Dynamic Real-Time Optimization: Concepts in Modeling, Algorithms and Properties

L. T. Biegler
Chemical Engineering Department
Carnegie Mellon University
Pittsburgh, PA

November 28, 2007

Dynamic Optimization Outline

2

DAE Models in Process Engineering

Differential Equations

Conservation Laws (Mass, Energy, Momentum)

Algebraic Equations

Constitutive Equations, Equilibrium (physical properties, hydraulics, rate laws)
Semi-explicit form
Assume to be index one (i.e., algebraic variables can be solved uniquely by algebraic equations)
If not, DAE can be reformulated to index one (see Ascher and Petzold)

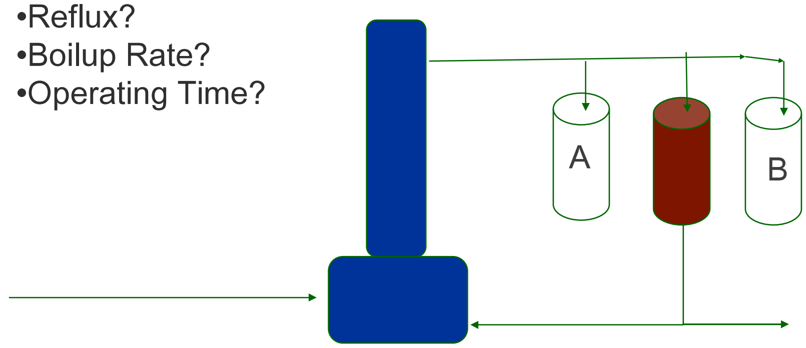
Characteristics

Large-scale models – not easily scaled
Sparse but no regular structure
Direct linear solvers widely used
Coarse-grained decomposition of linear algebra

3

Batch Distillation Multi-product Operating Policies

- Run between distillation batches
- Treat as boundary value optimization problem
  - When to switch from A to offcut to B?
  - How much offcut to recycle?
  - Reflux?
  - Boilup Rate?
  - Operating Time?



4

Parameter Estimation

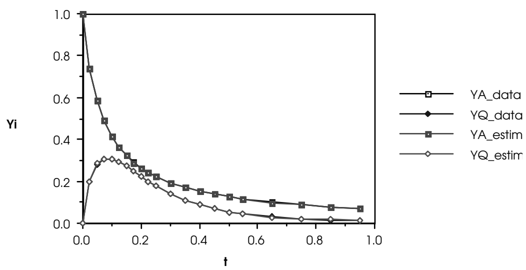
Catalytic Cracking of Gasoil (Tjoa, 1991)

$$A \xrightarrow{p_1} Q,\; Q \xrightarrow{p_2} S,\; A \xrightarrow{p_3} S$$

$$\dot{a} = -(p_1 + p_3)a^2$$

$$\dot{q} = -p_1 a^2 - p_2 q$$

$$a(0) = 1, \quad q(0) = 0$$



number of states and ODEs: 2
number of parameters:3
no control profiles
constraints: $p_L \le p \le p_U$

Objective Function: Ordinary Least Squares

$(p_1, p_2, p_3)^0 = (6, 4, 1)$
$(p_1, p_2, p_3)^* = (11.95, 7.99, 2.02)$
$(p_1, p_2, p_3)_{true} = (12, 8, 2)$

5

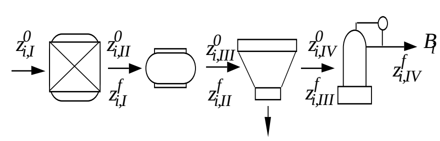
Batch Process Optimization

Optimization of dynamic batch process operation resulting from reactor and distillation column

DAE models:
$z' = f(z, y, u, p)$
$g(z, y, u, p) = 0$

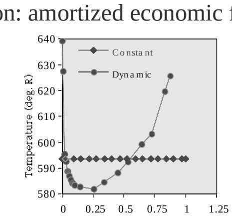
$A+B \rightarrow C$
$C+B \rightarrow P+E$
$P+C \rightarrow G$

number of states and DAEs: $n_z + n_y$
parameters for equipment design (reactor, column)
n_u control profiles for optimal operation

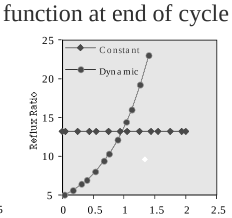


Constraints: $u_L \le u(t) \le u_U$ $\quad z_L \le z(t) \le z_U$
$y_L \le y(t) \le y_U$ $\quad p_L \le p \le p_U$

Objective Function: amortized economic function at end of cycle time t_f



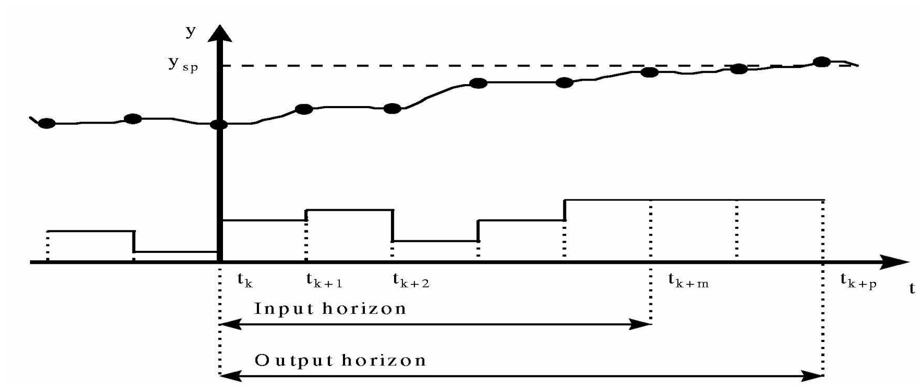
optimal reactor temperature policy



optimal column reflux ratio

6

Nonlinear Model Predictive Control (NMPC)



$$\min_{\mathbf{u}} \quad \sum \| y(t) - y^{sp} \|^2_{Q_y} + \sum \| \mathbf{u}(\mathbf{t}^k) - \mathbf{u}(\mathbf{t}^{k-1}) \|^2_{Q_u}$$

$$\begin{aligned} s.t. \quad & z'(t) = F(z(t), y(t), \mathbf{u}(t), t) \\ & 0 = G(z(t), y(t), \mathbf{u}(t), t) \\ & z(t) = z^{\text{init}} \\ & \text{Bound Constraints} \\ & \text{Other Constraints} \end{aligned}$$

7

Dynamic Optimization Problem

$$\min \quad \Phi\left(z(t),\ y(t),\ u(t),\ p,\ t_f\right)$$

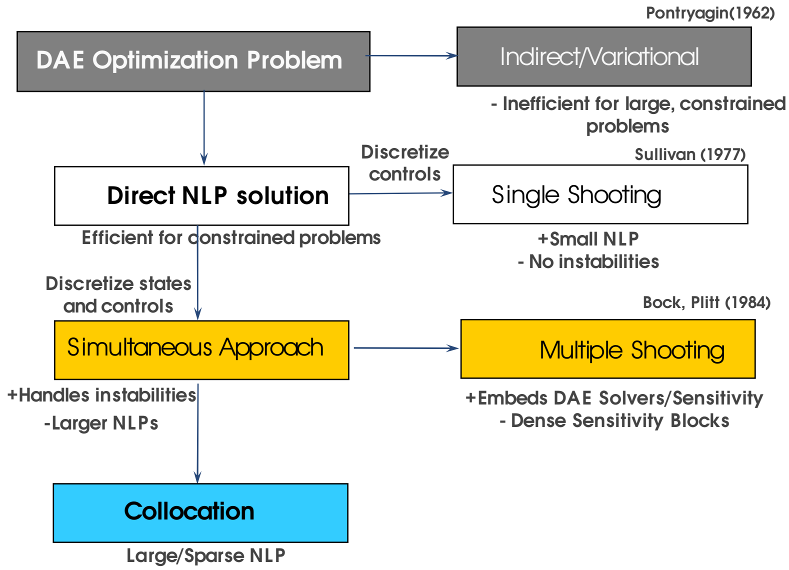
$$\begin{aligned} \textbf{s.t.} \quad & \frac{dz(t)}{dt} = f\left(z(t), y(t), u(t), t, p\right) \\ & g\left(z(t), y(t), u(t), t, p\right) = 0 \\ & z^o = z(0) \\ & z^l \le z(t) \le z^u \\ & y^l \le y(t) \le y^u \\ & u^l \le u(t) \le u^u \\ & p^l \le p \le p^u \end{aligned}$$

t, time
z, differential variables
y, algebraic variables

t_f, final time
u, control variables
p, time independent parameters

8

Dynamic Optimization Approaches



9

Sequential Approaches - Parameter Optimization

Consider a simpler problem without control profiles:

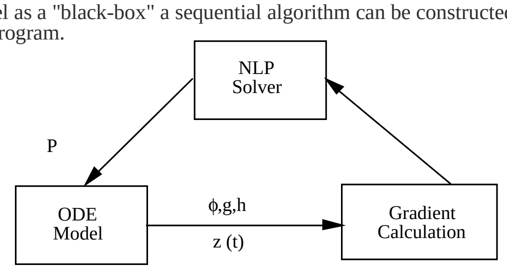
e.g., equipment design with DAE models - reactors, absorbers, heat exchangers

$$Min \quad \Phi(z(t_f))$$

$$z' = f(z, p),\ z(0) = z_0$$

$$g(z(t_f)) \leq 0,\ h(z(t_f)) = 0$$

By treating the ODE model as a "black-box" a sequential algorithm can be constructed that can be treated as a nonlinear program.



Task: How are gradients calculated for optimizer?

10

Gradient Calculation

Perturbation

Sensitivity Equations

Adjoint Equations

Perturbation

Calculate approximate gradient by solving ODE model (np + 1) times

Let $\psi = \Phi$, g and h (at $t = t_f$)

$$d\psi/dp_i = \{\psi (p_i + \Delta p_i) - \psi (p_i)\}/ \Delta p_i$$

Very simple to set up

Leads to poor performance of optimizer and poor detection of optimum unless roundoff error ($O(1/\Delta p_i)$ and truncation error ($O(\Delta p_i)$) are small.

Work is proportional to np (expensive)

11

Direct Sensitivity

From ODE model: $$\frac{\partial}{\partial p}\{z' = f(z, p, t), z(0) = z_0(p)\}$$

$$\text{define } s_i(t) = \frac{\partial z(t)}{\partial p_i} \; i = 1, \ldots \text{np}$$

$$s_i' = \frac{d}{dt}(s_i) = \frac{\partial f}{\partial p_i} + \frac{\partial f}{\partial z}^T s_i, \; s_i(0) = \frac{\partial z(0)}{\partial p_i}$$

(nz x np sensitivity equations)

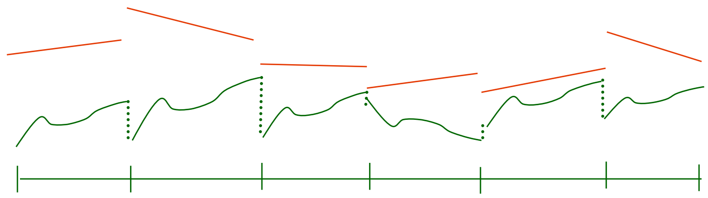
- z and s_i , i = 1,…np, an be integrated forward simultaneously.
- for implicit ODE solvers, $s_i(t)$ can be carried forward in time after converging on z
- linear sensitivity equations exploited in ODESSA, DASSAC, DASPK, DSL48s and a number of other DAE solvers

Sensitivity equations are efficient for problems with many more constraints than parameters (1 + ng + nh > np)

12

Multiple Shooting for Dynamic Optimization

Divide time domain into separate regions



Integrate DAEs state equations over each region

Evaluate sensitivities in each region as in sequential approach wrt u_{ij}, p and z_j

Impose matching constraints in NLP for state variables over each region

Variables in NLP are due to control profiles as well as initial conditions in each region

13

Multiple Shooting Nonlinear Programming Problem

$$\min_{u_{i,j},p} \psi\left(z(t_f), y(t_f)\right)$$

s.t.

$$z(z_j, u_{i,j}, p, t_{j+1}) - z_{j+1} = 0$$

$$z_k^{\ l} \le z(z_j, u_{i,j}, p, t_k) \le z_k^{\ u}$$

$$y_k^{\ l} \le y(z_j, u_{i,j}, p, t_k) \le y_k^{\ u}$$

$$u_i^{\ l} \le u_{i,j} \le u_i^{\ u}$$

$$p^l \le p \le p^u$$

$$\left(\frac{dz}{dt}\right) = f\left(z, y, u_{i,j}, p\right), \quad z(t_j) = z_j$$

$$g\left(z, y, u_{i,j}, p\right) = 0$$

$$z_0^{\ o} = z(0)$$

$$\min_{x \in \Re^n} f(x)$$

$$\text{s.t} \quad c(x) = 0$$

$$x^L \le x \le x^u$$

Solved Implicitly

14

Dynamic Optimization – Multiple Shooting Strategies

Larger NLP problem O(np+nu+NE nz)

- Use SNOPT, MINOS, etc.
- Second derivatives difficult to get

Repeated solution of DAE model and sensitivity/adjoint equations, scales with nz and np

- Dominant computational cost
- May fail at intermediate points

Multiple shooting can deal with unstable systems with sufficient time elements.

Discretize control profiles to parameters (at what level?)

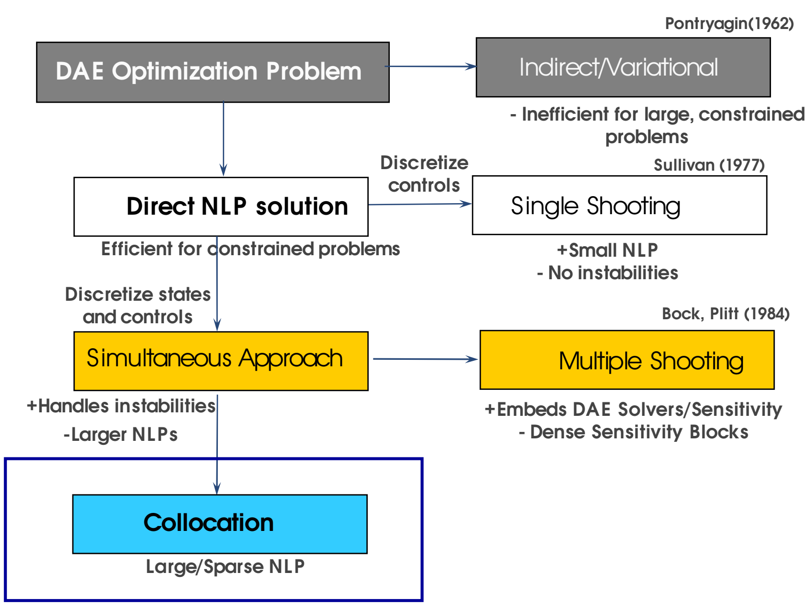
Path constraints are difficult to handle exactly for NLP approach

Block elements for each element are dense!

