Nonlinear Programming Strategies for State Estimation and Model Predictive Control

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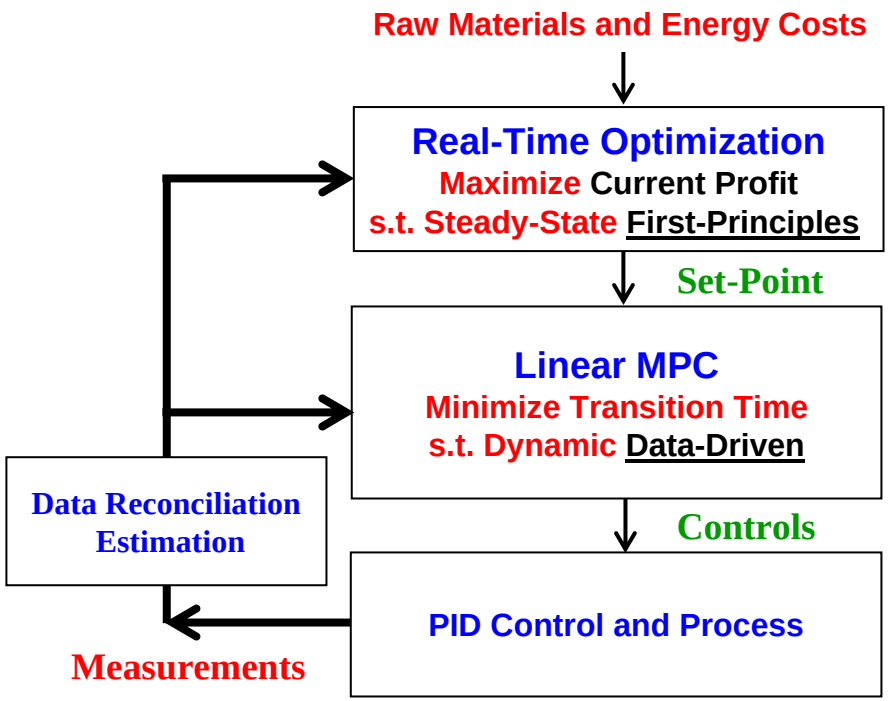
Overall Motivation

NMPC for Chemical Process Operations



NMPC
Maximize Future Profit
s.t. Dynamic First-Principles

- Challenge (This Work):

