Dynamic Real-Time Optimization: Linking Off-line Planning with On-line Optimization

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Overview

Introduction

- Pyramid of operations
- Off-line vs On-line Tasks
- Steady state vs Dynamics
- Enablers and open questions

On-line Issues

- Model predictive control
- Treatment of nonlinear model and uncertainty
- Benefits and successes

Advanced Step Controller

- Basic concepts and properties
- Performance for examples

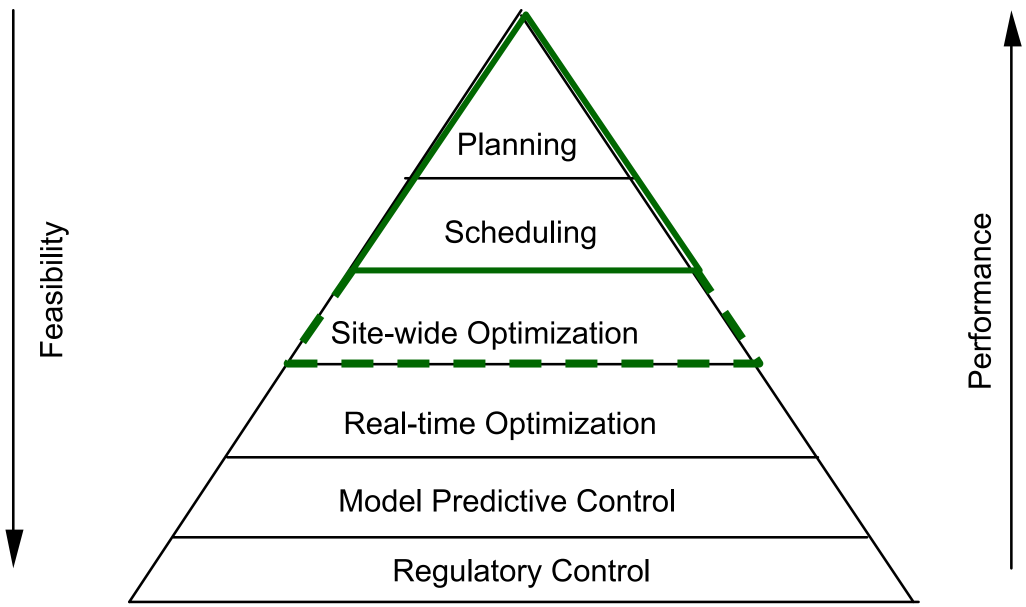
Future Work

Decision Pyramid for Process Operations

Goal: Bridge between planning, logistics (linear, discrete problems) and detailed process models (nonlinear, spatial, dynamic)

Planning and Scheduling

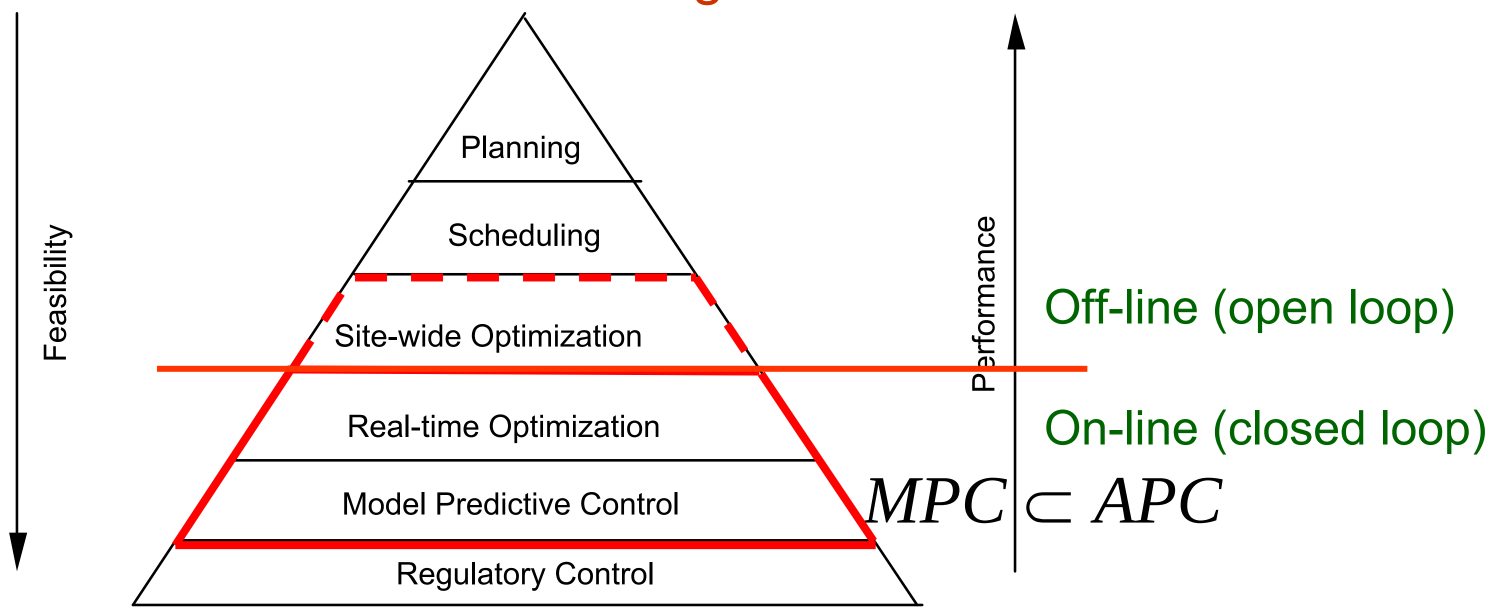
- Many Discrete Decisions
- Few Nonlinearities



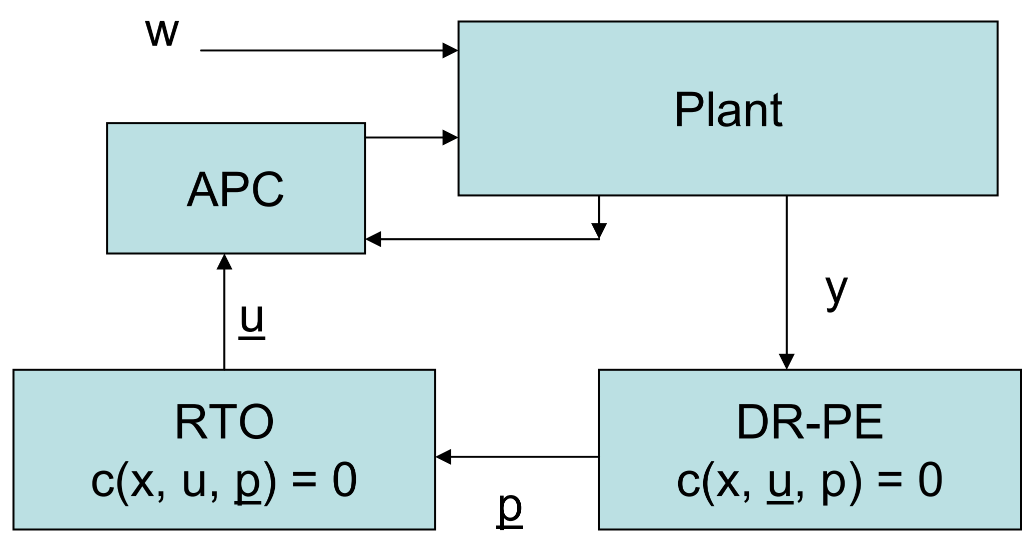
Decision Pyramid for Process Operations

Real-time Optimization and Advanced Process Control

- Fewer discrete decisions
- Many nonlinearities
- Frequent, "on-line" time-critical solutions
- Higher level decisions must be feasible
- Performance communicated for higher level decisions



Steady State RTO



On line optimization

- Nonlinear steady state model for states (x)
- Supply setpoints (u) to APC (control system) with Linear Dynamic Models
- Model mismatch, measured and unmeasured disturbances (w)

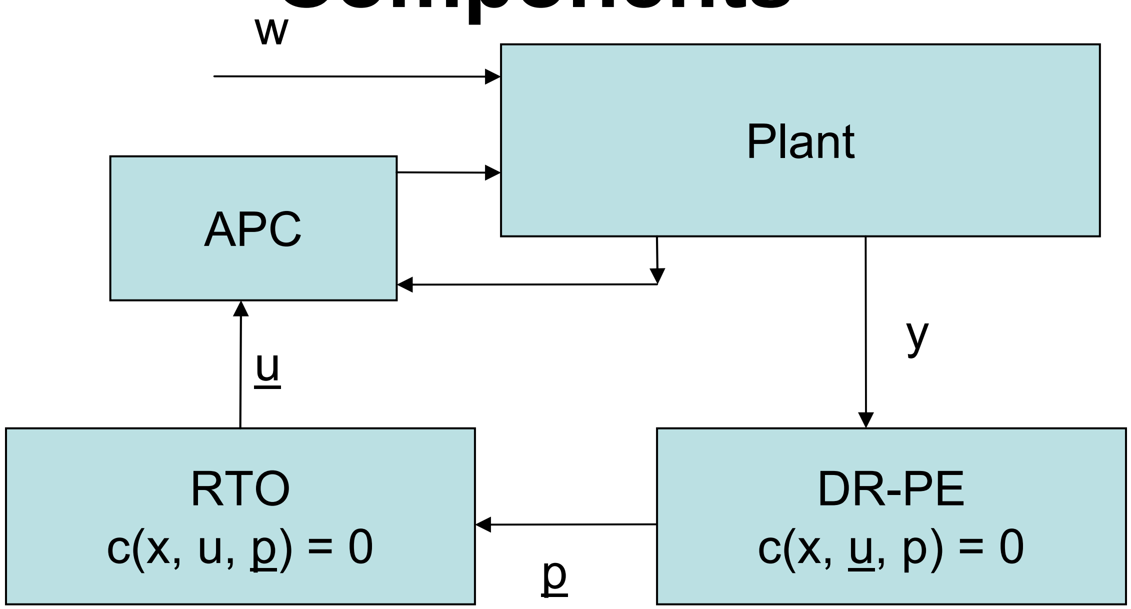
$$\mathrm{Min}_u \; F(x, u, w)$$
$$\text{s.t. } c(x, u, \underline{p}, w) = 0$$
$$x \in X,\ u \in U$$

Data Reconciliation & Parameter Identification

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

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

Steady-state On-line Optimization: Components

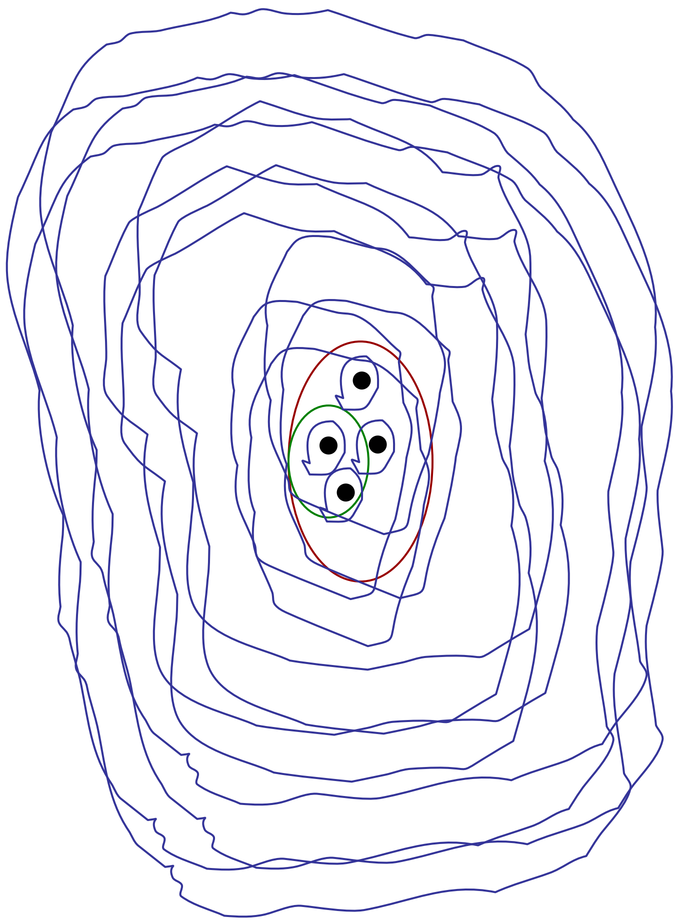


- Data reconciliation – identify gross errors and inconsistency in data
- Periodic update of process model identification
- Usually requires APC loops (MPC, DMC, etc.)
- RTO/APC interactions: <u>Assume decomposition of time scales</u>
    - APC to handle disturbances and fast dynamics
    - RTO to handle static operations
- Typical cycle: 1-2 hours, closed loop

- <u>What if steady state and dynamic models are inconsistent?</u>

Steady-state On-line Optimization: Properties
(Marlin and coworkers)

- Consistency of models and Stability of steady-state RTO
- Sensitivity of the optimum to disturbances and model mismatch? => NLP sensitivity
- Steady state test? Has the process changed?
  - Statistical test on objective function => change is within a confidence region satisfying a χ^2 distribution
  - Implement new RTO solution only when the change is significant
  - **<u>Assumes accurate model</u>**
- Are we optimizing on the noise? Model mismatch? Dynamics?
- Can lead to *<u>ping-ponging</u>*



Why Dynamic RTO?

