AACHENER VERFAHRENSTECHNIK

HD–MPC

Dynamic Real-Time Optimization

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AVT – Process Systems Engineering

RWTH Aachen University

HD-MPC Industrial Workshop

June 24, 2011

Leuven, Belgium

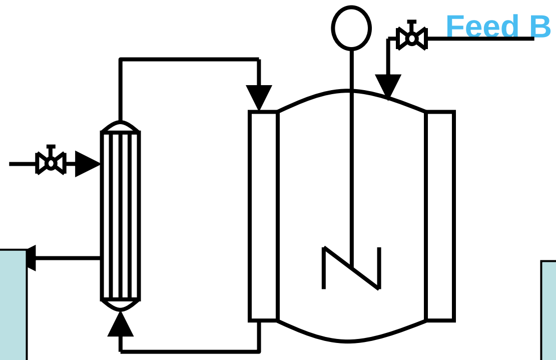
RWTH

Two „Optimisation Strategies“

What is the best feed rate B?

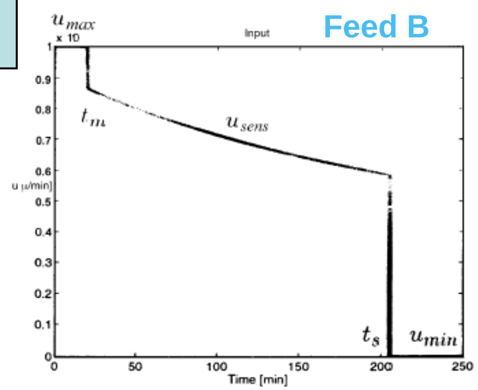
Simulation

Optimisation



Strategy 1:

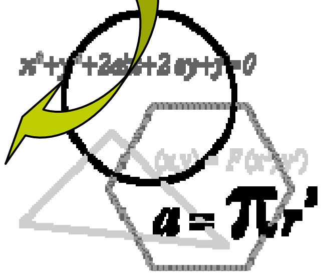
- Determine optimal and feasible feed rate by trial and error
- Study various trajectories by dynamic simulation scenarios
- Unsystematic approach, high human effort



“Exact” solution (Srinivasan et al., 2003)

Strategy 2:

- Determine optimal and feasible feed rate by means of dynamic optimisation
- Dynamic optimiser systematically searches for the best trajectory
- Systematic and efficient approach

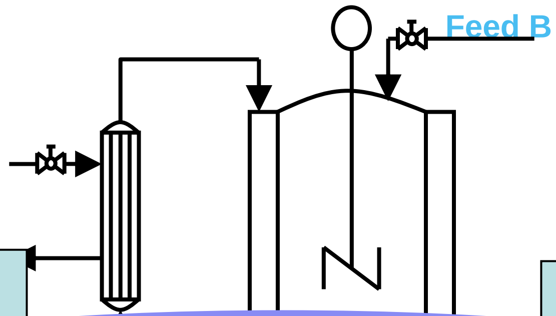


Two „Optimisation Strategies“

What is the best feed rate B?

Simulation

Optimisation



Strategy 1:

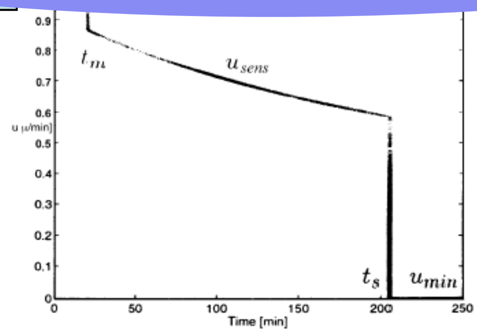
- Determine optimal and f… feed rate b…
- Stu… dyn…
- Unsystema… hu… effort

Strategy 2:

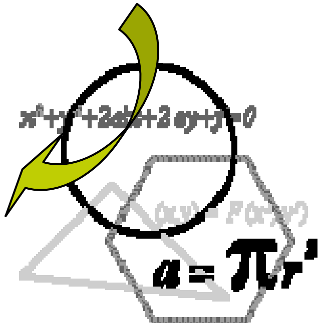
- …timal and feasible …lynamic
- …tically …rajectory
- …ystematic and efficient approach

Replace human effort by numerical algorithms!

Solve the inverse problem directly !



“Exact” solution (Srinivasan et al., 2003)



Outline

- Problem formulation for economically optimal control problems
- Efficient solution methods for optimal control problems
  - adaptive grid refinement
  - structure detection
  - software realization
- Optimal control online – Dynamic Real-Time Optimization (DRTO)
  - hierarchical MPC – time-scale decomposition
  - suboptimal NMPC – Neighboring Extremal Updates
  - software realization
- Distributed MPC – a new approach for DRTO

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Some Sample Problems

Large-scale industrial process (Shell):

- How fast can an intermediate chemicals plant be moved from operating point A to B ?

Olefine polymerization process (Novolen):

- Can we decide on a production schedule and optimize grade transitions simultaneously ?

Membrane bioreactor for waste water treatment (Koch Membrane Systems):

- Can we minimize energy demand and reduce membrane stress in real time?

Styrene-butylacrylate co-polymerization (BASF):

- Is real-time optimization ready for use in the chemical industries to increase productivity and improve process operability?

Mathematical Problem Formulation

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

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

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. specs.)

decision variables:

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

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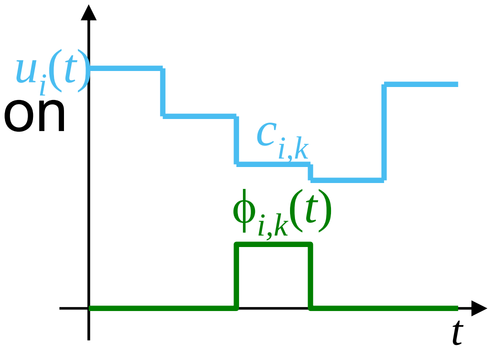
Sequential Solution Strategy

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)

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

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

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

DAE system solved by underlying numerical integration

Gradients for NLP solver typically obtained by integration of sensitivity systems

How to keep number of sensitivity integrations low?

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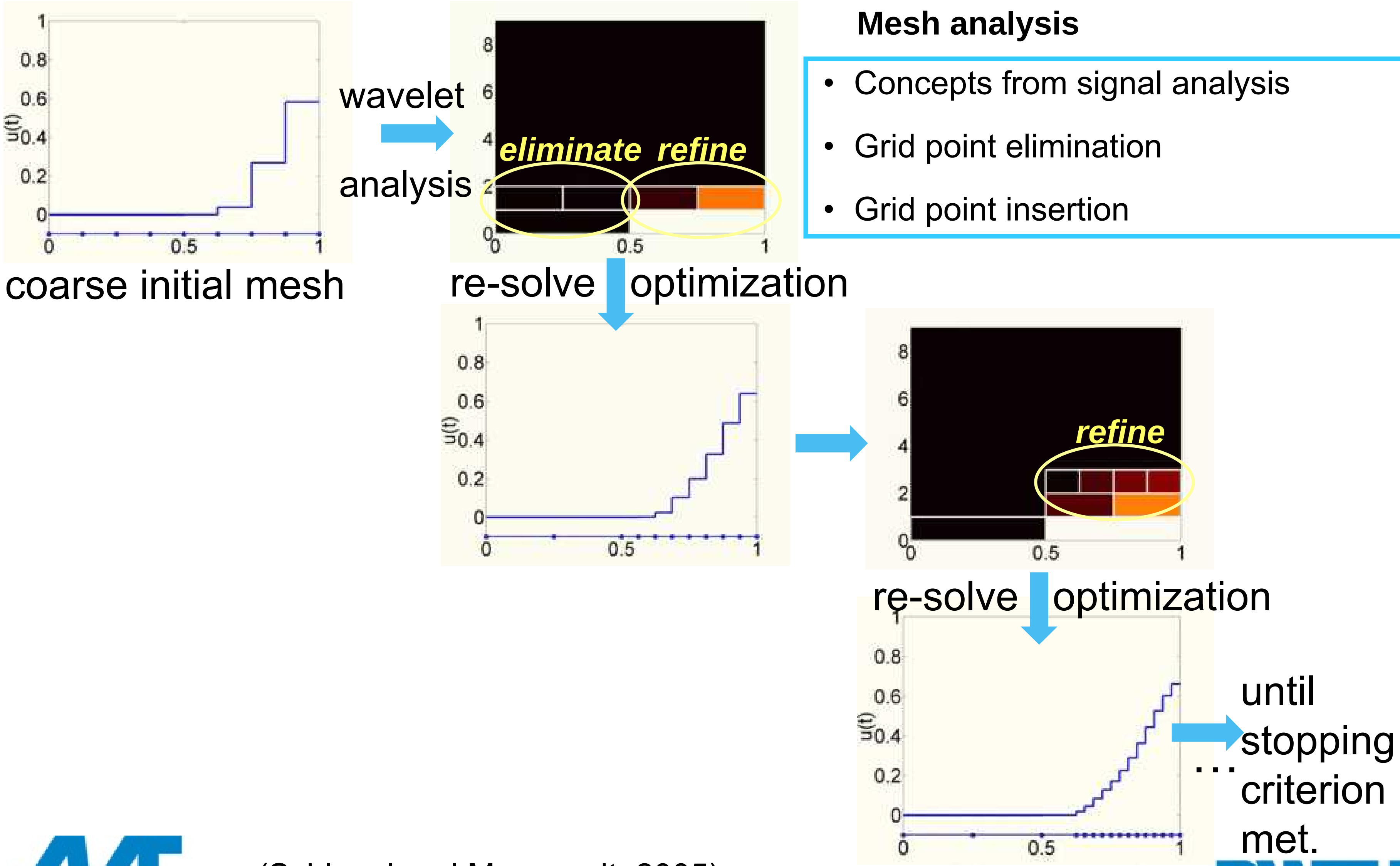
Adaptive Refinement of Control Parameterization

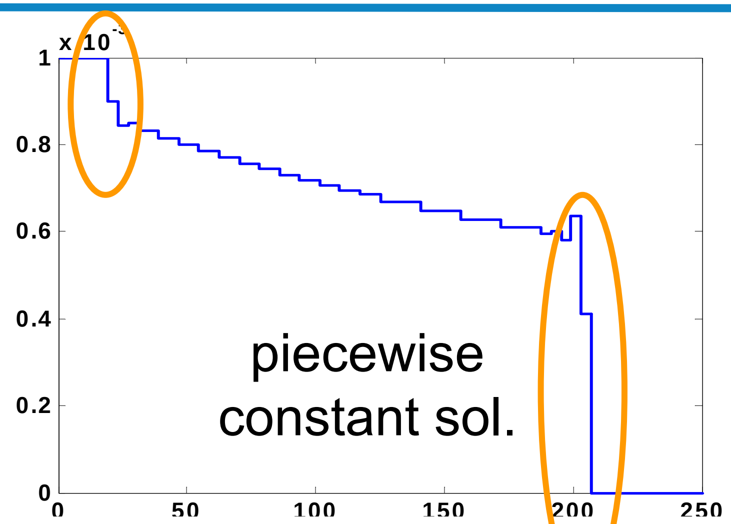
Mesh analysis

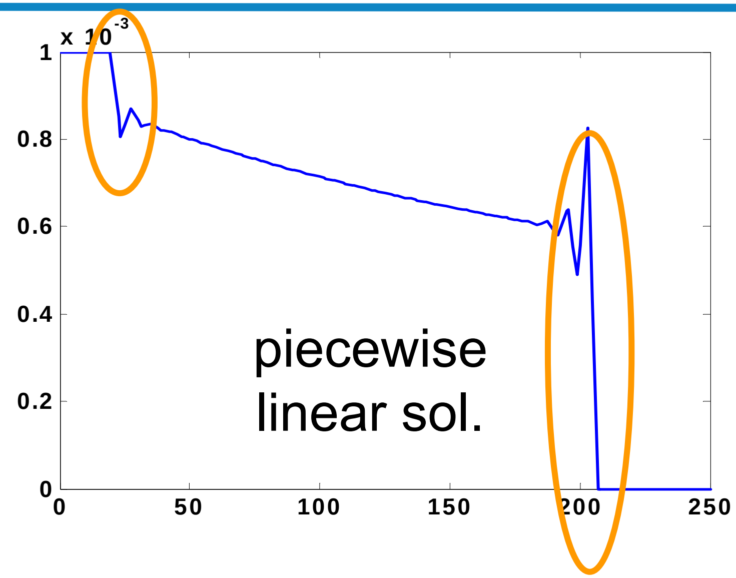
- Concepts from signal analysis
- Grid point elimination
- Grid point insertion

