A Nonlinear Programming Path to NMPC and Real-Time Optimization

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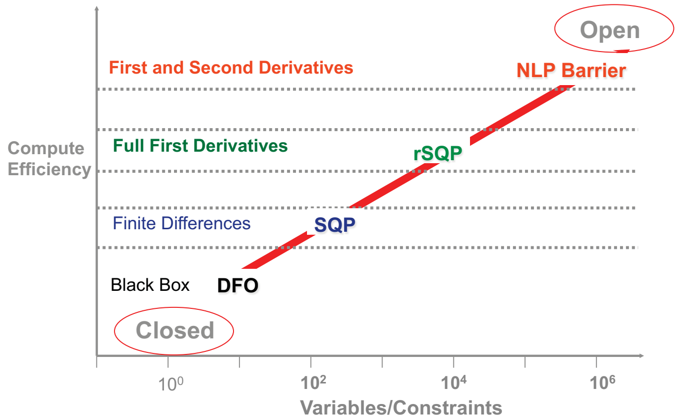
January, 2012

Overview

- Process Optimization – Why and How?
- Two Key Concepts
  - Newton Barrier NLP
  - NLP Sensitivity
- LDPE Case Study
  - Parameter Estimation
  - NMPC → asNMPC
  - MHE → asMHE
  - RTO → D-RTO
- Where to NMPC and NLP?
- Conclusions

Why Process Optimization?

How Process Optimization? Optimization Formulations and Models



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

$$\boldsymbol{a} \leq \boldsymbol{x} \leq \boldsymbol{b}$$

Barrier Approach

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

⇒As $\mu \rightarrow 0$, $x^*(\mu) \rightarrow x^*$ Fiacco and McCormick (1968)

Barrier Problem Solution

⇒ Newton Directions (KKT System)

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

$e^T = [1,1,1...]$, $X = diag(x)$

$A = \nabla c(x)$, $W = \nabla_{xx} L(x,\lambda,v)$

⇒ 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

IPOPT Features
(Wächter, Laird, B., 2002-2009)

Newton-Based Barrier Method

- Globally, superlinearly convergent (Wächter and B., 2005)
- Easily tailored to different problem structures

Line Search Globalization

- ℓ_2 exact penalty merit function
- augmented Lagrangian merit function
- **Filter method (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

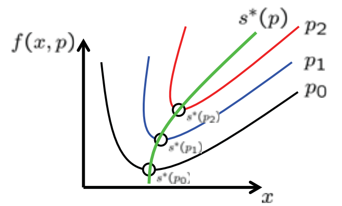
Widely Available

- Eclipse License and COIN-OR distribution: **http://www.coin-or.org**
- Solved on many thousands of test problems and applications
- Broad, growing user community

NLP Sensitivity

Parametric Program

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



Solution Triplet

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

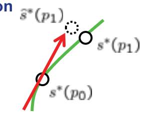
Optimality Conditions $\mathrm{P}(p)$

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

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

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

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



NLP Sensitivity with IPOPT
(Pirnay, Lopez Negrete, B., 2011)

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

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

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

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

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

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

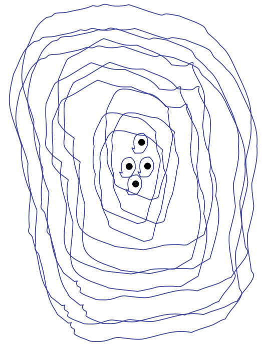
KKT Matrix IPOPT

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

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

NLP Sensitivity
Optimum change with parameters p?

- Identify sensitive parameters
- What is sensitivity of the optimum to disturbances and model mismatch?
- Information obtained essentially free (one backsolve for each perturbation)
- Starting point for parametric optimization problems



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NLP Sensitivity
Response Surface for Degrees of Freedom

- Reduced Hessian extraction from IPOPT
  - Not directly generated by solver, but easily extracted from KKT conditions
- Split *x* into degrees of freedom (*d*) and basic (*b*) variables

$$x^T = \left[b^T, d^T\right] \qquad A = \left[A_b | A_d\right] \qquad W = \begin{bmatrix} W_{bb} & W_{bd} \\ W_{db} & W_{dd} \end{bmatrix}$$

- Linearized KKT Conditions are:

$$\begin{bmatrix} W_{bb} & W_{bd} & A_b^T \\ W_{db} & W_{dd} & A_d^T \\ A_b & A_d & 0 \end{bmatrix} \begin{bmatrix} \Delta b \\ \Delta d \\ \Delta\lambda \end{bmatrix} = \begin{bmatrix} 0 \\ \mathbb{I}_{nd}(j,:) \\ 0 \end{bmatrix} \quad \textbf{Change RHS}$$

- The solution leads to

$$\Delta d = \left(\mathbb{Z}^T W \mathbb{Z}\right)^{-1}(:,j) \qquad Z = \begin{bmatrix} -A_b^{-1}A_d \\ I \end{bmatrix}$$

- *j*-th column of reduced Hessian inverse.
- requires single back-solve with KKT matrix already factorized!

