Optimization Strategies for NMPC: Properties and Algorithms

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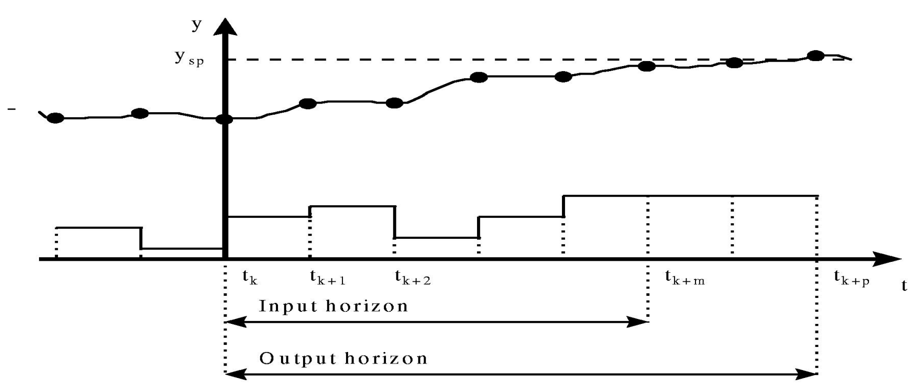
1

Nonlinear Model Predictive Control (NMPC)



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

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

$$z_0 = x(k)$$

Bounds and Constraints

2

MPC - Background

- Motivation: embed dynamic model in moving horizon framework to drive process to desired state
  - **Generic MIMO controller**
  - **Direct handling of input and output constraints**
  - Relatively slow time-scales in chemical processes

- Different Model types
  - Linear Models: Step Response (DMC) and State-space
  - Data-Driven Models: Neural Nets, Volterra Series
  - Hybrid Models: linear with binary variables, multi-models
  - **Nonlinear First Principle Models – direct link to off-line planning and optimization**

- Nonlinear MPC 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

3

MPC and NMPC

Optimization and Optimal Control
- Pontryagin (1959), Bryson and Ho (1969), Ray (1981), Sargent and coworkers (1970s),…

Model Predictive Control
- Evolution from LQ, Initial MPC (Kleinman, 1975; Kwon and Pearson, 1977).
- DMC (Cutler and Ramaker, 1979), QDMC (Garcia and Morshedi,1984) using step response models
- Concepts and Analysis: Allgöwer and coworkers (1989 -), Bordons and Camacho (2001), Rawlings and Mayne (2009), Grüne and Pannek (2011)
- LQ models ➔ solve quadratic programs on-line

Nonlinear NMPC – need to consider on-line solution of NLP.

4

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

5

Nonlinear Model Predictive Control – Air Separation Unit (Huang, B., 2011)

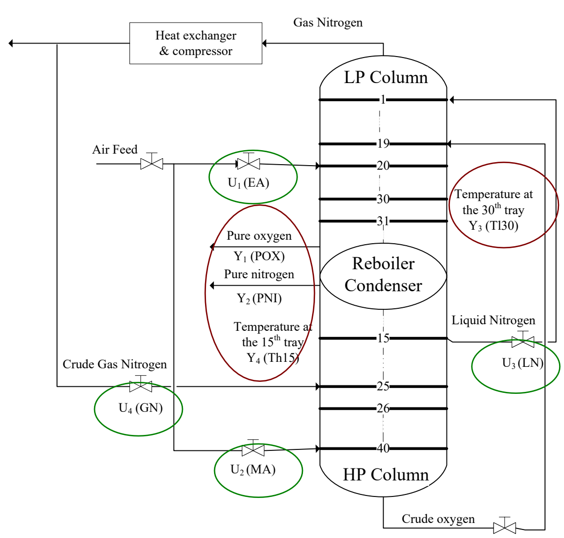
Objective: *minimize operating cost subject to demand specifications*

4 manipulated variables.
4 output variables.

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

DAEs: 1520

After Discretization:
Variables: 117,140
Constraints: 116,900



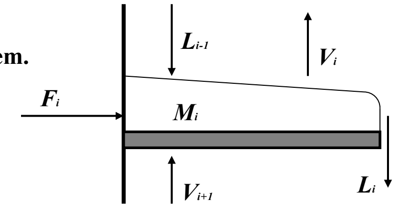
6

Case Study: Air Separation Unit

- **Mesh Equations for Distillation Column**

Assumption:

- **Vapor holdups are negligible.** **Index 2 system.**
- **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: $y_{i,j}p_i = \gamma_{i,j}x_{i,j}p^{sat}_{i,j}$

Summation: $1 = \sum_{j \in \mathrm{COMP}} y_{i,j}$

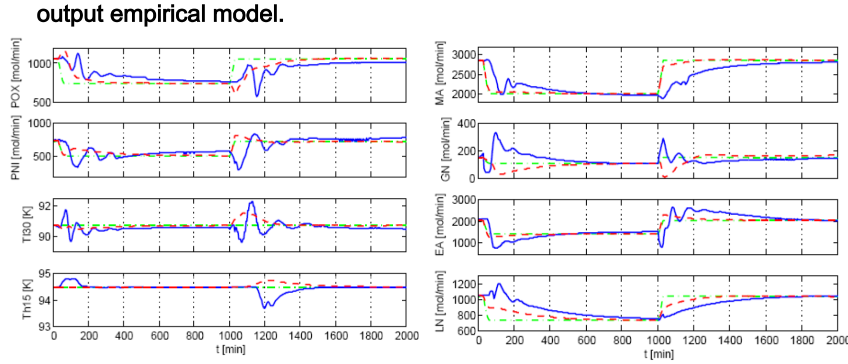
Hydrodynamics: $L_i = k_d M_i$

Reformulated index 1 system contains 320 ODEs, 1200 AEs.

7

ASU Nonlinear MPC - Case 1

t = 30-60 min, product rates are ramped down by 30%. t =1000-1030 min, they are ramped back. 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 NMPC profile.

All the tuning parameters are favored to the linear controller.
Horizon Solution Time: 200 CPUs, 6 IPOPT iters.

8

Finite Horizon Formulation for NMPC

$$J(x(k)) := \min_{v_l, z_l} \Phi(z_N) + \sum_{l=0}^{N-1} \psi(z_l, v_l)$$

$$\begin{aligned} s.t. \quad & z_{l+1} = f(z_l, v_l), l = 0, \ldots, N-1 \\ & z_0 = x(k) \\ & g(z_l) \le 0, l = 0, \ldots, N \\ & v_l \in U, l = 0, \ldots, N-1 \\ & z_N \in X_f \end{aligned}$$

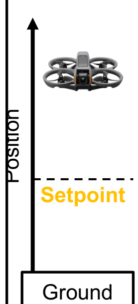
z_0 – initial value
$x(k)$ – measurement of state at t_k
ψ, Φ - (quadratic) stage and terminal costs
v_l - predicted manipulated variable
z_l - predicted state variable in finite horizon
z_N - terminal state, how defined?

How long is N to meet terminal conditions?

9

Determine horizon length and specify terminal conditions?

Drone hovering problem:

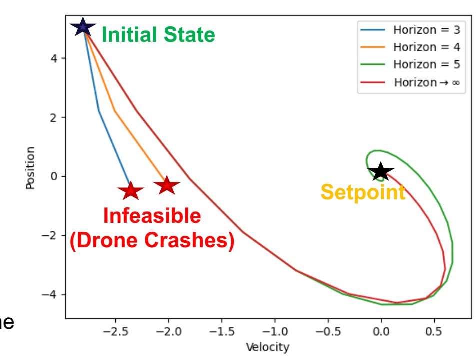


$$x_{k+1} = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} x_k + \begin{bmatrix} 0 \\ 1 \end{bmatrix} u_k$$

where $x_k = \begin{bmatrix} Position_k \\ Velocity_k \end{bmatrix}$;
$u_k = [acceleration_k]$

Constraints:
$\|x_k\|_\infty \le 5$; $\|u_k\|_\infty \le 0.5$ $\forall k \ge 0$

Tracking MPC Objective: Bring drone to new height (setpoint) without crashing to the floor.



Effect of N on closed-loop feasibility

Without terminal conditions in the formulation of the MPC (no terminal constraints or terminal cost, etc.), the closed-loop MPC is ***infeasible*** (the drone is descending too quickly and will crash) ***if*** the MPC's ***horizon is less than 5***.