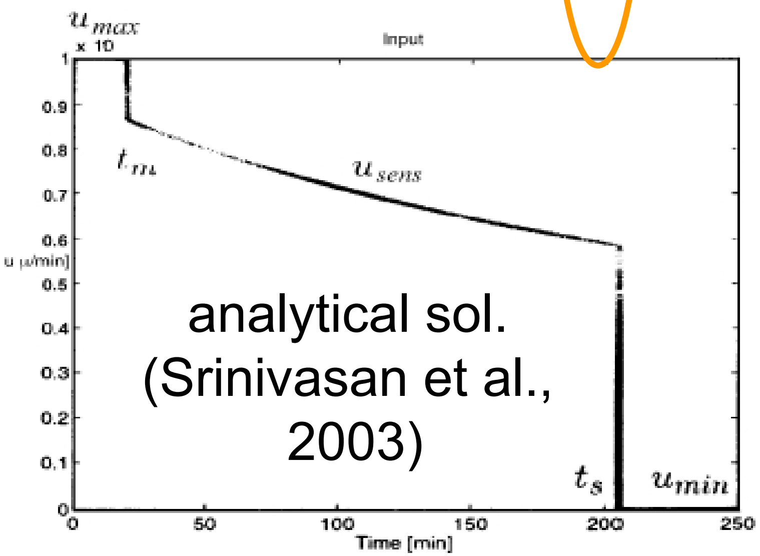


(Schlegel and Marquardt, 2005)

A typical input trajectory …





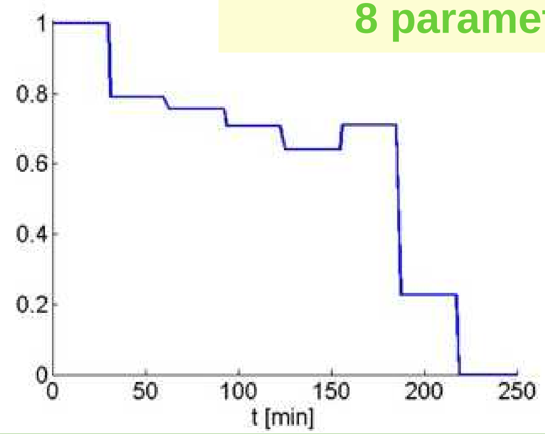


Obvious open issues

- how to capture switching points?
- how to avoid over-parameterization?

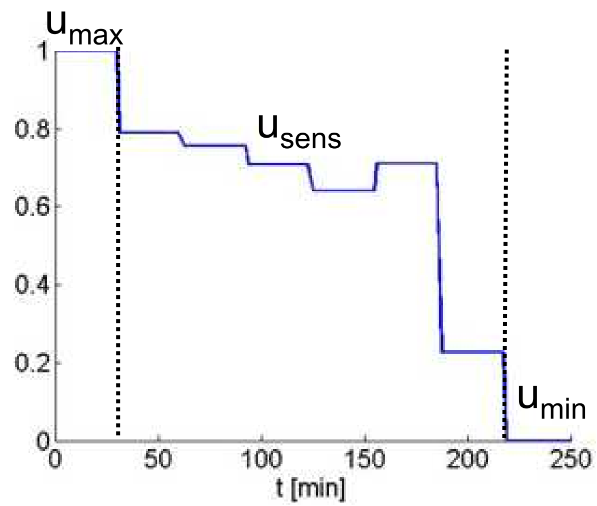
Is there a way to **detect switching structure** from numerical solution?

Switching Structure Detection

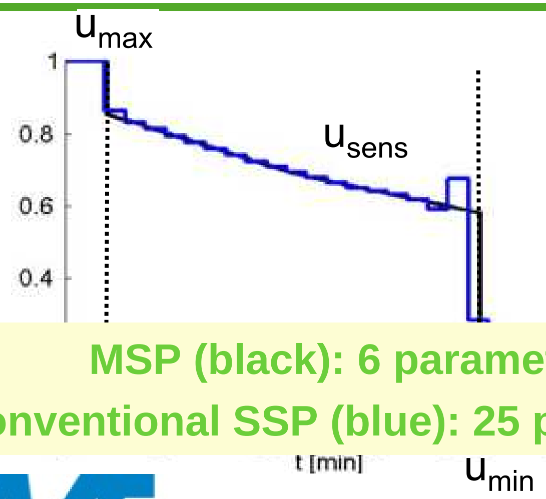


8 parameters

1. Solve coarsely discretized *single-stage* problem (SSP)



2. Determine the switching structure from NCO of NLP



3. Reformulate as a *multi-stage* problem (MSP) according to switching structure

MSP (black): 6 parameters!

Conventional SSP (blue): 25 parameters!

(Schlegel and Marquardt, 2006)

Does it Work? – Let's Try …

Continuous Polymerization Process (Bayer AG, Dünnebier et al., 2004)

- complex reaction mechanism
- large-scale model (~ 2000 equations)
- 3 input variables, 6 path constraints

process operation tasks:
- optimal load change
- optimal grade change

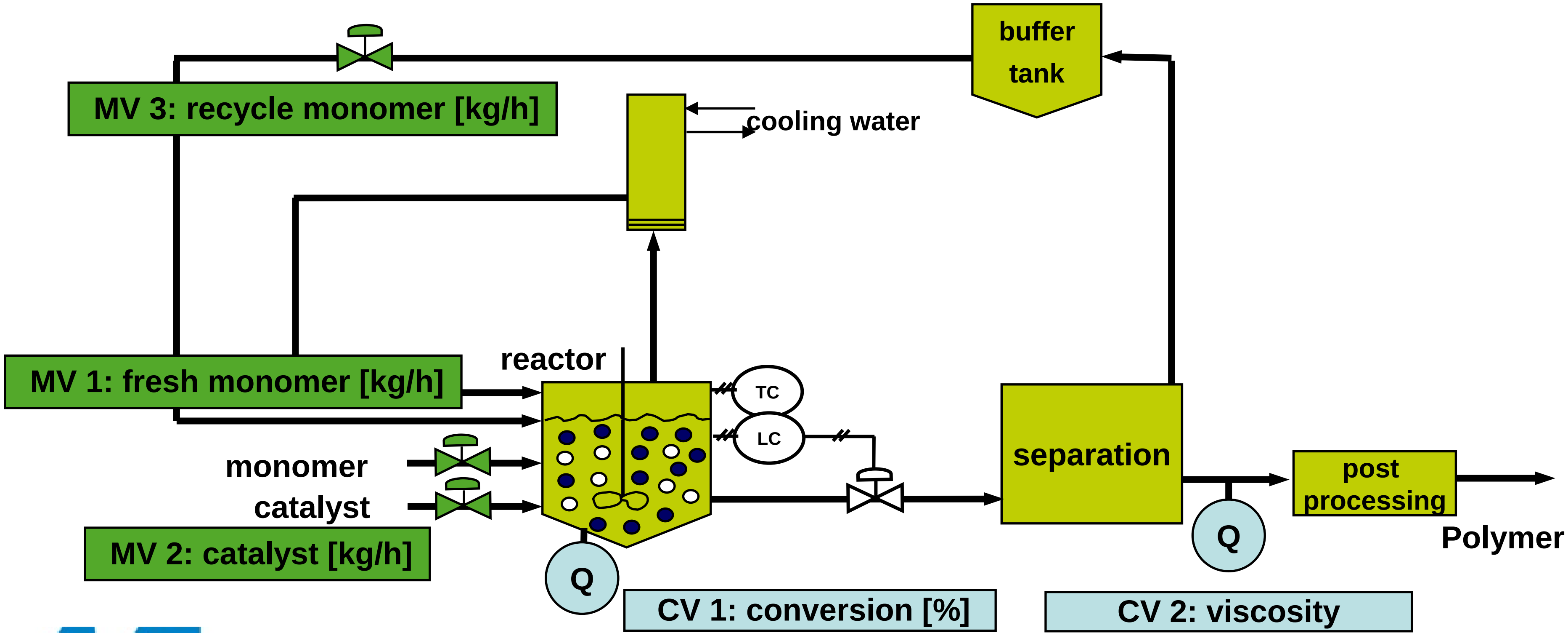
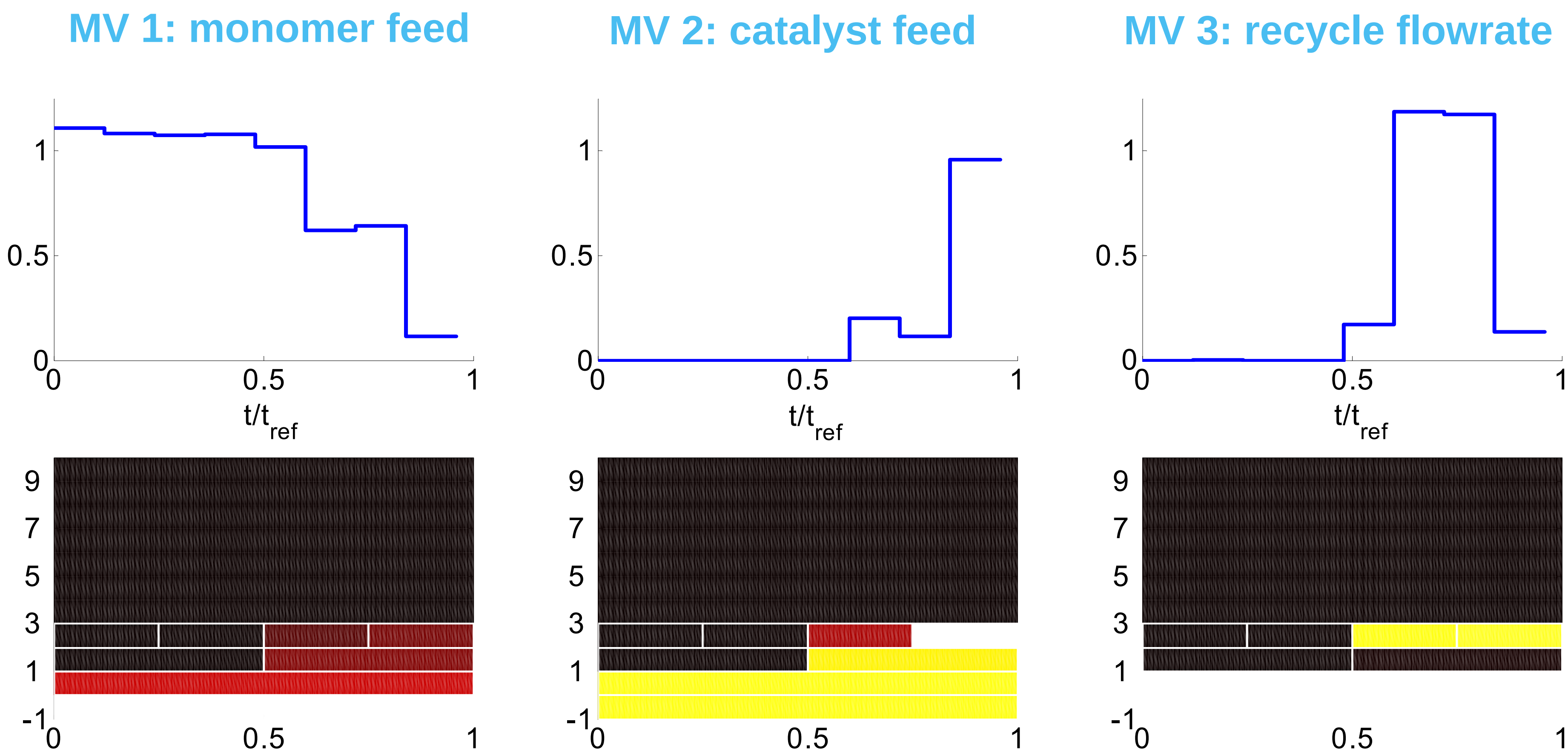