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NLP Sensitivity
Parameter and State Estimation

- Analyze sensitivity of estimates with changes in data

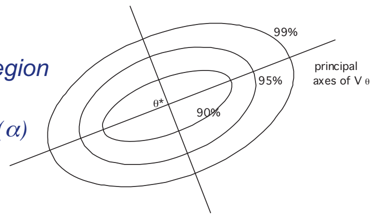
$$\min_{\theta,\gamma,y} \frac{1}{2}\left[(y-\hat{y})^T \hat{V}_y^{-1}(y-\hat{y}) + (\theta-\hat{\theta})^T \hat{V}_\theta^{-1}(\theta-\hat{\theta})\right]$$
$$\text{s.t.} \quad c(\theta,\gamma,y) = 0$$

- Introduce perturbations $\theta^* + \delta\hat{\theta}$, $\gamma^* + \delta\hat{\gamma}$ and $y^* + \delta\hat{y}$

$$\mathrm{Cov}\,(\theta) \approx \mathbb{E}\left\{\Delta\theta\Delta\theta^T\right\} = \left(\mathbb{Z}^T W \mathbb{Z}\right)^{-1}$$

Approximate Confidence Region

$$(\theta - \theta^*)^T V_\theta^{-1} (\theta - \theta^*) \le \chi(\alpha)$$



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Dynamic Optimization Problem

$$\min \ \psi\big(z(t), y(t), u(t), p, t_f\big)$$

$$\text{s.t.} \quad \frac{dz(t)}{dt} = F\big(z(t), y(t), u(t), t, p\big)$$

$$G\big(z(t), y(t), u(t), t, p\big) = 0$$

$$z^o = z(0)$$

$$z^l \le z(t) \le z^u$$

$$y^l \le y(t) \le y^u$$

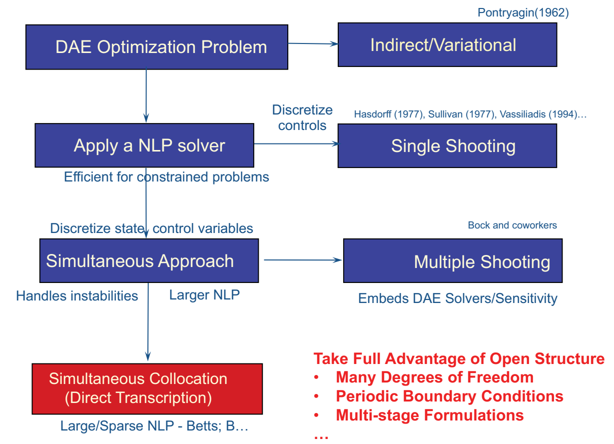
$$u^l \le u(t) \le u^u$$

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

t, time
z, differential variables
y, algebraic variables

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

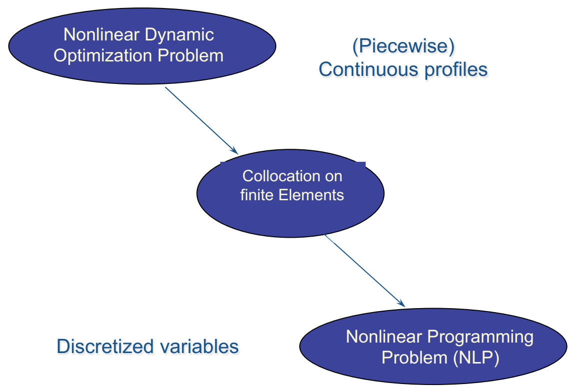
Dynamic Optimization Approaches



Take Full Advantage of Open Structure
- **Many Degrees of Freedom**
- **Periodic Boundary Conditions**
- **Multi-stage Formulations**

…

Nonlinear Programming Formulation



Nonlinear Programming Problem

$$\min \ \psi\big(z_i, y_{i,q}, u_{i,q}, p, t_f\big)$$

$$\text{s.t.} \quad \left(\frac{dz}{dt}\right)_{i,j} = F\left(z_{i-1}, \frac{dz}{dt}_{i,j}, z_i, y_{i,j}, u_{i,j}, p\right)$$