10

10

Lyapunov stability of NMPC

- Nominal stability
  - Basic idea
    - Perfect model, no uncertainty: $x^+ = f(x, u)$
    - Remain bounded and eventually achieve desired state
- Definition: Lyapunov Property

A function V: $R^n \rightarrow R_{\geq 0}$ is a Lyapunov function for a system

$$x(k+1) \quad = \quad f(x(k), u(k))$$

if there exist a set X, three $\mathcal{K}_\infty$ functions α_1,α_2,α_3 such that

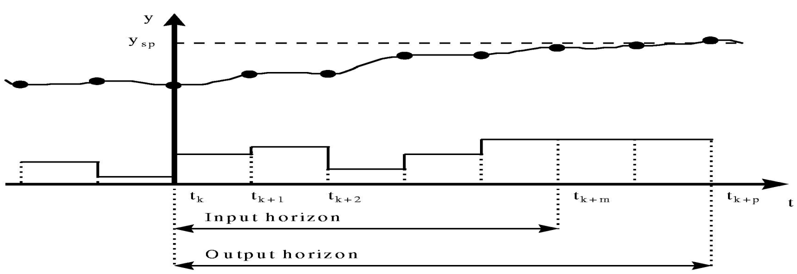
$$\alpha_1(|x|) \leq V(x) \leq \alpha_2(|x|)$$
$$V(f(x,u)) - V(x) \leq -\alpha_3(|x|)$$
$$\forall x \in X$$

- Can the objective function J_k serve as $V(x_k)$?

11

MPC Stability – Infinite Horizon

(Keerthi and Gilbert (1988)



$$J_k = \sum_{l=k}^{\infty} \| y(l) - y^{sp} \|^2_{Q^y} + \sum_{l=k}^{\infty} \| \boldsymbol{u}(l) - \boldsymbol{u}(l-1) \|^2_{Q^u}$$

$$J_k - J_{k+1} = \| y(k) - y^{sp} \|^2_{Q^y} + \| \boldsymbol{u}(k) - \boldsymbol{u}(k-1) \|^2_{Q^u}$$

$$J_1 \geq \sum_{k=1}^{\infty} (J_k - J_{k+1})$$

$$= \sum_{k=1}^{\infty} (\| y(k) - y^{sp} \|^2_{Q^y} + \| \boldsymbol{u}(k) - \boldsymbol{u}(k-1) \|^2_{Q^u})$$

$$\Rightarrow y(k) \rightarrow y_{sp}, u(k) \rightarrow u(k-1)$$

Nominal stability – perfect model

- m (input) = p (output)
- Based on discrete Lyapunov arguments with J(x) as Lyapunov function
- Infinite time horizon, ideal case
- Finite time horizon - need endpoint constraint ➔ $z(k+p)=0$
  <u>*Suffers End Effects*</u>
- Choice of terminal cost/constraints gives additional stability properties

12

Current Challenges of Nonlinear MPC Stability: Appropriate Terminal Conditions

Approaches	Advantages	Remaining Challenges	References
Sufficiently Long Horizon	•	• approach tationally expensive	Common Practice
Adaptive Horizon	• Computationally efficient	• A sufficiently long horizon is needed to initialize	Griffith et al. (2018), JPC
Terminal Cost	• Approximate an increasing horizon	• Nonlinear or constrained systems require long horizon (overly?) large terminal cost	Mayne et al. (2000), Pannocchia, Rawlings (2003) Faulwasser et al. (2018)
Terminal Constraint	• Simplified implementation	• Reachability? • Requires offline computation	Limon et al. (2006), IEEE TAC Griffith et al. (2018), JPC

$$V(x_k)\ (=J_k) =: \min_{v_l, z_l} \Phi(z_N) + \sum_{l=0}^{N-1} \psi(z_l, v_l)$$

$$s.t.\quad z_{l+1} = f(z_l, v_l),\ l = 0, \dots, N-1$$
$$z_0 = x(k)$$
$$g(z_l) \le 0,\ l = 0, \dots, N$$
$$v_l \in U,\ l = 0, \dots, N-1$$
$$z_N \in X_f$$

Main Objective: **Avoid all this!**
Develop an infinite horizon model predictive control using time transformation to enhance closed-loop stability and simplify implementation.

13

13

Infinite Horizon NMPC: Previous Work

- S. S. Keerthi and E.G. Gilbert (1988) - Classic NMPC paper with asymptotic stability properties for infinite horizon problems.
- P. Kunkel and O. Hagen (2000) – TPBVP with *exp* time transformation to determine optimal trajectories.
- L. Würth and W. Marquardt (2014, 2016) – *tanh* time transformation with sampling times determined by wavelet adaptations over entire horizon, ***open loop stable cases only***
- M. Muehlebach and R. D'Andrea (2016, 2017) - applied to LTI MPC with Galerkin approximations, applied to UAV with 100 Hz performance
- W. Greer and C. Sultan (2020) - divides LTI MPC problem into finite horizon part and infinite horizon part (with LQR control). Applied to very fast helicopter control.

14

14

Time Transformation: Infinite to Finite Horizon What's New?

Given continuous-time dynamic system:

$$\frac{dx}{dt} = f(x(t), u(t))$$

Time transformation - ***only*** applied to ***final sampling time*** in MPC horizon.

Converts infinite interval $t \in [0, \infty)$ to finite interval $\tau \in [0,1]$*

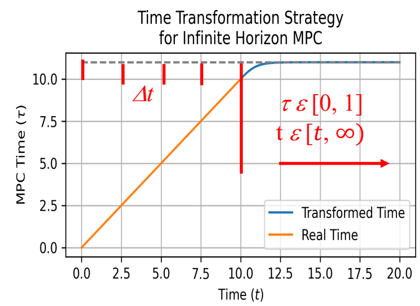
$$\tau = \tanh(\gamma t)$$

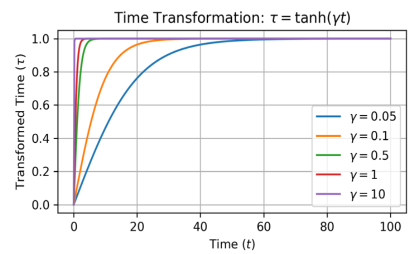
γ is the tuning parameter

Transformed continuous-time dynamic system:

$$\frac{dx}{d\tau} = \frac{f(x(\tau), u(\tau))}{\gamma(1-\tau^2)}; \quad x(t=0) = x(\tau=0)$$

*any transformation with bijective mapping in intervals can be applied





15

Infinite Horizon MPC with Time Transformation

Infinite horizon NMPC at $t_k = k\Delta t$:

$$V(x_k)(=J_k) = \min \sum_{l=0}^{N-1} \psi(z_l, v_l)\Delta t + \Phi(z_N)\,\Delta t$$
$$\text{s.t. } z_{l+1} = F(z_l, v_l),\ l = 0, \dots N-1$$
$$z_s = F(z_N, v)$$
$$z_0 = x_k$$
$$z_l \in \mathcal{X}, v_l \in \mathcal{U},\ l = 0, \dots N$$

Discretization for index-1 DAEs:

$$F(z_l, v_l) = z_l + \int_{t_k+\Delta t\, l}^{t_k+\Delta t\,(l+1)} f(z(t), v(t))dt$$

Last element, $t \in [t, \infty)$, $t = t_k + (N-1)\Delta t$:

$$F(z_N, v) = z_N + \int_t^{\infty} f(z(t), v(t))\, dt$$

Apply time transform $\tau = \tanh(\gamma(t - t))$:

$$F(z_N, v) = z_N + \int_0^1 \frac{f(z(\tau), v(\tau))}{\gamma(1-\tau^2)} d\tau$$

Terminal Cost $\Phi(z_N)$: designed to ***overestimate*** Riemann sum of last element (infinite length):

$$\Phi(z_N)\Delta t = \beta \int_t^{\infty} \psi(z(t), v(t))dt > \sum_{l=0}^{\infty} \boldsymbol{\psi(z_l, v_l)\Delta t}$$

where $\beta > \hat{\beta} \geq 1$ for some threshold $\hat{\beta}$.

➔ Leads to recursive feasibility for NMPC

Terminal constraints use (z_s, u_s) as boundary conditions which "pin down unstable modes"

➔ Allows unstable open-loop dynamics!