Extensive developments and applications by Bock and coworkers using MUSCOD code

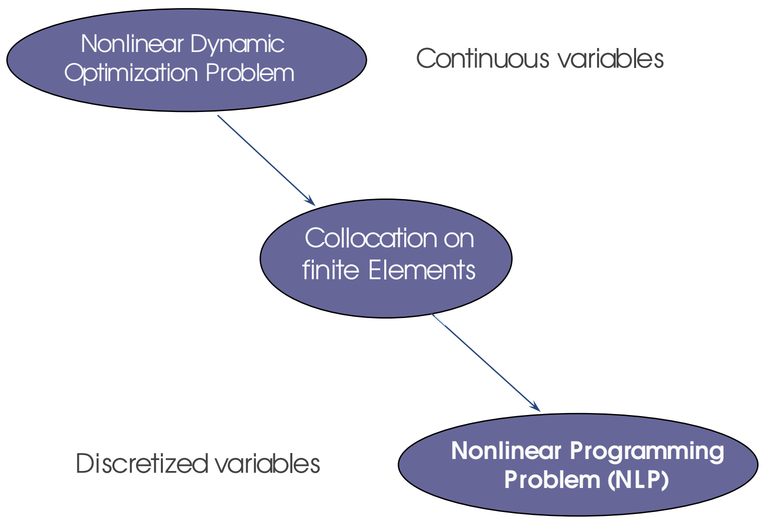
15

Dynamic Optimization Approaches



16

Nonlinear Programming Formulation



17

Discretization of Differential Equations
Orthogonal Collocation

Given: *dz/dt = f(z, u, p), z(0)=given*

Approximate *z* and *u* by Lagrange interpolation polynomials (order K+1 and K, respectively) with interpolation points, t_k

$$z_{K+1}(t) = \sum_{k=0}^{K} z_k \ell_k(t),\ \ell_k(t) = \prod_{\substack{j=0 \\ j \neq k}}^{K} \frac{(t - t_j)}{(t_k - t_j)} \Longrightarrow z_{N+1}(t_k) = z_k$$

$$u_K(t) = \sum_{k=1}^{K} u_k \ell_k(t),\ \ell_k(t) = \prod_{\substack{j=1 \\ j \neq k}}^{K} \frac{(t - t_j)}{(t_k - t_j)} \Longrightarrow u_N(t_k) = u_k$$

Substitute z_{N+1} and u_N into ODE and apply equations at t_k.

$$r(t_k) = \sum_{j=0}^{K} z_j \dot{\ell}_j(t_k) - f(z_k, u_k) = 0, \quad k = 1, \ldots K$$

18

Converted Optimal Control Problem Using Collocation

Min $\phi(z(t_f))$

s.t. $z' = f(z, u, p), z(0)=z_0$

$g(z(t), u(t), p) \le 0$

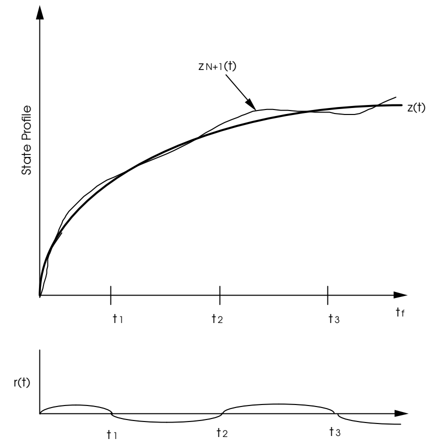
$h(z(t), u(t), p) = 0$

to Nonlinear Program

Min $\phi(z_f)$

$$\left.\begin{aligned}&\sum_{j=0}^{K} z_j \dot{\ell}_j(t_k) - f(z_k, u_k) = 0,\ z_0 = z(0)\\ &g(z_k, u_k) \le 0\\ &h(z_k, u_k) = 0\end{aligned}\right\} k = 1,\ldots K$$

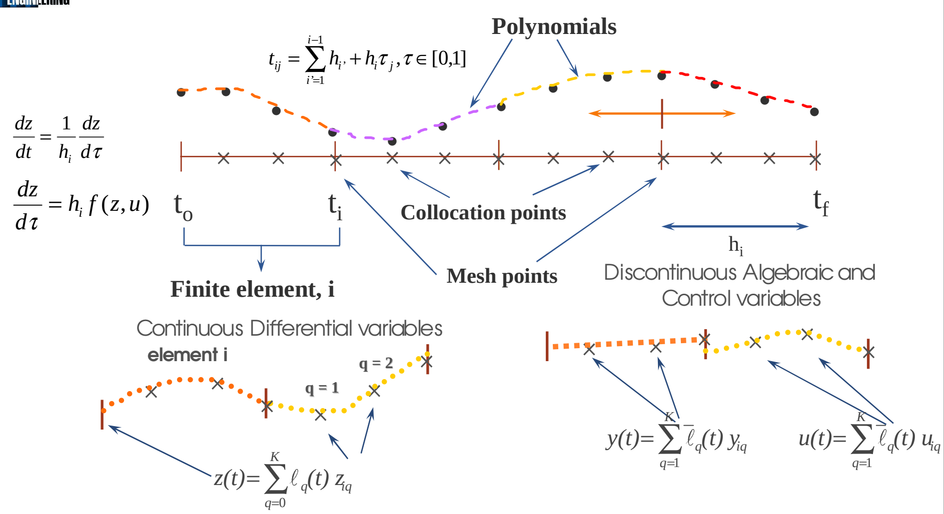
$$\sum_{j=0}^{K} z_j \ell_j(1) - z_f = 0$$



How accurate is approximation

19

Collocation on Finite Elements



$$r(t_{ik}) = \sum_{j=0}^{K} (z_{ij} \dot{\ell}_j(\tau_k)) - h_i f(z_{ik}, u_{ik}, p) = 0, \quad k = 1,..K, i = 1,..NE$$

20

Nonlinear Programming Problem

$$\min \ \psi\left(z_f\right)$$

s.t.

$$\sum_{j=0}^{K}(z_{ij}\dot{\ell}_j(\tau_k)) - h_i f(z_{ik}, u_{ik}, p) = 0$$

$$g\left(z_{i,k}, y_{i,k}, u_{i,k}, p\right) = 0$$

$$\sum_{j=0}^{K}(z_{i-1,j}\ell_j(1)) - z_{i0} = 0, \ i = 2,..NE$$

$$\sum_{j=0}^{K}(z_{NE,j}\ell_j(1)) - z_f = 0, \ z_{10} = z(0)$$

$$z_{i,j}^{\ l} \le z_{i,j} \le z_{i,j}^{\ u}$$

$$y_{i,j}^{\ l} \le y_{i,j} \le y_{i,j}^{\ u}$$

$$u_{i,j}^{\ l} \le u_{i,j} \le u_{i,j}^{\ u}$$

$$p^l \le p \le p^u$$

$$\min_{x \in \Re^n} f(x)$$

$$\text{s.t} \quad c(x) = 0$$

$$x^L \le x \le x^u$$

Finite elements, h_i, can also be variable to determine break points for $u(t)$.

Add $h_u \ge h_i \ge 0, \sum h_i = t_f$

Can add constraints $g(h, z, u) \le \varepsilon$ for approximation error

21

Theoretical Properties of Simultaneous Method

A. Stability and Accuracy of Orthogonal Collocation

- Equivalent to performing a *fully implicit* Runge-Kutta integration of DAE models at Gaussian (Radau) points
- 2K order (2K-1) method which uses K collocation points
- Algebraically stable (i.e., possesses A, B, AN and BN stability)

B. Analysis of the Optimality Conditions (Kameswaran, B., 2007)

- An equivalence has been established between the KKT conditions of NLP and the variational necessary conditions
- Rates of convergence have been established for the NLP method

22

Example: Batch reactor - temperature profile

Maximize yield of B after one hour's operation by manipulating a transformed temperature, u(t).

$\Rightarrow$ Minimize $-z_B(1.0)$

s.t.

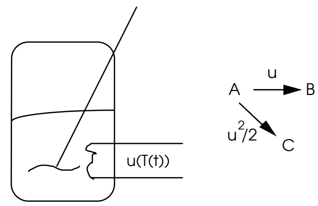
$z'_A = -(u+u^2/2)\, z_A$

$z'_B = u\, z_A$

$z_A(0) = 1$

$z_B(0) = 0$

$0 \le u(t) \le 5$



<u>Optimality conditions:</u>

$H = -\lambda_A(u+u^2/2)\, z_A + \lambda_B\, u\, z_A$

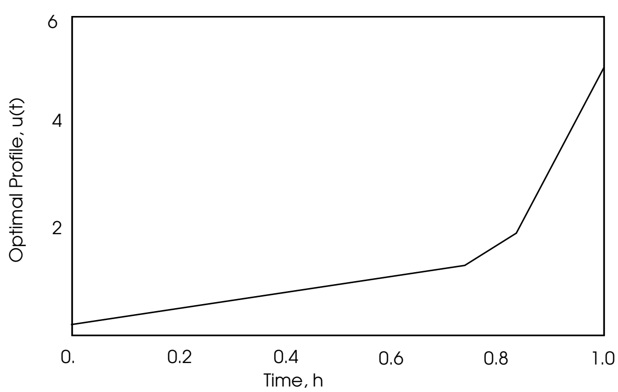
$\partial H/\partial u = \lambda_A\, (1+u)\, z_A + \lambda_B\, z_A$

$\lambda'_A = \lambda_A(u+u^2/2) - \lambda_B\, u, \quad \lambda_A(1.0) = 0$

$\lambda'_B = 0, \quad \lambda_B(1.0) = -1$

23

Batch Reactor Optimal Temperature Program Piecewise Linear



<u>Results:</u>

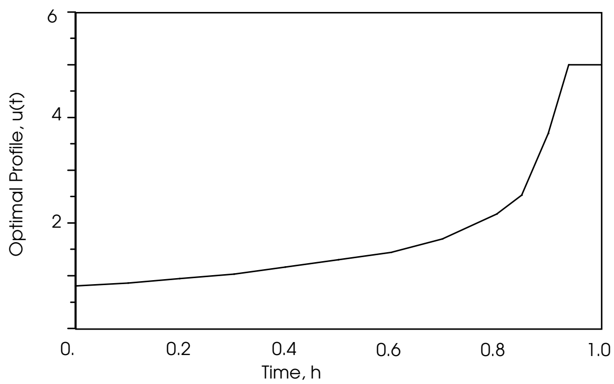
Piecewise Linear Approximation with Variable Time Elements

Optimum B/A: <u>0.5726</u>

Equivalent # of ODE solutions: <u>32</u>

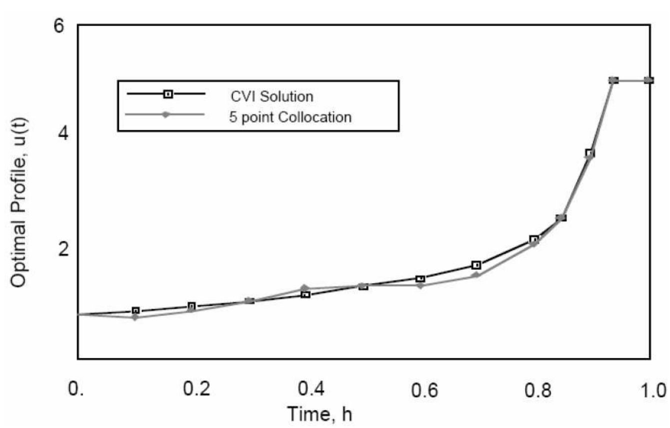
24

Batch Reactor Optimal Temperature Program
Indirect Approach



<u>Results:</u>
Control Vector Iteration with Conjugate Gradients
Optimum (B/A): <u>0.5732</u>
Equivalent # of ODE solutions: <u>58</u>

Results of Optimal Temperature Program
Batch Reactor (Revisited)



<u>Results</u> - NLP with Orthogonal Collocation
Optimum B/A - <u>0.5728</u>
# of ODE Solutions - <u>0.7</u> (Equivalent)

Dynamic Optimization Engines

Evolution of NLP Solvers:

➔ ***for dynamic optimization, control and estimation***

SQP

E.g., ***NPSOL*** and Sequential Dynamic Optimization - over 100 variables and constraints

27

Dynamic Optimization Engines

Evolution of NLP Solvers:

➔ ***for dynamic optimization, control and estimation***

SQP ⟶ rSQP

E.g, ***SNOPT*** and Multiple Shooting - over 100 d.f.s but over 10^5 variables and constraints

28

Dynamic Optimization Engines

Evolution of NLP Solvers:

➔ ***for dynamic optimization, control and estimation***

SQP ⟶ rSQP ⟶ Full-space Barrier

E.g., ***IPOPT*** - Simultaneous dynamic optimization over 1 000 000 variables and constraints

Object Oriented Codes tailored to structure, sparse linear algebra and computer architecture (e.g., IPOPT 3.3)

29

Barrier Methods for Large-Scale Nonlinear Programming

Original Formulation

$$\min_{x \in \Re^n} f(x)$$
$$\text{s.t} \quad c(x) = 0$$
$$x \geq 0$$

Can generalize for

$$a \leq x \leq b$$

Barrier Approach

$$\min_{x \in \Re^n} \varphi_\mu(x) = f(x) - \mu \sum_{i=1}^{n} \ln x_i$$
$$\text{s.t} \quad c(x) = 0$$

$\Rightarrow$As μ ➔ 0, $x^*(\mu)$ ➔ x^* Fiacco and McCormick (1968)

30

Solution of the Barrier Problem

⇒**Newton Directions (KKT System)**

$$\begin{aligned} \nabla f(x) + A(x)\lambda - v &= 0 \\ Xv - \mu e &= 0 \\ c(x) &= 0 \end{aligned}$$

$e^T = [1, 1, 1...]$

$X = diag(x)$

⇒**Solve**

$$\begin{bmatrix} W & A & -I \\ A^T & 0 & 0 \\ V & 0 & X \end{bmatrix} \begin{bmatrix} d_x \\ d_\lambda \\ d_v \end{bmatrix} = - \begin{bmatrix} \nabla f + A\lambda - v \\ c \\ Xv - \mu e \end{bmatrix}$$

IPOPT Code – www.coin-or.org

31

Solution of the Barrier Problem

⇒**Newton Directions (KKT System)**

$$\begin{aligned} \nabla f(x) + A(x)\lambda - v &= 0 \\ Xv - \mu e &= 0 \\ c(x) &= 0 \end{aligned}$$

$e^T = [1, 1, 1...]$

$X = diag(x)$

⇒ **Reducing the System**

$$d_v = \mu X^{-1} e - v - X^{-1} V d_x$$

$$\begin{bmatrix} W + \Sigma & A \\ A^T & 0 \end{bmatrix} \begin{bmatrix} d_x \\ \lambda^+ \end{bmatrix} = - \begin{bmatrix} \nabla \varphi_\mu \\ c \end{bmatrix} \qquad \Sigma = X^{-1} V$$

IPOPT Code – www.coin-or.org

32

IPOPT Algorithm – Features

Line Search Strategies for Globalization

- ℓ_2 exact penalty merit function
- augmented Lagrangian merit function
- **Filter method (adapted and extended from Fletcher and Leyffer)**

Hessian Calculation

- BFGS (full/LM and reduced space)
- SR1 (full/LM and reduced space)
- **Exact full Hessian (direct)**
- Exact reduced Hessian (direct)
- Preconditioned CG

Algorithmic Properties

Globally, superlinearly convergent (Wächter and B., 2005)

Easily tailored to different problem structures

Freely Available

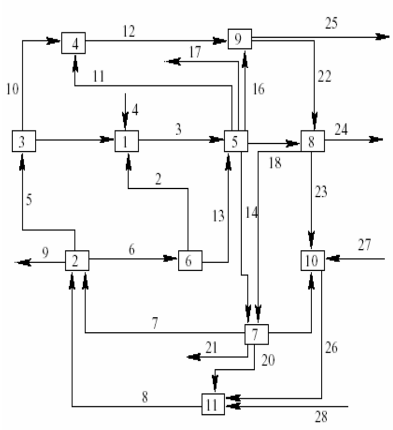
CPL License and COIN-OR distribution: **http://www.coin-or.org**

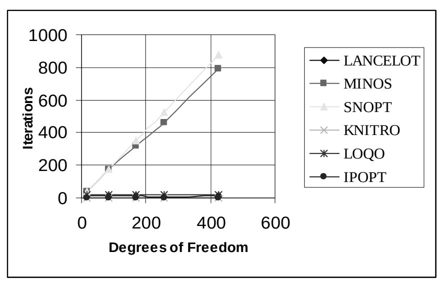
IPOPT 3.x recently rewritten in C++

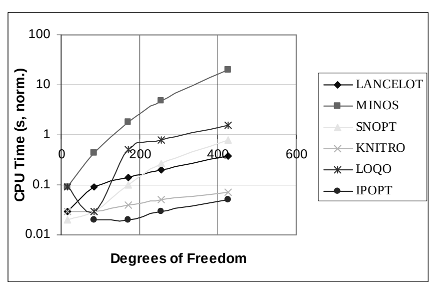
Solved on thousands of test problems and applications

