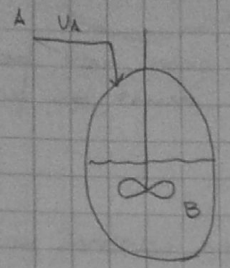
16.01.2012 Laboratory #12



u_A : flow rate

$A + B \to C$

state equations

$$\begin{cases} \dfrac{dm_A(t)}{dt} = u_A - k\dfrac{m_A(t)\,m_B(t)}{V(t)^2} \\[2ex] \dfrac{dm_B(t)}{dt} = -k\dfrac{m_A(t)\,m_B(t)}{V(t)^2} \quad \to \text{no inflow} \\[2ex] \dfrac{dm_C(t)}{dt} = k\dfrac{m_A(t)\,m_B(t)}{V(t)^2} \end{cases}$$

$$\frac{dV(t)}{dt} = Q_A\, u_A(t)$$

→ $V(t)$ changes with the volume of the feed

- Ordinary differential equations

$$\left.\begin{aligned} m_A(0) &= 0 \\ m_B(0) &= m_{B,0} \\ m_C(0) &= 0 \\ V(0) &= V_0 \end{aligned}\right\} \text{initial conditions}$$

- Fixing the control variables → state variables are automatically determined (by integration)
- Control variables $u_A(t)$
- Differential / state variables $m_A(t)$, $m_B(t)$, $m_C(t)$, $V(t)$
- If u_A is fixed then all state variables are also fixed by integration

OPTIMIZATION PROBLEM

- Maximize $\dfrac{m_B(3) - m_B(0)}{m_B(0)}$, 3 is the final time

$$\min \; -\frac{(m_B(3) - m_B(0))}{m_B(0)}$$

⇒ obj. function evaluated at the final time

s.t. ODEs , initial conditions

$$\underset{\substack{\downarrow \\ \text{const.}}}{\underline{u}} \le u_A(t) \le \underset{\substack{\downarrow \\ \text{const.}}}{\bar{u}}, \quad \forall t \in [0,3]$$

⇒ Bounds (can also be seen as Path Constrains)

$$m_A(t) \le \underset{\substack{\downarrow \\ \text{const}}}{\bar{r}} \cdot m_B(t), \quad \forall t \in [0,3]$$

* these constrains are called PATH CONSTRAINS (it must hold during the whole time interval)

- the objective function is usually only evaluated at the final time

- u_A : only degree of freedom, other variables can not be freely manipulated (the control variable must be fixed)

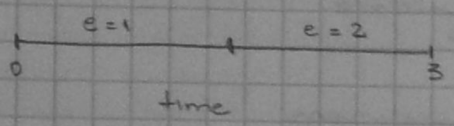
New aspects in dynamic optimization:

- all variables are time-dependent : state and control variables
- all constrains are time dependent
- the objective function is time dependent

HOW TO SOLVE ?

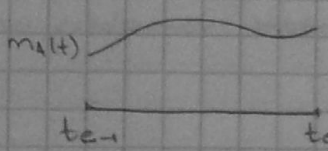
- Full discretization approach (also called early discretization, simultaneous approach)

STEP 1 : split the time horizon $[0,3]$ into $E = 2$ parts, so-called finite elements



→ 2 finite elements

STEP 2 : Approximate the ODEs at $[0, 1{,}5]$ and $[1{,}5, 3]$



⇒ finite element e

$$\frac{dm_A(t)}{dt} = u_A(t) - k \frac{m_A(t)\, m_B(t)}{V(t)}$$

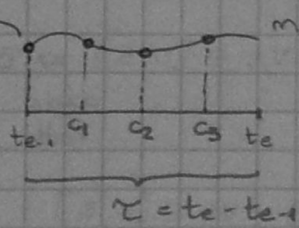
$\boxed{A}$ Explicit Euler

$$m_A(t_e) = m_A(t_{e-1}) + (t_e - t_{e-1}) \left[\frac{-k \cdot (m_A(t_{e-1})\, m_B(t_{e-1})}{V(t_{e-1})^2} + u_A(t_{e-1}) \right]$$