Additional assumptions: Weak controllability

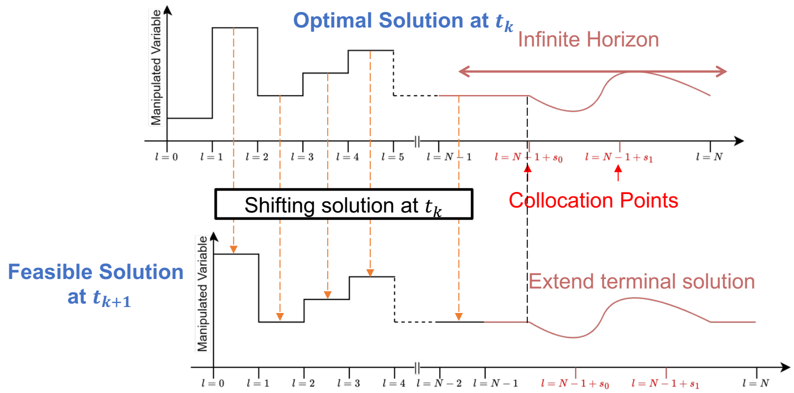
$$0 \leq \psi(x, u) \leq \alpha_1(\|x\|)$$
$$0 \leq \Phi(x) \leq \alpha_2(\|x\|)$$

$\alpha_1(\|x\|), \alpha_2(\|x\|)$ are $\mathcal{K}_\infty$ functions of $\|x\|$

16

16

Recursive Feasibility of Time-Transformed Infinite Horizon MPC



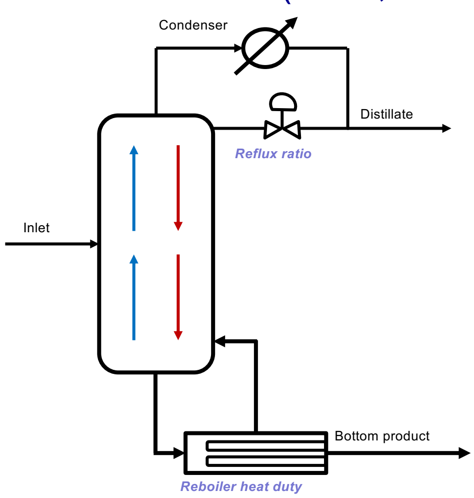
- Final Element Discretization: <u>Orthogonal collocation on finite elements</u>
- Zero-order hold: <u>not applied</u> for MVs in last (infinite) element
- To ensure recursive feasibility:
  - First collocation point of the last element fixed at previous time step solution
  - First collocation point must be larger than Δt, i.e., $tanh^{-1}(\gamma \Delta t) > \tau_{1,1}$
- **<u>Leads to Asymptotic Stability of NMPC</u>**

17

17

Case Study: Distillation Column

(Diehl, 2001; Lin, 2023)



Model description

1. High-purity distillation column
2. Separate methanol and n-propanol
3. Controls: Reboiler heat duty Q_r, Reflux ratio R
4. States: Mole fraction x, Liquid molar holdup M
5. *Differential-algebraic model with 84 differential and 503 algebraic equations.*

Control Task

Stage cost: maintain product mole fractions at 0.98.

18

18

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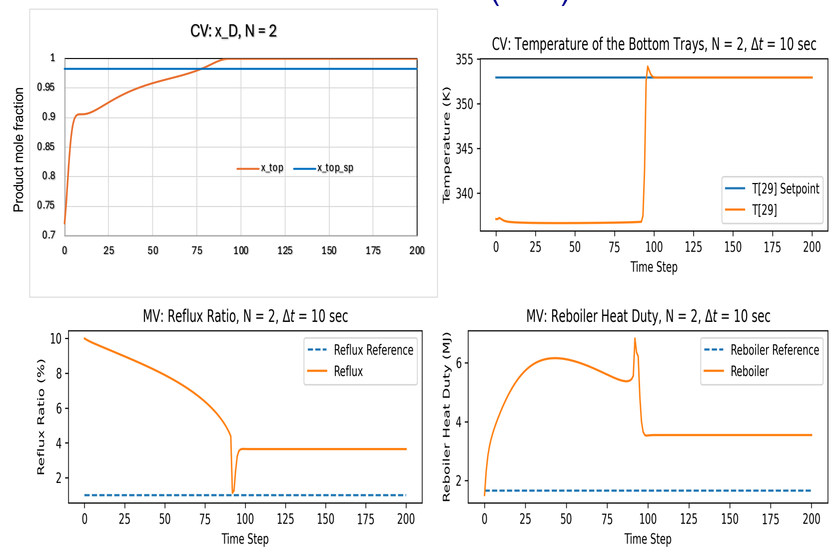
Distillation Column Case Study: Short Finite Prediction Horizon (N=2)



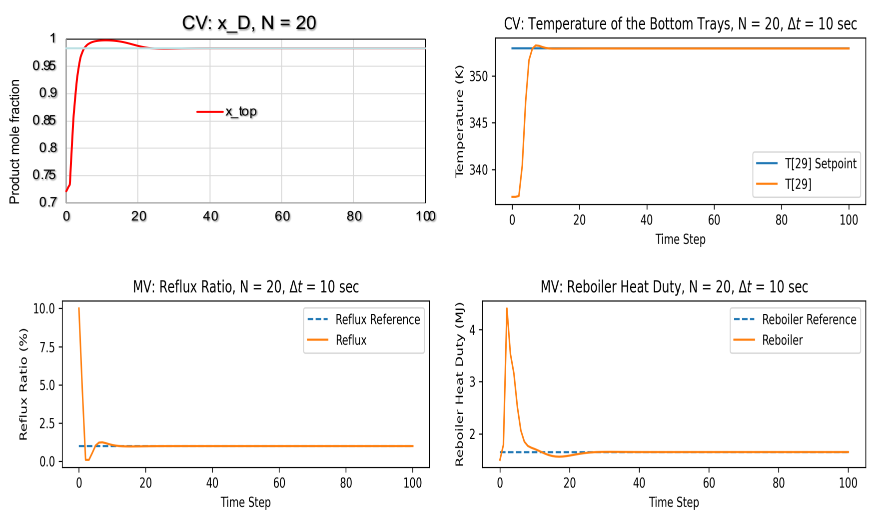
Tracking MPC - unable to achieve new setpoint if prediction horizon is too short

19

19

Chemical ENGINEERING

Distillation Column Case Study: Long Finite Prediction Horizon (N=20)

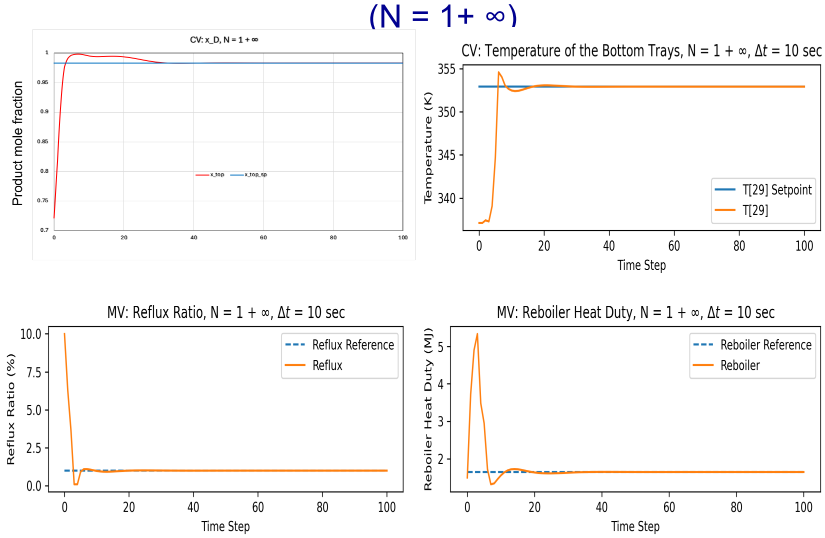


Extending horizon improves closed-loop stability - at much higher computational cost

20

20

Distillation Column Case Study: Short Finite Prediction Horizon with Augmented Infinite Horizon (N = 1+ ∞)



Infinite horizon MPC achieves closed-loop stability w/ two-element prediction horizon. First element is finite; second element is the time-transformed infinite horizon.

21

21

Lyapunov stability of NMPC

- Robust stability
  - Basic idea
    - Uncertainty in model: $x^+ = f(x, u, w)$, where w could be additive disturbance or uncertain parameters;
    - Remain stable in the presence of disturbances.

A function V(.) is called an ISS-Lyapunov function for a system

$$x(k+1) = f(x(k), u(k)) + q(x(k), w(k))$$

if there exist a set X, $\mathcal{K}_\infty$ functions α_1,α_2,α_3 and a $\mathcal{K}$ function σ such that

$$\alpha_1(|x|) \le V(x) \le \alpha_2(|x|)$$
$$V(f(x,u,w)) - V(x) \le -\alpha_3(|x|) + \sigma(|w|)$$
$$\forall x \in X,\ \forall \omega \in W$$

22

Proof of robust stability for NMPC

- Additional Assumptions:
  - $|q(x,w)| \leq |q(x,0)| + L_g|w|$
  - $|q(x,0)| \leq \rho\alpha_p(|x|)/\zeta$, *and* $|q(x,0)| \leq q_{max,}$ *where* $\rho \in (0,1)$.

$$
\begin{aligned}
& J(x(k+1)) - J(x(k)) \\
= \;& J(f(x(k),u(k))) - J(x(k)) + J(x(k+1)) - J(f(x(k),u(k))) \\
\leq \;& -\psi(x(k),u(k)) + L_J\,|q(x(k),w(k))| \\
\leq \;& -\alpha_p(|x(k)|) + L_J \frac{\rho}{\varsigma}\alpha_p(|x(k)|) + L_J L_g\,|w(k)| \\
\leq \;& (\rho-1)\alpha_p(|x(k)|) + \sigma\,|w(k)|
\end{aligned}
$$

23

Nonlinear programming (NLP) formulation for NMPC

$$
\begin{aligned}
J_N(x(k)) := \quad & \min_{v_l, z_l} \Phi(z_N) + \sum_{l=0}^{N-1} \psi(z_l, v_l) \\
s.t. \quad & z_{l+1} = f(z_l, v_l), l = 0, \ldots, N-1 \\
& z_0 = x(k) \\
& g(z_l) \leq 0, l = 0, \ldots, N \\
& v_l \in U, l = 0, \ldots, N-1
\end{aligned}
$$

z_0 – initial value

$x(k)$ – measurement of state at t_k

ψ, Φ - (quadratic) stage and terminal costs

v_l - predicted controlled variable

z_l - predicted manipulated variable

How will NLP formulation satisfy assumptions of NMPC stability properties?

