Robust Model Predictive Control and Dynamic Real-time Optimization: Applications to Energy Processes

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Overview

1. Dynamic Optimization and Nonlinear MPC
   - Vehicle for dynamic optimization on-line
   - Need fast on-line computations
   - Need to enforce stability and robustness

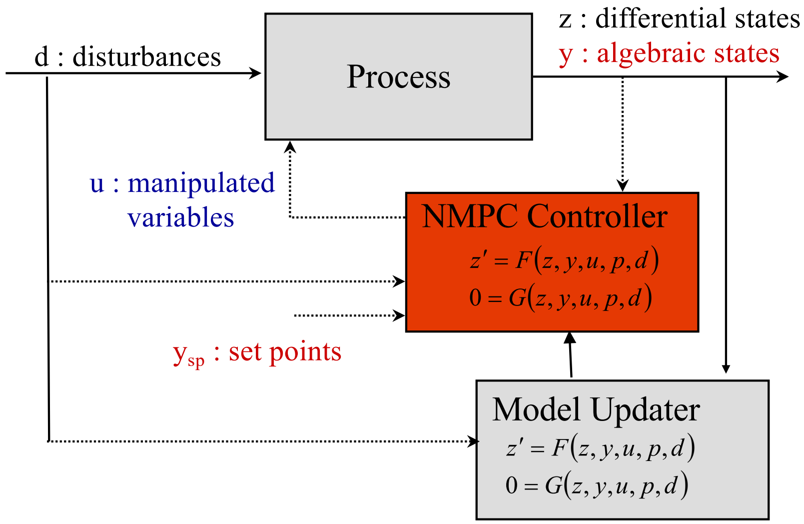
2. NMPC for CO_2 Adsorption/Capture
   - Time critical PDE modeling and control
   - Fast NMPC and MHE with advanced-step concepts

3. Economic NMPC for Distillation
   - Concepts for dynamic optimization and stability
   - Ensuring (robustly) stable eNMPC formulations
   - Performance comparisons

4. Hydraulic fracturing and NMPC
   - Solution strategies for multistage NMPC under uncertainty model properties
   - Guaranteed performance under uncertainty

Nonlinear Model Predictive Control (NMPC)

NMPC Estimation and Control



Why NMPC?

- Track a profile
- Severe nonlinear dynamics (e.g, sign changes in gains)
- Operate process over wide range (e.g., startup and shutdown)

NMPC Subproblem

$$\min_{\boldsymbol{u}} \quad \sum_j \| y(\boldsymbol{t}_{k+j}) - y^{sp} \|^2_{Q_y} + \sum_j \| \boldsymbol{u}(\boldsymbol{t}_{k+j}) - \boldsymbol{u}(\boldsymbol{t}_{k+j-1}) \|^2_{Q_u}$$

$$s.t. \quad z'(t) = F(z(t), y(t), \boldsymbol{u}(t), t)$$

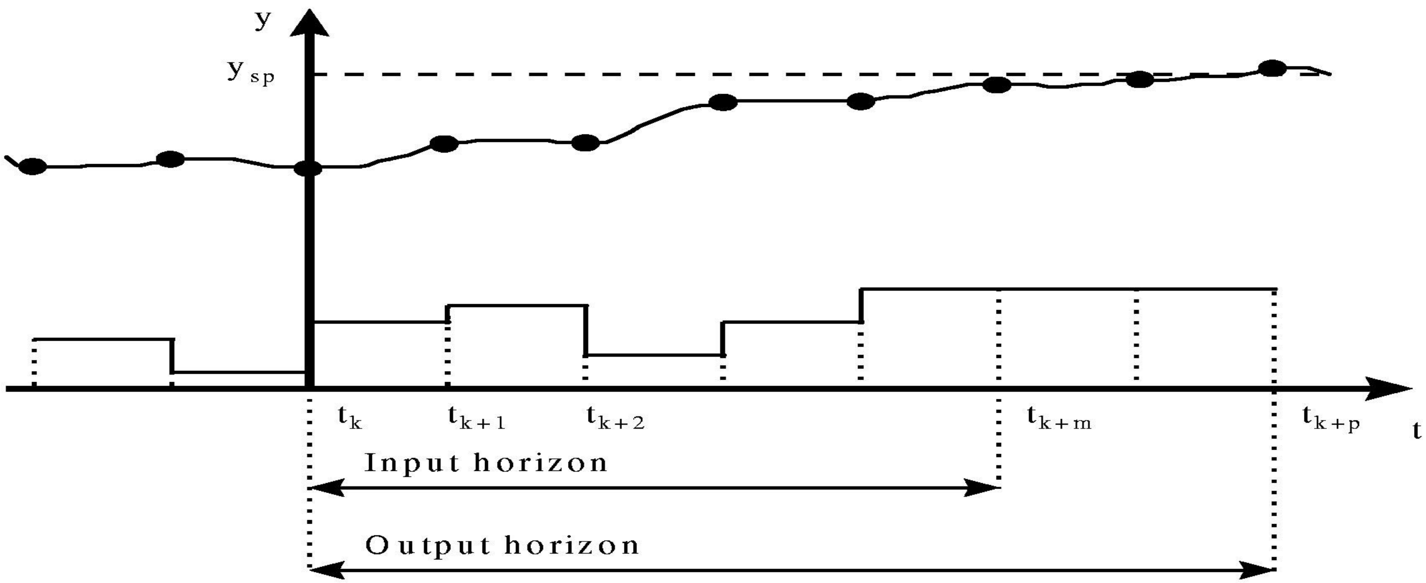
$$0 = G(z(t), y(t), \boldsymbol{u}(t), t)$$

$$z(t) = z(t_k)$$

Bound Constraints

Other Constraints

Nonlinear Model Predictive Control (NMPC)



$$\min_{\boldsymbol{u}} \quad \sum_j \| y(\boldsymbol{t_{k+j}}) - y^{sp} \|^2_{Q_y} + \sum_j \| \boldsymbol{u}(\boldsymbol{t_{k+j}}) - \boldsymbol{u}(\boldsymbol{t_{k+j-1}}) \|^2_{Q_u}$$

$$s.t. \quad \begin{aligned} z'(t) &= F(z(t), y(t), \boldsymbol{u}(t), t) \\ 0 &= G(z(t), y(t), \boldsymbol{u}(t), t) \end{aligned}$$

$$z(t) = z(t_k)$$

Bound Constraints

Other Constraints

MPC - Background

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
- Empirical 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

