Frameworks for On-Line Direct Transcription

Lorenz T. Biegler and Victor M. Zavala

Department of Chemical Engineering
Carnegie Mellon University

vzavala@cmu.edu

http://numero.cheme.cmu.edu

SIAM Conference on Optimization
May 11th 2008

Carnegie Mellon

CAPD CENTER

Outline

1. DAE-Constrained Optimization in On-Line Applications
2. Direct Transcription and General Interior-Point NLP Solvers
3. <u>Add-On Capabilities for Interior-Point Solvers</u>
4. Case Study
5. Conclusions and Future Work

DAE-Constrained Optimization in On-Line Applications

$$\min_{u(t),p(t),z_0} \int_{t_0}^{t_f} \varphi(z(t),y(t),u(t),p(t))dt$$

Objective –Least-Squares, Complex Economic-

$$\frac{dz}{dt} = \mathbf{f}(z(t),y(t),u(t),p(t))$$

Conservation Equations

$$0 = \mathbf{g}(z(t),y(t),u(t),p(t))$$

Physical and Thermodynamic Properties

$$0 \geq \mathbf{h}(z(t),y(t),u(t),p(t))$$

Physical and Operational Limits

$$z(0) = z_0$$

Current Trend

- **Dynamic Models <u>as Detailed as Possible</u> for <u>On-line</u> Economic Optimization and Control**

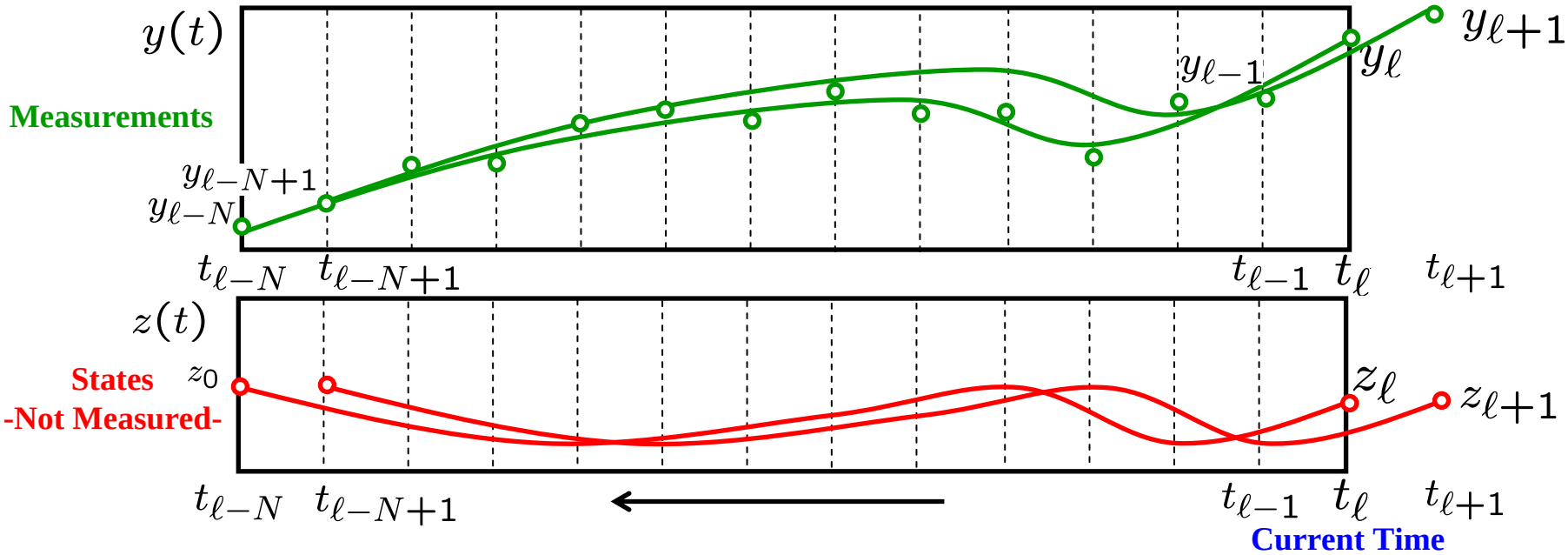
Manageable Problem Dimensions

~ 1,000-10,000 DAEs -Mostly Algebraic, Many Degrees of Freedom-

Related Tasks:

- **Off-Line: Parameter Estimation, Trajectory Design**
- **On-Line: State Estimation, Control**

Moving Horizon Estimation

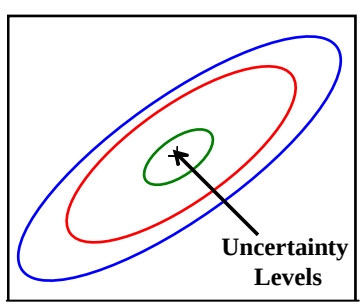


$$\min_{p(t),\, z_0} \sum (y(t_k) - y_{\ell-k+N})^T \mathbf{V}_y^{-1} (y(t_k) - y_{\ell-k+N})$$

$$\begin{aligned} \frac{dz}{dt} &= \mathbf{f}\left(z(t), w(t), u(t), p(t)\right) \\ 0 &= \mathbf{g}\left(z(t), w(t), u(t), p(t)\right) \\ y(t) &= \chi(z(t), w(t), u(t), p(t)) \\ z(0) &= z_0 \quad \textbf{Uncertain} \end{aligned}$$

$$\min_{p(t),\, z_0} \sum (y(t_k) - y_{\ell-k+N+1})^T \mathbf{V}_y^{-1} (y(t_k) - y_{\ell-k+N+1})$$

$$\begin{aligned} \frac{dz}{dt} &= \mathbf{f}\left(z(t), w(t), u(t), P(t)\right) \\ 0 &= \mathbf{g}\left(z(t), w(t), u(t), P(t)\right) \\ y(t) &= \chi(z(t), w(t), u(t), P(t)) \\ z(0) &= z_0 \end{aligned}$$



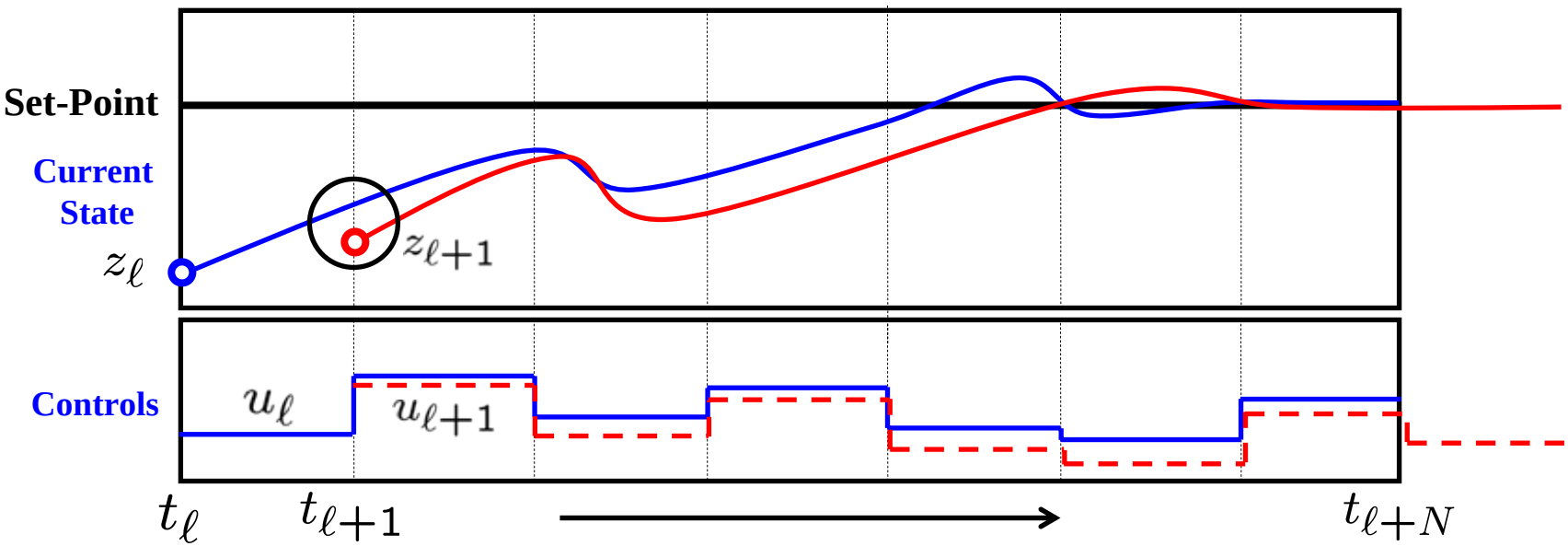
$$\mathbf{\Pi}_\ell \to 0$$

How Uncertain in Current State z_ℓ ?

