Dynamic Real-time Optimization with Direct Transcription and NLP Sensitivity

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Introduction

- RTO State of Art → D-RTO
- Challenges for dynamic optimization → direct transcription

Nonlinear Model Predictive Control (NMPC)

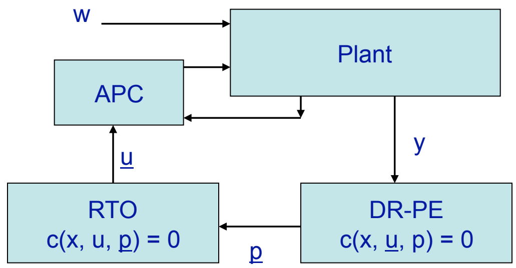
- Fast NMPC
- Problem formulation and NLP Sensitivity
- Moving Horizon Estimation (MHE)

ASU Optimization Case Study

- Fast NMPC
- NMPC + MHE
- Dynamic Optimization (periodic conditions)

Conclusions

RTO – State of the Art



Real-time optimization

- Steady state model for states (x)
- Supply setpoints (u) to APC (control system)
- Model mismatch, measured and unmeasured disturbances (w)

$\mathrm{Min}_u \; F(x, u, w)$
s.t. $c(x, u, \underline{p}, w) = 0$
$x \in X, u \in U$

Data Reconciliation & Parameter Identification

- Estimation problem formulations
- Steady state model
- Maximum likelihood objective functions considered to get parameters (p)

$\mathrm{Min}_p \; \Phi(x, y, p, w)$
s.t. $c(x, \underline{u}, p, w) = 0$
$x \in X, p \in P$

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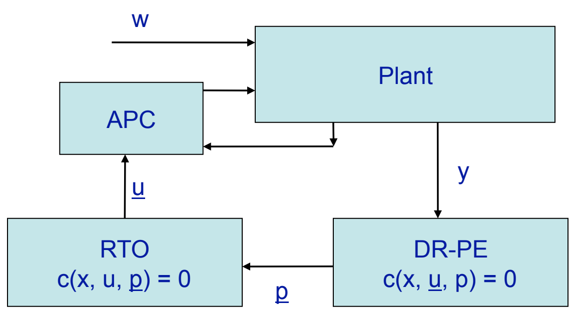
RTO Characteristics



- Data reconciliation – identify gross errors and consistency in data
- Periodic update of process model identification
- Usually requires APC loops (MPC, DMC, etc.)
- RTO/APC interactions: Assume decomposition of time scales
  - APC to handle disturbances and fast dynamics
  - RTO to handle static operations
- Typical cycle: 1-2 hours, closed loop
- State of art operation - widely implemented in refineries and petrochemical plants

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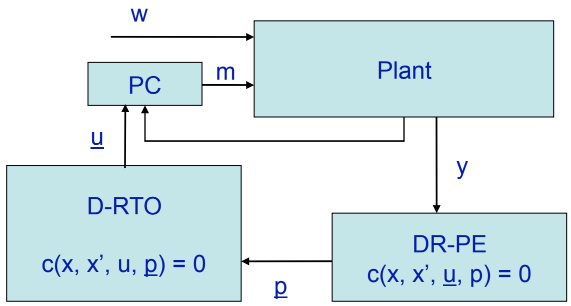
Dynamic On-line Optimization:



Integrate On-line Optimization with APC

- Consistent, first-principle dynamic models
- Consistent, feed-forward optimization
- Increase in computational complexity
- Time-critical calculations

Essential for:

- Feed changes
- Nonstandard operations
- Optimal disturbance rejection

Dynamic Optimization Problem

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

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

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

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

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

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

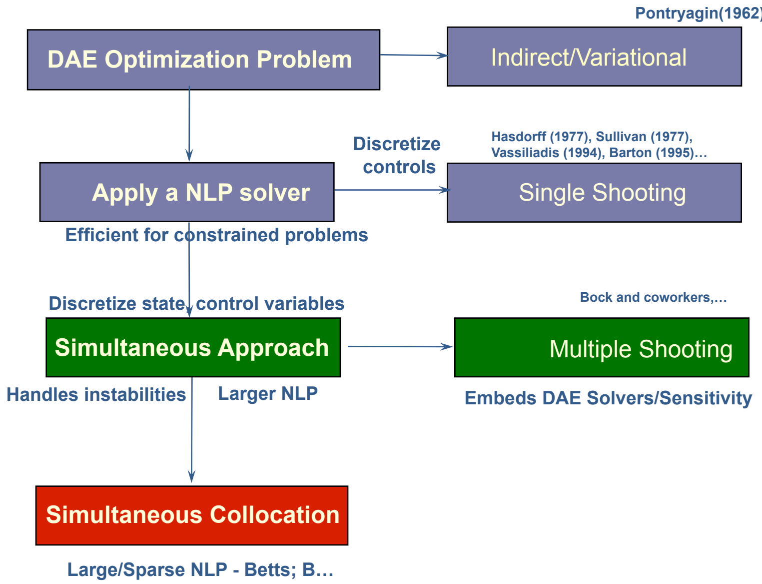
$$u^l \le u(t) \le u^u$$

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

t, time
z, differential variables
y, algebraic variables

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

Dynamic Optimization Approaches



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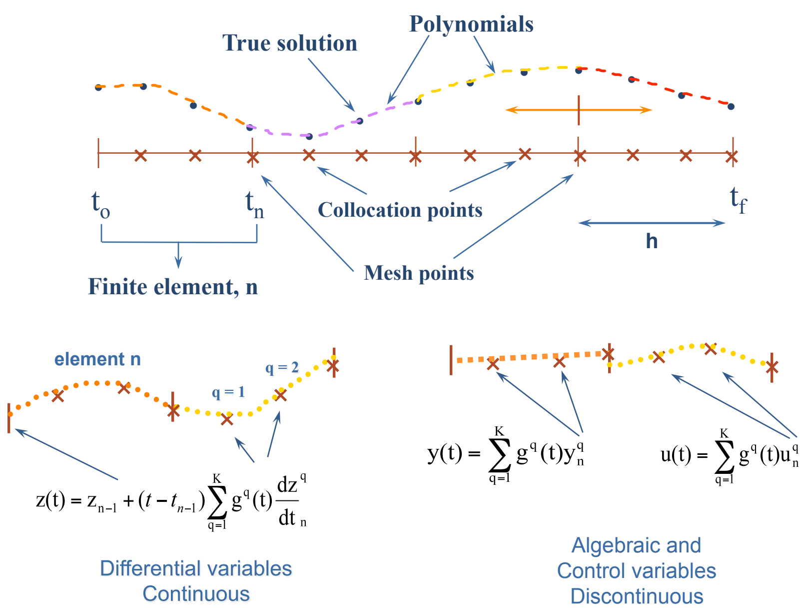
Radau Collocation on Finite Elements



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Nonlinear Programming Problem

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

s.t.

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

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

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

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

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

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

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

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

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

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

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

Need large-scale NLP code!
➔ IPOPT

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

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 rewritten in C++

Solved on many thousands of test problems and applications

Wide and growing user community

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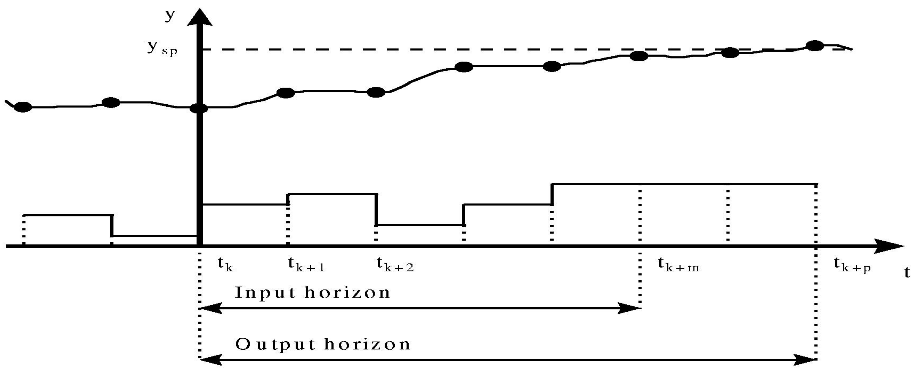
Nonlinear Model Predictive Control (NMPC)



$$\min_{u} \quad J(x(k)) = \sum_{l=0} \psi(z_l, u_l) + E(z_N)$$

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

$$z_0 = x(k)$$

Bounds

$$z' = F(z, y, u, p, d)$$

$$0 = G(z, y, u, p, d)$$

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MPC - Background

Motivate: embed dynamic model in moving horizon framework to drive process to desired state

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

Different types

- Linear Models: Step Response (DMC) and State-space
- Empirical Models: Neural Nets, Volterra Series
- Hybrid Models: linear with binary variables, multi-models
- **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**

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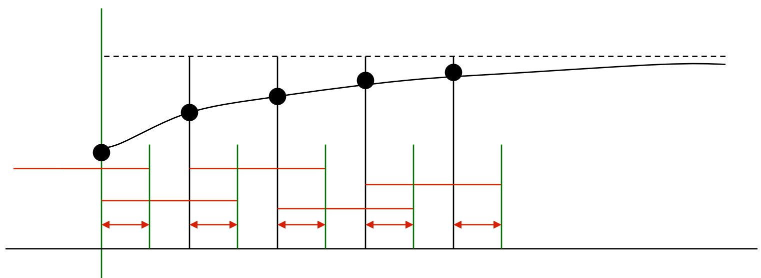
What about Fast NMPC?