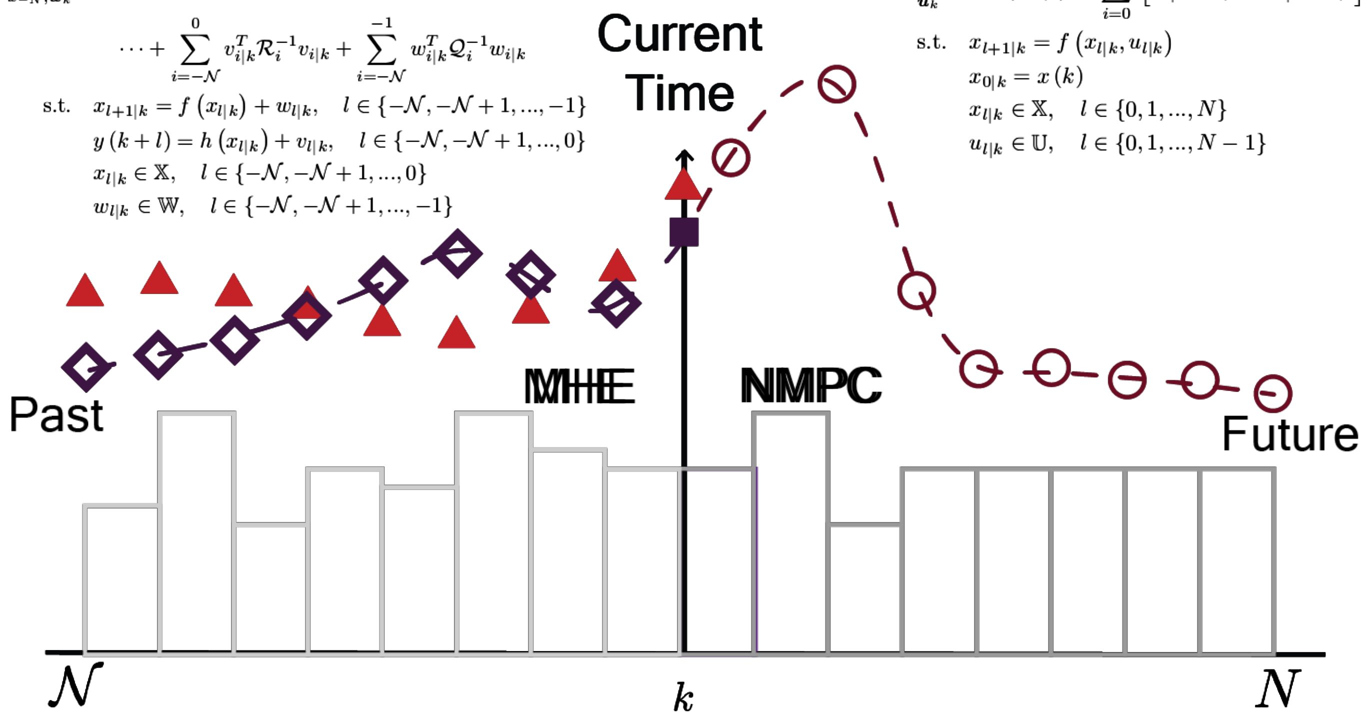
Model-based Estimation and Control: MHE and NMPC

$$\mathcal{M}\left(\Pi_{-N|k-1}, \hat{x}_{-N|k-1}, y(k), \ldots, y(k-\mathcal{N})\right):$$

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

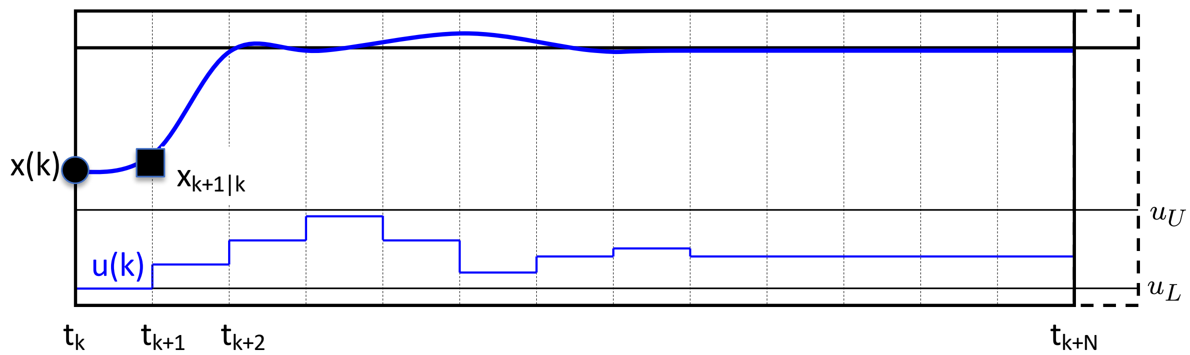
$$\mathcal{P}\left(x(k)\right):$$

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



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

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



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

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

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

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

Solve NLP(k) in <u>background</u> (between t_k and t_{k+1})

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

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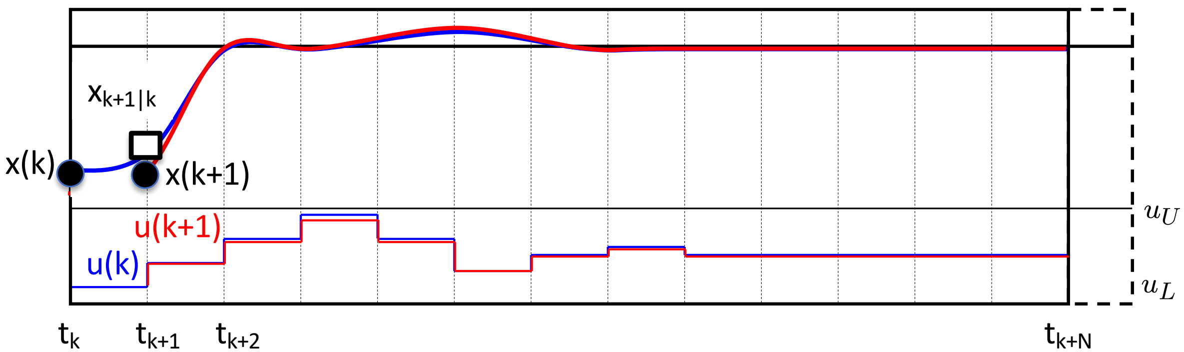


$$\begin{bmatrix} W_k & A_k & -I \\ A_k^T & 0 & 0 \\ Z_k & 0 & X_k \end{bmatrix} \begin{bmatrix} \Delta \mathbf{x} \\ \Delta \lambda \\ \Delta z \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ x_{k+1|k} - x(k+1) \\ 0 \end{bmatrix}$$

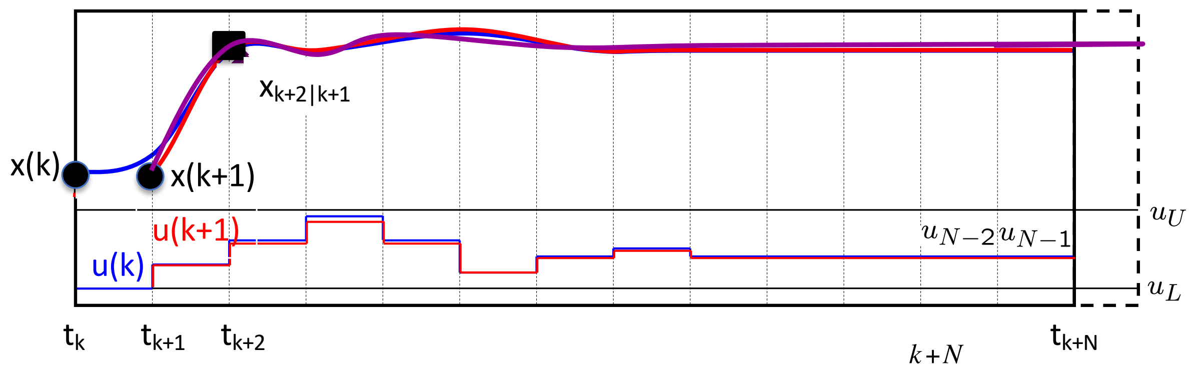
Solve NLP(k) in background (between t_k and t_{k+1})

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



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

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

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

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

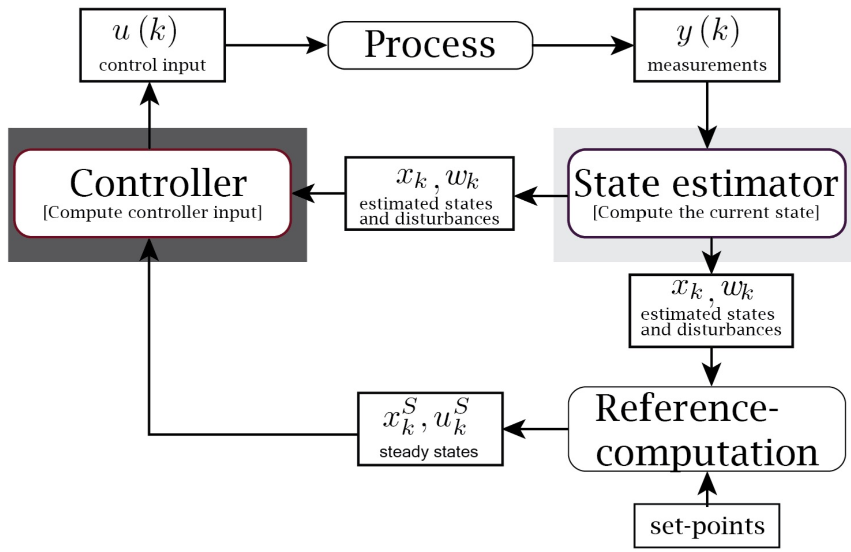
Also extends to Advanced Step MHE to update $\hat{x}_{N|k-1}$ and $\Pi_{N|k-1}$