Computationally Intensive Optimization Problems, Time-Critical Solutions

Sampling Times: 1-10 Minutes, Dynamic Models: 1,000 – 10,000 DAEs

Outline

Industrial Polyethylene Process

First-Principles Model for MHE-NMPC Framework

Large-Scale PDE-Constrained Optimization

Computational Framework

Full-Discretization + Interior-Point Optimizers

Numerical Linear Algebra

Advanced Step MHE-NMPC

Fast Feedback in Large Applications

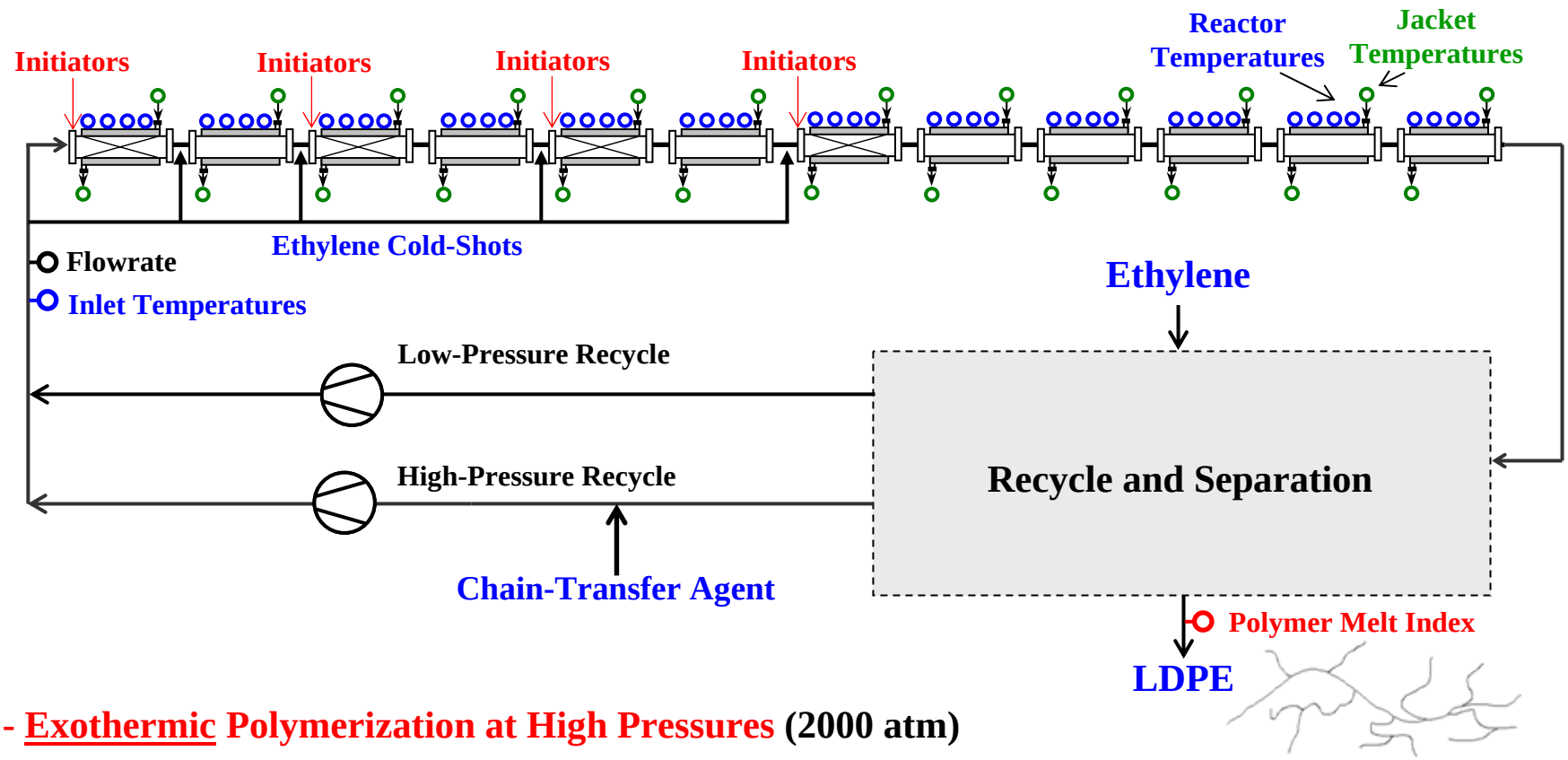
Results Polyethylene Process

NMPC to Improve Process Profitability

Conclusions and Future Work

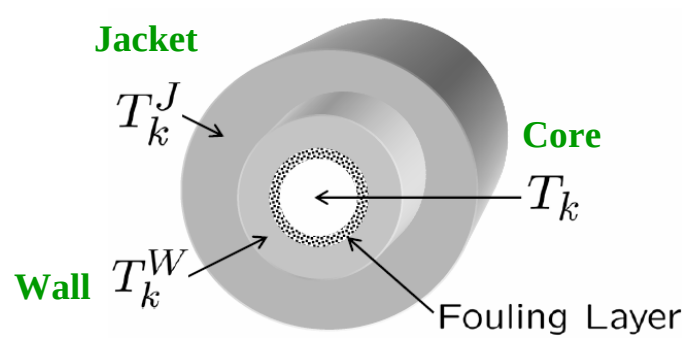
Industrial Polyethylene Process

Low-Density Polyethylene (LDPE) Process

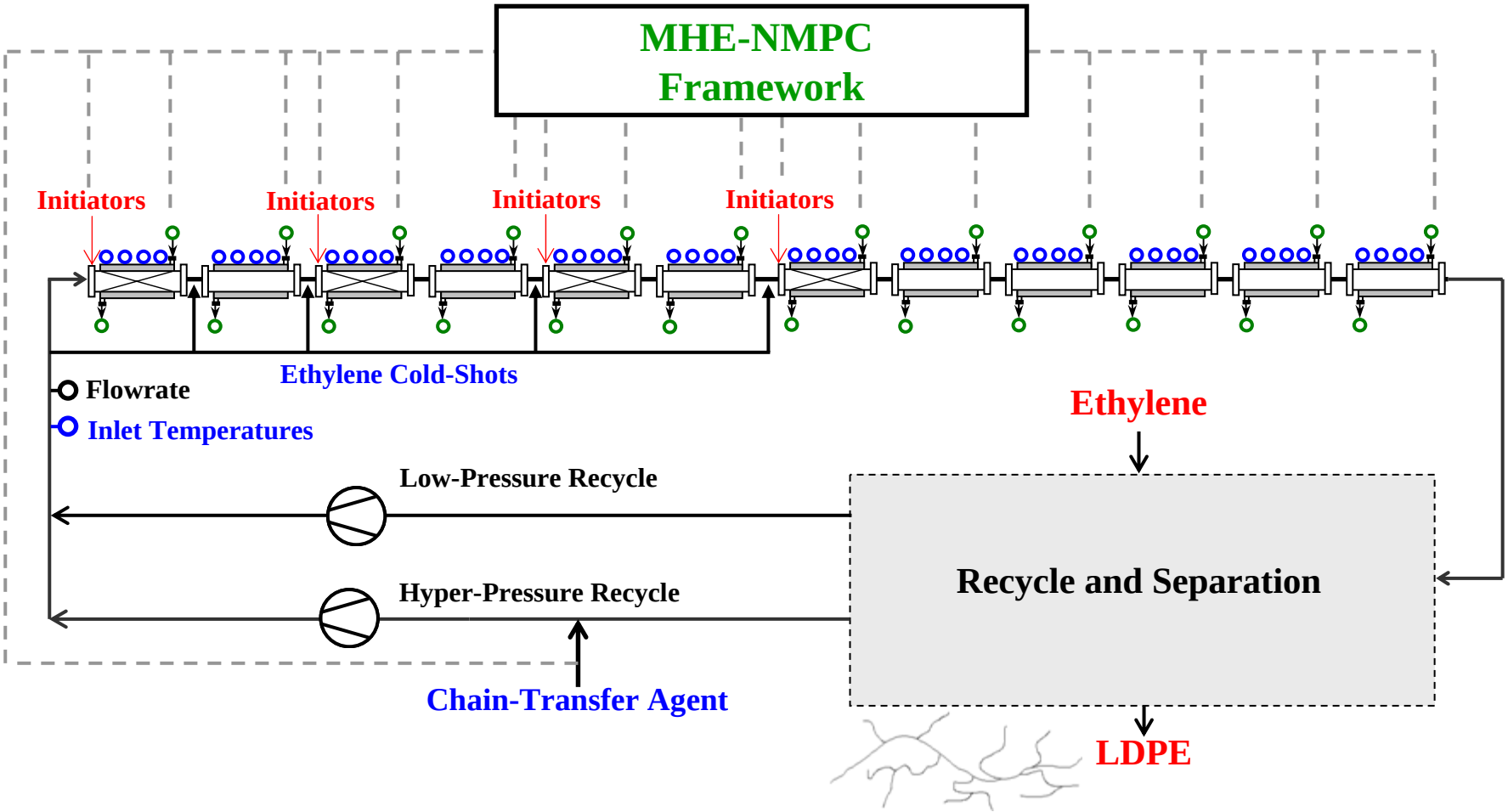


- **Exothermic Polymerization at High Pressures** (2000 atm)
- **Multi-Product Operations** (Wide Operating Window)
- **Production Strongly Affected by Aging Disturbances -Fouling-**

  Potential Benefits of 1% More Production = + 4,500,000 $/yr



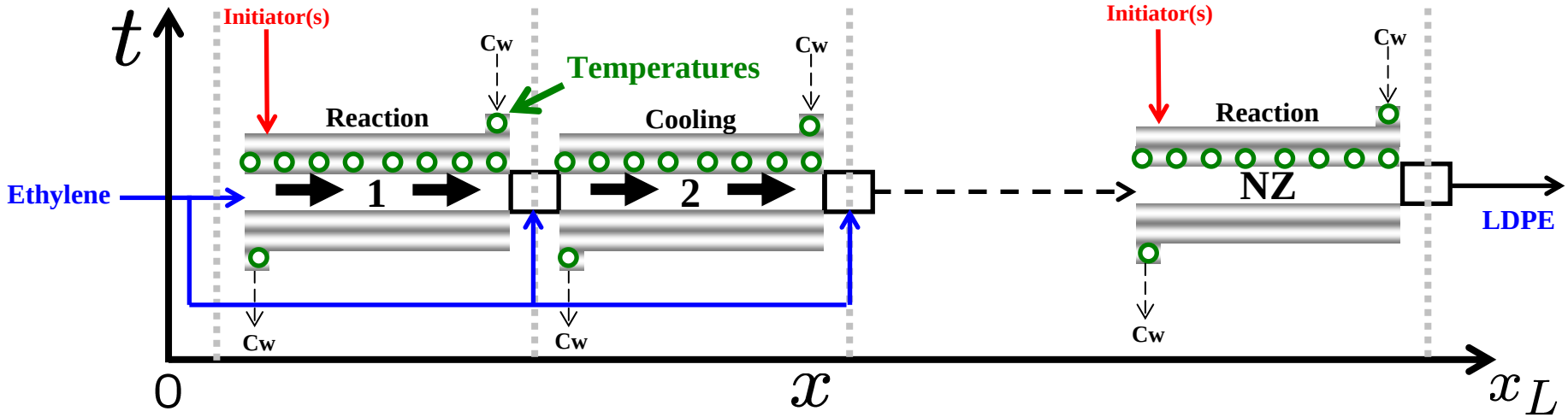
Low-Density Polyethylene (LDPE) Process



Framework Objectives:

- Capture Multivariable Coupling Between Zones
- Monitor and Reject Aging Disturbances

LDPE Dynamic Model



States Controls Parameters (Heat Transfer)

$$\left\{\frac{\partial z}{\partial t} + \phi(x,t)\frac{\partial z}{\partial x}\right\} = \mathbf{F}\left(z(x,t), w(x,t), u(t), p(t)\right)$$ **Conservation**

$$0 = \mathbf{G}\left(z(x,t), w(x,t), u(t), p(t)\right)$$ **Physical Properties**

Measured Outputs → $$y(t) = \chi\left(z(x,t), w(x,t), u(t), p(t)\right)$$ **Output Mapping**

$$z(x,0) = z_0(x)$$ **Initial Conditions**

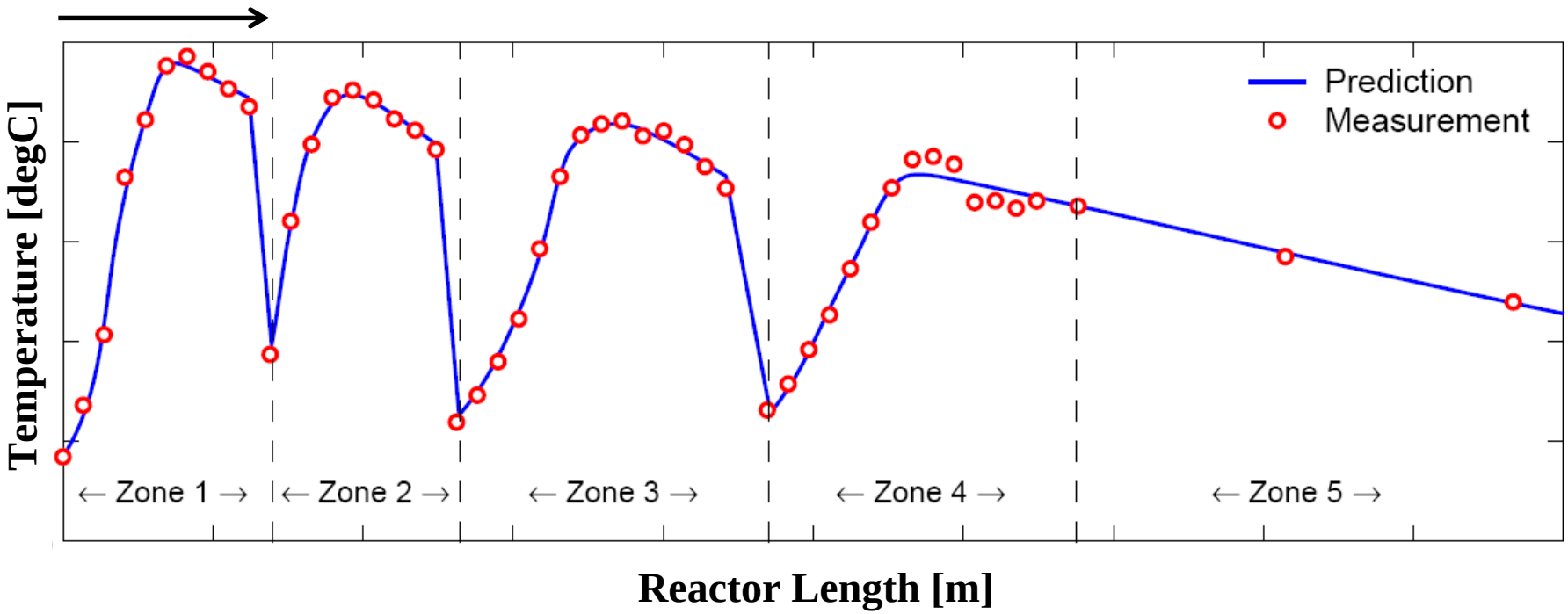
$$0 = \varphi\left(z(t,0), z(t,x^L), \frac{\partial z}{\partial x}(t,0), \frac{\partial z}{\partial x}(t,x^L), w(t,0), u(t)\right)$$ **Boundary Conditions**

- Large Set of PDEs ~ 9,000 DAEs, 50 Controls, 30 Parameters, 100 Measured Outputs