24

Nonlinear Programming
(note notation change)

Problem: $Min_x\ f(x)$
s.t. $g(x) \leq 0$
$h(x) = 0$

where:
- $f(x)$ - scalar objective function
- x - n vector of variables
- $g(x)$ - inequality constraints, m vector
- $h(x)$ - meq equality constraints.

Sufficient Condition for Global Optimum
- $f(x)$ must be convex, and
- feasible region must be convex,
  i.e. $g(x)$ are all convex
  $h(x)$ are all linear

Except in special cases, there is no guarantee that a local optimum is global if sufficient conditions are violated.

25

Optimality conditions for local optimum

Necessary First Order Karush Kuhn - Tucker Conditions

$\nabla L(x^*, u, v) = \nabla f(x^*) + \nabla g(x^*)\, u + \nabla h(x^*)\, v = 0$
(Balance of Forces)
$u \geq 0$ (Inequalities act in only one direction)
$g(x^*) \leq 0$, $h(x^*) = 0$ (Feasibility)
$u_j\, g_j(x^*) = 0$ (Complementarity: either $g_j(x^*) = 0$ or $u_j = 0$)
u, v are "weights" for "forces," known as KKT multipliers, shadow prices, dual variables

"To guarantee that a local NLP solution satisfies KKT conditions, a constraint qualification is required. E.g., the Linear Independence Constraint Qualification (LICQ) requires active constraint gradients, $[\nabla g_A(x^*)\ \nabla h(x^*)]$, to be linearly independent. Also, under LICQ, KKT multipliers are uniquely determined."

Necessary (Sufficient) Second Order Conditions
- Positive curvature in "constraint" directions.
- $p^T \nabla^2 L(x^*)\, p \geq 0$ ($p^T \nabla^2 L(x^*)\, p > 0$)
  where p are the constrained directions: $\nabla h(x^*)^T p = 0$
  for $g_i(x^*)=0$, $\nabla g_i(x^*)^T p = 0$, for $u_i > 0$, $\nabla g_i(x^*)^T p \leq 0$, for $u_i = 0$

26

Constraint Qualifications

- Linear Independence Constraint Qualification (LICQ):
  $[\nabla h(x^*),\ \nabla g_j(x^*)]$ is linearly independent, where
  $j \,\varepsilon\, J=\{j|g_j(x^*)=0\}$

➔ *KKT multipliers (u,v) are bounded and unique.*

- Mangasarian-Fromovitz Constraint Qualification (MFCQ): $\nabla h(x^*)$ is linearly independent and exists y such that

$$\nabla h(x^*)^T y = 0,\ \nabla g_j(x^*)^T y < 0,\ j \,\varepsilon\, J$$

➔ *KKT multipliers (u,v) are bounded.*

- Constant Rank Constraint Qualification (CRCQ): all subsets of $[\nabla h(x),\ \nabla g_j(x)]$, $j \,\varepsilon\, J$ have constant rank in neighborhood of x^*

27

Second Order Conditions

(easy to satisfy for NMPC)

- Strong Second Order Sufficient Conditions (SSOSC): At KKT point with LICQ,

$$p^T\ \nabla_{xx}L\ (x^*, u^*, v^*)\ p\ > 0\ ,$$

  where $\nabla h(x^*)^T p = 0,\ \nabla g_j(x^*)^T p = 0,\ j \,\varepsilon\, J_+=\{j|g_j(x^*)=0,\ u_j^* > 0\}$

- Generalized Strong Second Order Sufficient Conditions (GSSOSC): At KKT point with MFCQ,

$$p^T\ \nabla_{xx}L\ (x^*, u^*, v^*)\ p\ > 0\ ,$$

for all u^*, v^* *satisfying KKT conditions where* $\nabla h(x^*)^T p = 0,$ $\nabla g_j(x^*)^T p = 0,\ j \,\varepsilon\, J_+$

- Strict Complementarity (SC): $u_j^* - g_j(x^*) > 0$, *for all* j.

28

NLP Sensitivity Properties

- Theorem (Kojima, 1985):
  - *If f(•, •), ψ(•, •), Ψ(•) are twice continuously differentiable and MFCQ and GSSOSC satisfied*
  - *Then exists $L_J > 0$ with $|J(p)-J(p_0)| \le L_J |p-p_0|$, where p is an input parameter*
- **MFCQ, GSSOSC** – Lipschitz continuity of objective functions and primal variables wrt *p*. (Kojima, 1985)
- MFCQ, GSSOSC, CRCQ → ($D_{\Delta p}x^*$) directional derivatives calculated with additional LP and QP steps (Ralph and Dempe, 1995)
- LICQ, SOSC, SC → (*dx*/dp*), derivatives can be calculated (Fiacco, 1983)

29

Reformulating NLP with Soft State Constraints

- Disturbances may lead to infeasibility of the NLP
- Dependent active sets can make system unstable under perturbations

- Formulation
  - If s* = 0, stability of the mixed constraint problem is same as original NLP

$$
\begin{aligned}
J(x(k)) := \quad & \min_{v_l, z_l} \Phi(z_N) + \rho s_N^T e + \sum_{l=0}^{N-1} \psi(z_l, v_l) + \sum_{l=0}^{N-1} \rho s_l^T e \\
s.t. \quad & z_{l+1} = f(z_l, v_l), l = 0, \ldots, N-1 \\
& z_0 = x(k) \\
& g(z_l) \le s_l, s_l \ge 0, l = 0, \ldots, N \\
& v_l \in U, l = 0, \ldots, N-1 \\
& e = [1,1,1,1 \ldots 1]^T
\end{aligned}
$$

If *g(z)* is linear, MFCQ and CRCQ are always satisfied at KKT point.

de Oliveira, N. M. C. and Biegler, L. T. [1998], 'Constraint handling and stability properties of model-predictive control', *Process Systems Engineering* ***40, 1138–1155.***

30

A Nonrobust NMPC Example (Grimm et al., 2004)

$$\min_{x,u} \; g(\mathbf{x}_{10}) + \rho_g s_N + \sum_{l=0}^{10-1} l(\mathbf{x},u) + \rho_l s_l$$

$$s.t. \quad x_1(k+1) = f_1(\mathbf{x},u) = \frac{-(x_1^2(k)+x_2^2(k))^{1/2}u(k) + x_1(k)}{1+(x_1^2(k)+x_2^2(k))u^2(k) - 2x_1(k)u(k)}$$

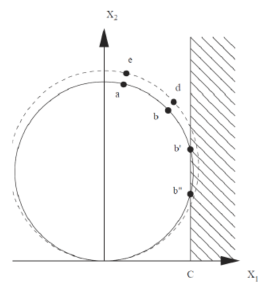
$$x_2(k+1) = f_2(\mathbf{x},u) = \frac{x_2(k)}{1+(x_1^2(k)+x_2^2(k))u^2(k) - 2x_1(k)u(k)}$$

$$x_{1,i} \le c + s_i, i = 0,\dots,N-1, |\mathbf{x}_N| \le \varepsilon + s_N$$

$$u \in [-1,1], \kappa_f(\mathbf{x}) = -1$$

$$g(x) = |\mathbf{x}| \cos^{-1} \frac{(x_2 - |\mathbf{x}|)(-|\mathbf{x}|)}{|\mathbf{x}|\sqrt{x_1^2 + (x_2 - |\mathbf{x}|)^2}}$$

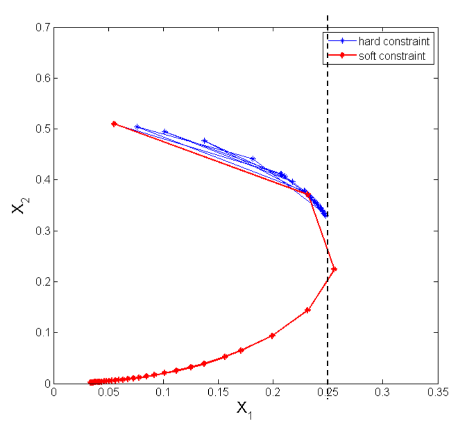
$$l(x,u) = |\mathbf{x}| \cos^{-1} \frac{x_1 f_1(\mathbf{x},-1) + (x_2 - |\mathbf{x}|)(f_2(\mathbf{x},-1) - |\mathbf{x}|)}{\sqrt{x_1^2 + (x_2 - |\mathbf{x}|)^2}\sqrt{f_1(\mathbf{x},-1)^2 + (f_2(\mathbf{x},-1) - |\mathbf{x}|)^2}}$$