- Batch processes
- Grade transitions
- Cyclic reactors (coking, regeneration…)
- Cyclic processes (PSA, SMB…)
- Continuous processes are never in steady state:
  - Feed changes
  - Nonstandard operations
  - Optimal disturbance rejections

- Simulation environments (e.g., ACM, gPROMS) and first principle dynamic models are widely used for off-line studies

Some DRTO Case Studies

- Integrated grade transitions
  - MINLP of scheduling with dynamics (Flores & Grossmann, 2006, Prata et al., 2007)
  - *Significant reduction in transition times*
- Dynamic Predictive Scheduling
  - Processes and supply chains need to optimally respond to disturbances through dynamic models
  - *Reduction in energy cost by factor of two*
- Cyclic Process Optimization
  - Decoking scheduling
  - SMB optimization
  - PSA optimization
  - *Productivity increases by factor of 2-3*

Dynamic Optimization Problem

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

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

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

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

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

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

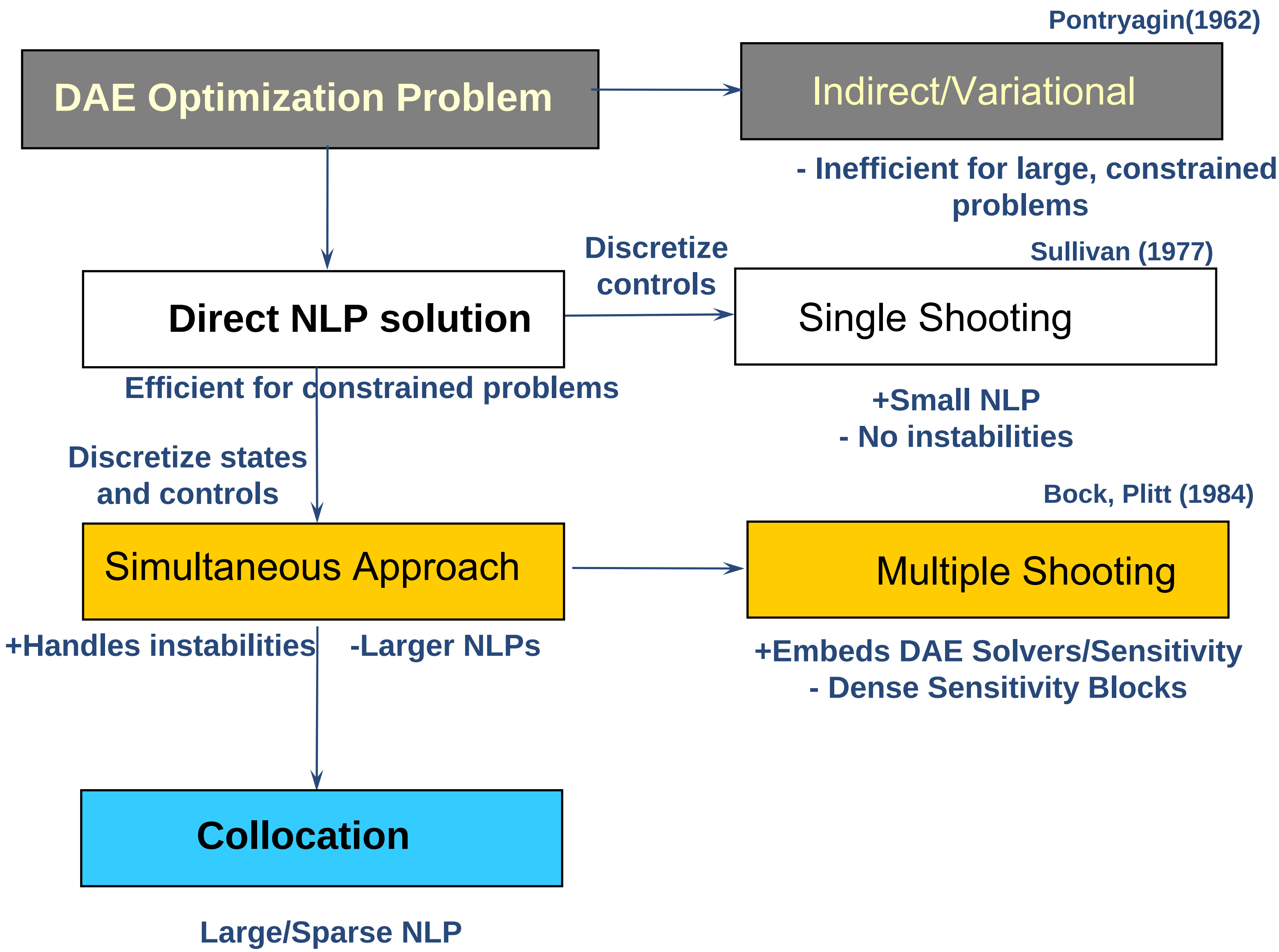
$$u^l \le u(t) \le u^u$$

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

t, time
z, differential variables
y, algebraic variables

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

Dynamic Optimization Approaches



Dynamic Optimization Engines

Evolution of NLP Solvers:

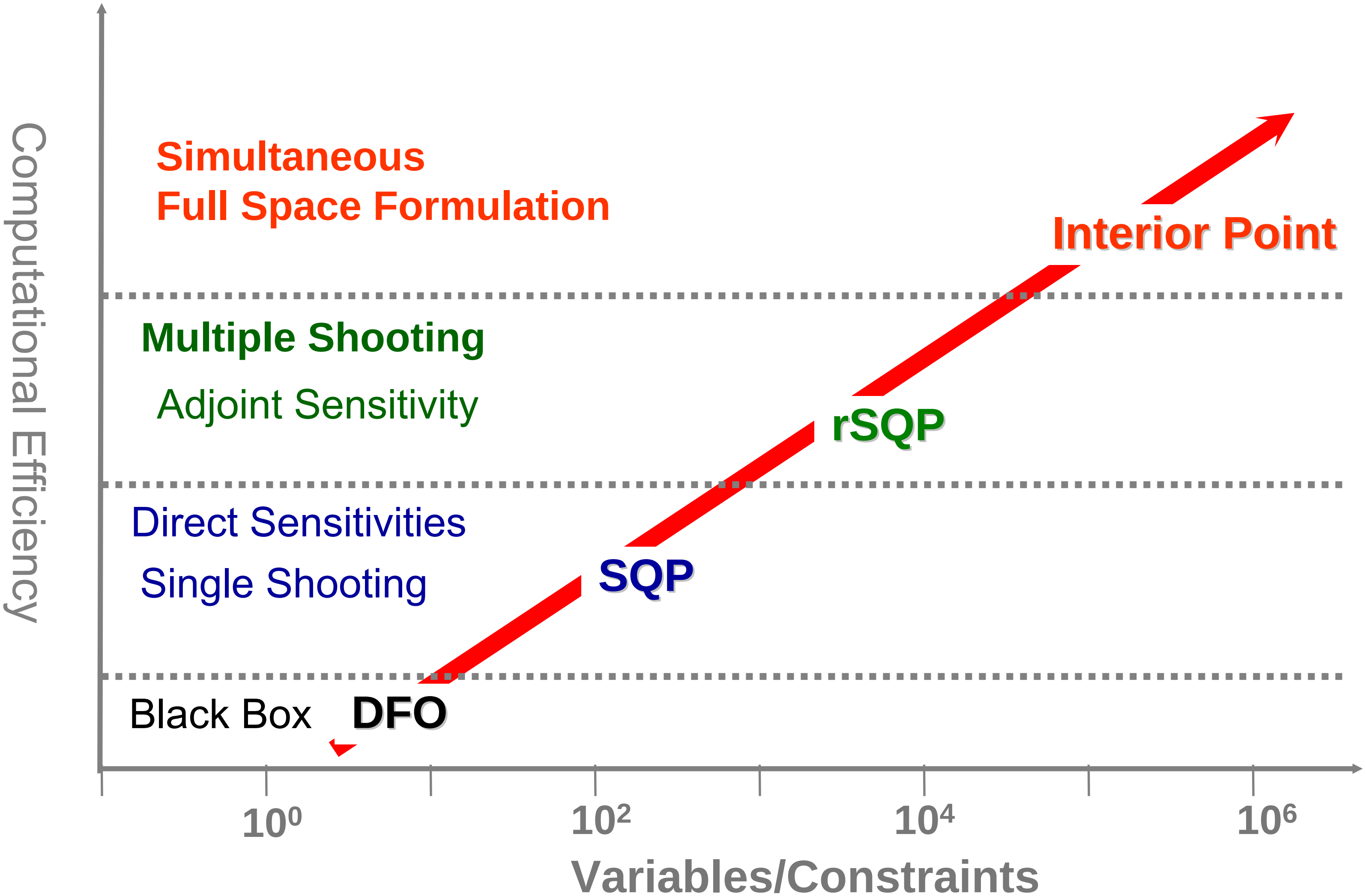
➔ ***for dynamic optimization, control and estimation***

SQP ⟶ rSQP ⟶ Full-space Barrier

E.g., ***IPOPT*** - Simultaneous dynamic optimization over 1 000 000 variables and constraints

Object Oriented Codes tailored to structure, sparse linear algebra and computer architecture (e.g., IPOPT 3.2)

Hierarchy of Nonlinear Programming for Dynamic Optimization Formulations



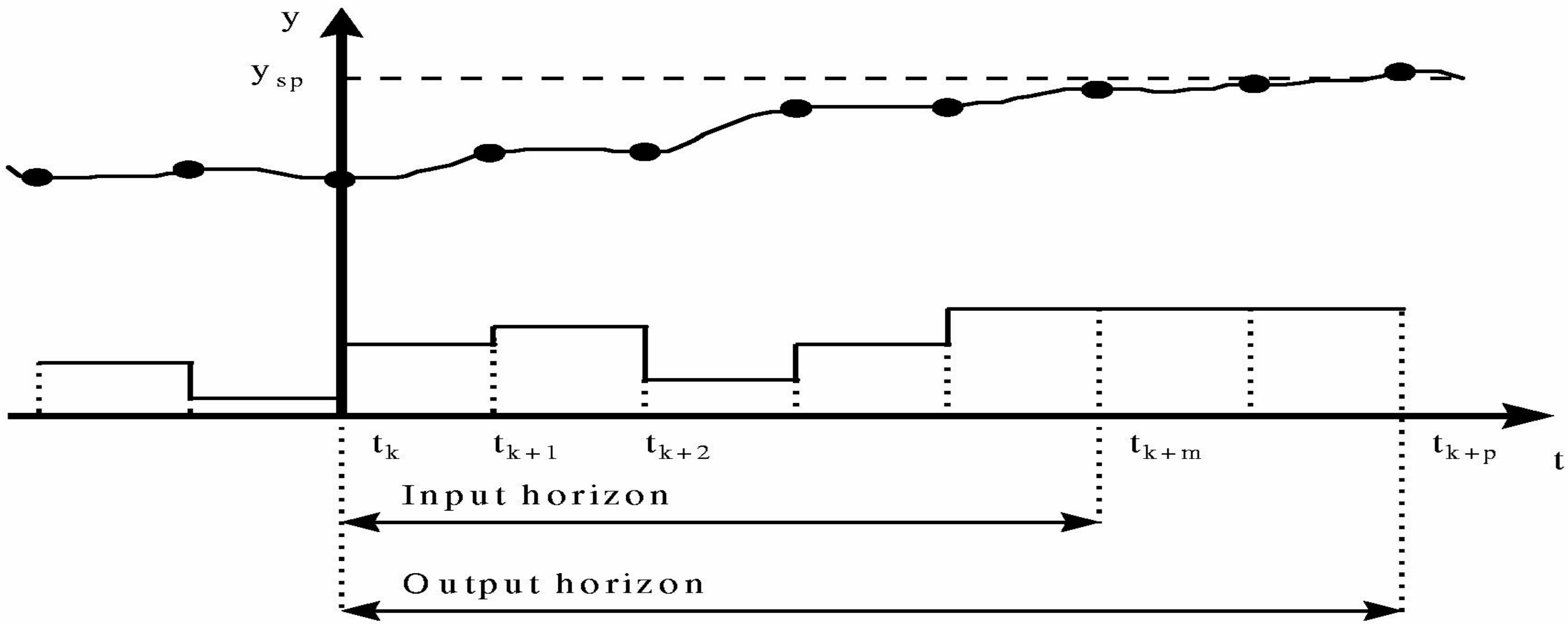
Comparison of Computational Complexity

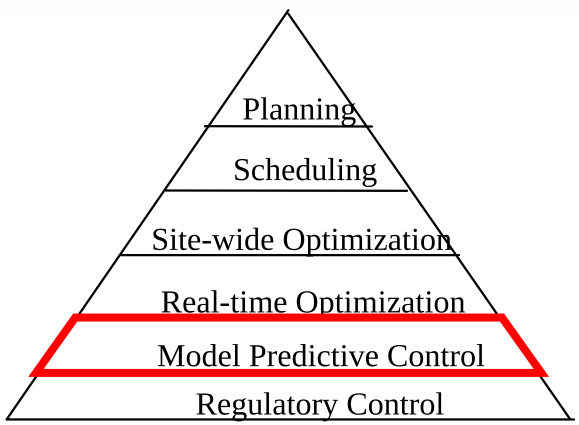
($\alpha \in [2, 3]$, $\beta \in [1, 2]$, n_w, n_u - assume $N_m = O(N)$)