33

Comparison of NLP Solvers: Data Reconciliation
(Poku, Kelly, B. (2004))







34

Comparison of Computational Complexity

($\alpha \in [2, 3]$, $\beta \in [1, 2]$, n_w, n_u - assume $N_m = O(N)$)

	Single Shooting	Multiple Shooting	Simultaneous
DAE Integration	$n_w^\beta N$	$n_w^\beta N$	---
Sensitivity	$(n_w N)(n_u N)$	$(n_w N)(n_u + n_w)$	$N(n_u + n_w)$
Exact Hessian	$(n_w N)(n_u N)^2$	$(n_w N)(n_u + n_w)^2$	$N(n_u + n_w)$
NLP Decomposition	---	$n_w^3 N$	---
Step Determination	$(n_u N)^\alpha$	$(n_u N)^\alpha$	$((n_u + n_w)N)^\beta$
Backsolve	---	---	$((n_u + n_w)N)$
	$O((n_u N)^\alpha + N^2 n_w n_u + N^3 n_w n_u^2)$	$O((n_u N)^\alpha + N n_w^3 + N n_w (n_w + n_u)^2)$	$O((n_u + n_w)N)^\beta$

35

Simultaneous DAE Optimization

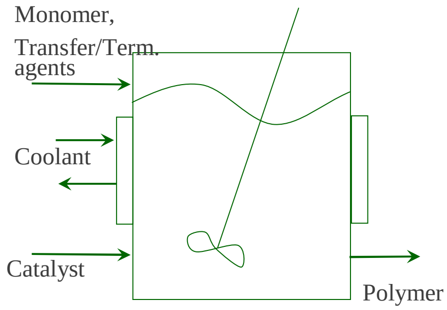
Case Studies

- Reactor - Based Flowsheets
- Fed-Batch Penicillin Fermenter
- Temperature Profiles for Batch Reactors
- Parameter Estimation of Batch Data
- Synthesis of Reactor Networks
- Batch Crystallization Temperature Profiles
- Ramping for Continuous Columns
- Reflux Profiles for Batch Distillation and Column Design
- Air Traffic Conflict Resolution
- Satellite Trajectories in Astronautics
- Batch Process Integration
- Source Detection for Municipal Water Networks
- **Optimization of Simulated Moving Beds**
- **Grade Transition of Polymerization Processes**
- **Parameter Estimation of Tubular Reactors**
- **Nonlinear MPC**

36

Production of High Impact Polystyrene (HIPS)

Startup and Transition Policies (Flores et al., 2005a)



Initiation reactions

Thermal

$$3M_S \xrightarrow{k_{i0}} 2R_S^1$$

Chemical

$$I \xrightarrow{f_1 k_d} 2R$$
$$R + M_S \xrightarrow{k_{i1}} R_S^1$$
$$R + B_0 \xrightarrow{k_{i2}} B_R$$
$$B_R + M_S \xrightarrow{k_{i3}} B_{RS}^1$$

Propagation reactions

$$R_S^j + M_S \xrightarrow{k_p} R_S^{j+1}$$
$$B_{RS}^j + M_S \xrightarrow{k_p} B_{RS}^{j+1}$$

Definite termination reactions

Homopolymer

$$R_S^j + R_S^m \xrightarrow{k_t} P^{j+m}$$

Grafting

$$R_S^j + B_R \xrightarrow{k_t} B_P^j$$
$$R_S^j + B_{RS}^m \xrightarrow{k_t} B_P^{j+m}$$

Crosslinking

$$B_R + B_R \xrightarrow{k_t} B_{EB}$$
$$B_{RS}^j + B_R \xrightarrow{k_t} B_{PB}^j$$
$$B_{RS}^j + B_{RS}^m \xrightarrow{k_t} B_{PB}^{j+m}$$

Transfer reactions

Monomer

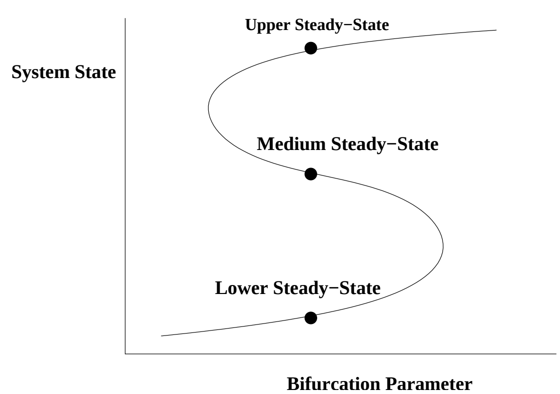
$$R_S^j + M_S \xrightarrow{k_{fs}} P^j + R_S^1$$
$$B_{RS}^j + M_S \xrightarrow{k_{fs}} B_P^j + R_S^1$$

Grafting sites

$$R_S^j + B_0 \xrightarrow{k_{fb}} P^j + B_R$$
$$B_{RS}^j + B_0 \xrightarrow{k_{fb}} B_P^j + B_R$$

Phase Diagram of Steady States

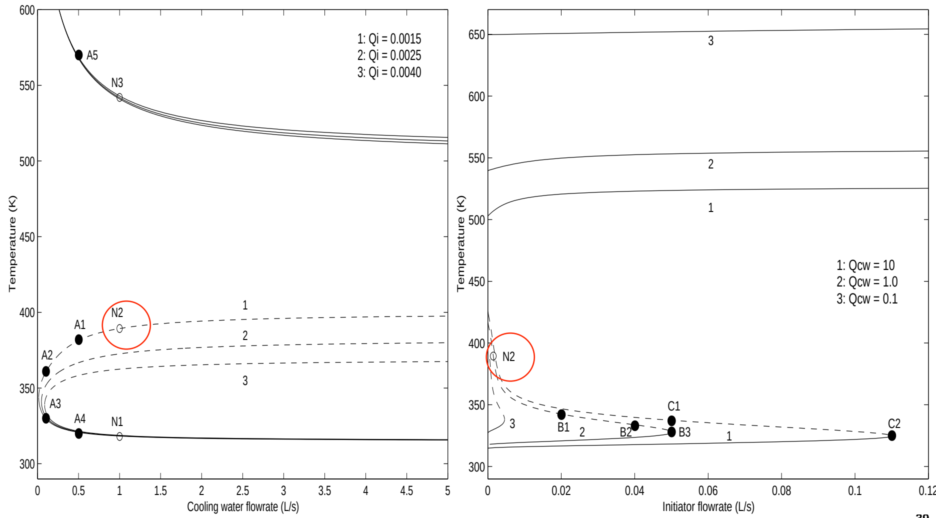
Transitions considered among all steady state pairs



38

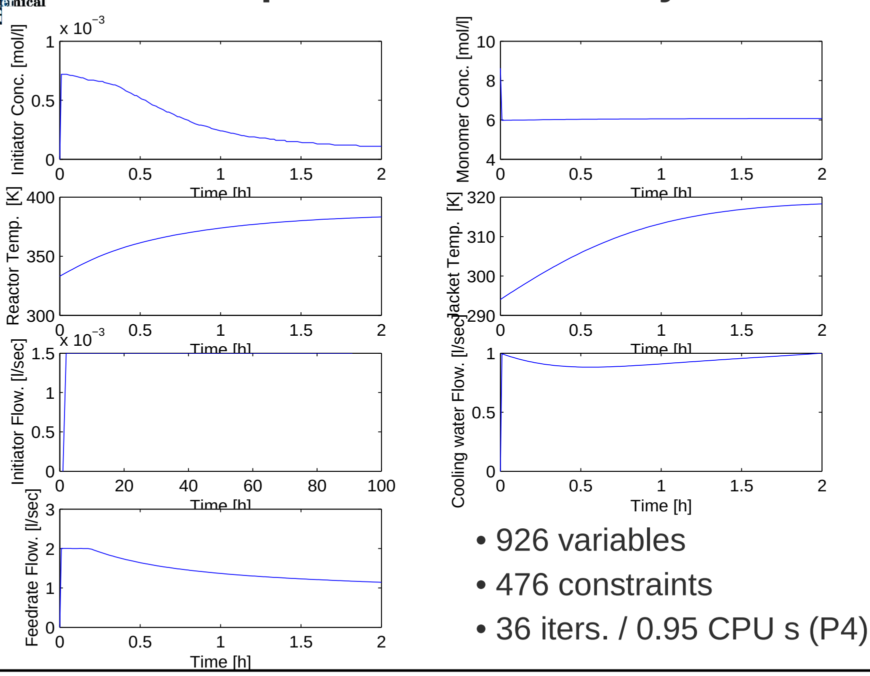
Phase Diagram of Steady States

Transitions considered among all steady state pairs



39

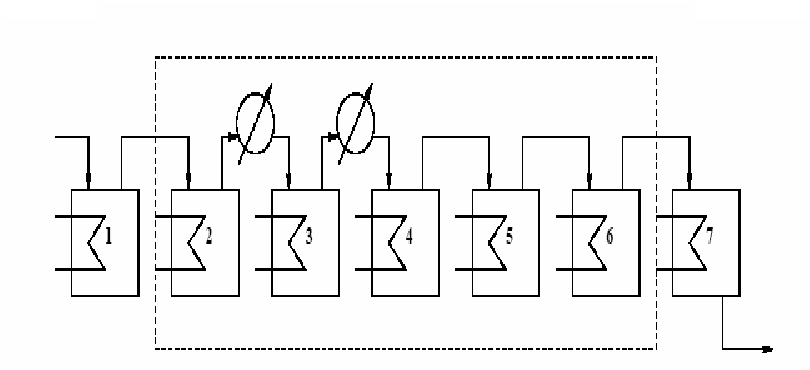
Startup to Unstable Steady State



- 926 variables
- 476 constraints
- 36 iters. / 0.95 CPU s (P4)

40

HIPS Process Plant (Flores et al., 2005b)



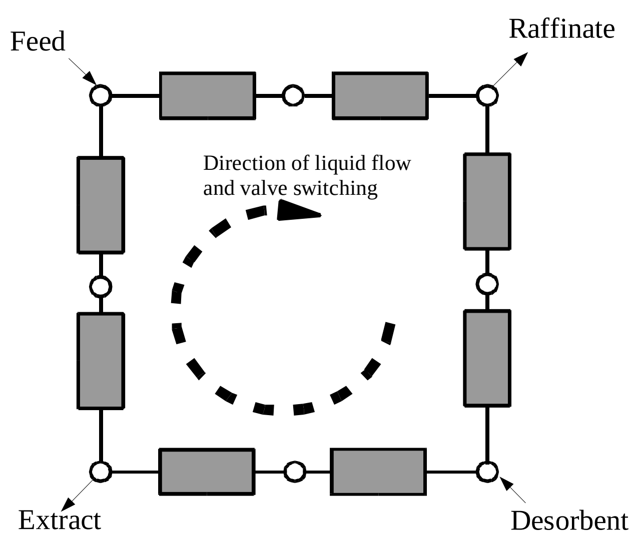
•Many grade transitions considered with stable/unstable pairs

•1-6 CPU min (P4) with IPOPT

•Study shows benefit for sequence of grade changes to achieve wide range of grade transitions.

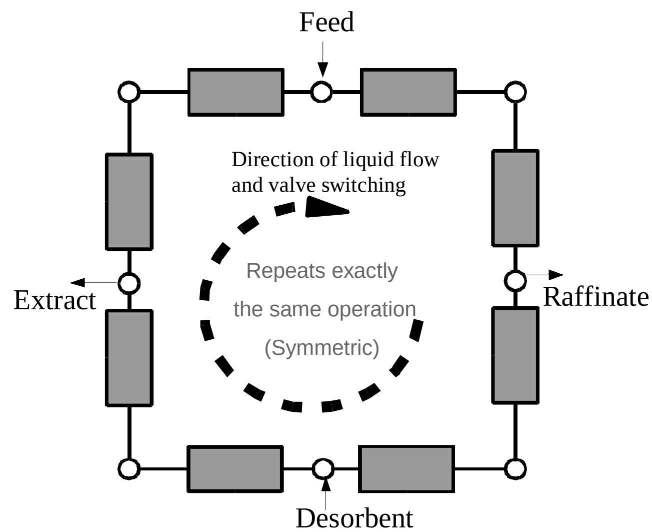
41

Simulated Moving Bed Optimization
(Kawajiri, B., 2005-2007)



42

Simulated Moving Bed Optimization
(Kawajiri, B., 2005-2007)



43

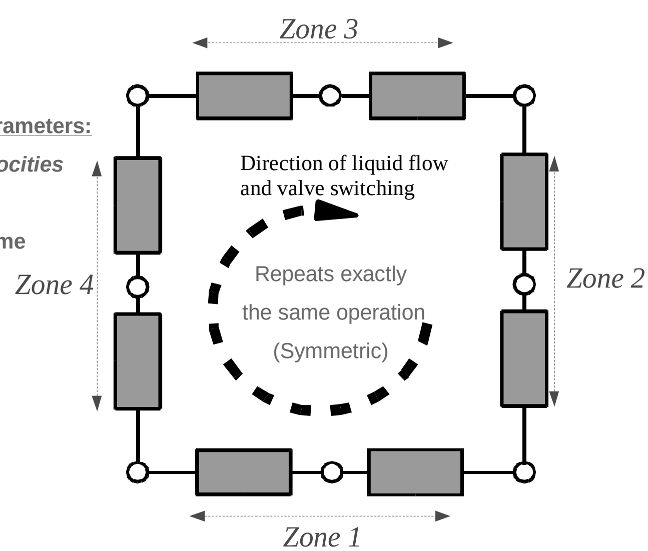
Simulated Moving Bed Optimization
(Kawajiri, B., 2005-2007)

Operating parameters:

4 Zone velocities

+

Step time



44

Formulation of Optimization Problem

Zone velocities Step time

$$\max_{u_I(t),u_{II}(t),u_{III}(t),u_{IV}(t),t_{step}} \quad \bar{u}_F := \frac{1}{t_{step}} \int_0^{t_{step}} u_F(t)dt$$

(Maximize average feed velocity)

Product requirements

$$(Extract \quad Product \quad Purity) = \frac{\int_0^{t_{step}} u_E(t) C_{E,k}(t)dt}{\sum_{i=1}^{Nc} \int_0^{t_{step}} u_E(t) C_{E,i}(t)dt} \geq Pur_{min}$$

$$(Extract \quad Product \quad Recovery) = \frac{\int_0^{t_{step}} u_E(t) C_{E,k}(t)dt}{\int_0^{t_{step}} u_F(t) C_{F,k}(t)dt} \geq Rec_{min}$$

Bounds on liquid velocities

$$u_l \leq u_m(t) \leq u_u \qquad m = I, II, III, IV$$

SMB model

$$\epsilon \frac{\partial C_i(x,t)}{\partial t} + (1-\epsilon)\frac{\partial q_i(x,t)}{\partial t} + u_m \frac{\partial C_i(x,t)}{\partial x} = 0$$

$$(1-\epsilon)\frac{\partial q_i(x,t)}{\partial t} = K_{app\,i}(C_i(x,t) - C_i^{eq}(x,t))$$

$$q_{n,i}(x,t) = K_i C_{n,i}^{eq}(x,t)$$

CSS constraint

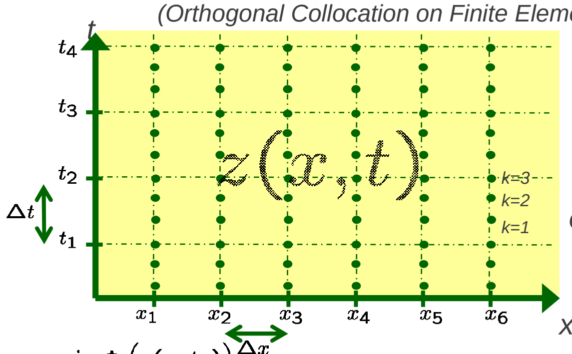
$$C_i(x,t) = C_i(x, t + t_{step})$$

$$q_i(x,t) = q_i(x, t + t_{step})$$

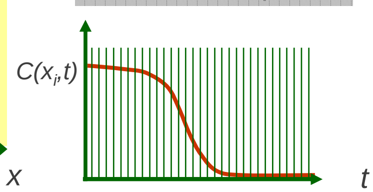
45

Treatment of PDEs: Simultaneous Approach

(Orthogonal Collocation on Finite Elements)