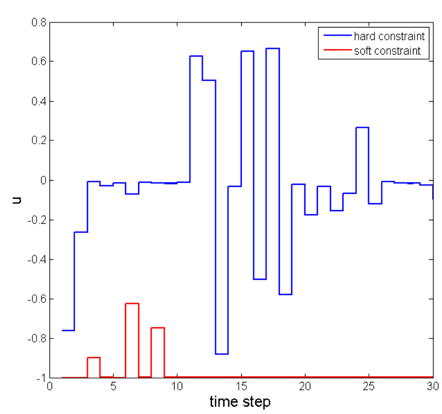


Grimm, G., Messina, M. J., Tuna, S. and Teel, A. [2004], 'Examples when nonlinear model predictive control is nonrobust', *Automatica* ***40, 523–533.***

31

Nonrobust NMPC Example

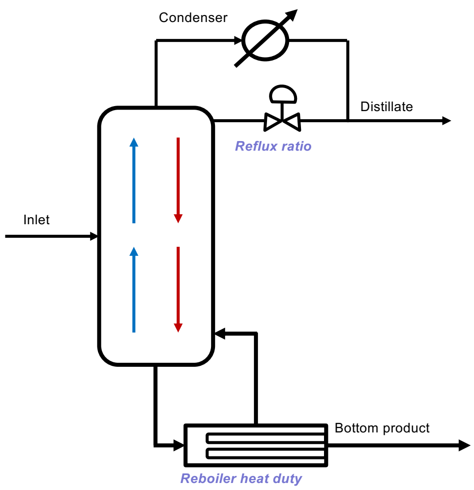




- The constraint $x_1 \le c$ prevents the trajectory from going beyond x_1=c
- Soft constraint allows the trajectory to go beyond x_1=c and then converge

32

Infinite Horizon: Distillation Column
(Diehl, 2001; Lin, 2023)



Model description

1. High-purity distillation column
2. Separate methanol and n-propanol
3. Controls: Reboiler heat duty Q_r, Reflux ratio R
4. States: Mole fraction x, Liquid molar holdup M
5. *Differential-algebraic model with 84 differential and 503 algebraic equations.*

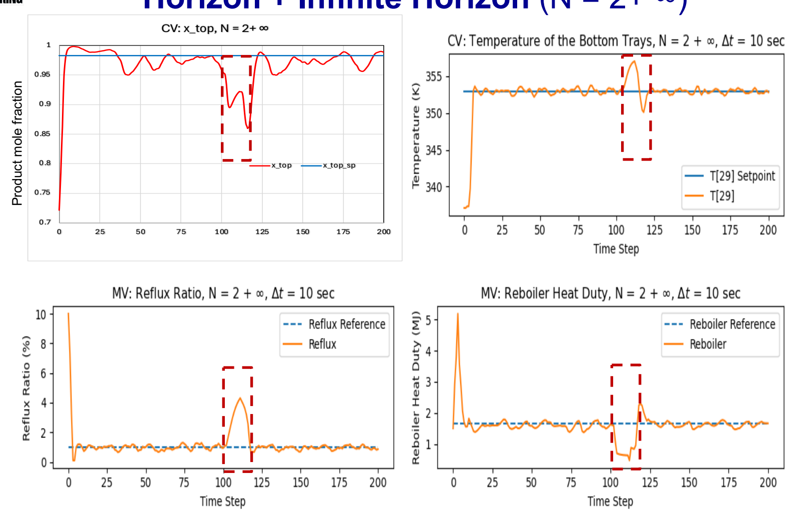
Control Task

Stage cost: maintain product mole fractions at 0.98.

33

33

Distillation Case w/ Disturbance : Short Prediction Horizon + Infinite Horizon (N = 2+ ∞)



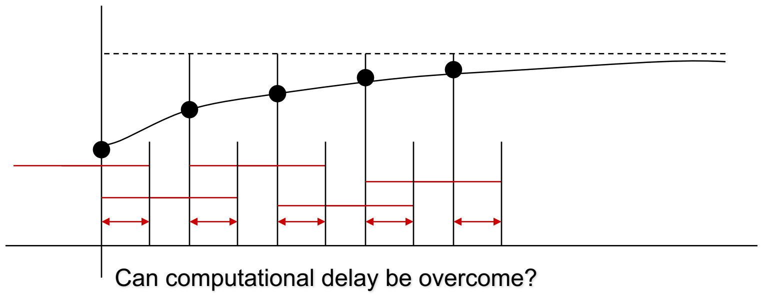
- Disturbances: The feed concentration fluctuates 10% around its nominal values. At the 100th time step, a large *unscheduled disturbance* drops feed concentration to 30% its nominal values for 10 time steps.
- Infinite horizon MPC keeps the CVs in bounded regions around the setpoints and is able to bring the system back from the unplanned large disturbance.

34

34

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



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

35

NMPC – Can we avoid on-line optimization?

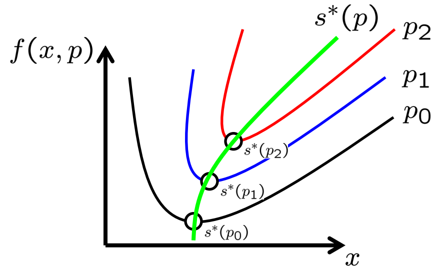
- **Divide Dynamic Optimization Problem** (Diehl, Bock et al., 2002)**:**
  - preparation, feedback response and transition stages
  - solve complete NLP in background (‘between’ sampling times) as part of preparation and transition stages
  - solve perturbed problem on-line
  - > two orders of magnitude reduction in on-line computation
- **Based on NLP sensitivity of z_0 for dynamic systems**
  - Extended to Collocation approach – Zavala et al. (2008, 2009)
  - Similar approach for MH State and Parameter Estimation – Zavala et al. (2008)
- **Stability Properties** (Zavala et al., 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

36

NLP Sensitivity

Parametric Program

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



Solution Triplet

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

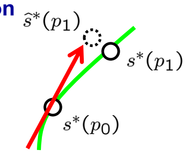
Optimality Conditions $\mathbf{P}(p)$

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

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

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

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



37

NLP Sensitivity with IPOPT (Pirnay, Lopez Negrete, B., 2011)

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

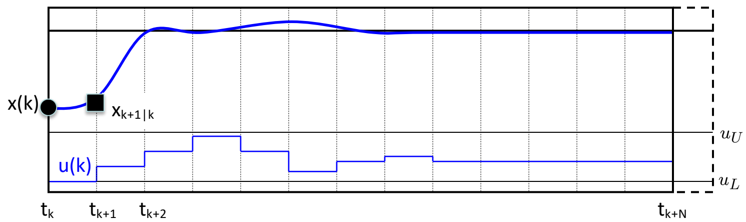
$$\begin{bmatrix} W(x_k,\lambda_k) & A(x_k) & -I \\ A(x_k)^T & 0 & 0 \\ V_k & 0 & X_k\end{bmatrix}$$

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

38

Advanced Step Nonlinear MPC (Zavala, B., 2009)

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



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

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

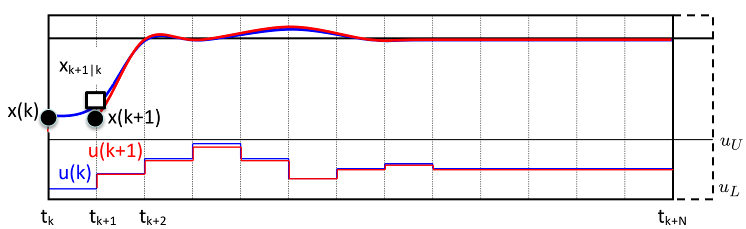
$$x_{l+1|k} = f(x_{l|k}, v_{l|k}), \quad l = k+1, \ldots k+N-1$$

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

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

Advanced Step Nonlinear MPC (Zavala, B., 2009)

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

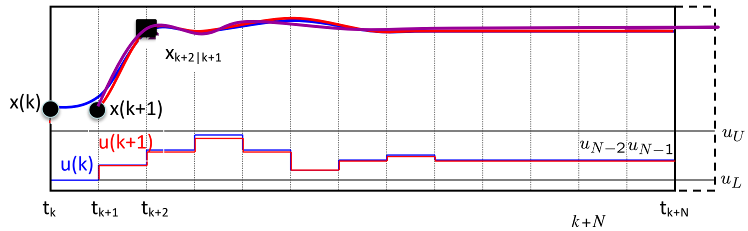


$$\begin{bmatrix} W_k & A_k & -I \\ A_k^T & 0 & 0 \\ Z_k & 0 & X_k \end{bmatrix} \begin{bmatrix} \Delta \mathbf{x} \\ \Delta \lambda \\ \Delta z \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ x_{k+1|k} - x(k+1) \\ 0 \end{bmatrix}$$