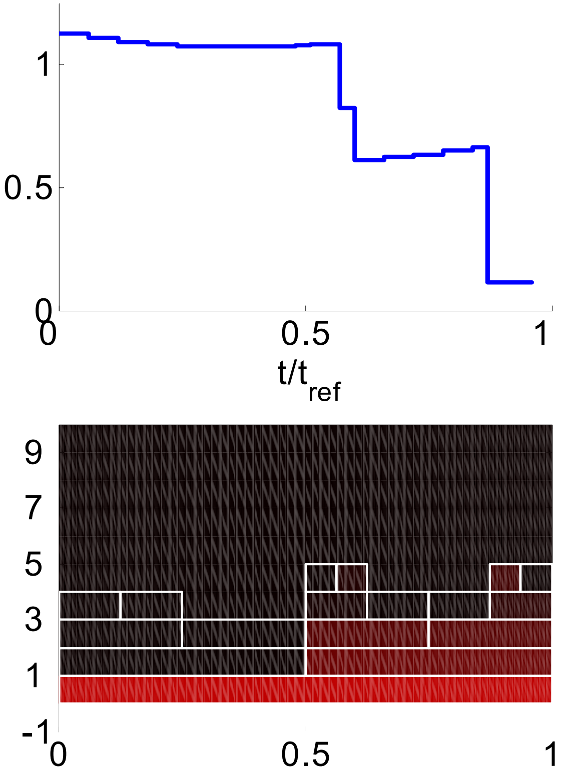
Illustration of Adaptation Strategy



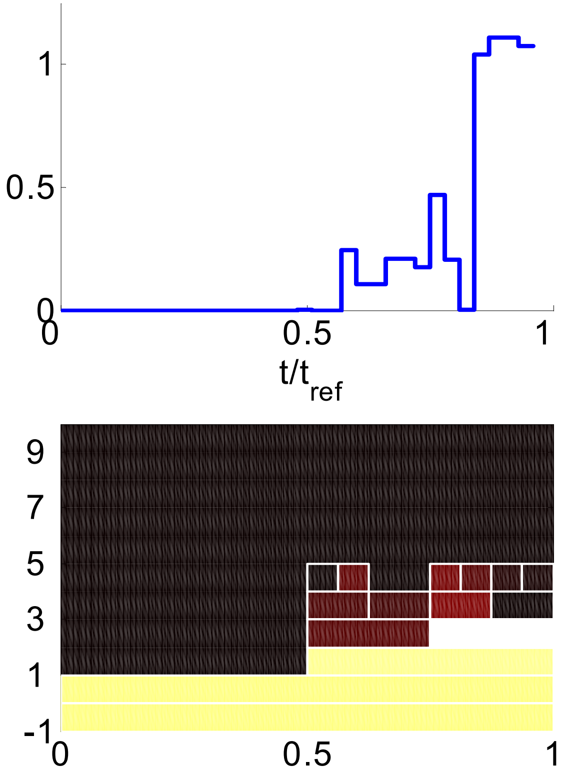
Iteration 1

Illustration of Adaptation Strategy

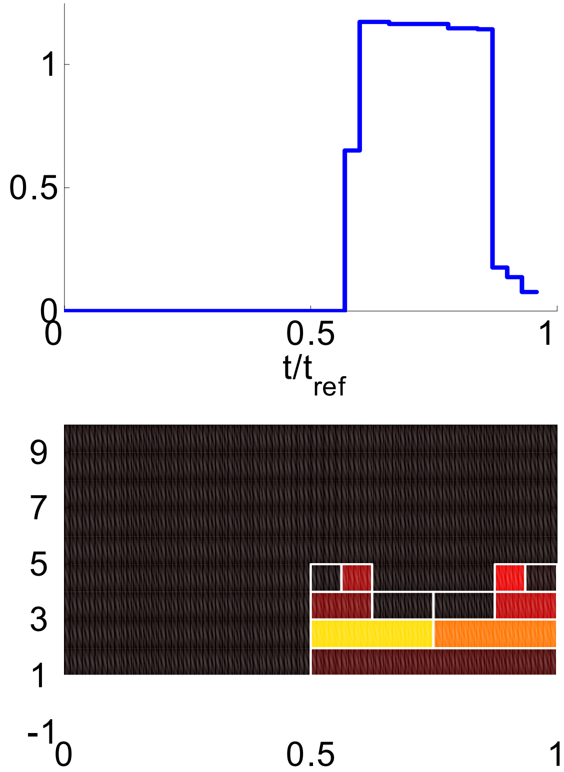
MV 1: monomer feed



MV 2: catalyst feed



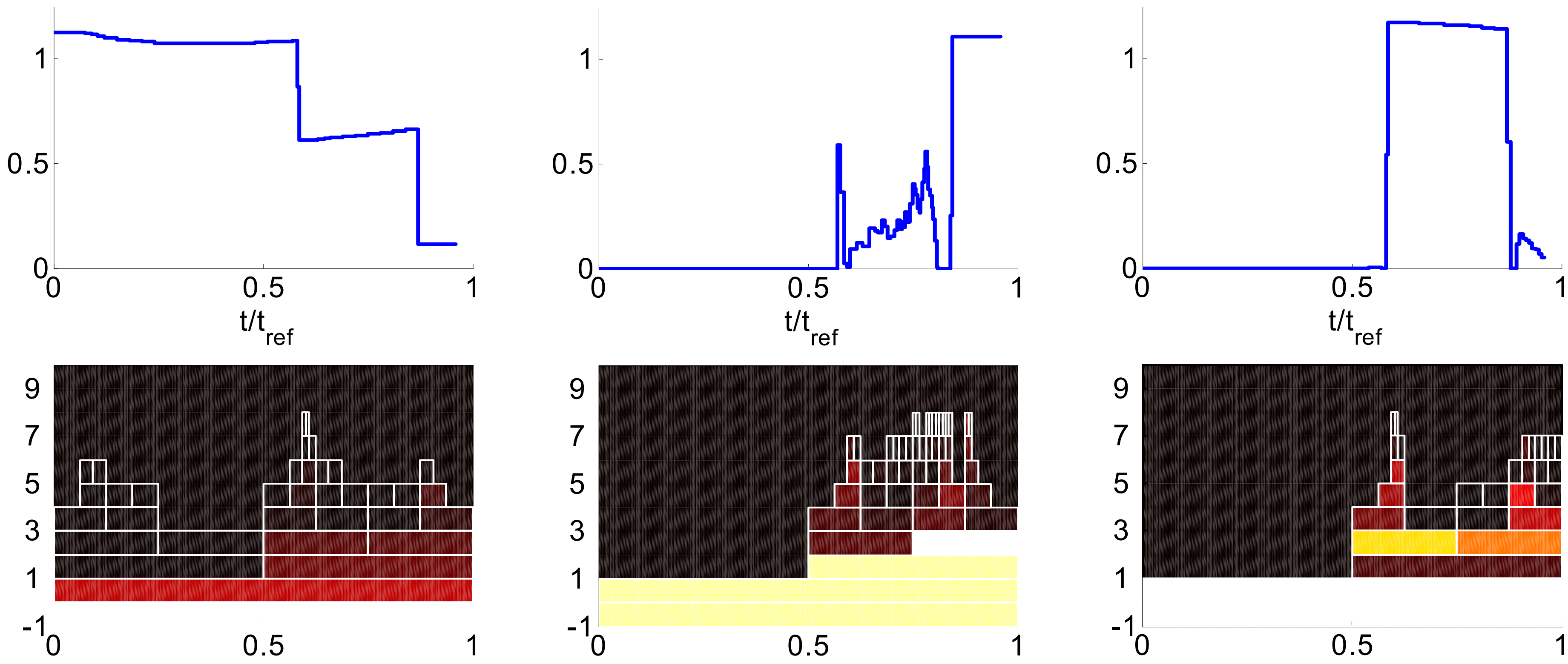
MV 3: recycle flowrate



Iteration 3

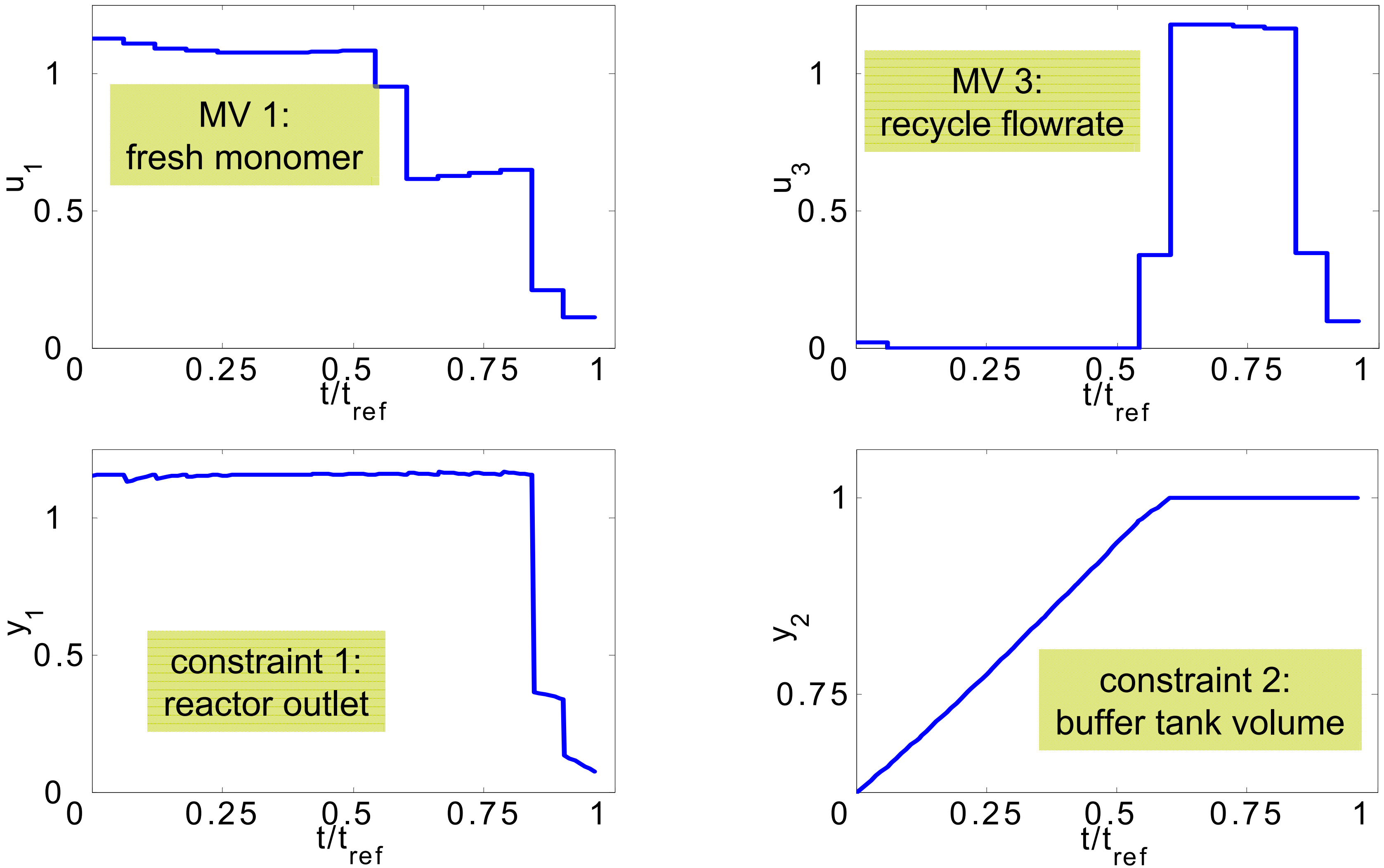
Illustration of Adaptation Strategy

MV 1: monomer feed | MV 2: catalyst feed | MV 3: recycle flowrate

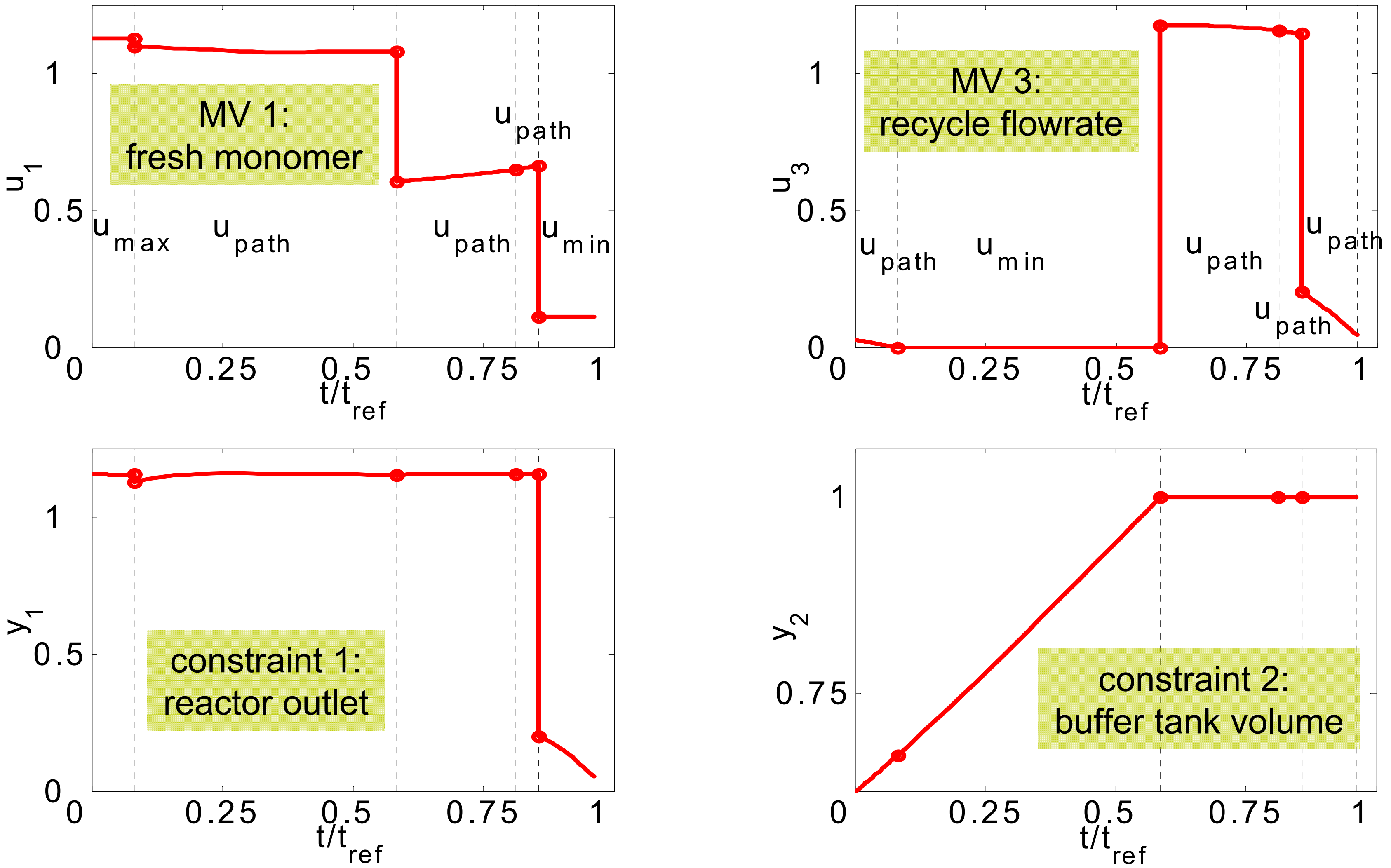


Iteration 6

Non-adaptive Algorithm

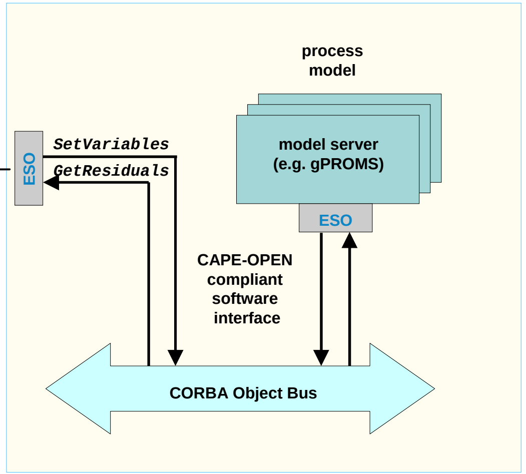


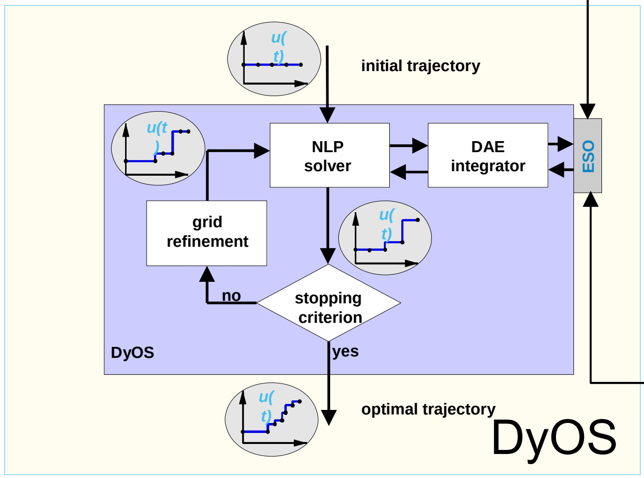
Adaptive Algorithm with Structure Detection