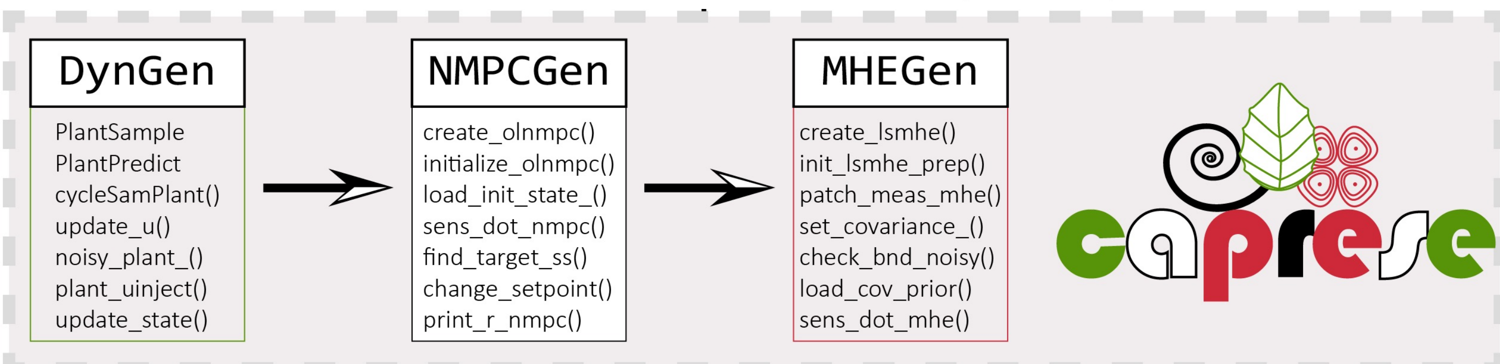
Solve NLP(k) in <u>background</u> (between t_k and t_{k+1})

Sensitivity to update problem <u>on-line</u> to get (u(k+1))

Solve NLP(k+1) in <u>background</u> (between t_{k+1} and t_{k+2})

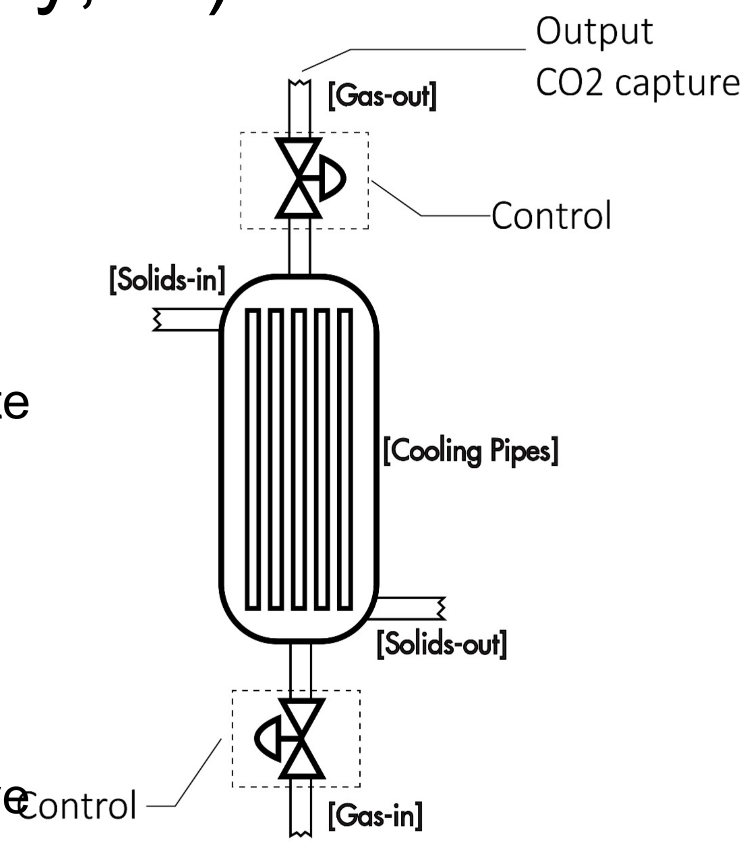
CAPRESE: Control and Adaptation with PREdictive SEnsitivity (David Thierry)



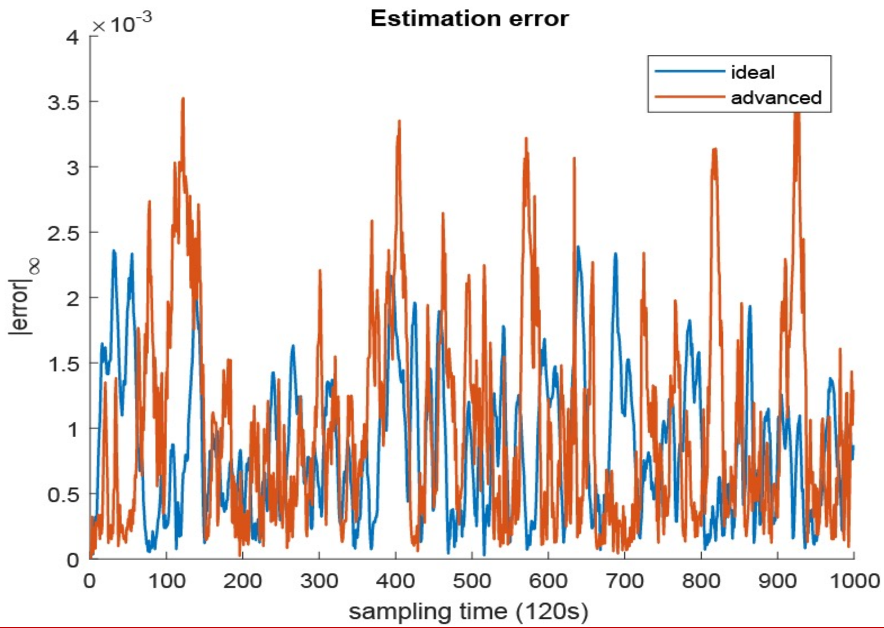


NMPC for CO_2 Capture (Bubbling Fluid Bed) (Thierry, B.)

- 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.