- **Analysis Covariance Matrix $\mathbf{\Pi}_\ell$**
- **Penalize z_0 as Confidence Increases**

Moving Horizon Control

Mismatch (Model,Disturbances)



Economic-Tracking

$$\min_{u(t)} \int_{t_\ell}^{t_{\ell+N}} \varphi(z(t), y(t), u(t), p(t))dt$$

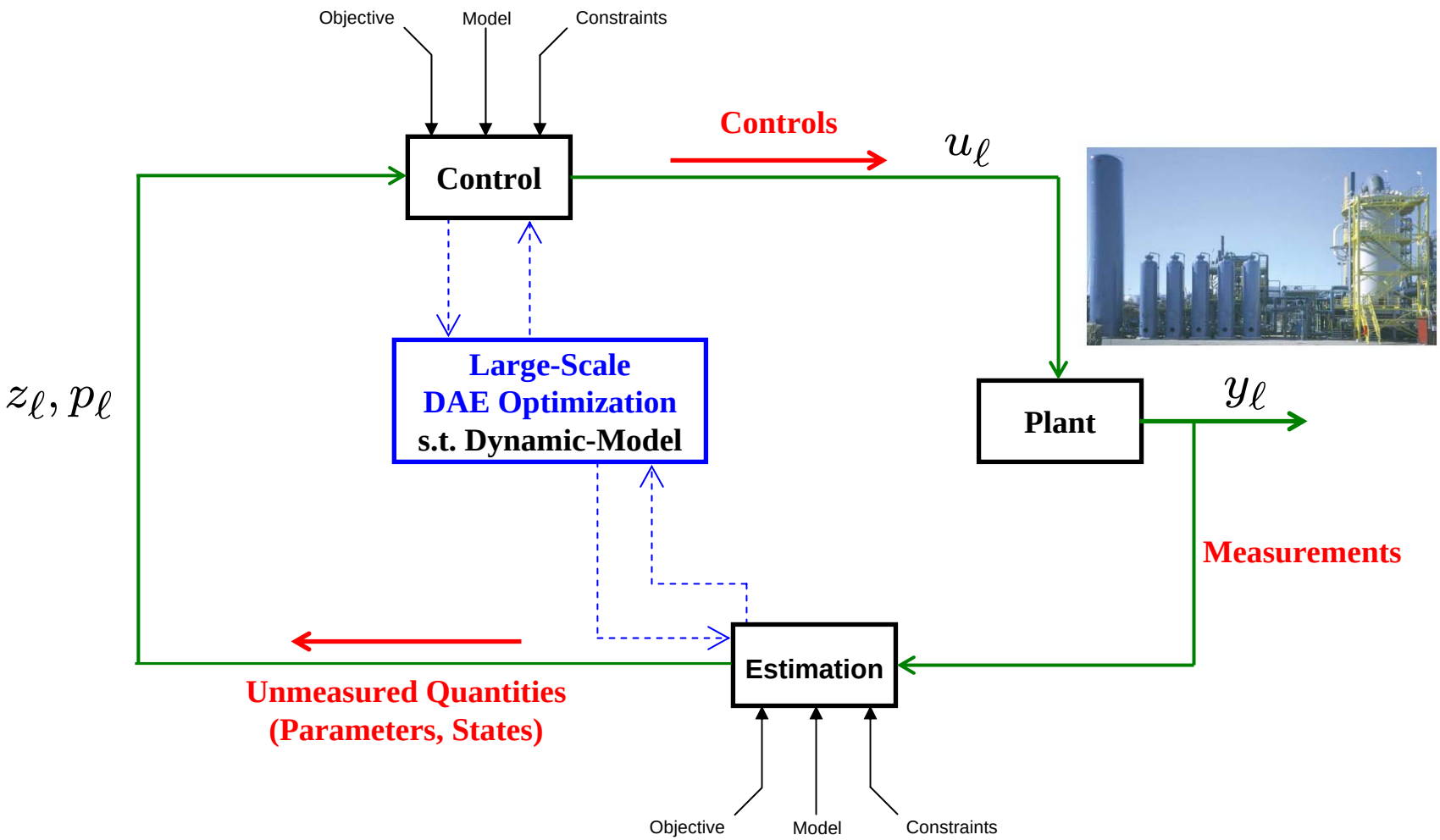
$$\begin{aligned} \frac{dz}{dt} &= \mathbf{f}(z(t), y(t), u(t), p(t)) \\ 0 &= \mathbf{g}(z(t), y(t), u(t), p(t)) \\ 0 &\geq \mathbf{h}(z(t), y(t), u(t), p(t)) \\ \boxed{z(0) = z_\ell} \end{aligned}$$

$$\min_{u(t)} \int_{t_{\ell+1}}^{t_{\ell+N+1}} \varphi(z(t), y(t), u(t), p(t))dt$$

$$\begin{aligned} \frac{dz}{dt} &= \mathbf{f}(z(t), y(t), u(t), p(t)) \\ 0 &= \mathbf{g}(z(t), y(t), u(t), p(t)) \\ 0 &\geq \mathbf{h}(z(t), y(t), u(t), p(t)) \\ \boxed{z(0) = z_{\ell+1}} \end{aligned}$$

+ MPC Stabilizes Complex Multivariable Systems

DAE-Constrained Optimization in On-Line Applications



Time-Critical Applications

Feedback Delay = Solution Time Estimation + Control = Destabilizes Process

Outline

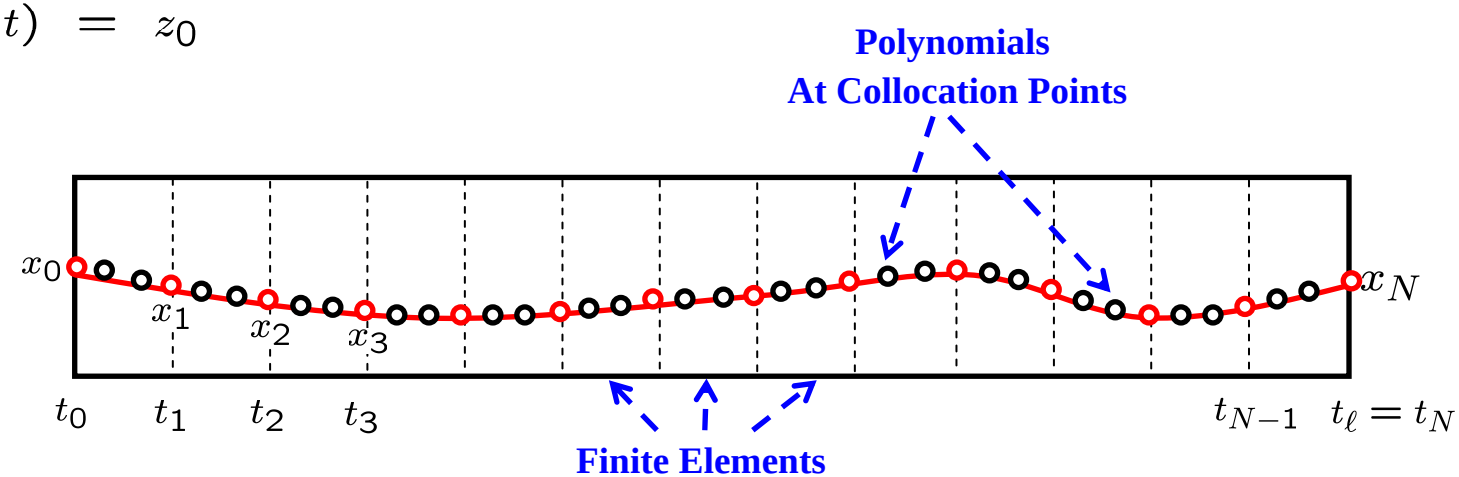
1. DAE-Constrained Optimization in On-Line Applications
2. Direct Transcription and General Interior-Point NLP Solvers
3. Add-On Capabilities for Interior Point Solvers
4. Case Study
5. Conclusions and Future Work

Direct Transcription

$$\min_{u(t),p(t),z_0} \quad \int_{t_0}^{t_f} \varphi(z(t),y(t),u(t),p(t))dt$$

$$\left.\begin{aligned} \frac{dz}{dt} &= \mathbf{f}(z(t),y(t),u(t),p(t)) \\ 0 &= \mathbf{g}(z(t),y(t),u(t),p(t)) \end{aligned}\right\} \text{Algebraic Representation of Continuous-Time DAE Model}$$

$$\begin{aligned} 0 &\geq \mathbf{h}(z(t),y(t),u(t),p(t)) \\ z(t) &= z_0 \end{aligned}$$



$$\begin{aligned} \min \quad & f(x) \\ \text{s.t.} \quad & c(x) = 0 \\ & x \geq 0 \end{aligned}$$

Large-Scale and Sparse NLP

- **Radau and Gauss Collocation** -Accuracy, Constraint Handling-
- **Cheap Exact First and Second Derivatives Through Modeling Platforms**

Full-Space NLP Solvers

Knitro, LOQO, *IPOPT* *Wächter, Biegler 2006*

$$\begin{aligned} \min \quad & f(x) \\ \text{s.t.} \quad & c(x) = 0 \\ & x \geq 0 \end{aligned} \quad \text{NLP} \quad \rightarrow \quad \begin{aligned} \min \quad & f(x) - \mu \sum_{i=1}^{nx} \ln\left(x^{(i)}\right) \\ \text{s.t.} \quad & c(x) = 0 \end{aligned} \quad \text{Barrier Problem}$$

Solve Sequence of BPs with $\mu \rightarrow 0$

$$\begin{aligned} \nabla_x f(x) + \nabla_x c(x)\,\lambda - \nu &= 0 \\ c(x) &= 0 \\ XVe - \mu\, e &= 0 \end{aligned} \xrightarrow[\text{Exact Derivatives}]{\text{Newton's Method}} \begin{bmatrix} H_k & A_k & -I \\ A_k^T & 0 & 0 \\ V_k & 0 & X_k \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta\lambda \\ \Delta\nu \end{bmatrix} = -\begin{bmatrix} \nabla f(x_k) + A_k\lambda_k - \nu_k \\ c(x_k) \\ X_k V_k e - \mu e \end{bmatrix}$$

