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

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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.
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Operational Strategies – the Status

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

Corporate objectives

Units, group of units, plant, group of plants, ...

Market

Supply chain

Environment

Production planning system

Operation support system

Purchasing & procurement

Supplier

Marketing & sales

Customer
Manufacturing in the Future

Real-time Business Decision Making in the Process Industries

- Operational strategies
- Reengineering the plant
- Synchronous or asynchronous
- Rolling window prediction adaptation
- Performance indicators
- Feedback

- The plant as part of the supply chain
- The disturbances
- Delivery on demand
- Varying quality specs
- Fluctuating prices
- Time-varying environment
- Corporate strategy
- Advancing technologies
- Saturating global markets
- Tightening legal regulations
- ... 

- Flexible production
- Smooth dynamics
- Lean inventories
- High capital productivities
- Sustainable production
- ... 

...
General Operational Objectives

Optimal operation of chemical processes

Why should they be constant over time?

Process model:

\[ 0 = f(x, u, p, d) \]

\[ x(t_0) = x_0 \]

\[ y = g(x) \]
Optimization-based Control and Operations

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.

$$0 = f(\eta, x_r, u_r, d_r)$$
$$y_r = g(x_r)$$
$$x_r(t_r) = x_r,0$$
$$u_r = U(u_c(\cdot))$$
$$0 \geq h_r(x_r, d_r)$$
$$t \in [t_r, t_c]$$

Dynamic optimization (open/closed loop)

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

s.t.

$$0 = f(\eta, x_c, u_c, d_c)$$
$$y_c = g(x_c)$$
$$x_c(t_c) = x_r(t_c)$$
$$d_c = D(d_r(\cdot))$$
$$0 \geq h_c(x_c, u_c)$$
$$t \in [t_c, t_f]$$

2 coupled problems!
Direct Solution Approach

• solution of optimal control reconciliation problems at controller sampling frequency

• computationally demanding

• model complexity limited \Rightarrow \text{large models}

• lack of transparency, redundancy and reliability

(\text{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 $\Delta d(t)$

$u_c(t) = u_c(t) + \Delta u(t)$

$\Phi, h$

$
\begin{align*}
\eta_0(t) & \xrightarrow{\delta_0} \text{long time scale dynamic data reconciliation} \\
\Delta \eta(t) & \xrightarrow{\delta_c} \text{short time scale dynamic data reconciliation} \\
\text{time scale separator} & \\
\text{optimizing feedback control system} & \\
\end{align*}
$

$\text{decision maker}$

$\text{optimal trajectory design}$

$\text{tracking controller}$

$\text{process including base control}$

Real-time Business Decision Making in the Process Industries
Real-time Dynamic Optimization

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

Real-time Business Decision Making in the Process Industries
Mathematical problem formulation

\[
\min_{u(t), p, t_f} \Phi(x(t_f)) \quad \text{objective function (e.g. cost)}
\]

s.t.

\[
\begin{align*}
M &\Leftrightarrow F(x, u, p, t), \quad t \in [t_0, t_f], \\
0 &= x(t_0) - x_0, \\
0 &\geq P(x, u, p, t), \quad t \in [t_0, t_f], \\
0 &\geq E(x(t_f))
\end{align*}
\]  \quad \text{DAE system (process model)}

\quad \text{path constraints (e.g. temp. bound)}

\quad \text{endpoint constraints (e.g. prod. spec.)}

Degrees of freedom: \quad u(t) \quad \text{time-variant control variables}

\quad p \quad \text{time-invariant parameters}

\quad t_f \quad \text{final time}
Sequential Approach (Single Shooting)

Control vector parameterization
\[ u_i(t) \approx \sum_{k \in \Lambda_i} c_{i,k} \phi_{i,k}(t) \]

Parameterization functions
\[ \phi_{i,k}(t) \]

Parameters
\[ c_{i,k} \]

Reformulation as nonlinear programming problem (NLP)
\[
\begin{align*}
\min_{c,p,t_f} \Phi(x(c, p, t_f)) \\
\text{s.t.} \quad & 0 \geq P(x, c, p, t_i), \quad \forall t_i \in T, \\
& 0 \geq E(x(t_f))
\end{align*}
\]

DAE system solved by underlying numerical integration

Gradients for NLP solver typically obtained by integration of sensitivity systems
**Real-time Business Decision Making in the Process Industries**

**Improved Algorithms – Sequential Approach**

- **Sensitivity integration** is expensive
  - Improve efficiency of sensitivity integration
  - New solver for sensitivity integration

- **State integration** is expensive
  - Reduce number of sensitivity parameters
  - Reduce model complexity

- **Methods for model reduction**

- **Control grid adaptation strategy**
Different **representations** of the same function ...