Bubble Fluid Bed MHE Results: Ideal vs. asMHE



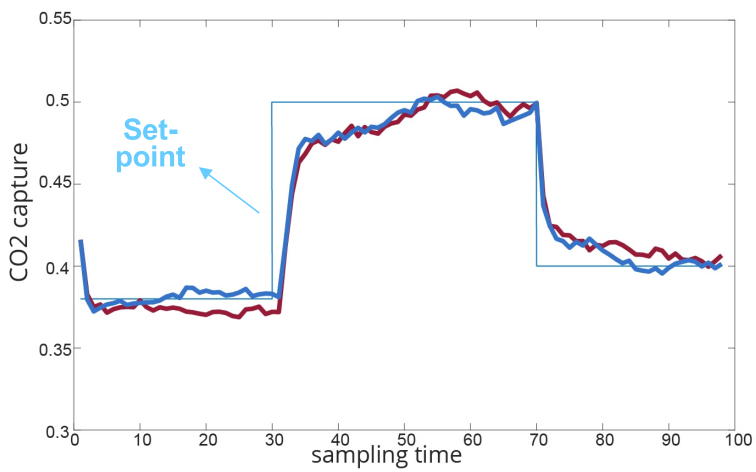
	Average CPUs	
	Ideal MHE	asMHE
IPOPT	9.23	9.23
k_aug (rH)	13.02	13.02
k_aug (sens)	0	12.99
dot_(online)	0	2.4
Online Cost	22.25	2.4

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

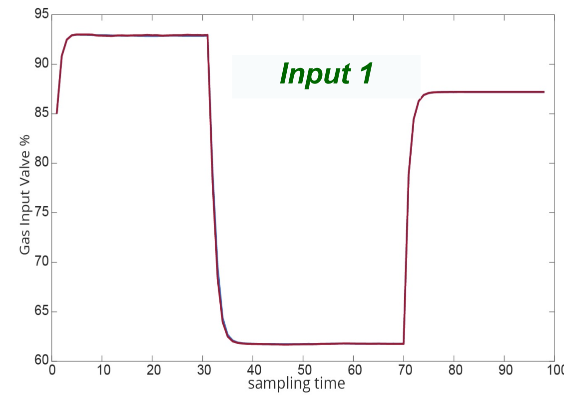
- **asMHE: similar performance at ~10% online cost**

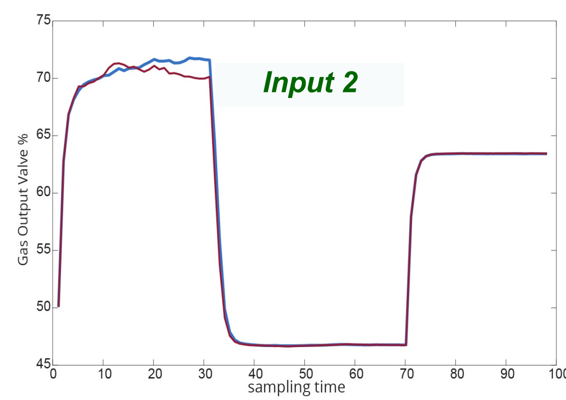
asNMPC vs Ideal NMPC (noise: $\sigma = 1\%$)

BFB Results: asNMPC: similar performance



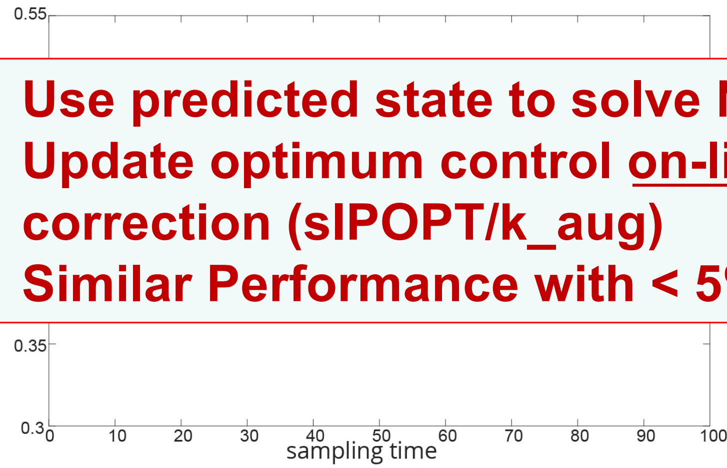
	Average CPUs	
	Ideal NMPC	asNMPC
IPOPT	6.37	6.37
k_aug (rH)	0	0
k_aug (sens)	0	5.6
dot_sens (online)	0	0.3
Online	6.37	0.3



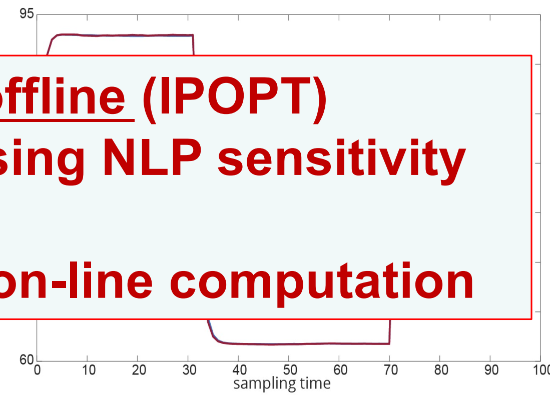


asNMPC vs Ideal NMPC (noise: $\sigma = 1\%$)

BFB Results: asNMPC: similar performance



- **Use predicted state to solve NLP <u>offline</u> (IPOPT)**
- **Update optimum control <u>on-line</u> 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
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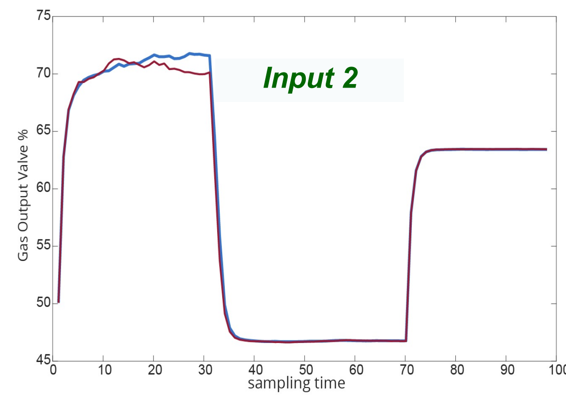
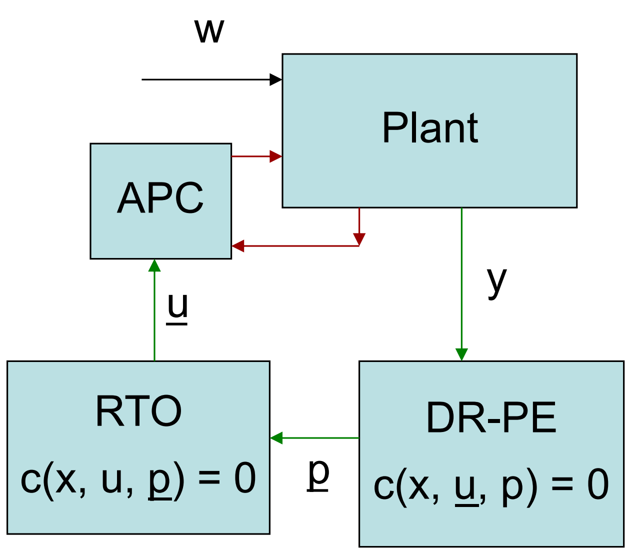


D-RTO with Economic Objectives → Beyond NMPC Tracking

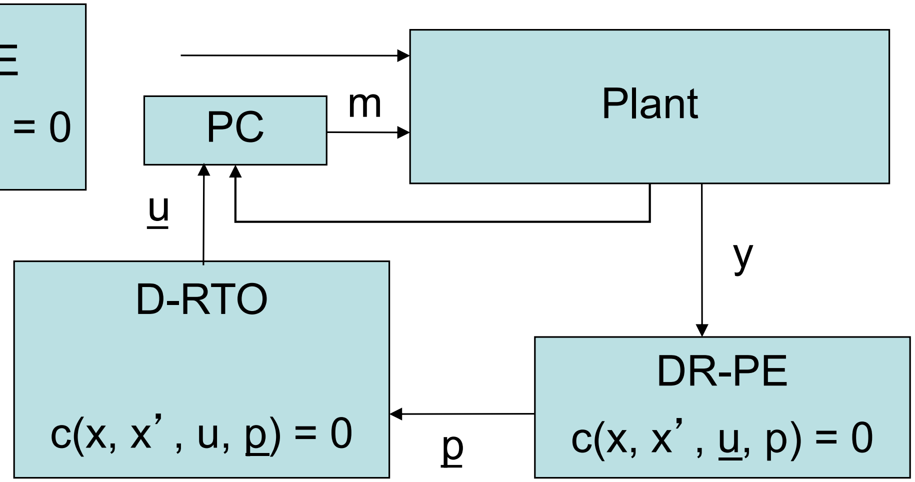


Benefits of combining RTO with NMPC?