- Solution of KKT System Most Expensive Step -Seconds/Minutes-

General Direct Sparse Factorization	Tailored Riccati Decomposition	Tailored Reduced Space Decomposition
$O(N(n_z + n_y + n_u))^{1,2}$	$O(N(n_z + n_y + n_u)^3)$	$O(N(n_z + n_y)^{1,2} + (Nn_u)^3)$

- General Interior-Point NLP Solvers

- **Favorable Overall Complexity, Exploit Recent Algorithmic Advances**

- Practical Issues

- **Analysis of Solution (e.g. Controllability, Observability, Covariance of States)**
- **Bottlenecks in On-Line Applications: Factorization Time, Warm-Starts**

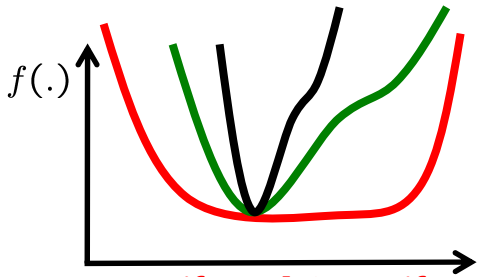
Outline

1. DAE-Constrained Optimization in On-Line Applications
2. Direct Transcription and General Interior-Point NLP Solvers
3. **Add-On Capabilities for Interior Point Solvers**
4. **Case Study**
5. **Conclusions and Future Work**

Post-Optimal Analysis

Reduced Hessian $Z^T H Z$

- $(Z^T H Z)^{-1}$ **Closely Related to <u>Covariance</u>** $\mathbf{\Pi}_\ell$ *Z., Biegler 2007*
- **Singularity & Controllability Optimal Control Problems** *Kameswaran, 2007*
- **<u>Never Formed</u> in Full-Space <u>IPOPT</u>**



<u>Verify and Quantify</u>
Second-Order Conditions

- **KKT System at Solution**

Full Hessian $\qquad x = [\bar{x}\ u]$

Already Factorized

$$\begin{bmatrix} H & A \\ A^T & \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta \lambda \end{bmatrix} = -\begin{bmatrix} \nabla_x \mathcal{L}(x^*, \lambda^*) \\ c(x^*) \end{bmatrix}$$

- **Split Variables into Basic and Non-Basic (e.g.; Degrees of Freedom)**

Already Factorized

$$\left[\begin{array}{cc|c} H_{\bar{x}\bar{x}} & H_{\bar{x}u} & A_{\bar{x}} \\ H_{u\bar{x}} & H_{uu} & A_u \\ \hline A_{\bar{x}}^T & A_u^T & \end{array}\right] \left[\begin{array}{c} \bar{X} \\ U \\ \hline \Lambda \end{array}\right] = -\left[\begin{array}{c} 0 \\ \mathbf{I}_{n_u} \\ \hline 0 \end{array}\right]$$

$\mathbf{K}^*$

- $U = (Z^T H Z)^{-1}$ **with** $Z = \begin{bmatrix} -A_{\bar{x}}^{-1} A_u \\ \mathbf{I}_u \end{bmatrix}$ *Z. & Biegler, 2007*

- **<u>Reduced Hessian</u> Can be Extracted Through <u>Backsolves</u> with Full-Space KKT Matrix**

NLP Sensitivity

Fast Approximate Solutions of Parametric NLPs

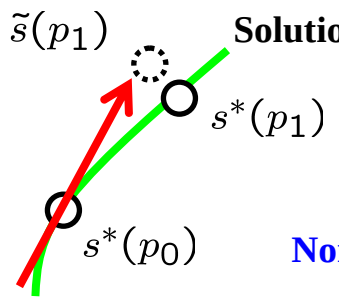
$$\left.\begin{array}{ll} \min & f(x,p) \\ \text{s.t.} & c(x,p)=0 \\ & x \geq 0 \end{array}\right\} \mathrm{P}(p)$$

$\uparrow$ **On-Line Moving Data**

Solution Triplet

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

Existence and Differentiability of Continuous Solution Path - *Fiacco, 1983*



Perturbed Newton Step

Nominal Solution -Second Order Conditions-

KKT System at Nominal Solution

Already Factorized

$$\mathbf{K}^* \ \underset{\substack{\uparrow \\ (\tilde{s}(p_1) - s^*(p_0))}}{\Delta s} = -\nabla_s \mathcal{L}(s^*(p_0), \overset{\substack{p_1 \\ \swarrow}}{p_0})$$

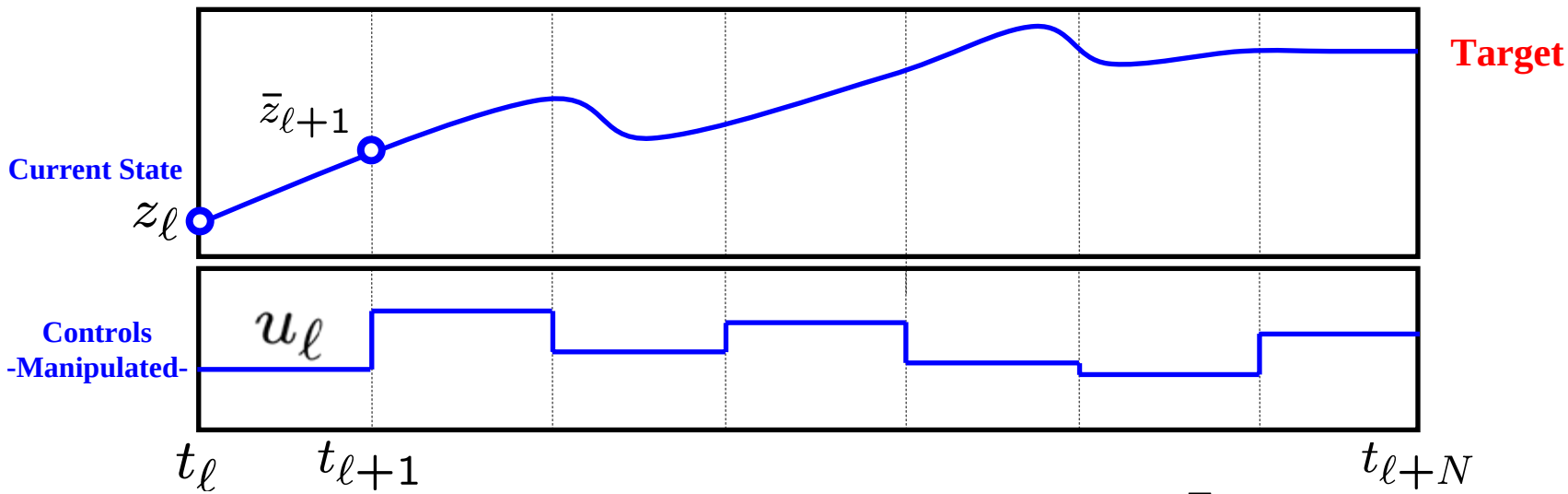
+ **Bounded Approximation Error** $|\tilde{s}(p_1) - s^*(p_1)| \leq L|p_1 - p_0|^2$

+ **Fast Approximate Solution with One Backsolve using Factorized KKT Matrix**

- **Assumes Active-Set Preserved**

Fast Moving Horizon Control

Advanced-Step Controller *Z. & Biegler 2007*



Having z_ℓ and u_ℓ I Can <u>Predict</u> Process Will Go To $\bar{z}_{\ell+1}$

$$\mathrm{P}(\bar{z}_{\ell+1})$$

Predicted Problem

$$\begin{aligned}
\min_{u(t)} \quad & \int_{t_{\ell+1}}^{t_{\ell+N+1}} \varphi(z(t), y(t), u(t), p(t))dt \\
\frac{dz}{dt} &= \mathbf{f}(z(t), y(t), u(t), p(t)) \\
0 &= \mathbf{g}(z(t), y(t), u(t), p(t)) \\
0 &\geq \mathbf{h}(z(t), y(t), u(t), p(t)) \\
\boxed{z(0) = \bar{z}_{\ell+1}}
\end{aligned}$$