$$G\left(z_{i-1}, \frac{dz}{dt}_{i,j}, z_i, y_{i,j}, u_{i,j}, p\right) = 0$$

$$z_i = f\left(\frac{dz}{dt}_{i-1,j}, z_{i-1}\right)_i$$

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

$$z_i^{\,l} \le z_i \le z_i^{\,u}$$

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

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

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

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

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

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

Some Case Studies with Simultaneous Collocation

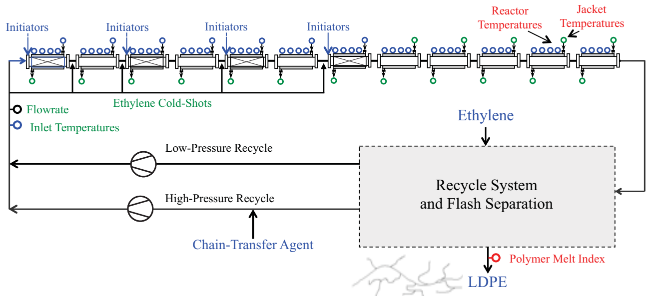
Off-line Case Studies

- Dynamic Bioprocess Optimization
- Parameter Estimation of Batch Data
- Synthesis of Reactor Networks
- Crystallization Temperature Profiles
- Optimal Batch Distillation Operation
- Satellite Trajectories in Astronautics
- Batch Process Integration
- Simulated Moving Bed Optimization
- Optimization of Polymerization Processes
- Optimal Pressure Swing Adsorption

On-line Case Studies

- NMPC of Tenn. Eastman Process
- Source Detection of Water Networks
- Cross-directional Sheet-forming Processes
- Thermo-mech. Pulping NMPC
- D-RTO for Gas Pipelines
- Air Traffic Conflict Resolution
- NMPC for Refinery Distillation
- Ramping for Air Separation Columns
- Startup for Combined Cycle Power Generation
- **Cyclic Operation for LDPE Process**

Low-Density Polyethylene Process



- Free-Radical Polymerization at Supercritical Conditions (2000 - 3000 atm)
- Multi-Zone Tubular Reactor (2 Km Long Pipe)
- Highly Exothermic, Keep Low Conversions (20-35%)
- High Throughput (300,000 Ton/yr)
- Multi-Product Operations (> 20 Grades)
- Inputs/ Outputs for control and optimization

Large-Scale Parameter Estimation

- Complex Kinetic Mechanisms

Initiator decomposition

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

Chain Initiation

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

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

$$P_{r,s} + S_i \xrightarrow{k_{s_i1}} P_{1,0} + M_{r,s}$$
$$Q_{r,s} + S_i \xrightarrow{k_{s_i2}} Q_{0,1} + M_{r,s}$$

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

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

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

Large-Scale Parameter Estimation

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

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

Least-Squares

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

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

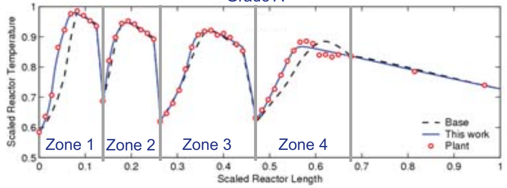
Bottleneck - Memory Requirements In KKT Factorization Step (Handled through blockwise decomposition of KKT matrix)

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

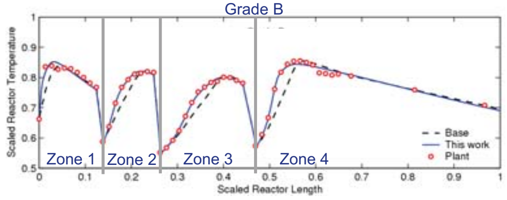
LDPE Parameter Estimation

Improved Prediction Core Temperature Profile

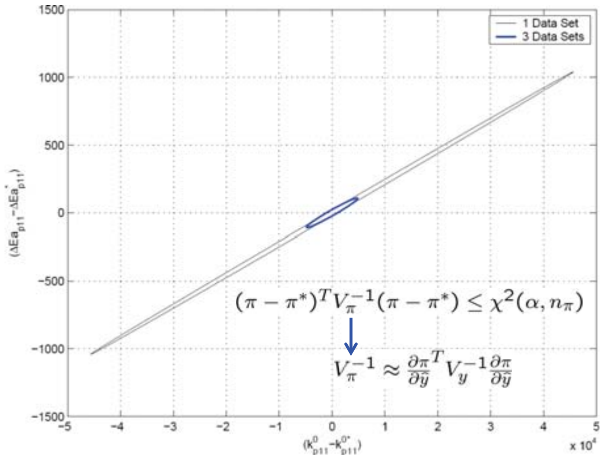
Grade A



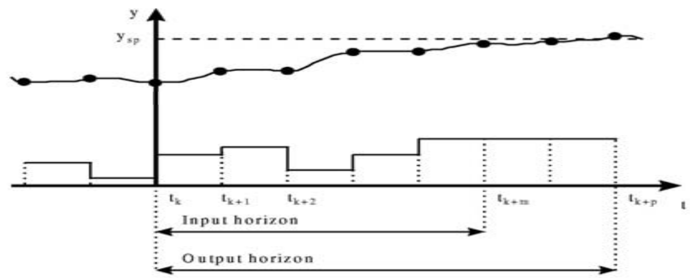
Grade B



Sensitivity-based Confidence Regions



On-line Issues: Model Predictive Control (NMPC)



$$\min_u \; J(x(k)) = \sum_{l=0} \psi(z_l, u_l) + F(z_N)$$

$$s.t. \quad z_{l+1} = f(z_l, u_l))$$

$$z_0 = x(k)$$

Bounds

MPC - Background

Motivate: embed dynamic model in moving horizon framework to drive process to desired state (Rawlings and Mayne, 2009)

