Centre for Process Systems Engineering

Imperial College London

From Multi-Parametric Programming Theory to MPC-on-a-chip Multi-scale Systems Applications

Stratos Pistikopoulos

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hy2seps
CONNECT
PRISM
EPSRC
erc MOBILE
MARIE CURIE ACTIONS
PROMATCH
AIR PRODUCTS

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ParOS
Advanced control technology on a chip

Outline

- Key concepts & historical overview
- Recent developments in multi-parametric programming and mp-MPC
- MPC-on-a-chip applications
- Concluding remarks & future outlook

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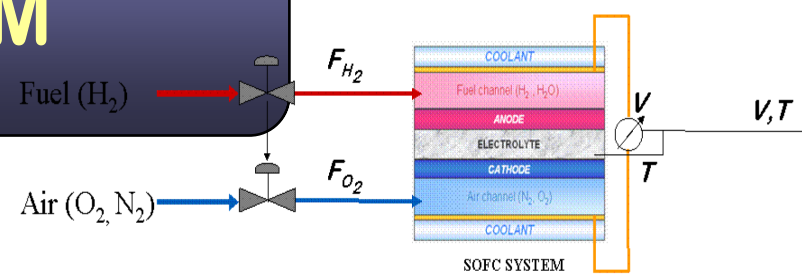
What is On-line Optimization?

MODEL/OPTIMIZER

Control Actions

Data - Measurements

SYSTEM



What is Multi-parametric Programming?

- Given:
  - a performance criterion to minimize/maximize
  - a vector of constraints
  - a vector of parameters

$$z(x) = \min_{u} f(u,x)$$
$$\text{s.t.}\ \ g(u,x) \le 0$$
$$x \in \mathbb{R}^n$$
$$u \in \mathbb{R}^s$$

What is Multi-parametric Programming?

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$$\text{s.t. } g(u,x) \le 0$$
$$x \in \mathbb{R}^n$$
$$u \in \mathbb{R}^s$$

- Obtain:
  - the performance criterion and the optimization variables as a function of the parameters
  - the regions in the space of parameters where these functions remain valid

Multi-parametric programming

$$z(x) = \min_{u} f(u,x)$$

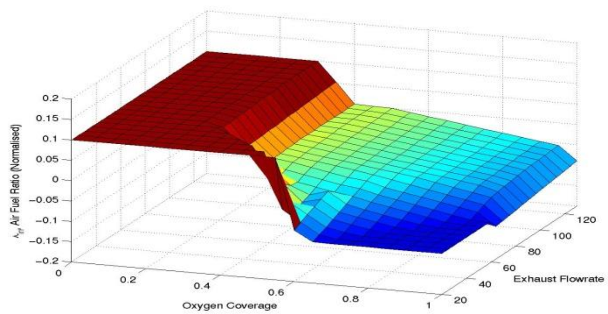
$$\text{s.t. } g(u,x) \le 0$$

$$x \in \mathbb{R}^n$$

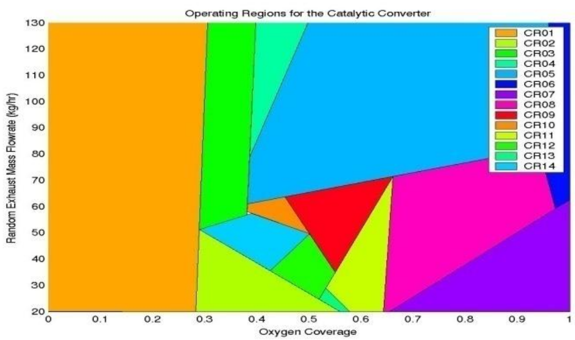
$$u \in \mathbb{R}^s$$

$$u(x)$$

(1) Optimal look-up function



(2) Critical Regions



Obtain optimal solution *u(x)* as a function of the parameters *x*

Multi-parametric programming

Problem Formulation

$$\min_{\mathbf{u}_1,\mathbf{u}_2} \left(-3\mathbf{u_1} - 8\mathbf{u_2}\right)$$

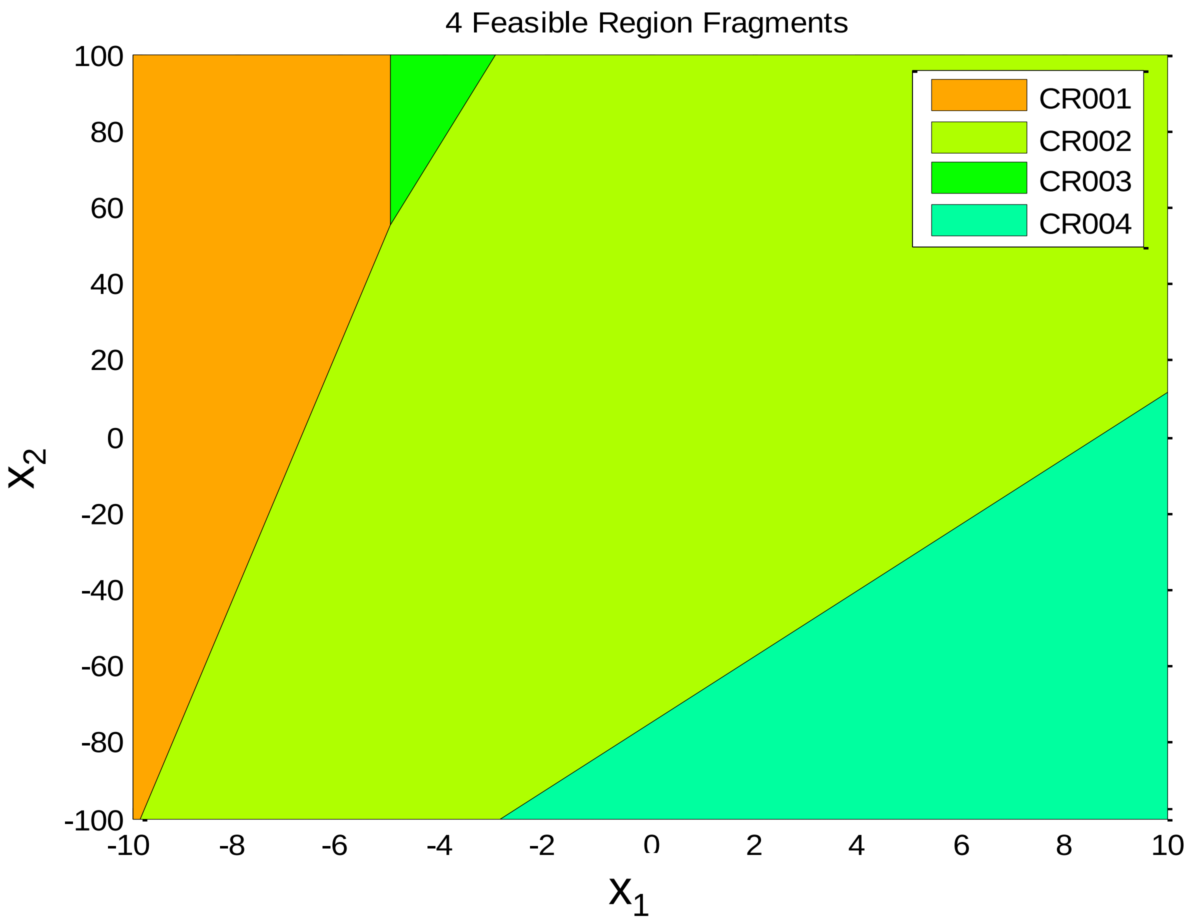
$$st.$$

$$\begin{bmatrix} 1 & 1 \\ 5 & -4 \\ -8 & 22 \\ -4 & -1 \end{bmatrix} \cdot \begin{bmatrix} \mathbf{u_1} \\ \mathbf{u_2} \end{bmatrix} + \begin{bmatrix} -1 & 0 \\ 0 & 0 \\ 0 & -1 \\ 0 & 0 \end{bmatrix} \cdot \begin{bmatrix} \mathbf{x_1} \\ \mathbf{x_2} \end{bmatrix} + \begin{bmatrix} -13 \\ -20 \\ -121 \\ 8 \end{bmatrix} \leq \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$-10 \leq \mathbf{x_1} \leq 10 \qquad -100 \leq \mathbf{x_2} \leq 100$$

Multi-parametric programming

Critical Regions



Multi-parametric programming

Multi-parametric Solution

$$
\mathbf{U} = \begin{cases}
\begin{bmatrix} -0.33 & 0 \\ 1.33 & 0 \end{bmatrix} \cdot \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix} + \begin{bmatrix} -1.67 \\ 14.67 \end{bmatrix} & \textbf{if} \begin{bmatrix} 1 & -0.031 \\ 1 & 0 \\ -1 & 0 \\ 0 & -1 \\ 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix} \le \begin{bmatrix} -6.71 \\ -5 \\ 10 \\ 100 \\ 100 \end{bmatrix} \\
\begin{bmatrix} 0.73 & -0.03 \\ 0.26 & 0.03 \end{bmatrix} \cdot \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix} + \begin{bmatrix} 5.5 \\ 7.5 \end{bmatrix} & \textbf{if} \begin{bmatrix} 1 & -0.115 \\ -1 & 0.031 \\ -1 & 0.045 \\ 1 & 0 \\ 0 & -1 \\ 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix} \le \begin{bmatrix} 8.65 \\ 6.71 \\ 7.5 \\ 10 \\ 100 \\ 100 \end{bmatrix} \\
\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \cdot \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix} + \begin{bmatrix} 0 \\ 13 \end{bmatrix} & \textbf{if} \begin{bmatrix} 1 & -0.045 \\ -1 & 0 \\ 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix} \le \begin{bmatrix} -7.5 \\ 5 \\ 100 \end{bmatrix} \\
\begin{bmatrix} 0 & 0.05 \\ 0 & 0.06 \end{bmatrix} \cdot \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix} + \begin{bmatrix} 11.8 \\ 9.8 \end{bmatrix} & \textbf{if} \begin{bmatrix} -1 & 0.11 \\ 1 & 0 \\ 0 & -1 \end{bmatrix} \cdot \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix} \le \begin{bmatrix} -8.65 \\ 10 \\ 100 \end{bmatrix}
\end{cases}
$$

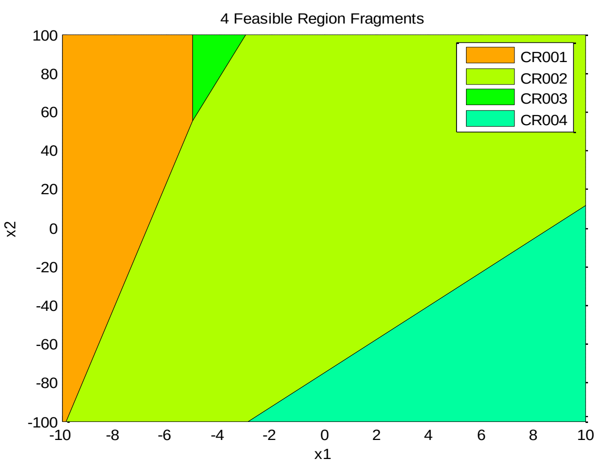
Multi-parametric programming

$$\min_u \left(-3u_1 - 8u_2\right)$$

$$st.$$

$$\begin{bmatrix} 1 & 1 \\ 5 & -4 \\ -8 & 22 \\ -4 & -1 \end{bmatrix} \cdot \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} + \begin{bmatrix} -1 & 0 \\ 0 & 0 \\ 0 & -1 \\ 0 & 0 \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} -13 \\ -20 \\ -121 \\ 8 \end{bmatrix} \le \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

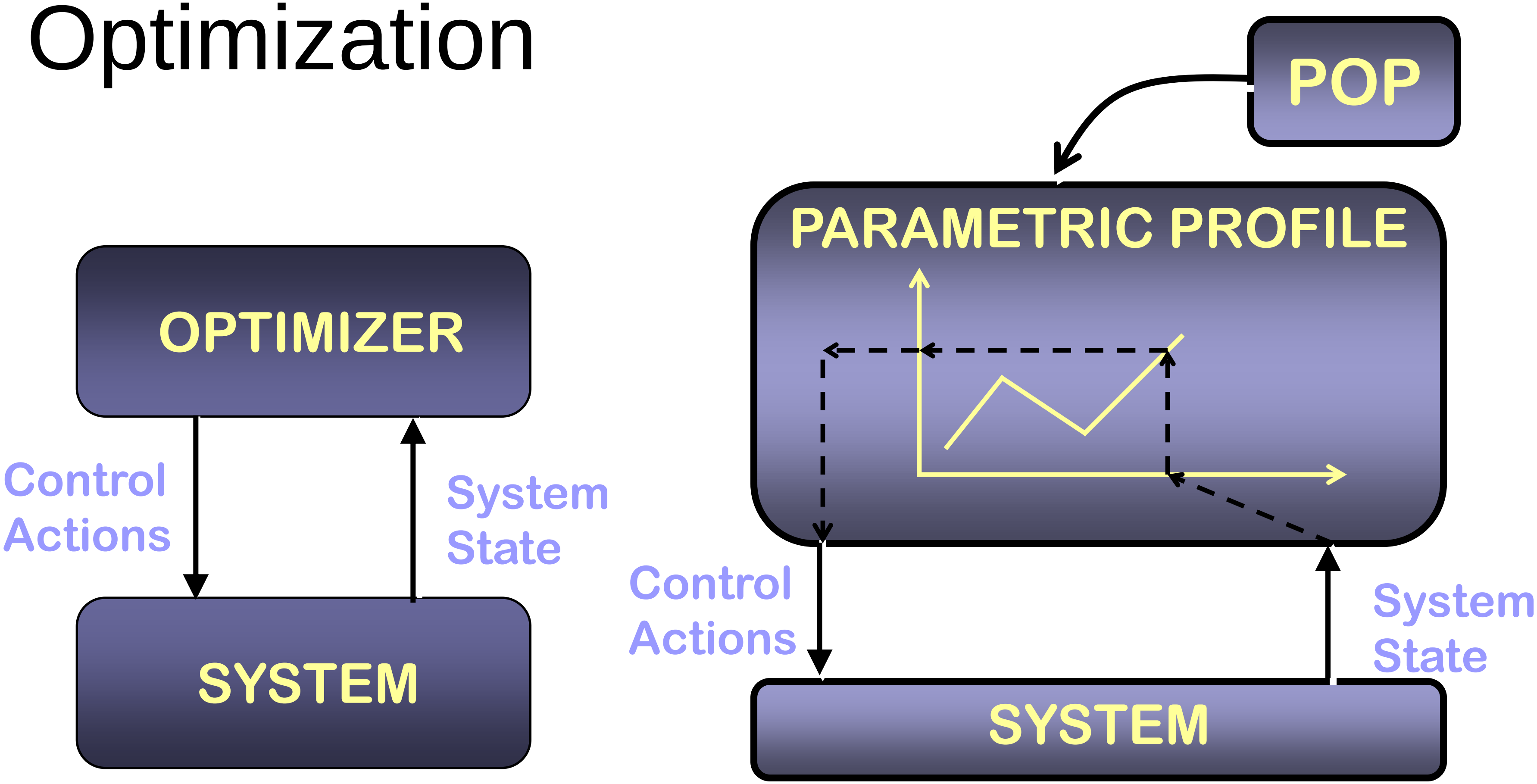
$$-10 \le x_1 \le 10, -100 \le x_2 \le 100$$



$$U = \begin{cases} \begin{bmatrix} -0.333 & 0 \\ 1.333 & 0 \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} -1.6667 \\ 14.6667 \end{bmatrix} & \textbf{if} \begin{bmatrix} 1 & -0.03125 \\ 1 & 0 \\ -1 & 0 \\ 0 & -1 \\ 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \le \begin{bmatrix} -6.71875 \\ -5 \\ 10 \\ 100 \\ 100 \end{bmatrix} \\ \begin{bmatrix} 0.7333 & -0.0333 \\ 0.26667 & 0.03333 \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} 5.5 \\ 7.5 \end{bmatrix} & \textbf{if} \begin{bmatrix} 1 & -0.115385 \\ -1 & 0.03125 \\ -1 & 0.0454545 \\ 1 & 0 \\ 0 & -1 \\ 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \le \begin{bmatrix} 8.65385 \\ 6.71875 \\ 7.5 \\ 10 \\ 100 \\ 100 \end{bmatrix} \\ \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} 0 \\ 13 \end{bmatrix} & \textbf{if} \begin{bmatrix} 1 & -0.0454545 \\ -1 & 0 \\ 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \le \begin{bmatrix} -7.5 \\ 5 \\ 100 \end{bmatrix} \\ \begin{bmatrix} 0 & 0.05128 \\ 0 & 0.0641 \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} 11.8462 \\ 9.80769 \end{bmatrix} & \textbf{if} \begin{bmatrix} -1 & 0.115385 \\ 1 & 0 \\ 0 & -1 \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \le \begin{bmatrix} -8.65385 \\ 10 \\ 100 \end{bmatrix} \end{cases}$$

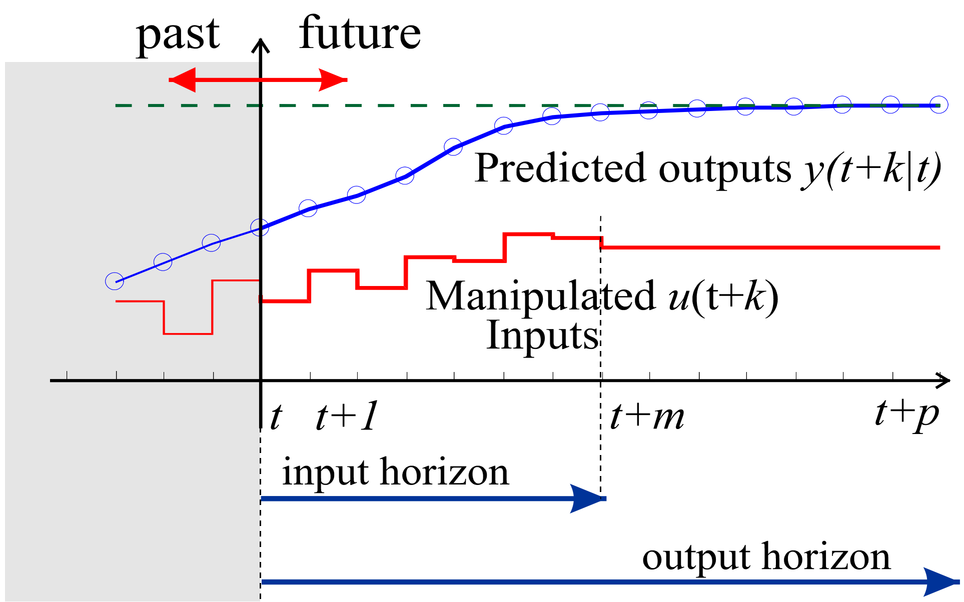
Only 4 optimization problems solved!