Start Solving <u>Predicted Problem Now</u>, Between Sampling Times

At Solution, <u>Hold KKT System</u>

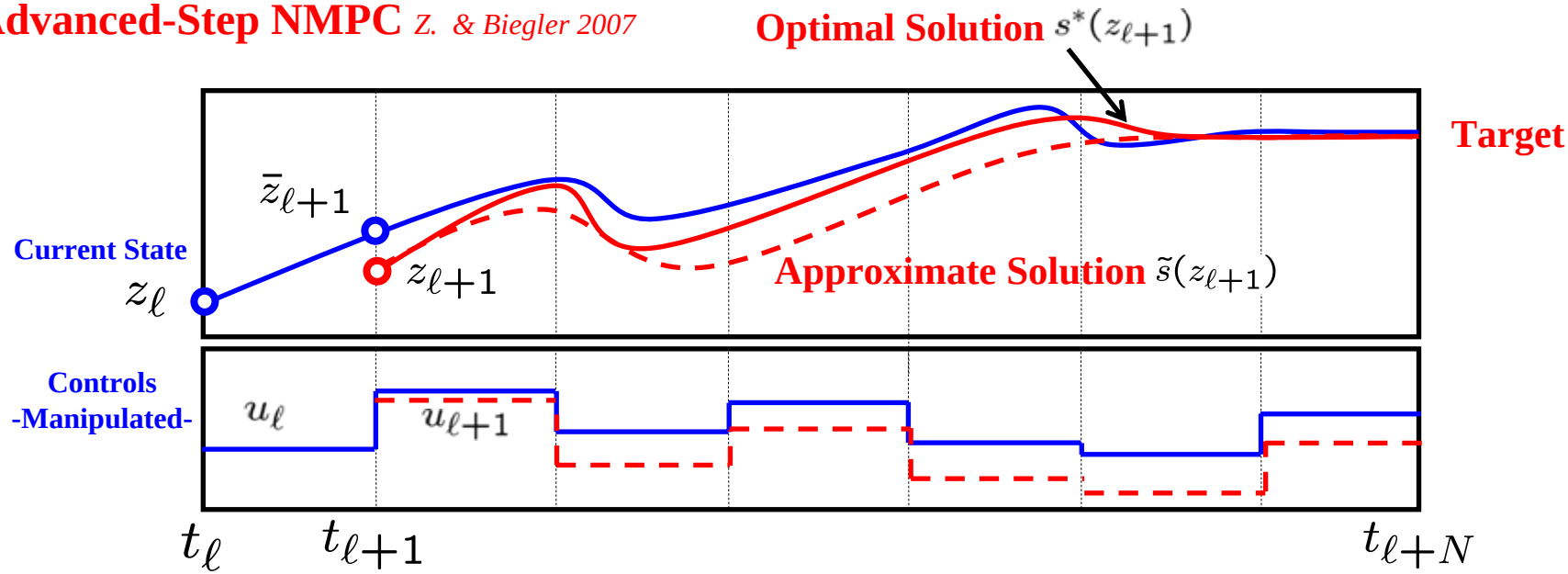
$$\begin{bmatrix} H^* & A^* \\ A^* & \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta\lambda \end{bmatrix} = -\begin{bmatrix} \nabla_x \mathcal{L}(x^*, \lambda^*) \\ c(x^*, \bar{z}_{\ell+1}) \end{bmatrix}$$

K*

Contains Predicted State

Fast Moving Horizon Control

Advanced-Step NMPC *Z. & Biegler 2007*



Once True Plant State $z_{\ell+1}$ Is Estimated

Fast <u>On-Line Correction</u> of KKT System with <u>True State</u>

$$\begin{bmatrix} H^* & A^* \\ A^* & \mathbf{K^*} \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta \lambda \end{bmatrix} = - \begin{bmatrix} \nabla_x \mathcal{L}(x^*, \lambda^*) \\ c(x^*, \bar{z}_{\ell+1}) \end{bmatrix}$$

Predicted State $\bar{z}_{\ell+1}$ → **True State** $z_{\ell+1}$

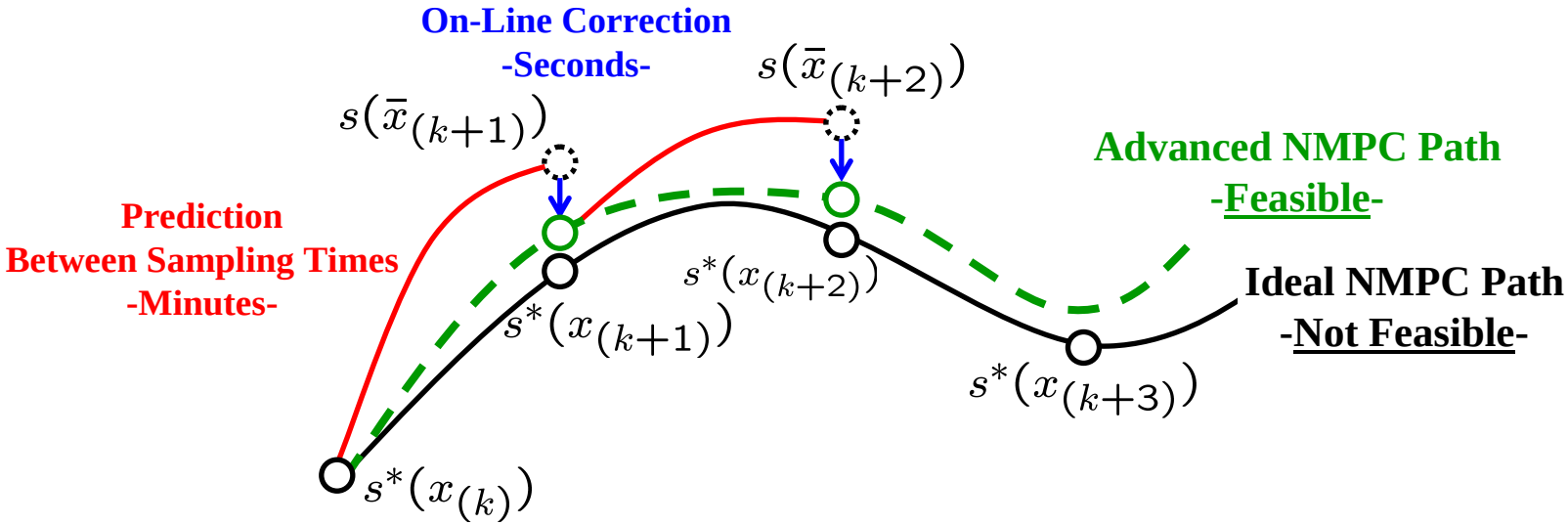
Approximation Error ~ Bound on <u>Uncertainty</u> Description

$$\|\tilde{s}(z_{\ell+1}) - s^*(z_{\ell+1})\| \leq L \|\bar{z}_{\ell+1} - z_{\ell+1}\|^2$$

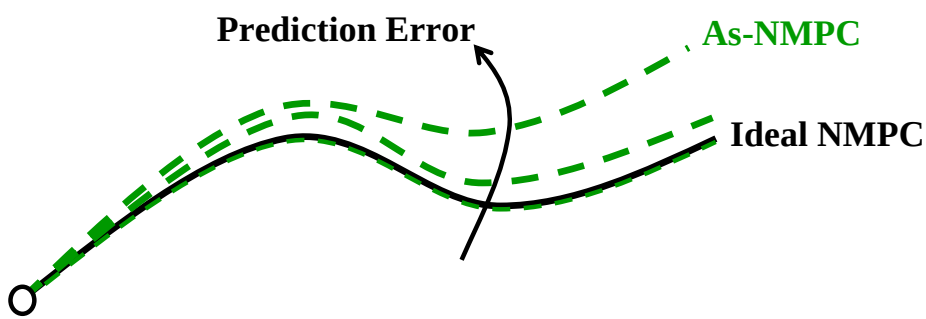
Fast Moving Horizon Control

Advanced-Step NMPC

- Analogy Predictor-Corrector Methods from Bifurcation Analysis



Effect of Prediction Error on Approximation Error



+ Principle Applicable to Estimation -Predict Measurement, Correct On-line-

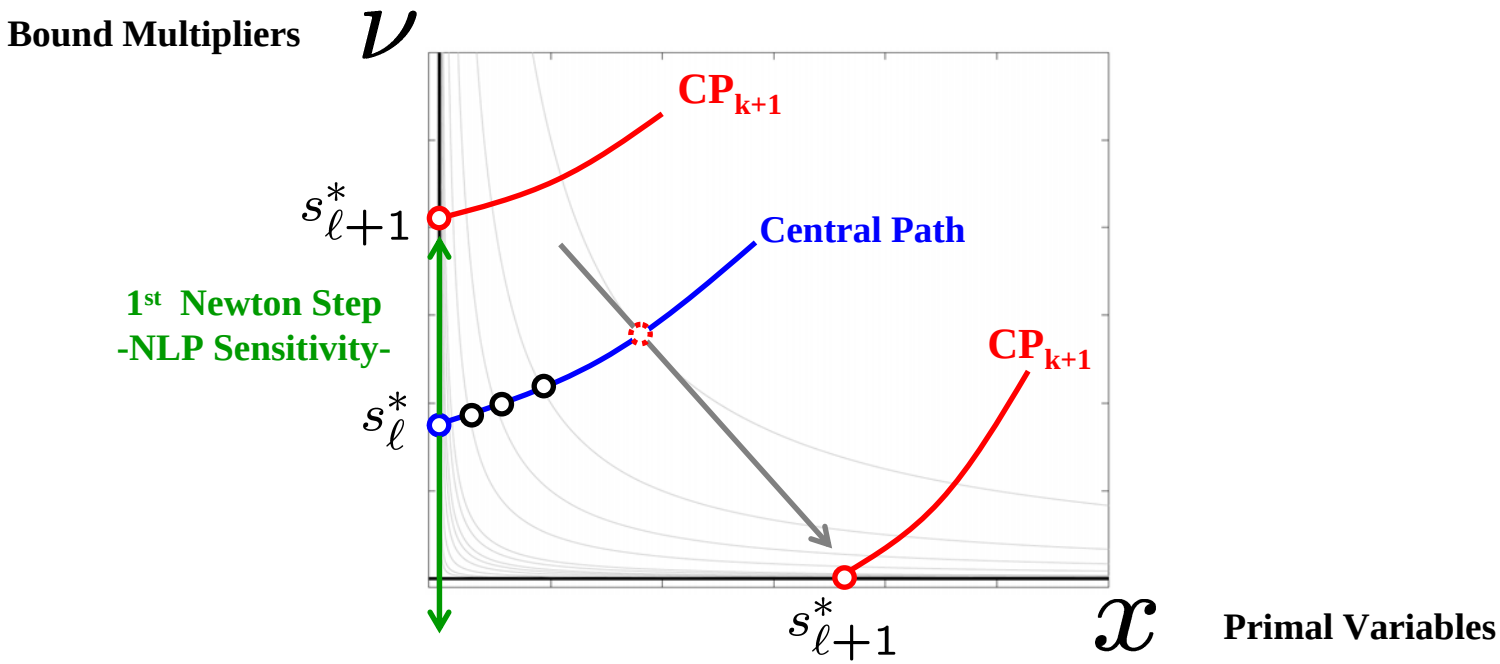
- What if Perturbation Induces Active-Set Change ?