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

Advanced Step Nonlinear MPC (Zavala, B., 2009)

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



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

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

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

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

Solve NLP(k) in 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})

41

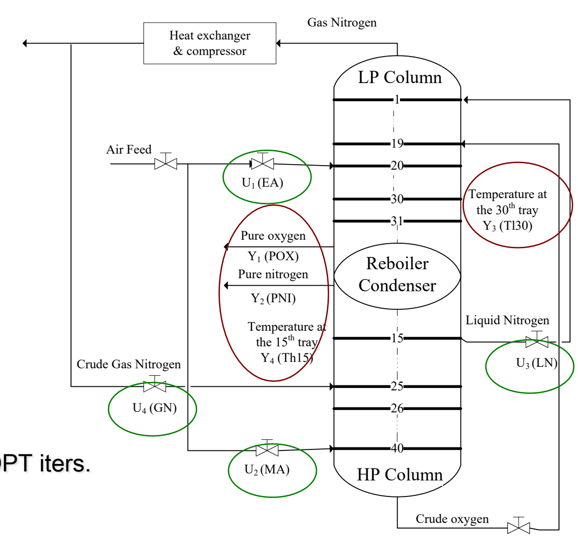
Nonlinear Model Predictive Control – Air Separation Unit (Huang, B., 2011)

Objective: *minimize operating cost subject to demand specifications*

4 manipulated variables.
4 output variables.

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

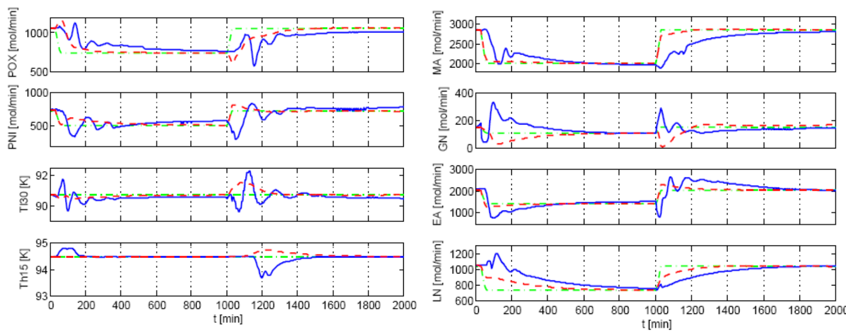
DAEs: 1520
Variables: 117,140
Constraints: 116,900
Background: 200 CPUs, 6 IPOPT iters.
Online: 1 CPUs



42

ASU Nonlinear MPC - Case 1

t = 30-60 min, product rates are ramped down by 30%. t =1000-1030 min, they are ramped back. asNMPC 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 NMPC profile.

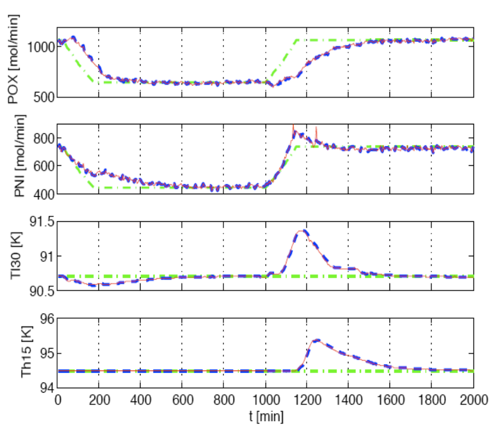
All the tuning parameters are favored to the linear controller.

43

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.



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

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.

44

asNMPC: Concepts and Properties

- Interpretation: Fast linear MPC controller using *linearization of nonlinear model at previous step*.
- NLP solved between samples, "instantaneous" sensitivity update at sampling time
- On-line computation 2-3 orders of magnitude faster;
  - ➔ Computational delay virtually eliminated
- Second order errors compared to ideal NMPC
  - ➔ Nominal and ISS stability (Zavala, B., 2009)
- ISpS stability when coupled with embedded state estimators (Huang, Patwardhan, B., 2009a,b, 2010a-c, 2012)

45

On-Line Optimization with Uncertainty

Jung, Nie, Lee, LTB (2015); Jang, Lee, LTB (2016), Holtorf, Mitsos, LTB (2018)

D-RTO through NMPC

- Detailed dynamic model
- Economic NMPC (t_f)
- Key Issues
  - Uncertainty-tolerant optimization formulations
  - Time critical optimization (large-scale NLP)
  - Accelerate with advanced step (sensitivity-based) strategies

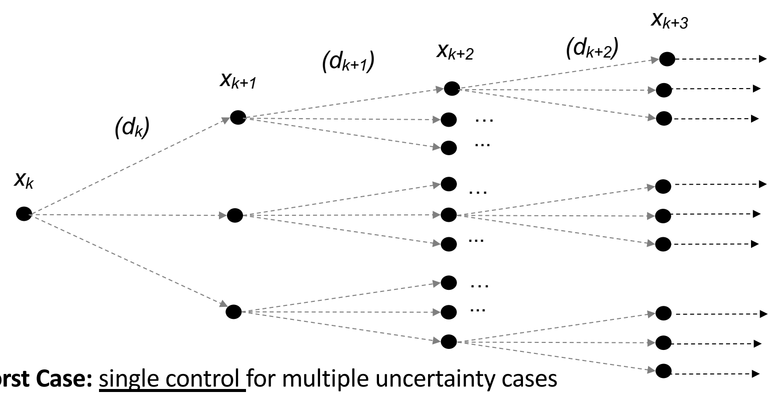
Incorporation of Uncertainty

- From states, parameters, measurement noise
- State estimation with expanding batch horizon, …
- NMPC with shrinking batch horizon...
- Off-line multi-model approach (Bonvin et al., 2003)
- Stochastic, Multi-stage Programs within NMPC for disturbances with delayed realization (**Lucia, Engell**, 2014; Puschke, Mitsos, 2018)

46

Handling of Uncertain Dynamic Systems? Multi-model Approach – Worst Case Control (Bonvin et al., 2003)

Scenario branching: effect of uncertainty while optimizing control input



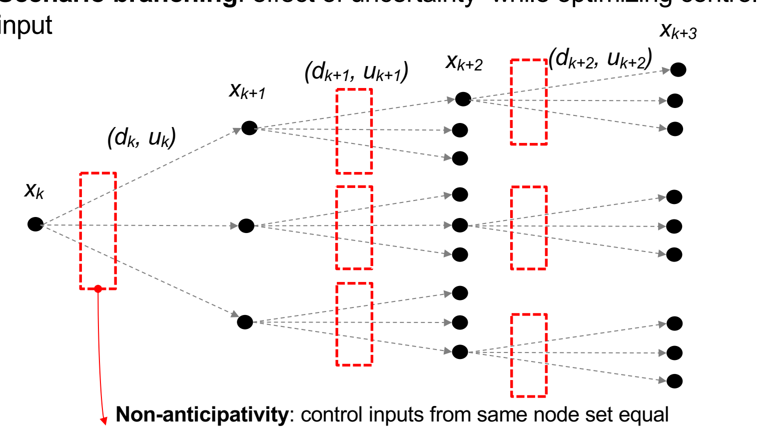
- **Worst Case:** single control for multiple uncertainty cases
- Large-scale, highly constrained NLP
- Feasible, but conservative performance

47

Handling of Uncertain Dynamic Systems?