+ Sparse and Highly Structured

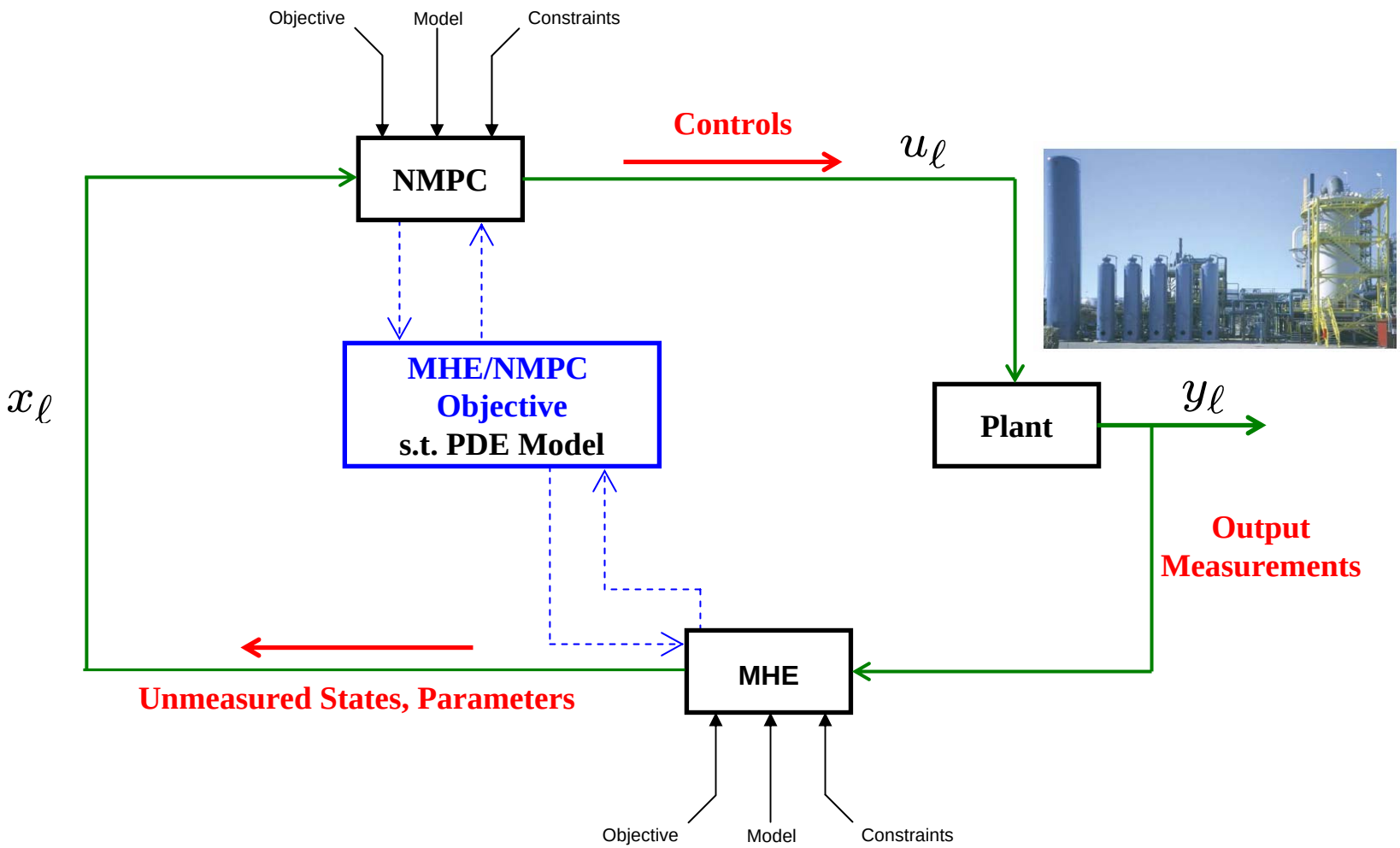
LDPE Dynamic Model

Off-Line Prediction of Core Temperature Profile



Good Off-Line Predictions but Aging Phenomena Needs to be Estimated On-line

MHE-NMPC Application



Feedback Delay = Solution Time MHE + NMPC

Is MHE-NMPC Framework Feasible?

Computational Framework

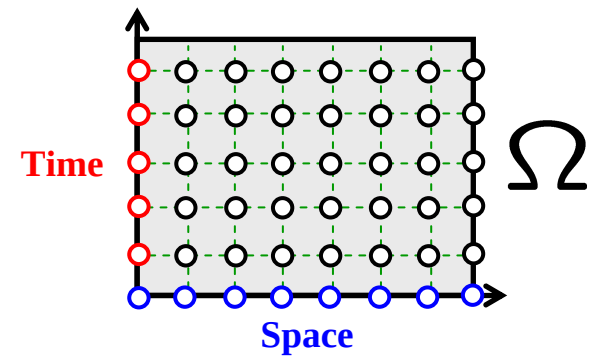
Full-Discretization Approach

PDE-Constrained Optimization (MHE,NMPC)
(Economic, Least-Squares Objectives)

$$\min_{u(t),\, z_0(x),\, p(t)} \quad \int_0^{t_N}\int_0^{x_L} \varphi(z(x,t), w(x,t), u(t), p(t))\,dx\,dt$$

$$\begin{aligned}
\left\{\frac{\partial z}{\partial t} + \phi(x,t)\frac{\partial z}{\partial x}\right\} &= \mathbf{F}\left(z(x,t), w(x,t), u(t), p(t)\right) \\
0 &= \mathbf{G}\left(z(x,t), w(x,t), u(t), p(t)\right) \\
y(t) &= \chi\left(z(x,t), w(x,t), u(t), p(t)\right) \\
0 &\leq \mathbf{H}\left(z(x,t), w(x,t), u(t), p(t)\right) \\
z(x,0) &= z_0(x) \\
x, t &\in \Omega
\end{aligned}$$

PDEs → Algebraic Equations



Optimization ⇔ **Discretized PDE Model** ⟷

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

Nonlinear Programming (NLP)

+ Avoid Repetitive Simulations of Large PDE Model

+ Cheap <u>Exact Derivatives</u> (Favorable Convergence Properties)

Efficient NLP Solvers Required

Interior-Point Solvers

Knitro, LOQO, IPOPT *Wächter, Biegler 2006*

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

NLP

$\rightarrow$

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

Barrier Subproblem

Solve Barrier Subproblems with $\mu \rightarrow 0$

Karush-Kuhn-Tucker (KKT) Conditions

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

Newton's Method $\longrightarrow$

KKT Matrix

$$\begin{bmatrix} W_k & A_k \\ A_k^T & \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta \lambda \end{bmatrix} = - \begin{bmatrix} r(x_k, \lambda_k, \nu_k) \\ c(x_k) \end{bmatrix}$$

K

Newton Step

- Decomposition (Factorization) Time of KKT Matrix → Feedback Delay

+ KKT Matrix Inherits Sparsity and Structure of Dynamic Model

Tailored Riccati Decomposition

$$O(N(n_z + n_u)^3)$$

Horizon **States** **DOF**

(Initial States, Controls)

General Direct Sparse Factorization

$$O(N(n_z + n_u))^{1,2}$$

Factorization of KKT Matrix

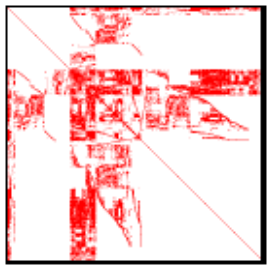
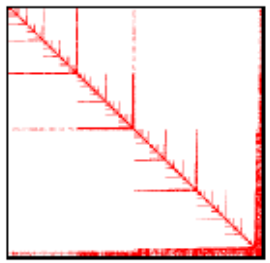
KKT Matrix

$$\mathbf{K} \begin{bmatrix} W_k & A_k \\ A_k^T & \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta \lambda \end{bmatrix} = - \begin{bmatrix} r(x_k, \lambda_k, \nu_k) \\ c(x_k) \end{bmatrix}$$

- General Sparse Linear Solvers -MA57 from Harwell-

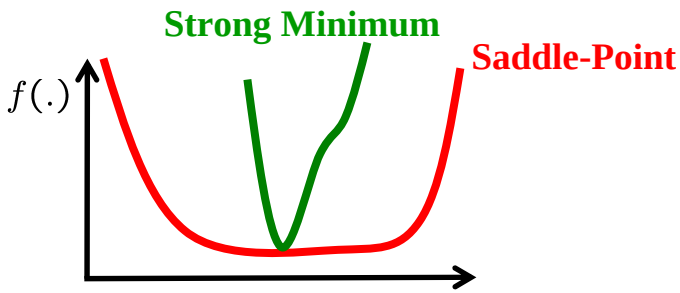
Phase I: Reordering to Preserve Sparsity **Phase II: Numerical Factorization**

Original **Reordered**

$\mathbf{K}$  **Phase I** $\longrightarrow$  **Phase II** $\longrightarrow$ $L^T B L$

- Nested Dissection Reordering Highly Efficient for Structured Matrices *Gould, 2004, Karypis, 1999*

- Eigenvalues of B are Eigenvalues of $\mathbf{K}$ (Sylvester's Law) *Nocedal & Wright 1999*



Check for Sufficient Second-Order Conditions (SSOC)
-e.g. Observability, Ill-Posed NMPC Formulations-

NLP Sensitivity

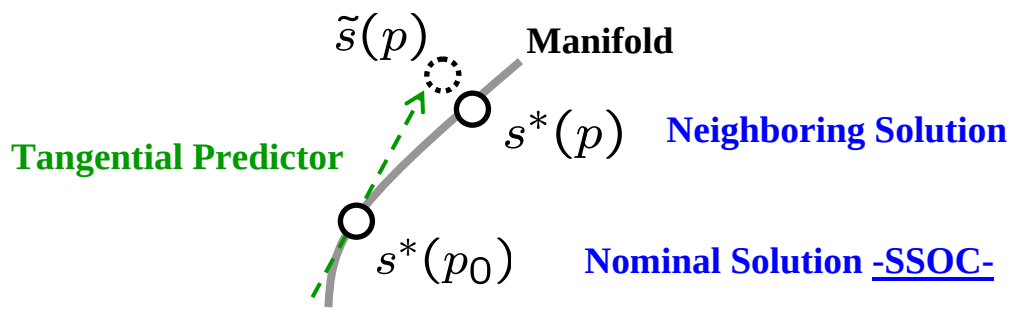
On-Line Factorization Time Will Always be a Bottleneck - Reuse Factorizations!