NLP Sensitivity with Active-Set Changes

Fundamental Issue Interior-Point Methods

- **Starting from Nominal Solution…**

  First Newton Step Towards New Solution is Tangential to Complementarity Relaxation



- **Sensitivity Approximation Inconsistent if Active-Set Change**
- **Alternative: Unblocking Strategy** *Grothey et.al, 2003*
  - **Select Solution of Interior Barrier Problem**
  - **Trial and Error, Store Multiple KKT Matrices**
  - **On-Line Problems Far from Central Path!**

NLP Sensitivity with Active-Set Changes

Fix-Relax Strategy

Start from Nominal Active-Set and Perturb Value of Internal Primal and Dual Variables

$y^*(p_0) \rightarrow y_d$

$x = [\bar{x}\ y]$

Already Factorized

$$\begin{bmatrix} H(p_0) & A(p_0) \\ A(p_0)^T & \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta\lambda \end{bmatrix} = -\begin{bmatrix} \nabla_x \mathcal{L}(s^*(p_0), p_0) \\ c(x^*(p_0), p_0) \end{bmatrix}$$

$\mathbf{K}^*$

$$\begin{aligned} H_{\bar{x}\bar{x}}\Delta\bar{x} + H_{\bar{x}y}\Delta y + A_{\bar{x}}\Delta\lambda &= -\nabla_{\bar{x}}\mathcal{L}(s^*(p_0), p_0) \\ \text{Relax}\ \boxed{\Delta\sigma} + \cancel{H_{y\bar{x}}\Delta\bar{x} + H_{yy}\Delta y + A_y\Delta\lambda} &= \cancel{\nabla_{\bar{y}}\mathcal{L}(s^*(p_0), p_0)} \\ A_{\bar{x}}^T\Delta\bar{x} + A_y^T\Delta y &= -c(s^*(p_0), p_0) \\ \boxed{\Delta y = -(y_d - y^*(p_0))} & \quad \text{Fix} \end{aligned}$$

Augmented KKT System

$$\left[\begin{array}{c|c} \mathbf{K}^* & \mathbf{E}_\sigma \\ \hline \mathbf{E}_y^T & 0 \end{array}\right] \left[\begin{array}{c} \Delta s \\ \hline \Delta\sigma \end{array}\right] = -\left[\begin{array}{c} \nabla_s \mathcal{L}(s^*(p_0), p_0) \\ \hline y_d - y^*(p_0) \end{array}\right]$$

$$\mathbf{K}^* = \begin{bmatrix} H_k & A_k & -I \\ A_k^T & 0 & 0 \\ V_k & 0 & X_k \end{bmatrix}$$

Active-Set QP (Recursive Correction of Variables Violating Bounds, Negative Bound Multipliers)

- **+ Equivalent to First Active-Set SQP Iteration in Solution of New Problem**
- **+ Warm-Start Interior-Point Solvers**

Avoid Factorization Through Schur Complement *Betts & Frank 1994, Bartlett, et.al. 2006*

Outline

1. DAE-Constrained Optimization in On-Line Applications
2. Direct Transcription and General Interior-Point NLP Solvers
3. Add-On Capabilities for Interior Point Solvers
4. **Case Study**
5. **Conclusions and Future Work**

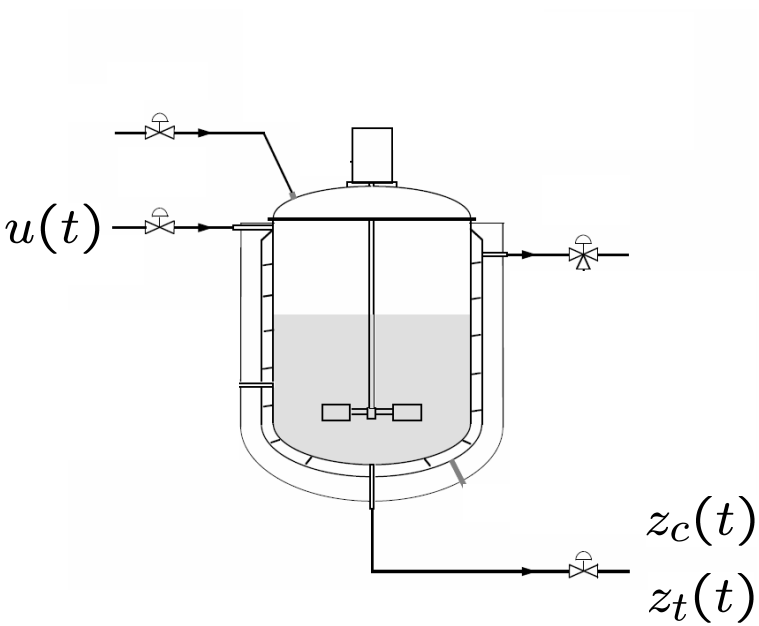
Case Study, Chemical Reactor

Chemical Reactor

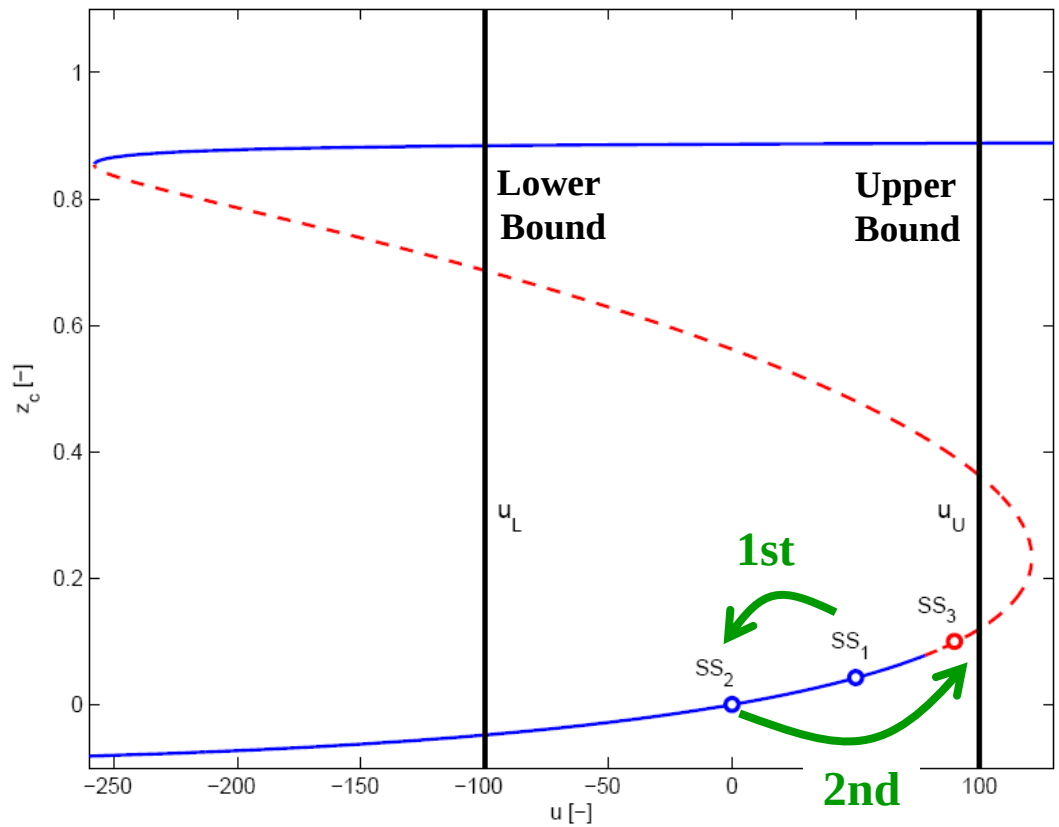
- Input: Cooling Water, Outputs: Temperature and Concentration

Illustrate Capabilities of IPOPT

- Covariance Analysis in State Estimation
- Fast Approximate Control Through NLP Sensitivity