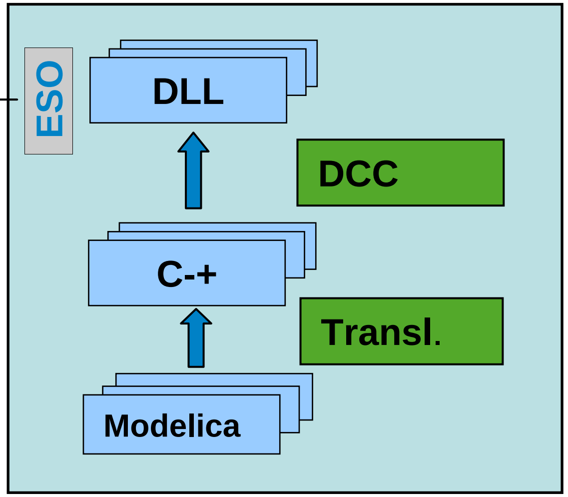


DyOS – Dynamic Optimization System

gPROMS
(PSE Ltd.)







AC-SAMMM (joint work with Uwe Naumann, RWTH Aachen):

Structured **A**utomatic **M**anipulation of **M**athematical **M**odels (Poster Session)

Modelica: Open source object-oriented modeling language

http://wiki.stce.rwth-aachen.de/bin/view/Projects/ERS/WebHome

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- **Optimal control online – Dynamic Real-Time Optimization (DRTO)**
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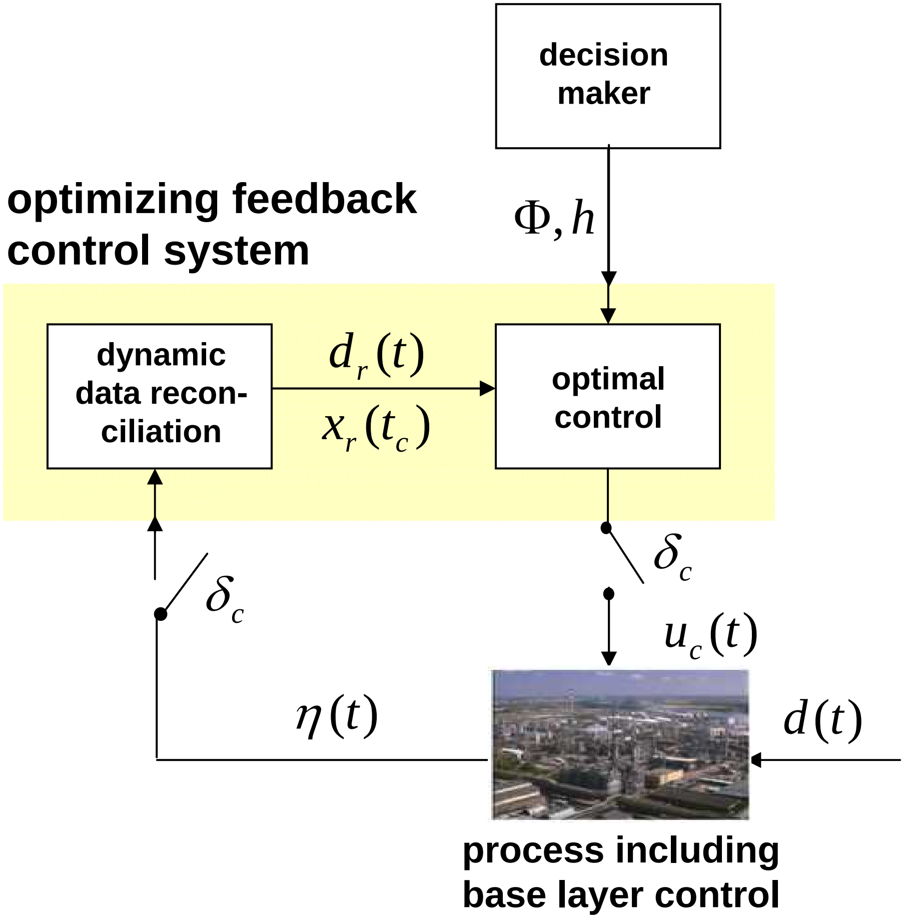
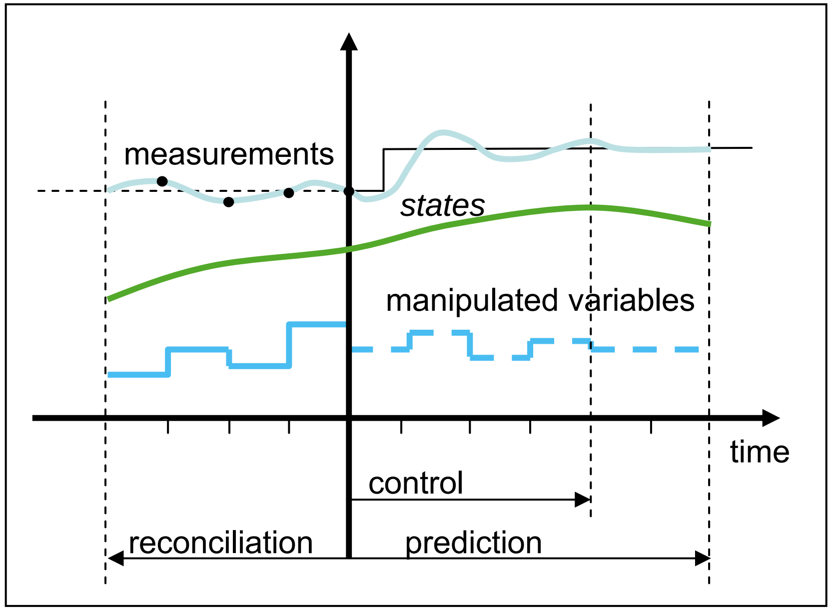
- Distributed MPC – a new approach for DRTO

