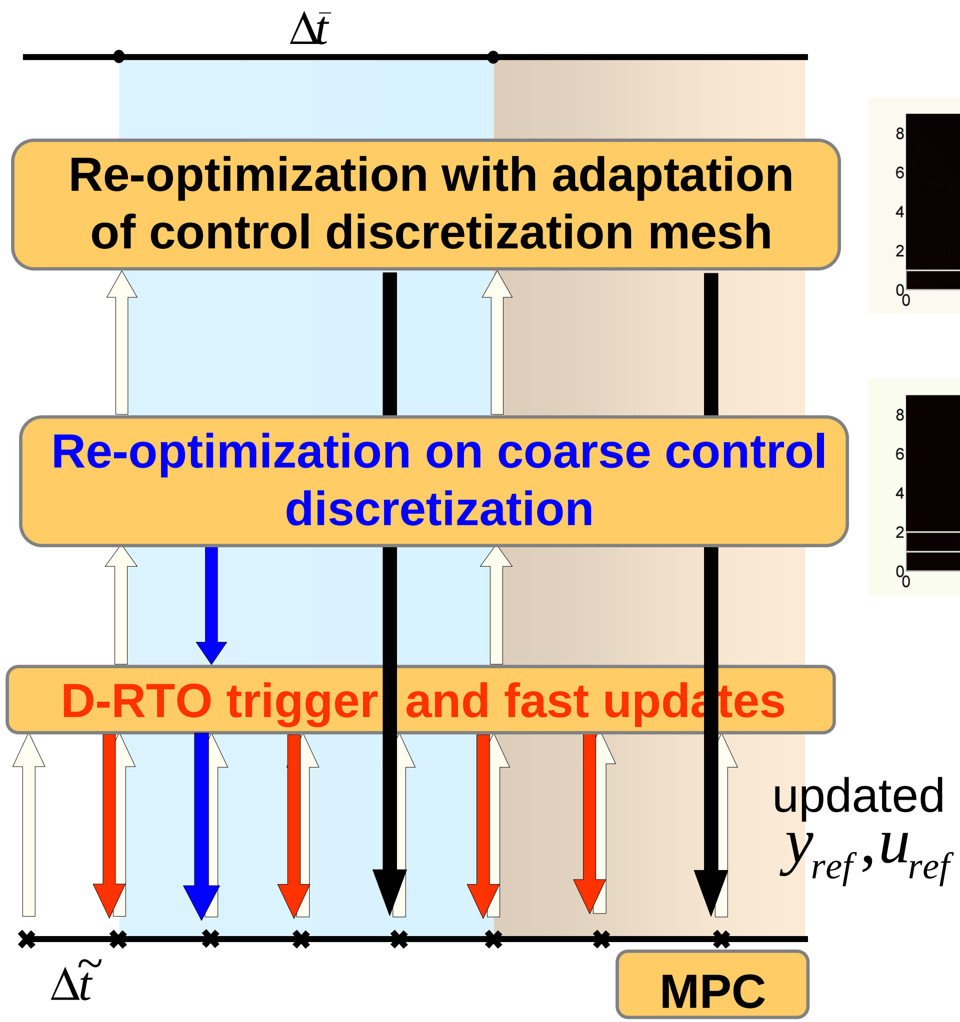
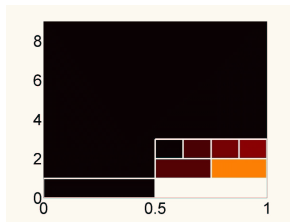
⇒ recently successfully applied to the Bayer INCOOP benchmark problem, a polymerization plant with 4 manipulated variables and ~ 2000 DAEs (joint work with Bonvin et al.)