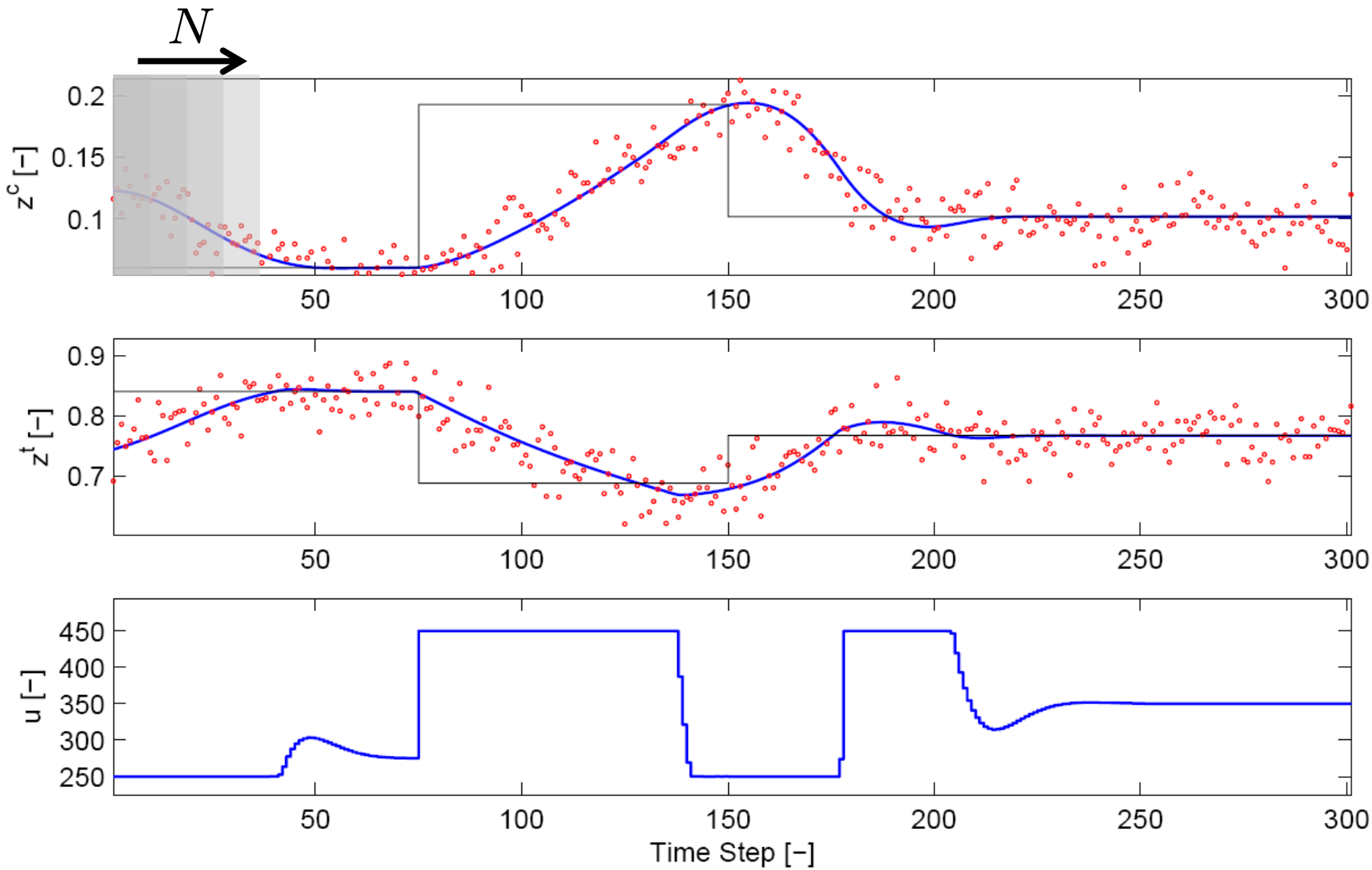


-Two Closed-Loop Transitions



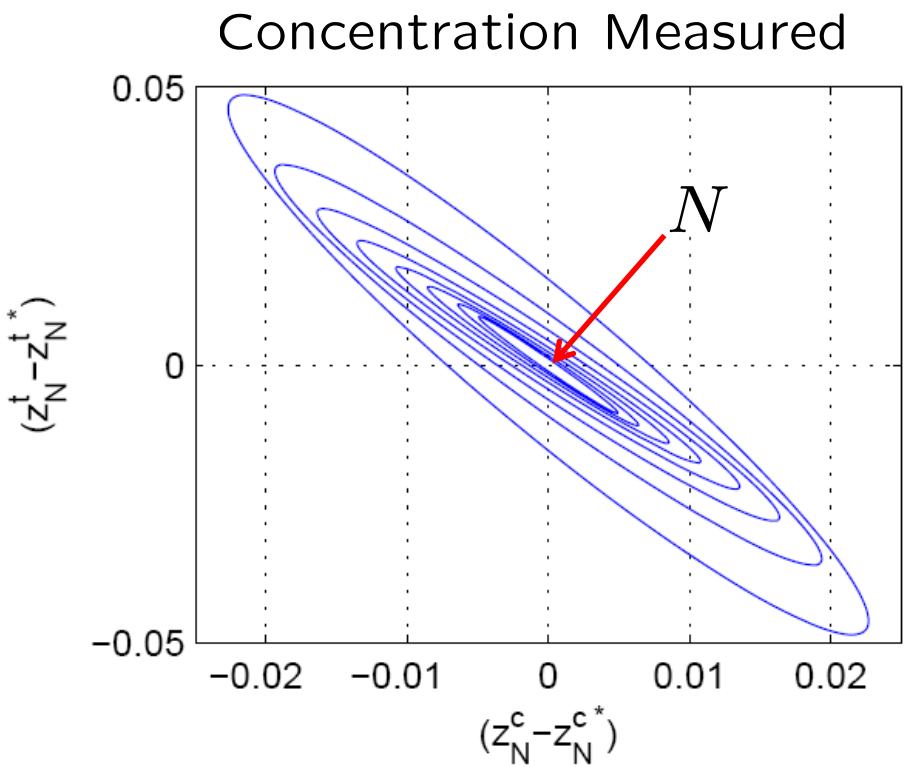
Case Study – Moving Horizon Estimation

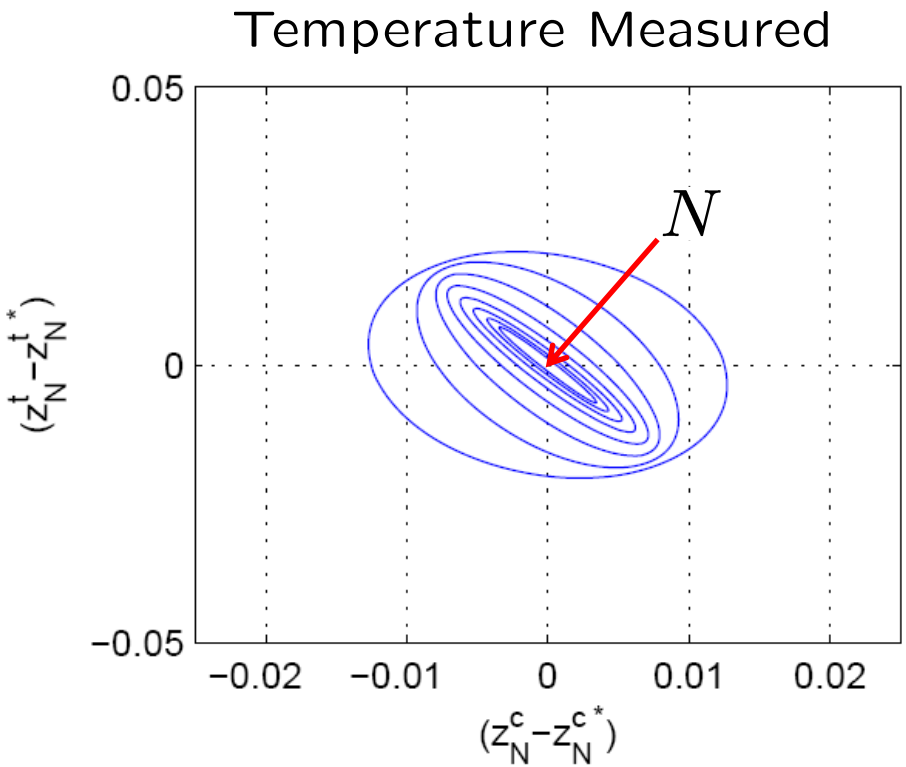
Measurements Generated with Gaussian Noise σ = 5%



