Optimization with Differential Algebraic Equations:

DAE Discretization and Pyomo DAE

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Outline

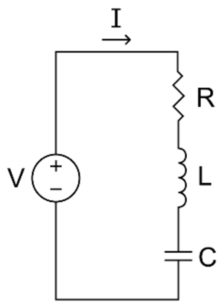
- Review: Differential Equations
- Optimization with DAEs
- Orthogonal Collocation

Review: Differential Equations

Differential Equations

- A *mathematical model* of a physical system.
- It is written in terms of the derivatives of some unknown function/s.
- To simulate the model, we need to find the “solution” to the differential equation, i.e. function/s that satisfy/ies the model.
- What we can do with the solution:
    - Graph it / plot it
    - Explore its properties
    - Interpret it in physical terms

> **“All models are wrong, but some are useful.”**
> – George Box



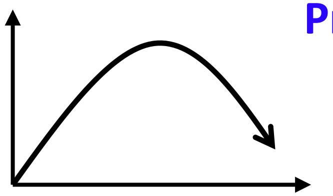
RLC Circuits

$$\frac{d^2 I}{dt^2} + \frac{R}{L}\frac{dI}{dt} + \frac{1}{LC} I = 0$$

Chemical Kinetics

$$\frac{dC_A}{dt} = \frac{F}{V}(C_{Af} - C_A) - k_1 C_A - k_3 C_A^2$$

$$\frac{dC_B}{dt} = -\frac{F}{V} C_B + k_1 C_A - k_2 C_B$$



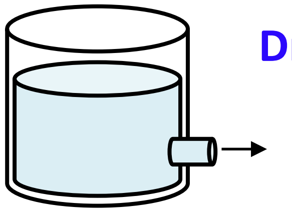
Projectile Motion

$$\frac{dv_x}{dt} = \mu v_x$$

$$\frac{dv_y}{dt} = -g - \mu v_y$$

Transport Equations

$$\frac{\partial c}{\partial t} = D\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right) - kc^2$$

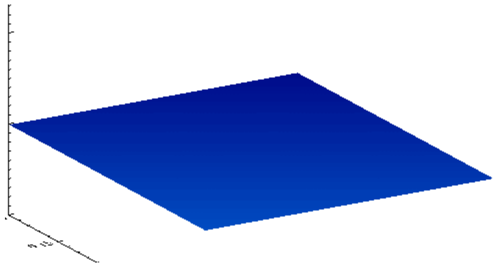


Draining a Tank

$$\frac{dh}{dt} = -C_v \sqrt{h}$$

Radioactive Decay

$$\frac{dA}{dt} = -kA$$



Shallow Water Equations

$$\frac{\partial(\rho\eta)}{\partial t} + \frac{\partial(\rho\eta u)}{\partial x} + \frac{\partial(\rho\eta v)}{\partial y} = 0,$$

$$\frac{\partial(\rho\eta u)}{\partial t} + \frac{\partial}{\partial x}\left(\rho\eta u^2 + \frac{1}{2}\rho g\eta^2\right) + \frac{\partial(\rho\eta uv)}{\partial y} = 0,$$

$$\frac{\partial(\rho\eta v)}{\partial t} + \frac{\partial(\rho\eta uv)}{\partial x} + \frac{\partial}{\partial y}\left(\rho\eta v^2 + \frac{1}{2}\rho g\eta^2\right) = 0.$$

Review: Differential Equations

Differential Algebraic Equations (DAEs)

General form of the DAE model with time:

$$\boxed{\begin{aligned}\dot{\mathbf{x}} &= \mathbf{f}(t, \mathbf{x}(t), \mathbf{u}(t)) \\ \mathbf{y} &= \mathbf{g}(t, \mathbf{x}(t), \mathbf{u}(t))\end{aligned}}$$

If we expand all vectors:

$$\dot{x}_1 = \frac{dx_1}{dt} = f_1(t, x_1(t), x_2(t), \dots, u_1(t), u_2(t), \dots)$$

$$\dot{x}_2 = \frac{dx_2}{dt} = f_2(t, x_1(t), x_2(t), \dots, u_1(t), u_2(t), \dots)$$

$$\vdots$$

$$y_1 = g_1(t, x_1(t), x_2(t), \dots, u_1(t), u_2(t), \dots)$$

$$y_2 = g_2(t, x_1(t), x_2(t), \dots, u_1(t), u_2(t), \dots)$$

$$\vdots$$

Models with higher-order derivatives $\left(\frac{d^n x}{dt^n}\right)$ can be cast into a **system of purely first-order DEs** using a <u>change of variables</u> (recall ES 204).