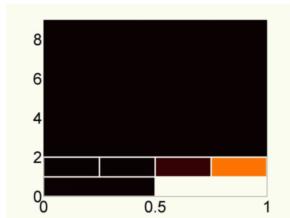
⇒ switching structure changes due to uncertainty, motivation for supervisory level

Alternative 2: LTV-MPC for Trajectory Tracking

dynamic real-time optimization (D-RTO), fast solution updates when possible, even for changing switching structure



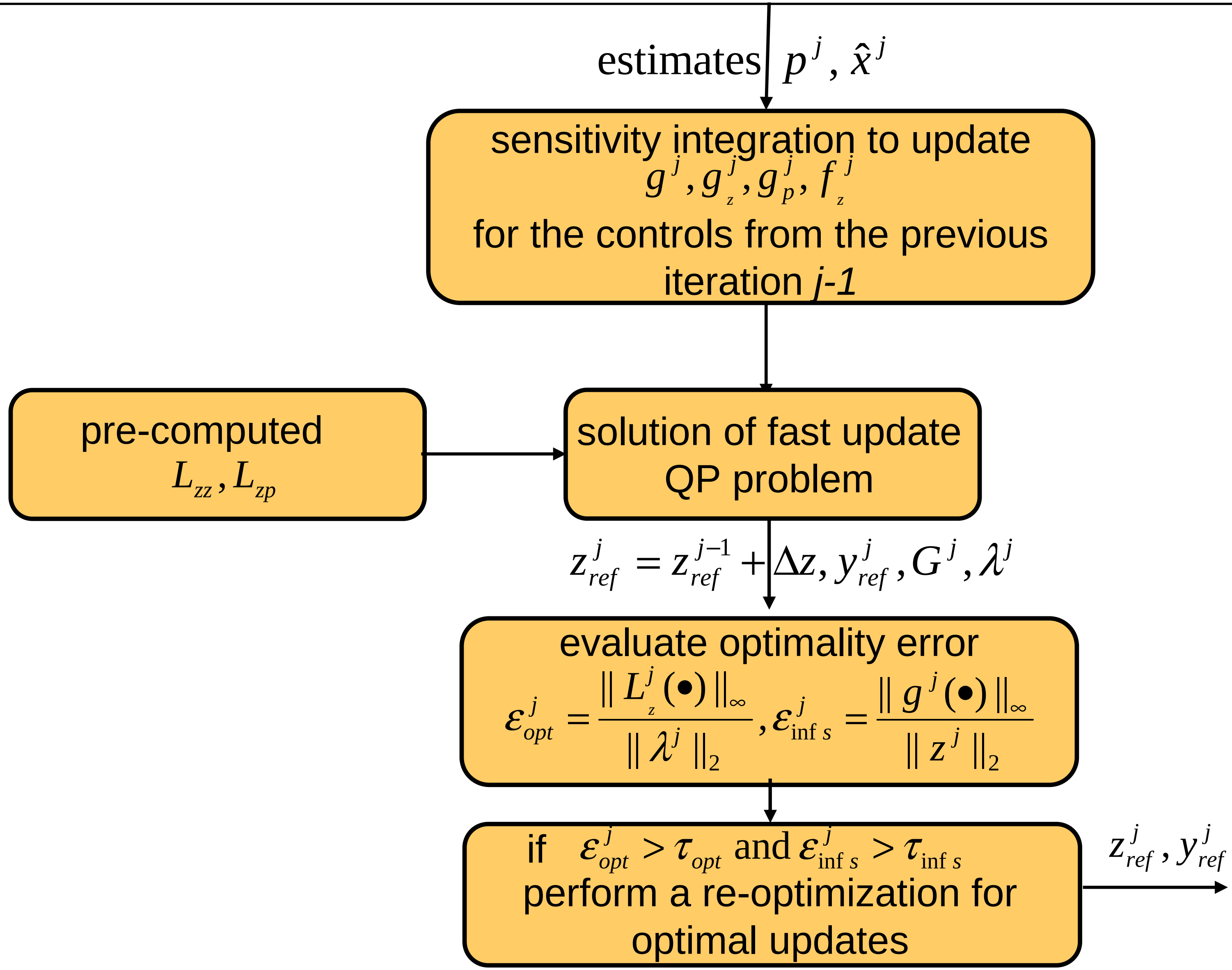




cheap sub-optimal feasible trajectory updates

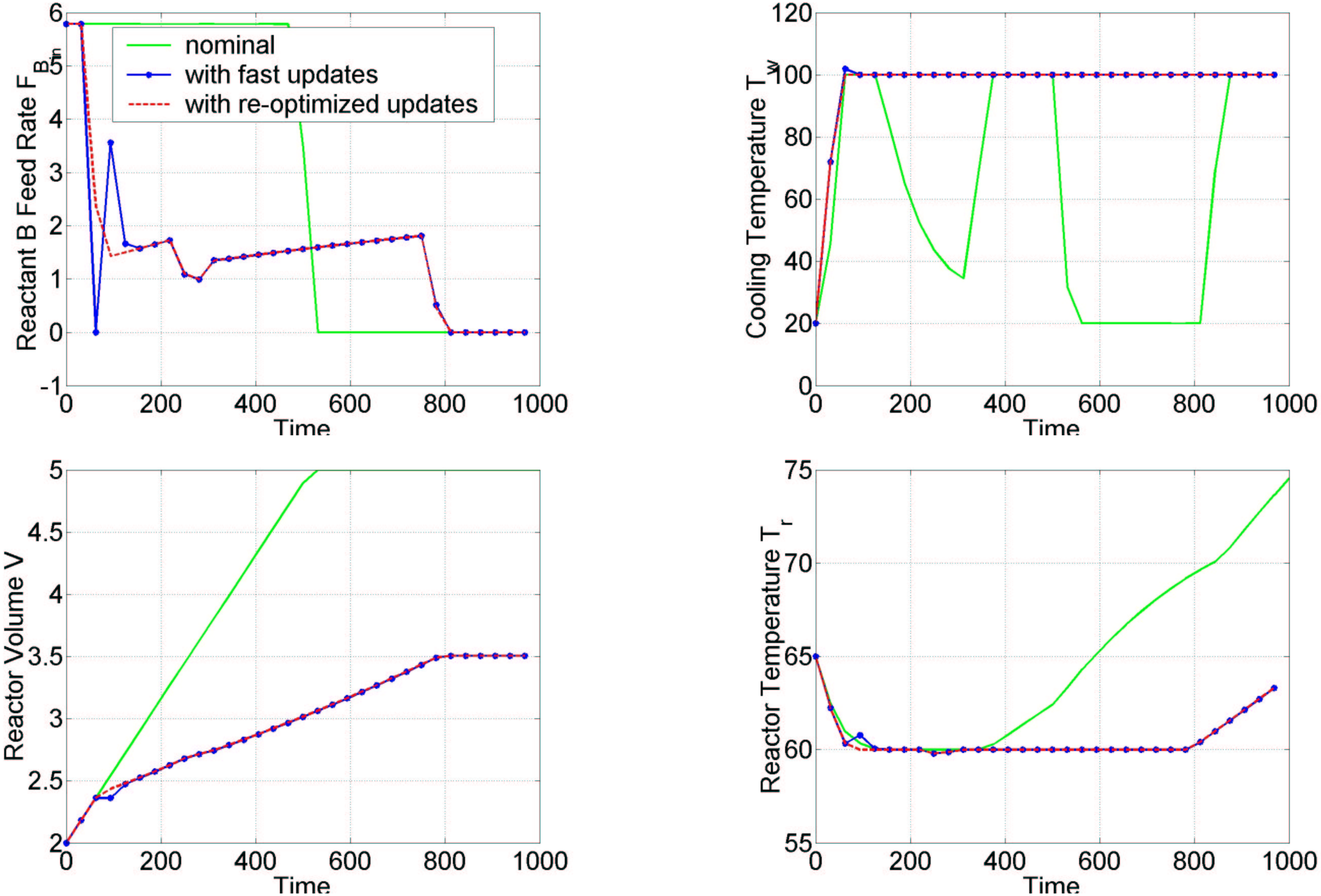
linear time-varying MPC in delta-mode for trajectory tracking, fast time-scale

