Product Dynamic Transitions Using A Derivative-Free Optimization Approach

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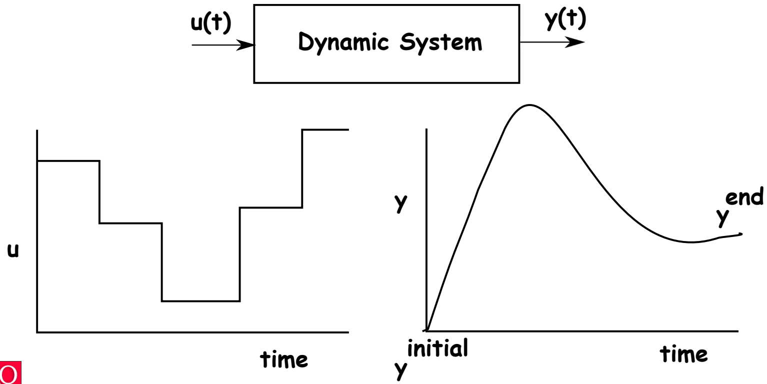
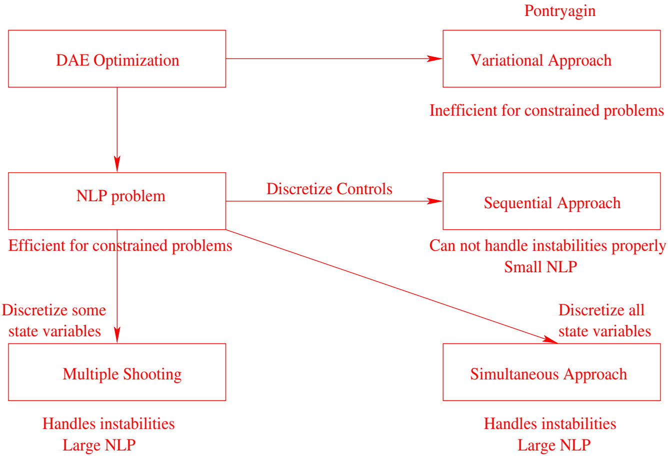
Traditional Optimal Model-based dynamic transitions

Take a dynamic system from an initial point to a final point in the best possible way



Common Approaches for Solving Dynamic Optimization Problems



Discretizing ODEs using Orthogonal Collocation

Given an ODE system:

$$\frac{dx}{dt} = f(x, u, p), \quad x(0) = x_{init}$$

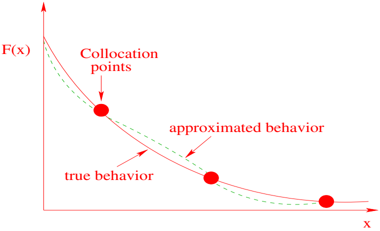
where $x(t)$ are the system states, $u(t)$ is the manipulated variable and p are the system parameters.

The aim is to approximate the behaviour of x and u by Lagrange interpolation polynomials (of orders $\mathcal{K}+1$ and $\mathcal{K}$, respectively) at collocation or discretization points t_k:

$$x_{k+1}(t) = \sum_{k=0}^{\mathcal{K}} x_k \ell_k^x(t), \quad \ell_k^x(t) = \prod_{\substack{j=0 \\ j\neq k}}^{\mathcal{K}} \frac{t - t_j}{t_k - t_j}$$

$$u_k(t) = \sum_{k=1}^{\mathcal{K}} u_k \ell_k^u(t), \quad \ell_k^u(t) = \prod_{\substack{j=1 \\ j\neq k}}^{\mathcal{K}} \frac{t - t_j}{t_k - t_j}$$

$$x_{N+1}(t_k) = x_k, \quad u_N(t_k) = u_k$$



Therefore replacing into the original ODE system, we get the system residual $\mathcal{R}(t_k)$:

$$\mathcal{R}(t_k) = \sum_{j=0}^{\mathcal{K}} x_j \frac{d\ell_j(t_k)}{dt} - f(x_k, u_k, p) = 0, \quad k = 1, .., \mathcal{K}$$