- Generic MIMO controller
- Direct handling of input and output constraints
- Slow process time-scales – consistent with dynamic operating policies

Different types

- Linear Models: Step Response (DMC) and State-space
- Empirical Models: Neural Nets, Volterra Series
- Hybrid Models: (QP/MIQP…), apply *parametric programming* and *Explicit MPC*
- **First Principle Models – direct link to off-line planning**

NMPC Pros and Cons

+ Operate process over wide range (e.g., startup and shutdown)
+ Vehicle for Dynamic Real-time Optimization
- Need Fast NLP Solver for time-critical, on-line optimization
- **Computational Delay from On-line Optimization degrades performance**

Some Related NMPC Research

Optimization and Optimal Control

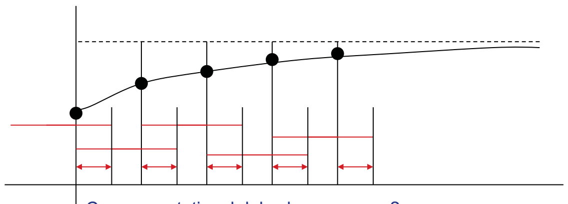
- Pontryagin (1959), Bryson and Ho (1969), Ray (1981), Sargent and coworkers (1970s),…

Model Predictive Control

- Evolution from LQ, MPC (Kleinman, 1975; Kwon and Pearson, 1977),
- DMC (Cutler and Ramaker, 1979), QDMC (Garcia and Morshedi,1984)
- Concepts and Analysis: Allgöwer and coworkers (1989 -), Bordons and Camacho (2001), Rawlings and Mayne (2009), Grüne and Pannek (2011)
- Real-time iteration (Diehl, Li, Ohtsuka, Oliveira, Santos, 1989 -)
- Neighboring extremal approaches (Bonvin, Marquardt, 2002 -)

What about Fast NMPC?

- Fast NMPC is not just NMPC with a fast solver (Engell, 2007)
- ***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 Rawlings and Mayne, 2009; Findeisen and Allgöwer, 2004; Santos et al., 2001)

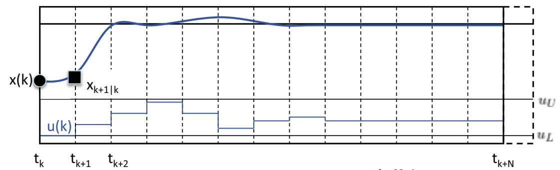


Can computational delay be overcome?

- Fast Newton-based NMPC
- Cheap NLP Sensitivity

Advanced Step Nonlinear MPC (Zavala, B., 2009)

Solve NLP in background (between steps, not on-line)
Update using sensitivity on-line



$$\min \quad J(x(k), u(k)) = F(x_{k+N|k}) + \sum_{l=k+1}^{k+N-1} \psi(x_{l|k}, v_{l|k})$$

$$s.t. \quad x_{k+1|k} = \boxed{f(x(k), u(k))}$$

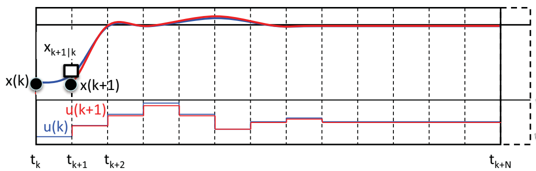
$$x_{l+1|k} = f(x_{l|k}, v_{l|k}), \quad l = k+1, .. k+N-1$$

$$x_{l|k} \in X, \quad v_{l|k} \in U, \quad x_{k+N|k} \in X_f$$

Solve NLP(k) in background (between t_k and t_{k+1})

Advanced Step Nonlinear MPC (Zavala, B., 2009)

Solve NLP in background (between steps, not on-line)
Update using sensitivity on-line

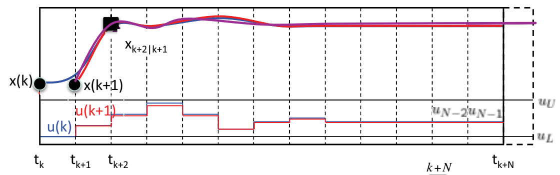


$$\begin{bmatrix} W_k & A_k & -I \\ A_k^T & 0 & 0 \\ Z_k & 0 & X_k \end{bmatrix}\begin{bmatrix}\Delta x\\ \Delta\lambda \\ \Delta z\end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ x_{k+1|k} - x(k+1) \\ 0\end{bmatrix}$$