Fast Update and D-RTO Trigger Algorithm



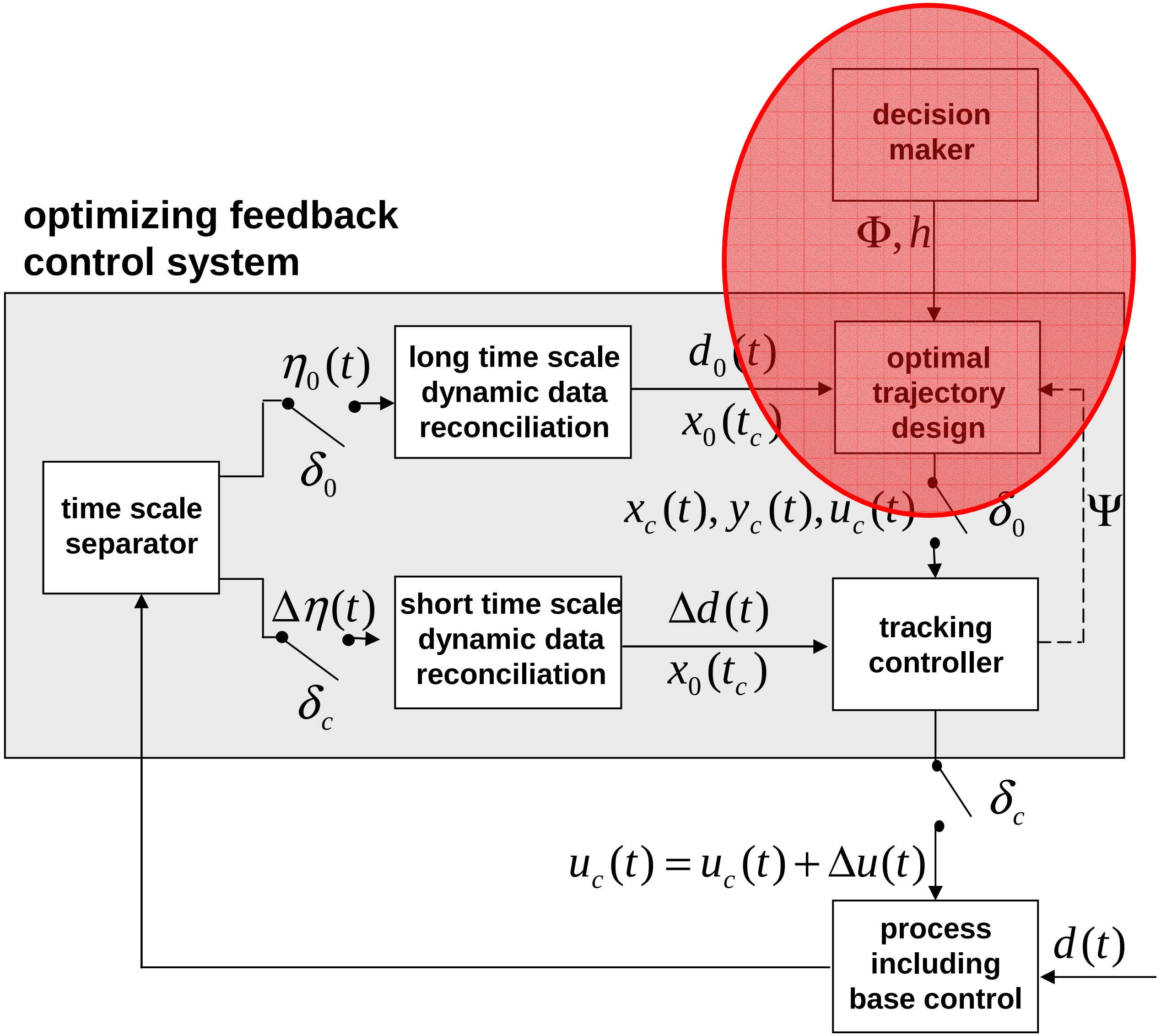
Closed-loop Optimization Results

Williams-Otto semi-batch reactor



$\Delta b_1 = +10\%$ and $\Delta T_{in} = -10^{\circ}\mathrm{C}$ at t = 250 sec

Real-time Planning and Scheduling



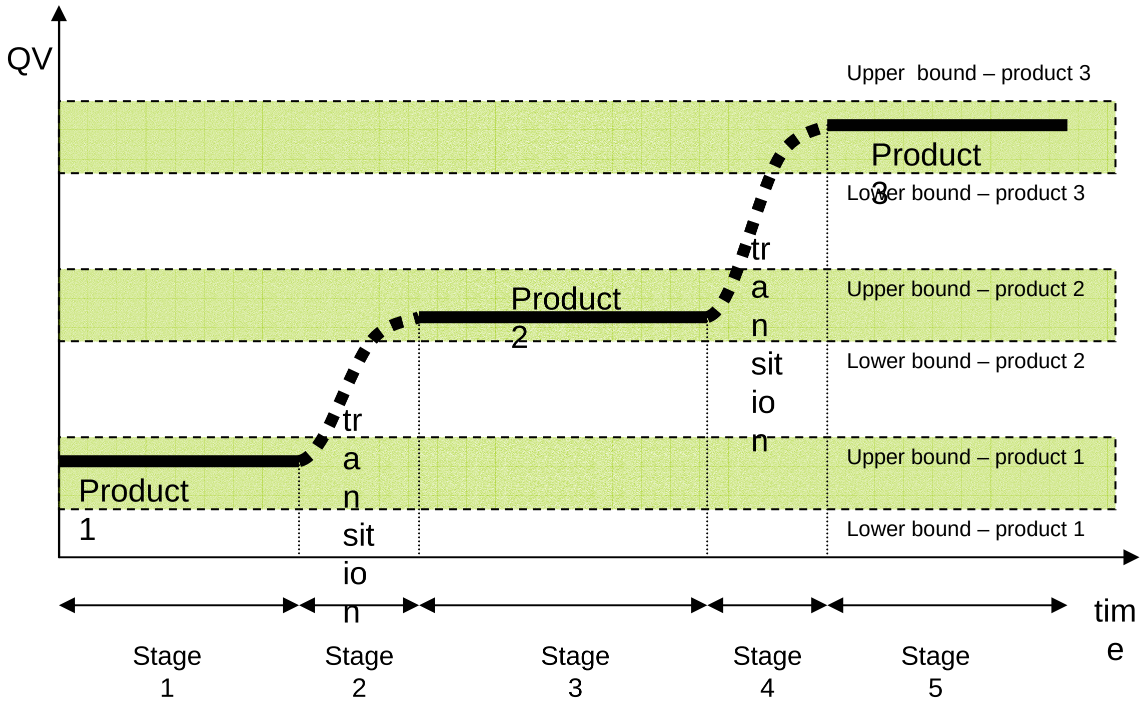
integration of planning & scheduling with model predictive control

- models, formulations, algorithms, ...
- integrated or decomposed problem formulations
- how to account for process performance and uncertainty on the planning level
- ...

An Illustrating Example

a typical problem

- scheduling of different polymer grades production
- optimization of grade transitions