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

Solution is Implicit Function $s^*(p)$

Moving Data MHE/NMPC

Continuity of Solution Manifold - *Fiacco, 1983*



IPOPT KKT System at Nominal Solution

Already Factorized

$$\begin{bmatrix} K^* \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta \lambda \end{bmatrix} = -\begin{bmatrix} r(s^*(p_0), p_0) \\ c(x^*(p_0), p_0) \end{bmatrix} \quad p_0 \to p$$

$$\tilde{s}(p) - s^*(p_0)$$

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

+ Fast Approximate Solutions (Active-Set Changes -- Schur Update Strategy)

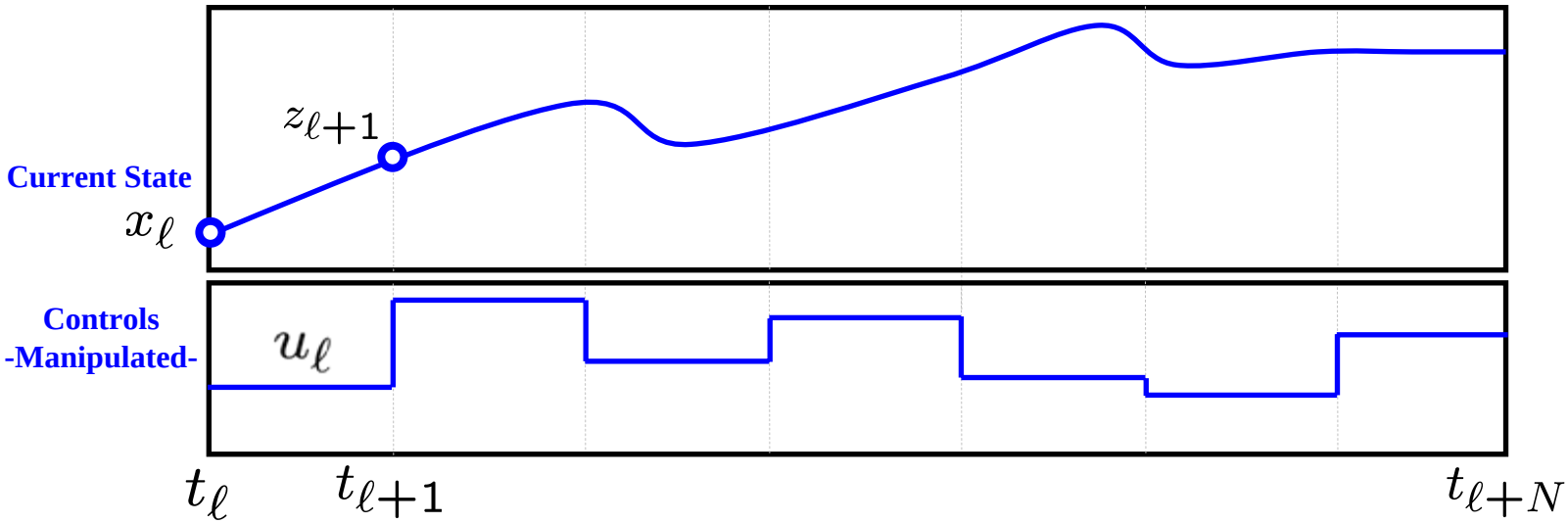
Advanced-Step NMPC and MHE

Separate Background and On-line Computation Tasks *Diehl, et. al. 2001*

Full Discretization + NLP Sensitivity to <u>Eliminate Feedback Delay</u>

Advanced-Step NMPC

Advanced-Step NMPC *Z. & Biegler 2007*



Having x_ℓ and u_ℓ I Can <u>Predict</u> Process Will Go To $z_{\ell+1}$

$$\min_{u(t)} \int_{t_{\ell+1}}^{t_{\ell+N+1}} \int_0^{x_L} \varphi(z(x,t), w(x,t), u(t), p(t))\,dx\,dt$$

$$\mathbf{P}(z_{\ell+1}) \quad \begin{aligned} \left\{\frac{\partial z}{\partial t} + \phi(x,t)\frac{\partial z}{\partial x}\right\} &= \mathbf{F}\left(z(x,t), w(x,t), u(t), p(t)\right) \\ 0 &= \mathbf{G}\left(z(x,t), w(x,t), u(t), p(t)\right) \\ y(t) &= \chi\left(z(x,t), w(x,t), u(t), p(t)\right) \\ \boxed{z(x, t_{\ell+1}) = z_{\ell+1}} \end{aligned}$$

Predicted Problem

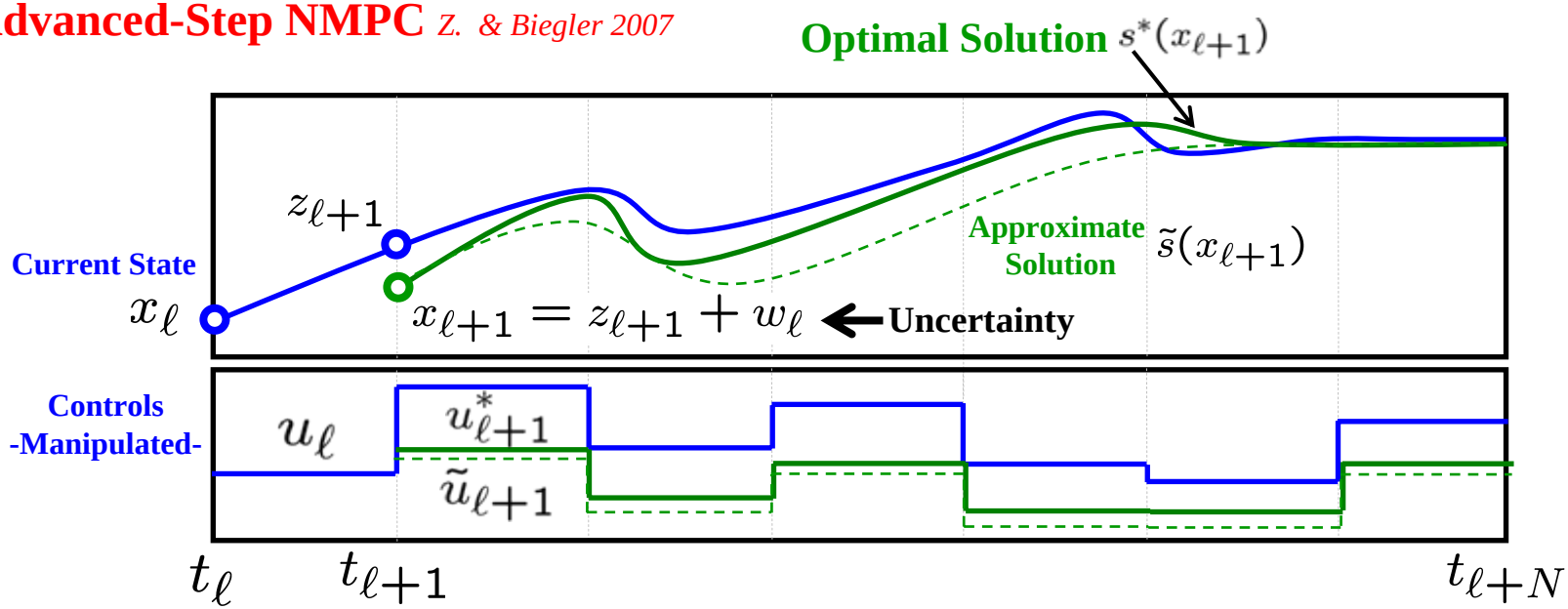
1) <u>Solve</u> Predicted Problem To Optimality and <u>Hold KKT System</u>

$$\begin{bmatrix} \mathbf{K}^* \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta \lambda \end{bmatrix} = -\begin{bmatrix} 0 \\ c(x^*, z_{\ell+1}) \end{bmatrix}$$

Contains Predicted State

Advanced-Step NMPC

Advanced-Step NMPC *Z. & Biegler 2007*



2) Once True/Estimated State $x_{\ell+1}$ Is Obtained

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

$$\begin{bmatrix} \mathbf{K}^* \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta \lambda \end{bmatrix} = -\begin{bmatrix} 0 \\ c(x^*, z_{\ell+1}) \end{bmatrix}$$

Predicted State $z_{\ell+1}$ → **True State** $x_{\ell+1}$

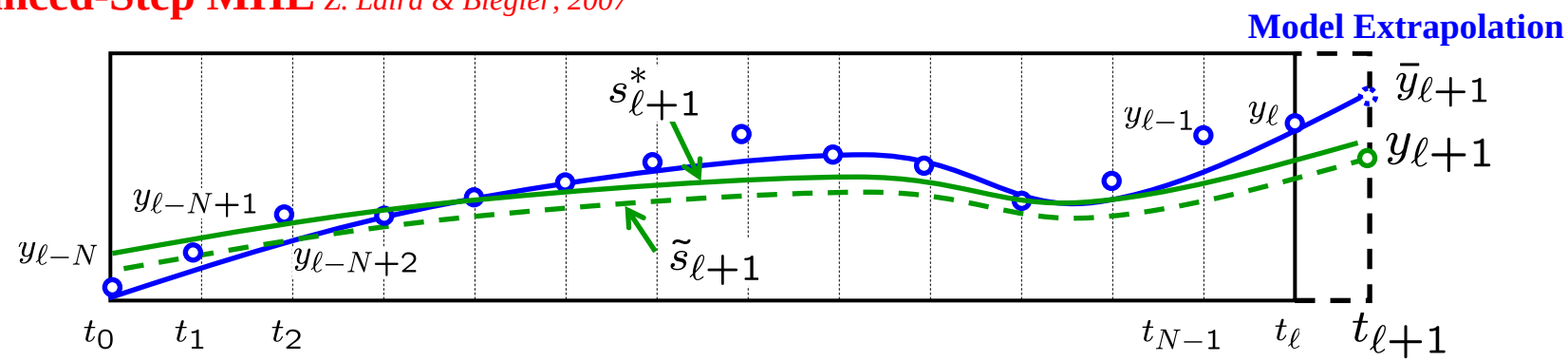
Approximation Error ~ <u>Uncertainty Bound</u>

$$\|\tilde{u}_{\ell+1} - u^*_{\ell+1}\| \leq L\|w_\ell\|^2$$

<u>Full Background Solutions</u> → Establish Nominal and Robust Stability Conditions