Transformation of a Dynamic Optimization problem into a NLP

Original dynamic optimization problem

$$\min_{x,u} \phi(x, u)$$

s.t.

$$\frac{dx(t)}{dt} = F\left(x(t), u(t), t, p\right)$$
$$x(0) = x^0$$
$$g(x(t), u(t), p) \leq 0$$
$$h(x(t), u(t), p) = 0$$
$$x^l \leq x \leq x^u$$
$$u^l \leq u \leq u^u$$

Discretized NLP

$$\min_{x_k, u_k} \phi(x_k, u_k)$$

s.t.

$$\sum_{j=0}^{\mathcal{K}} x_j \dot{\ell}_j(t_k) - F\left(x_k, u_k\right) = 0, \;\; k = 1, \ldots, \mathcal{K}$$
$$x_0 = x(0)$$
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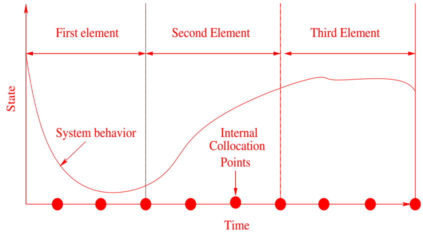
Approximation of a Dynamic Optimization Problem using Orthogonal Collocation on Finite Elements

Sometimes it is convenient to use Orthogonal Collocation on Finite Elements to approximate the behavior of systems exhibiting fast dynamics.



$$\min_{x_k, u_k} \phi(x, u)$$

s.t.

$$\sum_{j=0}^{\mathcal{K}} x_{ij} \dot{\ell}_j(\tau_k) - h_i F(x_{ik}, u_{ik}) = 0, \quad k \overset{i=1,\ldots,NE}{=} 1, \ldots, NC$$

$$x_{10} = x(0)$$

$$g(x_{ik}, u_{ik}, p) = 0, \quad i = 1, \ldots, NE; k = 1, .., NC$$

$$x_{ij}^{l} \leq x_{ij} \leq x_{ij}^{u}, \quad i = 1, \ldots, NE; k = 1, .., NC$$

$$u_{ij}^{l} \leq u_{ij} \leq u_{ij}^{u}, \quad i = 1, \ldots, NE; k = 1, .., NC$$

where NE is the number of finite elements, NC is the number of internal collocation points, h_i is the length of each element.

Example: Dynamic optimal transition between two steady-states: Hicks CSTR

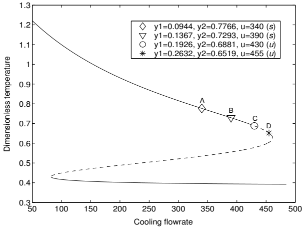
$$\frac{dC}{dt} = \frac{1-C}{\theta} - k_{10}e^{-N/T}C$$

$$\frac{dT}{dt} = \frac{y_f - T}{\theta} + k_{10}e^{-N/T}C - \alpha U(T - y_c)$$

Parameter values

θ	20	Residence time
T_f	300	Feed temperature
J	100	$(-\Delta H)/(\rho C_p)$
k_{10}	300	Preexponential factor
c_f	7.6	Feed concentration
T_c	290	Coolant temperature
α	1.95×10^{-4}	Heat transfer area
N	5	$E_1/(RJc_f)$

Desired Transition B $\rightarrow$ A



Desired dynamic transition

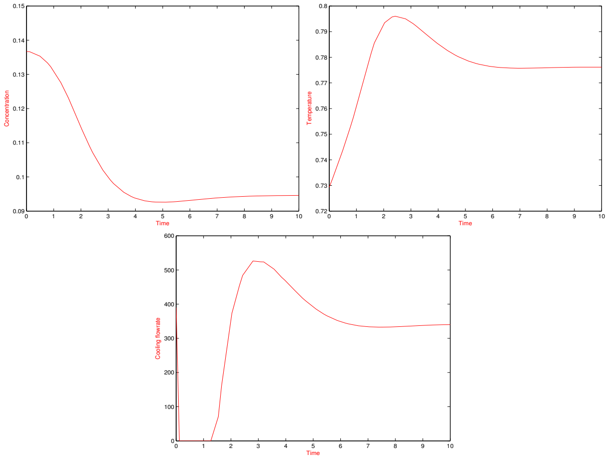
	C	T	U
Initial (B)	0.1367	0.7293	390
Final (A)	0.0944	0.7766	340

C = Concentration (c/c_f), T = temperature (T_r/Jc_f), y_c = Coolant temperature (T_c/Jc_f), y_f = feed temperature (T_f/Jc_f), U = Cooling flowrate. c and T_r are nondimensionless concentration and reactor temperature.