Solve NLP(k) in <u>background</u> (between t_k and t_{k+1})
Sensitivity to update problem <u>on-line</u> to get (u(k+1))

Advanced Step Nonlinear MPC (Zavala, B., 2009)

Solve NLP in background (between steps, not on-line)
Update using sensitivity on-line



$$\min \quad J(x(k+1), u(k+1)) = F(x_{k+N+1|k+1}) + \sum_{l=k+2}^{k+N} \psi(x_{l|k+1}, v_{l|k+1})$$

$$s.t. \quad x_{k+2|k+1} = f(x(k+1), u(k+1))$$

$$x_{l+1|k+1} = f(x_{l|k}, v_{l|k}), \quad l = k+2, ..k+N$$

$$x_{l|k+1} \in X, \quad v_{l|k+1} \in U, \quad x_{k+N+1|k+1} \in X_f$$

Solve NLP(k) in <u>background</u> (between t_k and t_{k+1})
Sensitivity to update problem <u>on-line</u> to get (u(k+1))
Solve NLP(k+1) in <u>background</u> (between t_{k+1} and t_{k+2})

Combining MHE & NMPC (Huang, Patwardhan, B., 2009)

Offset-free Formulation

- Apply MHE results as state and output corrections for NMPC problem
- Modify with an advanced step approach → *<u>as-MHE</u>*

$$\min \sum_{j=1}^{N_e} (\zeta^T_{k-N_e+j} \Pi_y \zeta_{k-N_e+j}) + \hat\theta_k^T \Pi_\theta \hat\theta_k + (\hat x_{k-N_e} - \bar x_{k-N_e})^T \Pi_0 (\hat x_{k-N_e} - \bar x_{k-N_e})$$

s.t. $\hat x_{k-N_e+j+1} = f(\hat x_{k-N_e+j}, u_{k-N_e+j}, \hat\theta_k)$

$\hat y_{k-N_e+j} = h(\hat x_{k-N_e+j})$

$\zeta_{k-N_e+j} = y_{k-N_e+j} - \hat y_{k-N_e+j}$

$\hat x_{k-N_e+j} \in \mathbb{X}, \zeta_{k-N_e+j} \in \Omega_\zeta, \hat\theta_k \in \Omega_\theta$

$j = 0, \ldots, N_e - 1.$

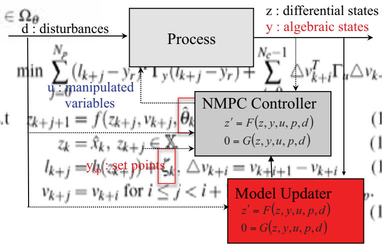
$$\min \sum_{j=0}^{N_p} (l_{k+j} - y_r)^T \Gamma_y (l_{k+j} - y_r) + \sum_{i=0}^{N_c-1} \Delta v_{k+i}^T \Gamma_u \Delta v_{k+i}$$

s.t $z_{k+j+1} = f(z_{k+j}, v_{k+j}, \hat\theta_k)$ (10a)

$z_k = \hat x_k, \; z_{k+j} \in \mathbb{X}$ (10b)

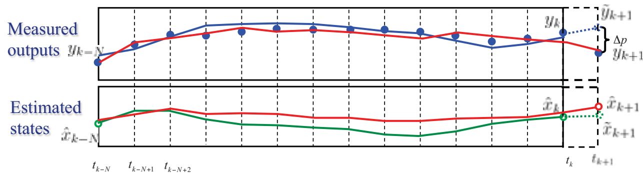
$l_{k+j} = h(z_{k+j}) + \zeta_k, \; \Delta v_{k+i} = v_{k+i+1} - v_{k+i}$ (10c)

$v_{k+j} = v_{k+i}$ for $i \le j < i + \ldots$ (10d)



Advanced-step MHE

(Zavala, Lopez Negrete, B. 2009 - 2011)



Background: At t_k, having x_k and u_k, <u>approximate</u> x_{k+1} and y_{k+1}. Solve the extended MHE problem from *k-N* to *k+1*. Let p_0 = *approximate* y_{k+1}.

On-line update: At t_{k+1}, obtain y_{k+1}. Set $p = y_{k+1}$ and use NLP sensitivity to get fast update x_{k+1}.

Iterate: Set *k = k+1* and go to background.