Case Study – Moving Horizon Estimation

95% Confidence Regions for $N = 5, 10, 15, \ldots, 30$

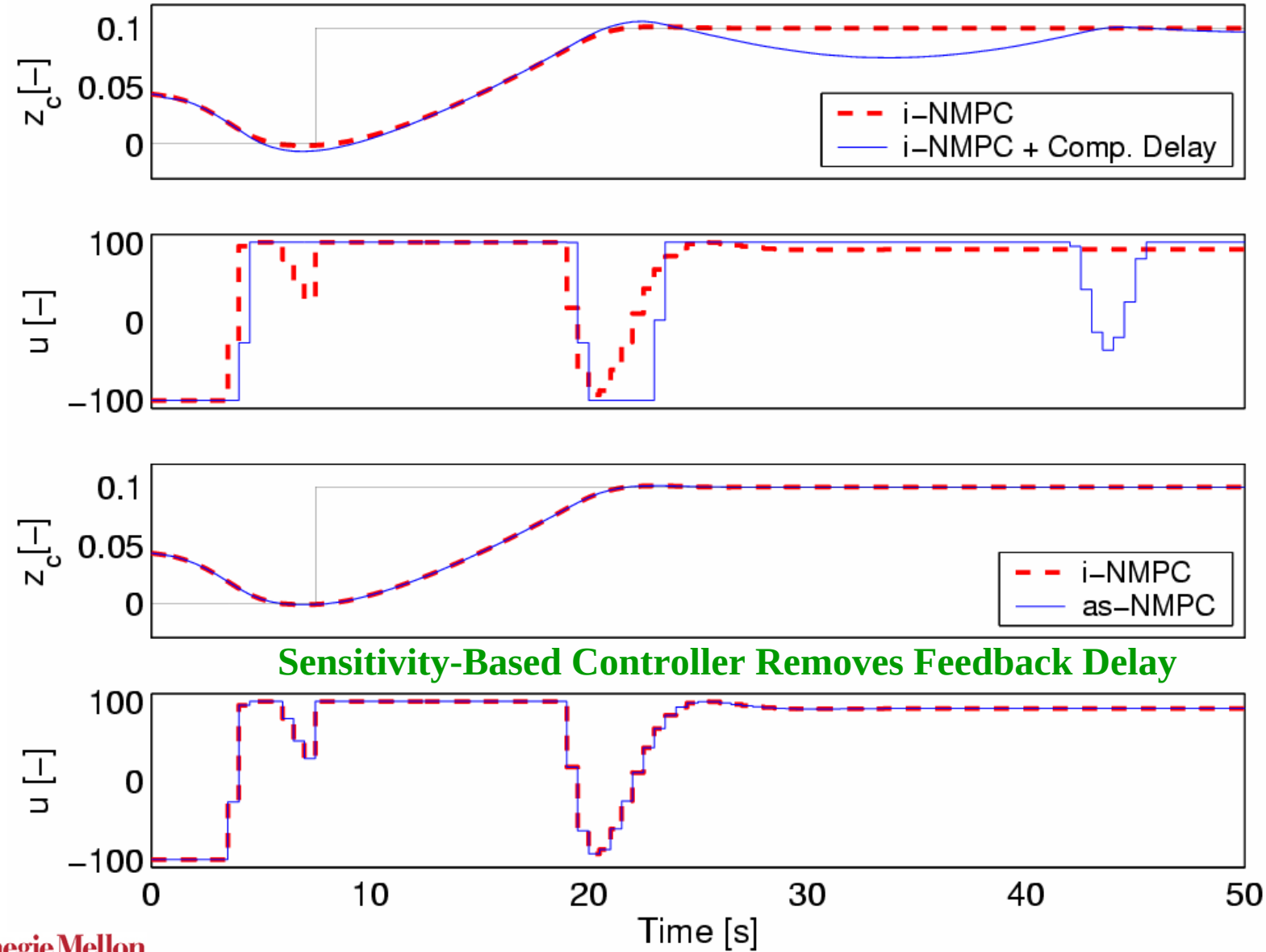




- System is Locally Observable
- Temperature is Most Informative Measurement
- Long Horizons Required To Decrease Confidence Levels

Case Study – Moving Horizon Control

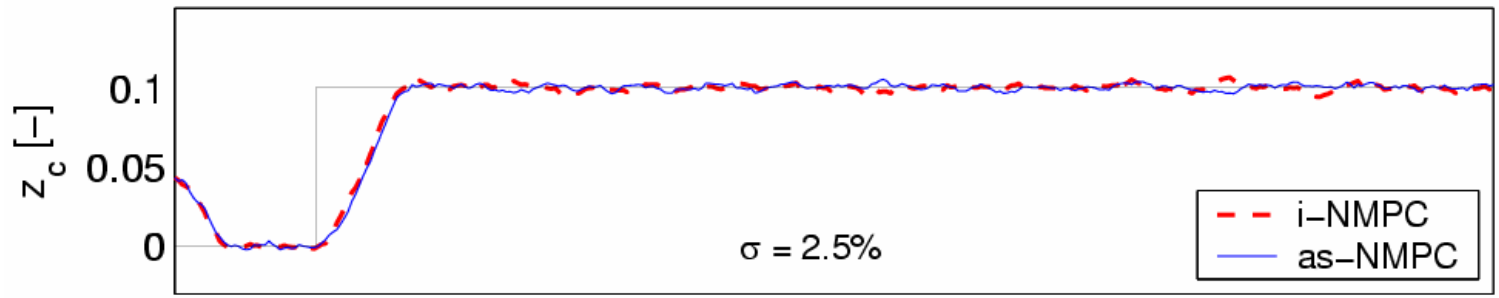
Effect of Feedback Delay on Controller Performance



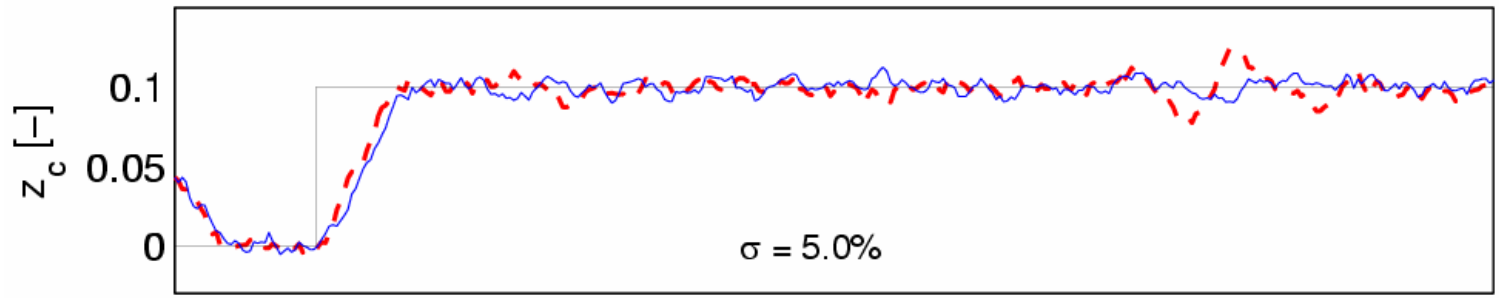
Sensitivity-Based Controller Removes Feedback Delay

Case Study – Moving Horizon Control

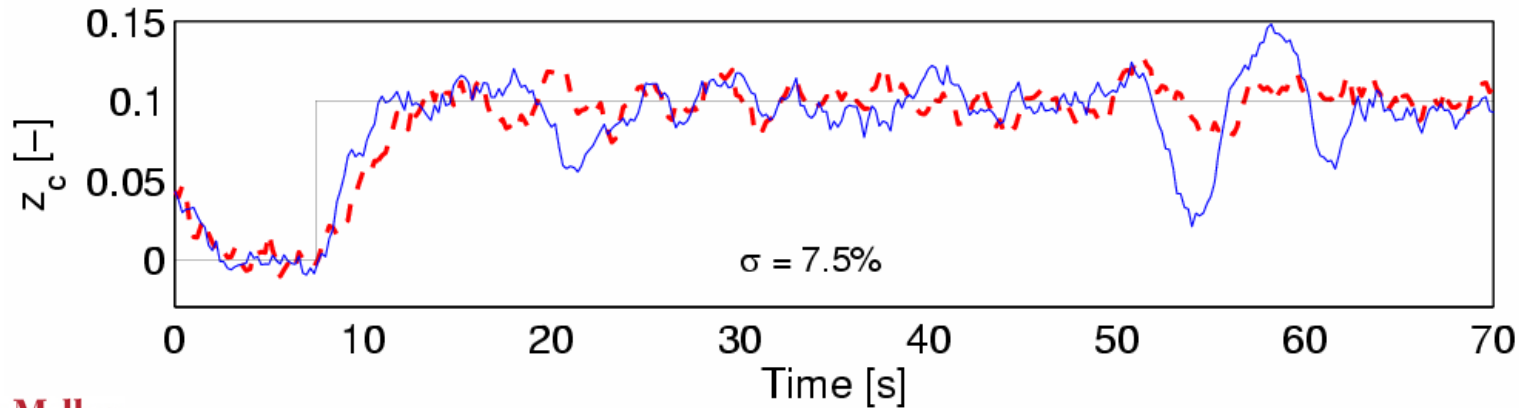
Effect of Perturbations on Approximation Errors (Model Mismatch + Noise)



+ Sensitivity Errors Negligible, Controller Tolerates Fairly Large Levels of Noise