Advanced-Step MHE

Advanced-Step MHE *Z. Laird & Biegler, 2007*



1) Solve Predicted Problem $\mathrm{P}(\bar{y}_{\ell+1})$ **with Measurement** $\bar{y}_{\ell+1} = \chi(z_{\ell+1})$

$$\begin{bmatrix} \mathbf{K}^* \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta \lambda \end{bmatrix} = -\begin{bmatrix} r(s^*, \bar{y}_{\ell+1}) \\ 0 \end{bmatrix}$$

2) At $t_{\ell+1}$ **Get True Measurement** $y_{\ell+1}$ **and Perturb KKT System**

$$\|\tilde{x}_{\ell+1} - x^*_{\ell+1}\| \leq L_1 \|y_{\ell+1} - \bar{y}_{\ell+1}\|^2$$

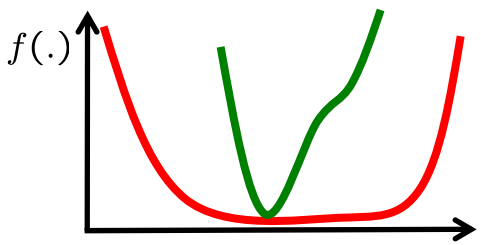
Approximation Error ~ Uncertainty

$$\|\tilde{x}_{\ell+1} - z_{\ell+1}\| \leq L_2 \|\mathbf{\Pi}_{\ell+1}\| \|y_{\ell+1} - \bar{y}_{\ell+1}\|$$

Correction Step

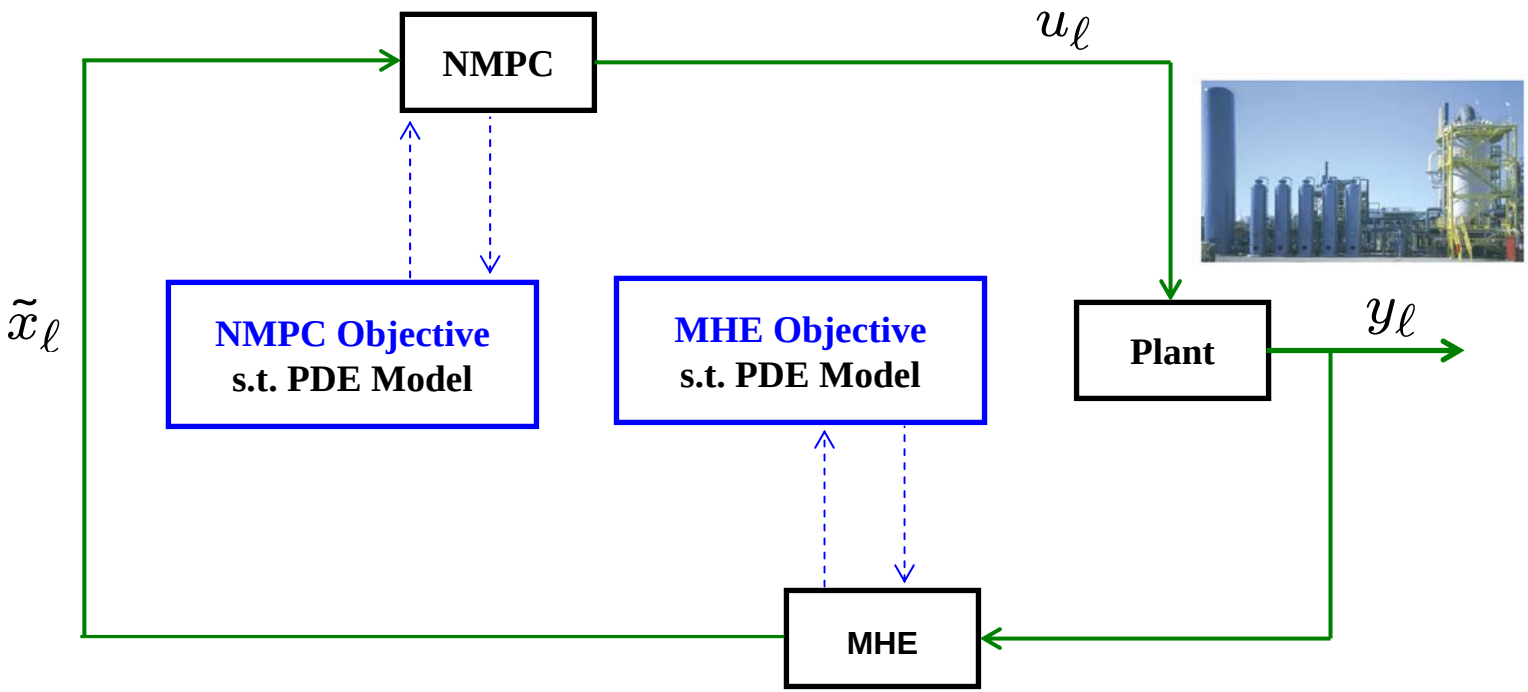
States Covariance

- **Strongly Observable** $\lambda_{max}(\mathbf{\Pi}_{\ell+1}) \to 0$ **→Approximation Error Small**
- **Weakly Observable** $\lambda_{max}(\mathbf{\Pi}_{\ell+1}) \gg 0$ **→ Approximation Error Large**



Advanced-Step MHE+NMPC

Advanced-Step Formulation <u>Decouples Background</u> Problems *Findeisen, et.al. 2002*