On-line Optimization via off-line Optimization



Function Evaluation!

Multi-parametric/Explicit Model Predictive Control



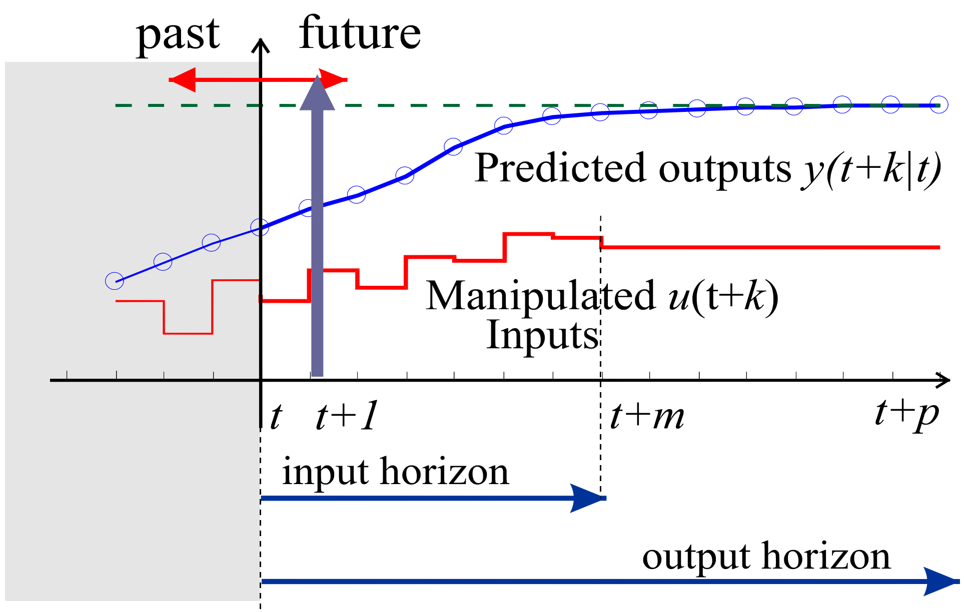
- Compute the optimal sequence of manipulated inputs which minimizes

tracking error = output – reference

subject to constraints on inputs and outputs

- On-line re-planning: Receding Horizon Control

Multi-parametric/Explicit Model Predictive Control



- Compute the optimal sequence of manipulated inputs which minimizes

Solve a QP at each time interval

- On-line re-planning: Receding Horizon Control

Multi-parametric Programming Approach

- State variables $\rightarrow$ Parameters
- Control variables $\rightarrow$ Optimization variables

- MPC $\rightarrow$ Multi-Parametric Programming problem
- Control variables $\rightarrow$ F(State variables)

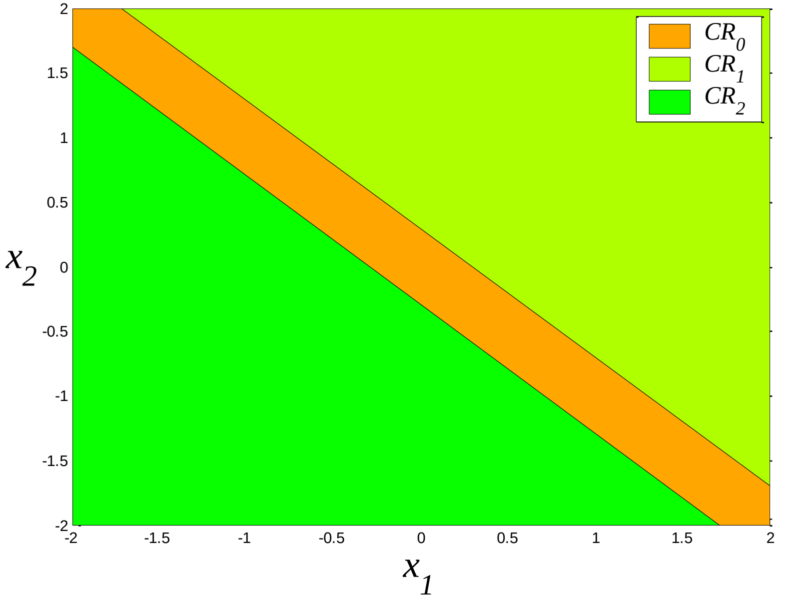
Multi-parametric Quadratic Program

Explicit Control Law

$$J(x(t)) = \min_{u_{t|t}, u_{t+1|t}} \sum_{j=0}^{1} \left\{ \mathbf{x}_{t+j|t}^T \mathbf{x}_{t+j|t} + 0.01\ \mathbf{u}_{t+j|t}^2 \right\} + \mathbf{x}_{t+2|t}^T P \mathbf{x}_{t+2|t}$$

$$\text{s.t} \quad \mathbf{x}_{t+j+1|t} = \begin{bmatrix} 0.7326 & -0.0861 \\ 0.1722 & 0.9909 \end{bmatrix} \mathbf{x}_{t+j|t} + \begin{bmatrix} 0.0609 \\ 0.0064 \end{bmatrix} \mathbf{u}_{t+j|t}$$

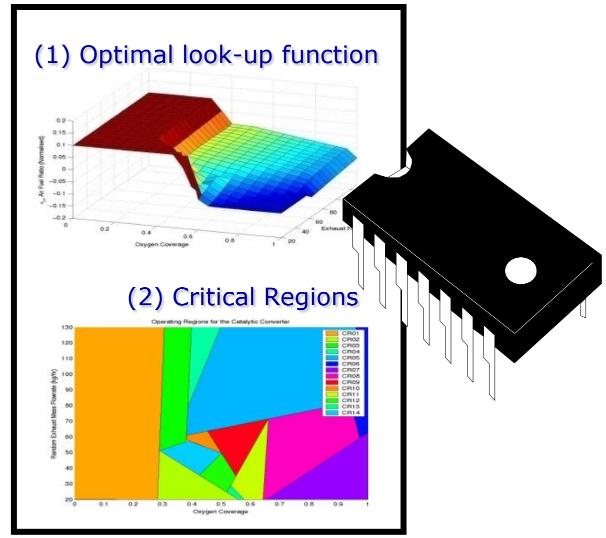
$$-2 \le \mathbf{u}_{t+j|t} \le 2 \quad \text{j} = 1,2 \quad \mathbf{x}_{t|t} = \mathbf{x}(t)$$



$$\mathbf{u}(t) = \begin{cases} [-6.8355 \ \ -6.8585]\,\mathbf{x}(t) & \textbf{if} \ \begin{bmatrix} 0.7059 & 0.7083 \\ -0.7059 & -0.7083 \end{bmatrix} \mathbf{x}(t) \le \begin{bmatrix} 0.2065 \\ 0.2065 \end{bmatrix} \\ -2 & \textbf{if} \ [-0.7059 \ \ -0.7083]\,\mathbf{x}(t) \le -0.2065 \\ 2 & \textbf{if} \ [0.7059 \ \ 0.7083]\,\mathbf{x}(t) \le -0.2065 \end{cases}$$

Multi-parametric Controllers

Optimization Model



Parametric Controller

Control Action

Measurements

SYSTEM

System Outputs

Input Disturbances

MPC-on-a-chip!

- **Explicit Control Law**
- **Eliminate expensive, on-line computations**
- **Valuable insights !**

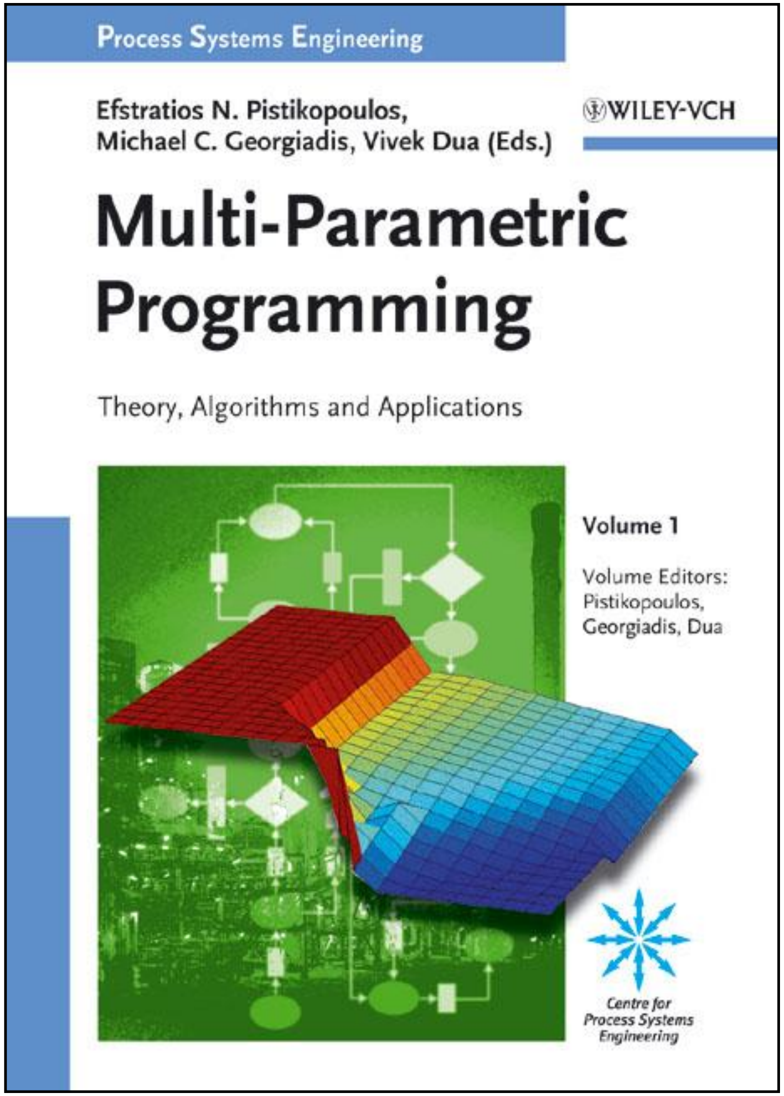
Key milestones-Historical Overview

AIChE J.,Perspective (2009)

- Number of publications

	Multi-Parametric Programming	Multi-Parametric MPC & applications
Pre-1999	**>100**	**0**
Post-1999	**~70**	**250+**

- 2002 Automatica paper ~ 580 citations
- Multi-parametric programming – until 1992 mostly analysis & linear models
- Multi-parametric/explicit MPC – post-2002 much wider attention


Process Systems Engineering
Efstratios N. Pistikopoulos,
Michael C. Georgiadis, Vivek Dua (Eds.)
WILEY-VCH
Multi-Parametric Programming
Theory, Algorithms and Applications
Volume 1
Volume Editors:
Pistikopoulos,
Georgiadis, Dua
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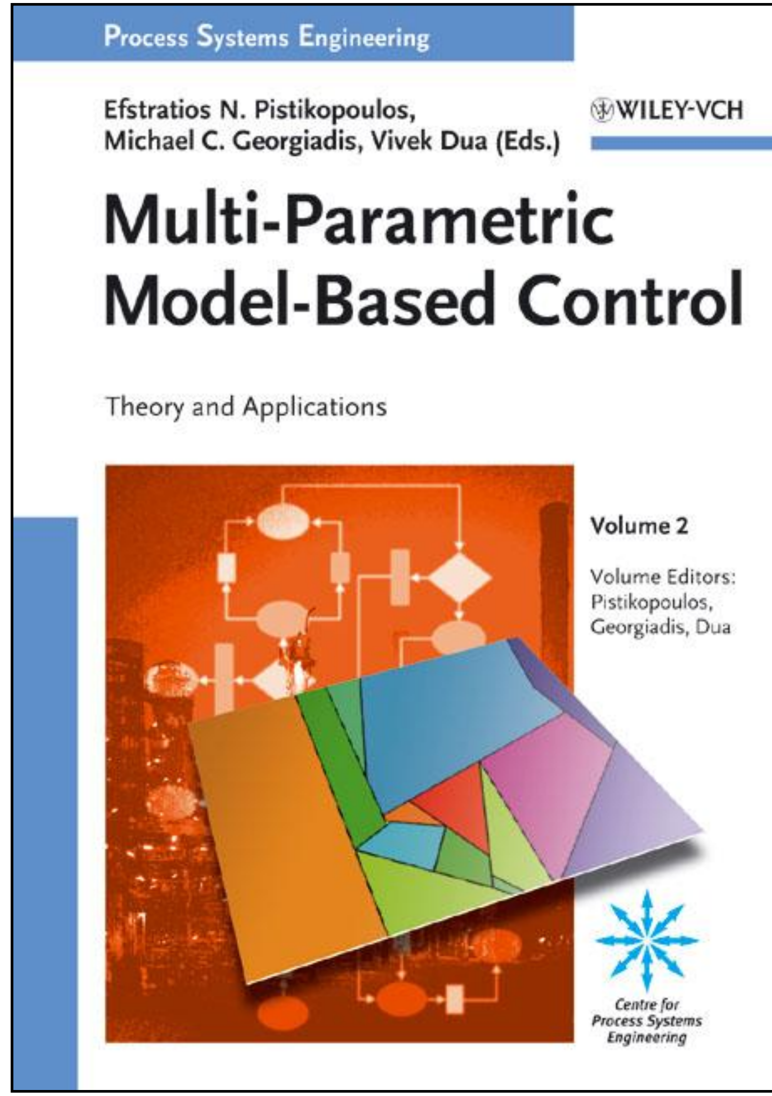
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WILEY-VCH
Multi-Parametric Model-Based Control
Theory and Applications
Volume 2
Volume Editors:
Pistikopoulos,
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Patented Technology

- Improved Process Control

  European Patent No EP1399784, 2004

- Process Control Using Co-ordinate Space

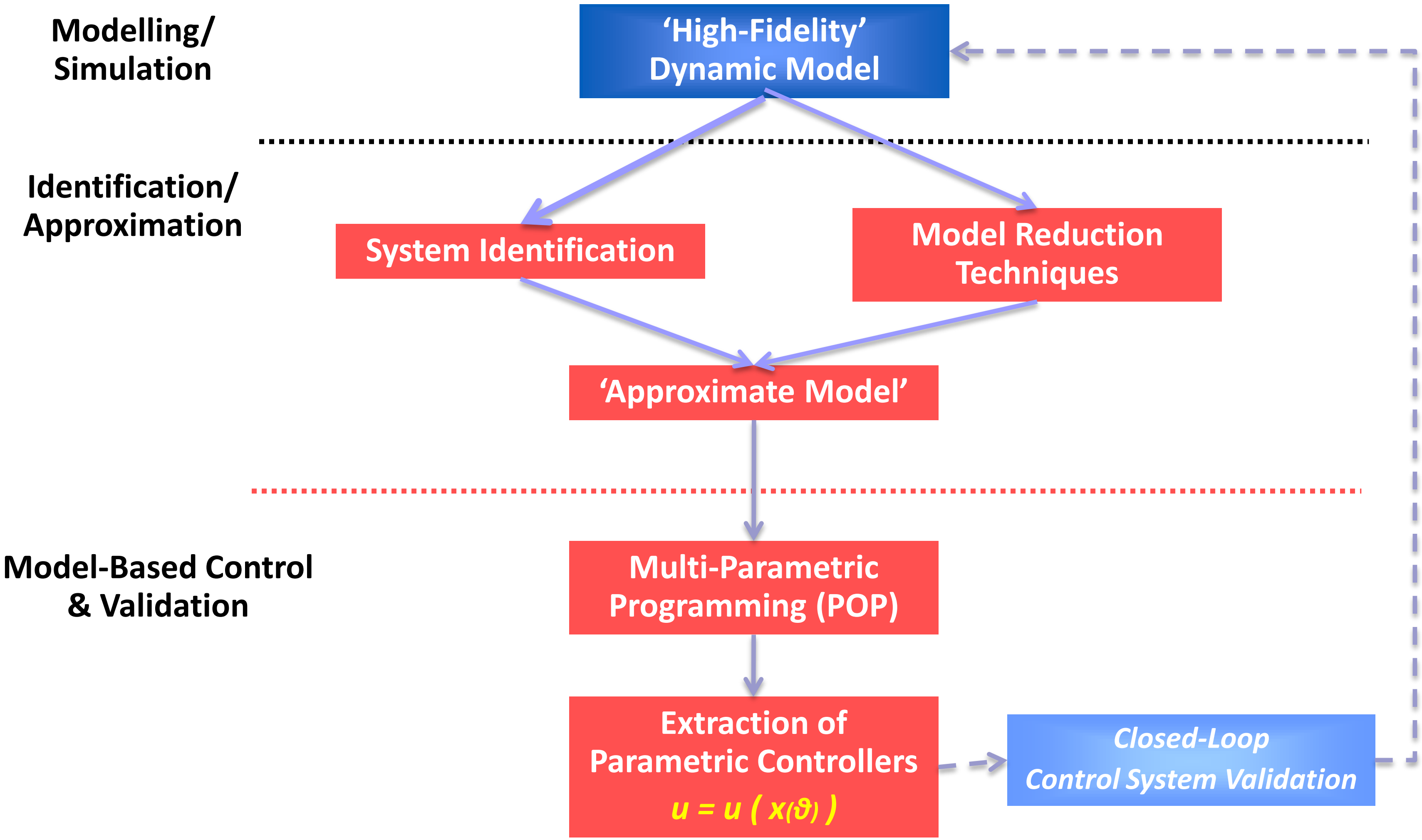
  United States Patent No US7433743, 2008

ParOS
Advanced control technology on a chip

Outline

- Key concepts & historical overview
- Recent developments in multi-parametric programming and mp-MPC
  - Model reduction/approximation
  - mp-NLP & explicit nonlinear mp-MPC
  - mp-MILP
  - Robust explicit mp-MPC
  - State estimation and mp-MPC
  - Framework for mp-MPC

