A Nonlinear Programming Path to NMPC and Real-Time Optimization

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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?

Parameter Estimation and Model Discrimination
Equipment and Flowsheet Design
Process Operations, Transients and Upsets
Better Results than with “Experience”
Consistent Results among all Practitioners
Support and Enhance Process Understanding
Reduce Cycle Time by Orders of Magnitude

How Process Optimization?

Optimization Formulations and Models

Compute Efficiency

Closed

Open

First and Second Derivatives
NLP Barrier

Full First Derivatives

Finite Differences

Black Box

DFO

Computational Efficiency
**Barrier Methods for Large-Scale Nonlinear Programming**

Original Formulation

\[
\begin{align*}
\min_{x \in \mathbb{R}^n} & \quad f(x) \\
\text{s.t.} & \quad c(x) = 0 \\
& \quad a \leq x \leq b \\
& \quad x \geq 0
\end{align*}
\]

Barrier Approach

\[
\begin{align*}
\min_{x \in \mathbb{R}^n} & \quad \phi_\mu(x) = f(x) - \mu \sum \ln x_i \\
\text{s.t.} & \quad c(x) = 0 \\
& \quad \mu \to 0, \quad x^\mu \to x^*
\end{align*}
\]

Fiacco and McCormick (1968)

**IPOPT Features**

(Wächter, Laird, B., 2002-2009)

**Newton-Based Barrier Method**
- Globally, superlinearly convergent (Wächter and B., 2005)
- Easily tailored to different problem structures

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

**Line Search Globalization**
- \( \ell \) exact penalty merit function
- augmented Lagrangian merit function
- Filter method (extended from Fletcher and Leyffer)

**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

**Barrier Problem Solution**

\[
\begin{align*}
\nabla f(x) + A(x) \lambda - \nu &= 0 \\
Xv - \mu \lambda &= 0 \\
A &= \nabla c(x), \quad W = \nabla L(x, \lambda, \nu)
\end{align*}
\]

Reducing the System

\[
\begin{align*}
\left[ W + \sum \frac{A}{A^T} \right] \left[ \begin{array}{c} d_x \\ A^{T} \end{array} \right] &= \left[ \begin{array}{c} \nabla \phi_\mu \\ c \end{array} \right] \\
\sum &= X^{-1}V
\end{align*}
\]

IPOPT Code – www.coin-or.org

**NLP Sensitivity**

Parametric Program

\[
\begin{align*}
\min & \quad f(x, p) \\
\text{s.t.} & \quad c(x, p) = 0 \\
& \quad x \geq 0
\end{align*}
\]

Solution Triplet

\[
s^*(p) = [x^T, \lambda^T, \nu^T]
\]

Optimality Conditions

\[
\begin{align*}
\nabla c(x(p)) + \nabla x(x(p)) \lambda &= 0 \\
c(x(p)) &= 0 \\
X\lambda &= \nu
\end{align*}
\]

NLP Sensitivity

Main Idea: Obtain \( \frac{\partial s^*(p)}{\partial p} \) and find \( s^*(p_1) \) by Taylor Series Expansion

\[
s^*(p_1) = s^*(p_0) + \left. \frac{\partial s^*(p)}{\partial p} \right|_{p_0} (p_1 - p_0)
\]
NLP Sensitivity with IPOPT
(Pirnay, Lopez Negrete, B., 2011)

Optimality Conditions of
\[
\begin{align*}
\nabla_c L &= \nabla_c f(x(p), p) + \nabla_c c(x(p), p) x(p) \quad \Rightarrow \quad \{ \nabla_c L, c(x(p), p) x(p) \} \\
\quad \text{and} \quad x(p) = i \\
Q(s, p) &= \nabla c(x(p), p) x(p)
\end{align*}
\]

Apply Implicit Function Theorem to
\[
Q(s, p) = \nabla c(x(p), p) x(p) \quad \Rightarrow \quad Q(s^*(p_0), p_0) = 0
\]

\[
\begin{bmatrix} W(x^*(p_0)) & A(x^*(p_0)) \\ A(x^*(p_0)) & X^*(p_0) \end{bmatrix} \begin{bmatrix} Z^{T} \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}
\]