Dynamic Transitions profiles for the Hicks CSTR example

As objective function the requirement of minimum transition time between the initial and final steady-states will be imposed:

$$\text{Min} \int_0^{t_f} \left\{ \alpha_1 (C(t) - C_{des})^2 + \alpha_2 (T(t) - T_{des})^2 + \alpha_3 (U(t) - U_{des})^2 \right\} dt$$



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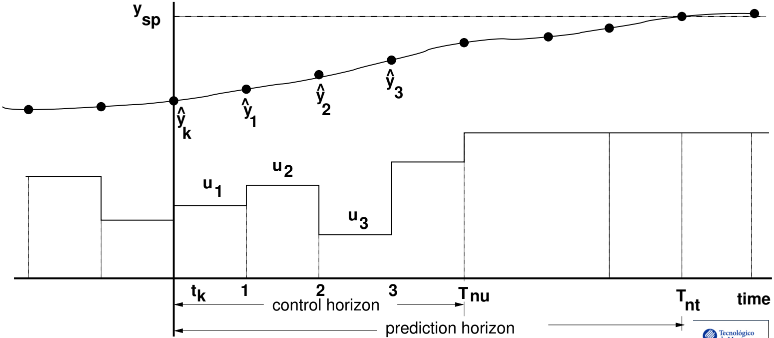

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$$\Delta x_i = x_i - x_{i-1}$$
$$\Delta u_i = u_i - u_{i-1}$$

In summary, the computation of optimal product dynamic transitions using a DFO approach can be cast as follows:

$$\min_{\mathbf{u}} \Omega = \sum_{i=1}^{N}[(x_i - x^f)^2 + (u_i - u^f)^2] + \lambda_x \sum_{i=1}^{N}[\Delta x_i]^2 + \lambda_u \sum_{i=1}^{N}[\Delta u_i]^2$$

$$\begin{aligned}
\text{s.t.} \qquad & x^l \le x_i \le x^u, & i = 1, \ldots, N \\
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where the l and u superscripts stand for lower and upper bounds, respectively.

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- Penalized state transition objective function, which includes the discretization of the dynamic mathematical model, reads:

$$\min \, \Omega = \frac{1}{2}\int_0^1 (y^2 + u^2)dt + \mathbf{F}(y, \dot{y}, \lambda)$$

where $\mathbf{F}(y, \dot{y}, \lambda)$ stands for a function which represents the discretized dynamic model as a function of the states (y), states derivates $(\dot{x})$ and penalty parameters (λ).

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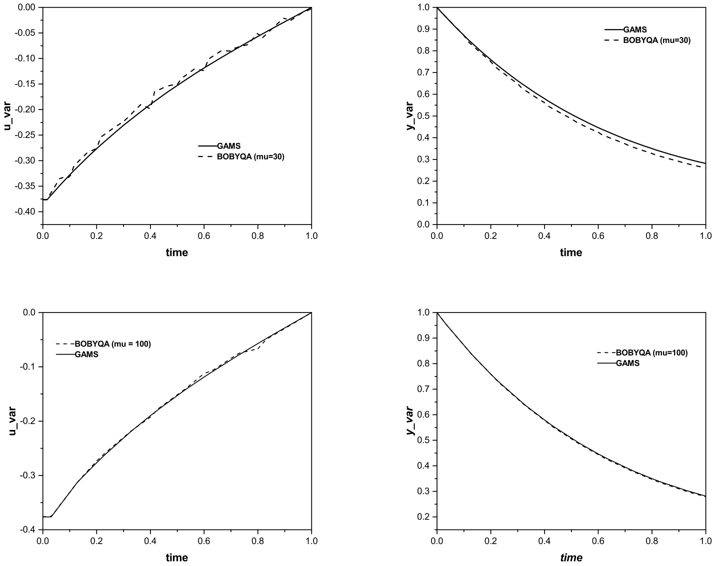

Upper: 10 finite elements and $\mu = 30$, Lower: 5 finite elements and $\mu = 100$.