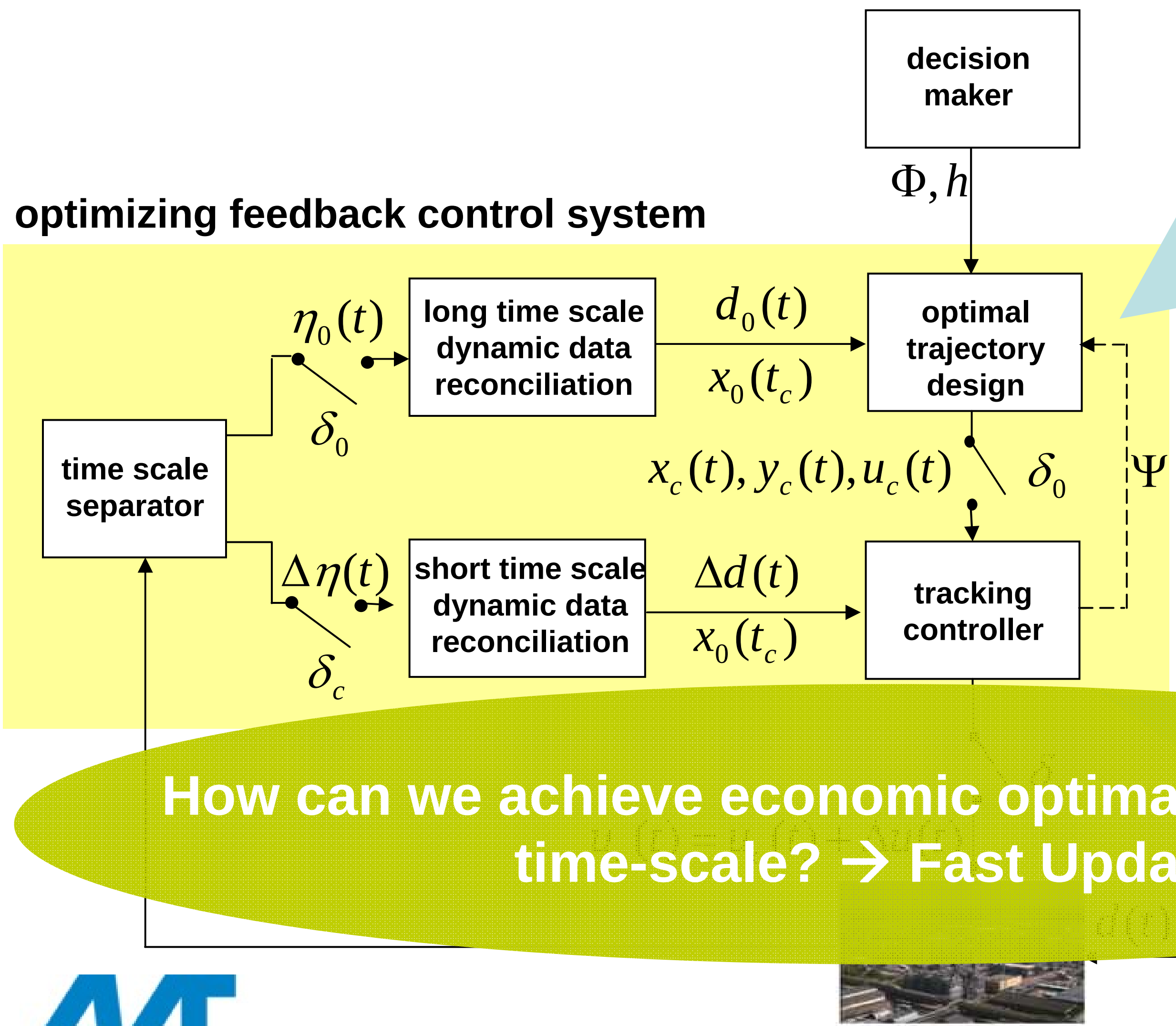
Dynamic Real-Time Optimization





- economical objectives & constraints
- optimal output feedback
- solution of optimization problems at sampling frequency
- computationally demanding, limited by model complexity

Time-Scale Decomposition



slow time-scale

- changing environment, process variations …
- most economical trajectory satisfying safety or equipment constraints!

fast time-scale

- measurement and process noise …
- trajectory tracking satisfying control …

How can we achieve economic optimality on the faster time-scale? → Fast Updates

Fast Neighboring Extremal Updates

(Kadam & Marquardt, 2004; Würth et al., 2009)

- parameterize uncertainty
- exploit sensitivity information of previously solved optimization problem to generate an approximation of the optimal update

Sensitivity system (Fiacco, 1983), invariant active set

$$\begin{bmatrix} L_{pp}(\cdot) & -g_p^{a,T}(\cdot) \\ g_p^{a,T}(\cdot) & 0 \end{bmatrix} \begin{bmatrix} p_\theta \\ \lambda_\theta \end{bmatrix} = -\begin{bmatrix} L_{p\theta}(\cdot) \\ g_\theta(\cdot) \end{bmatrix}$$

$$\Delta p := p(\theta) - p_0 = p_\theta(\theta_0)\Delta\theta$$

$$\Delta\lambda^a := \lambda^a(\theta) - \lambda_0^a = \lambda_\theta^a(\theta_0)\Delta\theta$$

$$\Delta\lambda^{ina} := \lambda^{ina}(\theta) - \lambda_0^{ina} = 0$$

L: Lagrange function
f: objective function
g: constraints
p: discretized controls
θ: uncertain param.

Changing active set (Ganesh & Biegler, 1987)

$$\min_{\Delta z} \; 0.5\Delta p^T L_{pp}^{ref}\Delta p + \Delta\theta^T L_{p\theta}^{ref}\Delta p + f_p^{T,ref}\Delta p$$

$$\text{s.t.} \quad g_p^{ref}\Delta p \geq -g_\theta^{ref}\Delta\theta + g^{ref}$$

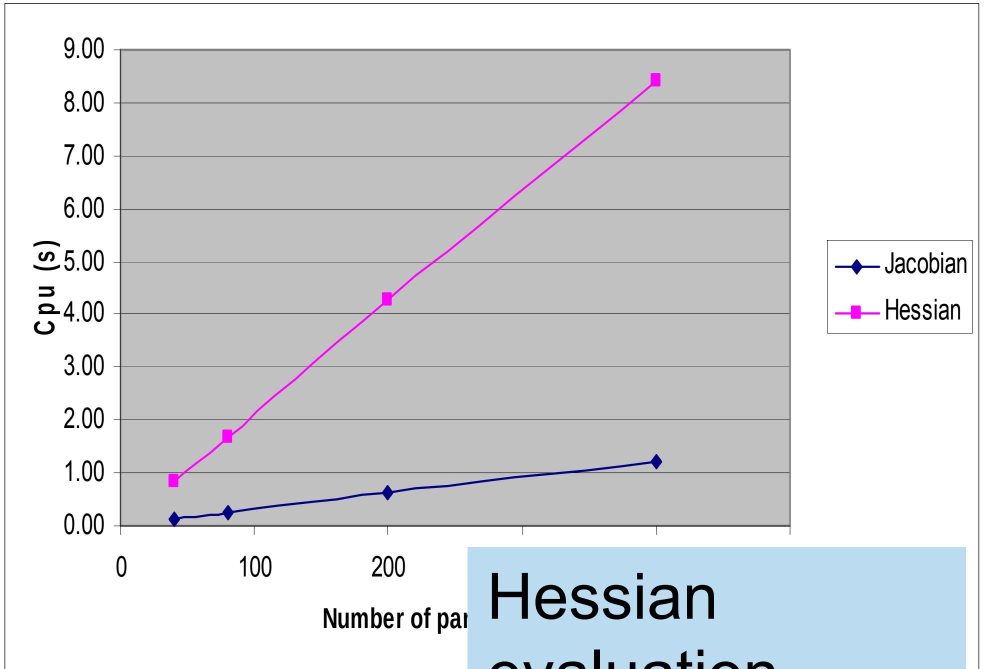
- compute first- and second-order derivatives $L_{pp}, L_{p\theta}, f_p, g_p, g_\theta$
- solve QP for fast update
- re-iterate if necessary

Efficient Computation of 2^{nd} order Sensitivities

HD-MPC

- finite differences and 2^{nd} order forward sensitivities (Vassiliadis et al., 1999) scale $O(n_p^2)$
- adjoint sensitivity analysis for problems without path constraints (Cao et al., 2003, Özyurt et al., 2005)
- 2^{nd} order adjoint sensitivity analysis for path-constrained problems (Hannemann & M., 2007, 2010) → **NIXE**

Williams-Otto benchmark problem

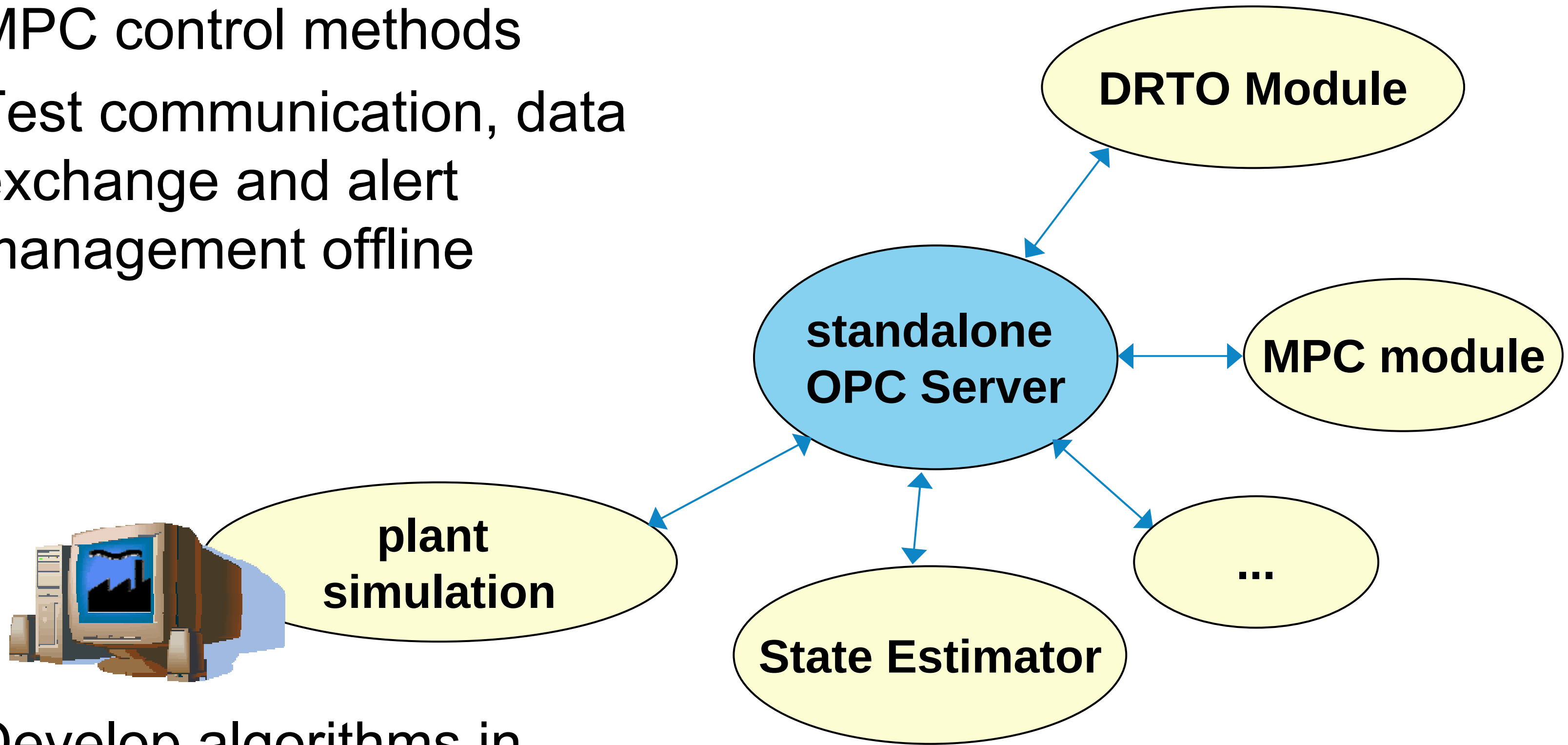


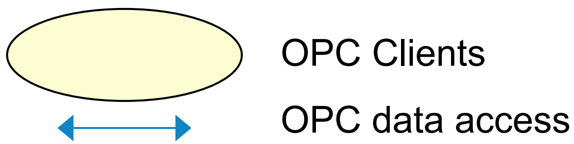
→ Superposition principle for the linear adjoint system: only one 2^{nd} order adjoint system

Hessian evaluation scales $\mathcal{O}(\mathbf{n_p})$!