	Single Shooting	Multiple Shooting	Simultaneous
DAE Integration	$n_w^\beta N$	$n_w^\beta N$	---
Sensitivity	$(n_w N)(n_u N)$	$(n_w N)(n_u + n_w)$	$N(n_u + n_w)$
Exact Hessian	$(n_w N)(n_u N)^2$	$(n_w N)(n_u + n_w)^2$	$N(n_u + n_w)$
NLP Decomposition	---	$n_w^3 N$	---
Step Determination	$(n_u N)^\alpha$	$(n_u N)^\alpha$	$((n_u + n_w)N)^\beta$
Backsolve	---	---	$((n_u + n_w)N)$

$O((n_u N)^\alpha + N^2 n_w n_u + N^3 n_w n_u^2)$	$O((n_u N)^\alpha + N n_w^3 + N n_w (n_w + n_u)^2)$	$O((n_u + n_w)N)^\beta$

On-line Issues: Model Predictive Control (NMPC)





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

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

$$z_0 = x(k)$$

$$Bounds$$

MPC - Background

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

- 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**

Stability properties

- Nominal – remain bounded and eventually achieve desired state without noise and with perfect model
- Robust – remain stable with model mismatch and noise

On-line Issues: Stability is Forever

$$\min_{\boldsymbol{u}} \quad J_k = \sum_{l=0}^{N} \varphi(z_l, u_l) + E(z_N)$$

$$s.t. \quad \begin{aligned} z_{l+1} &= f(z_l, u_l)) \\ z_0 &= x(k) \\ &Bounds \end{aligned}$$

$$J_{k-1} - J_k \geq \varphi(x(k-1), u(k-1)) + \{E(z_{N|k-1}) - \varphi(z_{N|k}, v_{N|k}) - E(z_{N|k})\}$$

$$\geq \varphi(x(k-1), u(k-1))$$

$$J_0 \geq \sum_{k=1}^{\infty} (J_{k-1} - J_k) = \sum_{k=1}^{\infty} \varphi(x(k-1), u(k-1))$$

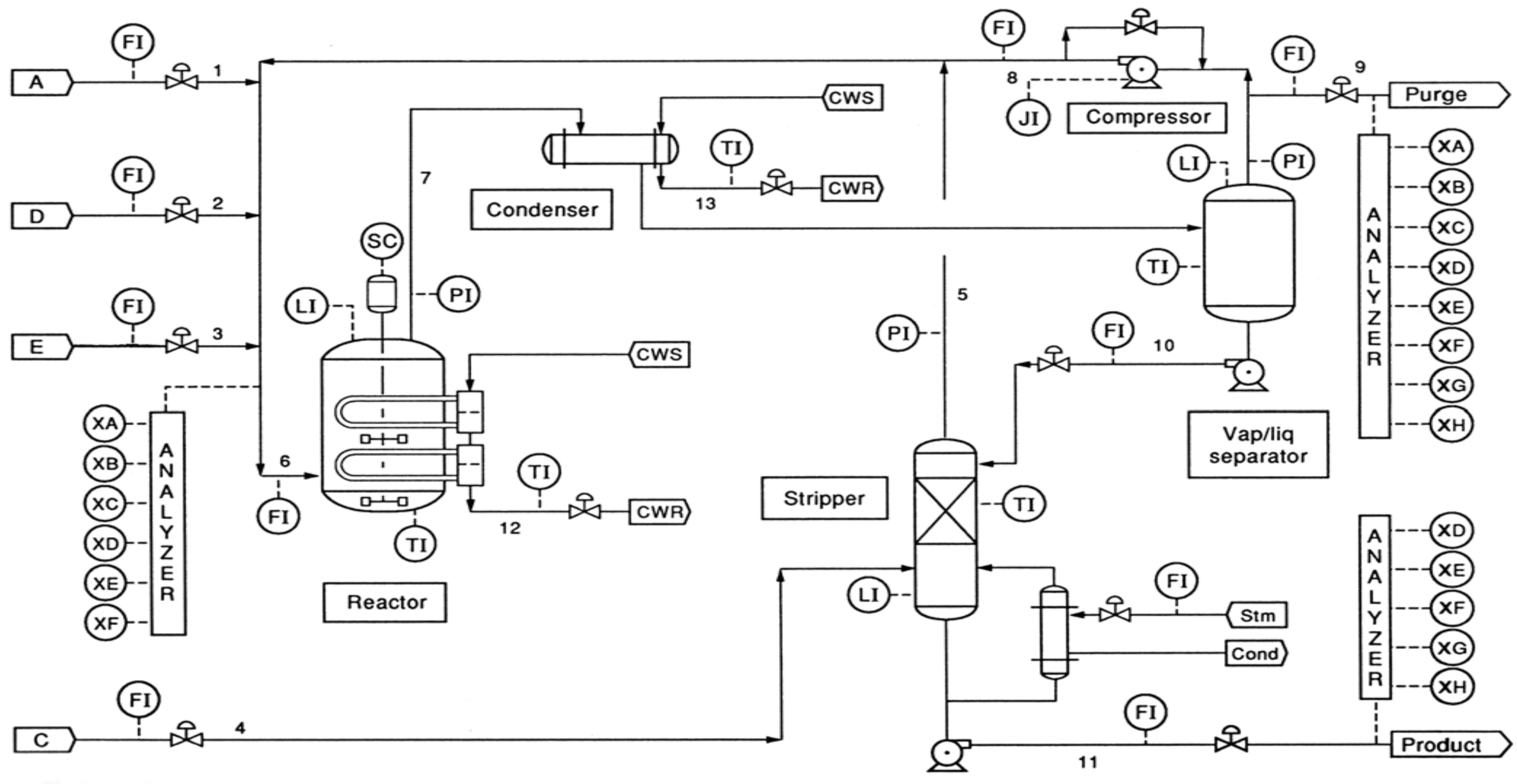
$$\Rightarrow x(k) \to 0, u(k) \to 0$$

Discrete Lyapunov stability proof

- Nominal case – no noise: perfect model
- General formulation with local asymptotic controller for t → ∞
- Robust case – keep (J_{k-1} – J_k) sufficiently positive in presence of noise/mismatch

NMPC for Tennessee Eastman Process

(Jockenhövel, Wächter, B., 2003)



Unstable Reactor

11 Controls; Product, Purge streams

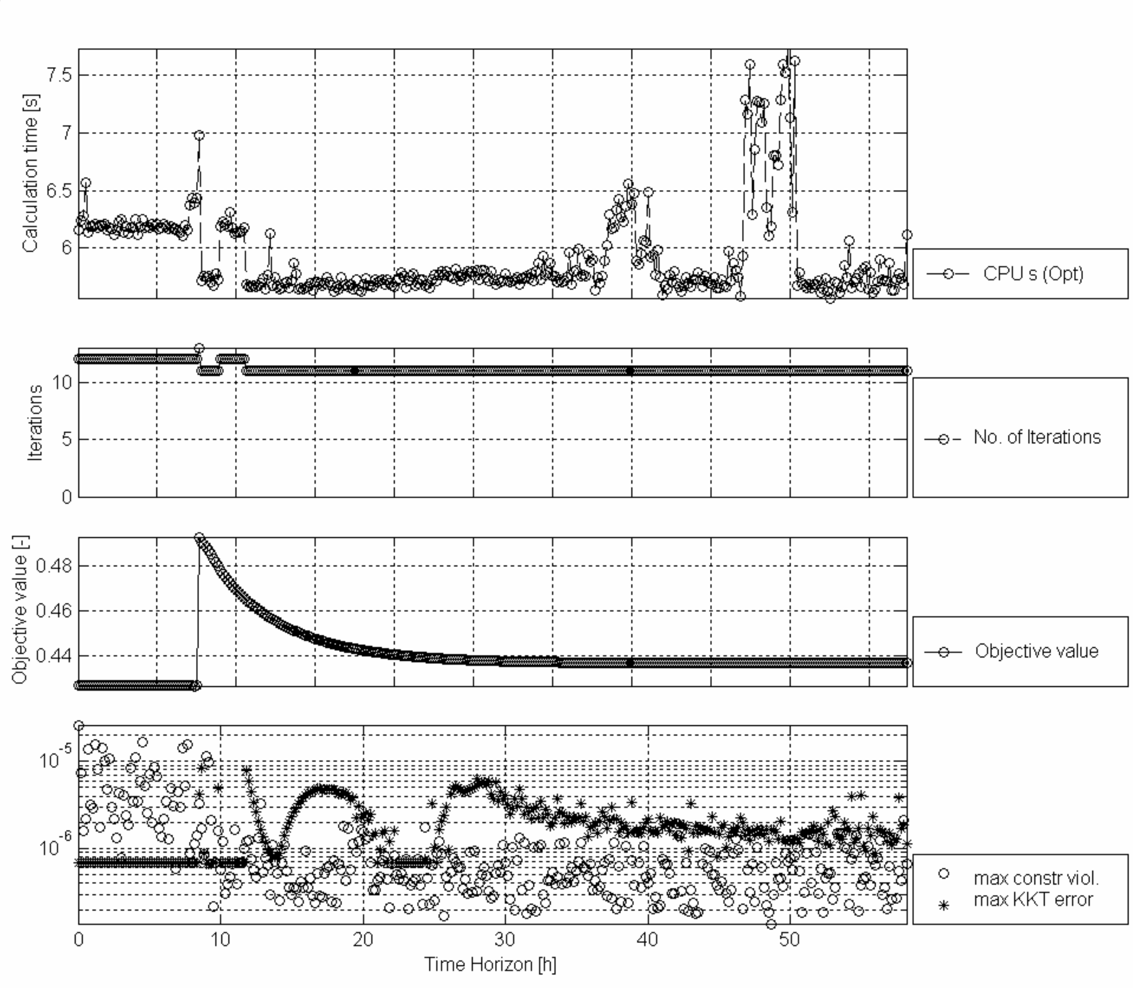
171 DAEs: Model extended with energy balances

After discretization

10920 variables

660 degrees of freedom

NMPC Results – Tennessee Eastman Problem



Optimization with IPOPT

Warm start with $\mu = 10^{-4}$

350 Optimizations

5-7 CPU seconds

11-14 Iterations

Optimization with SNOPT

Uses approximate (dense) reduced Hessian updates

Could not be solved within sampling times

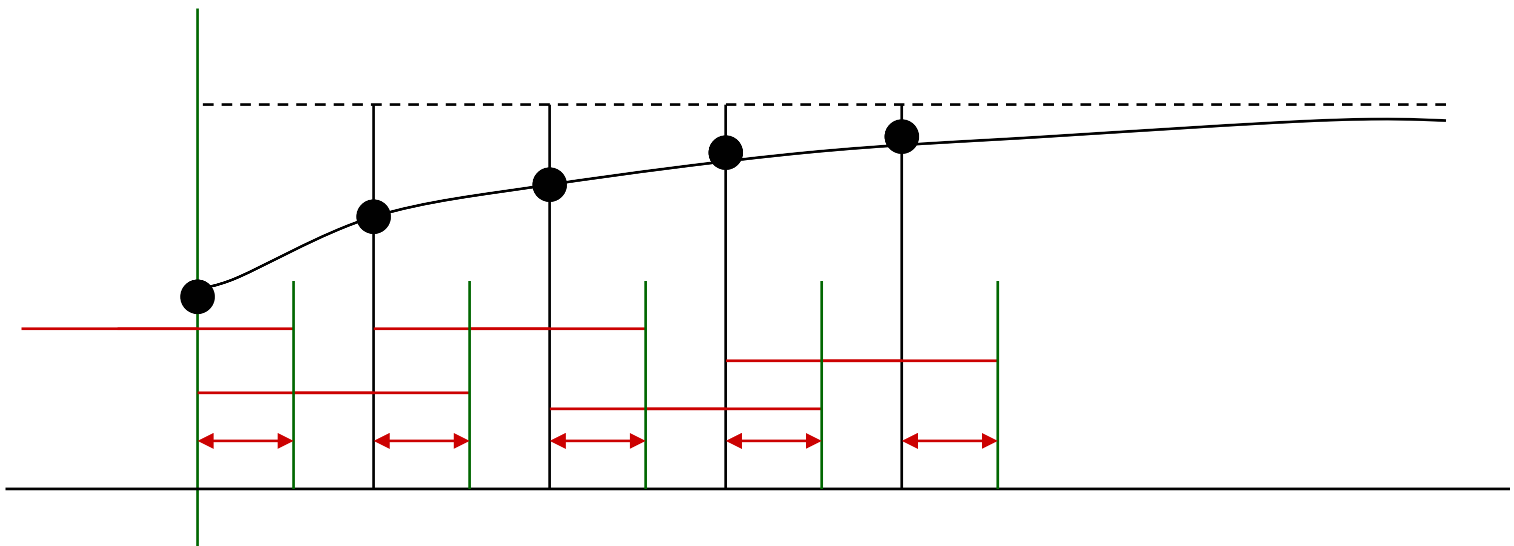
> 100 Iterations

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?