Fast NMPC is not just NMPC with a fast solver

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?

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NMPC – Can we avoid on-line optimization?

Divide Dynamic Optimization Problem:

- preparation, feedback response and transition stages (Bock, Diehl et al., 1998-2006)
- solve complete NLP in background ('between' sampling times)
  as part of preparation and transition stages
- solve perturbed problem on-line
- > two orders of magnitude reduction in on-line computation

Based on NLP sensitivity of z_0 for dynamic systems

- Extended to Collocation approach – Zavala et al. (2008, 2009)
- Similar approach for MH State and Parameter Estimation – Zavala et al. (2008)

Stability Properties (Zavala, B., 2009)

- Nominal stability – no disturbances nor model mismatch
  - Lyapunov-based analysis for NMPC
- Robust stability – some degree of mismatch
  - Input to State Stability (ISS) from Magni et al. (2005)
- Extension to economic objective functions

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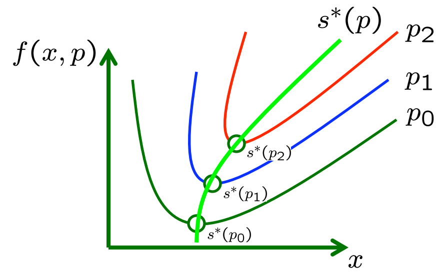
NLP Sensitivity

Parametric Programming

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



Solution Triplet

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

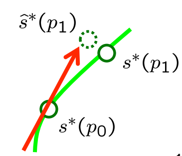
Optimality Conditions $\mathbf{P}(p)$

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

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

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

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



NLP Sensitivity

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

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

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

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

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

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

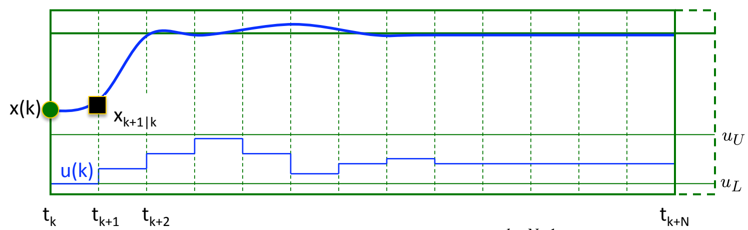
KKT Matrix IPOPT

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

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

Advanced Step Nonlinear MPC (Zavala, B., 2008)

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



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

$$\begin{aligned} s.t. \quad & x_{k+1|k} = \boxed{f(x(k), u(k))} \\ & x_{l+1|k} = f(x_{l|k}, v_{l|k}), \quad l = k+1, \ldots k+N-1 \\ & x_{l|k} \in X, \quad v_{l|k} \in U, \quad x_{k+N|k} \in X_f \end{aligned}$$

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

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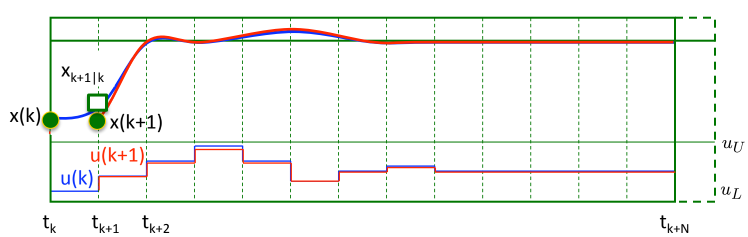
Advanced Step Nonlinear MPC (Zavala, B., 2008)

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 background (between t_k and t_{k+1})
Sensitivity to update problem on-line to get (u(k+1))

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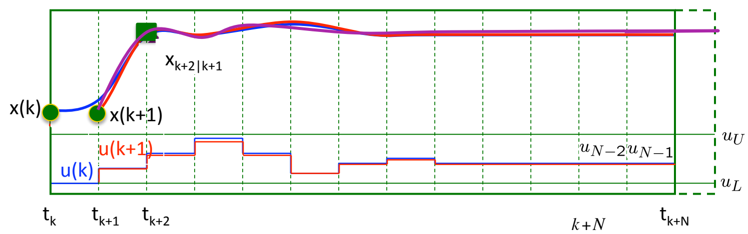
Advanced Step Nonlinear MPC (Zavala, B., 2008)

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



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

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

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

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

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})

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Stability Properties of *asNMPC*

x(k+1) = f(x(k), u(k)) – plant and model identical

Nominal Stability Theorem (Zavala, B., 2009)
<u>Assume</u> that the NLP can be solved within one sampling time, nominal stability assumptions hold for ideal NMPC (Mayne, 2000), and the nonlinear model is perfect without measurement noise. <u>Then</u> ideal NMPC controller performance and asNMPC controller performance are identical.
Ideal NMPC stability ➔ asNMPC stability.