<u>NLP Sensitivity used for State Approximation and Covariance Updates</u>

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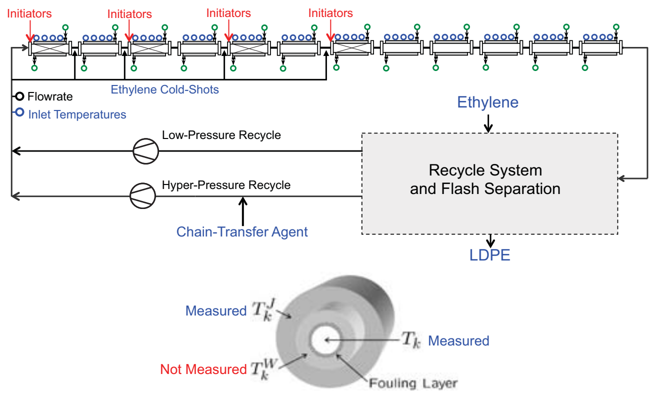
NMPC-MHE Scenario



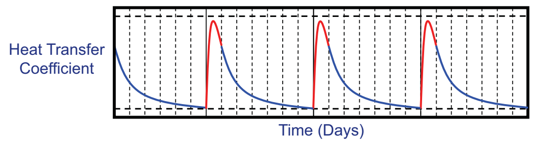
Fouling of reactor wall – treated as (imposed, unmeasured) disturbance

MHE+NMPC for LDPE Process

Fouling

Cannot Remove Heat of Reaction - Drop Production to Avoid Runaway

Defouling

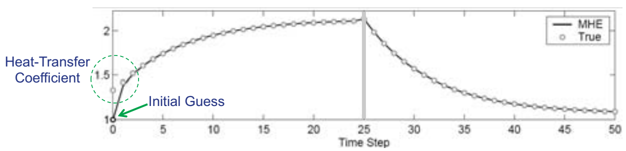


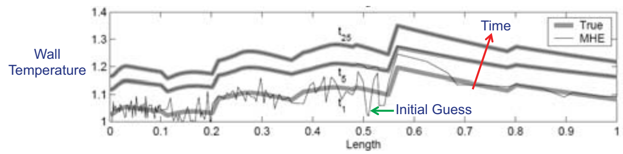
Centralized Control Framework Including PDAE Reactor Model

- Ramp Reactor Heat-Transfer Coefficients to Simulate Fouling-Defouling Behavior
- MHE to Infer Heat-Transfer and Model States (e.g. Wall Profile)
- NMPC to Stabilize Temperature Profile

NMPC-MHE Scenario

MHE Performance – Convergence to True State





MHE Recovers from Poor Initial Guesses in Few Time Steps

Distributed Temperature Measurements

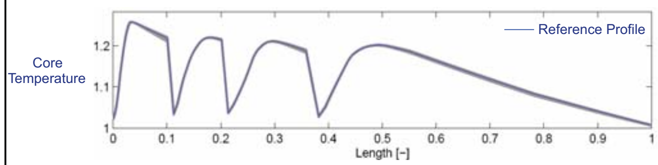
Make Reactor Strongly Observable *Zavala & B., 2010*

NMPC-MHE Scenario

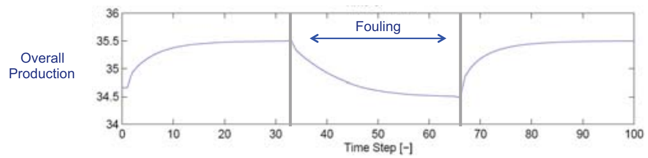
NMPC Performance – Tracking Objective

Minimize Transition Time

$$\min_{u(t)} \int_0^{t_f} \int_0^{x^L} (z(x,t) - z^{ref}(x))^T \mathbf{W} (z(x,t) - z^{ref}(x)) dx dt$$

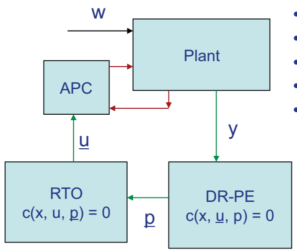


Controller Stabilizes Temperature Levels but Needs to Drop Production as Fouling Advances

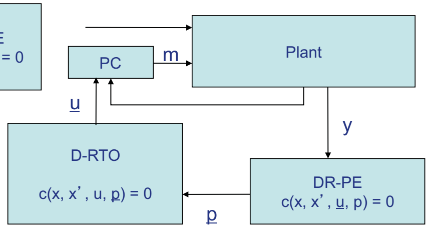


But… LDPE Reactor has Many Degrees of Freedom
-Not Fully Exploited with Conventional NMPC-

NMPC with Economic Objectives Beyond RTO and MPC Regulation → D-RTO



Benefits of combining RTO with NMPC?
- Direct, dynamic production maximization
- Remove artificial setpoint objective
- Remove artificial steady state problem
- Overcomes neglect of dynamic uncertainty
- Leads to significant improvements (**up to 10%**) over steady state RTO



Challenges with D-RTO

Replace regulation objective with economic objective in NMPC?