to be cast in a multi-stage dynamic optimization problem with logical constraints (a so-called MLDO problem)

Disjunctive Programming Formulation

- Objective: $\min_{z_k, u_k, p, Y} \quad \Phi := \sum_{k=1}^{n_s} \Phi_k\left(z_k(t_k), p, t_k\right) + \sum_{i=1}^{n_Y} b_i$ **(MLDO)**

- Dynamic model: $s.t. \quad f_k\left(\dot{z}_k, z_k, u_k, p, t\right) = 0, t \in [t_{k-1}, t_k], k \in K,$
- Constraints: $g_k\left(z_k, u_k, p, t\right) \le 0, t \in [t_{k-1}, t_k], k \in K,$
- Initial conditions: $l\left(\dot{z}_0, z_0, p\right) = 0,$
- Stage transition conditions: $z_{k+1}^d(t_k) - m_k\left(z_k(t_k), p\right) = 0, k \in K_m,$

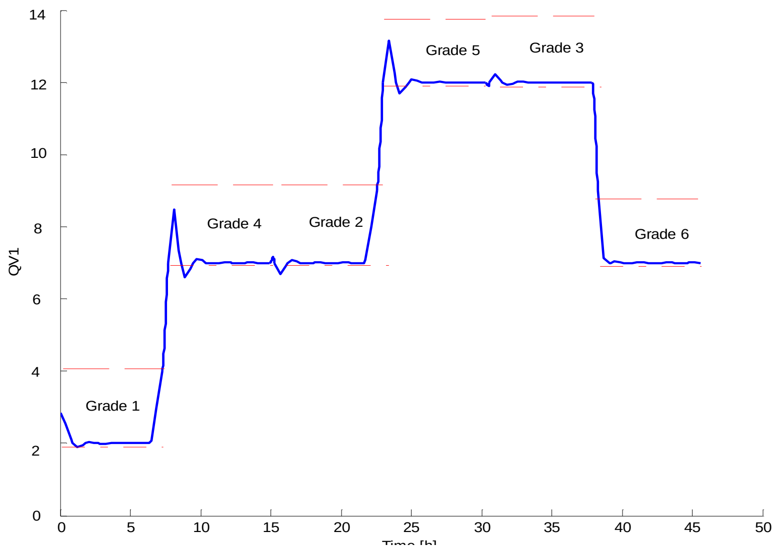
- Disjunctions:

$$\begin{bmatrix} Y_i \\ q_{k,i}\left(\dot{z}_k, z_k, u_k, p, t\right) = 0, \\ r_{k,i}\left(z_k, u_k, p, t\right) \le 0, \\ s_i\left(\dot{z}_0, z_0, p\right) = 0, \\ z_{k+1}^d(t_k) - v_k^i\left(z_k(t_k), p\right) = 0, \\ b_i = \gamma_i, \end{bmatrix} \vee \begin{bmatrix} \neg Y_i \\ B_{k,i}[u_k^T, p^T, \\ z_k(t_{k-1})]^T = 0, \\ b_i = 0, \end{bmatrix}$$

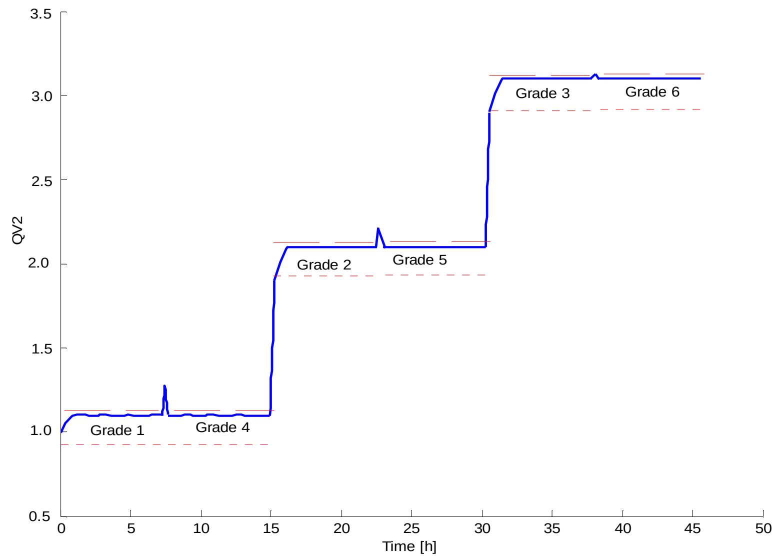
- Propositional logic: $\Omega(Y) = True.$

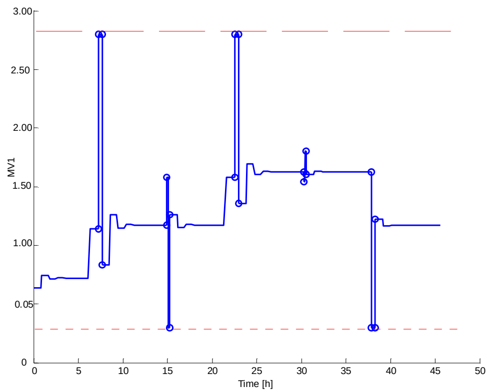
A Sample Result

quality variable 1



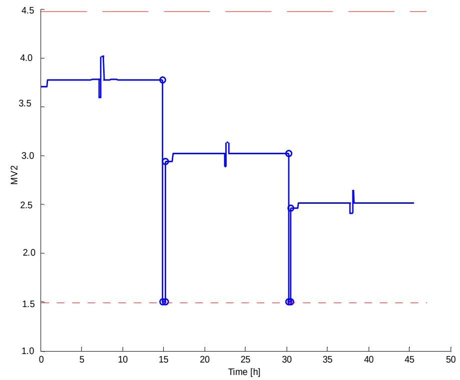
quality variable 2





manipulated variable 1

- polyolefine reactor, ca. 80 DAEs
- six grades production campaign
- no due dates constraints
- MLDO formulation
- solved by disjunctive programming in 4 major iterations in < 5 min CPU
- optimal sequence 1-2-4-6-3-5



manipulated variable 2

Conclusions

- **any-time economically optimal operation**
  - rather than set-point following and disturbance rejection
  - requires real-time business decision making (RT-BDM)

- **RT-BDM problems are dynamic optimization problems**

- RT-BDM **problem formulation, decomposition & analysis** are largely open fields

- dynamic optimization technology is a key enabler
  - how to deal with **uncertainty** ?
  - how to **decompose** and **re-integrate** ?
  - how to provide **consistent models** on different time-scales ?

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great opportunities for Systems and Control Community in theory and applications

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