# New Optimization Tools: The Julia Computing Environment

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August 31, 2016

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- Mainly focused on solving unconstrained optimization problems with simple box constraints

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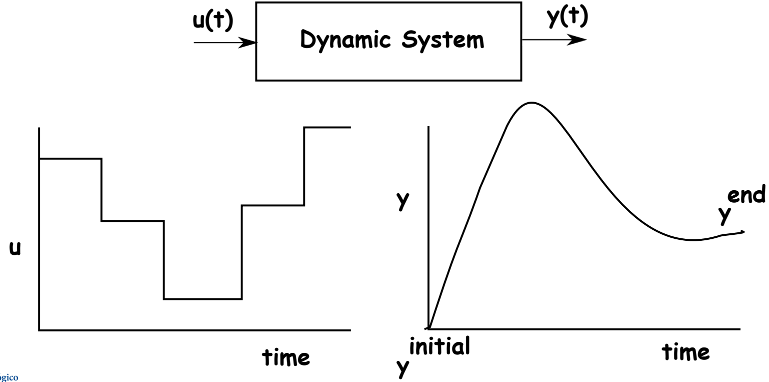
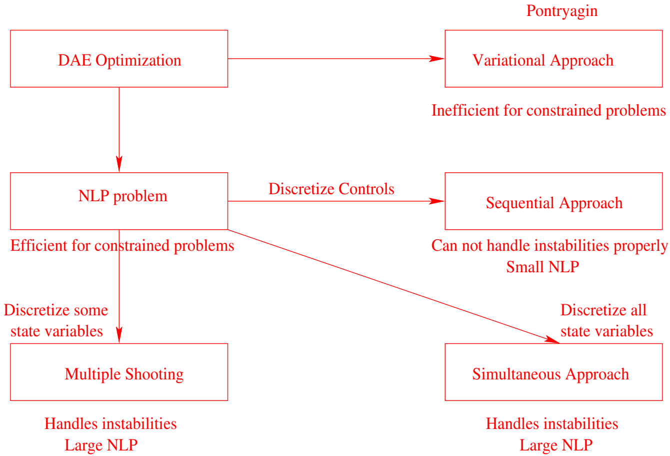
# Traditional Optimal Model-based dynamic transitions

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

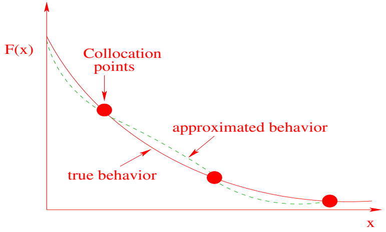
Given an ODE system:

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

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 $t_k$:

$$\begin{aligned} x_{k+1}(t) &= \sum_{k=0}^{\mathcal{K}} x_k \ell_k^x(t), \quad \ell_k^x(t) = \prod_{\substack{j=0 \\ j\neq k}}^{\mathcal{K}} \frac{t - t_j}{t_k - t_j} \\ u_k(t) &= \sum_{k=1}^{\mathcal{K}} u_k \ell_k^u(t), \quad \ell_k^u(t) = \prod_{\substack{j=1 \\ j\neq k}}^{\mathcal{K}} \frac{t - t_j}{t_k - t_j} \\ x_{N+1}(t_k) &= x_k, \quad u_N(t_k) = u_k \end{aligned}$$




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

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

$$\text{s.t.} \quad \frac{dx(t)}{dt} = F\left(x(t), u(t), t, p\right)$$

$$x(0) = x^0$$

$$g(x(t), u(t), p) \leq 0$$

$$h(x(t), u(t), p) = 0$$

$$x^l \leq x \leq x^u$$

$$u^l \leq u \leq u^u$$

Discretized NLP

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

$$\text{s.t.} \quad \sum_{j=0}^{\mathcal{K}} x_j \dot{\ell}_j(t_k) - F\left(x_k, u_k\right) = 0, \quad k = 1, \ldots, \mathcal{K}$$

$$x_0 = x(0)$$

$$g(x_k, u_k, p) \leq 0, \quad k = 1, \ldots, \mathcal{K}$$

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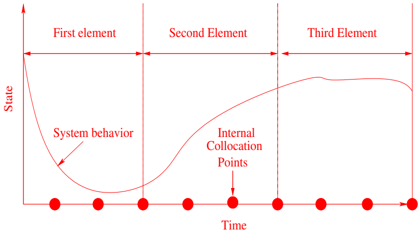
# Approximation of a Dynamic Optimization Problem using Orthogonal Collocation on Finite Elements