x(k+1) = f(x(k), u(k)) + <u>g(x(k), u(k), w(k))</u>
plant and model not identical

Robust Stability Theorem (Zavala, B., 2009)
<u>Assume</u> that the NLP can be solved within one sampling time, and that robust stability assumptions hold for ideal NMPC (Magni, Scattolini, 2007). <u>Then</u> there exist bounds on the noise, *w*, and model mismatch, *g*, for which the cost function $J_{N+1}(x)$, obtained from the asNMPC strategy, is an input-to-state (ISS)-Lyapunov function and the resulting closed-loop system is ISS stable.

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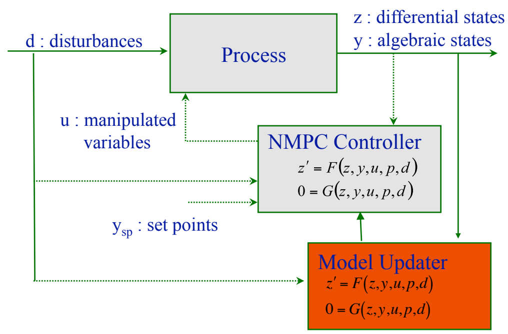
State and Parameter Estimation

NMPC Estimation and Control



Moving Horizon Estimation?

- Estimate a finite number of states and model parameters (unmeasured disturbances, rate constants, transport parameters)
- Compensate for process drifts and slowly changing conditions
- Allow better controller performance
- Alternatives to EKF, UKF…

$$\mathcal{M}_N(\eta^{mhe}(k)) \quad \min_{z_{0|k}, w_{l|k}} \phi(\eta^{mhe}(k)) = \Gamma(z_{0|k}) + L_N(z_{N|k}) + \sum_{l=0}^{N-1} L_l(z_{l|k}, w_{l|k})$$

$$\text{s.t. } z_{l+1|k} = f(z_{l|k}, w_{l|k}), \quad l = 0, ..., N-1$$

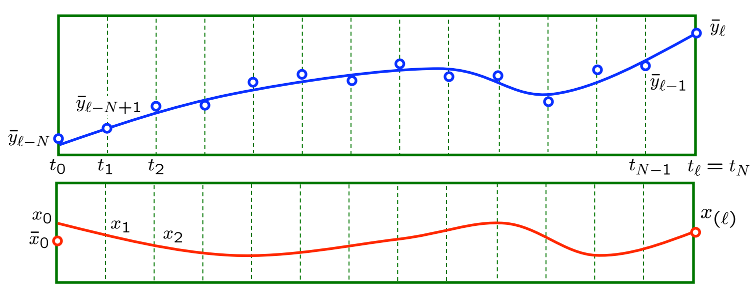
$$z_{l|k} \in \mathbb{Z},\ w_{l|k} \in \mathbb{W}.$$

$$\Gamma(z_{0|k}) = (z_{0|k} - \bar{z}_0(k))^T \bar{\Pi}_0^{-1}(k)(z_{0|k} - \bar{z}_0(k))$$

$$L_l(z_{l|k}, w_{l|k}) = (y(k-N+l) - \chi(z_{l|k}))^T R_l^{-1}(y(k-N+l) - \chi(z_{l|k})) + w_{l|k}^T Q_l^{-1} w_{l|k}$$

$$L_N(z_{N|k}) = (y(k) - \chi(z_{N|k}))^T R_N^{-1}(y(k) - \chi(z_{N|k})) \qquad (6.2)$$

Moving Horizon Estimation (MHE)



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
Can MHE be improved?

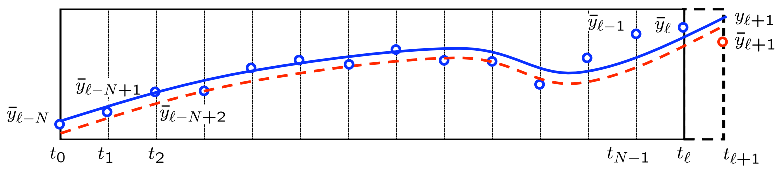
Large State Dimensionality $dim(x_k) \approx 100 - 10,000$

Degrees of Freedom $dim(x_0) + dim(w_k)N \approx (100 - 10,000) + (10 - 100)N$

Highly Nonlinear, Ill-Conditioned?