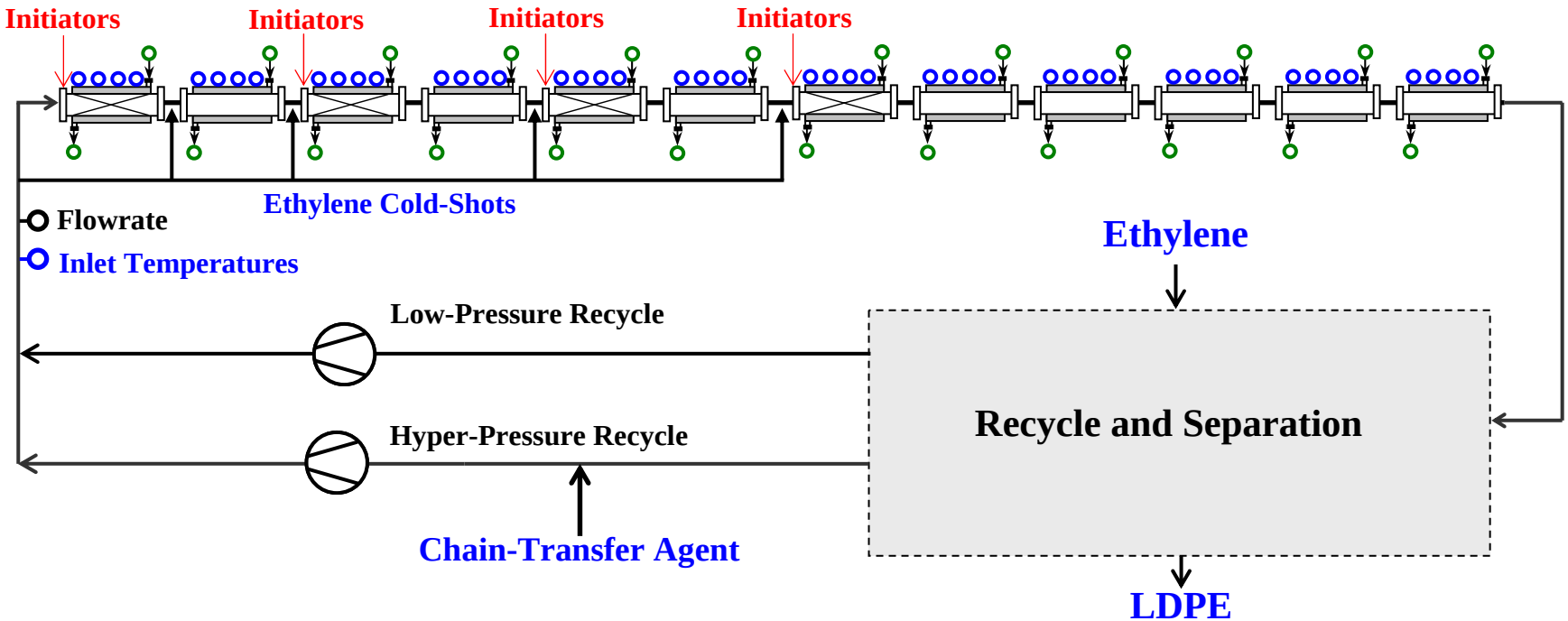


+ On-Line Cost = <u>2 Sequential Backsolves</u>

- However, MHE Approximation <u>Error Propagates</u> to NMPC

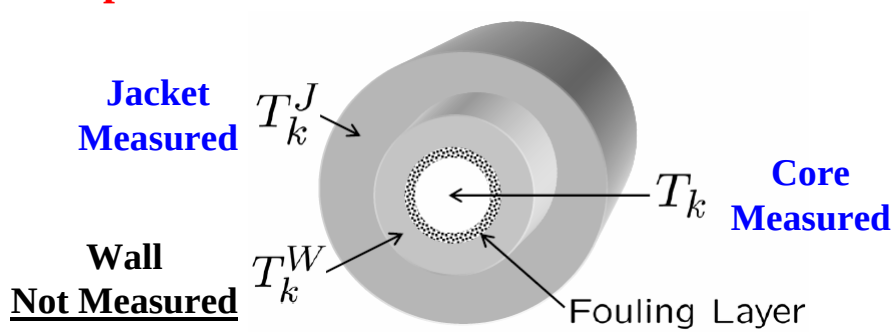
Results Industrial LDPE Process

MHE-NMPC Scenario LDPE



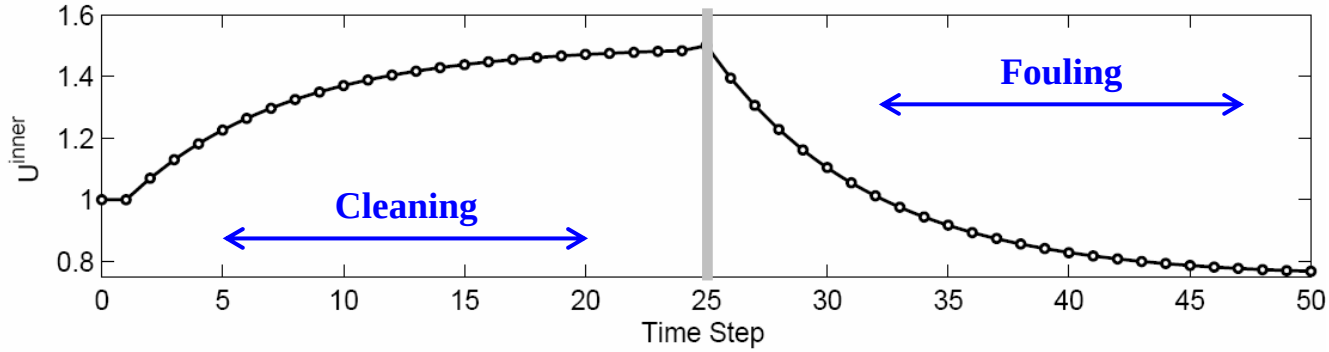
MHE-NMPC Framework with PDE Reactor Model

- Perturb Heat-Transfer Coefficients to Simulate Fouling Disturbances
- MHE to Infer Fouling Layer and States (e.g. Wall Axial Profile)
- NMPC to Stabilize Temperature Profile