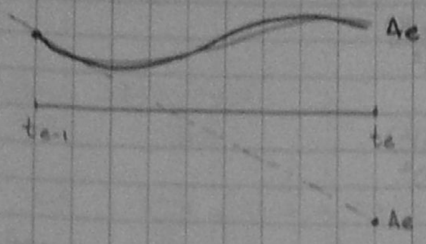
value of new time point = value of old time point + time duration · right hand side at old time

$\boxed{B}$ Collocation method (special case of the Runge-Kutta method for approximation of ODEs)

always choose also initial point



- choose $s+1$ points $(s = 3)$ (further discretization of the finite element)



$\Rightarrow$ collocation method

$\Rightarrow$ with explicit Euler

- the collocation method assumes that the approximation is a polynomial of degree s that includes all points c_i

$$A_e(t) = \alpha_s t^s + \alpha_{s-1} t^{s-1} + \dots + \alpha_1 t + \alpha_0$$

$\hookrightarrow$ TASK: determine the coefficients α_j, $j = 0, \dots, s$

- important: only the initial condition and the derivatives at the points c_j

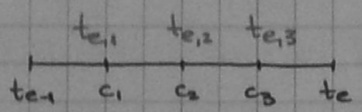
- one way:

$$\underbrace{A_e(t_{e-1})}_{=0} = 0 \quad , \quad \text{for } e = 1$$

$$\hookrightarrow \alpha_s \cdot 0 + \alpha_{s-1} \cdot 0 + \dots + \alpha_0 = 0$$

$$\alpha_0 = 0$$

$$\frac{dA_e(t_{e,j})}{dt} = u_A(t_{e,j}) - k\,\frac{A_e(t_{e,j})\,B_e(t_{e,j})}{V_e(t_{e,j})^2}$$

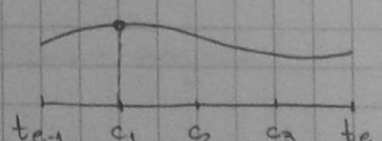


- the other way

$$A_e(t) = \sum_{j=0}^{s} L_j(t) \cdot A_e(t_{e,j}) \rightarrow$$ other way of expressing the polynomial $A_e(t_{e,j})$ as sum of the intermediary points times $L_j(t)$

$\hookrightarrow$ Legendre polynomial

$$L_j(t) = \frac{\prod_{i=0, i \neq j}^{s} (t - c_i)}{\prod_{i=0, i \neq j}^{s} (c_j - c_i)}$$



- in our case, $s = 3$ and $j = 1$

$$L_1(t) = \frac{(t - c_2)(t - c_3)(t - c_0)}{(c_1 - c_2)(c_1 - c_3)(c_1 - c_0)}$$

$$\hookrightarrow L_1(c_1) = 1$$
$$L_1(c_2) = 0$$

$$A_e(c_2) = \overset{0}{L_0(c_2)} \cdot A_e(t_{e,0}) + \overset{0}{L_1(c_2)} \cdot A_e(t_{e,1}) + \underbrace{L_2(c_2)}_{=1} \cdot A_e(t_{e,2}) + \overset{0}{L_3(c_2)} \cdot A_e(t_{e,3}) = A_e(t_{e,2})$$

$\downarrow$

exacly point at $t_{e,2}$ on the discretized time

$$\frac{dm_A(t)}{dt} \leftrightarrow \frac{dA_e(t)}{dt} = U_A(t) - k\,\frac{A_e(t)\,B_e(t)}{V_e(t)^2}$$

$$\sum_{j=0}^{3} \frac{dL_j(t)}{dt} A_e(t_{e,j}) = U_A(t) - k \cdot \frac{A_e(t)\,B_e(t)}{V_e(t)^2}$$

↳ from c_j it is possible to get an unique polynomial