... for problem discretization:

$$ u = \sum_{(j,k) \in \Lambda} c_{j,k} \phi_{j,k}(t) $$

... for grid point elimination analysis:

$$ u = c_{0,0} \phi_{0,0}(t) + \sum_{(j,k) \in \Psi} d_{j,k} \psi_{j,k}(t) $$

Real-time Business Decision Making in the Process Industries
Adaptive Refinement Algorithm

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

until stopping criterion met.
isothermal semi-batch reactor
(Srinivasan et al, 2003)

reactions: \( A + B \rightarrow C \), \( 2B \rightarrow C \)
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?
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 adaptive 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

Path constraint 1: heat

Path constraint 2: volume

Real-time Business Decision Making in the Process Industries
Results

MV 1: Feed rate

MV 2: Temperature

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 Business Decision Making in the Process Industries
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?
- ...

Real-time Business Decision Making in the Process Industries
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
Alternative 1: NCO Tracking

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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.)

Recent supervision control on dynamic optimization level
- check potential changes of switching structure
- quantitatively assess optimality loss

- track singular arc
- adjust switching times
- switch potential structure changes due to uncertainty, motivation for supervisory level
- trigger dynamic optimization and new switching structure detection
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.

Re-optimization with adaptation of control discretization mesh.

Re-optimization on coarse control discretization.

D-RTO trigger and fast updates.

Updated $y_{ref}, u_{ref}$.
Fast Update and D-RTO Trigger Algorithm

estimates \( p^j, \hat{x}^j \)

sensitivity integration to update \( g^j, g_z^j, g_p^j, f_z^j \) for the controls from the previous iteration \( j-1 \)

pre-computed \( L_{zz}, L_{zp} \)

solution of fast update QP problem

\[
\begin{align*}
\hat{z}_r^j &= \hat{z}_r^{j-1} + \Delta z, y_r^j, G^j, \lambda^j \\
\end{align*}
\]

evaluate optimality error

\[
\begin{align*}
\epsilon_{opt}^j &= \frac{\| L_z^j(\bullet) \|_{\infty}}{\| \lambda^j \|_2}, \epsilon_{inf}^j = \frac{\| g^j(\bullet) \|_{\infty}}{\| z^j \|_2} \\
\end{align*}
\]

if \( \epsilon_{opt}^j > \tau_{opt} \) and \( \epsilon_{inf}^j > \tau_{inf} \) perform a re-optimization for optimal updates

\[
\begin{align*}
\hat{z}_r^j, y_r^j \\
\end{align*}
\]
Closed-loop Optimization Results

Williams-Otto semi-batch reactor

\[ \Delta h_1 = +10\% \quad \text{and} \quad \Delta T_{in} = -10^\circ C \quad \text{at} \quad t = 250 \text{ sec} \]
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
- ...

Real-time Business Decision Making in the Process Industries
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

\[ \min_{z_k, u_k, p, Y} \Phi := \sum_{k=1}^{n} \Phi_k(z_k(t_k), p, t_k) + \sum_{i=1}^{m} b_i \] (MLDO)

- **Objective:**

- **Dynamic model:**

- **Constraints:**

- **Initial conditions:**

- **Stage transition conditions:**

- **Disjunctions:**

- **Propositional logic:**

\[ \Omega(Y) = \text{True.} \]
A Sample Result

quality variable 1

quality variable 2

manipulated variable 1

manipulated variable 2

- polyolefin 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

Real-time Business Decision Making in the Process Industries
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 ?
Conclusions

- any-time economically optimal operation
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Great opportunities for Systems and Control Community in theory and applications
Collaborators

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