Solution Time → *Order of Minutes*

Advanced Step Moving Horizon Estimation (asMHE)



$$\mathcal{M}_N(\eta^{mhe}(k)) \quad \min_{z_{0|k}, w_{l|k}} \phi(\eta^{mhe}(k)) = \Gamma(z_{0|k}) + L_N(z_{N|k}) + \sum_{l=0}^{N-1} L_l(z_{l|k}, w_{l|k})$$

$$\text{s.t. } z_{l+1|k} = f(z_{l|k}, w_{l|k}), \qquad l = 0, ..., N-1$$

$$z_{l|k} \in \mathbb{Z},\ w_{l|k} \in \mathbb{W}.$$

Given y_l, z_l, set "fake measurement" $z_{l+1} = f(z_l, w_l),\ \bar{y}_{l+1} \approx \chi(z_{l+1})$

Solve $\mathcal{M}_N$ in background (between t_l and t_{l+1})

Obtain measurement at t_{l+1}, use KKT sensitivity on-line to get z_{l+1}

Solve P(l+1) in background (between t_{l+1} and t_{l+2})

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NMPC for High Purity Distillation

Air Separation Unit in IGCC-based Power Plants
- Need for high purity O2
- Respond quickly to changes in process demand
- Large, highly nonlinear dynamic separation (MESH) models

Methanol distillation (Diehl, Bock et al., 2005)
- 40 trays, 210 DAEs, 19746 discretized equations

Argon Recovery Column
- 50 trays, 260 DAEs, 21306 discretized equations

Double Column ASU Case Study
- 80 trays, 1520 DAEs, 116,900 discretized equations

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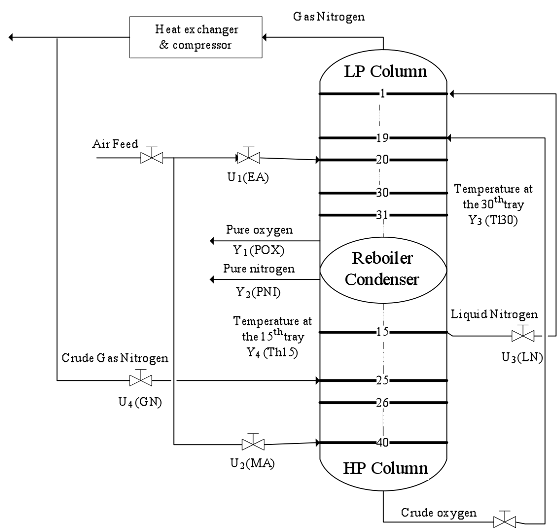
Nonlinear Model Predictive Control: Air Sep'n Unit
(Huang, B., 2008)

Objective: force the production rates to follow the set-points, while main their purities.
4 manipulated variables.
4 output variables.

Horizon: 100 minutes in 20 finite elements.
Sampling time: 5 minutes.



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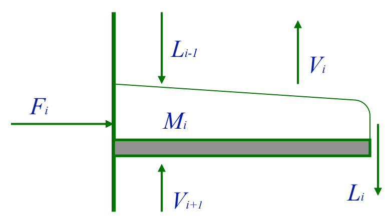
Case Study: Basic Air Separation Unit

MESH Equations for Distillation Column

Assumption:

- Vapor holdups are negligible.
- Ideal vapor phases.
- Well mixed entering streams.
- Constant pressure drop.
- Equilibrium stage model.



Mass balance: $\frac{dM_i}{dt} = L_{i-1} + V_{i+1} - L_i - V_i + F_i$

Component balance: $\frac{d(M_i x_{i,j})}{dt} = L_{i-1}x_{i-1,j} + V_{i+1}y_{i+1,j} - L_i x_{i,j} - V_i y_{i,j} + F_i x^f_{i,j}$

Energy balance: $\frac{d(M_i h^L_i)}{dt} = L_{i-1}h^L_{i-1} + V_{i+1}h^V_{i+1} - L_i h^L_i - V_i h^V_i + F_i h^f_i$

Phase equilibrium: $y_{ij} = K(x_i, T_i)_{ij} x_{ij}$

Summation: $\sum_j y_{ij} = \sum_j K(x_i, T_i)_{ij} x_{ij} = 1$

Index 2 system.

Hydrodynamics: $L_i = k_d M_i$

Enthalpy Definitions: $h^L_i = \varphi^L(x_i, T_i)$
$h^V_i = \varphi^V(y_i, T_i)$

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Air Separation Unit: Reformulate to Index 1