KKT Matrix IPOPT
\[
W(x^*(p_0)) \begin{bmatrix} A(x^*(p_0)) \\ X^*(p_0) \end{bmatrix} \begin{bmatrix} 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}
\]

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

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

- Linearized KKT Conditions are:

\[
\begin{bmatrix} W_{bb} & W_{bd} \\ W_{db} & W_{dd} \end{bmatrix} \begin{bmatrix} \Delta b \\ \Delta d \end{bmatrix} = \begin{bmatrix} \Delta b_d \\ \Delta d \end{bmatrix}
\]

- The solution leads to

\[
\Delta d = (Z^T W Z)^{-1} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad Z = \begin{bmatrix} -A_{b} \end{bmatrix}
\]

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

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

NLP Sensitivity
Parameter and State Estimation

- Analyze sensitivity of estimates with changes in data

\[
\min_{\theta, \gamma, a} \frac{1}{2} \left\{ (y - \bar{y})^T V_\theta^{-1} (y - \bar{y}) + \theta^T (\theta - \bar{\theta})^T V_{\theta}^{-1} (\theta - \bar{\theta}) \right\}
\]

s.t. \( c(\theta, \gamma, a) = 0 \)

- Introduce perturbations \( \theta^* + \delta \theta \) and \( \gamma^* + \delta \gamma \)

\[
\text{Cov} \left( \theta \right) \approx E \left\{ \Delta \theta \Delta \theta^T \right\} = (Z^T W Z)^{-1}
\]

Approximate Confidence Region

\[
(\theta - \theta^*)^T V_{\theta}^{-1} (\theta - \theta^*) \leq \chi^2(a)
\]
Dynamic Optimization Problem

\[
\begin{align*}
\text{min} & \quad \psi(z(t), y(t), u(t), p, t_f) \\
\text{s.t.} & \quad \frac{dz}{dt} = F(z(t), y(t), u(t), p) \\
& \quad G(z(t), y(t), u(t), p) = 0 \\
& \quad z^0 = z(0) \\
& \quad z^f = z(t_f) \\
& \quad y^0 = y(0) \\
& \quad u^0 = u(t) \\
& \quad p^0 = p
\end{align*}
\]

\(t_f\), final time
\(u\), control variables
\(p\), time independent parameters
\(t\), time
\(z\), differential variables
\(y\), algebraic variables

Dynamic Optimization Approaches

**DAE Optimization Problem**

- Discretize controls
- Efficient for constrained problems

**Single Shooting**

**Multiple Shooting**

- Embeds DAE Solvers/Sensitivity
- Handles instabilities
- Larger NLP

**Simultaneous Approach**

- Embeds DAE Solvers/Sensitivity
- Takes full advantage of open structure
- Many degrees of freedom
- Periodic boundary conditions
- Multi-stage formulations

Nonlinear Programming Formulation

**Nonlinear Dynamic Optimization Problem**

- (Piecewise)
- Continuous profiles

- Collocation on finite elements

**Discretized variables**

**Nonlinear Programming Problem (NLP)**

Nonlinear Programming Problem

\[
\begin{align*}
\text{min} & \quad \psi(z_i, y_i, u_i, p, t_f) \\
\text{s.t.} & \quad \left( \frac{dz_i}{dt} \right)_j = F(z_i, y_i, u_i, p) \\
& \quad G(z_i, y_i, u_i, p) = 0 \\
& \quad z_i^0 = z(0) \\
& \quad z_i^f = z(t_f) \\
& \quad y_i^0 = y(0) \\
& \quad u_i^0 = u(t) \\
& \quad p^0 = p
\end{align*}
\]

\(x^L \leq x \leq x^U\)

Nonlinear Programming Problem
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-RTD 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

### Large-Scale Parameter Estimation
- Complex Kinetic Mechanisms
  - Chain Transfer to Polymer
  - Chain Transfer to Solvent
  - Chain Initiation
  - Chain Propagation
  - Chain Termination
  - Chain Transfer to Monomer
  - Chain Termination by Disproportionation
  - Chain Transfer to Initiator
  - Chain Transfer to Initiator

  \[ k = k_0 \exp \left( \frac{E_a}{RT} \right) \approx 35 \text{ Elementary Reactions} \]