NMPC – Can we avoid on-line optimization?

Divide Dynamic Optimization Problem:

- preparation, feedback response and transition stages
- 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

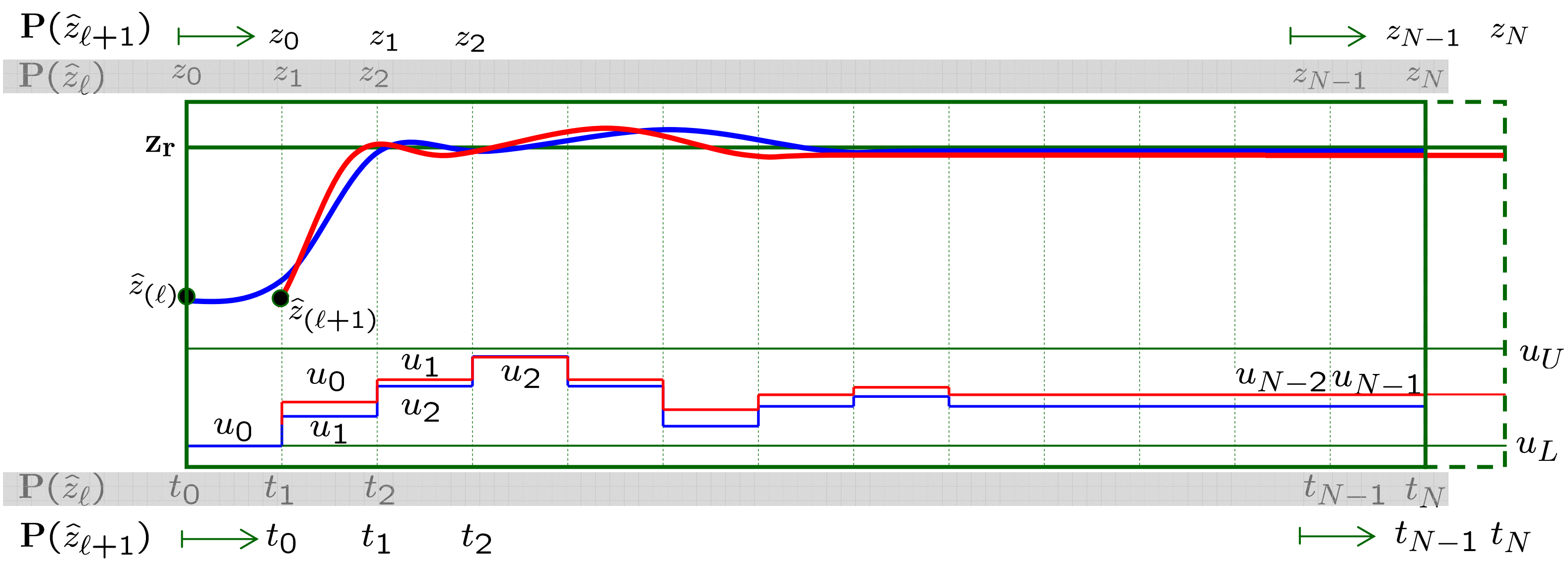
Based on NLP sensitivity of z_0 for dynamic systems

- Extended to Collocation approach – Zavala et al. (2006)
- Three computational variants developed
- Similar approach for MH State and Parameter Estimation – Zavala et al. (2007)

Stability Properties for Advanced Step Controller

- Nominal stability – can be shown from standard Lyapunov analysis
- Robust stability – apply results for input to state stability (ISS) from Magni et al. (2005)

Nonlinear Model Predictive Control – Parametric Problem



$$
\left.
\begin{array}{llrcl}
\mathcal{P}(x(k),N) & \min\limits_{v_{l|k}} & J(x(k),N) & = & F(z_{k+N|k}) + \sum\limits_{l=k}^{k+N-1} \psi(z_{l|k}, v_{l|k}) \\
 & \text{s. t.:} & z_{l+1|k} & = & f(z_{l|k}, v_{l|k}), \quad l = k, \ldots k+N-1 \\
 & & \boxed{z_{k|k}} & \boxed{=} & \boxed{x(k) = p_0} \\
 & & z_{l|k} & \in & \mathbb{X},\ z_{k+N|k} \in \mathbb{X}_f,\ v_{l|k} \in \mathbb{U}.
\end{array}
\right\} \mathrm{P}(p_0)
$$

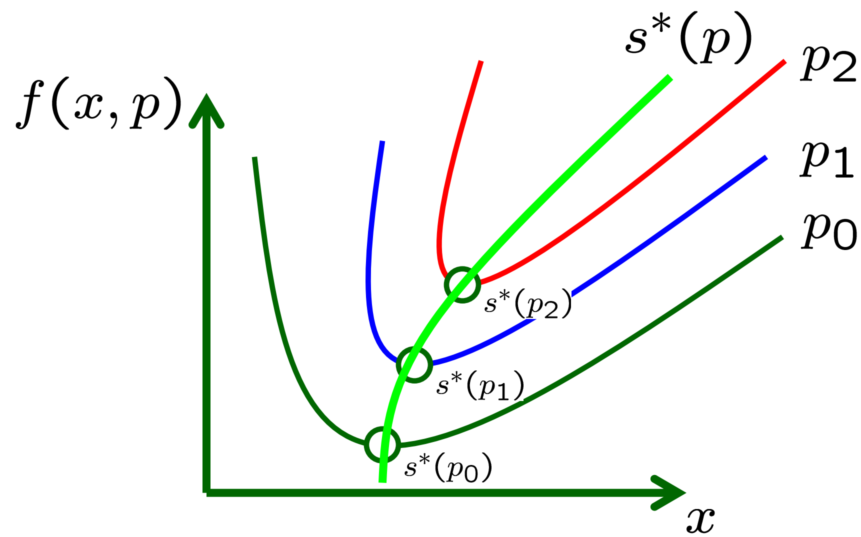
$$\mathrm{P}(p)$$

$$
\begin{array}{llrcl}
\mathcal{P}(x(k+1),N) & \min\limits_{v_{l|k+1}} & J(x(k+1),N) & = & F(z_{k+N+1|k+1}) + \sum\limits_{l=k+1}^{k+N} \psi(z_{l|k+1}, v_{l|k+1}) \\
 & \text{s. t.:} & z_{l+1|k+1} & = & f(z_{l|k+1}, v_{l|k+1}), \quad l = k+1, \ldots k+N \\
 & & \boxed{z_{k|k+1}} & \boxed{=} & \boxed{x(k+1) = p} \\
 & & z_{l|k+1} & \in & \mathbb{X},\ z_{k+N+1|k+1} \in \mathbb{X}_f,\ v_{l|k} \in \mathbb{U}.
\end{array}
$$

NLP Sensitivity

Parametric Programming

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



Solution Triplet

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

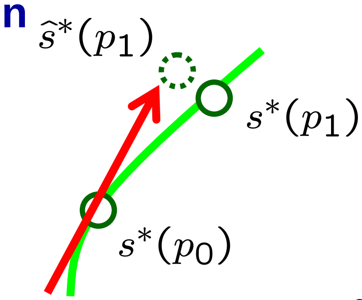
Optimality Conditions $\mathrm{P}(p)$

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

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

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

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

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

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

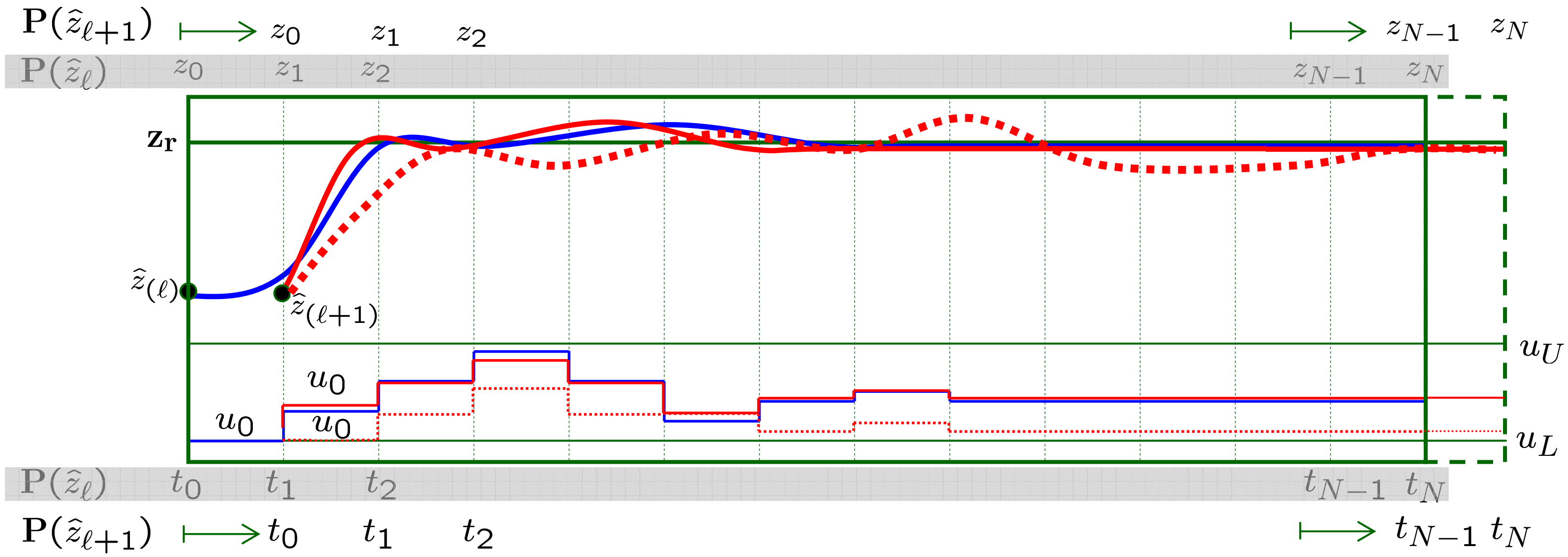
$$\begin{bmatrix} W(s^*(p_0)) & A(x^*(p_0)) & -I \\ A(x^*(p_0))^T & 0 & 0 \\ V^*(p_0) & 0 & X^*(p_0) \end{bmatrix} \begin{bmatrix} \frac{\partial x}{\partial p} \\ \frac{\partial \lambda}{\partial p} \\ \frac{\partial \nu}{\partial p} \end{bmatrix} + \begin{bmatrix} \nabla_{x,p}\mathcal{L}(s^*(p_0))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

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**

NMPC: Direct Sensitivity Variant



Assume:

Optimal Solution $\mathrm{P}(\hat{z}_{\ell})$ → $u_0 = u_L$

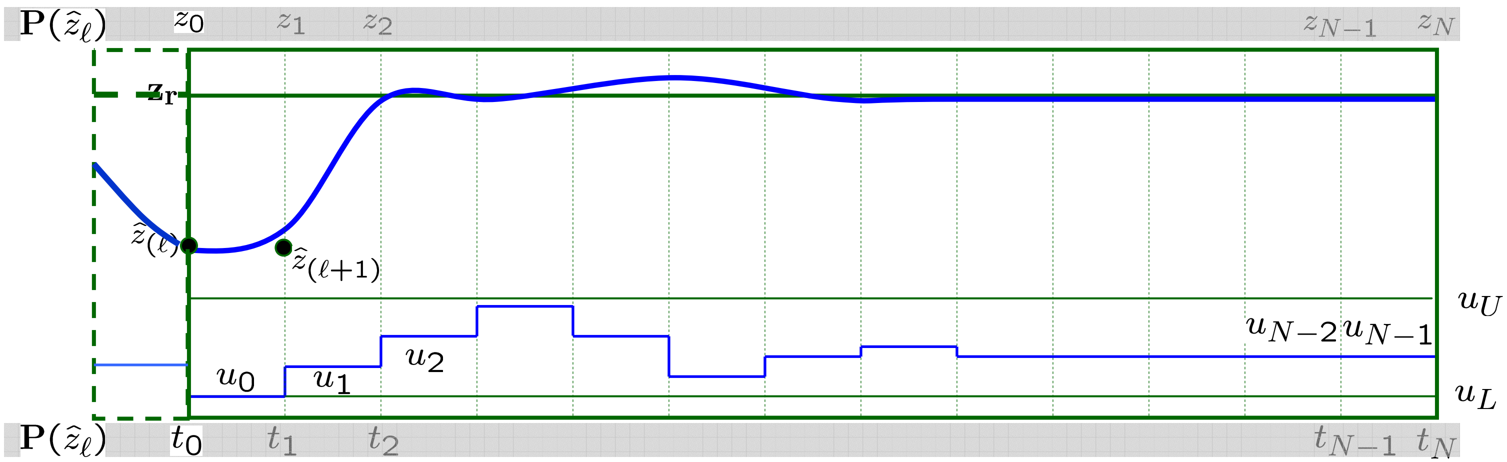
Optimal Solution $\mathrm{P}(\hat{z}_{\ell+1})$ → $u_0 > u_L$