•Direct, dynamic production maximization

•Remove artificial tracking objective

•Remove artificial steady state problem



Economic NMPC (eNMPC)

NLP formulation

$$\min_{v_l, z_l} \quad \Psi(z_N) + \sum_{l=0}^{N-1} \psi(z_l, v_l)$$

$$s.t. \quad z_{l+1} = f(z_l, v_l), l = 0, \ldots, N-1$$

$$z_0 = x(k)$$

$$z_l \in X, v_l \in U, l = 0, \ldots, N-1, z_N \in X_N$$

where ψ(x, u), Ψ(x) are economic terms

Challenge: $\alpha_p(|x|) \leq \psi(x, u) \leq \alpha_q(|x|)$ no longer holds

NMPC Stability Results do not carry over to eNMPC

Can be overcome by regularizing stage costs, compromise D-RTO

Reformulation of eNMPC with Stability Constraints

(Yang, Griffith, Zavala, B., 2019)

$$\min_{z_l, v_l} \sum_{l=0}^{N-1} \psi^{ec}(z_i, v_i)$$

$$\text{s.t. } z_{l+1} = f(z_l, v_l, 0) \quad l = 0, \ldots, N-1$$

$$z_0 = x_k$$

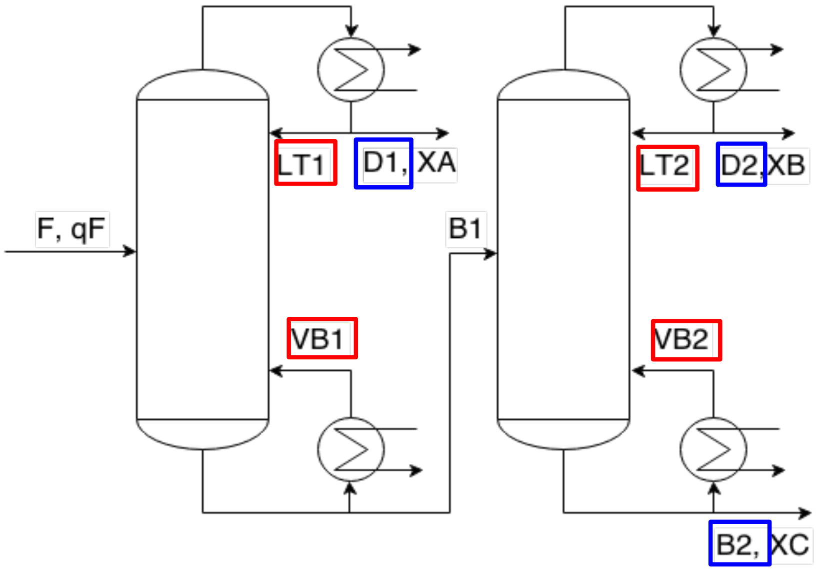
$$z_l \in \mathbb{X},\ v_l \in \mathbb{U} \quad l = 0, \ldots, N-1$$

$$z_N = x_s$$

$$\sum_{l=0}^{N-1} \psi^{tr}(z_l, v_l) - V(k-1, \mathbf{w}_{k-1}, x_0) \leq -\delta\, \psi^{tr}(x_{k-1}, u_{k-1})$$

- Add strict decrease of tracking Lyapunov function
- No regularization applied, no modification of economic stage costs
- Leads to nominal and ISS (robust) stability results!

Economic NMPC: Two Column Distillation (Yu, Griffith, B., 2020)



- 41 trays, 246 states
- 4 manipulated variables: LT1, VB1, LT2, VB2
- 3 output variables: D1, D2, B2
- Additive noise in model
- Hessian of Lagrange function of steady state problem has λ_{min} = -1.414
- Min *–(Net sales)*

$$\min_u \; J(u) = p_F F + p_V(VB1 + VB2) - (p_A D1 + p_B D2 + p_C B2)$$
$$s.t. \; Massbalance, \; Equilibrium$$
$$x_A \geq x_{A,min}, \; x_B \geq x_{B,min}, \; x_C \geq x_{C,min}$$
$$0 \leq LT1, LT2 \leq LT_{max}, \; 0 \leq VB1, VB2 \leq VB_{max}$$

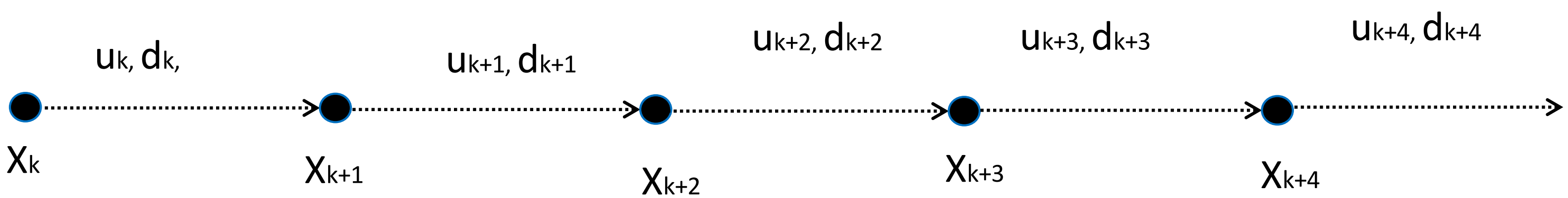
R.. B. Leer. Self-optimizing control structures for active constraint regions of a sequence of distillation columns. Master's thesis, NTNU, 2012.

Comparison of eNMPC Reformulations

- Baseline tracking to steady state optimum
- Pure economic NMPC has best economic performance, but no steady state nor stability guarantee
- eNMPC-sc similar to pure economic case, goes to steady state, robustly stable!
- Regularization of stage costs (eNMPC-rr, eNMPC-fr) improves over tracking with intermediate results

K = 9, N = 25	$\sum_{k=0}^{K}(\psi^{ec}(x_k,u_k) - \psi^{ec}_{ss})$	Average CPU sec.
Tracking	-20.7330	69.0
eNMPC-fr	-22.6650	72.0
eNMPC-rr	-26.2324	181.8
eNMPC-sc, $\delta = 0.01$	-28.6706	309.2
Economic	-28.6458	272.3

Standard NMPC – Treatment of Uncertainty?

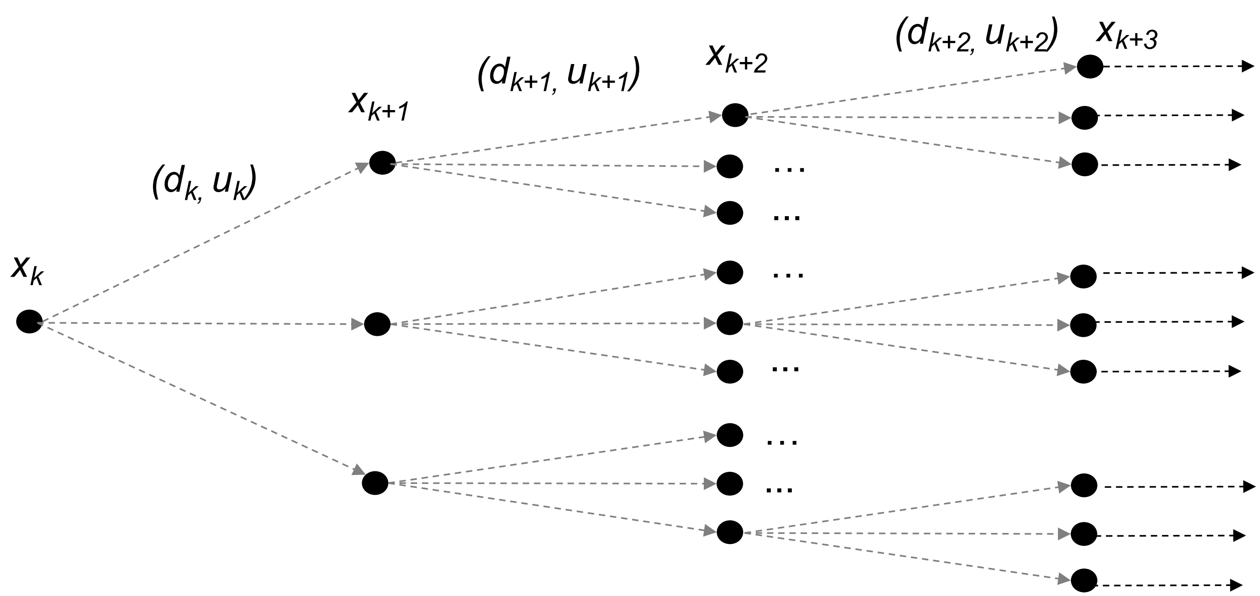


Nominal models with optimal performance

Sensitive to disturbances, model mismatch, uncertain inputs, etc.