- 100 Kinetic Parameters

### Large-Scale Parameter Estimation
- Use Rigorous Model to Match Plant Data Directly
- Least-Squares Formulation
- Special Case of Multi-Stage Dynamic Optimization Problem
- Solve using Simultaneous Collocation-Based Approach
  - 1 data set
  - 6 data sets
  - 500 ODEs $\times 6$
  - 3000 ODEs
  - 1000 AEs $\rightarrow$ 3000 AEs

### 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

- Polymer Melt Index (PMI)
- Recycle System and Flash Separation
- Ethylene
- Recycle
- Limited Low-Pressure Recycle
- High-Pressure Recycle
- Chain-Transfer Agent
- 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

- Multi-Zone Tubular Reactor – Quasi Steady-State
- LDPE Parameter Estimation
- Multi-Zone Tubular Reactor – Quasi Steady-State
- Improved Prediction Core Temperature Profile
- Grade A
- Grade B

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

Results
- Zonal Assumptions
- Characteristic Lengths
- Zonal Temperatures
- Zonal Energy Equations
- Boundary Conditions
- Continuity and Mass Conservation
- Kinetics

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

Sensitivity-based Confidence Regions

On-line Issues: Model Predictive Control (NMPC)

\[
\min_u J(x(k)) = \sum_{i=0}^{N} y(z_i, u_i) + F(z_N) \\
\text{s.t. } z_{i+1} = f(z_i, u_i) \\
\text{Bounds}
\]
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

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; Findelen and Allgöwer, 2004; Santos et al., 2001)

![Diagram](image1)

Can computational delay be overcome?
- Fast Newton-based NMPC
- Cheap NLP Sensitivity

Some Related NMPC Research

Optimization and Optimal Control

Model Predictive Control
- Evolution from LQ, MPC (Kleinman, 1975; Kwon and Pearson, 1977),
- DMC (Cutler and Ramaker, 1979), QDMC (Garcia and Morshed, 1984)
- Real-time iteration (Diehl, Li, Ohtsuka, Oliveira, Santos, 1989 - )
- Neighboring extremal approaches (Bonvin, Marquardt, 2002 - )

Advanced Step Nonlinear MPC (Zavala, B., 2009)
Solve NLP in background (between steps, not on-line)
Update using sensitivity on-line

\[
\begin{align*}
\min & \quad J(x(k), u(k)) = F(x_{k+N}^*) + \sum_{l=k}^{k+N} \psi(x_l, v_l) \\
\text{s.t.} & \quad x_{k+l} = f(x_l, v_l), \quad l = k + 1, \ldots, k + N - 1 \\
& \quad x_{k+l} \in X, \quad v_l \in U, \quad x_{k+N} \in X_f
\end{align*}
\]

Solve NLP(k) in background (between \(t_k\) and \(t_{k+N}^*\))
Advanced Step Nonlinear MPC (Zavala, B., 2009)

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

Update using sensitivity on-line

\[ \min \ J(x(k+1), u(k+1)) = F(x_{k+1}, t_{k+1}) + \sum_{l=k+2}^{k+N} p(x_{l_{k+1}}, v_{l_{k+1}}) \]

s.t. \( x_{l_{k+1}} = f(x_{l_{k+1}}, v_{l_{k+1}}) \), \( l = k+2, \ldots, k+N \)

\( x_{l_{k+1}} \in X, f_{l_{k+1}} \in U, x_{l_{k+1}} \in X_f \)

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

Sensitivity to update problem on-line to get (\( u(k+1) \))

Solve NLP(k+1) in background (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 \( \Rightarrow \) as-MHE

\[ \min \sum_{j=t_0}^{t_{k+1}} \left( \sum_{i=0}^{l} \left( q_{ij}^T x_{ij} + n_{ij}^T n_{ij} \right) + q_{ij}^T u_{ij} \right) \]

s.t. \( x_{ij+1} = f(x_{ij+1}, x_{ij}, u_{ij}, \theta) \)

\( \Delta x_{ij+1} = f(x_{ij+1}, x_{ij}, u_{ij}, \theta) \)

\( x_{ij+1}, x_{ij} \in X, \Delta x_{ij+1} \subseteq \Omega, \theta \subseteq \Theta \)