Approximate $\mathrm{P}(\hat{z}_{\ell+1})$ **by Perturbing** $\mathrm{P}(\hat{z}_{\ell})$ → $u_0 = u_L$

NLP Sensitivity → Approximate Solution Retains Active Set of Nominal Problem

This is fast but active set is inconsistent because it does not shift

Nonlinear Model Predictive Control – Equivalence to Previously Solved Problem



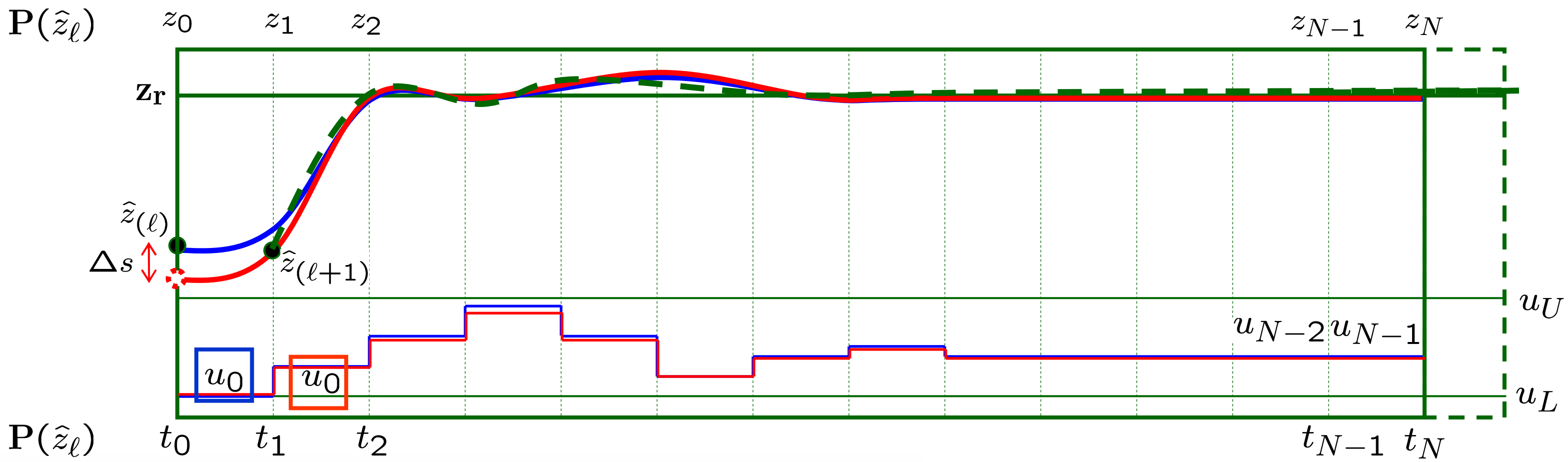
$$
\begin{array}{llrcl}
\mathcal{P}(x(k),N) & \min\limits_{v_{l|k}} & J(x(k),N) & = & F(z_{k+N|k}) + \sum\limits_{l=k}^{k+N-1} \psi(z_{l|k}, v_{l|k}) \\
& \text{s. t.:} & z_{l+1|k} & = & f(z_{l|k}, v_{l|k}), \quad l = k, \dots k+N-1 \\
& & z_{k|k} & = & x(k) = p_0 \\
& & z_{l|k} & \in & \mathbb{X},\ z_{k+N|k} \in \mathbb{X}_f,\ v_{l|k} \in \mathbb{U}.
\end{array}
$$

Solutions to both problems are equivalent in nominal case (ideal models, no disturbances)

$$
\begin{array}{llrcl}
\bar{\mathcal{P}}(x(k-1),N+1) & \min\limits_{v_{l|k}} & J(x(k-1),N) & = & F(z_{k+N|k-1}) + \sum\limits_{l=k}^{k+N-1} \psi(z_{l|k}, v_{l|k}) \\
& \text{s. t.:} & z_{l+1|k-1} & = & f(z_{l|k}, v_{l|k}), \quad l = k, \dots k+N-1 \\
& & z_{k|k-1} & = & f[x(k-1), u(k-1)] \\
& & z_{l|k} & \in & \mathbb{X},\ z_{k+N|k-1} \in \mathbb{X}_f,\ v_{l|k} \in \mathbb{U}.
\end{array}
$$

Advanced Step NMPC

Combine delay concept with sensitivity to solve NLP in background (between steps) – not on-line



$$
\begin{aligned}
\min_{v_{l|k}} \quad J(x(k),N) &= F(z_{k+N|k}) + \sum_{l=k}^{k+N-1} \psi(z_{l|k}, v_{l|k}) \\
\text{s. t.:} \quad z_{l+1|k} &= f(z_{l|k}, v_{l|k}), \quad l = k, \ldots k+N-1 \\
z_{k|k} &= z_0 \\
z_{l|k} &\in \mathbb{X},\ z_{k+N|k} \in \mathbb{X}_f,\ v_{l|k} \in \mathbb{U}.
\end{aligned}
$$

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

$$\mathbf{K}\Delta v = 0$$

$$
\boxed{
\left[\begin{array}{c|c} \mathbf{K} & \mathbf{E_0} \\ \hline \mathbf{E_1}^T & 0 \end{array}\right]
\left[\begin{array}{c} \Delta v \\ \hline \Delta s \end{array}\right]
= - \left[\begin{array}{c} 0 \\ \hline \hat{z}(\ell+1) - z_1^* \end{array}\right]
}
$$

Solve $P(z_\ell)$ in background

Sensitivity to updated problem to get (z_0, u_0)

Solve $P(z_{\ell+1})$ in background with new (z_0, u_0)

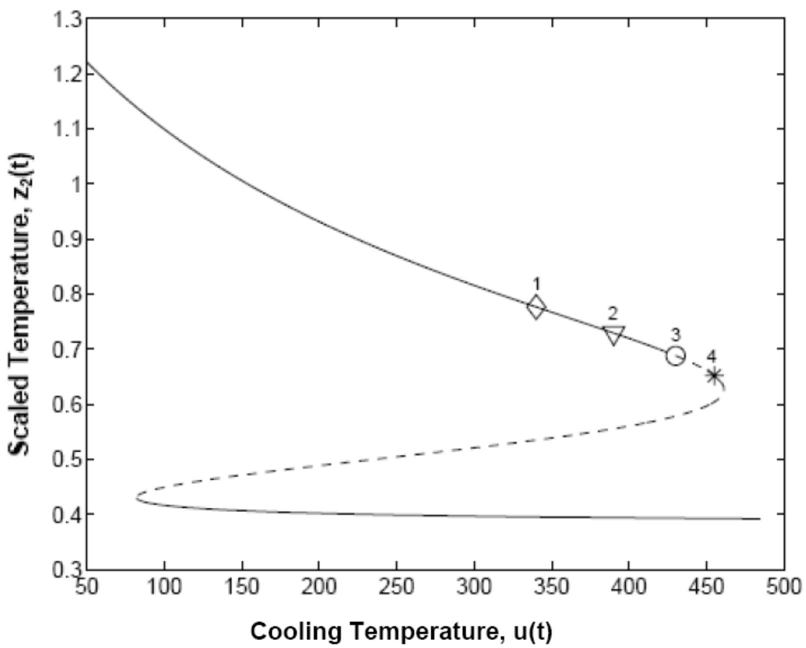
CSTR NMPC Example (Hicks and Ray)

$$\min_{v_{l|k}} \sum_{l=k}^{k+N-1} Q_c(z^c_{l|k})^2 + Q_t(z^t_{l|k})^2 + R(v_{l|k})^2$$

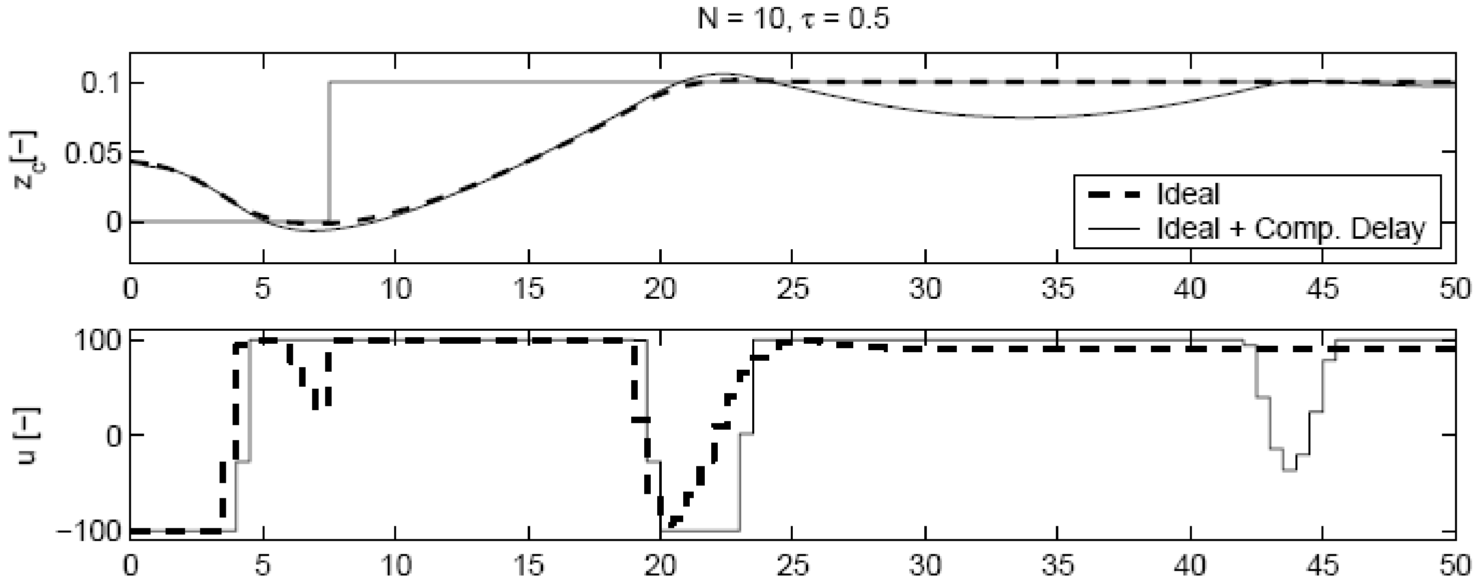
$$\begin{aligned}
\text{s.t.} \quad z^c_{l+1|k} &= \frac{1}{\theta}(1-(z^c_{l|k}+z^c_{ss})) - k_0 exp\left(-\frac{E_a}{z^t_{l|k}+z^t_{ss}}\right)(z^c_{l|k}+z^c_{ss}) \\
z^t_{l+1|k} &= \frac{1}{\theta}(t_f-(z^t_{l|k}+z^t_{ss})) + k_0 exp\left(-\frac{E_a}{z^t_{l|k}+z^t_{ss}}\right) z^c_{l|k} - \alpha(v+v_s s)((z^t_{l|k}+z^t_{ss})-t_c) \\
z^c_{k|k} &= x^c(k), \quad z^t_{k|k} = x^t(k) \\
z^c_{k+N|k} &= 0 \quad z^t_{k+N|k} = 0, \quad u^U \le v_{l|k} \le u^L.
\end{aligned}$$

Maintain unstable setpoint
Close to bound constraint
Final time constraint for stability (N is short)

Study effects of:
- Computational Delay
- Advanced Step NMPC
- Measurement Noise
- Model Mismatch