A framework for multi-parametric programming & MPC *(Pistikopoulos 2008, 2009)*



Model Reduction/Approximation

$$\dot{x} = f(x,u)$$
$$x = g(\dot{x}, x, u)$$
$$y = g(x,u)$$

Replace discrete dynamical System with a set of affine algebraic models

N-step ahead prediction- enables use of Linear MPC routines

$$\underset{\Delta u}{\text{Min}} \left\{ y^{*T}_{t+N} P y^{*T}_{t+N} + \sum_{k=0}^{N-1} y^{*T}_{t+k} Q y^{*}_{t+k} + \delta u^{T}_{t+k} R \delta u_{t+k} \right\}$$

st:

$$y^{*}_{t+k} = y_{t+k} - y_{sp},\ k = 1 \dots N$$

$$y_{t+k} = A_k x_t + B_k U + C_k,\ k = 1 \dots N$$

$$u_{t+k} = u_{t+k-1} + \delta u_{t+k},\ k = 1 \dots N$$

$$y_k \in \mathcal{Y},\ k = 0 \dots N$$

$$u_k \in \mathcal{U},\ k = 0 \dots N$$

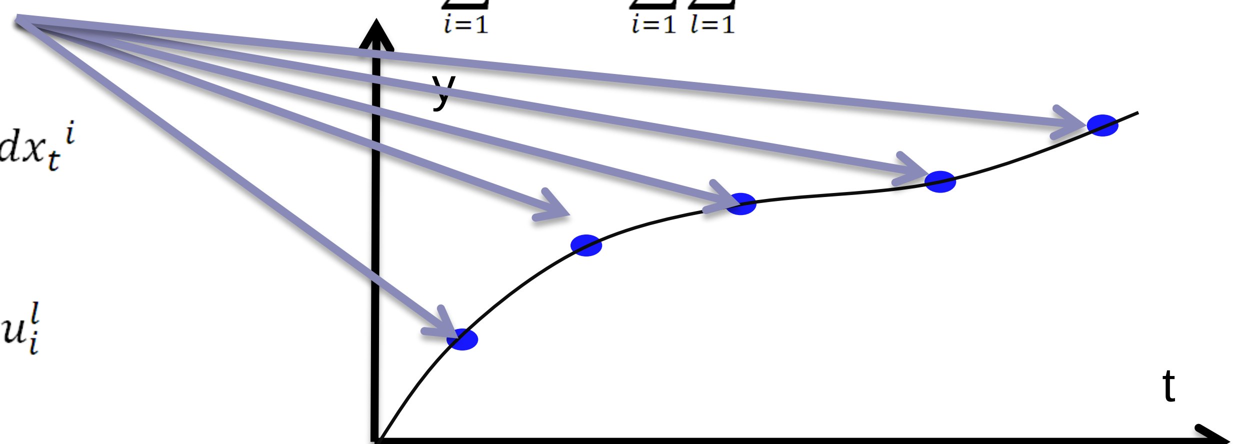
Model Reduction/Approximation

- N-step-ahead approximation based on initial conditions (measurements) and sequence of controls (constant control vector parameterization). Set of affine algebraic models
- For all j point over the time horizon - approximations are constructed as follows

$$y_j = f_j\left(x_t{}^1, x_t{}^2, \ldots, x_t{}^n, u_1, u_2, \ldots, u_j\right) \approx \alpha_0 + \sum_{i=1}^{n} \alpha_i x_t{}^i + \sum_{i=1}^{j}\sum_{l=1}^{m} \alpha_i^l u_i^l$$

$$\alpha_i = \int_0^1 f_i(x_t{}^i)\varphi_1(x_t{}^i)dx_t{}^i$$

$$\alpha_j^l = \int_0^1 f_j^l(u_i^l)\varphi_1(u_i^l)du_i^l$$



mp-NLP Algorithms for Explicit NMPC

Strategy: **Direct Approach**

Multi-parametric Nonlinear Dynamic Optimization Problem

↓

Discretize state and controls via Orthogonal Collocation Techniques

Approximate ↓

Multi-parametric Nonlinear Programming Problem (mp-NLP)

↙ ↘

Quadratic Approximation Based
Solve sequence of mp-QP's

Nonlinear Sensitivity based
Solve sequence of NLP's

↘ ↙

Partition state space recursively

mp-NLP Algorithms for Explicit NMPC

Key features: Two implementations for the characterization of the Parameter space

Quadratic Approximation based (General mp-NLP)

- Characterizes the parameter space by sub-partitioning CRs where the QA approximation provides “poor” solutions.

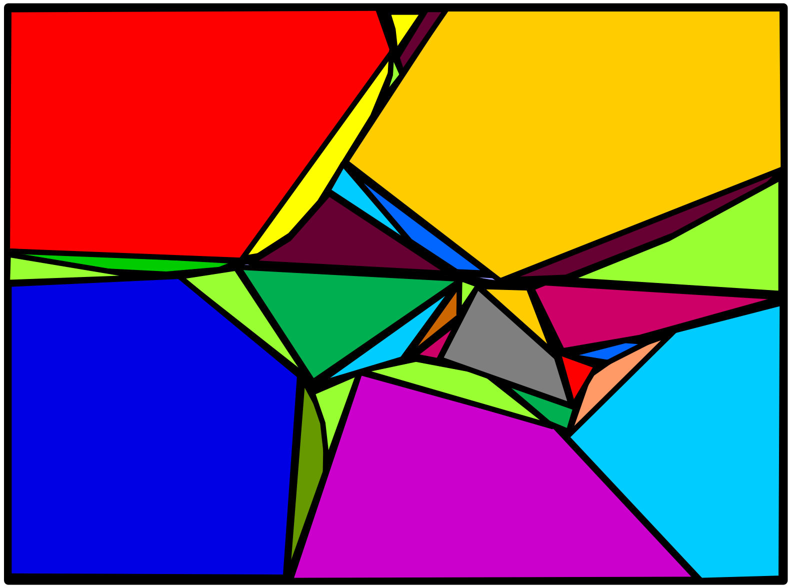
NLP Sensitivity Based (NMPC mp-NLP)

- Characterizes the parameter space using NLP sensitivity information and linearization of the constraints.

$$\begin{pmatrix} v(x) \\ \lambda(x) \\ \mu(x) \end{pmatrix} = \begin{pmatrix} v_0 \\ \lambda_0 \\ \mu_0 \end{pmatrix} - (M_0)^{-1} N_0 + (x - x_0) + \phi(||x||)$$

Validity of approximation:

$\phi(x) = O(||x||) \Rightarrow (x)/||x|| \rightarrow 0$ as $x \rightarrow 0$.



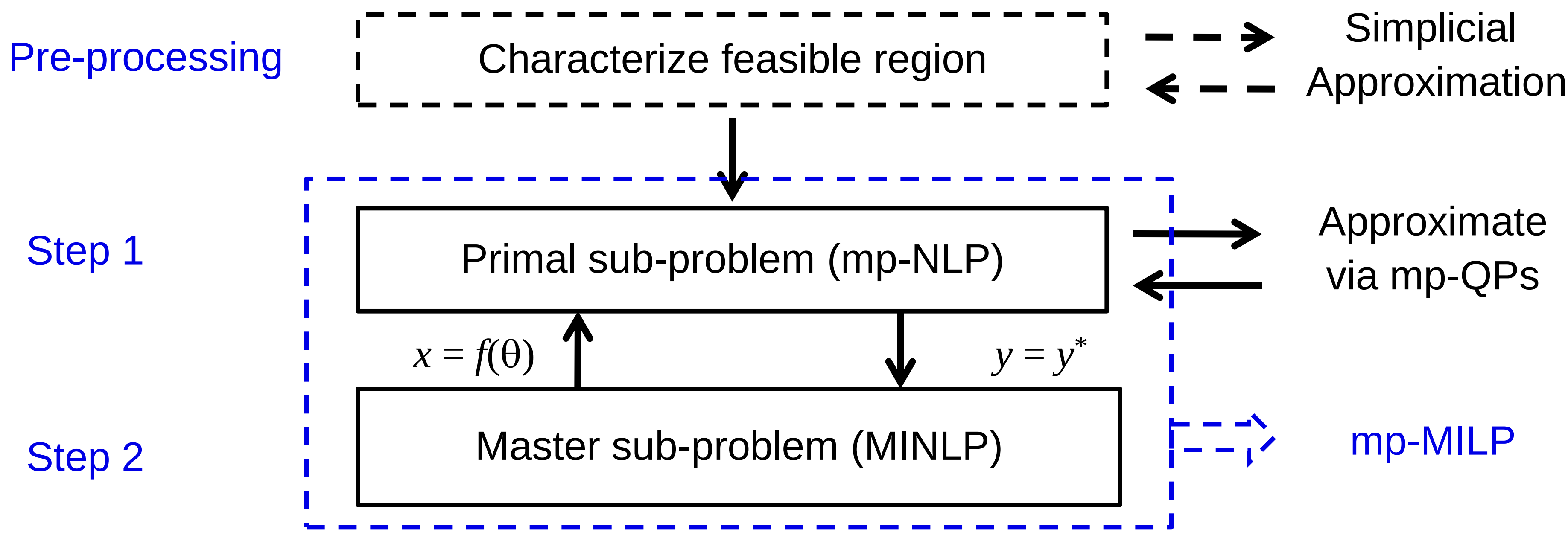
mp-NLP Algorithms for Explicit NMPC

Key Advantage: Fast implementation of the control laws

- State-of-the art multi-parametric solvers (e.g. mp-QP)
- Straightforward characterization of critical regions
- Complexity reduction through region merging
- Extension to address hybrid systems

Multiparametric Mixed-Integer Nonlinear Programming

Strategy: **Decompose mp-MINLP into two sub-problems**



Iterate until master sub-problem is infeasible

Explicit Solution of the general mp-MILP Problem

$$
\begin{aligned}
& z(\theta) := \min_{x,y} c(\theta)^T x + d(\theta)^T y \\
s.t. \quad & A(\theta)x + E(\theta)y \le b(\theta) \\
& x \in \mathbb{R}^n, x_{min} \le x \le x_{max}, \; y \in \{0,1\}^q \\
& \theta \in \mathbb{R}^p, \theta_{min} \le \theta \le \theta_{max}
\end{aligned}
$$

Applications

- **Pro-active Scheduling** under price, demand and processing time uncertainty *(seee poster & paper)*
- **Explicit Model Predictive Control** of **Hybrid Systems**: Control actions as *optimization variables*, states as *parameters*, input and model disturbances *as parameters*
- **Integration of scheduling & MPC**

Hybrid Approach - Two-Stage Method for mp-MILP[1]

Stage 1 – Reformulation

Partially robust RIM-mp-MILP* model;

Solutions are immunized against all *immeasurable parameters* and *complicating constraint matrix uncertainty*

↓

Stage 2 – Solution

Suitable multi-parametric programming algorithms *(e.g. Faisca et al. (2009))*

↓

Optimal partially robust solution; Upper bound on optimal objective function value

[1] *Wittmann-Hohlbein, Pistikopoulos (2011)*

*objective function coefficient and right hand side vector uncertainty

Global Optimization of mp-MILP[1]

Constraint matrix uncertainty poses major challenge ⟶ mp-MINLP

Multi-Parametric Global Optimization:

- Adaptation of strategies from the deterministic case to multi-parametric framework: *Parametric B&B procedure*
- Globally optimal solution is a piecewise affine function over polyhedral convex critical regions

Challenges in Global Optimization of mp-MILP Problems:

- *Comparison of parametric profiles*, not scalar values
- High computational requirements

↓

Can we find *"good solutions"* of an mp-MILP problem with less effort?

[1] *Wittmann-Hohlbein, Pistikopoulos; JOGO, submitted , 2011*

Robust Explicit mp-MPC

- Famous control problem: Dynamic Systems with Model Uncertainties (Mayne, *Rawlings, Rao & Scokaert, 2000*)

$$V(x) = \min_{U} \left\{ \sum_{k=0}^{N-1} (x_k' Q x_k + u_k' R u_k) + x_N' P x_N \right\}$$

$$x_{k+1} = \mathbf{A} x_k + \mathbf{B} u_k + W\theta_k$$

$$C x_k + D u_k \le d$$

$$M x_N \le \mu$$

$$u_{min} \le u \le u_{max}$$

$$x_0 = x$$

x: system states

u: control inputs

$U = [u_0' \quad \dots \quad u_{N-1}']'$

Parametric Uncertain System

$$A = [a_{ij}] \in \mathbb{R}^{n\times n},\ B = [b_{ij}] \in \mathbb{R}^{n\times m}$$

$$a_{ij} \in \left\{ a_{ij} : |a_{ij} - a_{ij,0}| \le \varepsilon a_{ij,0} \right\}$$

$$b_{ij} \in \left\{ b_{ij} : |b_{ij} - b_{ij,0}| \le \varepsilon b_{ij,0} \right\}$$

Exogenous Disturbance

$$\theta_{min} \le \theta \le \theta_{max}$$

- Uncertainty due to modelling, identification errors, measurement errors etc.
- Constraints represent safety, operational constraints
- It is very *critical* that the system does not violate them
- Immunize against uncertainty

Robust Explicit mp-MPC

- Robustification – robust reformulation step (*Ben-Tal & Nemirovski, 2000; Floudas& Co-workers, 2004-2007*)
- Dynamic Programming framework to Robust MPC
- Novel Multi-parametric Programming algorithm to constrained Dynamic Programming (*Faísca, Kouramas, Saraiva, Rustem & Pistikopoulos, 2008*)
  - Small mp-QP at each stage
  - No need for global optimization

MHE & mp-MPC

$$\min_{\bar{x}_0,\bar{u}_k} \left\| \bar{x}_{N_{MPC}} \right\|^2_{P_{MPC}} + \sum_{k=0}^{N_{MPC}} \left\| \bar{x}_k \right\|^2_{Q_{MPC}} + \sum_{k=0}^{N_{MPC}-1} \left\| \bar{u}_k \right\|^2_{R_{MPC}}$$

$$\text{s.t. } x_{k+1} = Ax_k + Bu_k + Gw_k \text{ (actual system)},$$

$$\bar{x}_{k+1} = A\bar{x}_k + B\bar{u}_k \text{ (nominal system)},$$

$$\hat{x}_{k+1} = A\hat{x}_k + Bu_k + t \text{ (estimated system step 1.3)},$$

$$u_0 = \bar{u}_0^* - K\left(\hat{x}_0^* - \bar{x}_0^*\right), \bar{u} \in \mathbf{U} \ominus K \cdot \bar{\mathbf{S}}, \bar{x}_{N_{MPC}} \in \bar{\mathbf{X}}_{\bar{T}},$$

$$\bar{x}_k \in \bar{\mathbf{X}} \equiv \mathbf{X} \ominus \mathbf{S}, k = 1 \ldots N_{MPC} - 1, \mathbf{S} = \mathbf{E}_x \oplus \bar{\mathbf{S}}, \hat{x}_0 \in \bar{x}_0 \oplus \bar{\mathbf{S}},$$

$$\bar{\mathbf{S}} \text{ is mRPI of } \hat{x}_{k+1} - \bar{x}_{k+1} = (A - BK)(\hat{x}_k - \bar{x}_k) + t.$$

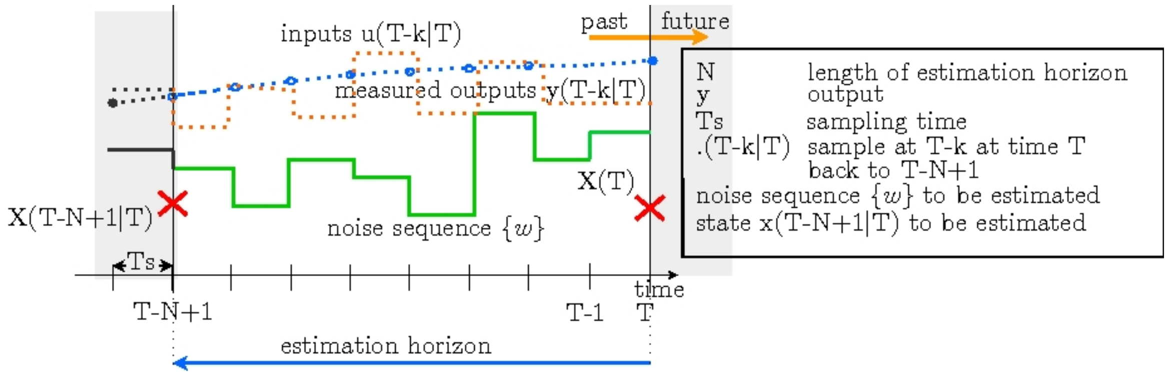
Main idea:

Step 1. Formulate the dynamics that govern the estimation error $e_T = f\left(e_{T-1}, w_{T-1}\right)$

Step 2. Use these dynamics to find the set that bounds the estimation error $e_T \in \bar{S}$

Step 3. Incorporate the bounding set into the controller to ‘robustify’ against the estimation error

Moving Horizon Estimation (MHE)



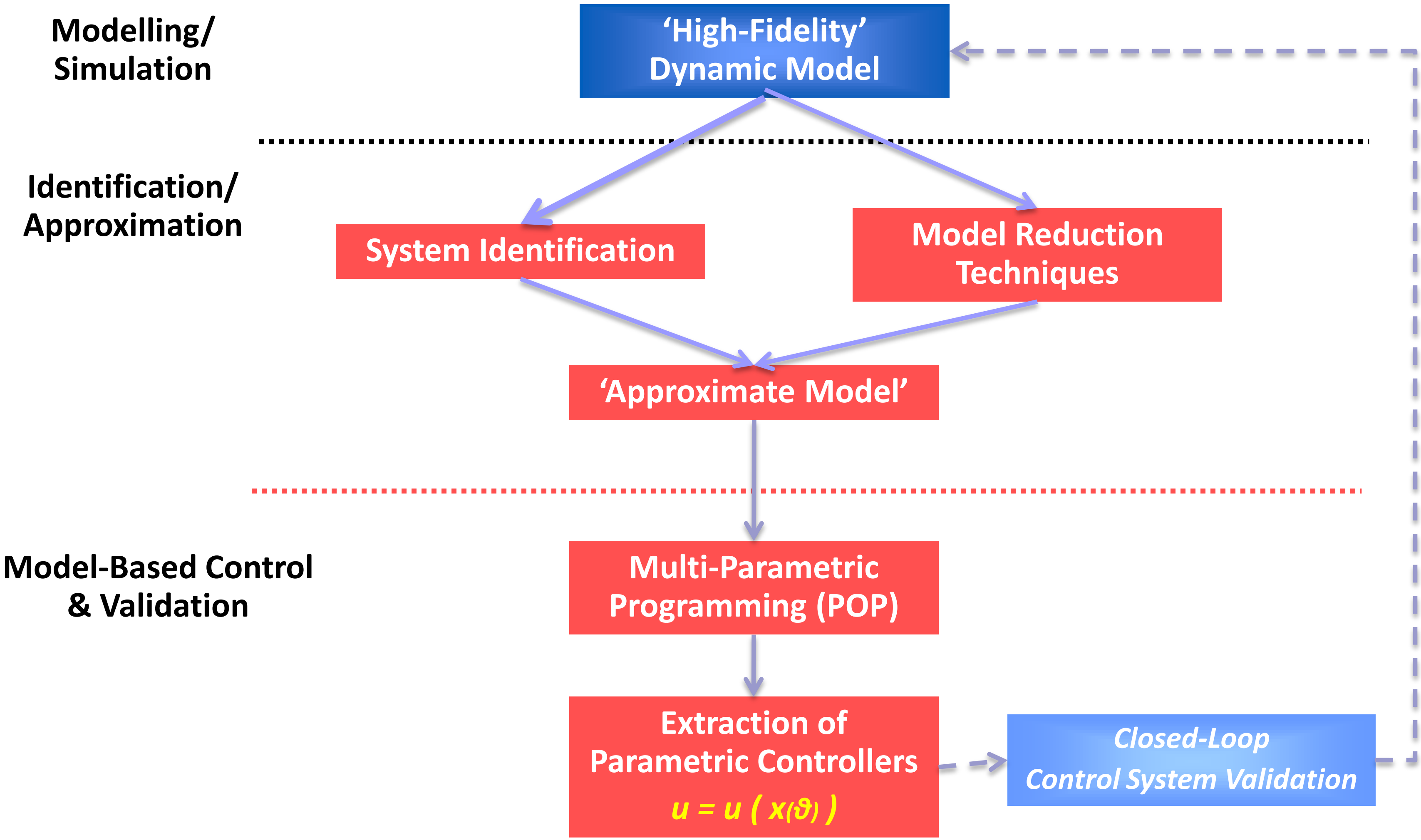
$$\min_{\hat{x}_{T-N|T},\hat{W}_{T-N|T}} \left\|\hat{x}_{T-N|T} - \underline{x}_{T-N|T}\right\|^2_{P^{-1}} - \left\|Y_{T-N}^{T-1} - \mathcal{O}\hat{x}_{T-N|T} - c\bar{b}U_{T-N}^{T-2}\right\|^2_{\mathcal{W}^{-1}} + \sum_{k=T-N}^{T-1}\left\|\hat{w}_k\right\|^2_{Q^{-1}} + \sum_{k=T-N}^{T}\left\|\hat{v}_k\right\|^2_{R^{-1}}$$

s.t. $\hat{x}_{k+1} = A\hat{x}_k + Bu_k + G\hat{w}_k, \quad \hat{y}_k = C\hat{x}_k + \hat{v}_k, \quad \hat{x}_k \in \mathbf{X}, \quad \hat{w}_k \in \mathbf{W}, \quad \hat{v}_k \in \mathbf{W}$

