

Index analysis:

$$A \Rightarrow B \Rightarrow C$$

$$\frac{dz_A}{dt} = -p_1 z_A(t) + p_2 z_B(t) \quad (1)$$

$$\frac{dz_B}{dt} = p_1 z_A(t) - (p_2 + p_3) z_B(t) + p_4 z_C(t), \quad (2)$$

$$1 = z_A(t) + z_B(t) + z_C(t), \quad (3)$$

$$z_A(0) = 1, \quad z_B(0) = 0. \quad (4)$$

Index Analysis:

Differentiate (3) and solve for $z_C'(t)$

$$\frac{dz_C}{dt} = -\frac{dz_A(t)}{dt} - \frac{dz_B(t)}{dt}.$$

We had to differentiate an equation in the DAE system once, so this is an index one DAE

Model Reformulation:

Substitute (4) into (3) at $t=0$

$$1 = 1 + 0 + z_C(0) \Rightarrow z_C(0) = 0,$$

so the consistent initial conditions are

$$z_A(0) = 1, \quad z_B(0) = 0, \quad z_C(0) = 0.$$

This yields the ODE system:

$$\frac{dz_A}{dt} = -p_1 z_A(t) + p_2 z_B(t),$$

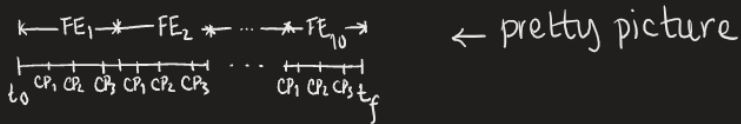
$$\frac{dz_B}{dt} = p_1 z_A(t) - (p_2 + p_3) z_B(t) + p_4 z_C(t),$$

$$\frac{dz_C}{dt} = -\frac{dz_A(t)}{dt} - \frac{dz_B(t)}{dt},$$

$$z_A(0) = 1, \quad z_B(0) = 0, \quad z_C(0) = 0.$$

Degrees of Freedom

Degrees of freedom calculation: e.g. w/ $NFE=10$ & $NCP=3$



Sets :

$$|\tau| = NFE \cdot NCP = 10 \cdot 3 + 1 = 31$$

Variables : $5|\tau|$

$$z_A(t), z_B(t), z_C(t), dz_A(t)/dt, dz_B(t)/dt$$

Constraints :

• What makes sense to me:

$$\frac{dz_A}{dt}, \frac{dz_B}{dt} : 2|\tau|$$

$$1 = z_A(t) + z_B(t) + z_C(t) : |\tau|$$

$$z_A(t=0) : 1$$

$$z_B(t=0) : 1$$

$$\text{no. constraints} = 3|\tau| + 2 = 95$$

• What Pyomo is doing

$$\frac{dz_A}{dt}, \frac{dz_B}{dt} : 2(|\tau|)$$

$$1 = z_A(t) + z_B(t) + z_C(t) : (|\tau|)$$

$$z_A(t=0) : 1$$

$$z_B(t=0) : 1$$

$$\frac{dz_A}{dt} - \text{disc}, \frac{dz_B}{dt} - \text{disc} : 2(|\tau| - 1)$$

$$\text{no. constraints} = 5|\tau|$$

Degrees of Freedom

$$\begin{aligned}\circ \text{My logic: } \text{DOF} &= 5|\tau| - 3|\tau| - 2 \\ &= 155 - 95 \\ &= 50\end{aligned}$$

$$\begin{aligned}\circ \text{Pyomo logic: } \text{DOF} &= 5|\tau| - 5|\tau| \\ &= 0\end{aligned}$$

The pyomo discretized constraints have one less element each (30) to account for the fact that we already specified an initial condition for both z_A and z_B .