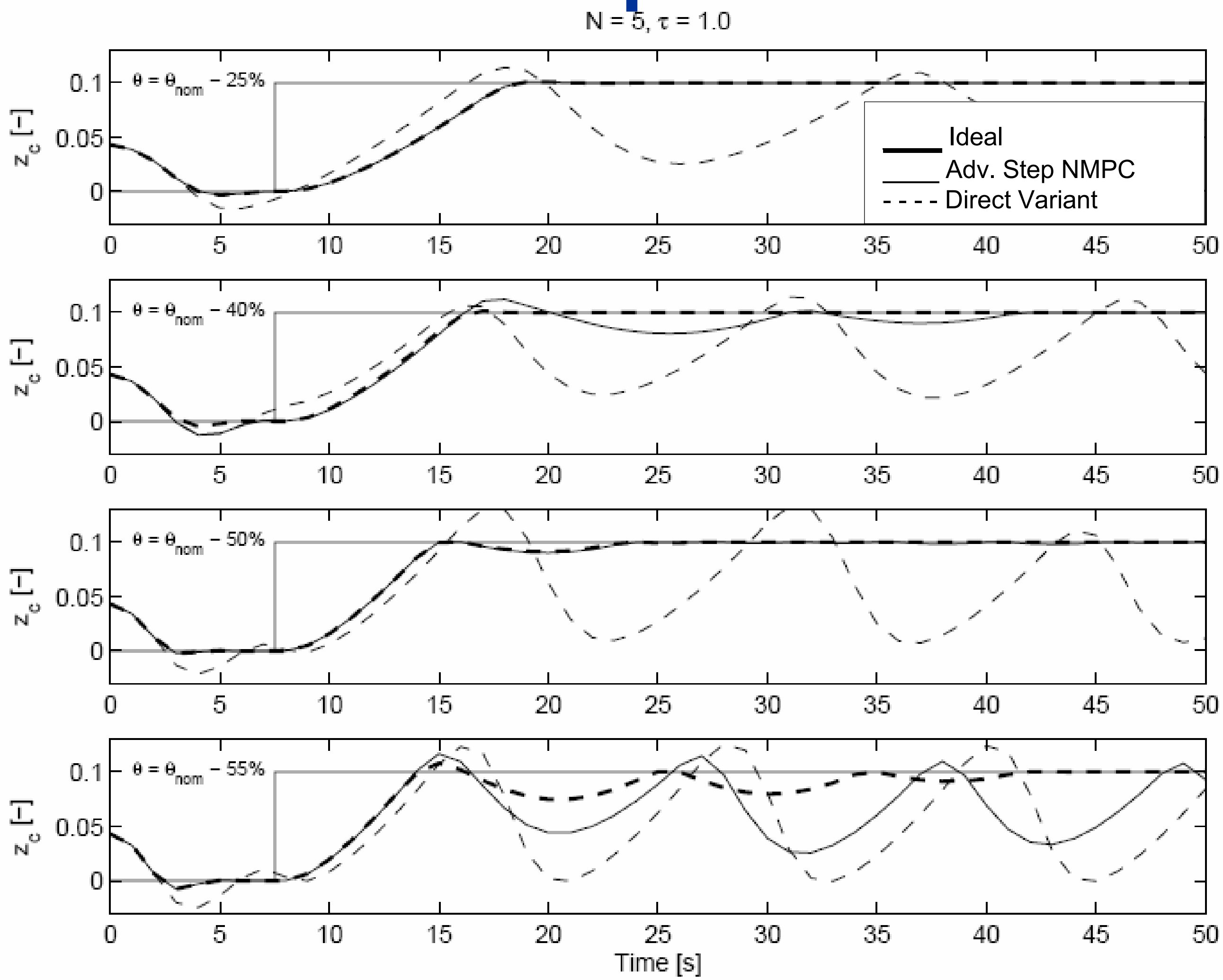


CSTR NMPC Example – Nominal Case



- NMPC applied with N = 10, τ = 0.5 sampling time
- Unstable steady state
- Steady state u close to upper bound
- Computational delay = 0.5, leads to instabilities
- Advanced Step Controller identical to ideal NMPC controller

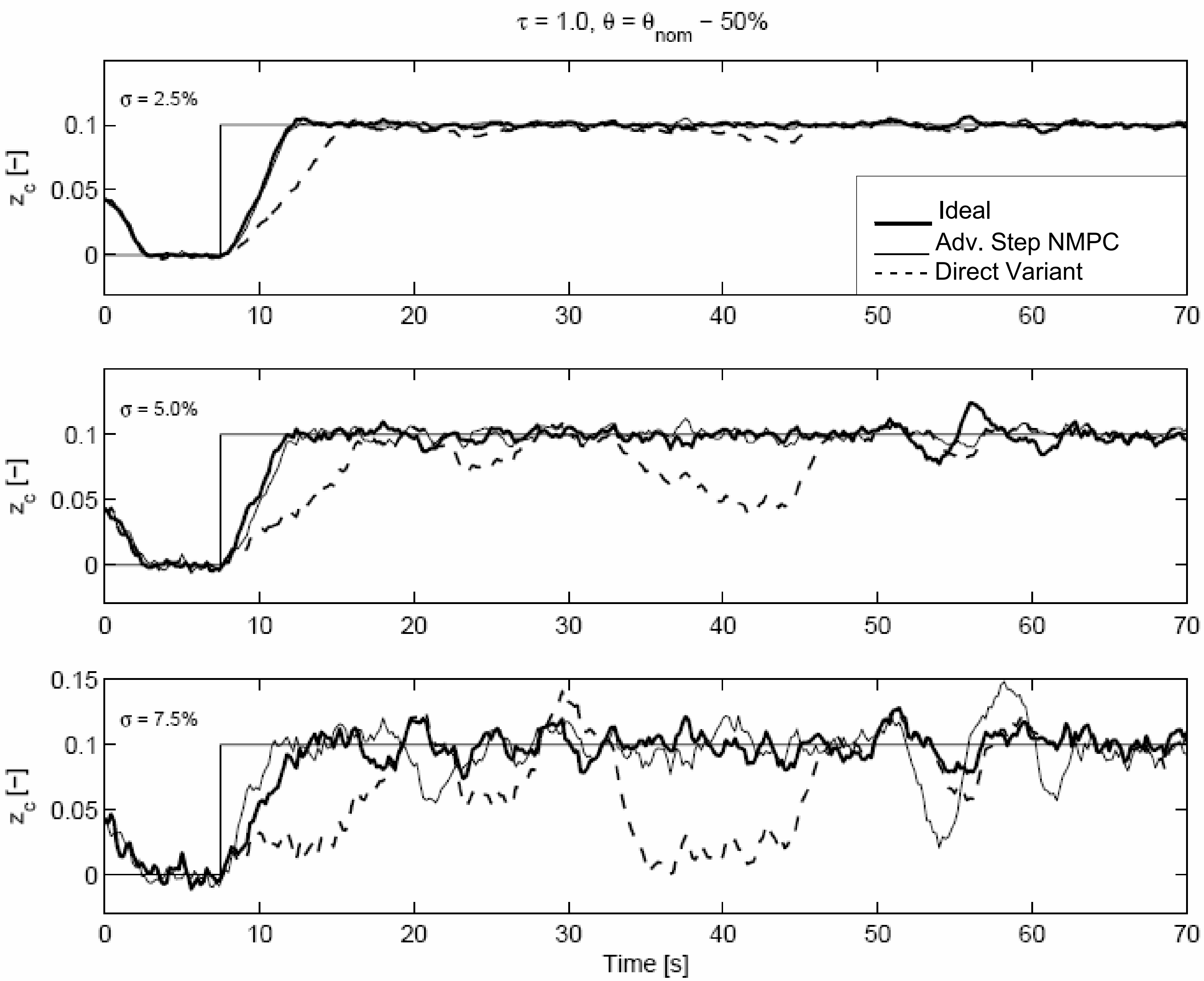
CSTR NMPC Example – Model Mismatch



Advanced Step NMPC not as robust as ideal - suboptimal selection of u(k)

Better than Direct Variant – due to better active set preservation

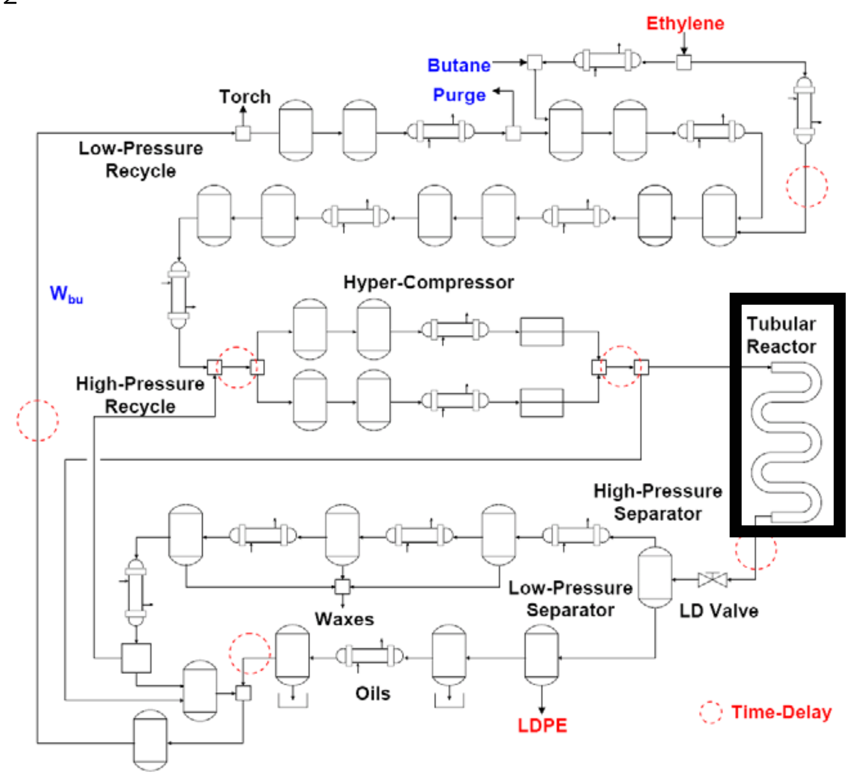
CSTR Example: Mismatch + Noise



Industrial Case Study – Grade Transition Control

Process Model: 289 ODEs, 100 AEs

$$
\begin{aligned}
\min \quad & \int_{t_\ell}^{t_\ell+t_p} \left(w_{C_4}(t) - w_{C_4}^r\right)^2 + \left(F_{C_4}(t) - F_{C_4}^r\right)^2 + \left(F_{pu}(t) - F_{pu}^r\right)^2 \\
\text{s.t.} \quad & \text{PDEs+ODEs} \\
& z(t = t_\ell) = \hat{z}(\ell) \\
& z_L \le z \le z_U \\
& y_L \le y \le y_U \\
& u_L \le u \le u_U
\end{aligned}
$$



Simultaneous Collocation-Based Approach

$$
\begin{aligned}
\min \quad & \sum_{m=0}^{M-1} \left\{ \sum_{k=0}^{K_m-1} \varphi_m^k \left(z_m^k, y_m^k, u_m^k, \pi_m, \Pi\right) \right\} \\
\text{s.t.} \quad & \\
z_m^{k+1} &= z_m^k + \mathrm{A}_m y_m^k \\
0 &= h_{m,k}\left(z_m^k, y_m^k, u_m^k, \pi_m, \Pi\right) \\
z_{m+1}^0 &= \bar{f}_m\left(z_m^{K_m}, y_m^{K_m}, u_m^{K_m}\right) \\
z_0^0 &= \hat{z}(\ell) = p \\
m &= 0, \ldots, M-1 \qquad k = 0, \ldots, K_m - 1
\end{aligned}
$$