Where:

$$\mathbf{x}(t) = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \end{bmatrix} = \text{state variables}$$

(those that appear in *time-derivative* terms)

$$\mathbf{u}(t) = \begin{bmatrix} u_1 \\ u_2 \\ \vdots \end{bmatrix} = \text{input variables}$$

(those that can be independently *adjusted*)

$$\mathbf{y}(t) = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \end{bmatrix} = \text{output variables}$$

(those that are physically *measured*)

$$\mathbf{f}(\cdot) = \text{state equations}$$

(expressions found in the differential equations)

$$\mathbf{g}(\cdot) = \text{output equations}$$

(expressions for computing the output variables)

Review: Differential Equations

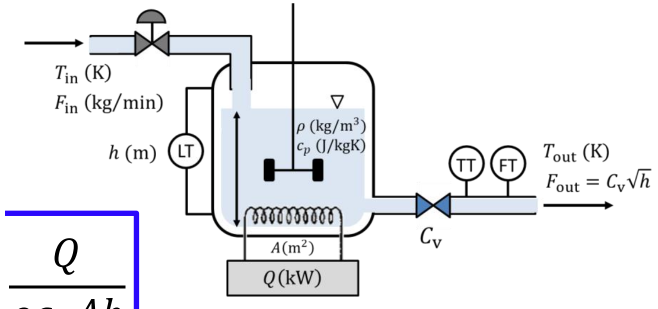
Differential Algebraic Equations (DAEs)

Example: Heated Stirred Tank

$$\frac{dx_1}{dt} \quad \frac{dh}{dt} = \boxed{\frac{1}{\rho A}\left(F_{\text{in}} - F_{\text{out}}\right)} \; f_1(t, \boldsymbol{x}, \boldsymbol{u})$$

$$\frac{dx_2}{dt} \quad \frac{dT_{\text{out}}}{dt} = \boxed{\frac{F_{\text{in}}}{\rho A h}\left(T_{\text{in}} - T_{\text{out}}\right) + \frac{Q}{\rho c_p A h}} \; f_2(t, \boldsymbol{x}, \boldsymbol{u})$$

$$y_1 \quad F_{\text{out}} = \boxed{C_{\text{v}}\sqrt{h}} \; g_1(t, \boldsymbol{x}, \boldsymbol{u})$$



State variables: $\boldsymbol{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} h \\ T_{\text{out}} \end{bmatrix}$

Input variables: $\boldsymbol{u} = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} = \begin{bmatrix} F_{\text{in}} \\ T_{\text{in}} \\ Q \end{bmatrix}$

Output variables: $\boldsymbol{y} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} F_{\text{out}} \\ T_{\text{out}} \\ h \end{bmatrix}$

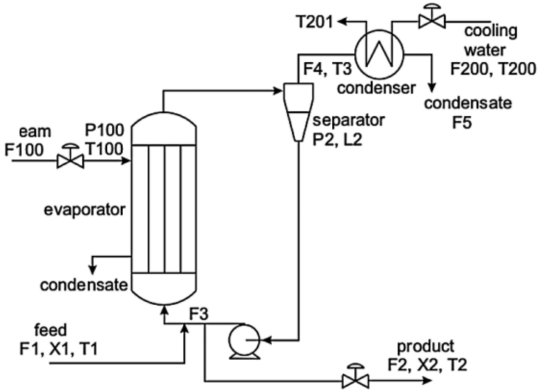
*Variables can be written in any order inside a vector, but you must consistently follow the same order all the time.