==> Non-conservative multi-stage NMPC

Scenario branching: effect of uncertainty while optimizing control input



Non-anticipativity: control inputs from same node set equal until uncertainty is realized

Lucia, Engell et al., *J. Process Control*, 2013

48

Multi-stage NMPC: Polyol Case Study

(Holtorf, Mitsos, LTB, 2018)

$$\min_{x^j_{k+1}, u^j_k, k=K,\dots,N_T-1, j=1,\dots,N_S(k)} \sum_{k=K}^{N_T-1} \left\{ \max_j \frac{\mathcal{L}(x^j_{k+1}, u^j_k)}{N_S(k)} \right\}$$

k : time index

j : scenario index

$\mathcal{L}(x^j_{k+1}, u^j_k) = \Delta t_b \ (+\mu P)$ **Economic cost function (processing time)**

$x^j_{k+1} = f\left(x^{p(j)}_k, u^j_k, d^j_k\right)$ Nonlinear dynamic model

$h(x^j_k, u^j_k, d^j_k) \leq 0$ Feasible domain

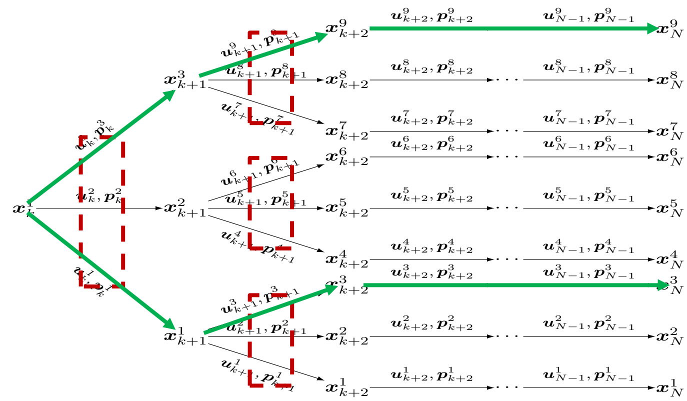
$u^j_k = u^l_k$ if $x^{p(j)}_k = x^{p(l)}_k$ Non-anticipativity constraints

- Assume uncertainties have monotonic effect on inequality constraints
- Identify worst case scenarios *a priori*
- Eliminate remaining scenarios

==> **Problem scales linearly with constraints, not exponentially with disturbances**

49

msNMPC- Adaptive Scenario Generation

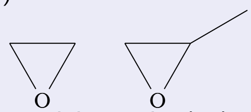


- Non-anticipativity constraints: $\boldsymbol{p_k}$ unknown at *k*, resolved at *k+1*
- **Much smaller (msNMPC):** $(\boldsymbol{n_{pc}} + \boldsymbol{n_e} + \mathbf{1})(\boldsymbol{n_{pc}} + \mathbf{1})^{\boldsymbol{N_R}}$ **scenarios**
  - Scales with path ($\boldsymbol{n_{pc}}$) and endpoint ($\boldsymbol{n_e}$) constraints, not $\boldsymbol{n_p}$
  - Scenarios updated with every NMPC shrinking horizon

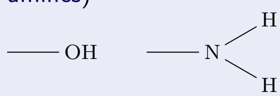
50

Dynamic Real-time Optimization Semi-Batch Polymer Process

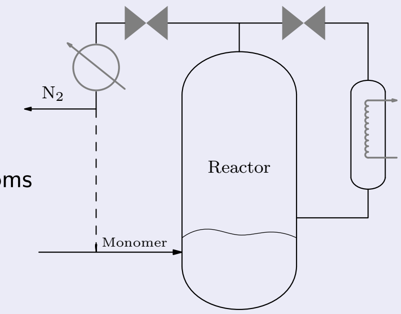
- Key ingredients
  - Epoxides (ethylene oxide (EO), propylene oxide (PO))



  - Molecules containing active hydrogen atoms (alcohols, amines)



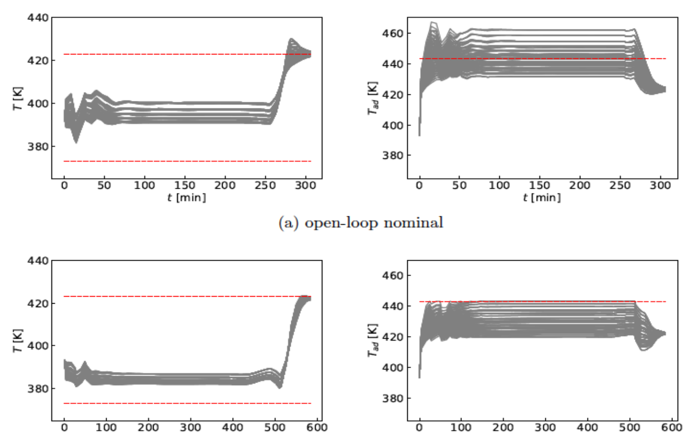
  - A basic catalyst (KOH)



- Basic procedures
  - Starters are first mixed with catalyst in the liquid phase
  - Alkylene oxides in the liquid phase are fed in controlled rates
  - The reactor temperature is controlled by the heat exchanger
  - Allowed maximum reactor pressure guarded by the vent system control valve

51

Nominal Trajectory: High Potential for Constraint Violations



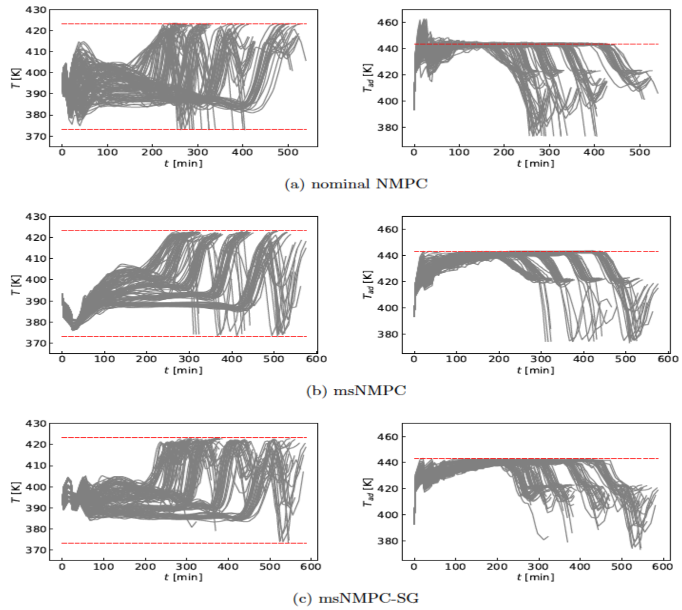
(a) open-loop nominal

(b) open-loop multi-model

Improved by Worst Case Multi-model Approach, but with High Conservatism

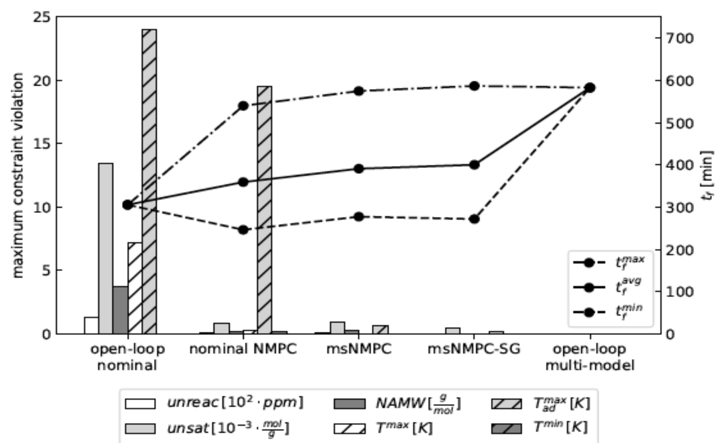
52

Infeasibilities Resolved with msNMPC & State Estimation



53

NMPC Strategies with (MHE) State Estimation



Computational Performance

- Nominal NMPC: 99% of problems solved **< 1 s**
- msNMPC: 99% of problems solved **< 10s**
- msNMPC-SG: 99% of problems solved **< 6s**
- **Implementable On-line**

54

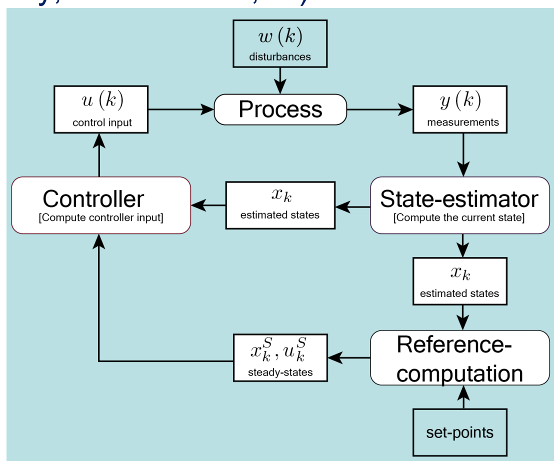
On-line Nonlinear State Estimation and Control Pyomo Optimization Framework

(D. Thierry, B. Nicholson, B.)