Differentiate $\sum_j K(x_i, T_i)_{ij} x_{ij} = 1$

Define dummy variables

$$\bar{T}_i := \frac{dT_i}{dt} = -\frac{\sum_{j \in \text{COMP}} \left[x_{i,j} \sum_{k \in \text{COMP}} \left(\frac{\partial K_{i,j}}{\partial x_{i,k}} \bar{x}_{i,k} \right) + K_{i,j} \bar{x}_{i,k} \right]}{\sum_{j \in \text{COMP}} x_{i,j} \partial K_{i,j} / \partial T_i}$$

$$\bar{x}_{i,j} := \frac{dx_{i,j}}{dt} = \frac{L_{i-1}(x_{i-1,j} - x_{i,j}) + V_{i+1}(y_{i+1,j} - x_{i,j}) - V_i(y_{i,j} - x_{i,j}) + F_i(x^f_{i,j} - x_{i,j})}{M_i}$$

Energy balance:

$$M_i\left(\frac{\partial h^L_i}{\partial T_i} \bar{T}_i + \sum_{j \in \text{COMP}} \frac{\partial h^L_i}{\partial x_{i,j}} \bar{x}_{i,j}\right) = L_{i-1}(h^L_{i-1} - h^L_i) + V_{i+1}(h^V_{i+1} - h^L_i) - V_i(h^V_i - h^L_i) + F_i(h^f_i - h^l_i)$$

Summation: $\sum_j K(x_i, T_i)_{ij} x_{ij} = 1$

Reformulated index 1 system contains 320 ODEs, 1200 AEs.

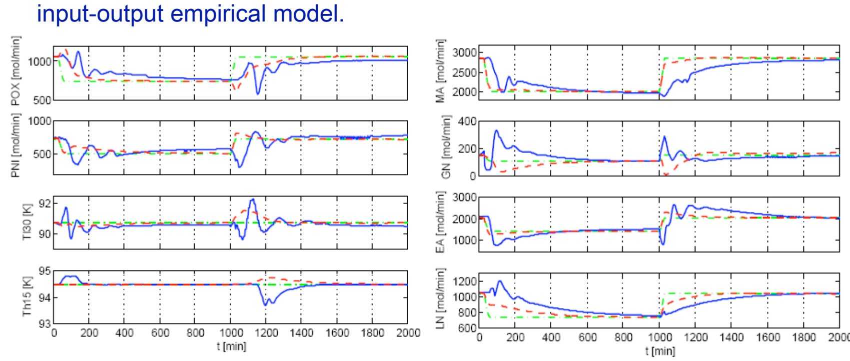
<u>Eliminate following ODEs</u>

Energy balance: $\frac{d(M_i h^L_i)}{dt} = L_{i-1} h^L_{i-1} + V_{i+1} h^V_{i+1} - L_i h^L_i - V_i h^V_i + F_i h^f_i$

<u>One</u> Component balance: $\frac{d(M_i x_{i,j})}{dt} = L_{i-1} x_{i-1,j} + V_{i+1} y_{i+1,j} - L_i x_{i,j} - V_i y_{i,j} + F_i x^f_{i,j}$

ASU Nonlinear MPC - Case 1

t = 30-60 min, product rates are ramped down by 30%. t =1000-1030 min, they are ramped back. AS-NMPC is compared to MPC with linear input-output empirical model.



Output Variables | Manipulated Variables

The green dot-dashed lines are the set-points, the blue dashed lines are the linear controller profiles and red solid lines are AS-NMPC profile.

All the tuning parameters are favored to the linear controller.

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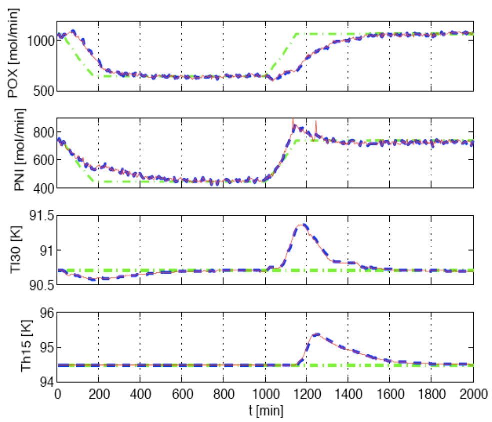
NMPC of Air Separation Unit – Case 2

(Huang, B., 2009)

At t = 30-60 min, product rates are ramped down by 40%.
At t =1000-1030 min, they are ramped back. 5% disturbance is added to M_i.



N = 20, K = 3
320 ODEs, 1200 AEs.
Variables: 117,140
Constraints: 116,900

400 NLPs solved
Background: 200 CPUs, 6 iters.
Online: 1 CPUs

Computational Feedback Delay
Reduced from 200 → 1 second.