Example: Newell-Lee Evaporator

$$\frac{dx_1}{dt} \quad \boxed{\frac{dL_2}{dt} = \frac{F_1 - F_4 - F_2}{20}} \; f_1(t, \boldsymbol{x}, \boldsymbol{u})$$

$$\frac{dx_2}{dt} \quad \boxed{\frac{dX_2}{dt} = \frac{F_1 X_1 - F_2 X_2}{20}} \; f_2(t, \boldsymbol{x}, \boldsymbol{u})$$

$$\frac{dx_3}{dt} \quad \boxed{\frac{dP_2}{dt} = \frac{F_4 - F_5}{4}} \; f_3(t, \boldsymbol{x}, \boldsymbol{u})$$



$$\begin{aligned}
T_2 &= 0.5616 P_2 + 0.3126 X_2 + 48.43 \\
T_3 &= 0.507 P_2 + 55.0 \\
F_4 &= \frac{Q_{100} - 0.07 F_1 (T_2 - T_1)}{38.5} \\
T_{100} &= 0.1538 P_{100} + 90.0 \\
Q_{100} &= 0.16 (F_1 + F_3)(T_{100} - T_2) \\
F_{100} &= Q_{100}/36.6 \\
Q_{200} &= \frac{0.9576 F_{200} (T_3 - T_{200})}{0.14 F_{200} + 6.84} \\
T_{201} &= T_{200} + Q_{200}/0.07 F_{200} \\
F_5 &= Q_{200}/38.5
\end{aligned}$$

$g_n(t, \boldsymbol{x}, \boldsymbol{u})$

States: $\boldsymbol{x} = \begin{bmatrix} L_2 \\ P_2 \\ X_2 \end{bmatrix}$

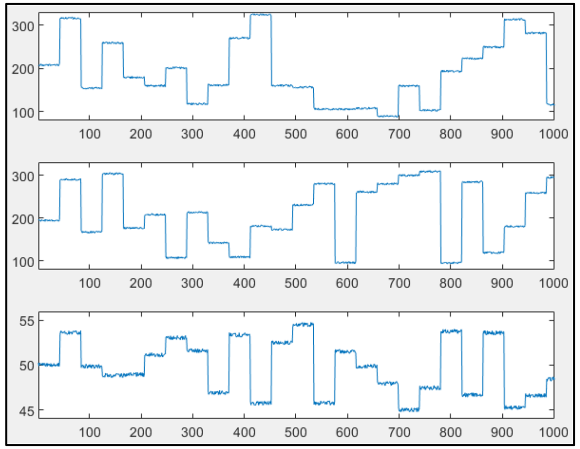
Inputs: $\boldsymbol{u} = \begin{bmatrix} P_{100} \\ F_{200} \\ F_2 \end{bmatrix}$

Outputs: $\boldsymbol{y} = \begin{bmatrix} L_2 \\ P_2 \\ \vdots \end{bmatrix}$

Review: Differential Equations

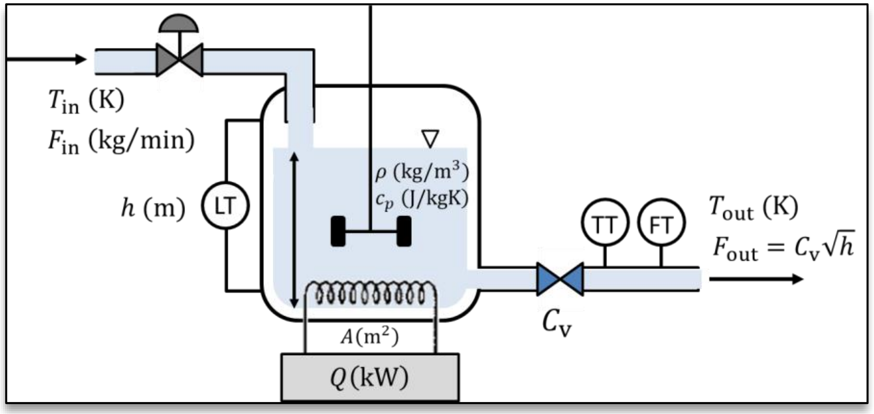
What do we mean by “Simulate a DAE”?