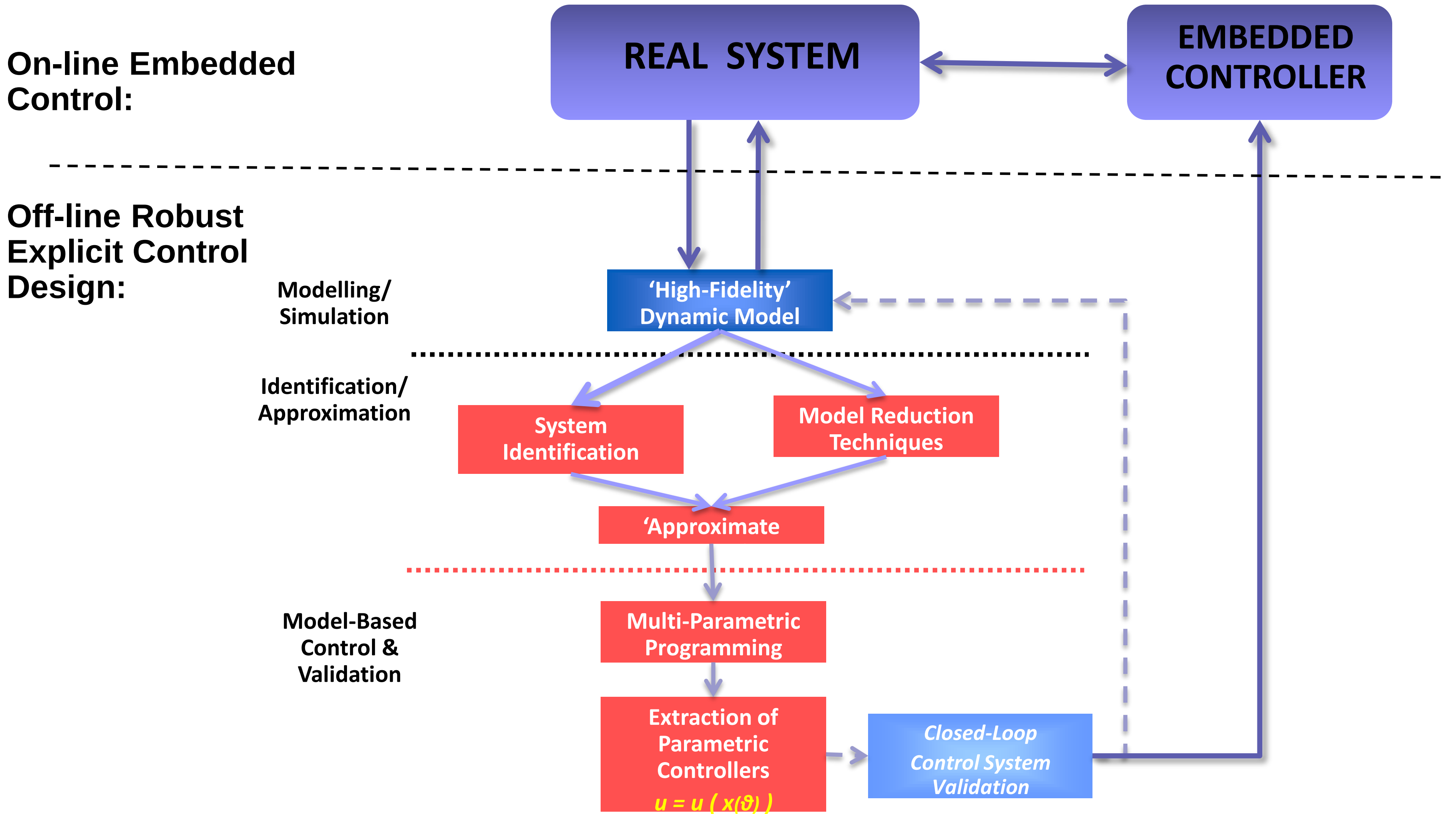
$\underline{x}_{T-N|T} = A\hat{x}^*_{T-N-1|T-1} + Bu_{T-N-1|T-1} + G\hat{w}^*_{T-N-1|T-1}$ (smoothed update of arrival cost)

- Model-based state estimator
- Obtains current state estimate x_T
- Main advantage: incorporates system constraints
- MHE is dual to MPC: *backwards MPC*

A framework for multi-parametric programming & MPC *(Pistikopoulos 2008, 2009)*



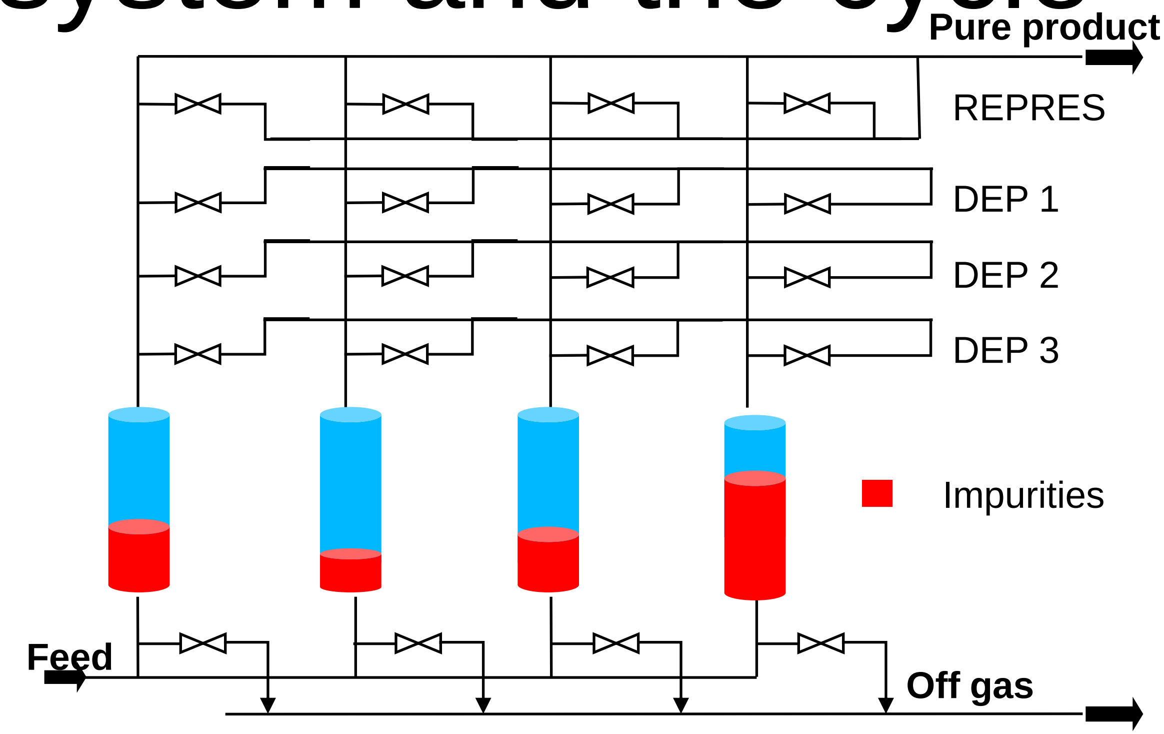
A framework for multi-parametric programming and MPC *(Pistikopoulos 2010)*



Outline

- Key concepts & historical overview
- Recent developments in multi-parametric programming and mp-MPC
- MPC-on-a-chip applications
  - PSA system
  - Fuel Cell system
  - Biomedical systems

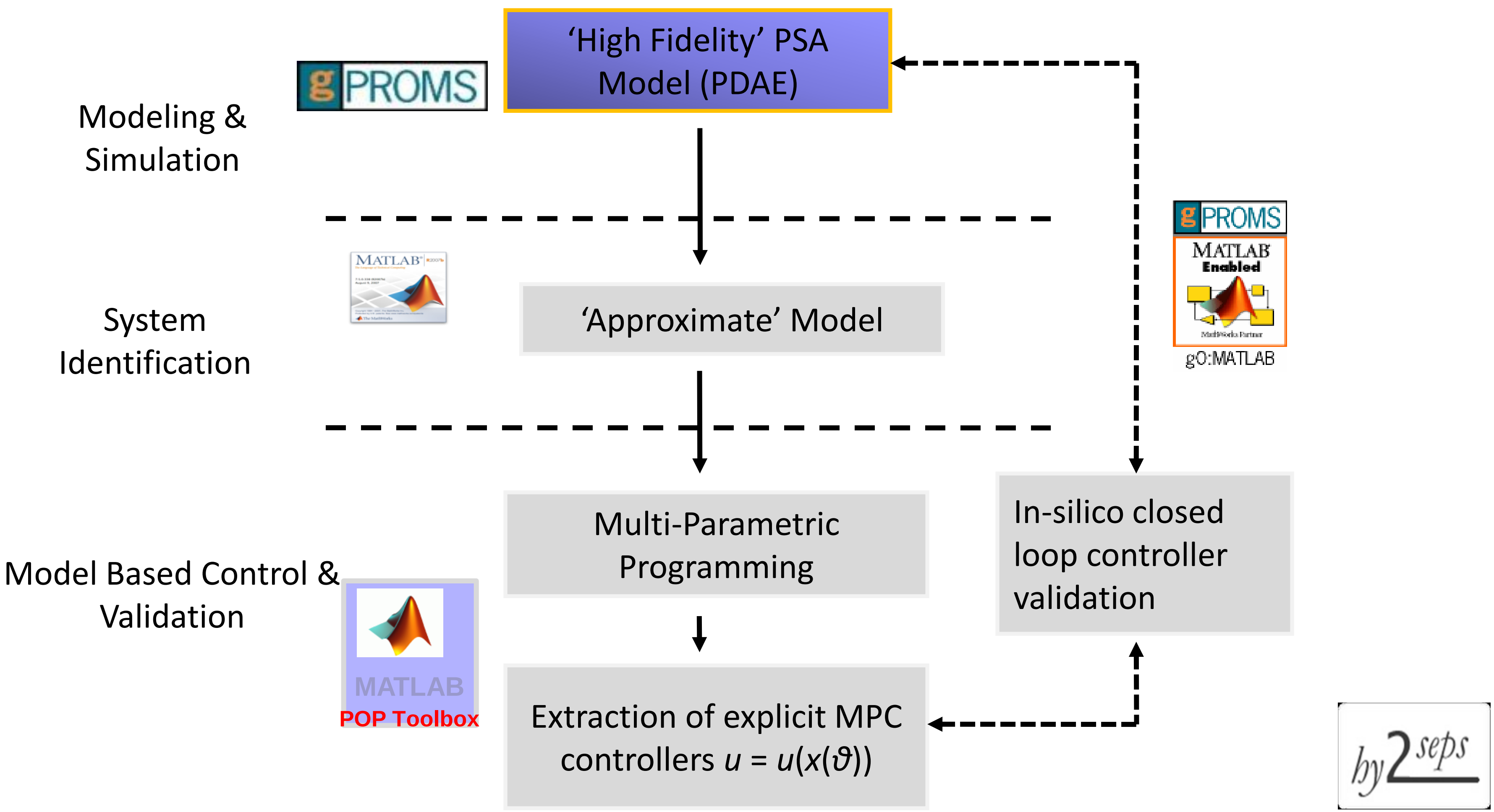
PSA system and the cycle



BED 1	FEED			DEP 1	DEP 2	DEP 3	Bd	Pu	PE 1	PE 2	REPRES
BED 2	PE 2	REPRES		FEED			DEP 1	DEP 2	DEP 3	Bd	Pu	PE 1
BED 3	Bd	Pu	PE 1	PE 2	REPRES		FEED			DEP 1	DEP 2	DEP 3
BED 4	DEP 1	DEP 2	DEP 3	Bd	Pu	PE 1	PE 2	REPRES		FEED		

Time →

A framework for multi-parametric programming and mp-MPC for PSA



Modelling - internal Bed

Mass balance

Species Accumulation

Mass transfer with adsorbent

$$(\varepsilon_b + (1-\varepsilon_b)\varepsilon_p)\frac{\partial C_i}{\partial t} + \frac{\partial U C_i}{\partial Z} + \rho_p (1-\varepsilon_b)\frac{\partial \bar{Q}_i}{\partial t} = \varepsilon_b D_{Zi} \frac{\partial^2 C_i}{\partial Z^2}$$

Bulk fluid convection

Dispersion in axial direction

- Radial effects neglected
- Transport properties independent of state variables
- Axial mass dispersion (Wakao and Funazkri, 1978), velocity dependent neglected

Energy balance

Energy accumulation in gas phase — Energy accumulation in adsorbed phase — Energy accumulation in solid phase

$$(\varepsilon_b + (1-\varepsilon_b)\varepsilon_p) \sum_{i=1}^{NCOMP} C_{v_i} C_i \frac{\partial T}{\partial t} + (1-\varepsilon_b)\rho_p \sum_{i=1}^{NCOMP} C_{v_i} \bar{Q}_i \frac{\partial T}{\partial t} + (1-\varepsilon_b) C_{ps} \rho_p \frac{\partial T}{\partial t} +$$

$$U \sum_{i=1}^{NCOMP} C_{p_i} C_i \frac{\partial T}{\partial Z} - (\varepsilon_b + (1-\varepsilon_b)\varepsilon_p) RT \sum_{i=1}^{NCOMP} \frac{\partial C_i}{\partial t} - (1-\varepsilon_b)\rho_p \sum_{i=1}^{NCOMP} \frac{\partial \bar{Q}_i}{\partial t}(-\Delta H_i) = \lambda \frac{\partial^2 T}{\partial Z^2}$$

Energy convection — Heat of adsorption — Heat dispersion

- Lumped energy balance on gas and solid phase
- Radial effects neglected
- Specific heat, transport properties independent of state variables
- Axial mass dispersion (Wakao et.al., 1978), velocity dependent neglected

Momentum balance & adsorption characteristics

$$-\frac{\partial P}{\partial Z} = \frac{150\mu(1-\varepsilon)^2}{\varepsilon^3 d_p^2} U + \frac{1.75(1-\varepsilon)\sum_{i=1}^{NCOMP} C_i MW_i}{\varepsilon^3 d_p} |U| U$$

Ergun's equation, steady state pressure drop

$$\frac{\partial \bar{Q}_i}{\partial t} = K_{LDF_i}\left(Q_i^* - \bar{Q}_i\right)$$

LDF Rate expression

$$\frac{Q_i^*}{Q_i^{max}} = a_i K_i C_i RT \left[1 - \sum_{i=1}^{NCOMP} \frac{Q_i^*}{Q_i^{max}}\right]^{a_i}$$

$$K_i = K_{\infty_i} \exp\left(\frac{-\Delta H_i}{RT}\right)$$

Nitta et.al. (1984), Ribeiro et.al. (2008), multisite Langmuir adsorption isotherm (multi-component mixture)

Valve Equation (for boundary conditions)

Chou and Huang (1994), Nilchan and Pantelides (1998)

$$U = \begin{cases} \phi C_V \sqrt{1 - \left(\dfrac{P_{High} - P_{Low}}{P}\right)^2} & if \ \dfrac{P_{Low}}{P_{High}} < P_{critical} \\ C_V \dfrac{P_{High}}{P} & Otherwise \end{cases}$$

$$P_{critical} = \left(\frac{2}{1+\gamma}\right)^{\frac{\gamma}{1-\gamma}} \qquad \gamma = \frac{C_p}{C_v}$$

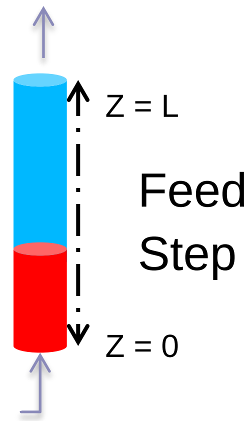
$P = P_{High}$ if gas leaving the bed

$= P_{Low}$ if gas entering the bed

- Prictical constant since Cp and Cv are assumed constant
- For REPRES and DEP Cp and Cv calculated at $y_{H_2} = 0.7$, $y_{CH_4} = 0.3$
- For blowdown and purge (off gas) Cp and Cv calculated at $y_{H_2} = 0.5$, $y_{CH_4} = 0.5$