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

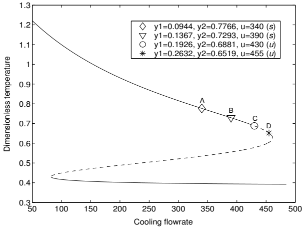
$$\frac{dC}{dt} = \frac{1 - C}{\theta} - k_{10} e^{-N/T} C$$

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

Parameter values

| | | |
|---|---|---|
| $\theta$ | 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 |
| $\alpha$ | $1.95 \times 10^{-4}$ | 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.

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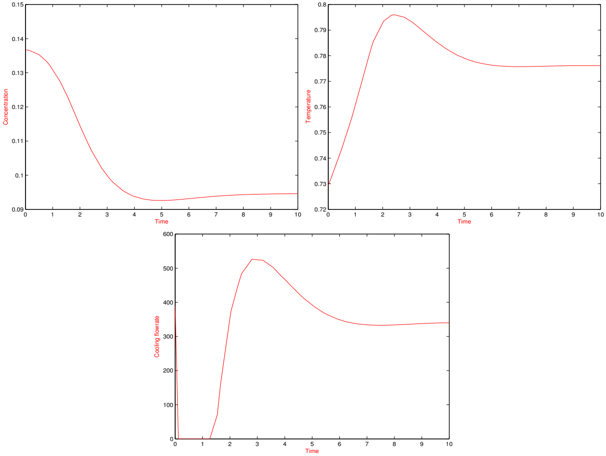
# Dynamic Transitions profiles for the Hicks CSTR example

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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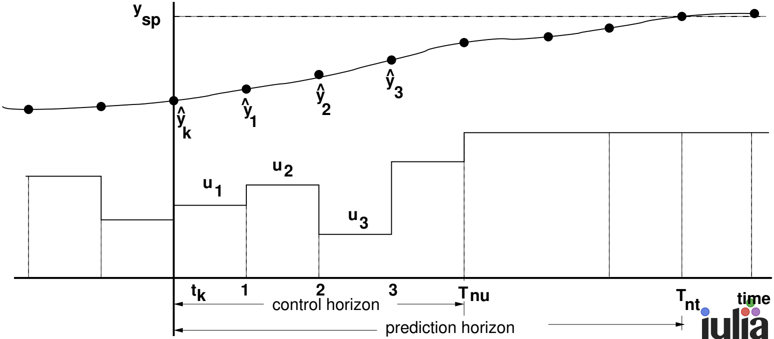

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- The aim of the last two terms is to penalize for large changes in both the states and manipulated variable values.

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

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

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

$$\begin{aligned} \text{s.t.} \qquad & x^l \leq x_i \leq x^u, & i = 1, \ldots, N \\ & u^l \leq u_i \leq u^u, & i = 1, \ldots, N \\ & \Delta x^l \leq \Delta x_i \leq \Delta x^u, & i = 1, \ldots, N \\ & \Delta u^l \leq \Delta u_i \leq \Delta u^u, & i = 1, \ldots, N \end{aligned}$$

where the $l$ and $u$ superscripts stand for lower and upper bounds, respectively.

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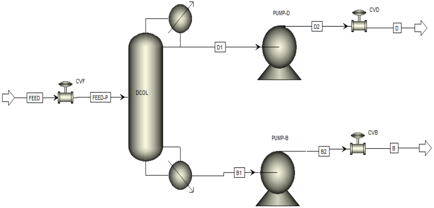


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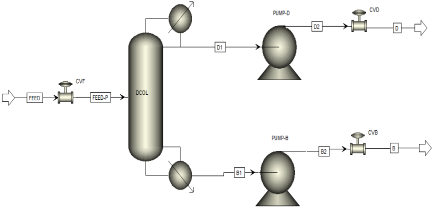


- A first-order dynamic model of a benzene/toluene binary distillation column was built using the ASPEN Dynamics simulation environment.
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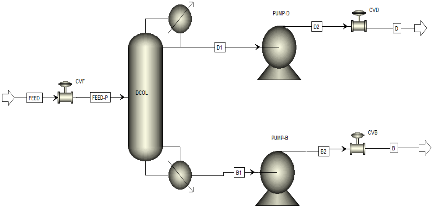