Multi-stage MPC (msNMPC) – Stochastic Programming Formulation (Lucia, Engell et al., 2013)

Scenario branching: effect of uncertainty while optimizing control input



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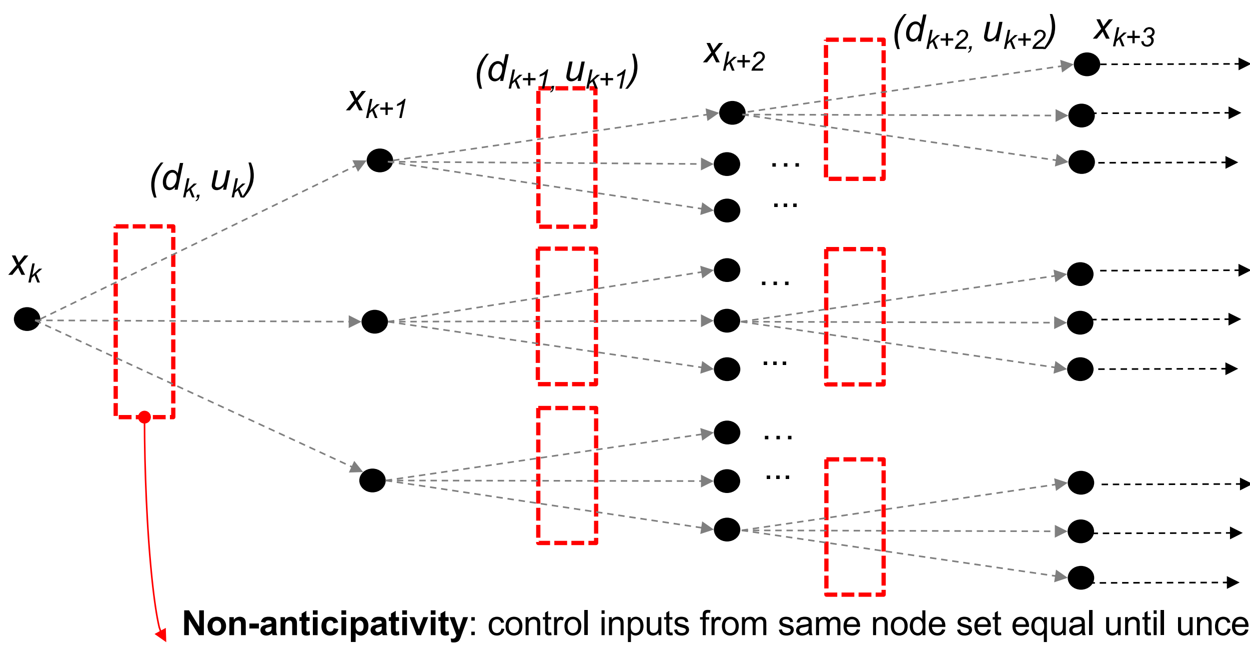

Non-anticipativity: control inputs from same node set equal until uncertainty is realized

Parallel KKT Decomposition for Stochastic Optimal Control

SOC problems become very large very quickly.

- Problem size (spatial discretization) x time discretization x # scenarios

Parallelize solution with Schur-Complement decomposition

- Schur-Complement based interior point algorithm using PyNumero and Parapint
- Exploits structure of KKT system induced by scenarios
- Parallel implementation using MPI

Can be accelerated through scenario generation and sensitivity assisted decomposition

Newton Step

$$\begin{bmatrix} \mathbf{K}_0 & & \dots & & N_0 \\ & \mathbf{K}_1 & \dots & & N_1 \\ \vdots & \vdots & \ddots & & \vdots \\ & & & \mathbf{K}_c & N_c \\ N_0^T & N_1^T & \dots & N_c^T & \end{bmatrix} \begin{bmatrix} \Delta \mathbf{s}_0 \\ \Delta \mathbf{s}_1 \\ \vdots \\ \Delta \mathbf{s}_c \\ \gamma \end{bmatrix} = - \begin{bmatrix} r_0 \\ r_1 \\ \vdots \\ r_c \\ 0 \end{bmatrix}$$

Schur Complement

$$\sum_{c \in \mathbb{C}} (N_c^T \mathbf{K}_c^{-1} N_c)\gamma = -\sum_{c \in \mathbb{C}} (N_c^T \mathbf{K}_c^{-1} r_c)$$

Backsolve

$$\mathbf{K}_c \Delta \mathbf{s}_c = -(r_c + N_c \gamma), \ \forall c \in \mathbb{C}$$

Rodriguez, J., Parker, R., Laird, C., Nicholson, B., Siirola, J., Bynum, M., “Scalable Parallel Nonlinear Optimization with PyNumero and Parapint”, under review, http://www.optimization-online.org/DB_HTML/2021/09/8596.html.

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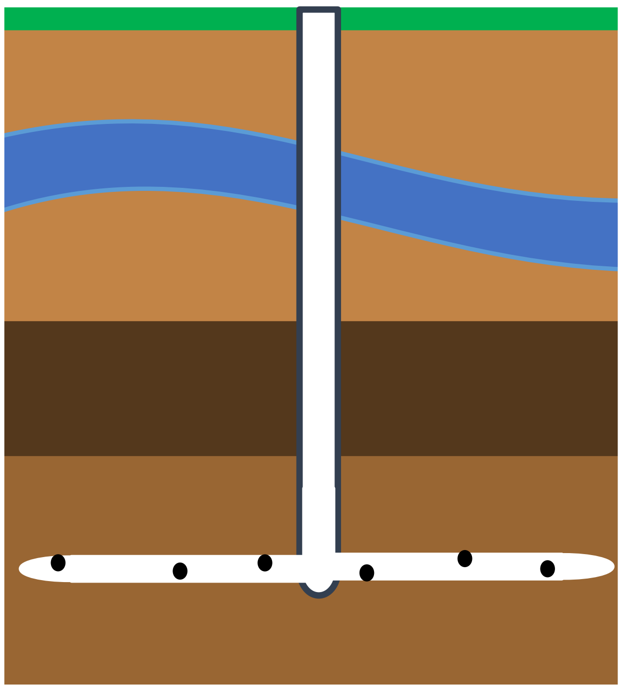
eNMPC under Uncertainty:
Hydraulic Fracturing for Natural Gas Extraction
(Lin, B., 2022)



- Advantages
  1. Increase production of hydrocarbons
  2. Considerable economic benefits

- Difficulties and concerns
  1. Extremely high pressure (625 atm)
  2. Rock formation is nonhomogeneous