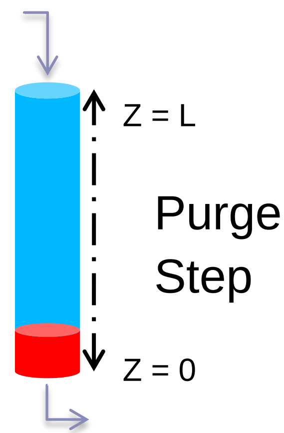
Constraints - Boundary conditions

Z = 0	Z = L
$UA = Q_{SLPM}(P_{FEED}, T_{FEED})$	$P = P_{PRODUCT}$
$C_i = \frac{PY_{Feed_i}}{RT}$	$\frac{\partial C_i}{\partial Z} = 0$
$T = T_{Feed}$	$\frac{\partial T}{\partial Z} = 0$



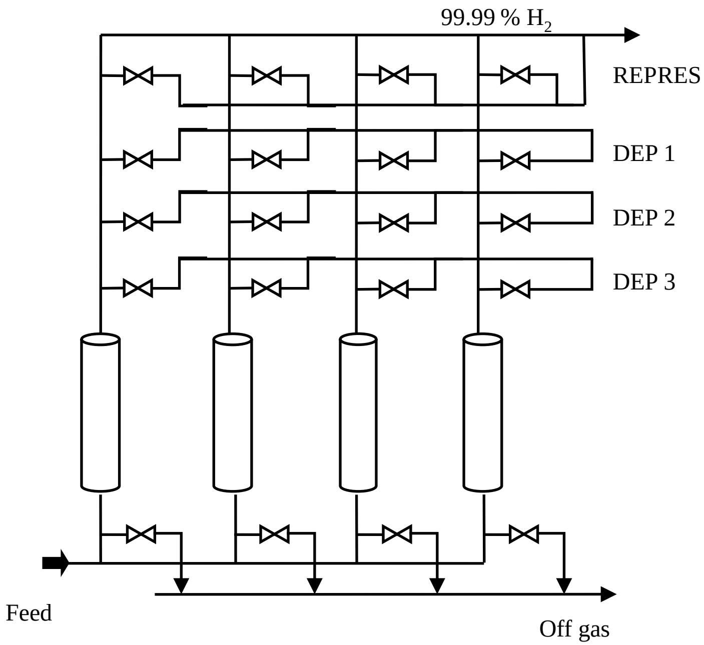
A boundary condition for each process step

Z = 0	Z = L
$U = f_{Valve}\left(P_{PURGE}, P_{CODEP}, Cv_{PURGE}\right)$	$U = \frac{\left(U \Sigma_i C_i\right)_{CODEP}}{\Sigma_i C_i}$
$\frac{\partial C_i}{\partial Z} = 0$	$C_i = \frac{PC_{CODEP_i}}{RT \Sigma_i C_{CODEP_i}}$
$\frac{\partial T}{\partial Z} = 0$	$T = T_{CODEP}$



Base case system

Number of Beds	4	Adsorbent	Activated Carbon
Feed pressure	7 bars	Bed length	1 m
Blowdown pressure	1.01325 bars	Bed diameter	0.12 m
Bed Porosity	0.4	Feed temperature	303.15 K
Feed Composition	70 % H_2, 30 %CH_4	Feed flow rate	8.0 SLPM



<table>
<tr><td>BED 1</td><td colspan="3">FEED</td><td>DEP 1</td><td>DEP 2</td><td>DEP 3</td><td>Bd</td><td>Pu</td><td>PE 1</td><td>PE 2</td><td colspan="2">REPRES</td></tr>
<tr><td>BED 2</td><td>PE 2</td><td colspan="2">REPRES</td><td colspan="3">FEED</td><td>DEP 1</td><td>DEP 2</td><td>DEP 3</td><td>Bd</td><td>Pu</td><td>PE 1</td></tr>
<tr><td>BED 3</td><td>Bd</td><td>Pu</td><td>PE 1</td><td>PE 2</td><td colspan="2">REPRES</td><td colspan="3">FEED</td><td>DEP 1</td><td>DEP 2</td><td>DEP 3</td></tr>
<tr><td>BED 4</td><td>DEP 1</td><td>DEP 2</td><td>DEP 3</td><td>Bd</td><td>Pu</td><td>PE 1</td><td>PE 2</td><td colspan="2">REPRES</td><td colspan="3">FEED</td></tr>
</table>

$$t_{FEED} = t_{DEP1} = t_{DEP2} = t_{DEP3} = t_{Bd} = t_{Pu} = t_{PE1} = t_{PE2} = t_{REPRES} = \tau$$ Adsorption time

Objective and process variables

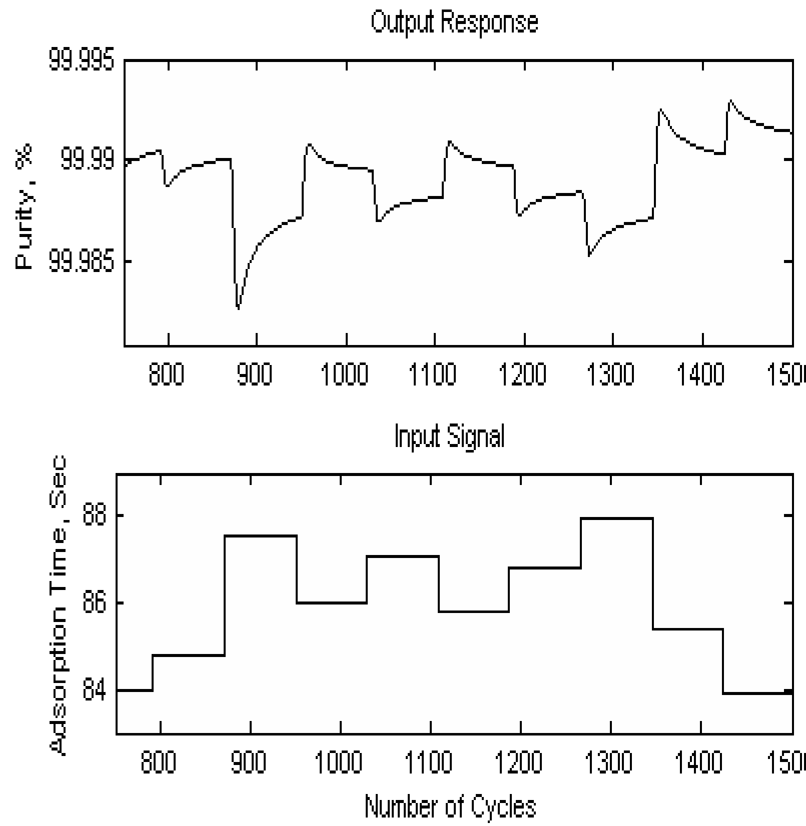
- Changes in adsorption time effects purity the most
  - Adsorption time – Manipulated variable

- Purity – Controlled variable

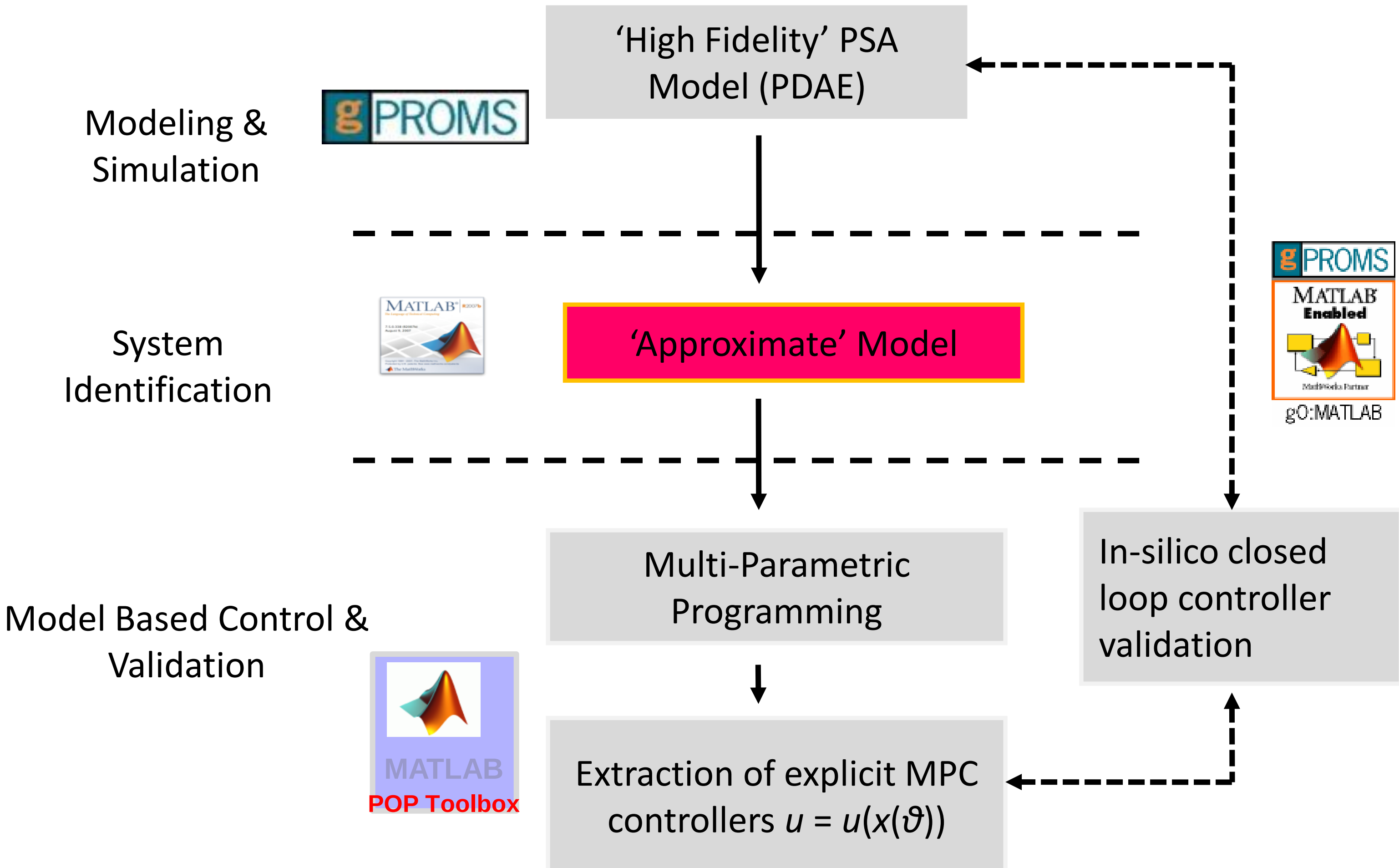
- Fast tracking of H_2 purity to the set point **99.99**%

- Regulate changes in adsorption time
  - Avoid bed saturation
  - Avoid high fluid inlet velocities as it causes mechanical damage

- Hard constraints on adsorption time has to be satisfied for safe and economical operation



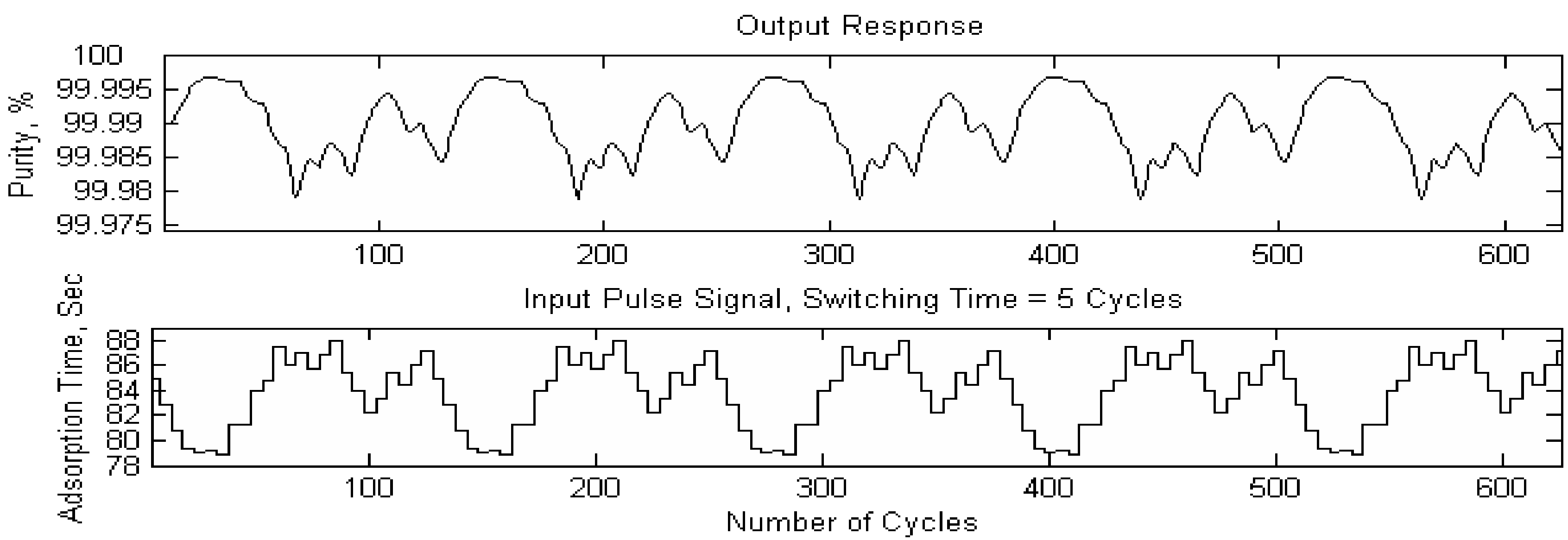
A framework for multi-parametric programming and MPC



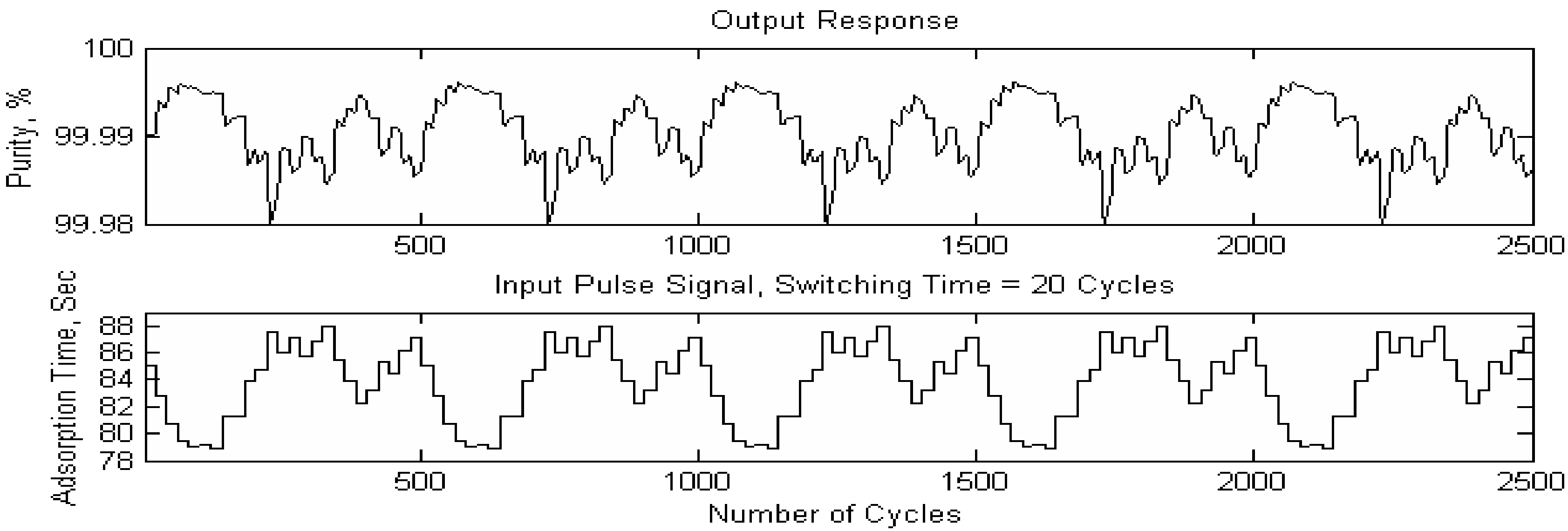
System Identification - Approximation

- PDAE model not suitable for current model based control approaches
  - Process model approximations are needed
- Input – Adsorption time
- Output – H_2 purity
- Sampling time – 1 PSA cycle

- Input signal design for system perturbation
  - Random pulse employed for persistent excitation
    - Maximum amplitude decided by hit and trial studies
    - Pulse duration (constant) calculation based on closed loop response