Bartusiak, Young et al. (2007)
Chachuat et al. (2008),
Dadhe and Engell (2008), Engell (2007, 2009)
Busch, Kadam Marquardt et al. (2008)
Odloak, Zanin, Tvrzska de Gouvea (2002)
Zanin, Tvrzska de Gouvea Odloak (2000)
Diehl, Amrit and Rawlings (2010)
Angeli and Rawlings (2010)
Angeli, Amrit and Rawlings (2011)

Robust Stability of Lyapunov function → must be $\mathcal{K}_\infty$ function (e.g., strong convexity of stage cost)

$$Min \sum_i \{\text{Profit}_i\} + \text{Profit}_N$$

Many open Stability/Robustness Questions Still Remain
- does optimum go to a steady state or not?
- how do we enforce optimal steady state?
- how to consider cyclic problems?

Remedy: Regularize economic objective with $\mathcal{K}_\infty$ function for stage cost?

Economic NMPC Stability Analysis (Huang, Harinath, B., 2011)

- Nominal Stability – ensure $L_i(\bar{z},\bar{v}) \geq \beta_\infty(|\bar{z}-0|)$.

For the rotated stage costs (transformed Lagrange function), $\bar{L}_i(0,0)=0$

$$\begin{aligned}\bar{L}_i(\bar{z},\bar{v}) &= \bar{L}_i(0,0) + \nabla\bar{L}_i(0,0)^T \begin{bmatrix}\bar{z}\\ \bar{v}\end{bmatrix} + 1/2\int_0^1 [\bar{z}^T\ \bar{v}^T]\nabla^2\bar{L}_i(\tau\bar{z},\tau\bar{v})\begin{bmatrix}\bar{z}\\ \bar{v}\end{bmatrix} d\tau \\ &\geq 1/2\int_0^1 [\bar{z}^T\ \bar{v}^T]\nabla^2\bar{L}_i(\tau\bar{z},\tau\bar{v})\begin{bmatrix}\bar{z}\\ \bar{v}\end{bmatrix} d\tau \geq \gamma_L(|\bar{z}|^2+|\bar{v}|^2) \geq \beta_\infty(|\bar{z}|).\end{aligned}$$

If $\bar{L}_i(\bar{z},\bar{v})$ is strongly convex, then the stage cost assumption is satisfied. If not, add regularization terms to rotated stage costs.

Allows straightforward extension to ISS stability

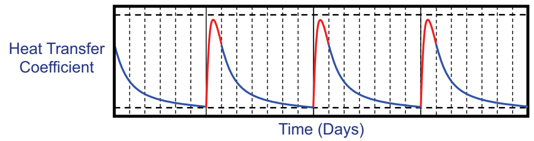
Strong convexity property can be checked/corrected off-line
- Related to strong duality (Diehl et al., 2011)
- Related to dissipativity (Angeli et al., 2011)

Dynamic RTO for LDPE Process (Zavala, B., 2010)

Fouling

Cannot Remove Heat of Reaction - Drop Production to Avoid Runaway

Defouling



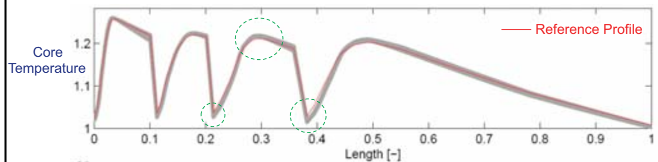
Persistent Dynamic Disturbances – Strong Effect on Profitability
Potential Economic Benefits of 1% Production Increase
0.01 x (300,000 Ton/yr) x (1,500 \$/Ton) = 4,500,000 \$/yr

D-RTO for LDPE Process

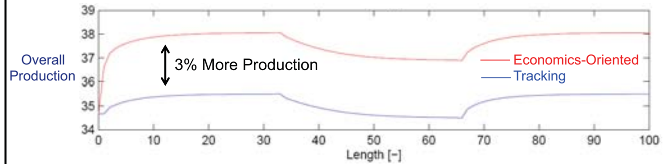
NMPC Performance – Regularized Economic Objective

Minimize Transition Time — Maximize Production

$$\min_{u(t)} \int_0^{t_f}\int_0^{x^L} \left[(z(x,t)-z^{ref}(x))^T \mathbf{W}(z(x,t)-z^{ref}(x)) - \text{Production}(x^L,t)\right] dx\,dt$$



Economics-Oriented NMPC Moves Away from Suboptimal Reference Profile



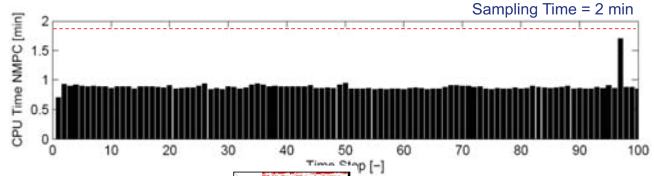
Distributes Production Along Reactor Efficiently
e.g. More Production in Less Fouled Zones