Software Realization – DRTO Toolbox (1)

- Use plant simulator for development of advanced MPC control methods
- Test communication, data exchange and alert management offline

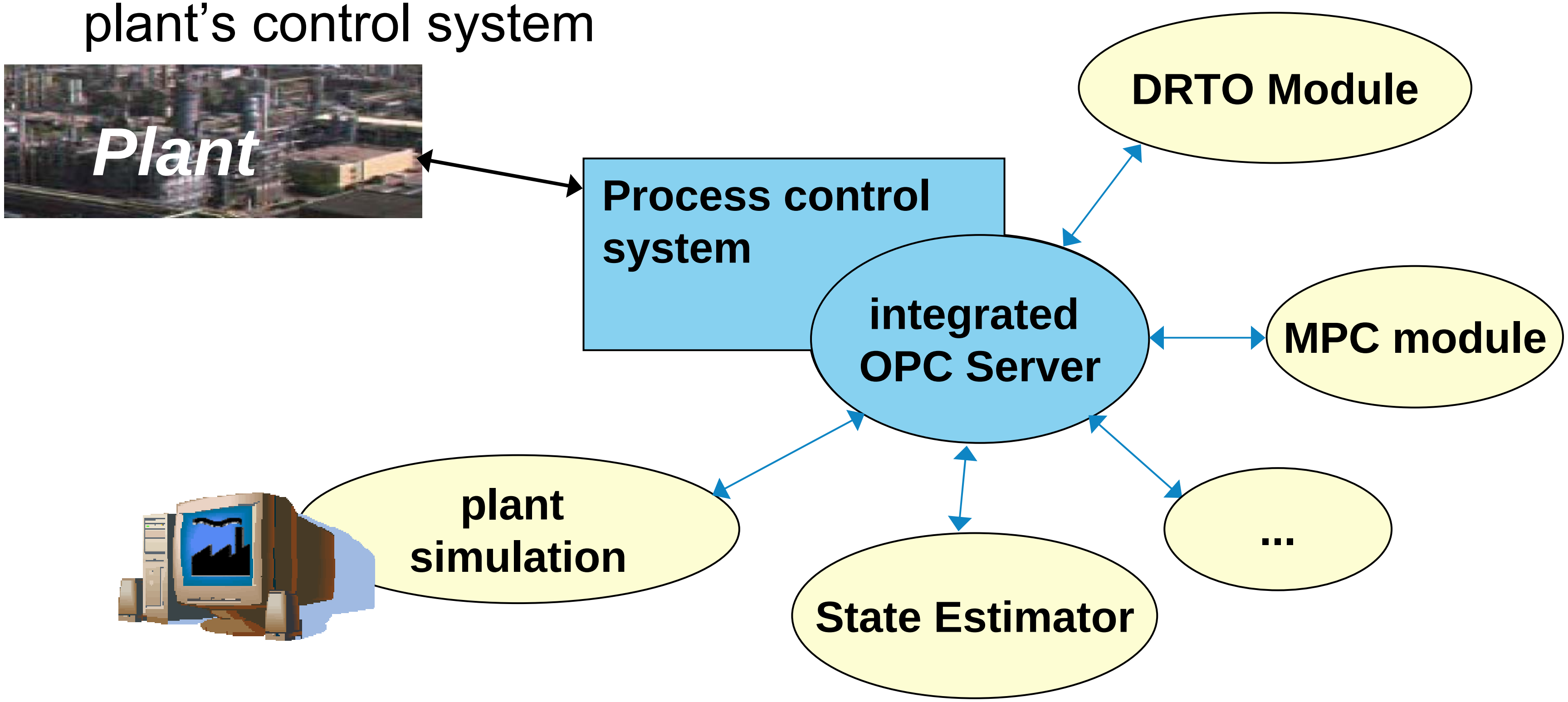




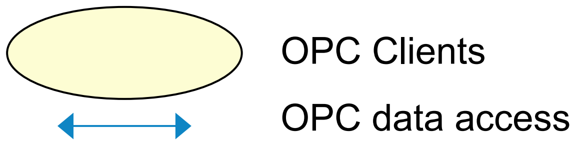
- Develop algorithms in Matlab, gPROMS, C++, ...

Software Realization – DRTO Toolbox (2)

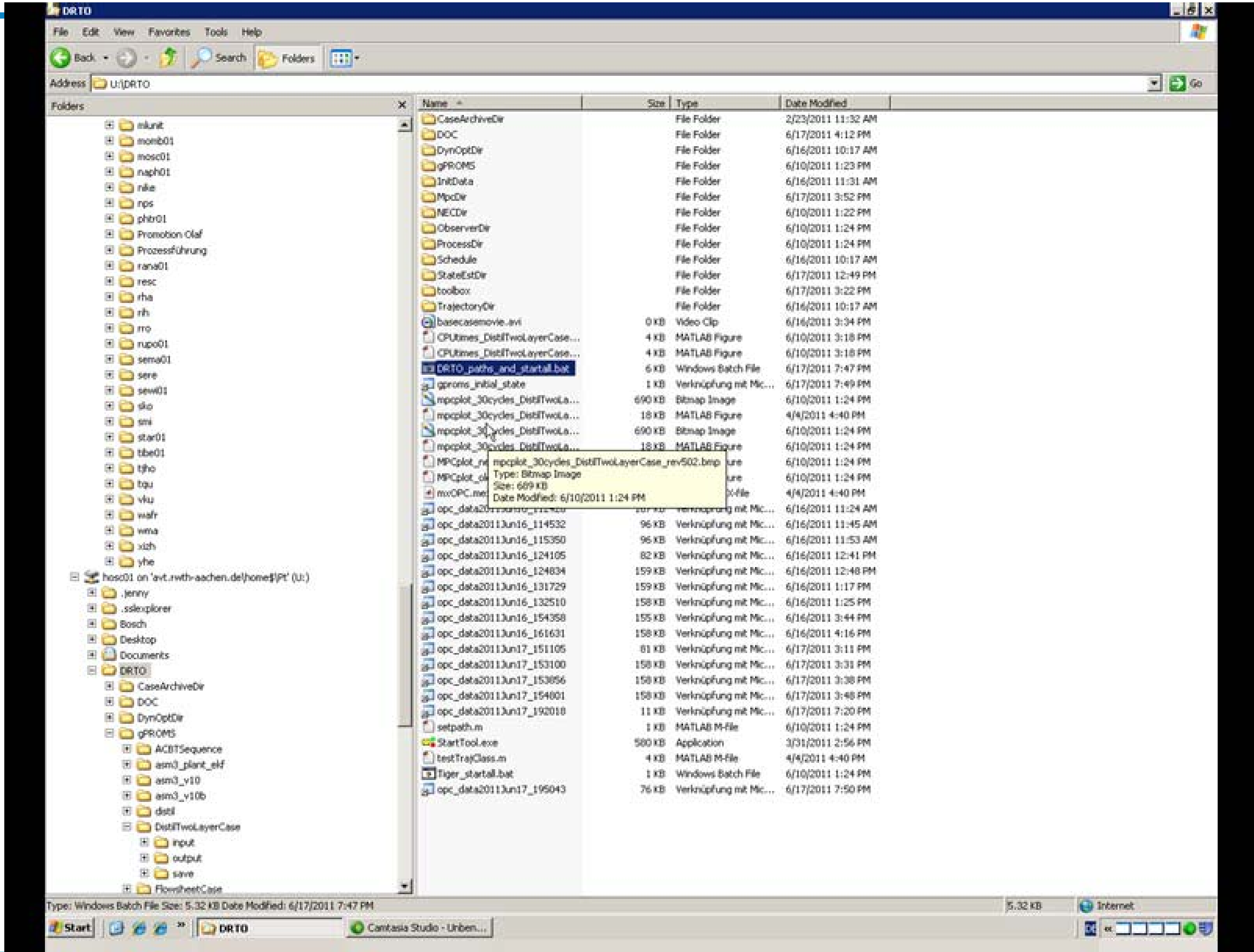
- Connect the control methods to the real control process through the plant's control system



- (Data structure in plant simulation should be the same as in PCS)

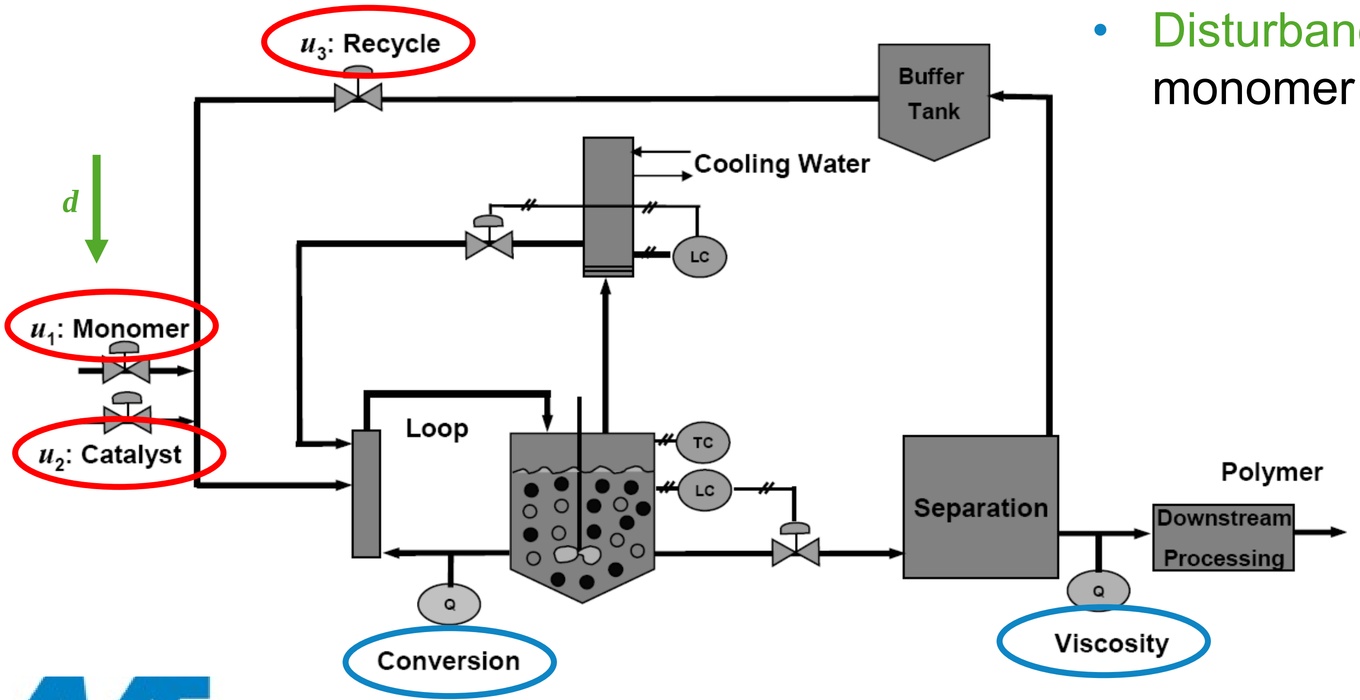


Software Realization – DRTO Toolbox (3)