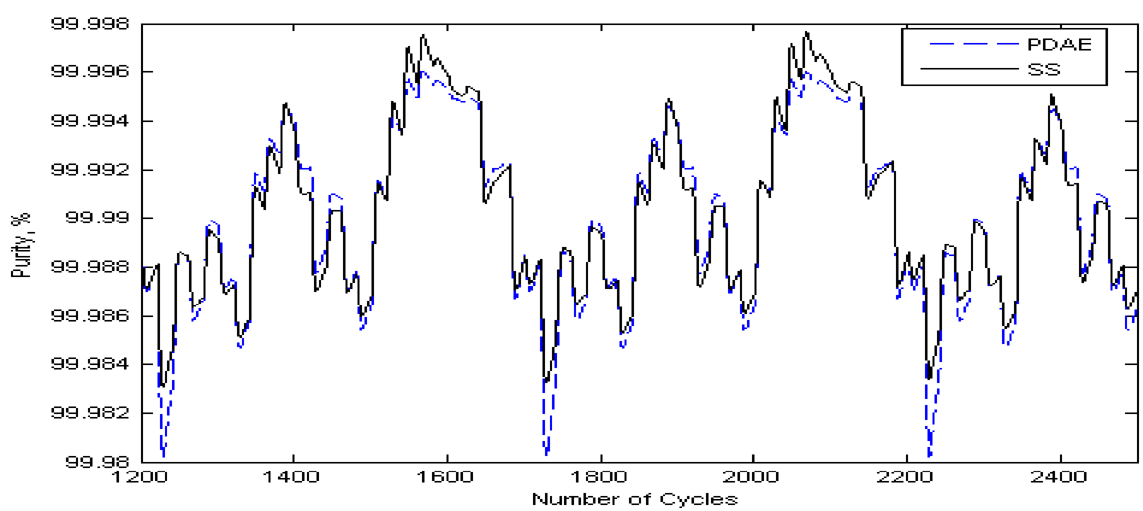
System identification



Model fit to the input output data above by an 8^{th} order state space system

$$x_{k+1} = Ax_k + Bu_k$$

$$y_k = Cx_k$$



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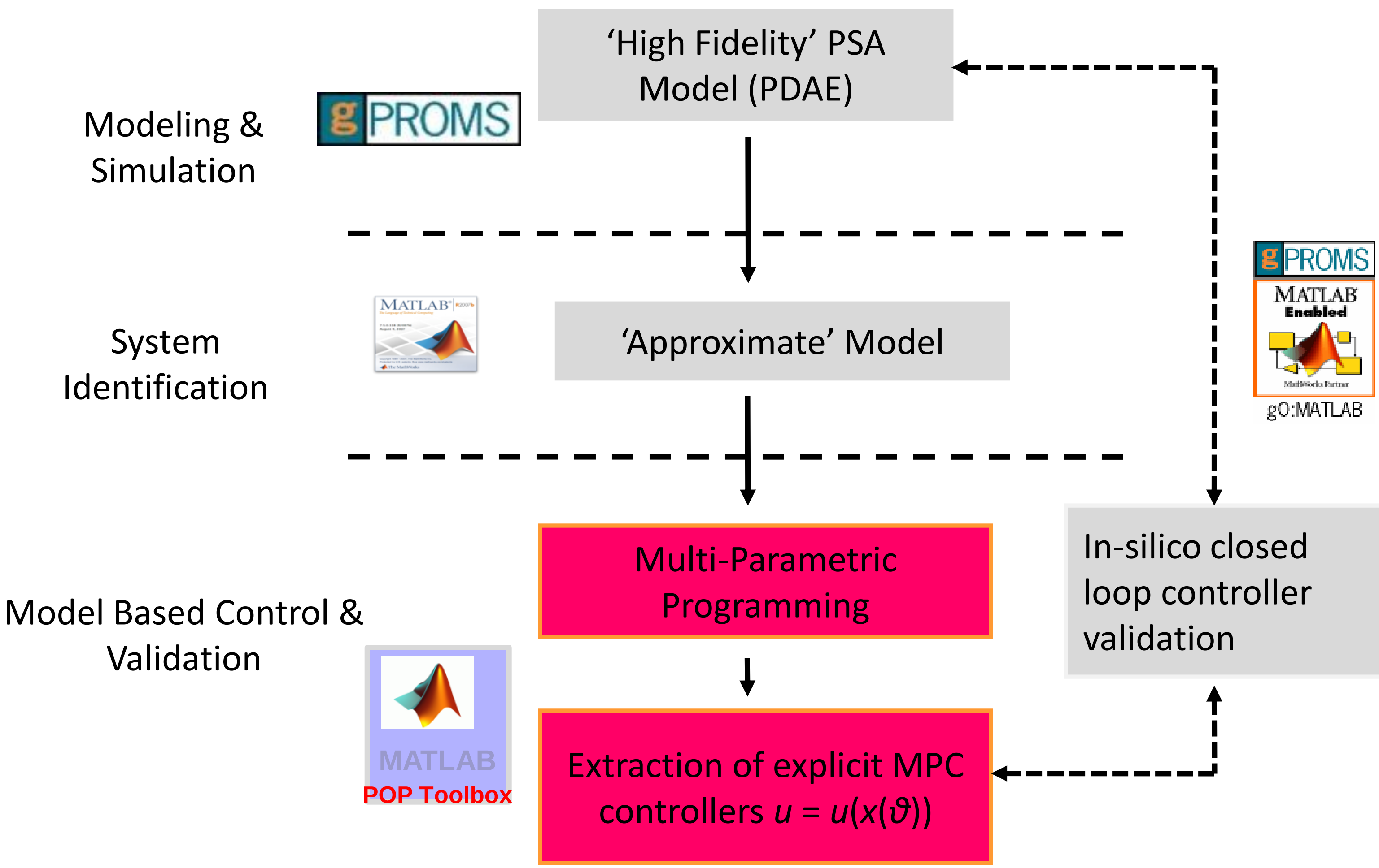


MPC Formulation for PSA

$$\min_{u} Z = \sum_{k=1}^{N-1} \left(y_k - y_k^R\right)' Q \left(y_k - y_k^R\right) + \sum_{k=0}^{M-1} \Delta u_k' R \Delta u_k$$

$$s.t.$$

$$x_{k+1} = Ax_k + Bu_k$$

$$y_k = Cx_k + y_{mismatch}$$

$$u_{low} \le u_k \le u_{high}$$

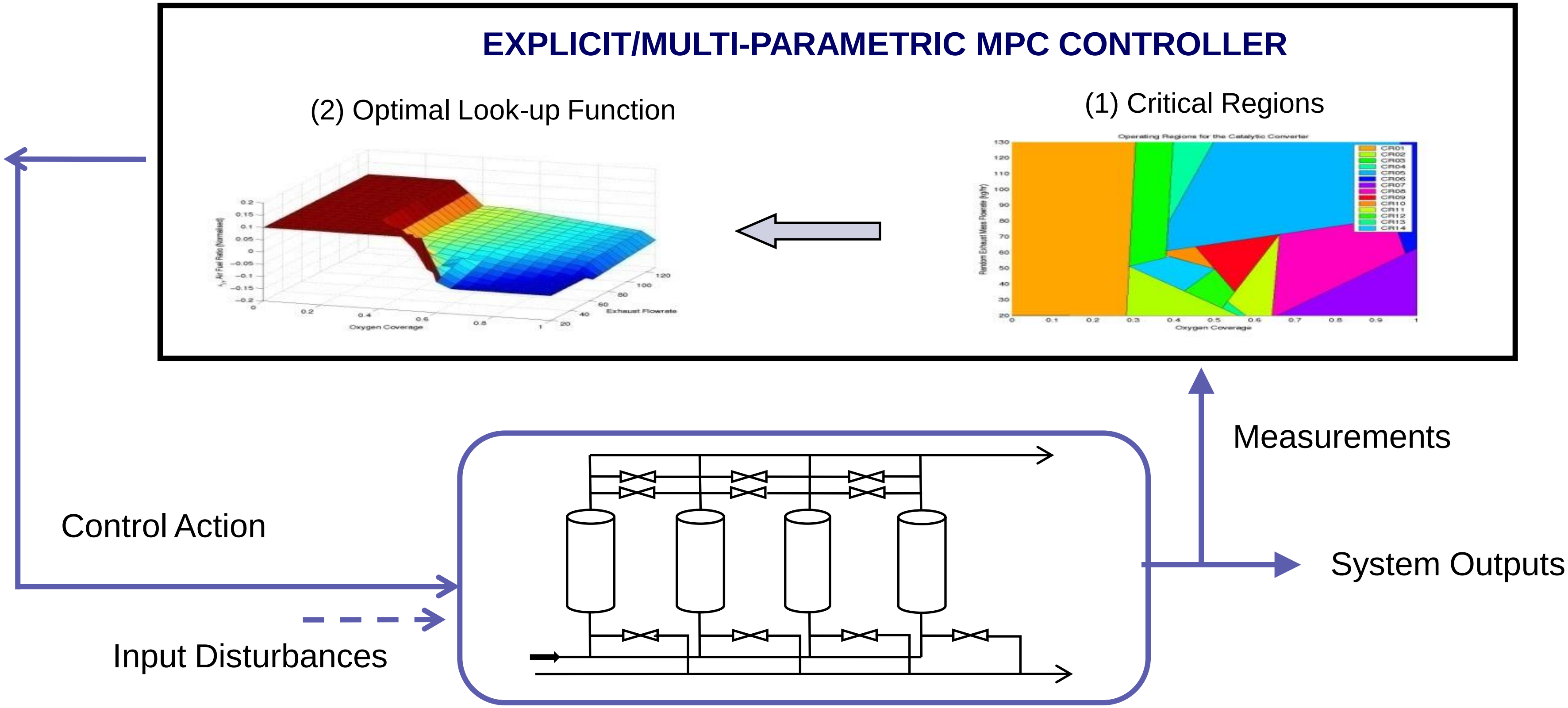
$$y_k \le 1$$

- y = hydrogen purity at the end of adsorption stage
- u = adsorption time, sec
- N = **4**, M = **2** Q = **1**
- 2 optimization variables u_0, u_1
- Optimal R based on the closed loop response

Constraints on u

- Low u: low adsorption time/cycle time, fast PSA cycles
  - More ON/OFFs of the switch valves per unit time
    - Extra wear and tear of manipulative variable hardware
  - Fast loading-unloading of adsorbent leading to its degradation
- High u: high adsorption time/cycle time, long PSA cycles
  - Risk of over saturation, or irreversible adsorption of adsorbent

mp-MPC for PSA control



MPC on a chip

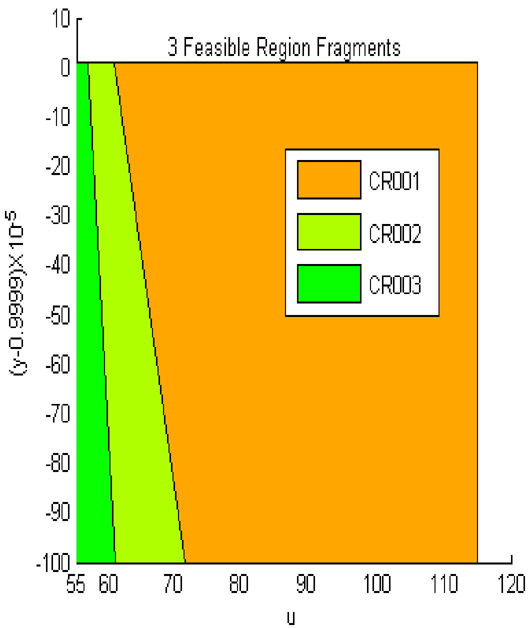
- Explicit Control Law →Eliminate expensive, on-line computations
- Valuable insights!

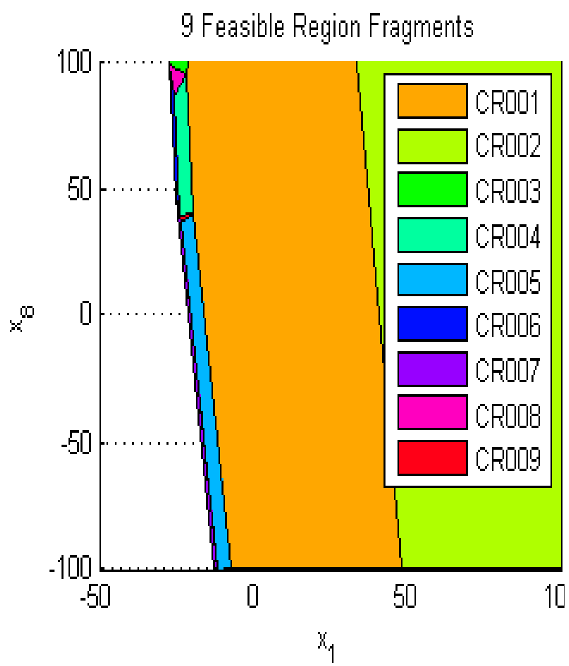
by2seps

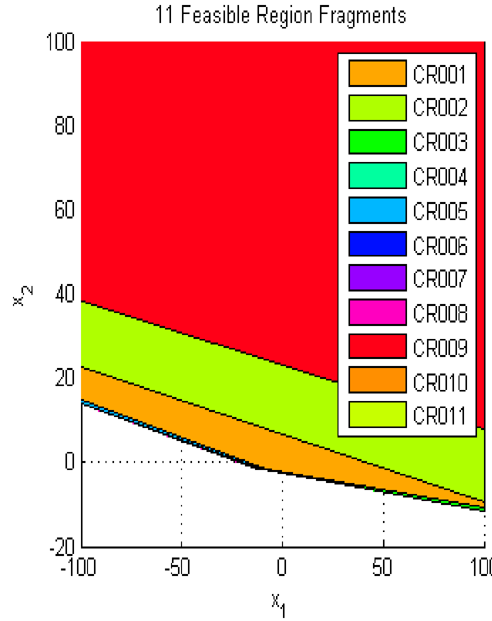
Explicit/Multi-Parametric MPC Design

Critical Regions from POP software

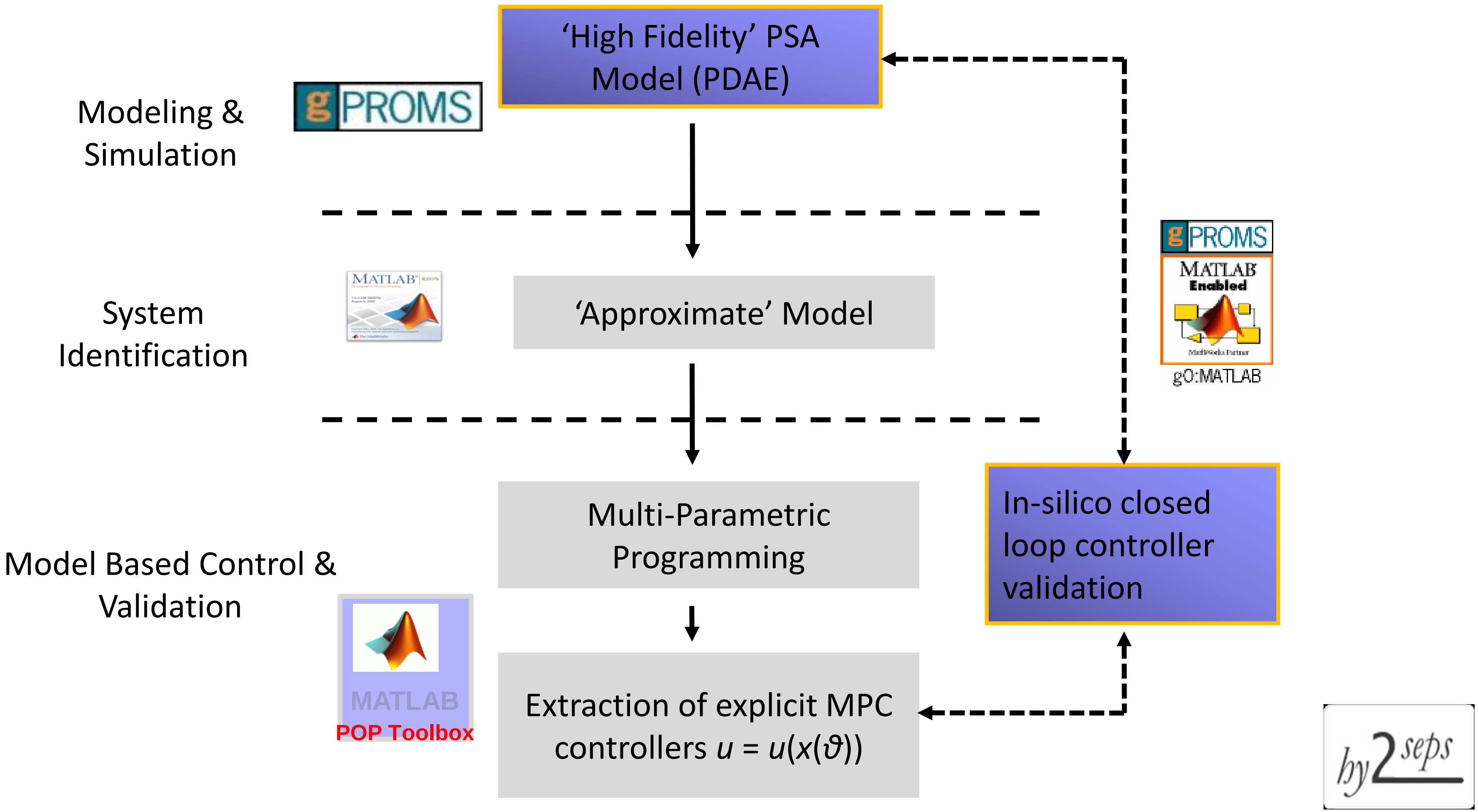
Solve the mp-optimization problem for all values of the parameters to obtain the explicit control laws ($u = D_1 x + u_0$) and the corresponding critical region maps ($D_2 x. \leq q$).







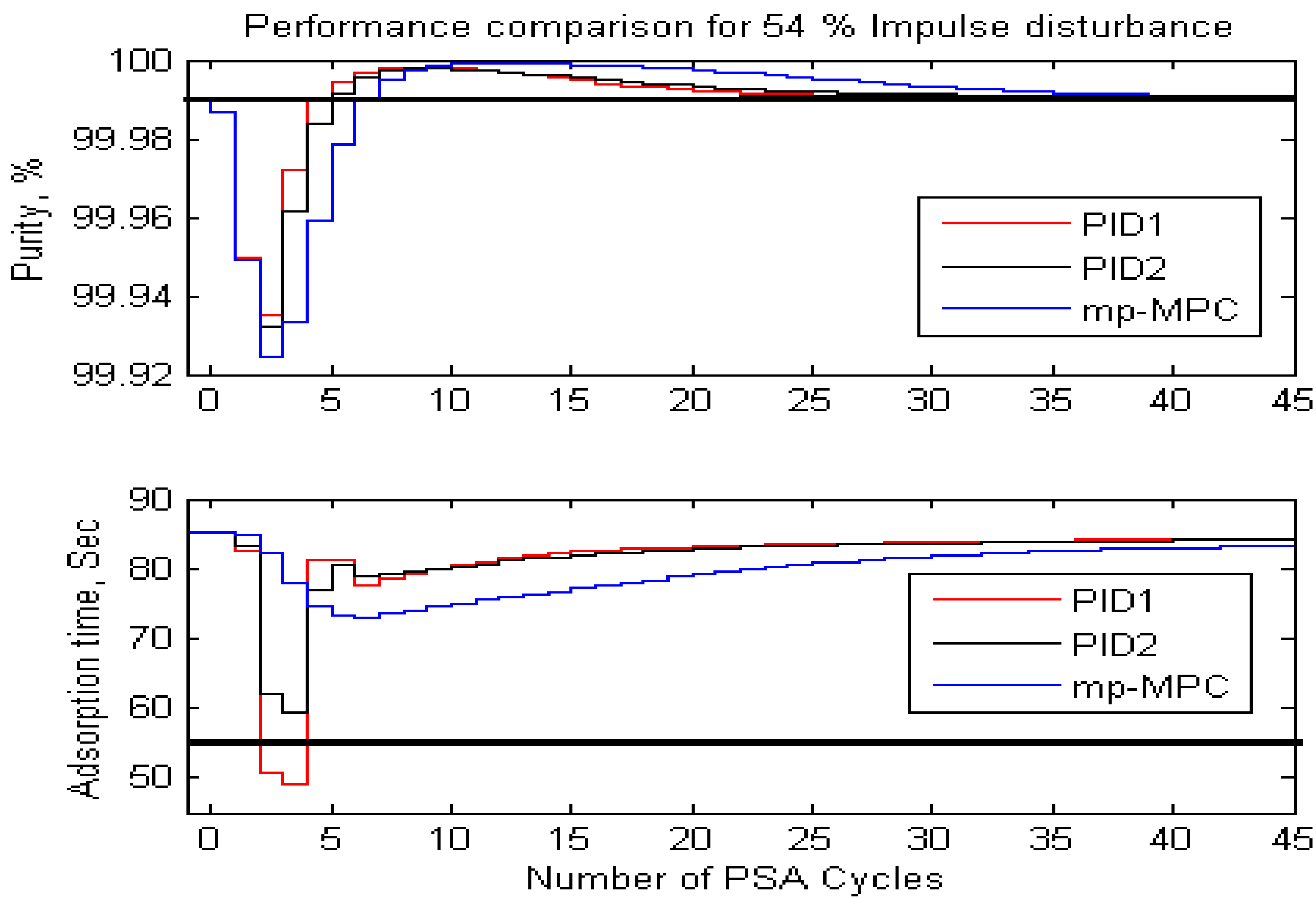
A framework for multi-parametric programming and MPC