- Pyomo.DAE - dynamic system with DAE model

$$\frac{dx}{dt} = F(x,y,u,w)$$
$$0 = G(x,y,u,w)$$
$$\downarrow$$
$$x(k+1) = f\big(x(k),u(k),w(k)\big)$$
$$y(k) = h\big(x(k)\big)$$

- State Estimator: Moving Horizon Estimation (MHE)
- Controller: Nonlinear Model Predictive Control (NMPC)

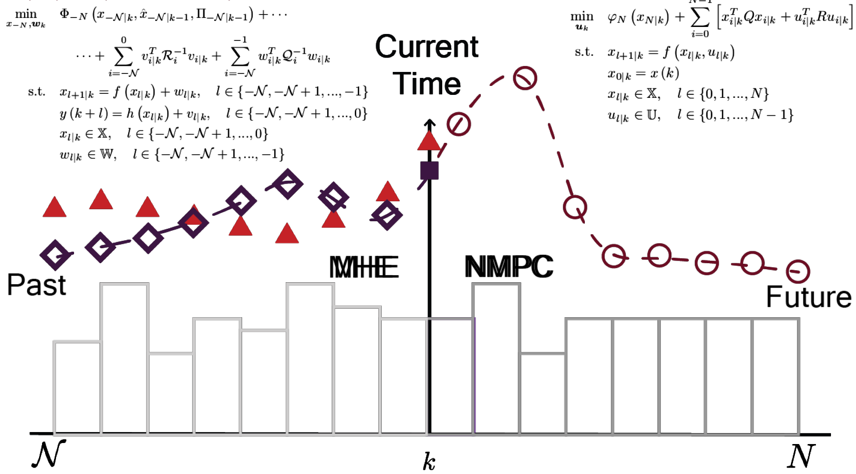


55

Model-based Estimation (MHE) and Control (NMPC)

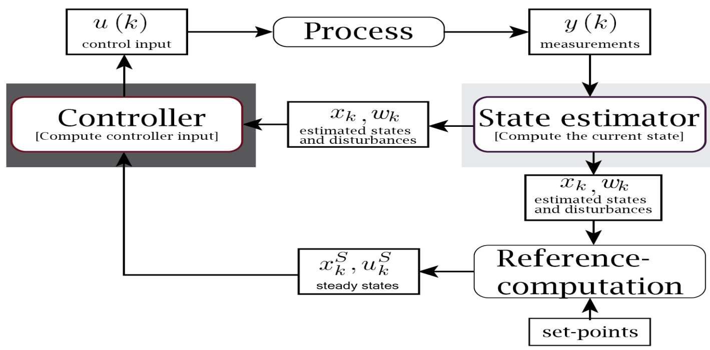
$$\mathcal{M}\left(\Pi_{-N|k-1}, \hat{x}_{-N|k-1}, y(k), ..., y(k-\mathcal{N})\right):$$
$$\begin{aligned} \min_{x_{-N}, \boldsymbol{w}_k} \quad & \Phi_{-N}\left(x_{-\mathcal{N}|k}, \hat{x}_{-\mathcal{N}|k-1}, \Pi_{-\mathcal{N}|k-1}\right) + \cdots \\ & \cdots + \sum_{i=-\mathcal{N}}^{0} v_{i|k}^T \mathcal{R}_i^{-1} v_{i|k} + \sum_{i=-\mathcal{N}}^{-1} w_{i|k}^T \mathcal{Q}_i^{-1} w_{i|k} \\ \text{s.t.} \quad & x_{l+1|k} = f\left(x_{l|k}\right) + w_{l|k}, \quad l \in \{-\mathcal{N}, -\mathcal{N}+1, ..., -1\} \\ & y(k+l) = h\left(x_{l|k}\right) + v_{l|k}, \quad l \in \{-\mathcal{N}, -\mathcal{N}+1, ..., 0\} \\ & x_{l|k} \in \mathbb{X}, \quad l \in \{-\mathcal{N}, -\mathcal{N}+1, ..., 0\} \\ & w_{l|k} \in \mathbb{W}, \quad l \in \{-\mathcal{N}, -\mathcal{N}+1, ..., -1\} \end{aligned}$$

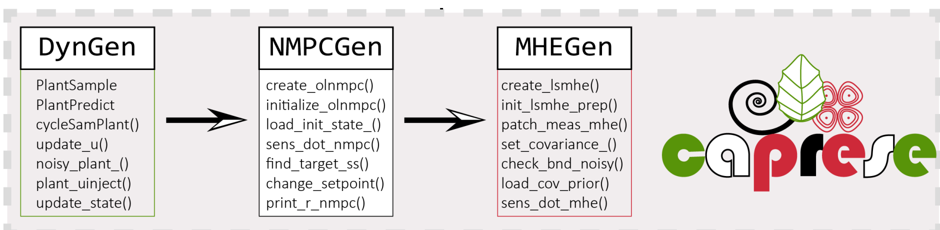
$$\mathcal{P}(x(k)):$$
$$\begin{aligned} \min_{\boldsymbol{u}_k} \quad & \varphi_N\left(x_{N|k}\right) + \sum_{i=0}^{N-1}\left[x_{i|k}^T Q x_{i|k} + u_{i|k}^T R u_{i|k}\right] \\ \text{s.t.} \quad & x_{l+1|k} = f\left(x_{l|k}, u_{l|k}\right) \\ & x_{0|k} = x(k) \\ & x_{l|k} \in \mathbb{X}, \quad l \in \{0, 1, ..., N\} \\ & u_{l|k} \in \mathbb{U}, \quad l \in \{0, 1, ..., N-1\} \end{aligned}$$



56

Model-based Estimation and Control: IDAES Dynamic Optimization and NMPC

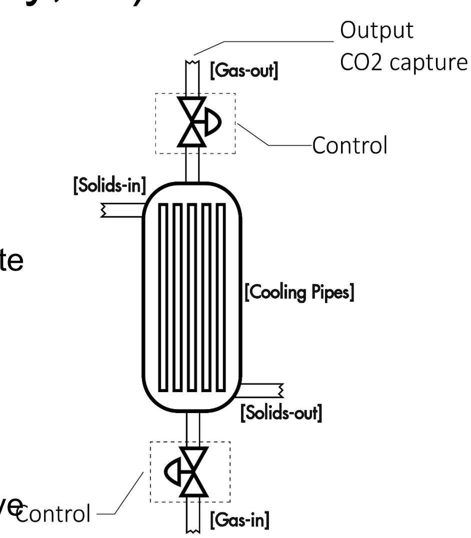




57

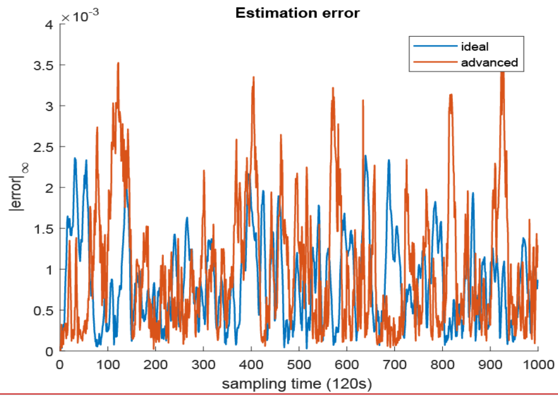
NMPC for CO_2 Capture (BFB) (Thierry, B.)

- Set-point on CO_2 removal fraction
- Controls: valve opening inlet and outlet gas
- Discretized with 5 spatial finite elements and 3 point Radau collocation in time
- 315 states for the current discretization
- Full-state feedback control, stage cost tracked in objective
- 46510 var. / 46500 eqns.



58

BFB Results: Ideal vs. asMHE



	Average CPUs	
	Ideal MHE	asMHE
IPOPT	9.23	9.23
k_aug (rH)	13.02	13.02
k_aug (sens)	0	12.99
dot_(online)	0	2.4
Online Cost	22.25	2.4

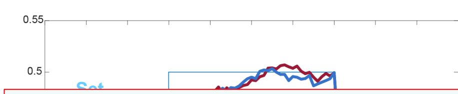
- **Use predicted measurement to solve NLP offline (IPOPT)**
- **Update optimum estimated state on-line using NLP sensitivity correction (sIPOPT/k_aug)**

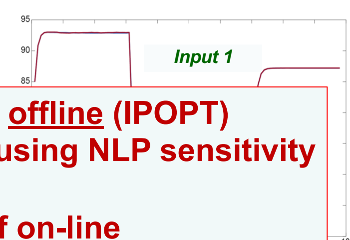
- **asMHE: similar performance at ~10% online cost**

59

asNMPC vs Ideal NMPC (noise: $\sigma = 1\%$)

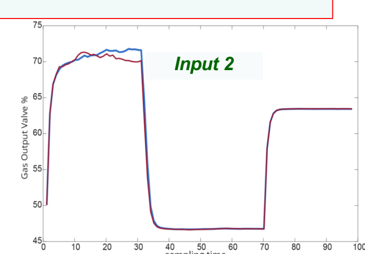
BFB Results: asNMPC: similar performance





- **Use predicted state to solve NLP offline (IPOPT)**
- **Update optimum control on-line using NLP sensitivity correction (sIPOPT/k_aug)**
- **Similar Performance with < 5% of on-line computation**

	Average CPUs	
	Ideal NMPC	asNMPC
IPOPT	6.37	6.37
k_aug (rH)	0	0
k_aug (sens)	0	5.6
dot_sens (online)	0	0.3
Online	6.37	0.3



60

Conclusions

NMPC has well-known stability/robustness guarantees
- Asymptotic / Robust stability based on NLP properties
- Can Avoid Unreachable Finite Horizons
- Infinite Horizon NMPC has asymptotic / robust stability

NMPC Computational Strategies
- Full-Discretization + Fast Sensitivity Calculations
- Large-scale nonlinear DAE models – case studies
- Sensitivity-based Nonlinear Estimation & Control

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

61

Some Recent Advances in NMPC

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78