Step size is determined a priori



Huge number of variables (handled by optimizer)

$$\min_p \Phi\left(z(x,t_f)\right)$$

$subject \quad to:$

$$f_{i,j,k}\left(p, \left(\frac{\Delta z}{\Delta x}\right)_{i,j,k}, \left(\frac{dz}{dt}\right)_{i,j,k}\right) = 0, \qquad \left(\frac{\Delta z}{\Delta x}\right)_{i,j,k} = \frac{z_{i+1,j,k} - z_{i-1,j,k}}{x_{i+1,j} - x_{i-1,j}}$$

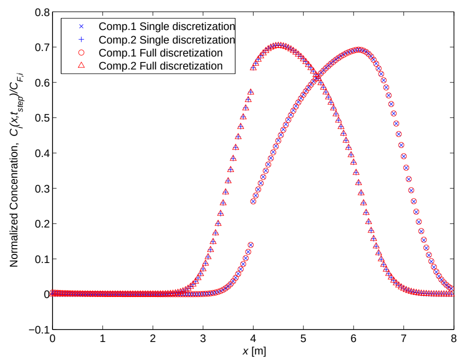
$$g\left(p, z(x,t)\right) \leq 0 \qquad z_{i,j,k} = z_{i,j}^0 + h_j \sum_{k=1}^{3} \Omega_{j,k} \left(\frac{dz}{dt}\right)_{i,j,k}$$

$$h\left(p, z(x,t)\right) = 0$$

PDE → Algebraic equations

46

Comparison of two approaches



(Linear isotherm, fructose/glucose separation)

Sequential and Simultaneous methods find same optimal solution

Initial feed velocity: 0.01 m/h

↓ Optimization

Optimal feed velocity: 0.52 m/h

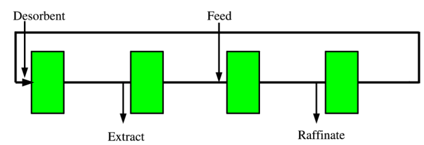
**On Pentium IV 2.8GHz*

	# of variables	CPU Time*	# of iteration
Sequential Approach *Implemented on gPROMS, solved using SRQPD*	644	*111.8 min* *(89% spent by integrator)*	49
Simultaneous Approach *Implemented on AMPL, solved using IPOPT*	33999	**1.53 min**	47

47

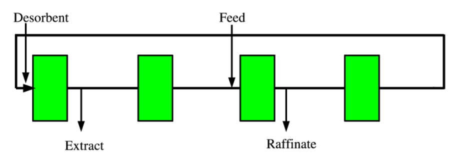
Nonstandard SMB: Addressed by Extended Superstructure NLP

- **Standard SMB**



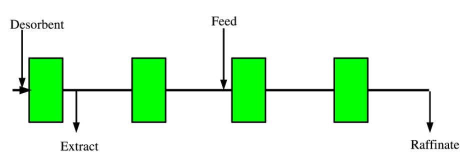
- **VARICOL**

(Asynchronous switching)



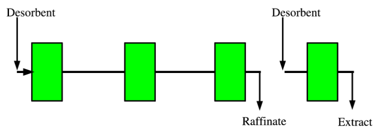
- **Three Zone**

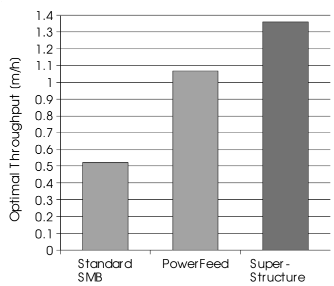
(Circulation loop is cut open)

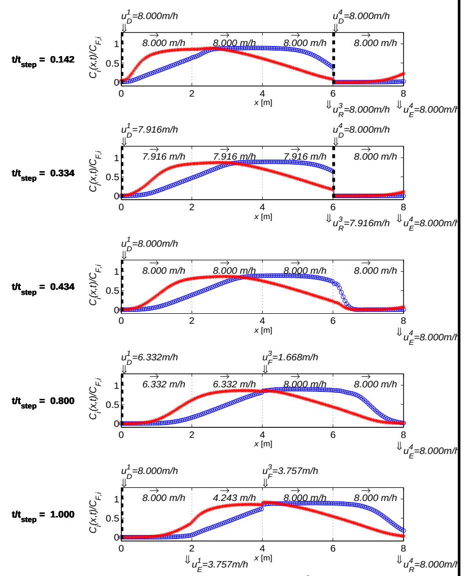


48

Optimal Operating Scheme:
Result of Superstructure Optimization





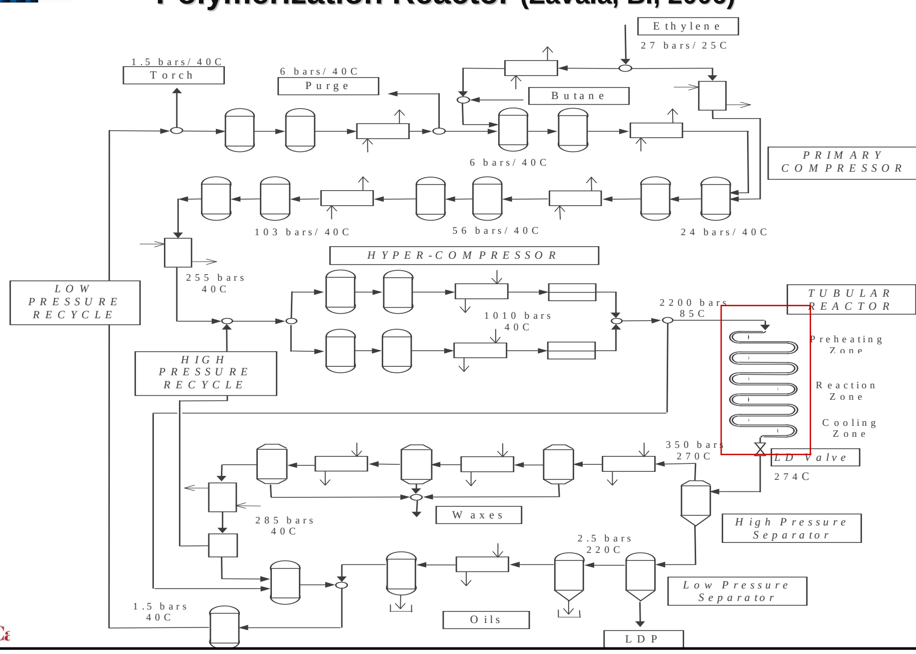


CPU Time for optimization: 9.03 min*

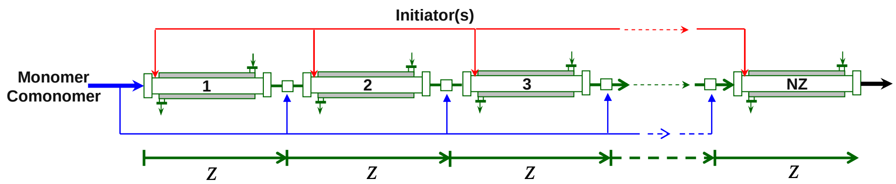
34098 variables, 34013 equations

*on Xeon 3.2 GHz

Large-Scale Parameter Estimation
Polymerization Reactor (Zavala, B., 2006)



Large-Scale Parameter Estimation



Material & Energy

$$\mathbf{F}_j \left[\frac{dy_j(z)}{dz}, y_j(z), w_j(z), z, \pi_j, \Pi \right] = 0$$

Physical Properties

$$\mathbf{G}_j \left[y_j(z), w_j(z), z, \pi_j, \Pi \right] = 0$$

Zone Transitions

$$y_j(0) = \phi(y_{j-1}(z_{L_{j-1}}), F_{f_j})$$

$$j \in \{1..NZ\}$$

500 ODEs

1000 AEs

Stiffness + Highly Nonlinear + Parametric Sensitivity + Algebraic Coupling

51

Large-Scale Parameter Estimation

- **Complex Kinetic Mechanisms**

Initiator decomposition

$$I_i \xrightarrow{k_{d_i}} 2R \quad i = 1, N_I$$

Chain Initiation

$$R^\cdot + M_1 \xrightarrow{k_{I_1}} P_{1,0}$$
$$R^\cdot + M_2 \xrightarrow{k_{I_2}} Q_{0,1}$$

Chain Propagation

$$P_{r,s} + M_1 \xrightarrow{k_{p11}} P_{r+1,s}$$
$$P_{r,s} + M_2 \xrightarrow{k_{p12}} Q_{r,s+1}$$
$$Q_{r,s} + M_1 \xrightarrow{k_{p21}} P_{r+1,s}$$
$$Q_{r,s} + M_2 \xrightarrow{k_{p22}} Q_{r,s+1}$$

Chain Transfer to Monomer

$$P_{r,s} + M_1 \xrightarrow{k_{fm11}} P_{1,0} + M_{r,s}$$
$$P_{r,s} + M_2 \xrightarrow{k_{fm12}} Q_{0,1} + M_{r,s}$$
$$Q_{r,s} + M_1 \xrightarrow{k_{fm21}} P_{1,0} + M_{r,s}$$
$$Q_{r,s} + M_2 \xrightarrow{k_{fm22}} Q_{0,1} + M_{r,s}$$

Chain Transfer to Solvent

$$P_{r,s} + S_i \xrightarrow{k_{si1}} P_{1,0} + M_{r,s}$$
$$Q_{r,s} + S_i \xrightarrow{k_{si2}} Q_{0,1} + M_{r,s}$$

Chain Transfer to Polymer

$$P_{r,s} + M_{x,y} \xrightarrow{k_{fp11}} P_{x,y} + M_{r,s}$$
$$P_{r,s} + M_{x,y} \xrightarrow{k_{fp12}} Q_{x,y} + M_{r,s}$$
$$Q_{r,s} + M_{x,y} \xrightarrow{k_{fp21}} P_{x,y} + M_{r,s}$$
$$Q_{r,s} + M_{x,y} \xrightarrow{k_{fp22}} Q_{x,y} + M_{r,s}$$

Termination by Combination

$$P_{r,s} + P_{x,y} \xrightarrow{k_{tc11}} M_{r+x,s+y}$$
$$P_{r,s} + Q_{x,y} \xrightarrow{k_{tc12}} M_{r+x,s+y}$$
$$Q_{r,s} + Q_{x,y} \xrightarrow{k_{tc22}} M_{r+x,s+y}$$

Termination by Disproportionation

$$P_{r,s} + P_{x,y} \xrightarrow{k_{td11}} M_{r,s} + M_{x,y}$$
$$P_{r,s} + Q_{x,y} \xrightarrow{k_{td12}} M_{r,s} + M_{x,y}$$
$$Q_{r,s} + Q_{x,y} \xrightarrow{k_{td22}} M_{r,s} + M_{x,y}$$

Backbitting

$$P_{r,s} \xrightarrow{k_{b1}} P_{r,s} \ or \ Q_{r,s}$$
$$P_{r,s} \xrightarrow{k_{b2}} Q_{r,s} \ or \ P_{r,s}$$

β-scission

$$P_{r,s} \xrightarrow{k_{\beta 1}} M^{=}_{r,s} + P_{1,0}$$
$$P_{r,s} \xrightarrow{k_{\beta 2}} M^{=}_{r,s} + Q_{0,1}$$

$$k = k_0 \ exp\left(-\frac{E_a + P\,E_v}{RT}\right)$$

~ 35 Elementary Reactions

~100 Kinetic Parameters

52

Large-Scale Parameter Estimation

- Parameter Estimation for Industrial Applications
  - Use Rigorous Model to Match Plant Data Directly
  - Start with Standard Least-Squares Formulation

$$\min_{\Pi,\pi_{k,j}} \sum_{k=1}^{NS}\sum_{j=1}^{NZ}\sum_{i=1}^{NM(j)} \left(y_{k,j}(z_i)-y^M_{k,j,i}\right)^T \mathbf{V}_{\mathbf{y}}^{-1}\left(y_{k,j}(z_i)-y^M_{k,j,i}\right) + \sum_{k=1}^{NS}\left(w_{k,NZ}-w^M_{k,NZ}\right)^T \mathbf{V}_{\mathbf{w}}^{-1}\left(w_{k,NZ}-w^M_{k,NZ}\right)$$

Least-Squares

$$s.t.$$

$$\mathbf{F}_{k,j}\left[\frac{dy_{k,j}(z)}{dz}, y_{k,j}(z), w_{k,j}(z), z, \pi_{k,j}, \Pi\right] = 0$$

$$\mathbf{G}_{k,j}\left[y_{k,j}(z), w_{k,j}(z), z, \pi_{k,j}, \Pi\right] 0$$

$$y_{k,j}(0) = \phi(y_{k,j-1}(z_{L_{k,j-1}}), F_{f_{k,j}})$$

$$j \in \{1..NZ\}, \quad k \in \{1..NS\}$$

Rigorous Reactor Model

- Special Case of Multi-Stage Dynamic Optimization Problem
  - Solve using Simultaneous Collocation-Based Approach

1 data set		6 data sets
500 ODEs	x 6 →	3000 ODEs
1000 AEs		6000 AEs

Large-Scale Parameter Estimation

- **Multi-Zone Tubular Reactor –** Quasi Steady-State
  - **Data Sets:** Operating Conditions and Properties for Different Grades
  - **Match:** Temperature Profiles and Product Properties
    - **On-line Adjusting Parameters →** Track Evolution of Disturbances
    - **Kinetic Parameters →** Development and Discrimination among Rigorous Models
- **Results**
  - **Single Data Set** (On-line Adjusting Parameters)

Grade	Constraints	Parameters	LB	UB	Iterations	CPUs	NZJ	NZH
A	11955	32	374	361	11	17.03	166425	87954
B	11283	32	374	361	8	10.06	138666	76890

  - **Multiple Data Sets** (On-line Adjusting Parameters + Kinetics)

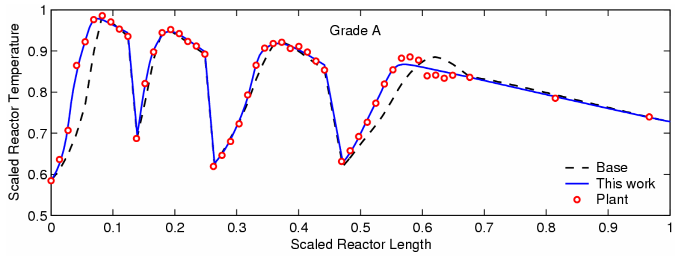
Data Sets	Constraints	DOF	LB	UB	Iterations	CPUs	NZJ	NZH
3	33900	121	1246	1207	68	451.51	520275	552738
6	68421	217	2467	2389	58	900.21	1058412	1119258

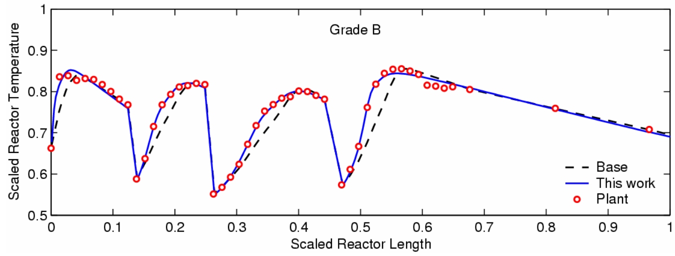
Bottleneck (Memory Requirements)
Factorization Step

$$\begin{bmatrix} W(x_k,\lambda_k) & A(x_k) & -I \\ A(x_k)^T & 0 & 0 \\ V_k & 0 & X_k \end{bmatrix}\begin{bmatrix} \Delta x \\ \Delta\lambda \\ \Delta\nu \end{bmatrix} = -\begin{bmatrix} \nabla f(x_k)+A(x_k)\lambda_k-\nu_k \\ c(x_k) \\ X_k V_k e - \mu_\ell e \end{bmatrix}$$