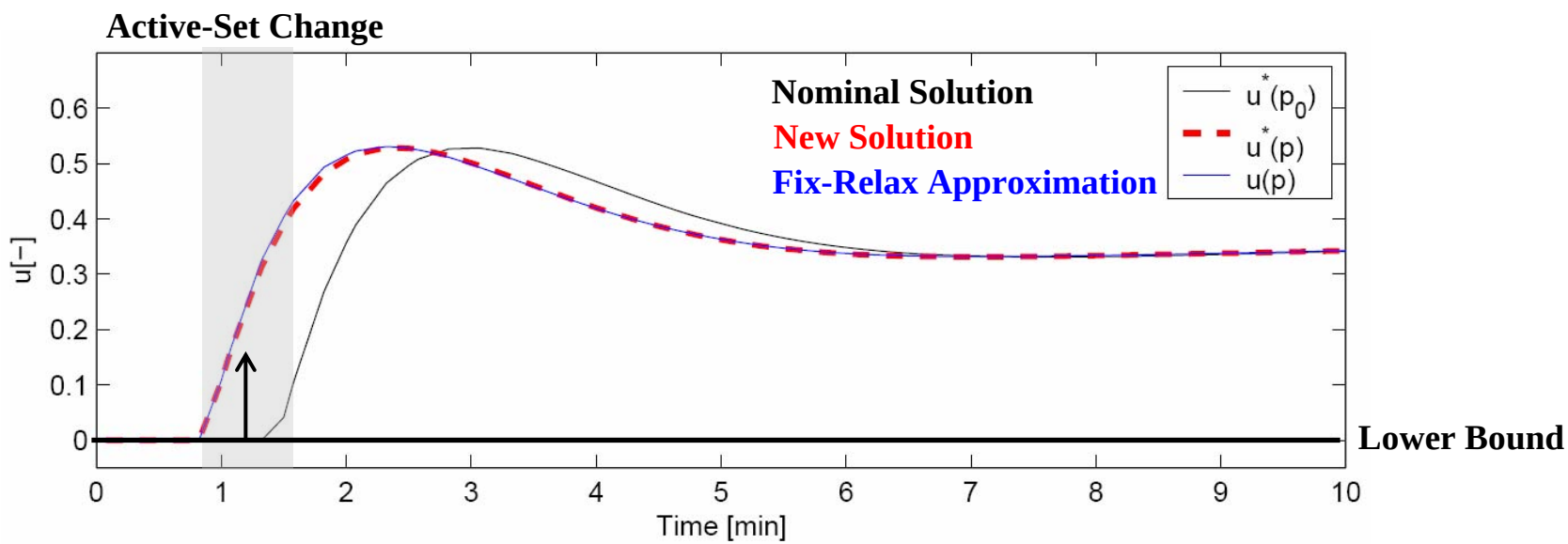


- Perturbations Induce Active-Set Changes and Destabilize System



Case Study – Active-Set

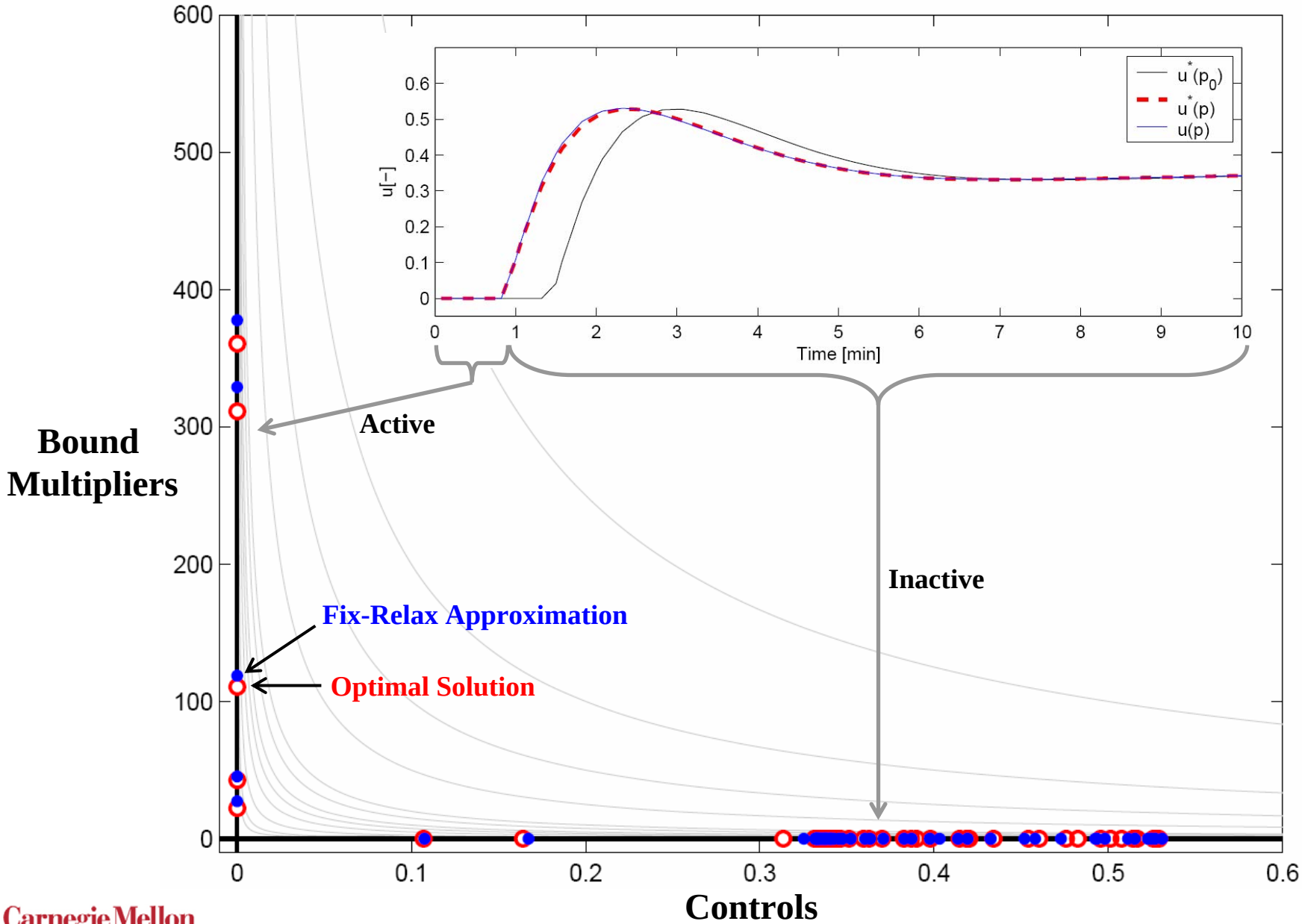
Correct Active-Set Through Fix-Relax Strategy



- Correction Requires 5 Backsolves
- Reuse Factorized KKT Matrix

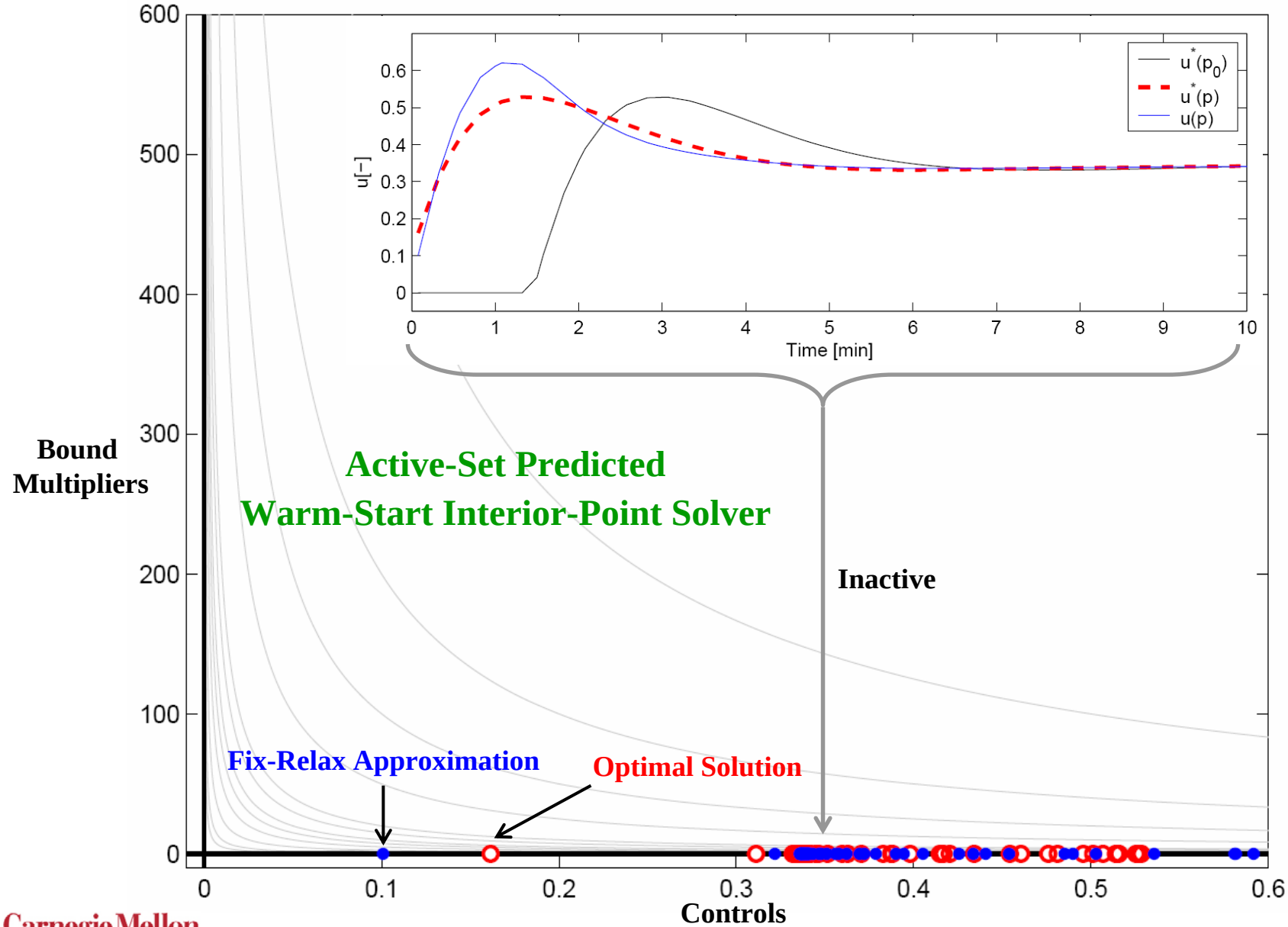
Case Study – Active-Set

Complementarity Products



Case Study – Active-Set

Complementarity Products -Stronger Perturbation-



Outline

1. DAE-Constrained Optimization in On-Line Applications
2. Direct Transcription and General Interior-Point NLP Solvers
3. Add-On Capabilities for Interior Point Solvers
4. Case Study
5. **Conclusions and Future Work**

Conclusions and Future Work

DAE-Constrained Optimization

Detailed Physics-Based Models for On-Line Tasks

Direct Transcription with General Interior-Point Solvers

+ Computational Complexity, Algorithmic Advances
- Hidden Problem Specifics for Analysis
- Solution Time Not Acceptable in On-line Applications

Add-On Capabilities in IPOPT

Reduced Hessian Information, NLP Sensitivity, Active-Set QP

<u>Reuse Factorization of KKT Matrix</u>

Future Work

Active-Set Warm-Start Strategy in IPOPT

Theoretical Analysis of Approximation Errors

Frameworks for On-Line Direct Transcription

Lorenz T. Biegler and Victor M. Zavala

Department of Chemical Engineering
Carnegie Mellon University

vzavala@cmu.edu

http://numero.cheme.cmu.edu

SIAM Conference on Optimization
May 2008

Carnegie Mellon

CAPD CENTER