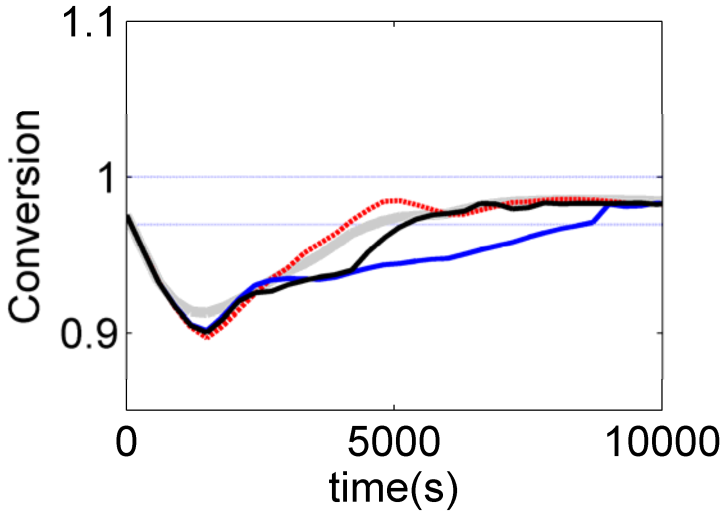
Case Study – Continuous Polymerization Process (1)

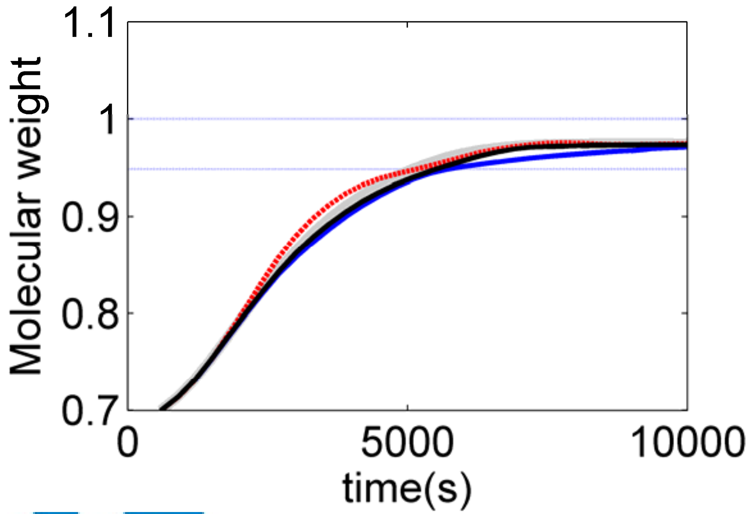
- Large-scale industrial process (Bayer AG, Dünnebier et al., 2004)
  - ~ 200 (dynamic) state variables
  - ~ 2000 algebraic variables
  - 3 manipulated variables
  - Task: Set point change from polymer A to B



- Disturbance: Ratio of monomer 1 and monomer 2

Case Study – Continuous Polymerization Process (2)

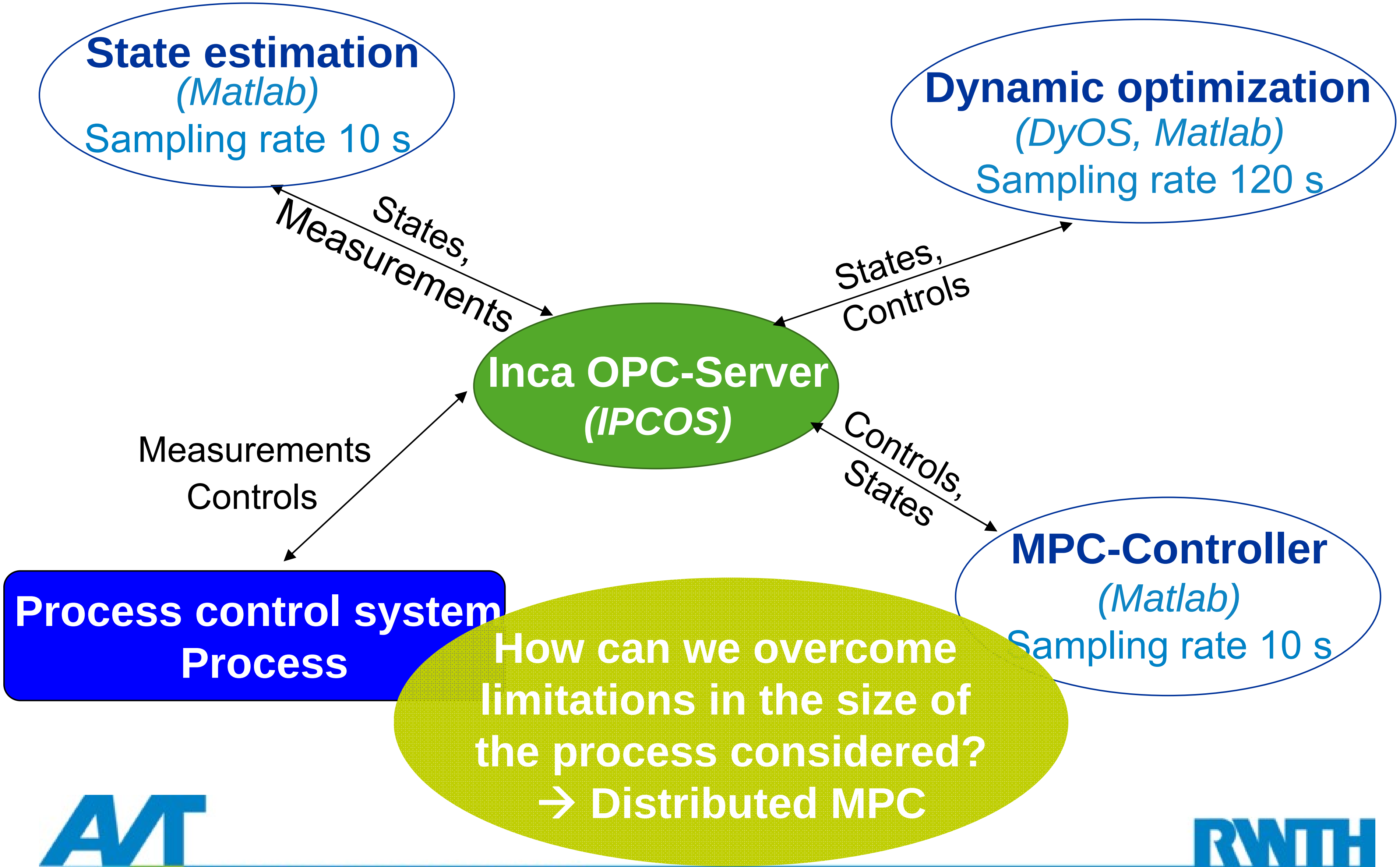




- Reference control strategy
  - Objective value: 0.59
  - Constraint violations: 1.6
- Delayed Single-Layer DRTO
  - Objective value: 1.18
  - Constraint violations: 16.2
- Single Layer: Neigboring Extremal Updates (NEU)
  - Objective value: 0.74
  - Constraint violations: 2.0
- Two-Layer (DRTO and NEU)
  - Objective value: 0.61
  - Constraint violations: 2.1

(Würth et al., 2011)

On-Site and Software Implementation



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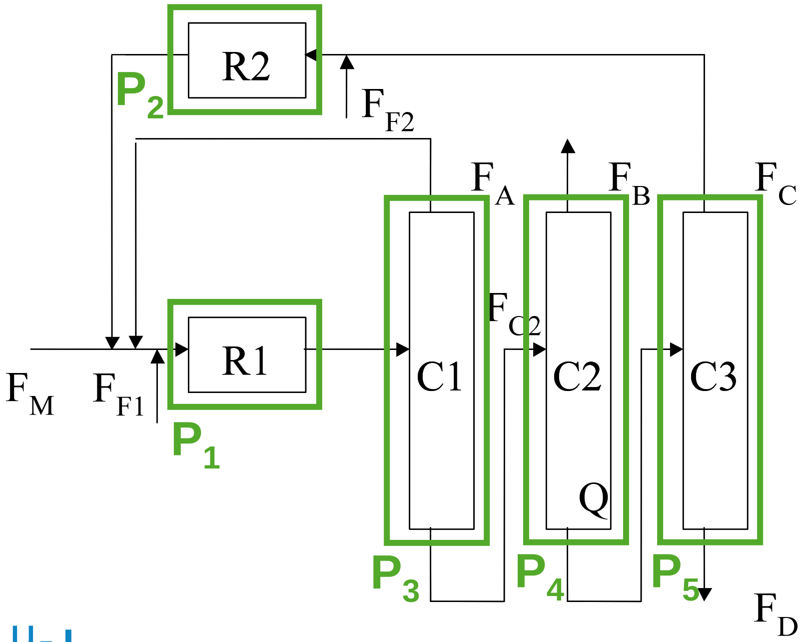
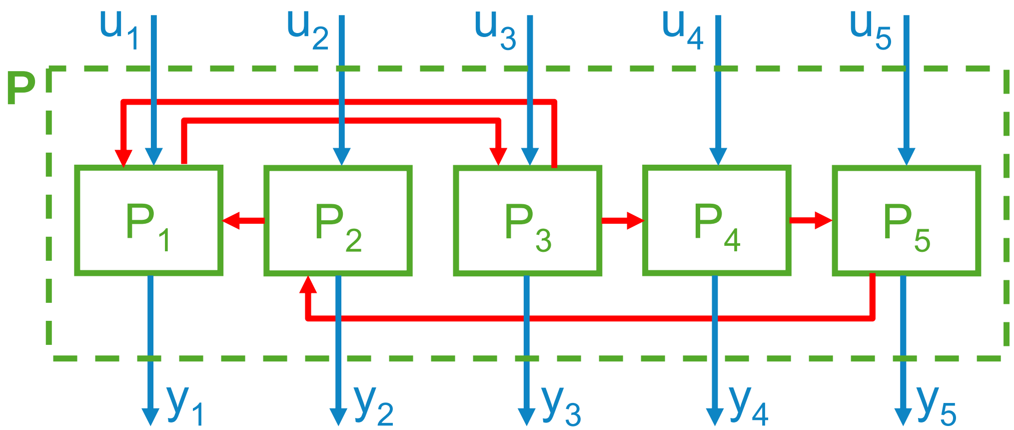
- **Distributed MPC – a new approach for DRTO**

Parellization via Problem Decomposition

- Applications can usually naturally be decomposed into subsystems
  - connected via interconnecting variables
  - local inputs
  - local outputs





Decomposition of Optimization Problem

$$\min_{u(t),p} \Phi(x(t_f)) = \sum_{i=1}^{N} \Phi_i(x_i(t_f))$$

separable objective function

$$M_i \dot{x}_i = F_i(x_i, u_i, p_i, t), \quad t \in [t_0, t_f],$$
$$0 = x_i(t_0) - x_{i,0},$$

separable DAE system

$$0 \geq P_i(x_i, u_i, p_i, t), \quad t \in [t_0, t_f],$$

separable path constraints

$$0 \geq E_i(t_f), \qquad i \in \{1, 2, \ldots, N\}$$

separable endpoint constraints

$$0 = m_i - H_i[x^T, u^T]^T$$

additional **nonseparable** interactions (here eq. constr.)