Example 2: Hicks reactor

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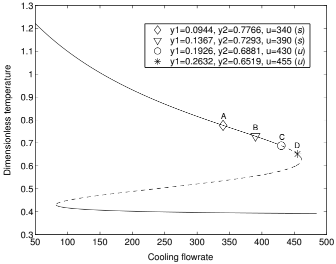
$$\frac{dy_1}{dt} = \frac{1 - y_1}{\theta} - k_{10} e^{-N/y_2} y_1$$
$$\frac{dy_2}{dt} = \frac{y_f - y_2}{\theta} - k_{10} e^{-N/y_2} y_1 - \alpha U (y_2 - y_c)$$

Parameter	Value	Description
θ	20	Residence time
J	100	$(-\Delta H)/(\rho C_p)$
c_f	27.6	Feed concentration
α	$1.95e^{-4}$	Dimensionless heat transfer area
T_f	300	Feed temperature
k_{10}	300	Preexponential factor
T_c	290	Coolant temperature
N	5	$E_1/(RJc_f)$



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where y_1 is the dimensionless concentration, y_2 is the dimensionless temperature and u is the cooling water flowrate, the superscript d stands for desired or target values. The term $\mathbf{F}(\mathbf{y}, \dot{\mathbf{y}}, \lambda)$ is a function representing the discretized dynamic model.

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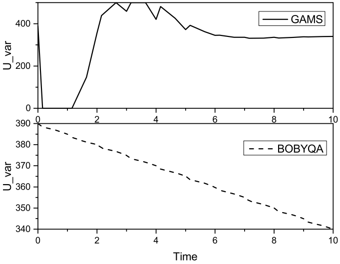
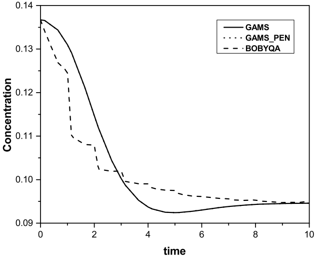
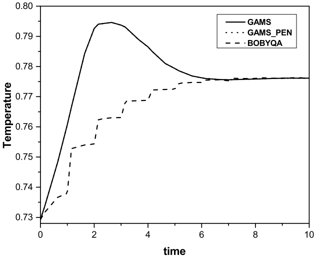

GAMS
BOBYQA
U_var
U_var
0
200
400
340
350
360
370
380
390
0
2
4
6
8
10
Time


GAMS
GAMS_PEN
BOBYQA
Concentration
0.09
0.10
0.11
0.12
0.13
0.14
0
2
4
6
8
10
time


GAMS
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Temperature
0.73
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time

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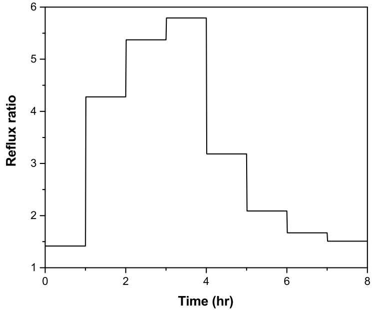
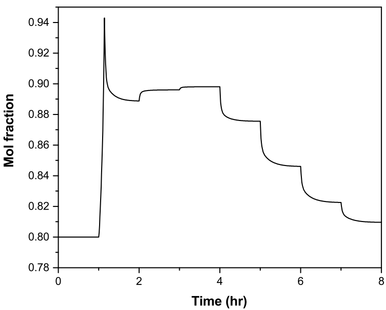


Reflux ratio
Time (hr)



Mol fraction
Time (hr)

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