27,135 constraints, 9630 LB & UB

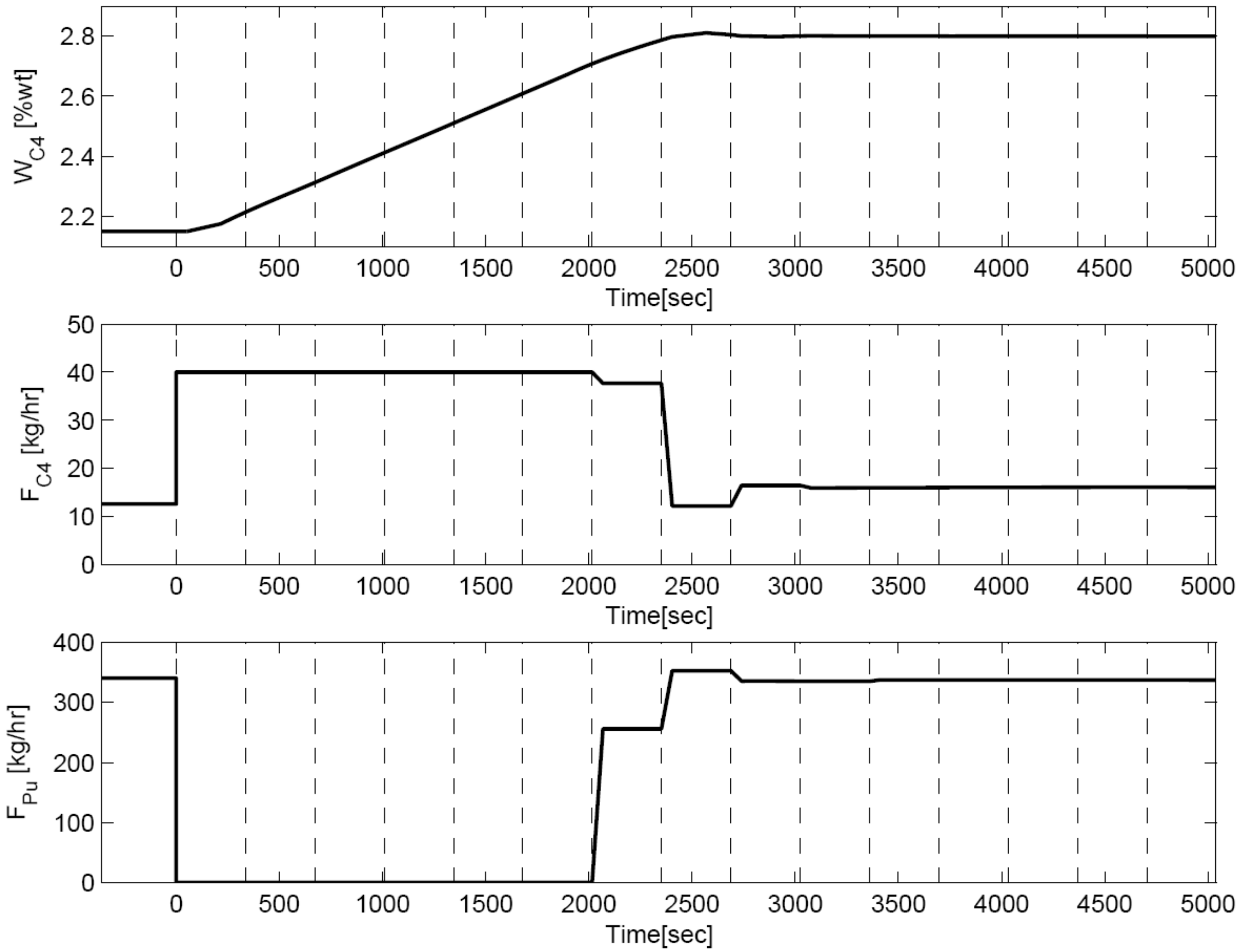
Off-line Solution with IPOPT

Algorithmic Step	CPU(s)
Full Solution (10 iterations)	351.5
Single Factorization of KKT Matrix	33.9
Step Computation (single backsolve)	0.94
Rest of Steps	0.12

Feedback Every 6 min

Nonlinear Model Predictive Control

- Optimal Feedback Policy → (On-line Computation 351 CPU s)

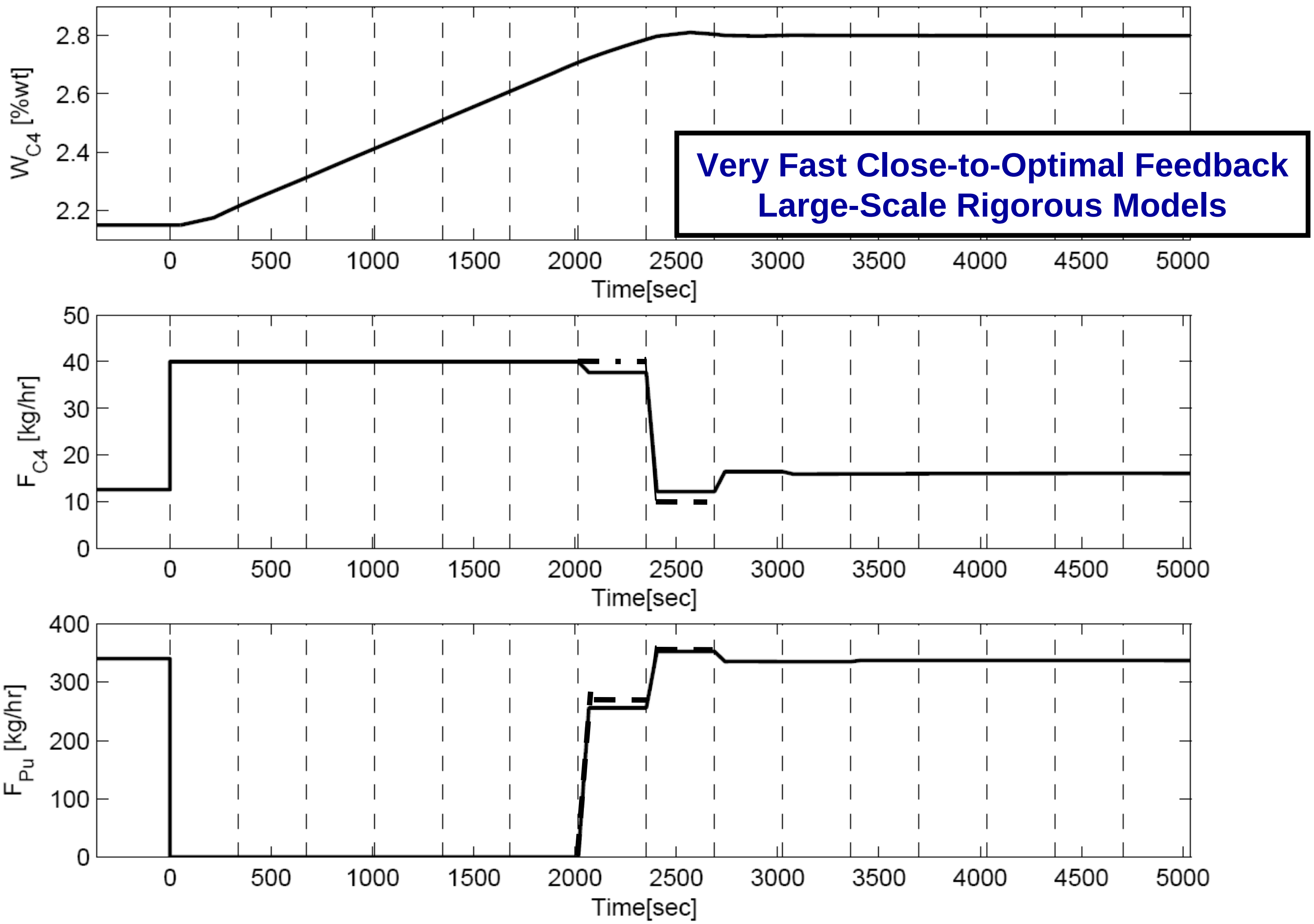


Ideal NMPC controller - computational delay not considered

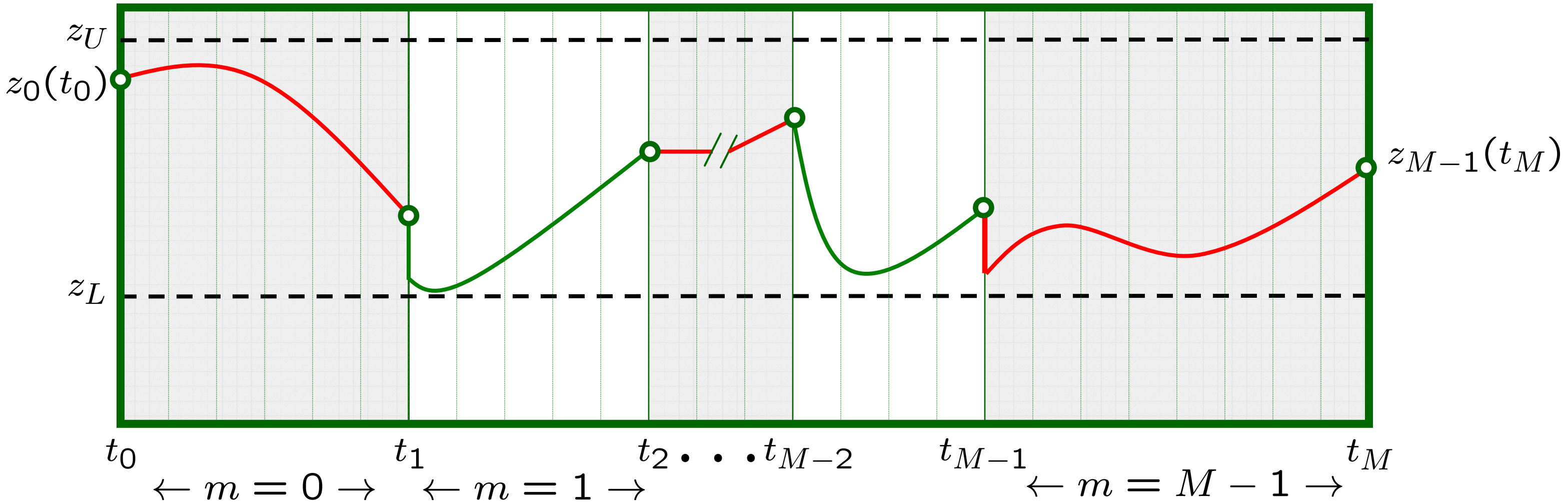
Time delays as disturbances in NMPC

Nonlinear Model Predictive Control

- Optimal Policy vs. NLP Sensitivity -Shifted → (On-line Computation 1.04 CPU s)



Future Work: Multi-Stage Dynamic Optimization



$$\min_{z_m(\cdot), y_m(\cdot), u_m(\cdot), \pi_m, \Pi, t_m} \sum_{m=0}^{M-1} \left\{ \int_{t_m}^{t_{m+1}} \varphi_m \left(z_m(t), y_m(t), u_m(t), \pi_m, \Pi \right) dt + E_m \left(x(t_{m+1}), y(t_{m+1}), \pi_m, \Pi \right) \right\}$$

DAE Model

Stage Transitions

Bounds

Path Constraints
Boundary Conditions

Multi-stage Optimization

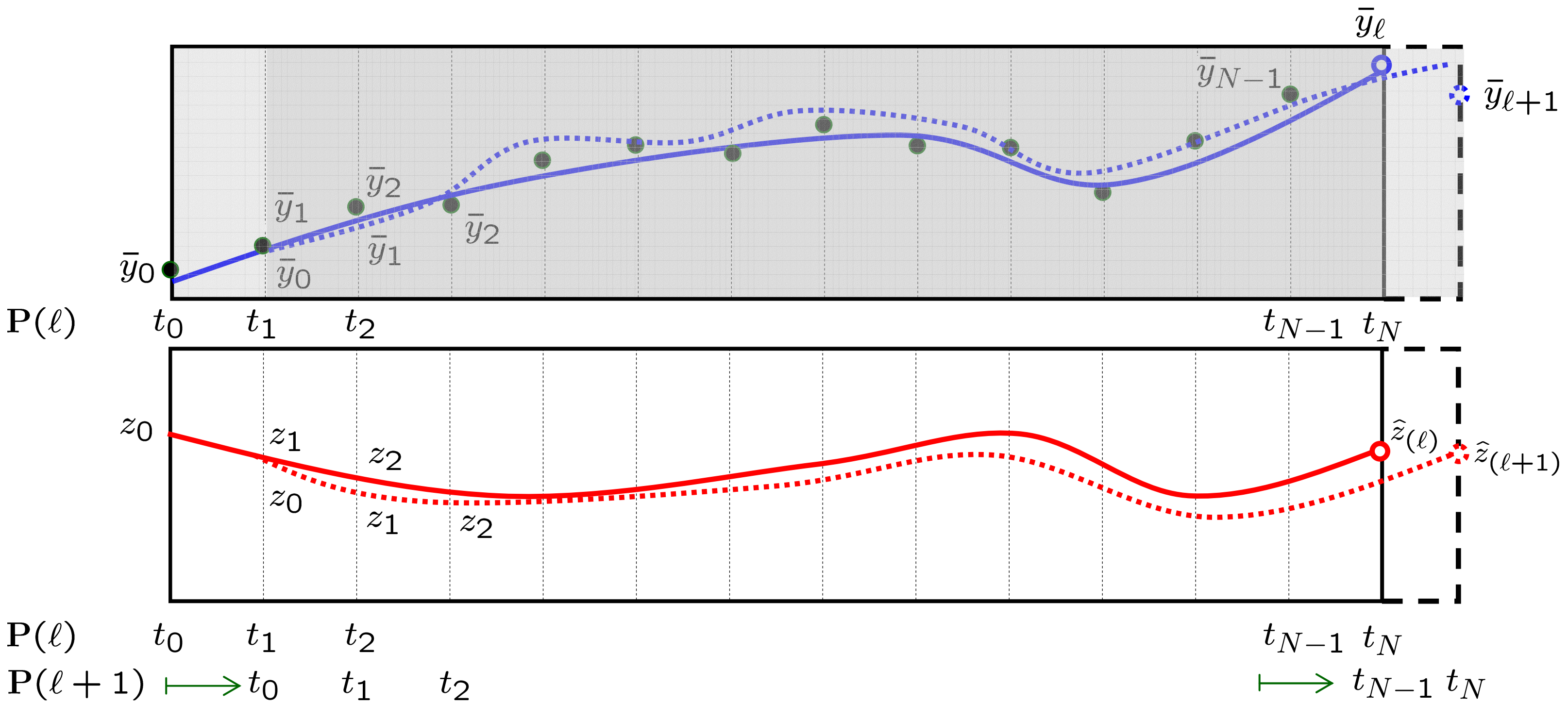
Determine Off-line policy

- Tracking problem for NMPC
- Nominal policy or incorporate uncertainty in conservative way (no recourse due to policy tracking)