Improving NMPC for LDPE

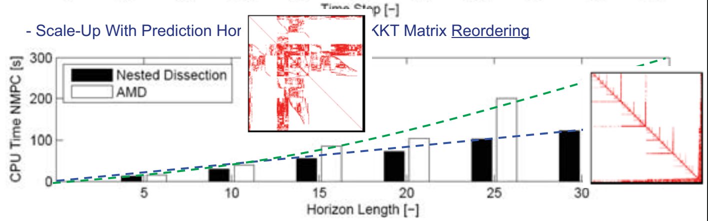
Background Computational Performance - NMPC

- Full-Discretization + IPOPT (MA57), Quad-Core Pentium IV
- Prediction Horizon 5 Time Steps, NLP ~ 50,000 Constraints, 300 DOF

Sampling Time = 2 min



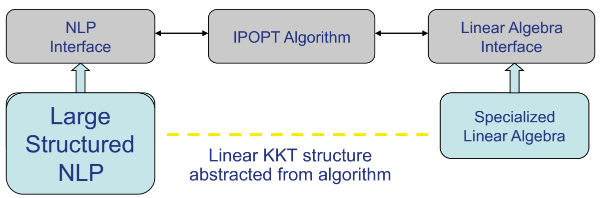
- Scale-Up With Prediction Horizon — KKT Matrix Reordering



NLP with 350,000 Constraints and 1,000 DOF Solved in ~ 2 Minutes

High Level NLP Design

(Laird, Wächter, 2006 -)



Optimization Models, NLP Interfaces

- AMPL, ASL (Gay et al., 1985)
- Optimica, JModelica (Åkesson, 2008)
- PyOMO (Sandia group, 2010)
- ACADO (Diehl et al., 2010)

Background NLP requires more than ΔT?

	Background Optimization	Online Update	NLP Type
Ideal	None	NLP	Various
Real-time Iteration	None	QP	Multiple shooting
Neighboring Extremal	Only once	KKT/ QP	Single shooting
asNMPC	Every step	KKT	Simultaneous Collocation

$$\begin{bmatrix} \mathbf{K} & \mathbf{E}_0 \\ \mathbf{E}_2^T & 0 \end{bmatrix}\begin{bmatrix} \Delta v \\ \Delta s \end{bmatrix} = -\begin{bmatrix} 0 \\ \hat{z}(\ell+2) - z_2^* \end{bmatrix}$$

Reuse L/U Factors of $\mathbf{K}$ with Schur Complement

$$-(E_2^T \mathbf{K}^{-1} E_0)\Delta s = \hat{z}(\ell+2) - z_2^*$$

Advanced Step Framework - Into the Future

- **Stability Properties for asNMPC** (Zavala, B., 2009)
  - Nominal stability – no disturbances nor model mismatch
  - Input to State Stability (ISS) - Assumes RPI set (no path constraints)
  - Guarantee specified level of uncertainty?
    - Adapt tube-based approaches for NMPC (Mayne et al., 2011)
    - Constraint relaxations
    - Direct calculation of RPI regions
- **Moving Horizon Estimation** (Lopez Negrete, Huang, B., 2010, 2011)
  - Fast sensitivity-based smoothed covariance of arrival cost
  - Robust stability for asMHE?
  - Statistical properties of arrival cost formulations?
- **Extension to economic objectives** (Huang, Harinath, B., 2011)
  - Nominal and ISS stability based on rotated stage costs
  - Extended to cyclic processes
  - Development of unbiased regularized stage costs?
  - Stability with incorporation of asMHE?

Conclusions

Bigger NLPs are not harder to solve

- Embrace and exploit size, sparsity and structure
- Exact first and second derivatives are essential
- Newton-based optimization is fast
- Optimal sensitivity is (nearly) free

Chemical Process Operations: RTO → D-RTO

- Essential for Batch Processes, Cyclic Processes, Transient Operations
- Need for First-Principles Dynamic Models
- Extension to On-Line Economic Decision-Making

NMPC and MHE Computational Strategies

- Full-Discretization + Fast Sensitivity Calculations
- Large-scale LDPE process with DAE model

From NMPC Setpoints to Economic Optimization

- Direct optimization in real-time
- Maintain stability and exploit uncertainties
- **Still many open questions**

For more information: http//:numero.cheme.cmu.edu
http//:capd.cheme.cmu.edu

Many Thanks to:

Research Colleagues

- Prof. Johan Åkesson
- Dr. Juan Arrieta
- Dr. Gilvan Fischer
- Prof. Antonio Flores
- Ajit Gopalakrishnan
- Eranda Harinath
- Dr. Rui Huang
- Prof. Carl Laird
- Dr. Rodrigo Lopez Negrete
- Prof. Andreas Wächter
- Dr. Victor Zavala
- Xue Yang

Lynne W. Biegler

and …

To the NPC community

In humble thanks for your award and recognition

For more details…

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