Hydraulic Fracturing Model

Fracture geometry by PKN model

Local mass balance

$$\frac{\partial q}{\partial x} + u + \frac{\partial A}{\partial t} = 0$$

Global mass balance

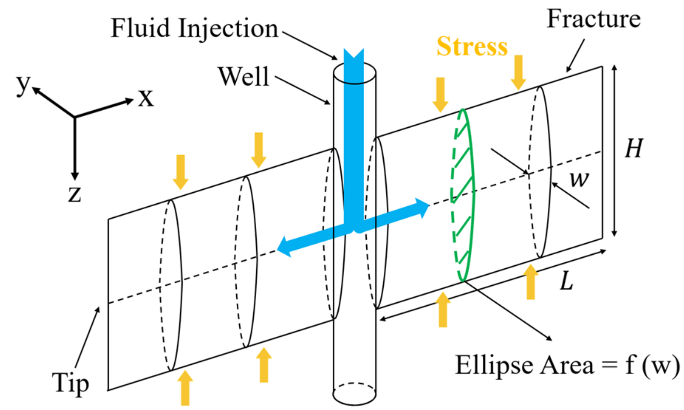
$$q_{leakoff} + q_{storage} = q_{total}$$

Mass transfer

- Proppant, C_p
- Friction reducer (FR), C_{FR}

Changes of fluid properties

- Density
- Viscosity



- Drag reduction caused by FR

$$\frac{1}{DR} = \frac{1}{DR_{lim}} + \frac{K_0}{Re\ C_{FR}} + \frac{K_1}{Re} + \frac{K_2}{C_{FR}}$$

- Wellhead pressure

$$P_{head} = P_{FR}(t, x=0) + \sigma - \rho g H_{well} + P_{frict}$$

Hydraulic Fracturing Model

- PKN model

$$-\frac{E}{2\mu H\pi^3(1-v^2)}\frac{\partial^2\overline{w}^4}{\partial x^2}+\frac{\partial\overline{w}}{\partial t}=0$$

$$\int_0^L \overline{w}\,dx=\frac{q_f t}{H}$$

- Mass transport

$$v_{slurry}=\frac{2E}{\pi^3\mu H(1-v^2)}\overline{w}^2\frac{\partial\overline{w}}{\partial x}$$

$$v_s=\frac{(1-C_p)^2(\rho_{sd}-\rho_{pf})\,g\,d^2}{10^{1.82\,C_p}\,18\,\mu}$$

$$v_c=v_{slurry}-(1-C_p)v_s$$

$$\frac{\partial(\overline{w}C_p)}{\partial t}+\frac{\partial(\overline{w}C_p v_c)}{\partial x}=0$$

$$\frac{\partial(\overline{w}C_{FR})}{\partial t}+\frac{\partial(\overline{w}C_{FR} v_c)}{\partial x}=0$$

- Changes of fluid properties

$$\mu=\mu_0\left(1-\frac{C_p}{C_{max}}\right)^{-\alpha}$$

$$\rho=C_p\rho_{sd}-(1-C_p)\rho_{pf}$$

- Drag reduction

$$\frac{1}{DR}=\frac{C_{FR}+K_2\,DR_{lim}}{DR_{lin}\,C_{FR}}$$

$$\Delta P_{head}=\Delta P_s\,(1-DR)$$

- Wellhead pressure

$$P_{fr}=\frac{16\mu q_f H_{well}}{\pi R^4}(1-DR)$$

$$P_s=\frac{2E}{\pi H(1-v^2)}\overline{w}+\sigma-\rho g H_{well}+P_{fr}$$

IC1: $L\,(t=0)=0$

IC2: $\overline{w}\,(t=0,x)=0$

IC3: $C_p\,(t=0,x)=0$

IC4: $C_{FR}(t=0,x)=0$

BC1: $\overline{w}\,(t,x=L)=0$

BC2: $q\,(t,x=0)=q_f$

BC3: $C_p(t,x=0)=\hat{C}_p$

BC4: $C_{FR}(t,x=0)=\hat{C}_{FR}$

Closed loop control of hydraulic fracturing process
Standard eNMPC

Goal: minimize operation time with the least amount of FR

$$\psi(v_l) = (W + q_f(l)\hat{C}_{FR}(l))h_k \qquad \text{for standard NMPC}$$

$$\psi(v_l^c) = (W + q_f^c(l)\hat{C}_{FR}^c(l))h_k^c \qquad \text{for multistage NMPC}$$

Control input: $q_f, \hat{C}_p, \hat{C}_{FR}$

Process state: $L, \bar{w}, C_p, C_{FR}, P_{head}$

Operating constraints

	Max.	Unit
P_{head}	6.34×10^7	Pa
qf	15.9	m^3/min
$\hat{C}_{propp}$	10.0	$ppga$
Δqf	3.18	m^3/min^2
$\Delta\hat{C}_{propp}$	1.25	$ppga/min$

- Endpoint constraints: $L, \bar{w}, M_p$
- Shrinking horizon:
  - Horizon shrinks one step at each time
  - $N = 35 - k$, h_k: sampling time
- Uncertain parameter:

  Young's modulus, E (Pa)

Deviation	E values (Pa)
-5%	2.28×10^{10}
Nominal	2.40×10^{10}
+5%	2.52×10^{10}

- Discretize the model
  - Space: finite difference
  - Time: implicit Euler discretization

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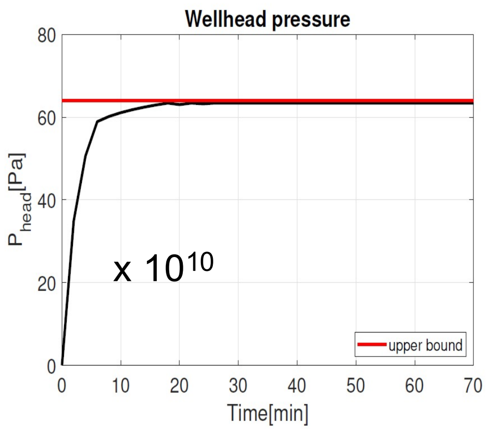
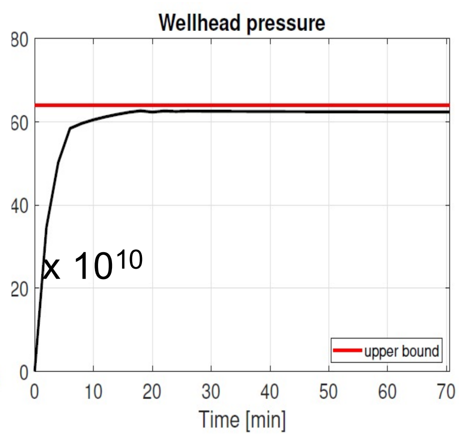
Standard NMPC under uncertainty

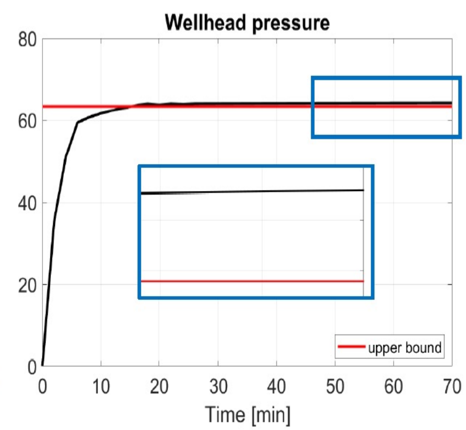
sNMPC, nom



sNMPC, min



sNMPC, max



	L	$\bar{w}$	$M_{p,k=N_0}$	$\sum_{k=0}^{N_0-1} h_k$	$\sum_{k=0}^{N_0-1} q_f(k)\hat{C}_{FR}(k)h_k$
unit	m	mm	ton	min	kg
Goal	**495.4**	–	**328.2**	–	–
sNMPC, nom	495.4	satisfied	328.2	70.00	4.416
sNMPC, E_{min}	494.7	satisfied	328.2	70.55	4.228
sNMPC, E_{max}	500.3	*not* satisfied	328.2	70.00	4.416