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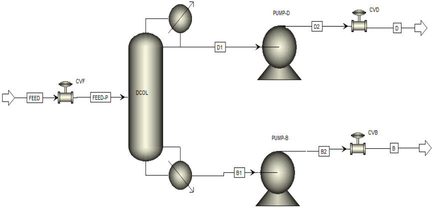


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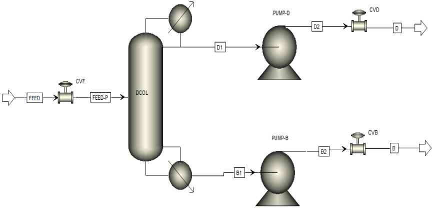


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- Two product dynamic transitions: (a) the initial steady-state is given by $[c_0, u_0]$=[0.8, 1.4116], whereas the target steady state is given by $[c^d, u^d]$=[0.9, 5.86] and (b) then the product transition in the opposite direction was done.

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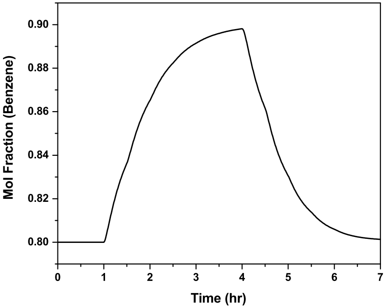
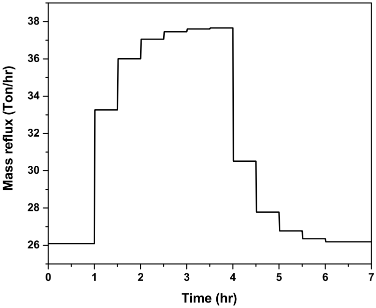
# One-point composition control of the distillate stream



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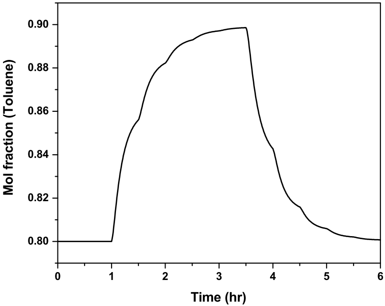
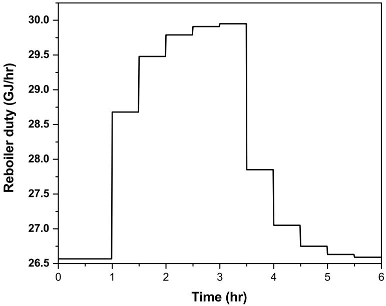
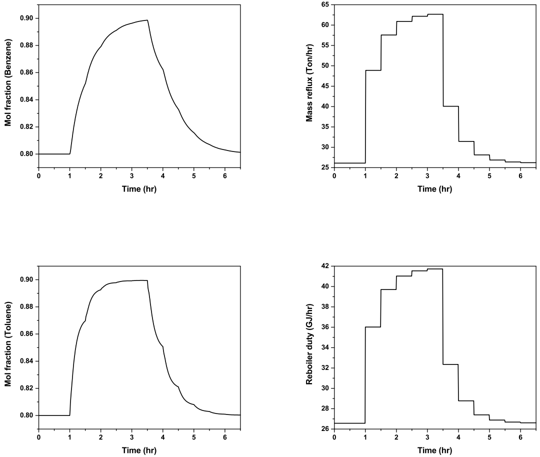
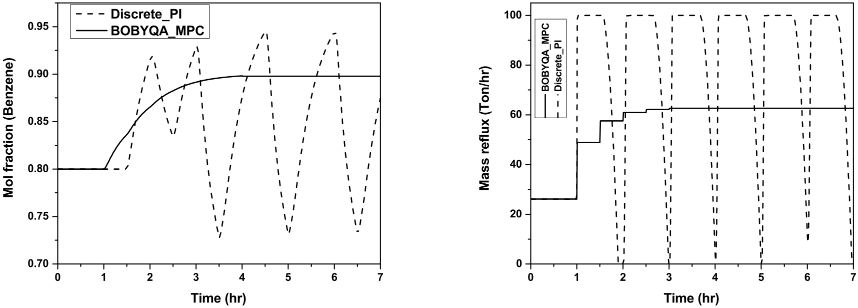


# Dual composition control of the distillate and bottoms streams



# Comparison against Proportional-Integral Controllers



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