Blue dashed lines are ideal NMPC profile
Red lines are AS-NMPC profile.
<u>In contrast, linearized controller is unstable</u>

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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>*

$$
\begin{aligned}
\min \ & \sum_{j=1}^{N_e} (\zeta^T_{k-N_e+j} \Pi_y \zeta_{k-N_e+j}) + \hat{\theta}_k^T \Pi_\theta \hat{\theta}_k \\
& + (\hat{x}_{k-N_e} - \bar{x}_{k-N_e})^T \Pi_0 (\hat{x}_{k-N_e} - \bar{x}_{k-N_e}) \\
\text{s.t.} \ & \hat{x}_{k-N_e+j+1} = f(\hat{x}_{k-N_e+j}, u_{k-N_e+j}, \hat{\theta}_k) \\
& \hat{y}_{k-N_e+j} = h(\hat{x}_{k-N_e+j}) \\
& \zeta_{k-N_e+j} = y_{k-N_e+j} - \hat{y}_{k-N_e+j} \\
& \hat{x}_{k-N_e+j} \in \mathbb{X}, \zeta_{k-N_e+j} \in \Omega_\zeta, \hat{\theta}_k \in \Omega_\theta \\
& j = 0, \ldots, N_e - 1.
\end{aligned}
$$

$$
\begin{aligned}
\min \ & \sum_{j=0}^{N_p} (l_{k+j} - y_r)^T \Gamma_y (l_{k+j} - y_r) + \sum_{i=0}^{N_c-1} \triangle v^T_{k+i} \Gamma_u \triangle v_{k+i} \\
\text{s.t} \ & z_{k+j+1} = f(z_{k+j}, v_{k+j}, \hat{\theta}_k), \ j = 0, \ldots, N_p - 1 && \text{(10a)} \\
& z_k = \hat{x}_k, \ z_{k+j} \in \mathbb{X} && \text{(10b)} \\
& l_{k+j} = h(z_{k+j}) + \zeta_k, \ \triangle v_{k+i} = v_{k+i+1} - v_{k+i} && \text{(10c)} \\
& v_{k+j} = v_{k+i} \text{ for } i \le j < i+1, \ v_{k+i} \in \mathbb{U}, \ N_c \le N_p. && \text{(10d)}
\end{aligned}
$$

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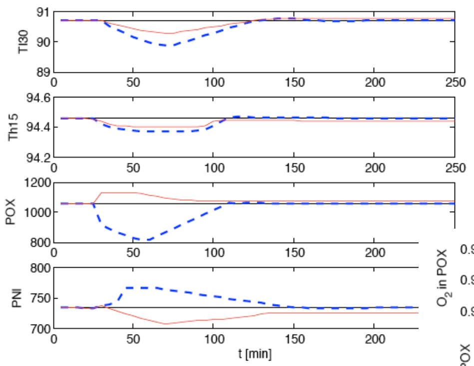
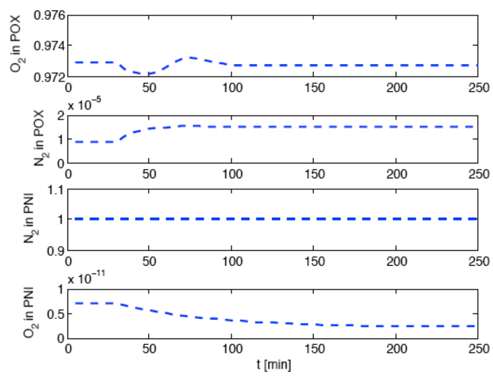
Combined MHE and NMPC for ASU
(Huang, B., 2009)



Change in model mismatch (hydraulic parameter)

- Setpoint
- MHE/NMPC with correction
- NMPC without correction

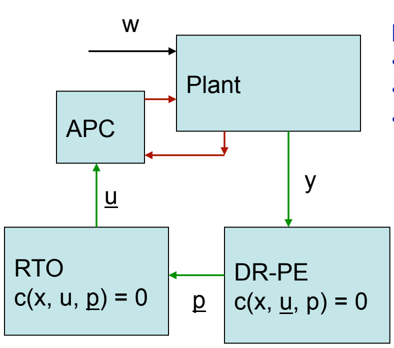


AMPL/IPOPT (DuoCore 2.4 GHz)
NMPC background (6 iter/200 CPUs)
MHE background (15 iter/90 CPUs)

- N=5, K=3
- 29,285 constraints
- 30,885 variables

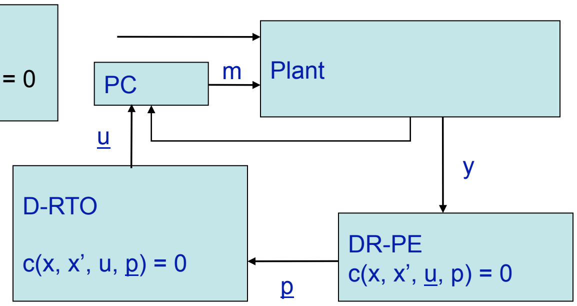
Online NMPC+MHE ~ 2 CPUs

D-RTO with Economic Objectives → Beyond NMPC Tracking



Benefits of combining RTO with NMPC?