Large-Scale Parameter Estimation

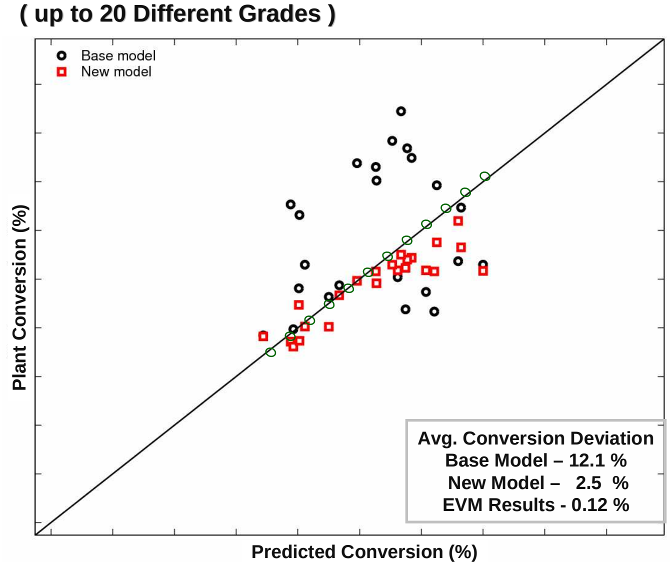
Improved Match of Reactor Temperatures Profile





Industial Case Study

- **Results - Reactor Overall Monomer Conversion (up to 20 Different Grades)**



Carnegie Mellon

Parameter Estimation in Parallel Architectures

Exploit Structure of KKT Matrix – *Laird, B. 2006*

$$\min_{\Pi, \pi_{k,j}} \sum_{k=1}^{NS}\sum_{j=1}^{NZ}\sum_{i=1}^{NM(j)} \left(y_{k,j}(z_i)-y^M_{k,j,i}\right)^T \mathbf{V}_\mathbf{y}^{-1}\left(y_{k,j}(z_i)-y^M_{k,j,i}\right) + \sum_{k=1}^{NS}\left(w_{k,NZ}-w^M_{k,NZ}\right)^T \mathbf{V}_\mathbf{w}^{-1}\left(w_{k,NZ}-w^M_{k,NZ}\right)$$

$s.t.$

$$\mathbf{F}_{k,j}\left[\frac{dy_{k,j}(z)}{dz}, y_{k,j}(z), w_{k,j}(z), z, \pi_{k,j}, \Pi\right]=0$$
$$\mathbf{G}_{k,j}\left[y_{k,j}(z), w_{k,j}(z), z, \pi_{k,j}, \Pi\right]=0$$
$$y_{k,j}(0)=\phi(y_{k,j-1}(z_{L_{k,j-1}}), F_{f_{k,j}})$$
$$j \in \{1..NZ\},\quad k \in \{1..NS\}$$

$$\min\ f(x) \quad \text{s.t.}\ c(x)=0,\ x \geq 0$$

$$\begin{bmatrix} H_k & A_k & -I \\ A_k^T & 0 & 0 \\ V_k & 0 & X_k \end{bmatrix}\begin{bmatrix} \Delta x \\ \Delta\lambda \\ \Delta\nu \end{bmatrix} = -\begin{bmatrix} r_x \\ r_\lambda \\ X_k V_k e - \mu_\ell e \end{bmatrix}$$

Direct Factorization MA27
Memory Bottlenecks
Factorization Time *Scales*
***Superlinearly* with Data sets**

$$\text{in}\ \sum_{k=1}^{N_S} f_k(x_k) \quad \text{s.t.}\ c_k(x_k,\Pi)=0,\ x_k,\Pi \geq 0$$

$$\begin{bmatrix} \mathbf{K}_1 & & & & Q_1 \\ & \mathbf{K}_2 & & & Q_2 \\ & & \ddots & & \vdots \\ & & & \mathbf{K}_N & Q_N \\ Q_1^T & Q_2^T & \dots & Q_N^T & D_\Pi \end{bmatrix}\begin{bmatrix} \Delta s_1 \\ \Delta s_2 \\ \vdots \\ \Delta s_N \\ \Delta\Pi \end{bmatrix} = -\begin{bmatrix} r_1 \\ r_2 \\ \vdots \\ r_N \\ r_\Pi \end{bmatrix}$$

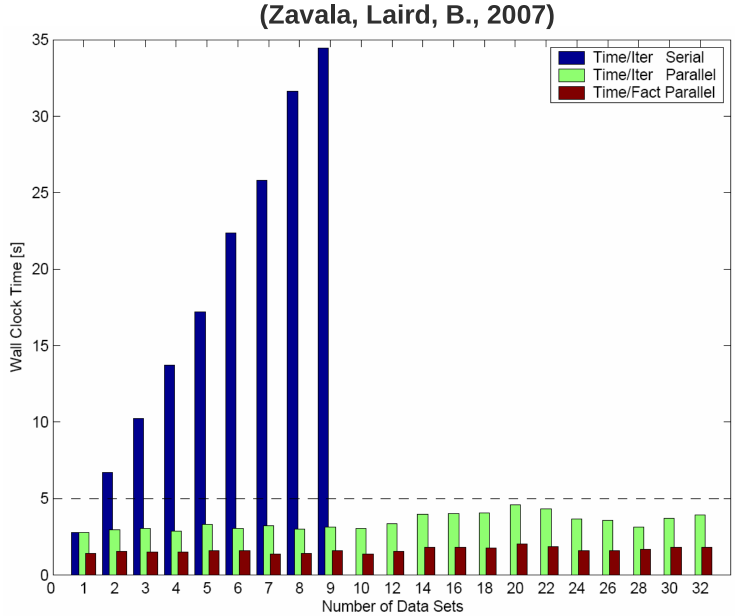
Block-bordered Diagonal Structure
Coarse-Grained Parallelization using Schur Complement Decomposition

IPOPT 3.x architecture supports tailored structured decompositions

57

Parameter Estimation in Parallel Architectures

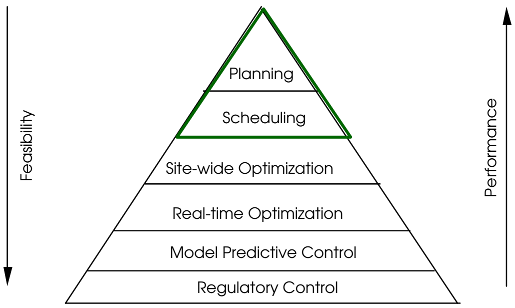
(Zavala, Laird, B., 2007)



Computational Results – LDPE Reactor EVM Problem

58

Decision-making in Chemical Industries



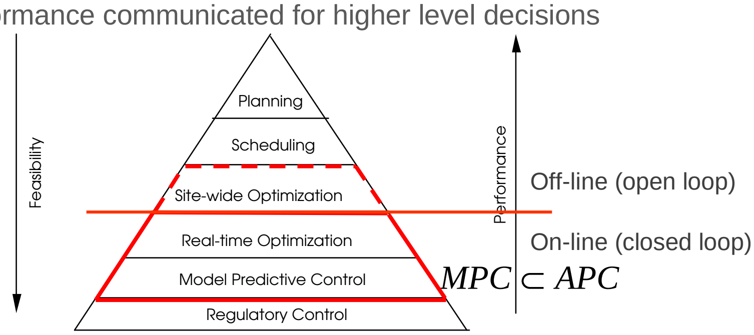
Supply Chain, Planning and Scheduling

- Large LP and MILP models
- Many Discrete Decisions
- Few Nonlinearities
- Essential link needed to process models
- ***Decisions need to be feasible at lower levels***

Decision Pyramid for Process Operations

Real-time Optimization and Advanced Process Control

- Fewer discrete decisions
- Many nonlinearities
- Frequent, “on-line” time-critical solutions
- Higher level decisions must be feasible
- Performance communicated for higher level decisions



Dynamic Real-time Optimization

Integrate On-line Optimization/Control with Off-line Planning

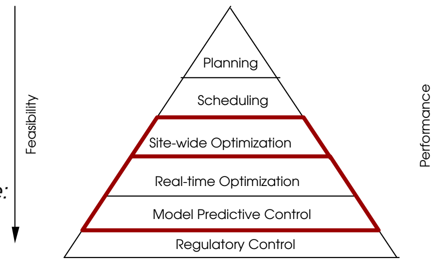
- Consistent, first-principle models
- Consistent, long-range, multi-stage planning
- Increase in computational complexity
- Time-critical calculations

Applications

- Batch processes
- Grade transitions
- Cyclic reactors (coking, regeneration…)
- Cyclic processes (PSA, SMB…)

Continuous processes are never in steady state:

- Feed changes
- Nonstandard operations
- Optimal disturbance rejections



Simulation environments and first principle dynamic models are widely used for off-line studies

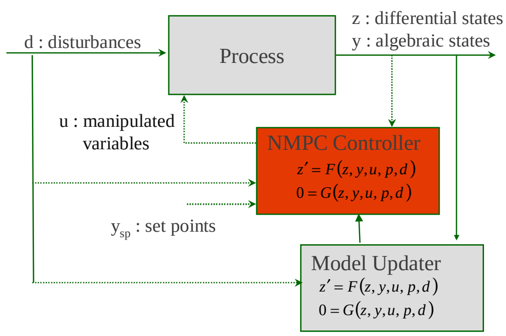
Can these results be implemented directly on-line for large-scale systems?

8

61

Nonlinear Model Predictive Control (NMPC)

NMPC Estimation and Control



Why NMPC?

- Track a profile
- Severe nonlinear dynamics (e.g, sign changes in gains)
- Operate process over wide range (e.g., startup and shutdown)

NMPC Subproblem

$$\min_{u} \sum \| y(t) - y^{sp} \|^2_{Q_y} + \sum \| \mathbf{u}(\mathbf{t}^k) - \mathbf{u}(\mathbf{t}^{k-1}) \|^2_{Q_u}$$

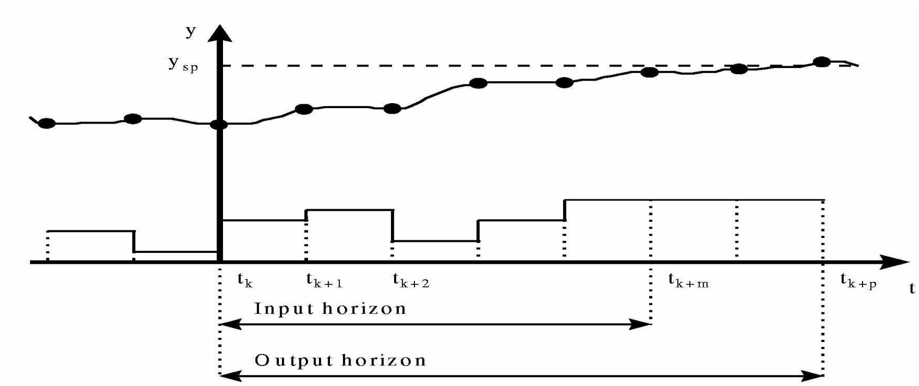
$$s.t. \quad z'(t) = F(z(t), y(t), \mathbf{u}(t), t)$$
$$0 = G(z(t), y(t), \mathbf{u}(t), t)$$
$$z(t) = z^{\text{init}}$$

Bound Constraints

Other Constraints

62

Nonlinear Model Predictive Control (NMPC)



$$\min_{\boldsymbol{u}} \quad \sum \| y(t) - y^{sp} \|^2_{Q_y} + \sum \| \boldsymbol{u}(t^k) - \boldsymbol{u}(t^{k-1}) \|^2_{Q_u}$$

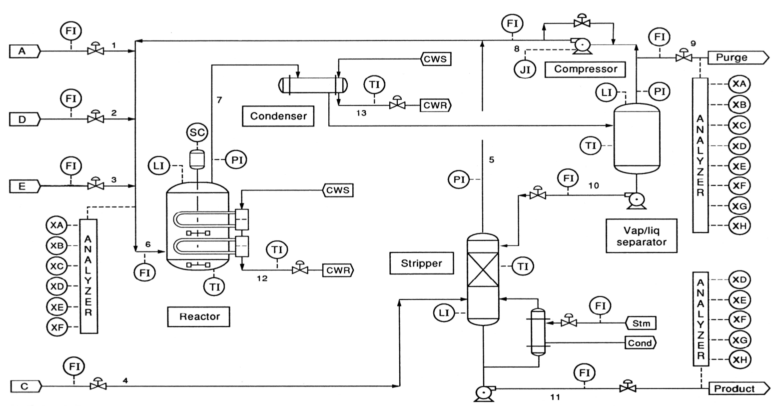
$$\begin{aligned} s.t. \quad & z'(t) = F(z(t), y(t), \boldsymbol{u}(t), t) \\ & 0 = G(z(t), y(t), \boldsymbol{u}(t), t) \\ & z(t) = z^{init} \end{aligned}$$

Bound Constraints

Other Constraints

63

Tennessee Eastman Process
(Downs and Vogel, 1993)



Unstable Reactor

11 Controls; Product, Purge streams

Model extended with energy balances

64

Tennessee Eastman NMPC Model
(Jockenhövel, Wächter, B., 2003)

DAE Model	
Number of differential equations	30
Number of algebraic variables	152
Number of algebraic equations	141
Difference (control variables)	11

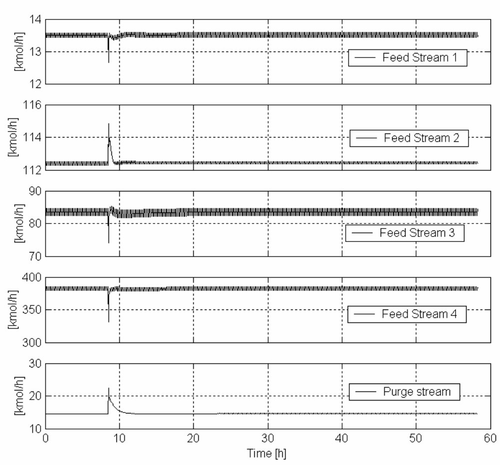
NLP Optimization problem	
Number of variables of which are fixed	10920 0
Number of constraints	10260
Number of lower bounds	780
Number of upper bounds	540
Number of nonzeros in Jacobian	49230
Number of nonzeros in Hessian	14700

Method of Full Discretization of State and Control Variables

Large-scale Sparse block-diagonal NLP

65

Case Study:
Change Reactor pressure by 60 kPa



Control profiles

All profiles return to their base case values

Same production rate

Same product quality

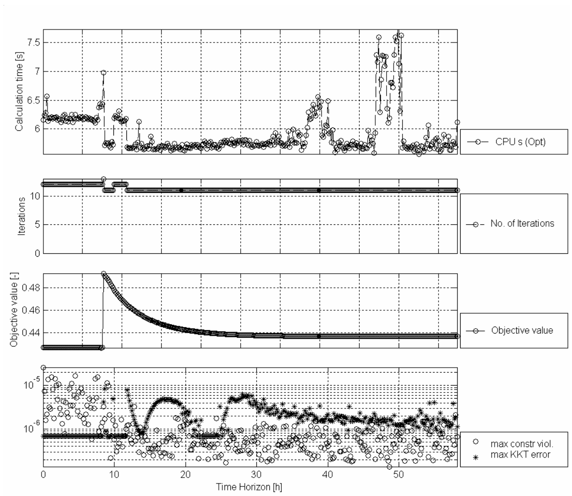
Same control profile

Lower pressure – leads to larger gas phase (reactor) volume

Less compressor load

66

Case Study: Change Reactor Pressure by 60 kPa



Optimization with IPOPT

1000 Optimization Cycles

5-7 CPU seconds

11-14 Iterations

Optimization with SNOPT

Often failed due to poor conditioning

Could not be solved within sampling times

> 100 Iterations

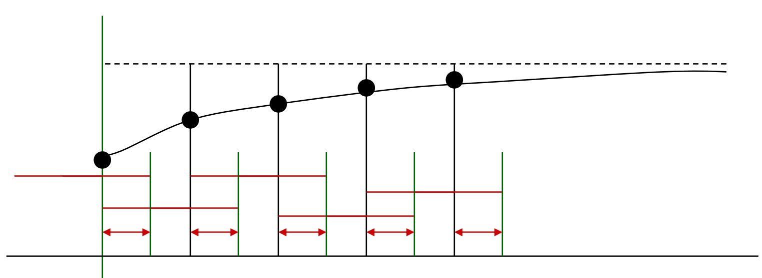
67

Limitations to NMPC Implementation

Issues: time-critical, more complex models, fast NLP solvers.