\( j = 0, \ldots, n_0 \)

\( \Delta x_{ij+1} \in \Omega, \Delta x_{ij} \subseteq \Omega \)

NMPC Controller

\( f(x_{k+1}, x_{k}, u_{k}, \theta) \)

\( \Delta x_{k+1} = f(x_{k+1}, x_{k}, u_{k}, \theta) \)

\( x_{k+1} = x_{k} + \Delta x_{k+1} \)

\( u_{k} = u_{k-1} \)

\( \Delta x_{k+1} = f(x_{k+1}, x_{k}, u_{k}, \theta) \)

\( x_{k+2} = x_{k+1} \)

Advanced-step MHE

Background: At \( t_0 \) having \( x_0 \) and \( u_0 \), approximate \( x_{k+1} \) and \( y_{k+1} \). Solve the extended MHE problem from \( k-N \) to \( k+1 \). Let \( \rho_2 = \) 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.

NLP Sensitivity used for State Approximation and Covariance Updates
**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

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

- MHE+NMPC for LDPE Process
  - Fouling
    - $T_{F,\text{MEA}} = \text{COLD}$
  - Defouling
    - $T_{F,\text{MEA}} = \text{HOT}$

Cannot Remove Heat of Reaction - Drop Production to Avoid Runaway

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

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

Minimize Transition Time

Zavala & B., 2010
**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

**Economic NMPC Stability Analysis**

(Huang, Harinath, B., 2011)

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

For the rotated stage costs (transformed Lagrange function), $T_i(0,0) = 0$

$$ L_i(\bar{z}, \bar{v}) = L_i(0,0) + \nabla \tilde{L}_i(0,\bar{v}) \bar{z} + \frac{1}{2} \int_0^{T_i} \| \nabla^2 \tilde{L}_i(t,\tau) \| \bar{z} \bar{v} + \frac{\bar{z}^T}{2} d\tau 
\geq \frac{1}{2} \int_0^{T_i} \| \nabla^2 \tilde{L}_i(t,\tau) \| \bar{z}^T \bar{v} + \bar{z}^T \geq \beta_m(|\bar{z}|).$$

If $\tilde{L}_i(\tau,\tau)_{||\bar{z}}$ 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)

**Challenges with D-RTO**

Replace regulation objective with economic objective in NMPC?

Bartusiak, Young et al. (2007)
Chachuat et al. (2008)
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)

$$ \min \sum_i \left[ \text{Profit}_i \right] + \text{Profit}_N $$

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?

**Dynamic RTO for LDPE Process**

(Zavala, B., 2010)

Fouling

$T_{Fouling} = COLL$

Cannot Remove Heat of Reaction - Drop Production to Avoid Runway

Defouling

$T_{Defouling} = HOT$

Heat Transfer Coefficient

Time (Days)

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

\[ \min_{u(t)} \int_0^T \int_0^T \left( c(x,t) - z^*(z) \right)^TW(z(x,t) - z^*(z)) - \text{Production}(z^*(t)) \, dt \]

Core Temperature

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 Hor

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?

<table>
<thead>
<tr>
<th>Background Optimization</th>
<th>Online Update</th>
<th>NLP Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ideal</td>
<td>None</td>
<td>NLP</td>
</tr>
<tr>
<td>Real-time Iteration</td>
<td>None</td>
<td>QP</td>
</tr>
<tr>
<td>Neighboring Extremal</td>
<td>Only once</td>
<td>KKT/QP</td>
</tr>
<tr>
<td>asNMPC</td>
<td>Every step</td>
<td>KKT</td>
</tr>
</tbody>
</table>

\[ \begin{bmatrix} K + F_0 \Delta s \end{bmatrix} = \begin{bmatrix} 0 \\ 2(t + 2) \end{bmatrix} \]

Reuse L/U Factors of \( K \) with Schur Complement

\[ -\left( E_2^T K^{-1} F_0 \right) \Delta s = \Delta z + 2(t + 2) \]
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?
    - Adapting 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?

---

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

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Conclusions

- 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

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Research Colleagues

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- Dr. Victor Zavala
- Xue Yang

Many Thanks to:

Lynne W. Biegler

and …

To the NPC community

In humble thanks for your award and recognition

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For more details…

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