- Direct, dynamic production maximization
- Remove artificial tracking objective
- Remove artificial steady state problem



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Challenges with D-RTO

Replace regulation objective with economic objective in NMPC?

Active ongoing activity:

- Bartusiak (2007)
- Chachuat et al. (2008)
- Dadhe and Engell (2008), Engell (2007, 2009)
- Diehl and Rawlings (2009), Rawlings and Amrit (2009)
- Kadam et al. (2008)
- Zavala, B. (2009)
- Swartz et al. (2010)

Need strict convexity of Lyapunov function for stability (i.e., $\mathcal{K}$ function)

$$Min \sum_{l} \{ w_l \varphi(z_l, u_l) \} + F(z_N)$$

Suggestion: Regularize economic objective so that NLP satisfies SSOC

Many Open Stability/Robustness Questions Still Remain

- need to find (and assume) an optimal steady state profit?

- how to consider cyclic problems?

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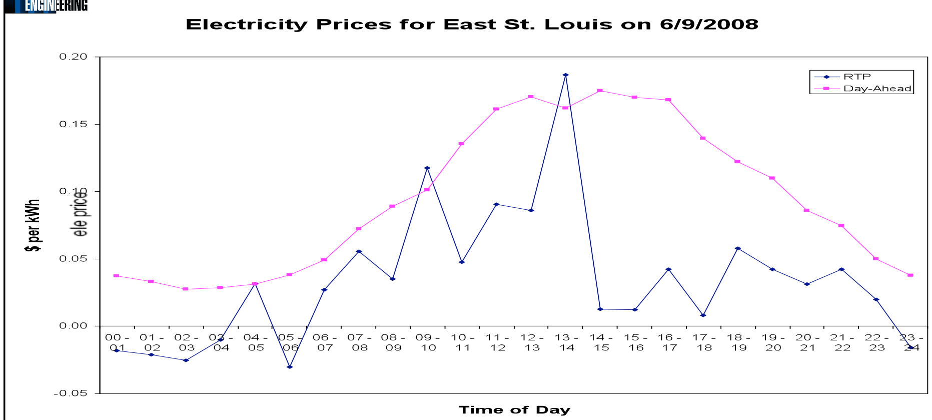
NMPC with Economic Objective



$$
\begin{aligned}
\min \quad & \sum_{i=0}^{N+K-1} l(z_i, v_i) \\
\text{s.t} \quad z_{i+1} &= f(z_i, v_i), \quad i = 0, \dots, N+K-1 \\
z_0 &= x_k, \; z_{N+K} = z_N, \\
z_i &\in \mathbb{X}, \; v_i \in \mathbb{U}
\end{aligned}
$$

- periodic boundary condition
- equivalent to endpoint constraint formulation for MPC
- $l(z,v)$ – strongly convex economic objective function (regularized)
- alternate infinite horizon formulation

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D-RTO: Preliminary ASU Results

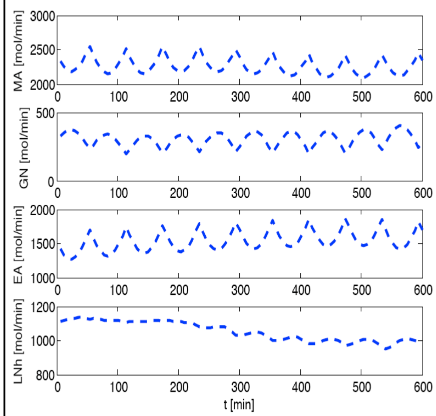

Figure 9: Input profile in the ASU study

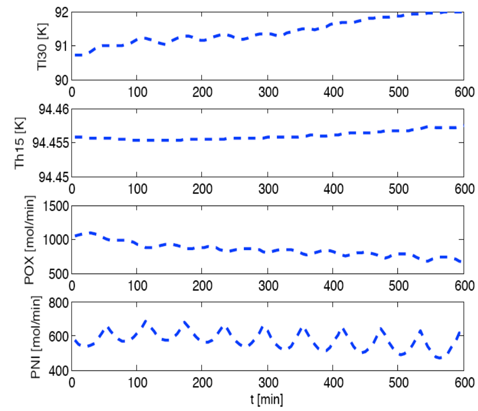

Figure 10: Output profile in the ASU study

- D-RTO results – cannot be obtained with two-tier strategy
- Computational Costs – comparable to as-NMPC
- Superior Performance over profile tracking – accommodates disturbances directly

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Conclusions

Dynamic optimization essential for many processes

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

Chemical Process Operations: RTO → D-RTO

- 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 Models

- ASU process with DAE model
- Advantages over linear MPC
- Extended to Uncertainties – NMPC + MHE Formulations
- Direct Dynamic Optimization

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Background References

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