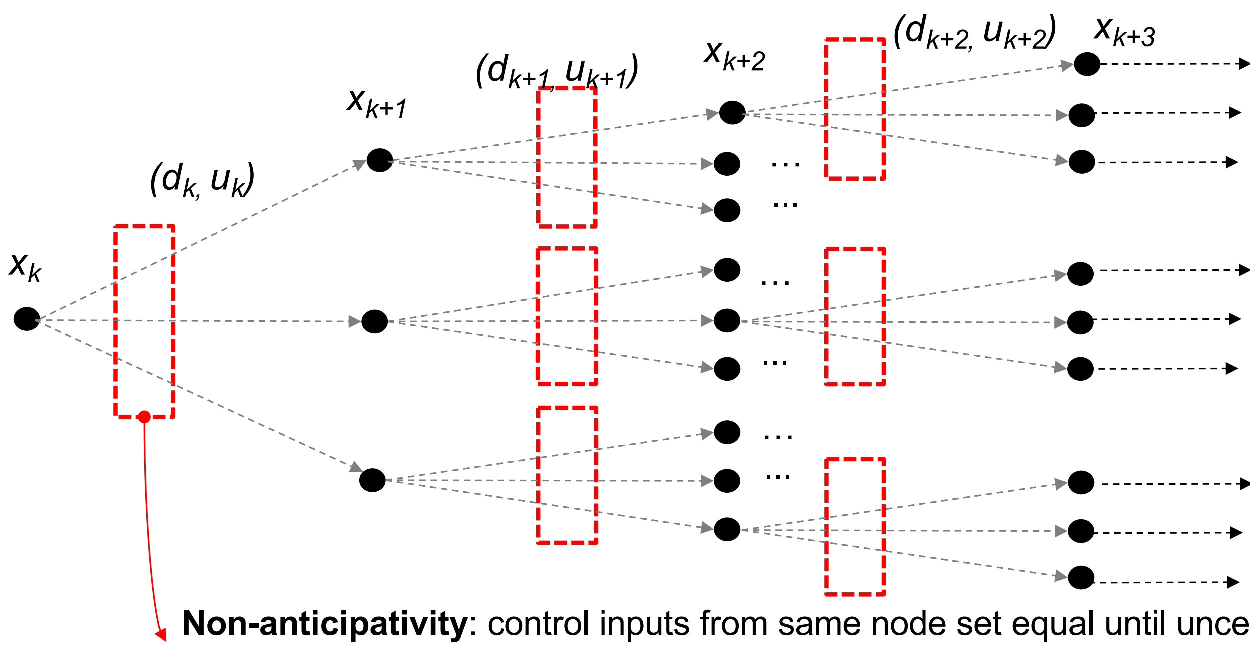
- Standard NMPC performs well without no process-controller mismatch
- All final requirements are satisfied
- Wellhead pressure remains within the bound

- When parameter mismatch exists, standard NMPC fails to meet the final requirements
- Pressure violation occurs in the max realization case

$\Rightarrow$ **Dangerous**

Multi-stage MPC (msNMPC) – Stochastic Programming Formulation (Lucia, Engell et al., 2013)

Scenario branching: effect of uncertainty while optimizing control input



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

Closed loop control of hydraulic fracturing process Multi-step eNMPC

Goal: minimize operation time with the least amount of FR

$$\psi(v_l) = (W + q_f(l)\hat{C}_{FR}(l))h_k \quad \text{for standard NMPC}$$

$$\psi(v_l^c) = (W + q_f^c(l)\hat{C}_{FR}^c(l))h_k^c \quad \text{for multistage NMPC}$$

Control input: $q_f, \hat{C}_p, \hat{C}_{FR}$

Process state: $L, \overline{w}, C_p, C_{FR}, P_{head}$

Operating constraints

	Max.	Unit
P_{head}	6.34×10^7	Pa
qf	15.9	m^3/min
$\hat{C}_{propp}$	10.0	$ppga$
Δqf	3.18	m^3/min^2
$\Delta\hat{C}_{propp}$	1.25	$ppga/min$

- Endpoint constraints: $L, \overline{w}, M_p$
- Shrinking horizon:
  - Horizon shrinks one step at each time
  - $N = 35 - k$, h_k: sampling time
- Uncertain parameters:

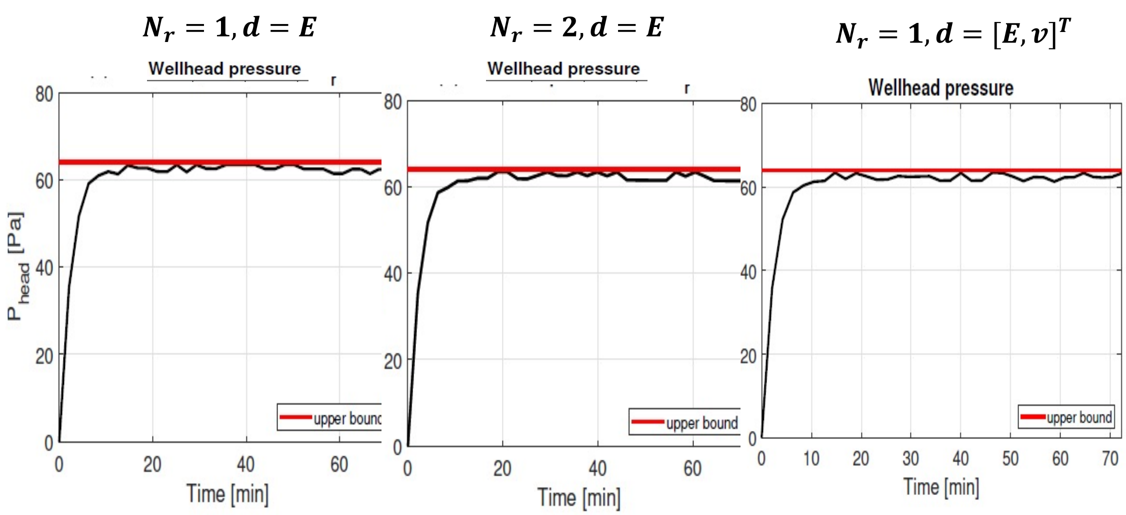
  Young's modulus, E (Pa)

  Poisson's ratio ν

Deviation	E values (Pa)	ν values
-5%	2.28×10^{10}	0.19
Nominal	2.40×10^{10}	0.20
+5%	2.52×10^{10}	0.21

- Discretize the model
  - Space: finite difference
  - Time: implicit Euler discretization

Guaranteed Performance under Uncertainty



	$L\ [m]$	$\bar{w}$	$M_p\ [ton]$	$\sum_{k=0}^{N} h_k\ [min]$	$\sum_{k=0}^{N} \hat{C}_{FR}(k)\ [ppm]$
Goal	495.4	–	328.2	–	–
$N_r = 1, d = E$	506.8	satisfied	328.2	72.17	179.51
$N_r = 2, d = E$	506.6	satisfied	328.2	72.16	181.44
$N_r = 1, d = [E, v]^T$	508.6	satisfied	328.2	72.22	195.06

- Multistage NMPC for probabilistic simulation performs well even when uncertainty is random and time-variant
- More degrees of freedom are required to maintain robustness when two uncertainties are involved
- No significant performance difference between robust horizons N_r = *1 or 2*

Summary and Conclusions

Dynamic optimization facilities implemented in IDAES

- Using PyomoDAE, CasADi and CAPRESE tools

Demonstrates advantages of full discretization optimization approach

- Leverages capabilities of large-scale decomposition & algorithms

Extends online dynamic optimization under uncertainty and robust NMPC

Demonstrated on challenging non-conventional energy applications

- CO_2 capture in BFBs (demanding first principle PDE models)
- Real-time dynamic optimization for distillation systems
- On-line optimization for Hydraulic Fracturing (uncertainty guarantees)