Computational delay – between receipt of process measurement and injection of control, determined by cost of dynamic optimization

Leads to loss of ***performance*** and ***stability*** (see Findeisen and Allgöwer, 2004; Santos et al., 2001)



As larger NLPs are considered for NMPC, can computational delay be overcome?

68

Avoid computational delay due to on-line optimization?

Real-time Iteration

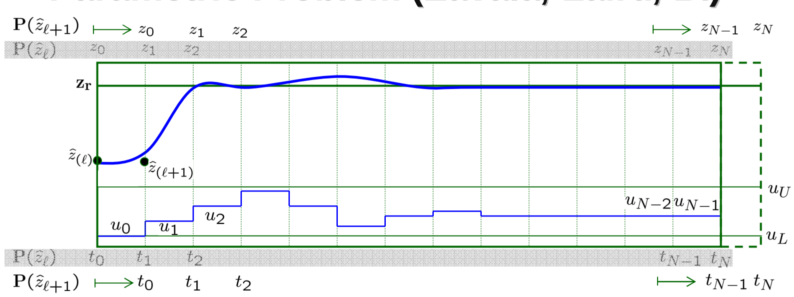
- preparation, feedback response and transition stages
- solve perturbed (linearized) problem on-line
  - Li, de Oliveira, Santos, B. (1990+)
  - Diehl, Findeisen, Bock, Allgöwer et al. (2000+)
  - > two orders of magnitude reduction in on-line computation
- solve complete NLP in background (‘between’ sampling times as part of preparation and transition stages

Based on NLP sensitivity for dynamic systems

- Extended to Simultaneous Collocation approach – Zavala et al. (2007)
- Develop Advanced Step NMPC
- Related to MPC with linearization constantly updated one step behind

69

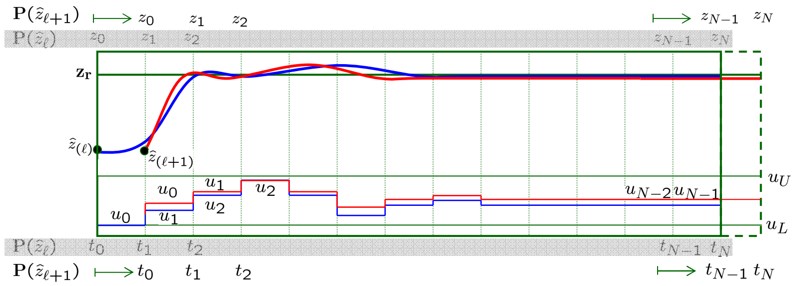
Nonlinear Model Predictive Control – Parametric Problem (Zavala, Laird, B.)



$$\left.\begin{array}{llcl} \mathcal{P}(x(k),N) & \min\limits_{v_{l|k}} J(x(k),N) & = & F(z_{k+N|k}) + \sum\limits_{l=k}^{k+N-1} \psi(z_{l|k}, v_{l|k}) \\ & \text{s. t.:} \quad z_{l+1|k} & = & f(z_{l|k}, v_{l|k}), \quad l = k, \ldots k+N-1 \\ & \boxed{z_{k|k} = x(k) = p_0} & & \\ & z_{l|k} & \in & \mathbb{X},\ z_{k+N|k} \in \mathbb{X}_f,\ v_{l|k} \in \mathbb{U}. \end{array}\right\} \mathrm{P}(p_0)$$

70

Nonlinear Model Predictive Control – Parametric Problem (Zavala, Laird, B.)



$$\mathcal{P}(x(k),N) \quad \min_{v_{l|k}} \; J(x(k),N) = F(z_{k+N|k}) + \sum_{l=k}^{k+N-1} \psi(z_{l|k}, v_{l|k})$$

$$\text{s. t.:} \quad z_{l+1|k} = f(z_{l|k}, v_{l|k}), \quad l = k, \ldots k+N-1$$

$$\boxed{z_{k|k} = x(k) = p_0}$$

$$z_{l|k} \in \mathbb{X}, \; z_{k+N|k} \in \mathbb{X}_f, \; v_{l|k} \in \mathbb{U}.$$

$\Bigg\}$ $\mathrm{P}(p_0)$

$\mathrm{P}(p)$

$$\mathcal{P}(x(k+1),N) \quad \min_{v_{l|k+1}} \; J(x(k+1),N) = F(z_{k+N+1|k+1}) + \sum_{l=k+1}^{k+N} \psi(z_{l|k+1}, v_{l|k+1})$$

$$\text{s. t.:} \quad z_{l+1|k+1} = f(z_{l|k+1}, v_{l|k+1}), \quad l = k+1, \ldots k+N$$

$$\boxed{z_{k|k+1} = x(k+1) = p}$$

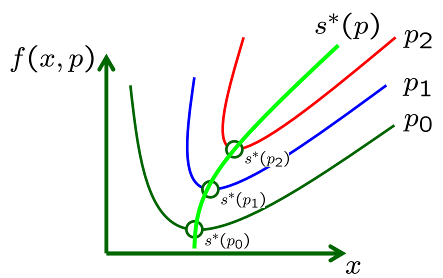
$$z_{l|k+1} \in \mathbb{X}, \; z_{k+N+1|k+1} \in \mathbb{X}_f, \; v_{l|k} \in \mathbb{U}.$$

71

NLP Sensitivity

Parametric Programming

$$\left.\begin{aligned} \min \quad & f(x,p) \\ \text{s.t.} \quad & c(x,p) = 0 \\ & x \geq 0 \end{aligned}\right\} \mathrm{P}(p)$$



Solution Triplet

$s^*(p)^T = [x^{*T} \; \lambda^{*T} \; \nu^{*T}]$

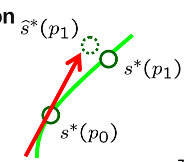
Optimality Conditions $\mathrm{P}(p)$

$$\begin{aligned} \nabla_x f(x,p) + \nabla_x c(x,p)\,\lambda - \nu &= 0 \\ c(x,p) &= 0 \\ XVe &= 0 \end{aligned}$$

NLP Sensitivity → Rely upon Existence and Differentiability of $s^*(p)$

→ Main Idea: Obtain $\left.\frac{\partial s}{\partial p}\right|_{p_0}$ **and find** $\hat{s}^*(p_1)$ **by Taylor Series Expansion**

$$\hat{s}^*(p_1) \approx s^*(p_0) + \left.\frac{\partial s}{\partial p}^T\right|_{p_0} (p_1 - p_0)$$



72

NLP Sensitivity

Obtaining $\left.\frac{\partial s}{\partial p}\right|_{p_0}$

Optimality Conditions of $\mathrm{P}(p)$

$$\left.\begin{aligned}\nabla_x \mathcal{L} = \nabla_x f(x,p) + \nabla_x c(x,p)\,\lambda - \nu &= 0\\ c(x,p) &= 0\\ XVe &= 0\end{aligned}\right\}\ \mathrm{Q}(s,p) = 0$$

Apply Implicit Function Theorem to $\mathrm{Q}(s,p) = 0$ **around** $(p_0, s^*(p_0))$

$$\frac{\partial \mathrm{Q}(s^*(p_0),p_0)}{\partial s}\left.\frac{\partial s}{\partial p}\right|_{p_0} + \frac{\partial \mathrm{Q}(s^*(p_0),p_0)}{\partial p} = 0$$

$$\begin{bmatrix} W(s^*(p_0)) & A(x^*(p_0)) & -I \\ A(x^*(p_0))^T & 0 & 0 \\ V^*(p_0) & 0 & X^*(p_0)\end{bmatrix}\begin{bmatrix}\frac{\partial x}{\partial p}\\ \frac{\partial \lambda}{\partial p}\\ \frac{\partial \nu}{\partial p}\end{bmatrix} + \begin{bmatrix}\nabla_{x,p}\mathcal{L}(s^*(p_0))\\ \nabla_p\, c(x^*(p_0))\\ 0\end{bmatrix} = 0$$

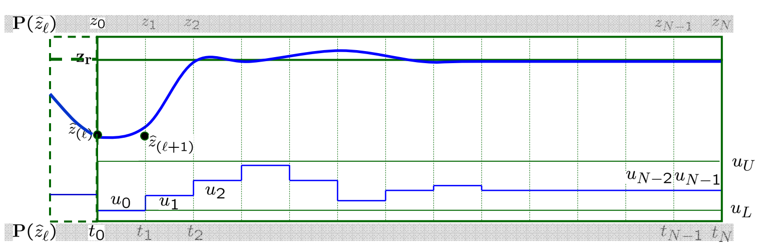
KKT Matrix IPOPT

$$\begin{bmatrix} W(x_k,\lambda_k) & A(x_k) & -I \\ A(x_k)^T & 0 & 0 \\ V_k & 0 & X_k\end{bmatrix}$$

- → **Already Factored at Solution**
- → **Sensitivity Calculation from Single Backsolve**
- → **Approximate Solution Retains Active Set**

73

Key Concept – Relate to Previous Horizon



$$\begin{aligned}\mathcal{P}(x(k),N) \quad \min_{v_{l|k}}\ J(x(k),N) &= F(z_{k+N|k}) + \sum_{l=k}^{k+N-1}\psi(z_{l|k},v_{l|k})\\ \text{s. t.:}\quad z_{l+1|k} &= f(z_{l|k},v_{l|k}),\quad l=k,\dots k+N-1\\ z_{k|k} &= x(k) = p_0\\ z_{l|k} &\in \mathbb{X},\ z_{k+N|k}\in\mathbb{X}_f,\ v_{l|k}\in\mathbb{U}.\end{aligned}$$

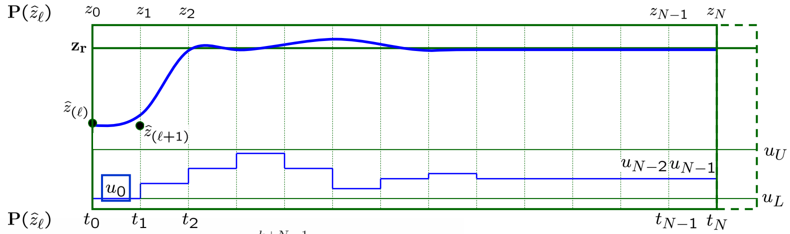
Solutions to both problems are equivalent in nominal case (ideal plant model, no disturbances)

$$\begin{aligned}\bar{\mathcal{P}}(x(k-1),N+1) \quad \min_{v_{l|k}}\ J(x(k-1),N) &= F(z_{k+N|k-1}) + \sum_{l=k}^{k+N-1}\psi(z_{l|k},v_{l|k})\\ \text{s. t.:}\quad z_{l+1|k-1} &= f(z_{l|k},v_{l|k}),\quad l=k,\dots k+N-1\\ z_{k|k-1} &= f[x(k-1),u(k-1)]\\ z_{l|k} &\in \mathbb{X},\ z_{k+N|k-1}\in\mathbb{X}_f,\ v_{l|k}\in\mathbb{U}.\end{aligned}$$

74

Advanced Step NMPC

Combine advanced step with sensitivity to solve NLP in background (between steps) – not on-line



$$
\begin{aligned}
\min_{v_{l|k}} \quad J(x(k),N) &= F(z_{k+N|k}) + \sum_{l=k}^{k+N-1} \psi(z_{l|k}, v_{l|k}) \\
\text{s. t.:} \quad z_{k+1|k} &= f(x(k), u(k)), \\
z_{l+1|k} &= f(z_{l|k}, v_{l|k}), \quad l = k+1, \dots k+N-1 \\
z_{k|k} &= z_0 \\
z_{l|k} &\in \mathbb{X}, \; z_{k+N|k} \in \mathbb{X}_f, \; v_{l|k} \in \mathbb{U}.
\end{aligned}
$$

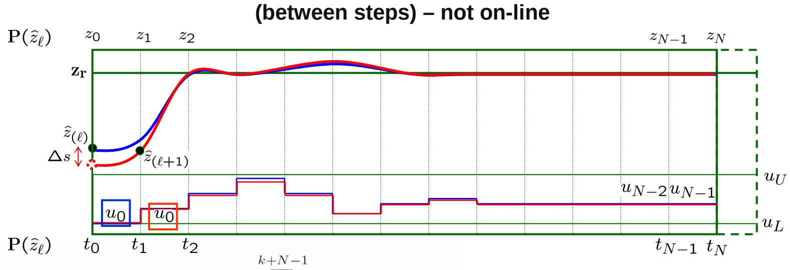
$$
\begin{bmatrix} W_k & A_k & -I \\ A_k^T & 0 & 0 \\ V_k & 0 & X_k \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta \lambda \\ \Delta \nu \end{bmatrix} = K \Delta v
$$

Solve P(z_ℓ) in background (between t_0 and t_1)

75

Advanced Step NMPC

Combine advanced step with sensitivity to solve NLP in background (between steps) – not on-line



$$
\begin{aligned}
\min_{v_{l|k}} \quad J(x(k),N) &= F(z_{k+N|k}) + \sum_{l=k}^{k+N-1} \psi(z_{l|k}, v_{l|k}) \\
\text{s. t.:} \quad z_{k+1|k} &= f(x(k), u(k)), \\
z_{l+1|k} &= f(z_{l|k}, v_{l|k}), \quad l = k+1, \dots k+N-1 \\
z_{k|k} &= z_0 + \Delta s \\
z_{k+1|k} &= z_1 = x(k+1) \\
z_{l|k} &\in \mathbb{X}, \; z_{k+N|k} \in \mathbb{X}_f, \; v_{l|k} \in \mathbb{U}.
\end{aligned}
$$

$$
\begin{bmatrix} W_k & A_k & -I \\ A_k^T & 0 & 0 \\ V_k & 0 & X_k \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta \lambda \\ \Delta \nu \end{bmatrix} = K \Delta v
$$

$$
\left[\begin{array}{c|c} \mathbf{K} & \mathbf{E_0} \\ \hline \mathbf{E_1}^T & 0 \end{array}\right] \begin{bmatrix} \Delta v \\ \Delta s \end{bmatrix} = - \begin{bmatrix} 0 \\ \hat{z}(\ell+1) - z_1^* \end{bmatrix}
$$

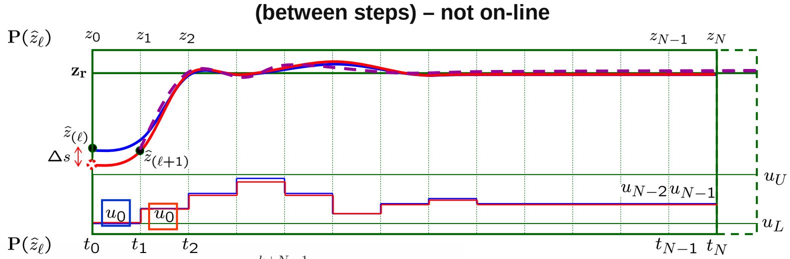
Solve P(z_ℓ) in background (between t_0 and t_1)