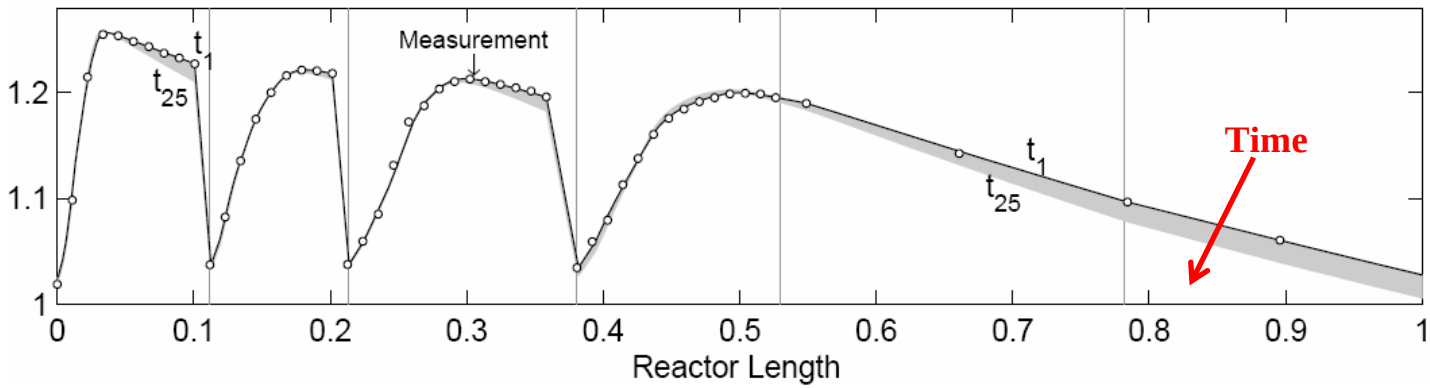


MHE-NMPC Scenario LDPE

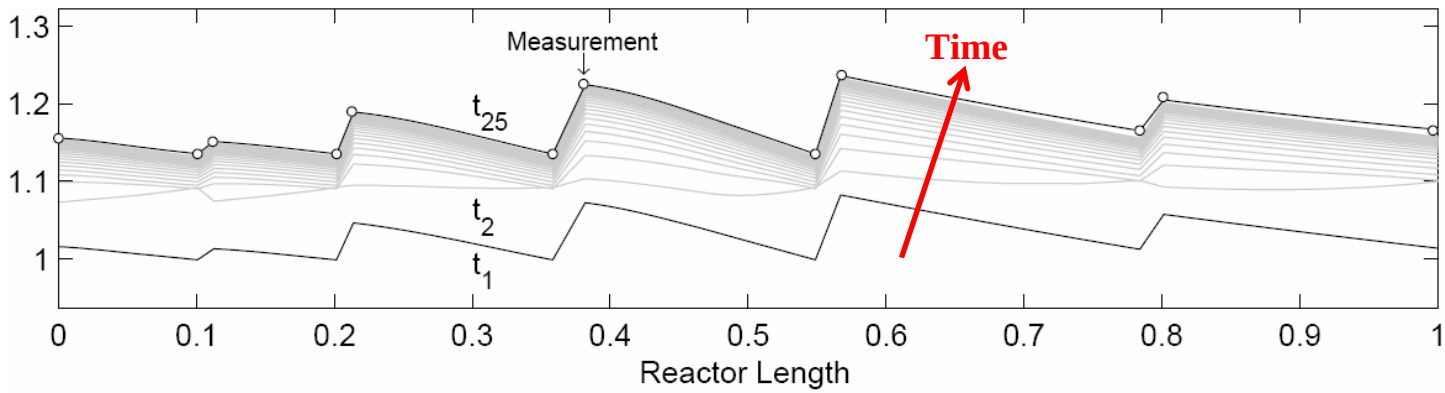
MHE – Scenario Description



Measured Core Temperature



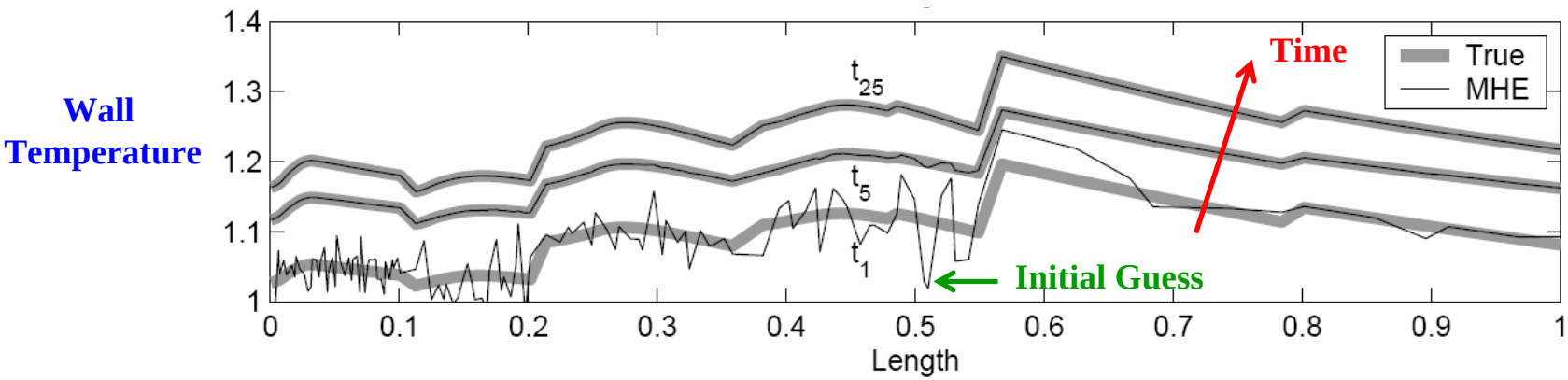
Measured Jacket Temperature



MHE-NMPC Scenario LDPE

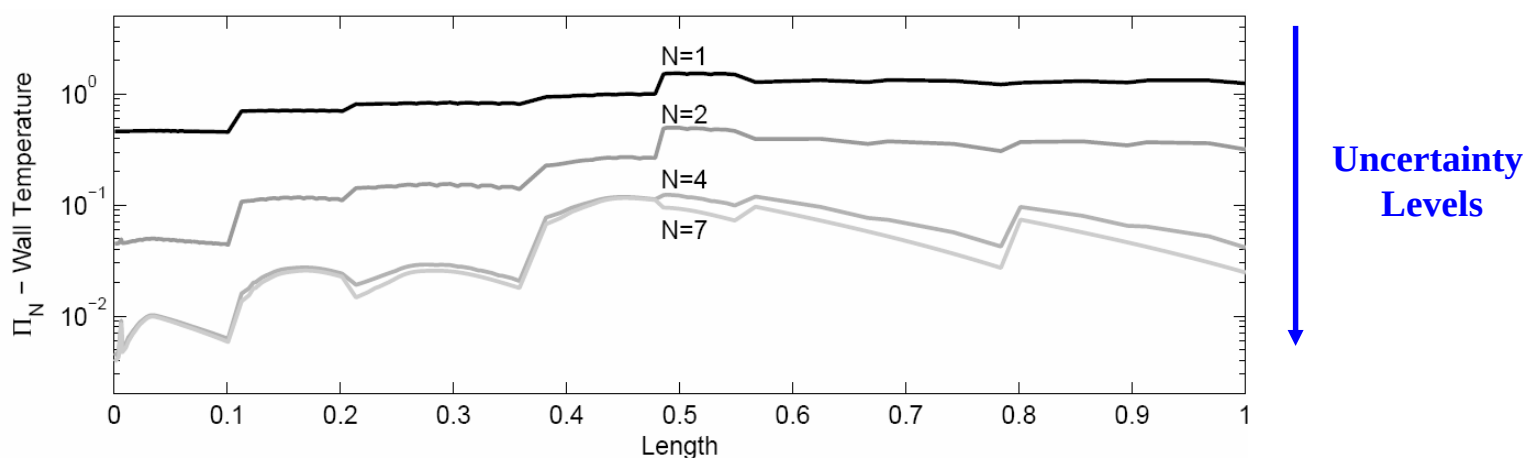
MHE – Convergence

Reconstruction of Wall Temperature Profile



Estimator Recovers Quickly from Poor Initial Guesses and Disturbances

Analysis of Covariance Matrix of Wall Temperature Profile



Distributed Temperature Measurements Make Reactor Strongly Observable

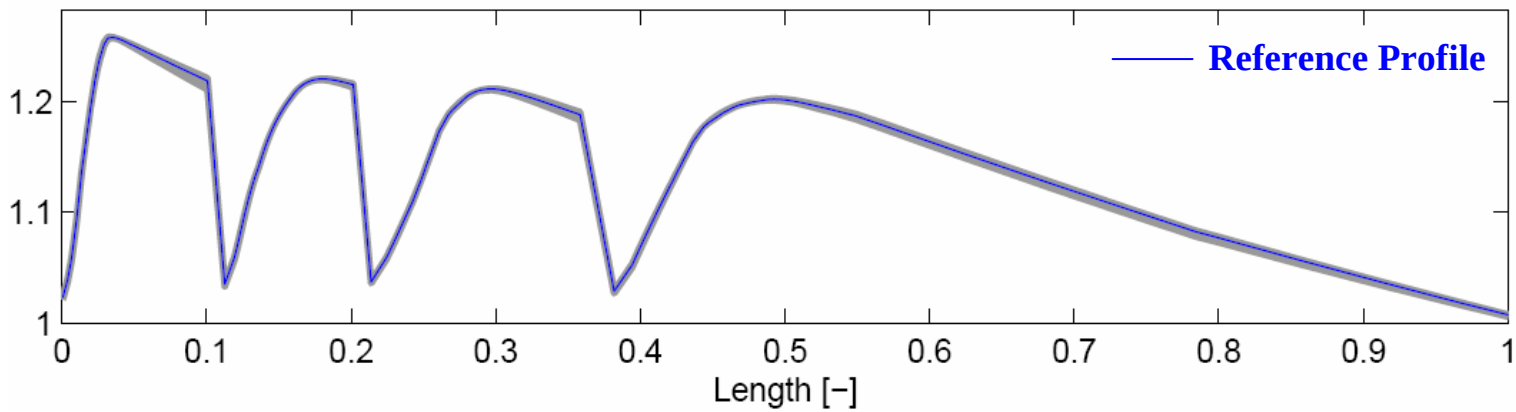
MHE-NMPC Scenario LDPE

NMPC – Tracking Objective

Minimize Transition Time

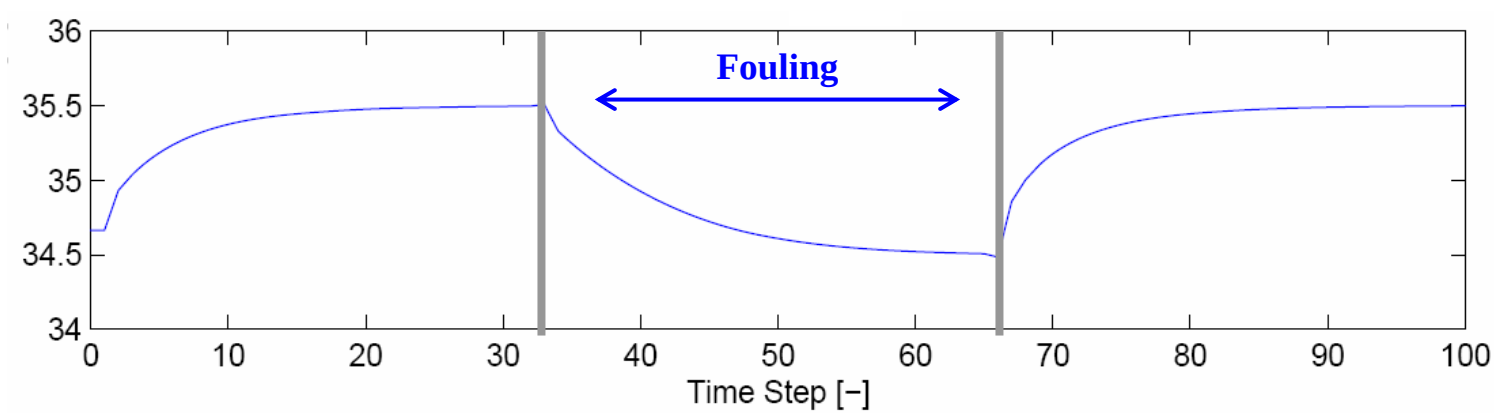
$$\min_{u(t)} \int_0^{t_f} \int_0^{x^L} (z(x,t) - z^{ref}(x))^T \mathbf{W} (z(x,t) - z^{ref}(x)) dx dt$$

Core Temperature



NMPC Stabilizes Profile but Needs to Drop Production as Fouling Advances

Overall Production



LDPE Reactors Have a Large Number of Degrees of Freedom

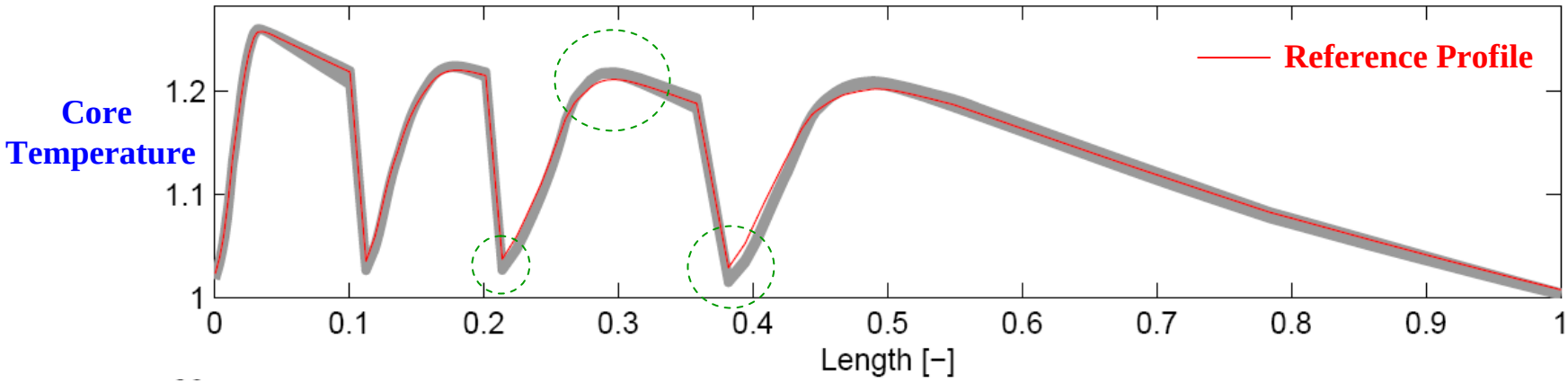
-Not Fully Exploited with Tracking NMPC-