MPC Vs PID

Step Disturbance in PSA feed rate – 10 % of Design			
Controller	Response time (Cycles)	Average ΔU (Seconds)	Maximum ΔU (Seconds)
mp-MPC	13	0.74	1.8
PID	25	0.84	5.09
Impulse Disturbance in PSA feed rate – 35 % of Design			
mp-MPC	7	0.75	1.6
PID	5	4.72	**12.12**
Open Loop	9		
Impulse Disturbance in PSA feed rate – 54 % of Design			
mp-MPC	7	1.77	4.18
PID1	4	17.11	32.29
PID2	5	9.44	**21.16**
Open Loop	10		

MPC Vs PID


Performance comparison for 54 % Impulse disturbance
Purity, %
100
99.98
99.96
99.94
99.92
0 5 10 15 20 25 30 35 40 45
PID1
PID2
mp-MPC
Adsorption time, Sec
90
80
70
60
50
0 5 10 15 20 25 30 35 40 45
Number of PSA Cycles
PID1
PID2
mp-MPC

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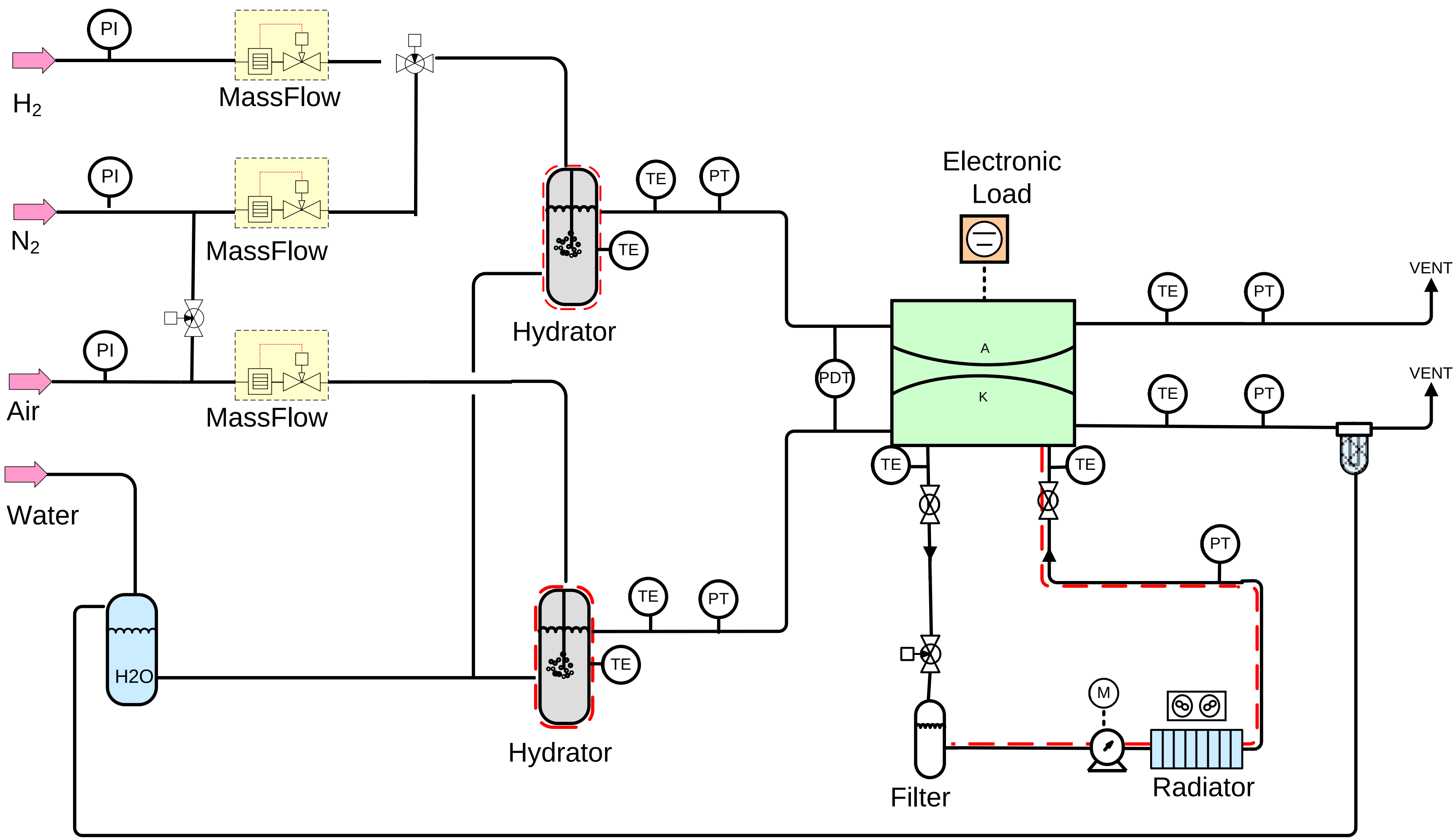
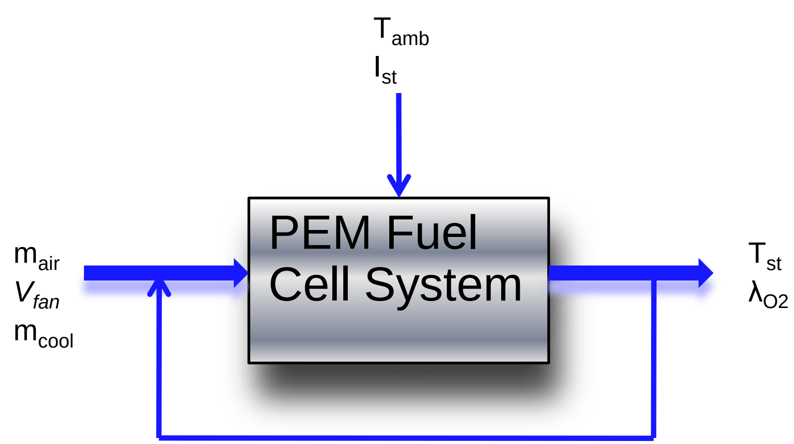
PEM Fuel Cell System



PEM Fuel Cell System

- Develop 1kW PEM fuel cell system
- Collect data for the PEM fuel cell, fan, hydrogen storage
- Design controller for the integrated system

u: $m_{air}, V_{fan}, m_{cool}$
d: T_{amb}, I_{st}
y: T_{st}, λ_{O2}
θ: $x_t, T_{amb}, I_{st}, T_{st}, T_{st,sp}$



PEM Fuel Cell System - Controller Design

- Optimized PID Controller

- Nominal MPC Controller

$$\min_{x,y,u} J = \sum_{k=1}^{N-1} (y_k - y_k{}^R)^T QR_k (y_k - y_k{}^R) + (y_N - y_N{}^R) P (y_N - y_N{}^R) + \sum_{k=0}^{M-1} (u_k - u^R)^T R_k (u_k - u^R)$$

Subject to:

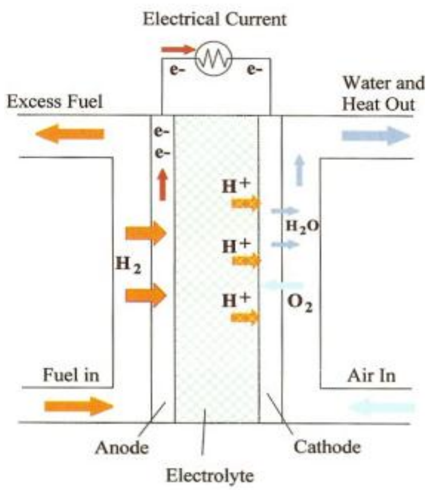
$$x_{t+1} = Ax_t + Bu_t$$

$$y_{t+1} = Cx_t$$

u: $m_{air}, V_{fan}, m_{cool}$
d: T_{amb}, I_{st}
y: T_{st}, λ_{O2}
θ: x_t, T_{amb}, I_{st}, T_{st}, $T_{st,sp}$

- Robust MPC Controller
  - Include in the controller design the model error

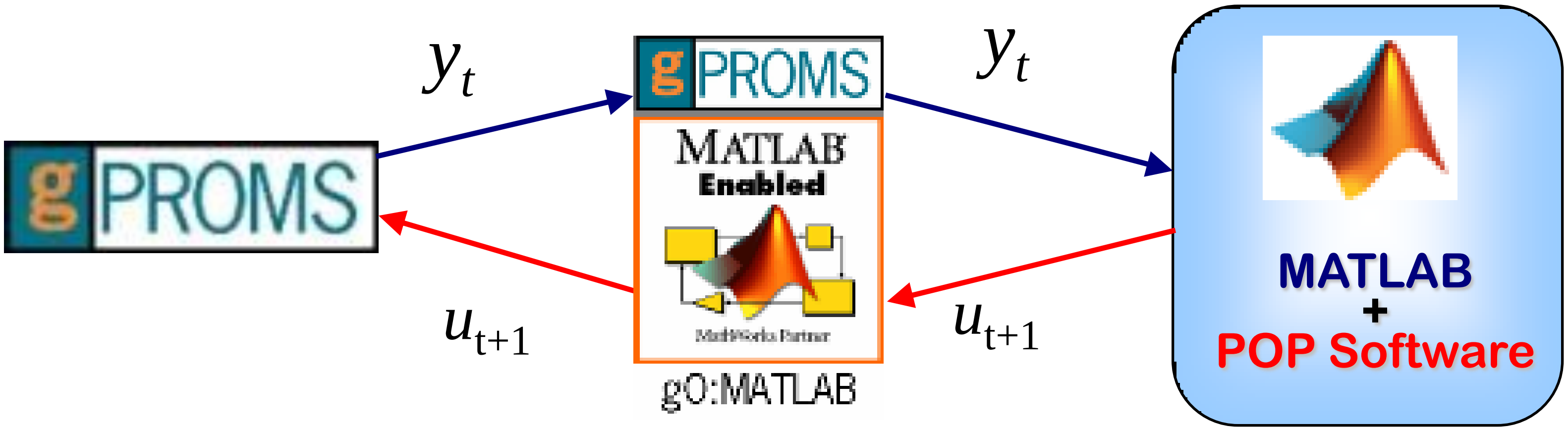
PEM fuel cell system



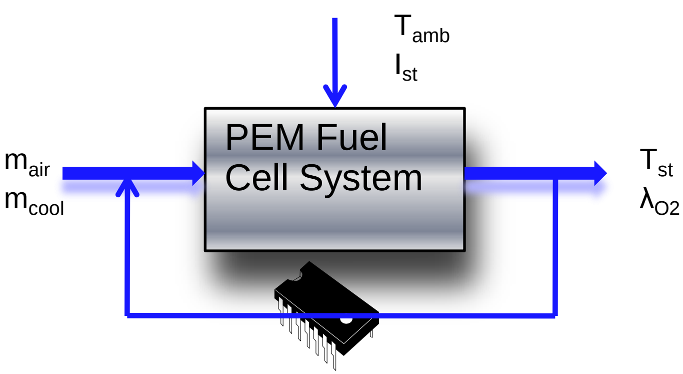
- ✓ Dynamic model
- ✓ Ideal and uniformly distributed gases
- ✓ The fuel and the oxidant are humidified
- ✓ No liquid can go into the membrane because it is waterproof
- ✓ Uniform temperature in the fuel cell stack
- ✓ Simplified mathematical models for humidifier, radiator and pump

Controller evaluation (*closed-loop simulation*)

➢Incorporate controller into high fidelity model and perform computational studies



➢Incorporate controller into the PEM Fuel Cell System - perform experiments



PEM Fuel Cell System

Unit Specifications

- Fuel Cell : 1.2kW
- Anode Flow : 5..10 lt/min
- Cathode Flow : 8..16 lt/min
- Operating Temperature : 65 – 75 °C
- Ambient Pressure

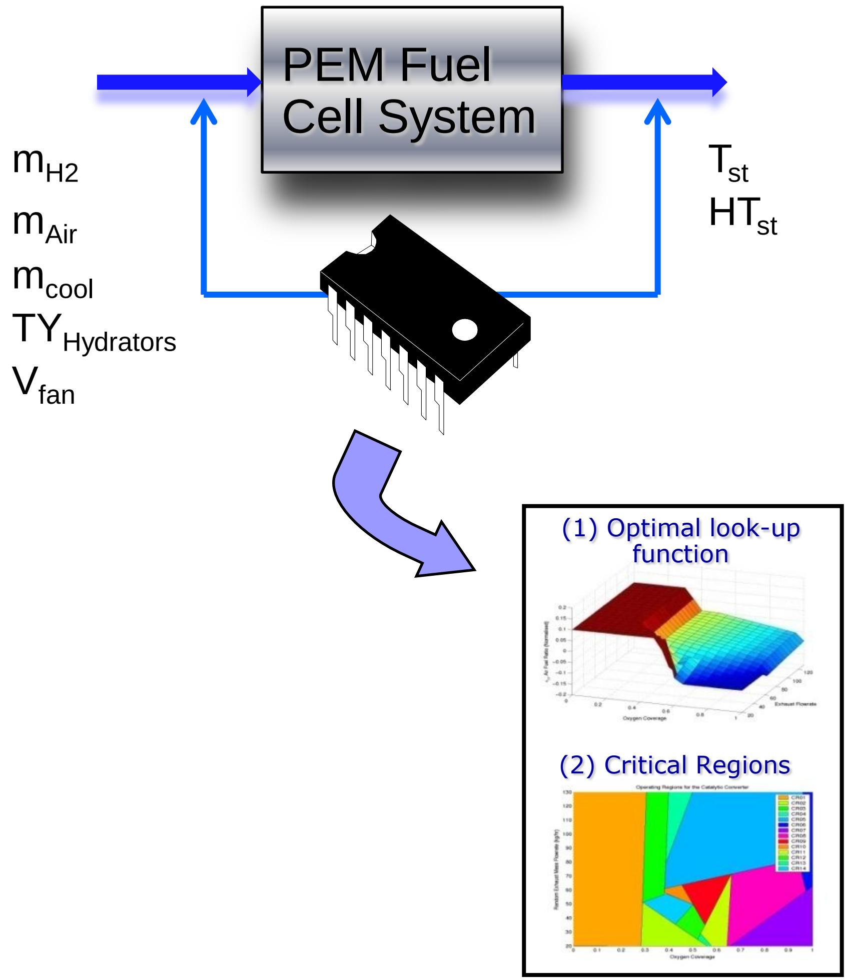
Control Strategy

<u>Start-up Operation</u>

- Heat-up Stage : Control of coolant loop

<u>Nominal Operation</u>

- Control Variables :
    - Mass Flow Rate of Hydrogen & Air
    - Humidity via Hydrators temperature
    - Cooling system via pump regulation
- Known Disturbance : Current



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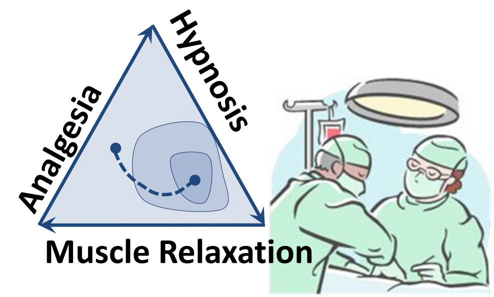
ERC MOBILE

Development of models and model based control and optimisation algorithms for biomedical systems

Anaesthesia

Provide hypnosis, analgesia and muscle relaxation while maintaining the vital functions

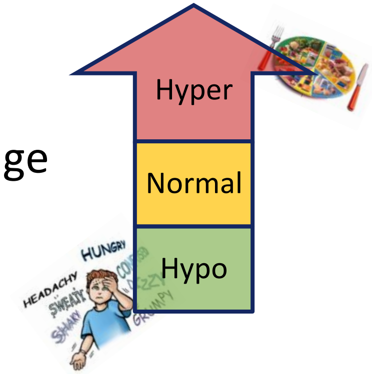
→ Multiple input multiple output model predictive control



Type 1 diabetes

Maintain blood glucose concentration within the normal range by optimising insulin delivery