Sensitivity to updated problem to get (z_0, u_0)

76

Advanced Step NMPC

Combine advanced step with sensitivity to solve NLP in background (between steps) – not on-line



$$\min_{v_{l|k}} J(x(k),N) = F(z_{k+N|k}) + \sum_{l=k}^{k+N-1} \psi(z_{l|k}, v_{l|k})$$

$$\begin{aligned} \text{s. t.:}\quad z_{k+1|k} &= f(x(k), u(k)), \\ z_{l+1|k} &= f(z_{l|k}, v_{l|k}), \quad l = k+1, \dots k+N-1 \\ z_{k|k} &= z_0 + \Delta s \\ z_{k+1|k} &= z_1 = x(k+1) \\ z_{l|k} &\in \mathbb{X},\ z_{k+N|k} \in \mathbb{X}_f,\ v_{l|k} \in \mathbb{U}. \end{aligned}$$

$$\begin{bmatrix} W_k & A_k & -I \\ A_k^T & 0 & 0 \\ V_k & 0 & X_k \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta \lambda \\ \Delta \nu \end{bmatrix} = K \Delta \upsilon$$

$$\left[\begin{array}{c|c} \mathbf{K} & \mathbf{E_0} \\ \mathbf{E_1}^T & 0 \end{array}\right] \begin{bmatrix} \Delta v \\ \Delta s \end{bmatrix} = -\begin{bmatrix} 0 \\ \hat{z}(\ell+1) - z_1^* \end{bmatrix}$$

Solve $P(z_\ell)$ in background (between t_0 and t_1)

Sensitivity to updated problem to get (z_0, u_0)

Solve $P(z_{\ell+1})$ in background with new (z_0, u_0)

77

AS-NMPC Stability Analysis

Nominal NMPC stability proof

- Nominal case – no noise: perfect model
- General formulation with local asymptotic controller for t → ∞
- Advanced step controller satisfies same relations, has same input sequence
  → shares identical stability property

Plant
$$x_{k+1} = \bar{f}(x_l, u_l)) = f(x_k, u_k)) + g(x_k, u_k, w_k))$$
$$\|g(x_k, u_k, w_k))\| \le L_J \|x_k\| + \sigma(\|w_k\|)$$

Model
$$z_{l+1} = f(z_l, u_l)), z_0 = x_k$$

Robust Stability Margins

- Analysis similar to Limon, Alamo, Camacho (2004), Magni and Scattolini (2005)
- Advanced step NMPC is ISS and tolerates some model mismatch
- ISS property (Jiang and Wang, 2001; Magni and Scattolini, 2005)
- Advanced step NMPC has smaller margin than Ideal NMPC,
  → but can be implemented without computational delay

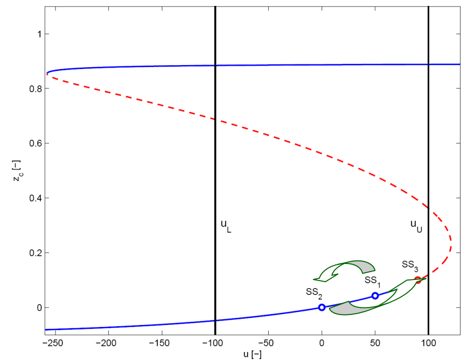
78

CSTR NMPC Example (Hicks and Ray)

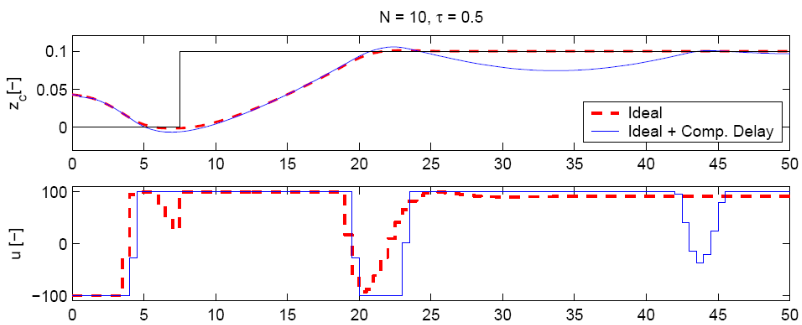
$$
\begin{aligned}
\min_{v_{l|k}} \quad & \sum_{l=k}^{k+N-1} Q_c(z^c_{l|k})^2 + Q_t(z^t_{l|k})^2 + R(v_{l|k})^2 \\
\text{s.t.} \quad z^c_{l+1|k} &= \frac{1}{\theta}(1-(z^c_{l|k}+z^c_{ss})) - k_0 exp\left(-\frac{E_a}{z^t_{l|k}+z^t_{ss}}\right)(z^c_{l|k}+z^c_{ss}) \\
z^t_{l+1|k} &= \frac{1}{\theta}(t_f-(z^t_{l|k}+z^t_{ss})) + k_0 exp\left(-\frac{E_a}{z^t_{l|k}+z^t_{ss}}\right) z^c_{l|k} - \alpha(v+v_s s)((z^t_{l|k}+z^t_{ss})-t_c) \\
z^c_{k|k} &= x^c(k), \;\; z^t_{k|k} = x^t(k) \\
z^c_{k+N|k} &= 0 \;\; z^t_{k+N|k} = 0, \;\; u^U \le v_{l|k} \le u^L.
\end{aligned}
$$

- Maintain unstable setpoint
- Close to bound constraint
- Final time constraint for stability

Effects of:
- Computational Delay
- Measurement Noise
- Model Mismatch
- Advanced Step NMPC

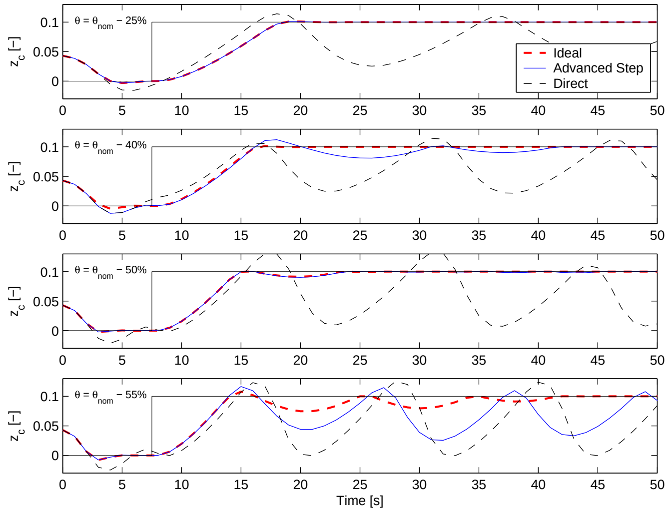


CSTR NMPC Example – Nominal Case



- NMPC applied with N = 10, τ = 0.5 sampling time
- Stable (z = 0) and unstable (z = 0.1) steady states
- u_2* close to upper bound
- Computational delay = 0.5, leads to instabilities

CSTR NMPC Example – Model Mismatch

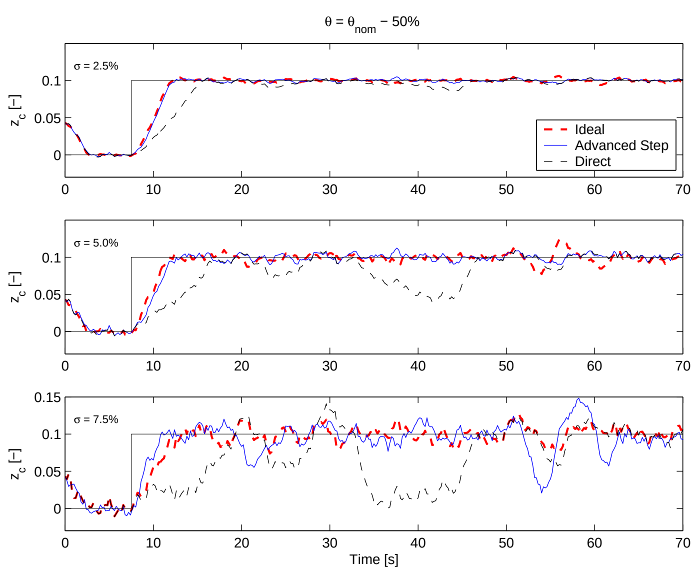


Advanced Step NMPC not as robust as ideal - suboptimal selection of u(k)

Better than Direct Variant – due to better active set preservation

81

CSTR Example: Mismatch + Noise

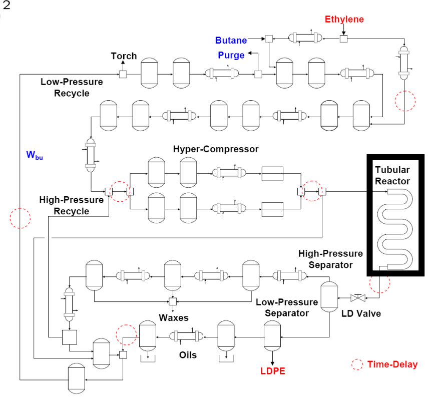


82

Industrial Case Study – Grade Transition Control

Process Model: 289 ODEs, 100 AEs

$$\begin{aligned} \min \quad & \int_{t_\ell}^{t_\ell+t_p} \left(w_{C_4}(t) - w^r_{C_4}\right)^2 + \left(F_{C_4}(t) - F^r_{C_4}\right)^2 + \left(F_{pu}(t) - F^r_{pu}\right)^2 \\ \text{s.t.} \quad & \text{PDEs+ODEs} \\ & z(t = t_\ell) = \hat{z}(\ell) \\ & z_L \le z \le z_U \\ & y_L \le y \le y_U \\ & u_L \le u \le u_U \end{aligned}$$



Simultaneous Collocation-Based Approach

$$\begin{aligned} \min \quad & \sum_{m=0}^{M-1} \left\{ \sum_{k=0}^{K_m-1} \varphi^k_m \left(z^k_m, y^k_m, u^k_m, \pi_m, \Pi\right) \right\} \\ \text{s.t.} \quad & \\ z^{k+1}_m &= z^k_m + \mathbf{A}_m y^k_m \\ 0 &= h_{m,k}\left(z^k_m, y^k_m, u^k_m, \pi_m, \Pi\right) \\ z^0_{m+1} &= \bar{f}_m\left(z^{K_m}_m, y^{K_m}_m, u^{K_m}_m\right) \\ z^0_0 &= \hat{z}(\ell) = p \\ m &= 0, \ldots, M-1 \qquad k = 0, \ldots, K_m - 1 \end{aligned}$$

27,135 constraints, 9630 LB & UB

Off-line Solution with IPOPT

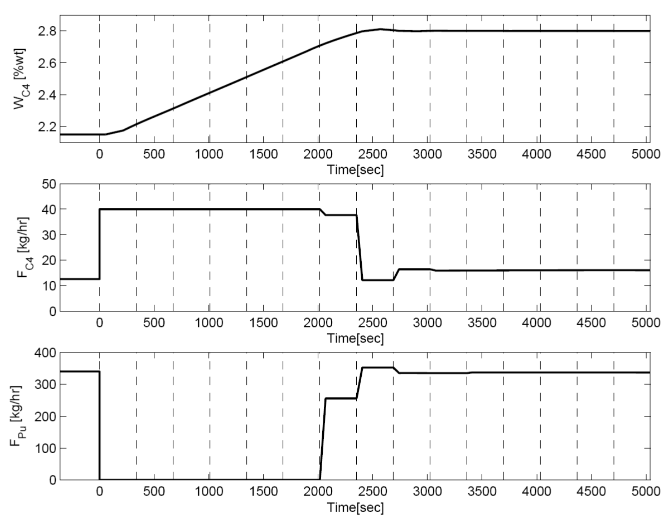
Algorithmic Step	CPU(s)
Full Solution (10 iterations)	351.5
Single Factorization of KKT Matrix	33.9
Step Computation (single backsolve)	0.94
Rest of Steps	0.12

→ **Feedback Every 6 min**

83

NMPC Case Study

- **Optimal Feedback Policy → (On-line Computation 351 CPU s)**



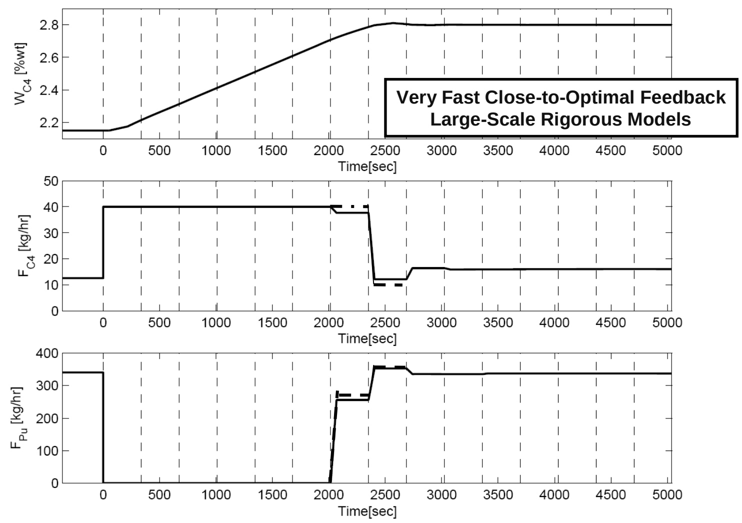
Ideal NMPC controller - computational delay not considered

Time delays as disturbances in NMPC

84

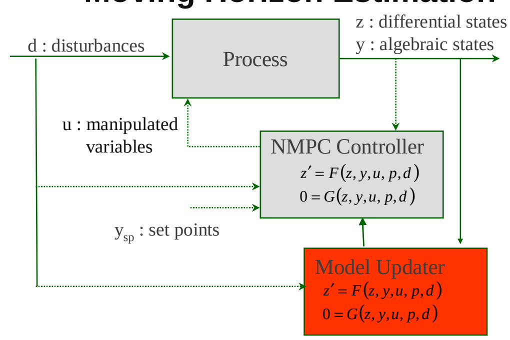
NMPC Case Study

- Optimal Policy vs. NLP Sensitivity -Shifted → (On-line Computation 1.04 CPU s)



85

Moving Horizon Estimation



Linear Systems, No inequalities → Kalman Filter for State Estimation

Nonlinear Systems: → Extended Kalman Filters in Practice

Moving Horizon Estimation:

+ directly captures nonlinear dynamics, statistical behavior

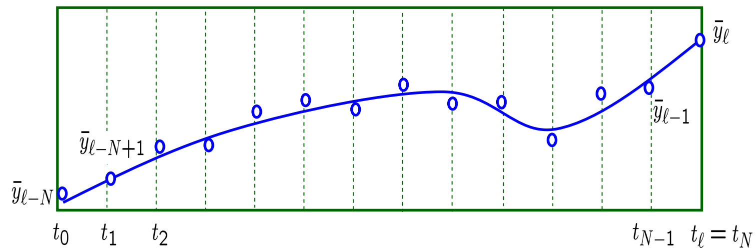
- need to solve NLP on-line

  Solution Time → Order of Minutes

Computational delay – between receipt of process measurement, estimation and injection of new control

Leads to loss of performance and stability

Moving Horizon Estimation



Linear Systems, No inequalities → Kalman Filter for State Estimation

Nonlinear Systems: → Extended Kalman Filters in Practice

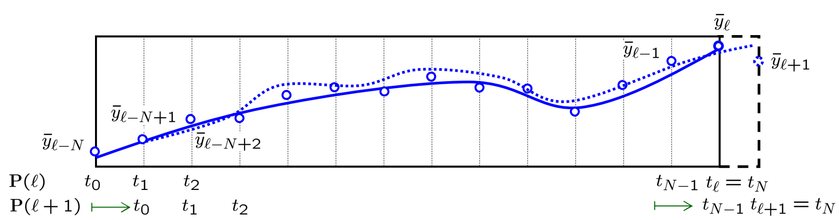
Moving Horizon Estimation:

- + directly captures nonlinear dynamics, statistical behavior
- - need to solve NLP on-line
  - Solution Time → Order of Minutes

Computational delay – between receipt of process measurement, estimation and injection of new control

Leads to loss of performance and stability

Moving Horizon Estimation



$$\underbrace{\begin{aligned} \min_{x_0, w_k} \quad & (x_0 - \boxed{\bar{x}_0^\ell})^T \Pi_0^{-1} (x_0 - \bar{x}_0^\ell) + \sum_{k=0}^{N} L_k(v_k, w_k) \\ s.t. \quad & x_{k+1} = f_k(x_k, w_k) \\ & \boxed{\bar{y}_{k+\ell-N}} = h_k(x_k) + v_k \end{aligned}}_{\mathrm{P}(\ell)}$$

Computational Delay **- MHE Impractical**

NLPs are *Parametric*

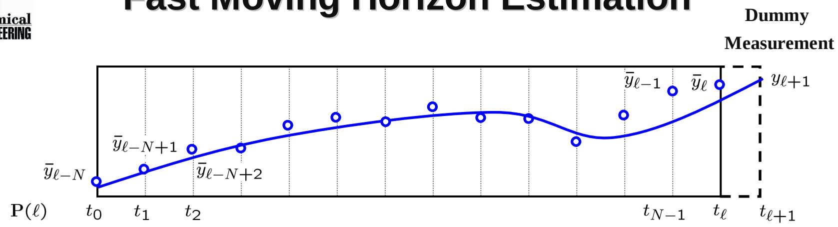
Solve $\mathrm{P}(\ell)$ in Background

Fast *Approximation* to $\mathrm{P}(\ell+1)$ *On-line*

$$\mathrm{P}(\ell+1) \left\{ \begin{aligned} \min_{x_0, w_k} \quad & (x_0 - \boxed{\bar{x}_0^{\ell+1}})^T \Pi_0^{-1} (x_0 - \bar{x}_0^{\ell+1}) + \sum_{k=0}^{N} L_k(v_k, w_k) \\ s.t. \quad & x_{k+1} = f_k(x_k, w_k) \\ & \boxed{\bar{y}_{k+\ell-N+1}} = h_k(x_k) + v_k \end{aligned} \right.$$

88

Fast Moving Horizon Estimation



1) Solve *Extended* Problem Between t_ℓ and $t_{\ell+1}$

$$\min_{x_0, w_k, y_{\ell+1}} \; (x_0 - \bar{x}_0^\ell)^T \Pi_0^{-1} (x_0 - \bar{x}_0^\ell) + \sum_{k=0}^{N} L_k(v_k, w_k) + L_{N+1}(v_{N+1}, w_{N+1})$$

$\bar{\mathrm{P}}(\ell)$

$$\begin{aligned} s.t. \quad x_{k+1} &= f_k(x_k, w_k), \quad k = 0, ..., N-1 \\ \bar{y}_{k+\ell-N} &= h_k(x_k) + v_k, \quad k = 0, ..., N \\ x_{N+1} &= f_N(x_N, w_N) \\ y_{\ell+1} &= h_{N+1}(x_{N+1}) + v_{N+1} \end{aligned}$$

Re-use KKT Matrix Available At Solution of $\bar{\mathrm{P}}(\ell)$

$$\begin{bmatrix} W(x_k, \lambda_k) & A(x_k) & -I \\ A(x_k)^T & 0 & 0 \\ V_k & 0 & X_k \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta \lambda \\ \Delta \nu \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

Analyze Terms due to Extended Horizon

$$\Delta \bar{\lambda}_{N+1} = 0$$

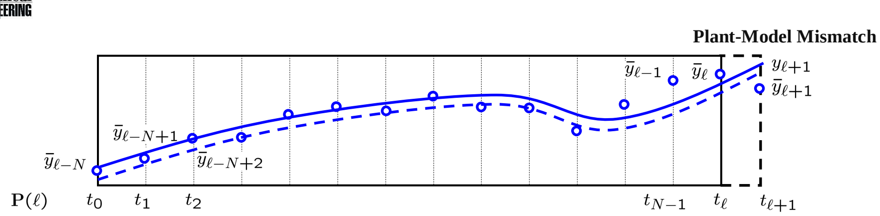
$$\mathrm{R}_{N+1}^{-1} \Delta v_{N+1} + \Delta \bar{\lambda}_{N+1} = 0$$

$$\Delta y_{\ell+1} - \nabla_x h_{N+1} \Delta x_{N+1} - \Delta v_{N+1} = 0$$

$y_{\ell+1}^* = h_{N+1}(x_{N+1}^*)$ **Dummy Measurement = Model Prediction at $t_{\ell+1}$**

89

Fast Moving Horizon Estimation



2) At $t_{\ell+1}$ once we know $\bar{y}_{\ell+1}$

$$\Delta \bar{\lambda}_{N+1} = 0$$

$$\mathrm{R}_{N+1}^{-1} \Delta v_{N+1} + \Delta \bar{\lambda}_{N+1} = 0$$

$$\Delta y_{\ell+1} - \nabla_x h_{N+1} \Delta x_{N+1} - \Delta v_{N+1} = 0$$

KKT System At Solution of $\bar{\mathrm{P}}(\ell)$

$$\begin{bmatrix} W(x_k, \lambda_k) & A(x_k) & -I \\ A(x_k)^T & 0 & 0 \\ V_k & 0 & X_k \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta \lambda \\ \Delta \nu \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\mathrm{K} \Delta s = 0$$

$\Delta \bar{\lambda}_{N+1} + \boxed{\Delta p} = 0$ **Relax Multiplier**

$\boxed{\Delta y_{\ell+1} = (y_{\ell+1}^* - \bar{y}_{\ell+1})}$ **Force Dummy to Measurement**

Find perturbation Δp that enforces

$$y_{\ell+1} = \bar{y}_{\ell+1}$$

Augmented KKT System

$$\begin{bmatrix} \mathrm{K} & \mathrm{E_p} \\ \mathrm{E_y}^T & 0 \end{bmatrix} \begin{bmatrix} \Delta s \\ \Delta p \end{bmatrix} = - \begin{bmatrix} 0 \\ \bar{y}_{\ell+1} - y_{\ell+1}^* \end{bmatrix}$$

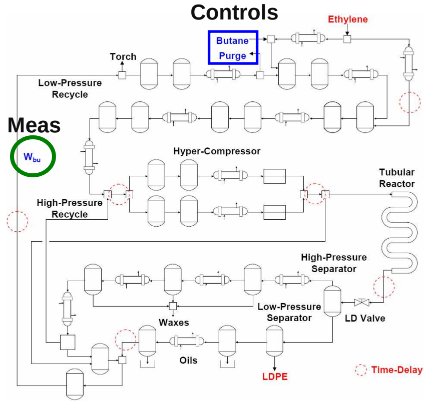
***K* is already factorized**
Solve as Schur complement problem
On-line Cost is a simple backsolve

90

MHE Case Study (Zavala, Laird, B.)

Controls

Meas



Single Measurement - Composition of Recycle Gas
Sampling Time ~ 6 min
Estimation Horizon N = 15

NLP Simultaneous Approach

$$\min_{x_0, w_k} \; (x_0 - \bar{x}_0^{\ell})^T \Pi_0^{-1} (x_0 - \bar{x}_0^{\ell}) + \sum_{k=0}^{N} L_k(v_k, w_k)$$

$$\begin{aligned} s.t. \quad x_{k+1} &= f_k(x_k, w_k) \\ \bar{y}_{k+\ell-N} &= h_k(x_k) + v_k \end{aligned}$$

27,121 Constraints, 9330 Bounds
294 Degrees of Freedom

Algorithmic Step	CPUs
Full Solution (6 iterations)	202.64
Single Factorization of KKT Matrix	33.77
Step Computation (single backsolve)	0.9-1.0
Rest of Steps	0.936

Computational Delay

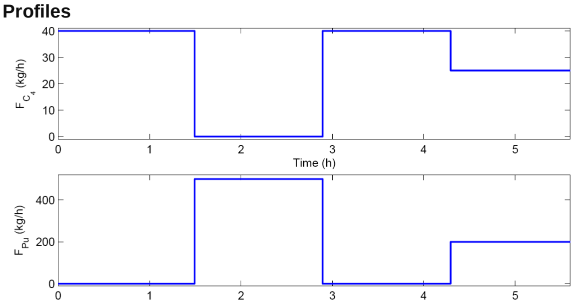
On-Line Calculation

K **has correct Inertia at Solution –** ***System Locally Observable***

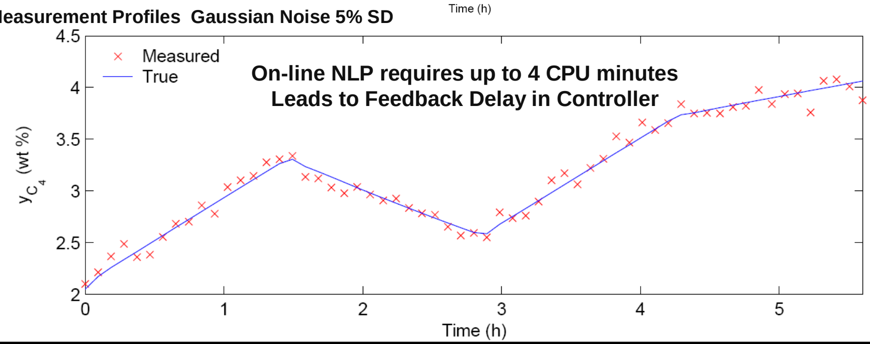
91

MHE Case Study

Simulated Control Profiles



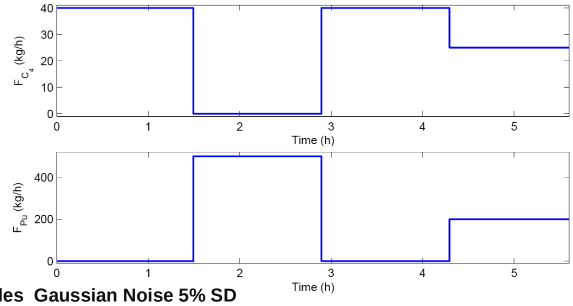
Measurement Profiles Gaussian Noise 5% SD



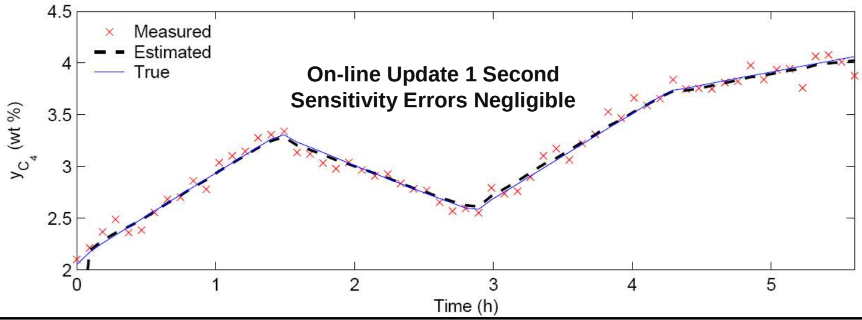
92

MHE Case Study

Simulated Control Profiles



Measurement Profiles Gaussian Noise 5% SD



93

Summary: Dynamic Optimization

<u>Sequential Approaches – Use DAE Integrators</u>

- Parameter Optimization
  - Gradients by: Direct (and Adjoint) Sensitivity Equations
- Optimal Control (Profile Optimization)
  - Variational Methods
  - NLP-Based Methods - Single and Multiple Shooting
- Require Repeated Solution of Model
- State Constraints are Difficult to Handle

<u>Simultaneous Collocation Approach</u>

- Discretize ODE's using orthogonal collocation on finite elements
- Straightforward addition of state constraints.
- Deals with unstable systems
- Solve model only once
- Avoid difficulties at intermediate points

<u>Large-Scale Extensions</u>

- Exploit structure of DAE discretization through decomposition
- Large problems solved efficiently with IPOPT

94

Summary: On-line Extensions

RTO and MPC widely used for refineries, ethylene and, more recently, chemical plants

- Inconsistency in models → operating problems?

Off-line dynamic optimization is widely used

- Polymer processes (especially grade transitions)
- Batch processes
- Periodic processes

NMPC provides link for off-line and on-line optimization

- Stability and robustness properties
- Advanced step controller leads to very fast calculations
  - Analogous stability and robustness properties
  - On-line cost is negligible

Multi-stage planning and on-line switches

- Avoids conservative performance
- Update model with MHE
- Evolve from regulatory NMPC to Large-scale DRTO

95

Acknowledgements

Funding

- Department of Energy
- National Science Foundation
- Center for Advanced Process Decision-making (CMU)

Research Colleagues

- Antonio Flores-Tlacuahuac
- Tobias Jockenhövel
- Shivakumar Kameswaran
- Yoshiaki Kawajiri
- Carl Laird
- Yi-dong Lang
- Andreas Wächter
- Victor Zavala

http://dynopt.cheme.cmu.edu

96

References – Dynamic Optimization

F. Allgöwer and A. Zheng (eds.), *Nonlinear Model Predictive Control*, Birkhaeuser, Basel (2000)

R. D. Bartusiak, "NLMPC: A platform for optimal control of feed- or product-flexible manufacturing," in *Nonlinear Model Predictive Control 05,* Allgower, Findeisen, Biegler (eds.), Springer, to appear

Biegler Homepage: http://dynopt.cheme.cmu.edu/papers.htm

Forbes, J. F. and Marlin, T. E.. Model Accuracy for Economic Optimizing Controllers: The Bias Update Case. *Ind.Eng.Chem.Res*. 33, 1919-1929. 1994

Forbes, J. F. and Marlin, T. E.. "Design Cost: A Systematic Approach to Technology Selection for Model-Based Real-Time Optimization Systems," *Computers Chem.Engng.* 20[6/7], 717-734. 1996

Grossmann Homepage: http://egon.cheme.cmu.edu/papers.html

M. Grötschel, S. Krumke, J. Rambau (eds.), *Online Optimization of Large Systems,* Springer, Berlin (2001)

K. Naidoo, J. Guiver, P. Turner, M. Keenan, M. Harmse "Experiences with Nonlinear MPC in Polymer Manufacturing," in *Nonlinear Model Predictive Control 05,* Allgower, Findeisen, Biegler (eds.), Springer, to appear

Yip, W. S. and Marlin, T. E. "Multiple Data Sets for Model Updating in Real-Time Operations Optimization," *Computers Chem.Engng*. 26[10], 1345-1362. 2002.

97

References – Recent DRTO Case Studies

Busch, J.; Oldenburg, J.; Santos, M.; Cruse, A.; Marquardt, W. Dynamic predictive scheduling of operational strategies for continuous processes using mixed-logic dynamic optimization, *Comput. Chem. Eng.,* **2007**, 31, 574-587.

Flores-Tlacuahuac, A.; Grossmann, I.E. Simultaneous cyclic scheduling and control of a multiproduct CSTR, *Ind. Eng. Chem. Res.*, **2006**, 27, 6698-6712.

Kadam, J.; Srinivasan, B., Bonvin, D., Marquardt, W. Optimal grade transition in industrial polymerization processes via NCO tracking. *AIChE J.*, **2007**, 53, 3, 627-639.

Oldenburg, J.; Marquardt, W.; Heinz D.; Leineweber, D. B., Mixed-logic dynamic optimization applied to batch distillation process design, *AIChE J.* **2003**, 48(11), 2900- 2917.

E Perea, B E Ydstie and I E Grossmann, A model predictive control strategy for supply chain optimization, *Comput. Chem. Eng.,* **2003**, 27, 1201-1218.

M. Liepelt, K Schittkowski, Optimal control of distributed systems with breakpoints, p. 271 in M. Grötschel, S. Krumke, J. Rambau (eds.), *Online Optimization of Large Systems*, Springer, Berlin (2001)

98