Determine On-line policy

- Solve consistent economic objective through on-line DRTO (NMPC that incorporates multi-stage with long horizons)
- Exploit uncertainty through recourse on trajectory optimization
  - Retain stability and robustness
  - Incorporate feedforward measurements
- Requires state and parameter estimation from plant
  - Use nonlinear model
  - Adopt Moving Horizon Estimation Formulation

Moving Horizon Estimation



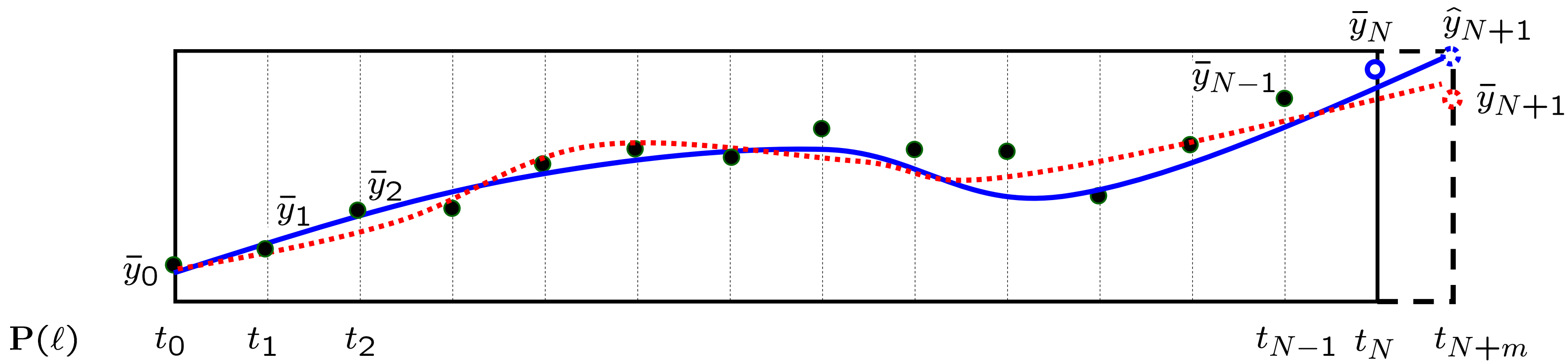
$$\min_{z_0, \pi} \quad \frac{1}{2}\left(\|z_0 - \bar{z}_0\|^2_{\mathbf{W}_z} + \|\pi - \bar{\pi}\|^2_{\mathbf{W}_\pi}\right) + \sum_{k=0}^{N} \frac{1}{2}\|y_k - \bar{y}_k\|^2_{\mathbf{W}_y}$$

$$\text{s.t.} \quad z_{k+1} = z_k + \mathbf{B}w_k, \quad k=0,\ldots,N-1$$

$$h(z_k, w_k, u_k, \pi) = 0, \quad k=0,\ldots,N-1$$

$$y_k - g(z_k) = 0, \quad k=0,\ldots,N$$

Real-Time Moving Horizon Estimation



$$\min_{z_0, \pi} \; \frac{1}{2}(\|z_0 - \bar{z}_0\|^2_{\mathbf{W}_z} + \|\pi - \bar{\pi}\|^2_{\mathbf{W}_\pi}) + \sum_{k=0}^{N} \frac{1}{2}\|y_k - \bar{y}_k\|^2_{\mathbf{W}_y}$$

s.t.

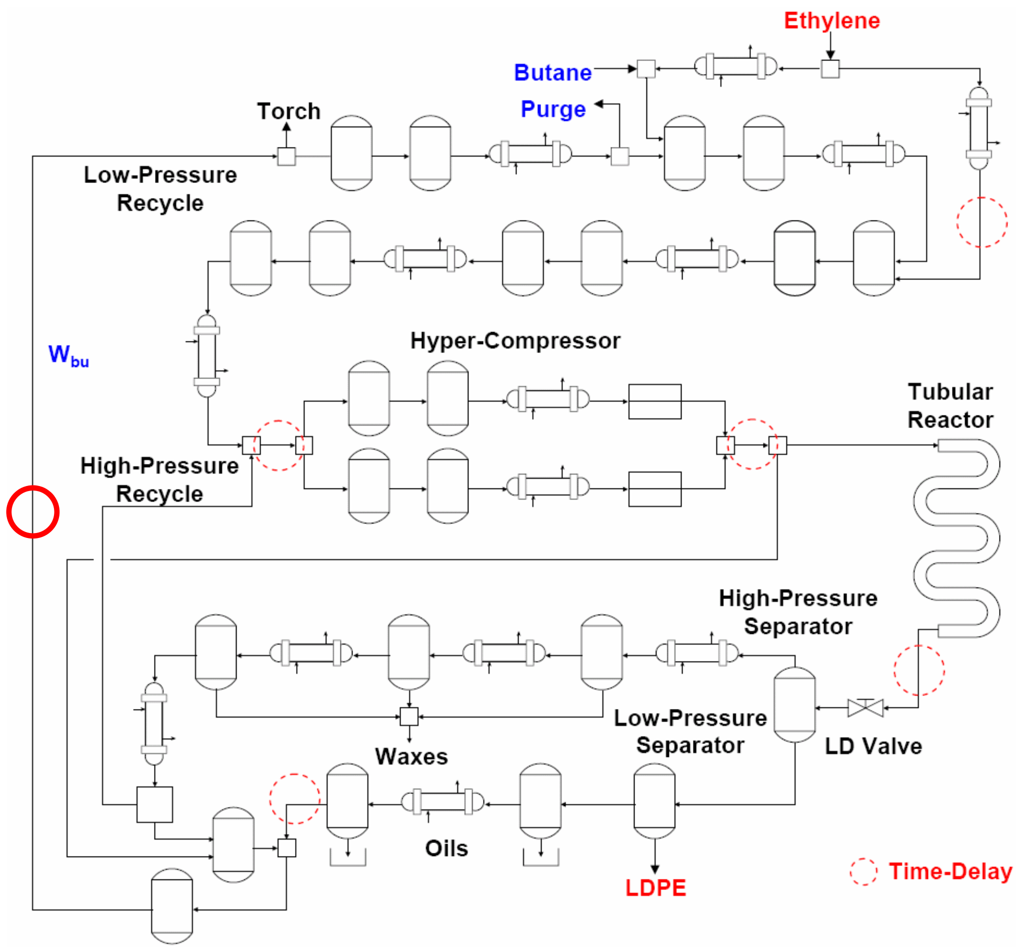
$$z_{k+1} = z_k + \mathrm{B}w_k, \quad {\scriptstyle k=0,\ldots,N+m-1}$$
$$h(z_k, w_k, u_k, \pi) = 0, \quad {\scriptstyle k=0,\ldots,N+m-1}$$
$$y_k - g(z_k) = 0, \quad {\scriptstyle k=0,\ldots,N+m}$$

$$\left.\begin{aligned} y_k &= \bar{y}_k - \hat{y}_k^* \\ \mathbf{W}_y(\Delta y_k - \Delta \hat{y}_k) + \sigma_{k-N} &= 0 \end{aligned}\right\} \; k = N+1, \ldots, N+j$$

$$\left[\begin{array}{c|c} \mathbf{K} & E_{s,j} \\ \hline E_j^T & 0 \end{array}\right] \left[\begin{array}{c} \Delta v \\ \hline \Delta p \end{array}\right] = \left[\begin{array}{c} 0 \\ \hline \bar{\mathbf{y}}_j - \hat{\mathbf{y}}_j^* \end{array}\right]$$

On-Line Calculation

Industrial Case Study



Single Measurement + Gaussian Noise
Composition of Recycle Gas

$$\min_{z_0,\pi} \; \tfrac{1}{2}(\|z_0-\bar{z}_0\|^2_{\mathbf{W}_z}+\|\pi-\bar{\pi}\|^2_{\mathbf{W}_\pi})+\sum_{k=0}^{N}\frac{1}{2}\|y_k-\bar{y}_k\|^2_{\mathbf{W}_y}$$

$$\text{s.t.} \quad z_{k+1}=z_k+\mathrm{B}w_k, \; {\scriptstyle k=0,\ldots,N-1}$$
$$h(z_k,w_k,u_k,\pi)=0, \; {\scriptstyle k=0,\ldots,N-1}$$
$$y_k-g(z_k)=0, \; {\scriptstyle k=0,\ldots,N}$$

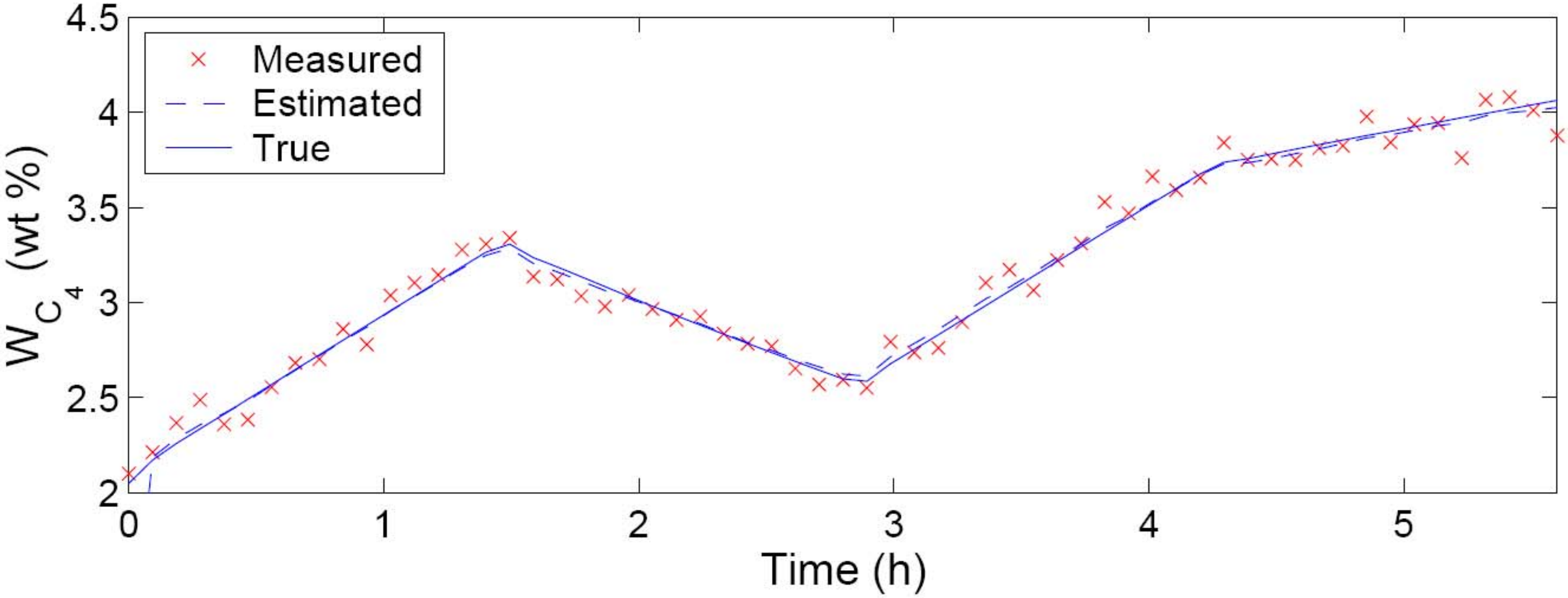
27,121 Constraints, 9330 Bounds
294 Degrees of Freedom

Real-Time Moving Horizon Estimation

Algorithmic Step	CPUs
Full Solution (6 iterations)	202.64
Single Factorization of KKT Matrix	33.77
Step Computation (single backsolve)	0.9-1.0
Rest of Steps	0.936

On-Line Calculation

Correct Inertia at Solution – System Observable



Summary

- RTO and MPC widely used for refineries, ethylene and, more recently, chemical plants
  - Inconsistency in models
  - Can lead to operating problems
- Off-line dynamic optimization is widely used
  - Polymer processes (especially grade transitions)
  - Batch processes
  - Periodic processes
- NMPC provides link for off-line and on-line optimization
  - Stability and robustness properties
  - Advanced step controller leads to very fast calculations
    - Analogous stability and robustness properties
    - On-line cost is negligible
- Multi-stage planning and on-line switches
  - Leads to exploitation of uncertainty (on-line recourse)
  - Avoids conservative performance
  - Update model with MHE
  - Evolve from regulatory NMPC to Large-scale DRTO

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