→ Model predictive control problem



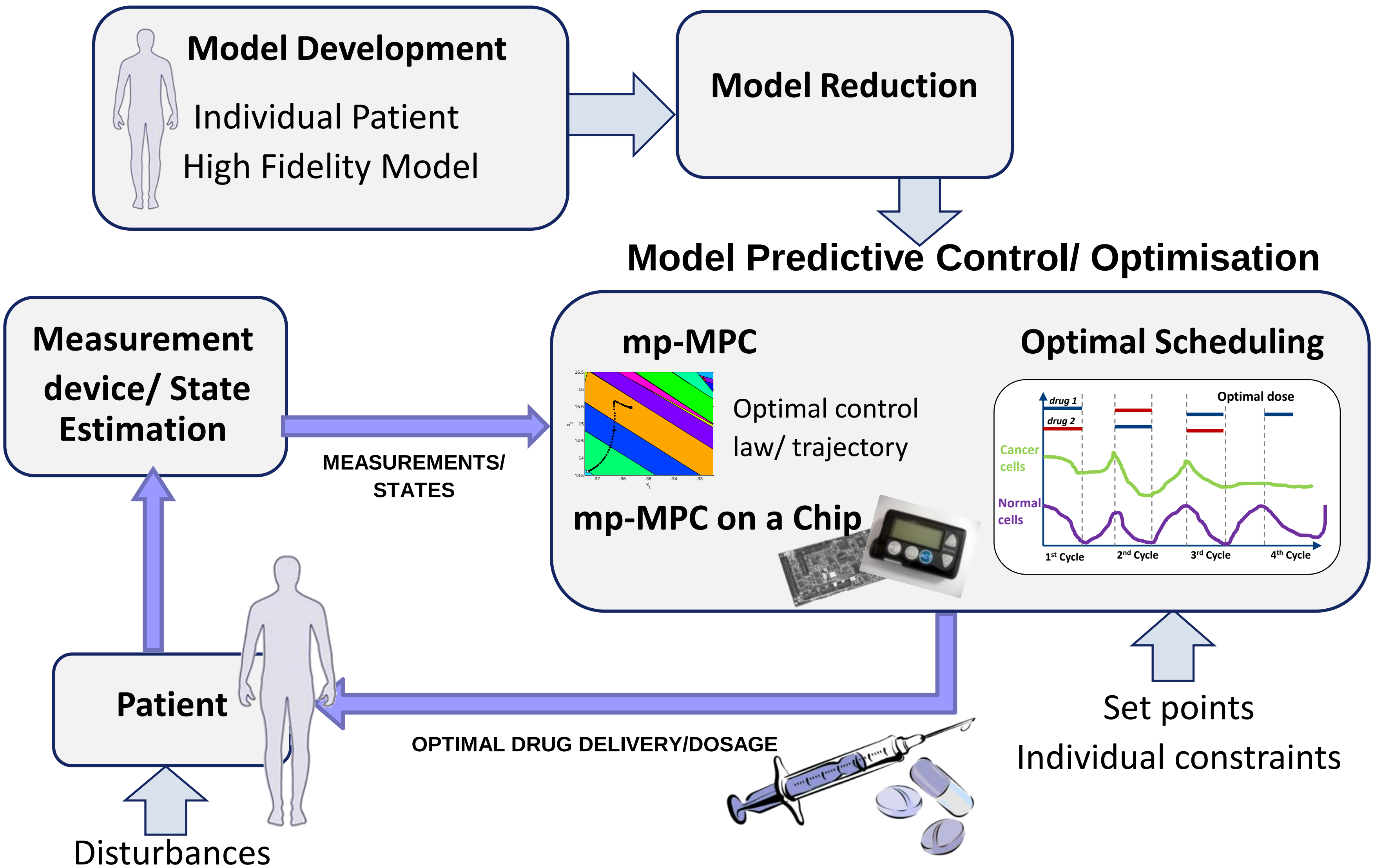
Acute Myeloid Leukaemia

Provide optimal chemotherapy dose to minimise the cancer cells

While keeping normal cells above a minimum level

→ Scheduling Problem

Framework towards optimal drug delivery systems



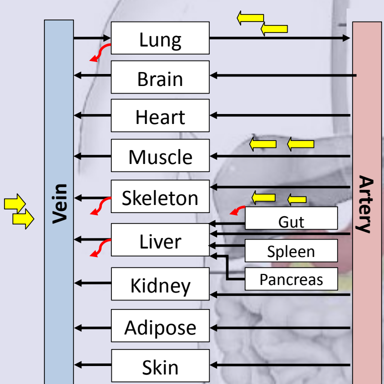
Mathematical Modelling

Model Development

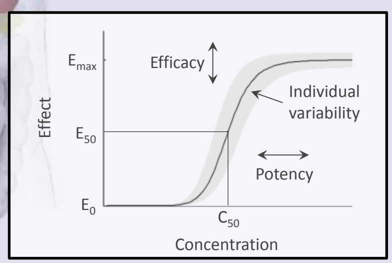
Individual Patient

High Fidelity Model

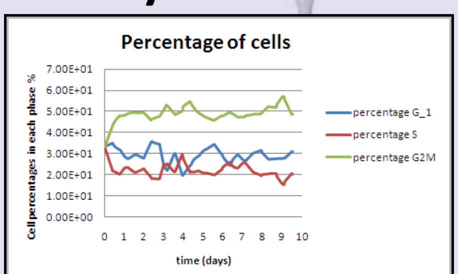
Pharmacokinetics

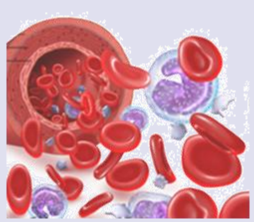


Pharmacodynamics

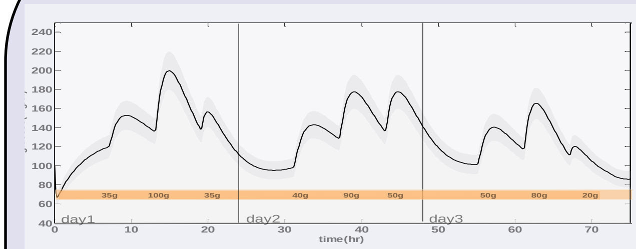


Cell Cycle





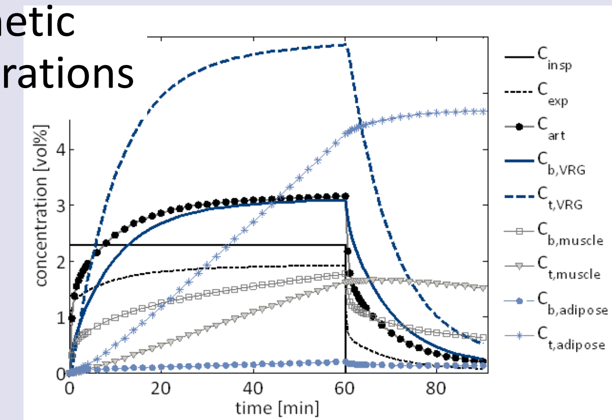
Diabetes Type I



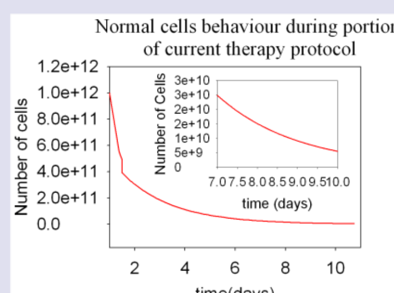
Glucose Profile

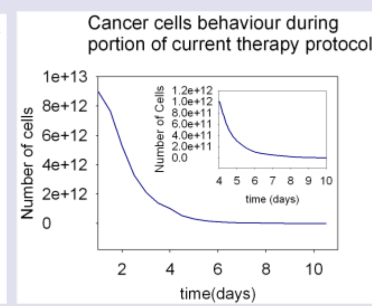
Anaesthesia

Anaesthetic concentrations



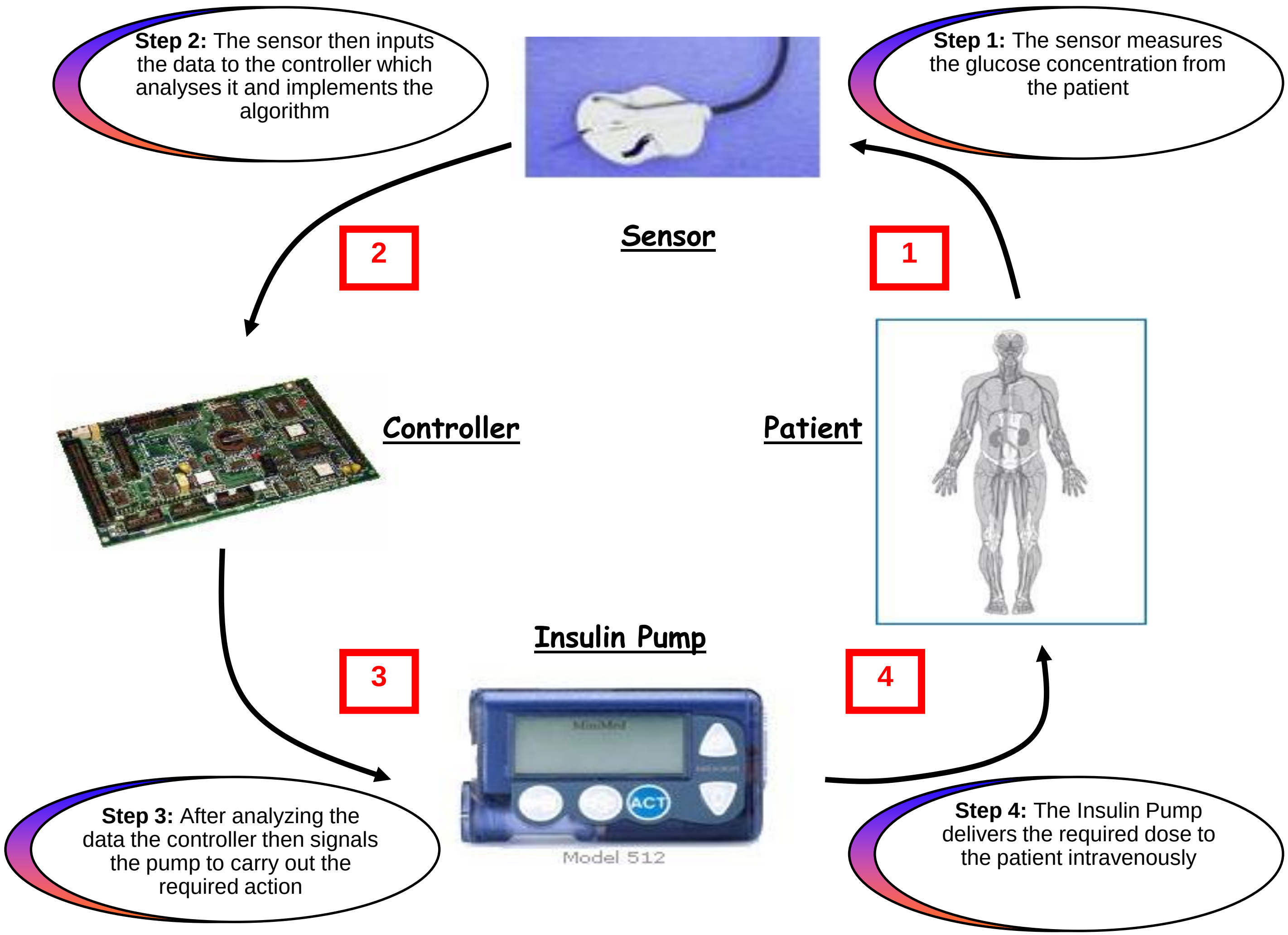
Leukaemia





Cell population profiles

ERC MOBILE


Step 2: The sensor then inputs the data to the controller which analyses it and implements the algorithm
Step 1: The sensor measures the glucose concentration from the patient
Sensor
2
1
Controller
Patient
Insulin Pump
3
4
ACT
Model 512
Step 3: After analyzing the data the controller then signals the pump to carry out the required action
Step 4: The Insulin Pump delivers the required dose to the patient intravenously

Outline

- Key concepts & historical overview
- Recent developments in multi-parametric programming and mp-MPC
- MPC-on-a-chip applications
- Concluding remarks & future outlook

MPC-on-a-chip technology – ***Reflections***

(10 years since 2002 Automatica paper appeared ..)

- Scientific/academic impact ?
- Application/industrial impact ?

MPC-on-a-chip technology – *Reflections*

(10 years since 2002 Automatica paper appeared ..)

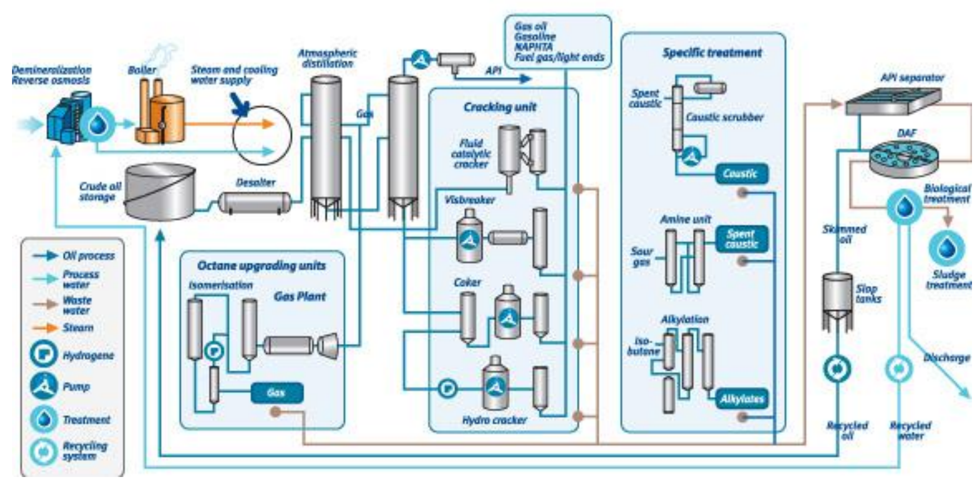
- Scientific/academic impact ? HIGH – many un-resolved issues ..
- Application/industrial impact ? Limited – not panacea to all MPC solutions ..

MPC-on-a-chip – Perspectives

- Application types for Multi-parametric Programming & MPC
  - **Type 1** - Large scale and expensive industrial processes with slow/medium dynamics
  - **Type 2** - Medium scale and cost industrial processes with medium/fast dynamics
  - **Type 3** - Small scale and inexpensive processes/equipment with medium/fast dynamics

MPC-on-a-chip – Perspectives

- **Type 1** – Large scale and expensive industrial processes with slow/medium dynamics

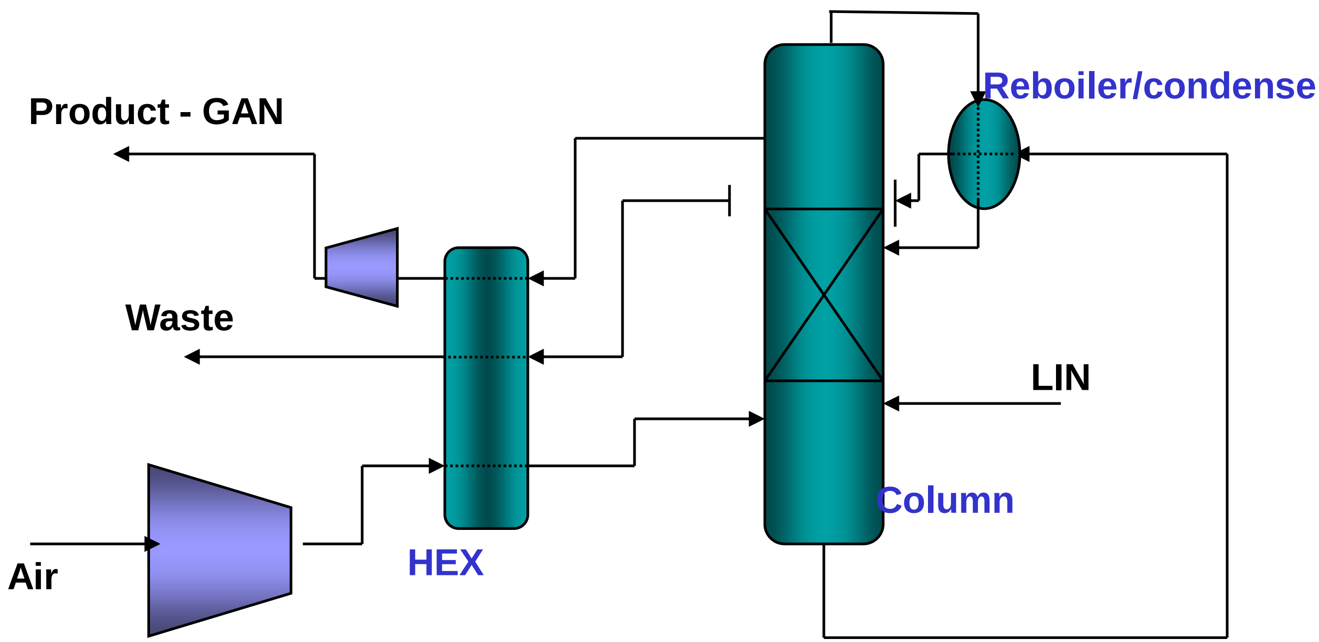


MPC-on-a-chip – Perspectives

- **Type 1** - Large scale and expensive industrial processes with slow/medium dynamics
  - Control hardware/software availability
  - MPC implementation mainly via online optimization
  - Explicit MPC **can play a role** for low level process control
  - Hybrid (on-line + off-line) approach possible – accelerate on-line dynamic optimization step

MPC-on-a-chip – Perspectives

- **Type 2** – medium scale and cost industrial processes with medium/fast dynamics

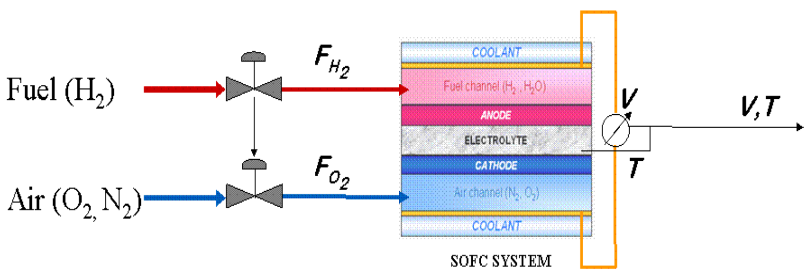


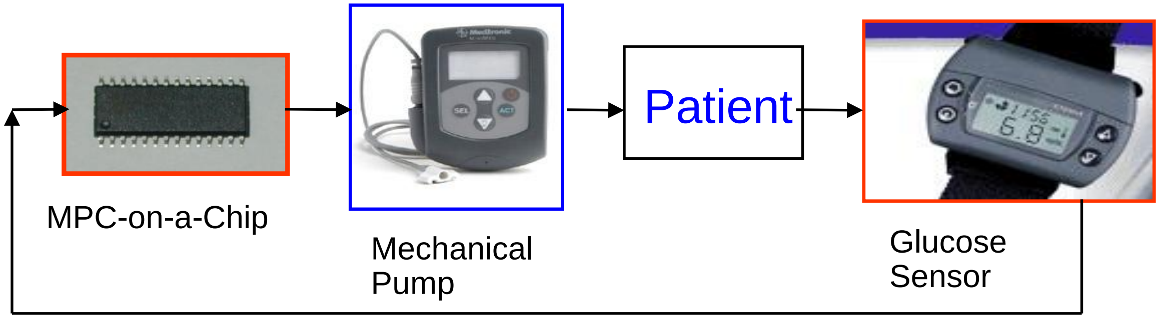
MPC-on-a-chip – Perspectives

- **Type 2** – medium scale and cost industrial processes with medium/fast dynamics
  - Limited Control hardware/software availability
  - Online optimization/MPC usually prohibitive
  - Multi-parametric MPC **ideal** – proved in previous applications (Air Separation, Automotive)

MPC-on-a-chip – Perspectives

- **Type 3** – small scale and inexpensive processes/equipment with medium/fast dynamics





MPC-on-a-chip – Perspectives

- **Type 3** – small scale and inexpensive processes/equipment with medium/fast dynamics
  - Available control hardware/software limited - not suitable for online MPC
  - Multi-parametric MPC technology **ideal/ essential**
  - MPC-on-a-Chip part of embedded (all-in-one) system
  - Suitable for new technologies (FPGA, wireless)

Centre for Process Systems Engineering

Imperial College London

From Multi-Parametric Programming Theory to MPC-on-a-chip Multi-scale Systems Applications

Stratos Pistikopoulos

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