MHE-NMPC Scenario LDPE

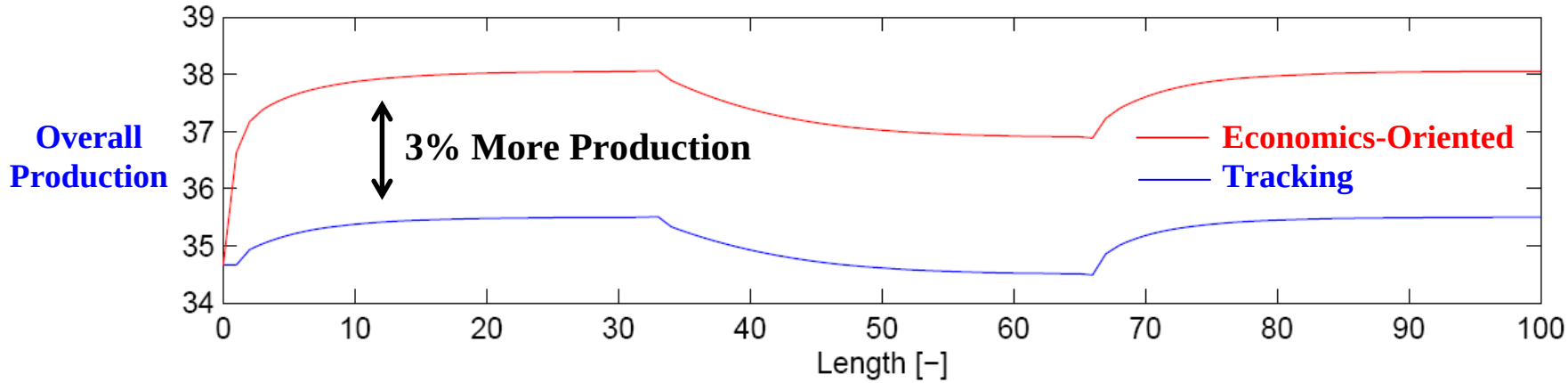
NMPC – Economic Objective

Minimize Transition Time **Maximize Production**

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



Economic-NMPC Moves Away from Suboptimal Reference Profile



Distributes Production Along Pipe Efficiently

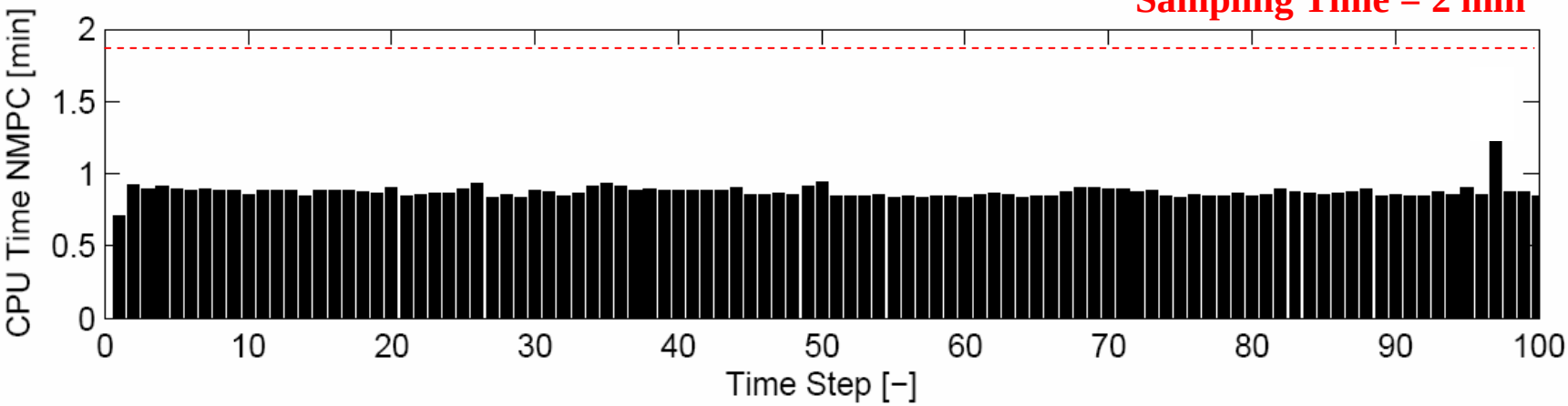
Purely Economic Objective Leads to Ill-Posedness *Huesman, et.al. 2007*

MHE-NMPC Scenario LDPE

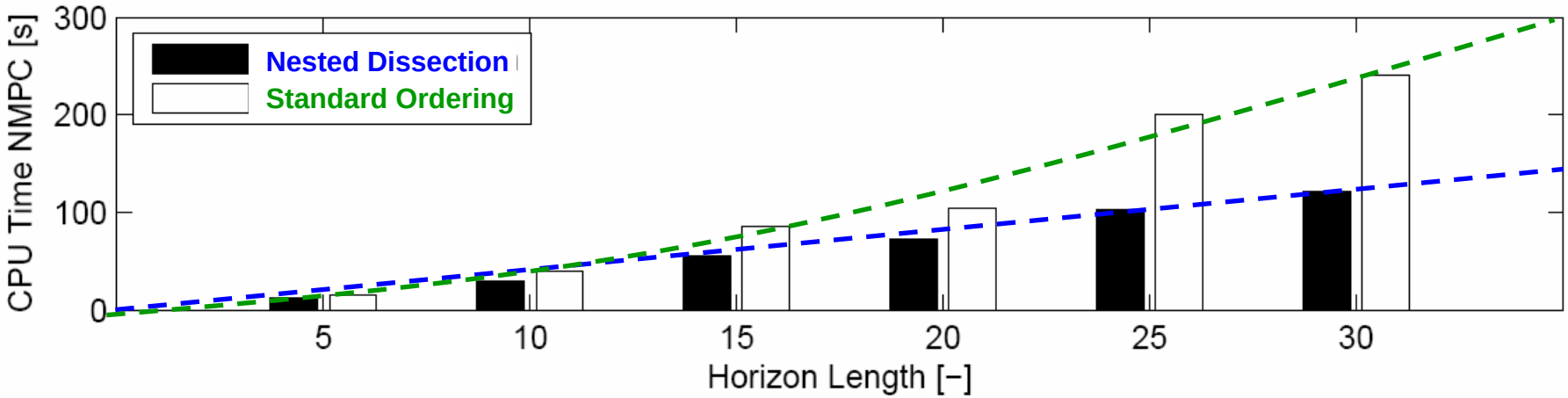
NMPC – Computational Performance

- Full-Discretization + IPOPT (MA57)
- NLP ~ 80,000 Constraints, 370 Degrees of Freedom (DOF)

Sampling Time = 2 min



- Scale-Up and Effect of KKT Matrix Reordering



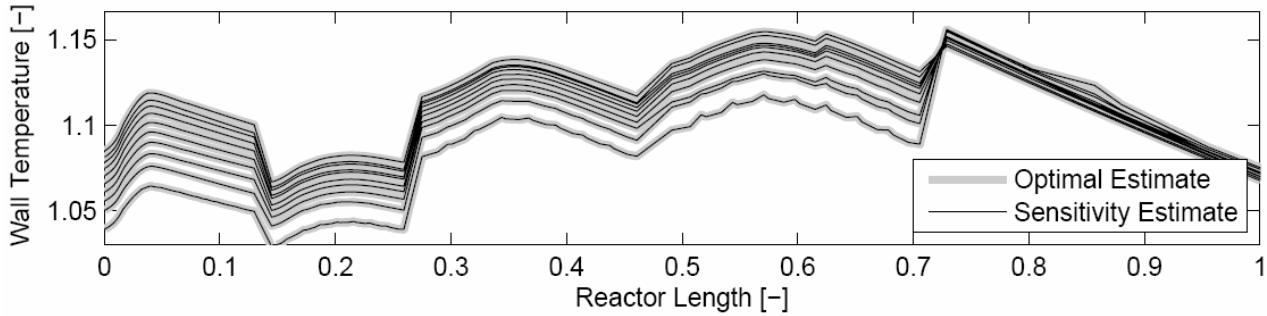
NLP with 350,000 Constraints and 1,000 DOF Solved in ~ 2 Minutes

MHE-NMPC Scenario LDPE

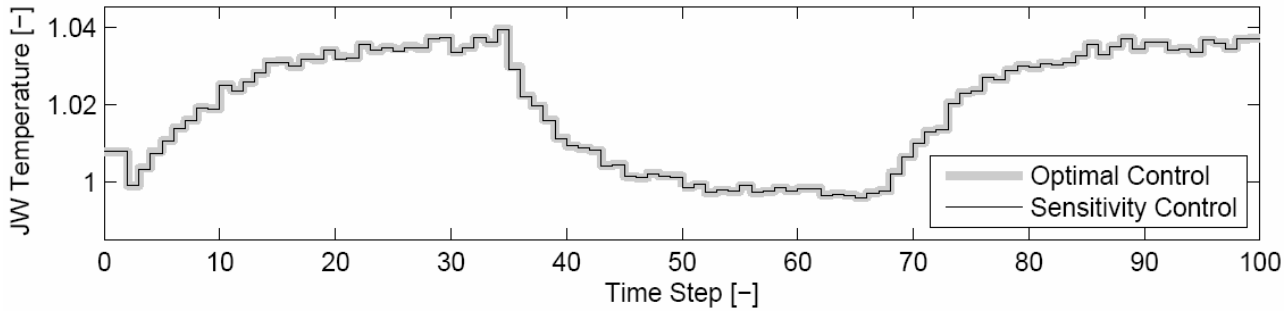
Feedback Delay MHE+NMPC ~ 4 min, Sampling Time = 4 min

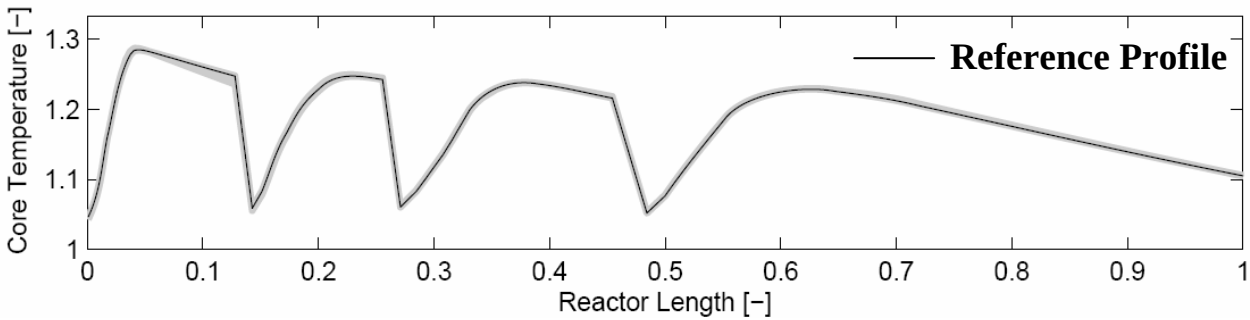
- Advanced-Step to Overcome Delays and Reduce Sampling Time

Advanced-Step MHE



Advanced-Step NMPC





+ Approximation Errors (In General) Negligible

+ Feedback Delay ~ <u>0.2 CPUs</u>, Sampling Time = 2 min

Conclusions and Future Work

Conclusions and Future Work

Chemical Process Operations

First-Principles Models for On-Line Decision-Making

Large-Scale On-Line Optimization

Computational Framework

Full-Discretization for Fast Background Solutions

Reuse KKT Matrix for Fast On-Line Calculations

Industrial Polyethylene Process

Complex PDE Model, Significant Benefits in Profit

Future Work

Faster Factorizations of KKT Matrix

Better Reorderings, Exploit Intuitive and Non-Intuitive Structures *Gondzio, et.al. 2003*

Emphasize on General Linear Solvers

Exploit Multi-Core Computer Technology *Gill, et.al. 2007*

Nonlinear Programming Strategies for State Estimation and Model Predictive Control

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