Solution Strategies for Decomposed Problems (1)

Reformulation as set of NLPs $i \in \{1,2,\ldots,N\}$

$$
\begin{aligned}
&\min_{c_i, p_i} \Phi_i(x_i(c_i, m_i, p_i)) \\
\text{s.t.}\quad & 0 \ge P_i(x_i, c_i, p_i, t_k), \quad \forall t_k \in T, \\
& 0 \ge E_i(x_i(t_f)),
\end{aligned}
$$

DAE system solved by underlying independent numerical integration

$$
0 = \sum_{i=1}^{N} h_i(x_i, c_i, m_i, t_k), \quad \forall t_k \in T,
$$

nonseparable interactions

Primal decomposition (Silverman 1972)

$$
\begin{aligned}
&\min_{c_i, p_i} \Phi_i(x_i(c_i, m_i, p_i)) \\
\text{s.t.}\quad & \vdots \\
& \gamma_i = h_i(x_i, c_i, m_i, t_k), \quad \forall t_k \in T,
\end{aligned}
$$

resource allocation s.t. $0 = \sum_{i=1}^{N} \gamma_i$

Dual decomposition (Lasdon 1970)

$$
\begin{aligned}
&\min_{c_i, p_i, m_i} L_i(x_i(c_i, m_i, p_i, \lambda)) \\
\text{s.t.}\quad & \vdots \\
& L_i(x_i(c_i, m_i, p_i, \lambda)) = \Phi_i(\ldots) + \lambda^T h_i(\ldots)
\end{aligned}
$$

price coordination s.t. $0 = \sum_{i=1}^{N} h_i$

Solution Strategies for Decomposed Problems (2)

- Sensitivity-Driven Distributed Model-Predictive Control (S-DMPC)
  (Scheu, Marquardt, 2011)
- Application of the linearized partial goal-interaction operator
  (Mesarovic et al.1970)

$$\Phi_i^{\text{S-DMPC}} = \Phi_i + \sum_{\substack{j=1 \\ j\neq i}}^{N} \Gamma'_{ij}(\tilde{u})u \; (u_i - \tilde{u}_i)$$

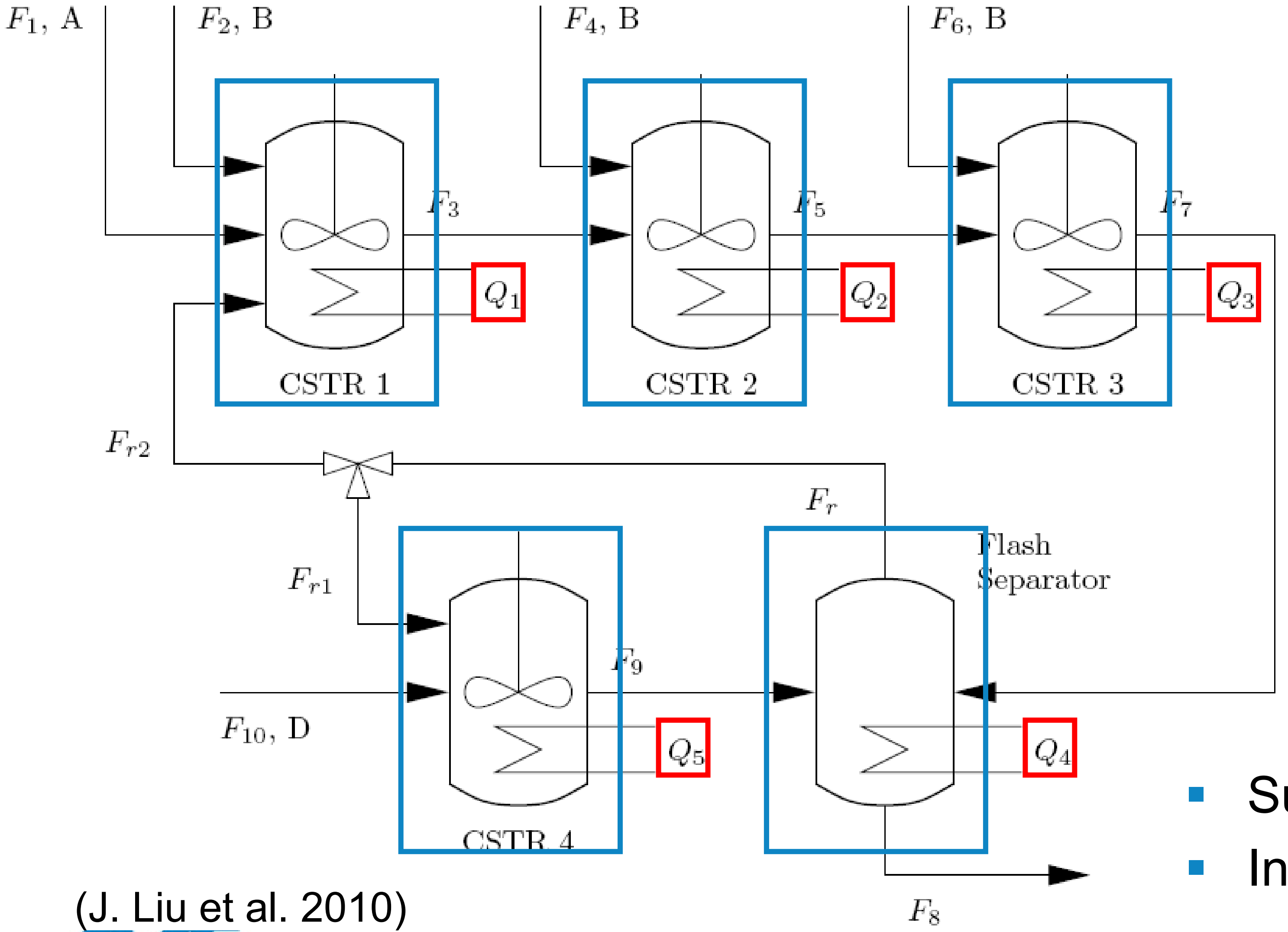
Cost function of the distributed controllers

$$= \boxed{\Phi_i} + \boxed{\left[\sum_{\substack{j=1 \\ j\neq i}}^{N} \left.\frac{\mathrm{d}\Phi_j}{\mathrm{d}u_i}\right|_{\tilde{u}}\right] (u_i - \tilde{u}_i)}$$

linearized information of nonlocal objective functions

copy of the local objective function

Alkylation of Benzene Process



- Subsystems
- Inputs

(J. Liu et al. 2010)

Mathematical model

For each subsystem:

- Mass balances for each species and energy balance

$$\begin{bmatrix} \frac{\mathrm{d}\, c_{Ai}}{\mathrm{d}t} \\ \frac{\mathrm{d}\, c_{Bi}}{\mathrm{d}t} \\ \frac{\mathrm{d}\, c_{Ci}}{\mathrm{d}t} \\ \frac{\mathrm{d}\, c_{Di}}{\mathrm{d}t} \\ \frac{\mathrm{d}\, T_i}{\mathrm{d}t} \end{bmatrix} = f_i(\ldots)$$

For CSTRs:

- reaction kinetics

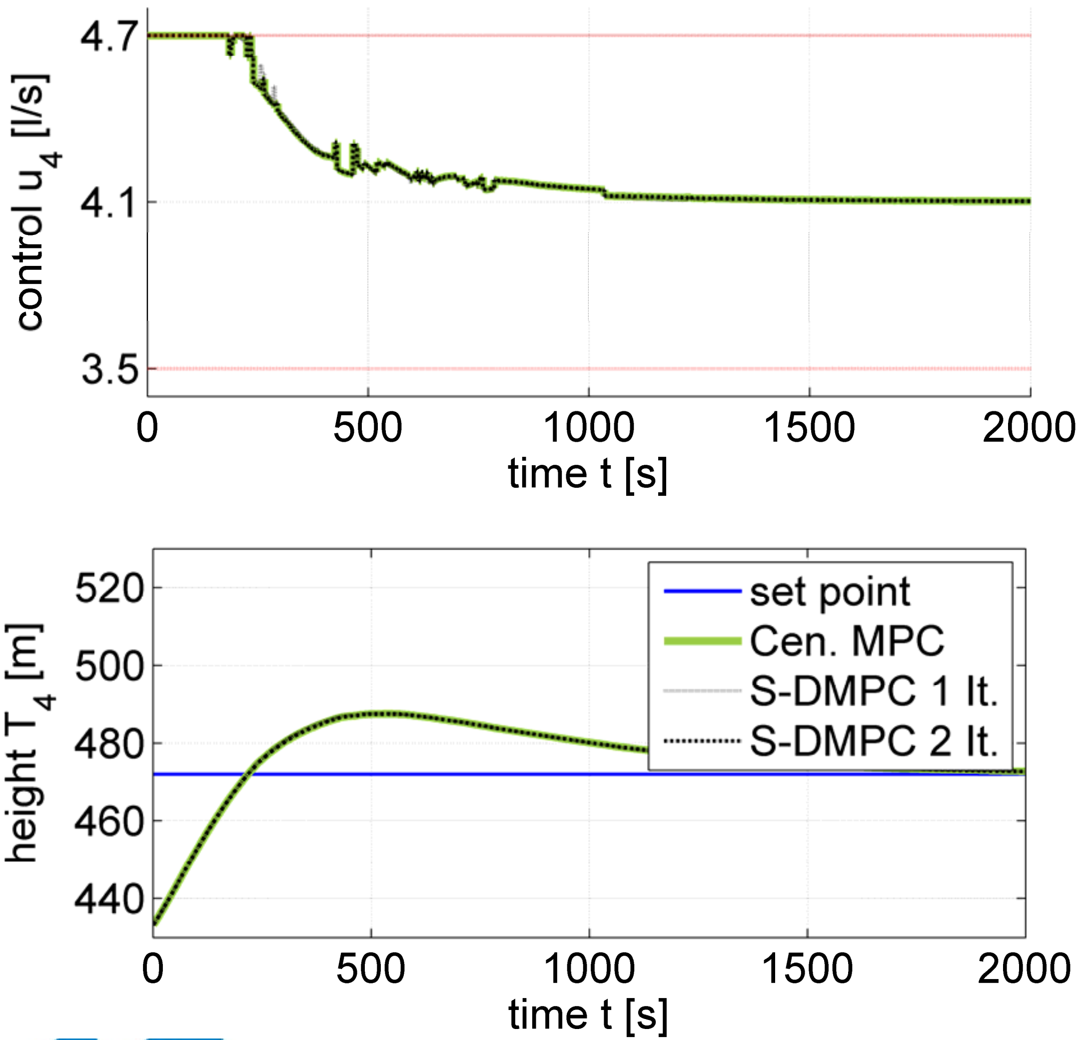
For flash separator:

- phase equilibrium descriptions

Medium scale DAE system:
- 25 differential equations
- ~100 algebraic equations

Results

(Scheu and Marquardt, 2011)



S-DMPC provides the same controller performance as a centralized MPC

Solve 5 small QP in parallel instead of 1 large QP

→ faster computation possible

Conclusions & Future Perspectives

- Algorithms for dynamic optimization are continuously maturing
  - basis for DRTO, reduce computing time
  - still many challenges ahead, e.g. discontinuous and mixed integer problems
- Hierarchical and distributed MPC are enabling technologies for real-time applications
- Hierarchical MPC Methods already successfully applied to large-scale industrial processes (simulation and experiments)
- Distributed MPC is a key technology to apply DRTO to even larger plants
  - methods are maturing
  - have to be integrated into DRTO toolbox

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