Inputs Data

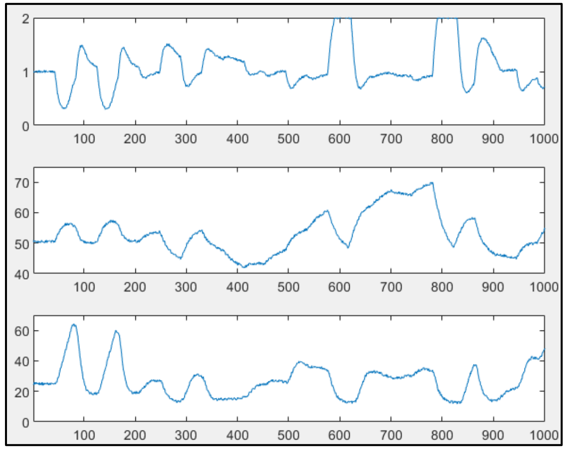


Process

(modeled as DAE)

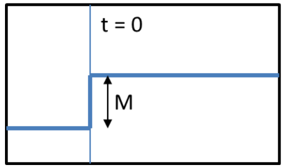


Outputs Data

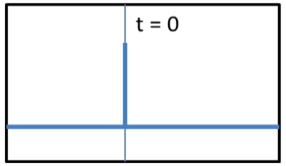


Input excitations → the only way to *perturb* the process away from steady-state and “simulate” its dynamic behavior.

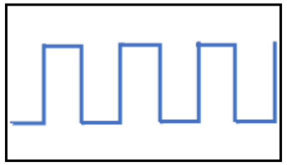
Step



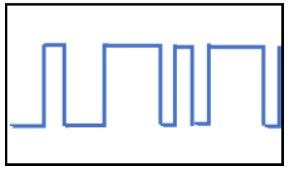
Impulse



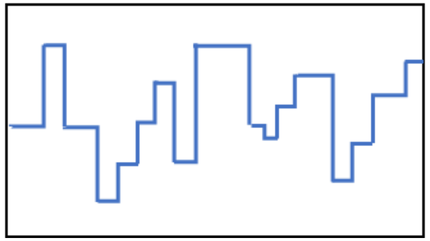
Rectangular



PRBS



APRBS (Amplitude-modulated Pseudo-random Binary Signals)



Output variations consist of:

- *Homogeneous part* (inherent behavior of the system)
- *Non-homogeneous part* (due to input excitations)
- Sensor Noise
- Process Noise

Optimization with DAEs

Standard NLP		
Minimize:	$f(\boldsymbol{x})$	
Subject to:	$h_i(\boldsymbol{x}) = 0$	$i = 1, 2, \ldots, l$
	$g_j(\boldsymbol{x}) \leq 0$	$j = 1, 2, \ldots, m$
and	$x_k^L \leq x_k \leq x_k^U$	$k = 1, 2, \ldots, n$

$\Rightarrow$

Optimization with DAE		
Minimize:	$\Psi(t, \boldsymbol{x}(t), \boldsymbol{y}(t), \boldsymbol{u}(t))$	
Subject to:	$\dot{\boldsymbol{x}} = \boldsymbol{f}\big(t, \boldsymbol{x}(t), \boldsymbol{u}(t)\big)$	States
	$\boldsymbol{y} = \boldsymbol{g}(t, \boldsymbol{x}(t), \boldsymbol{u}(t))$	Outputs
and	$h_i(t, \boldsymbol{x}, \boldsymbol{u}, \boldsymbol{y}) \leq 0$	$i = 1, 2, \ldots, m$

PARAMETER ESTIMATION

Given a real data set of $\boldsymbol{u}(t)$ and $\boldsymbol{y}(t)$, *find all parameter values* within $\boldsymbol{f}(\cdot)$ and $\boldsymbol{g}(\cdot)$ that fits the data.

DATA RECONCILIATION

Given a real data set of $\boldsymbol{u}(t)$ and $\boldsymbol{y}(t)$, and fully known $\boldsymbol{f}(\cdot)$ and $\boldsymbol{g}(\cdot)$, *reconcile* the *actual* $\boldsymbol{y}(t)$ with the *simulated* $\boldsymbol{y}(t)$.

OPTIMAL CONTROL

Given a fully known $\boldsymbol{f}(\cdot)$ and $\boldsymbol{g}(\cdot)$, *find* $\boldsymbol{u}(t)$ that achieves *a desired trajectory* in $\boldsymbol{y}(t)$ while satisfying other constraints.

OPTIMAL DESIGN

Find an operating point $\boldsymbol{x}(0), \boldsymbol{u}(0)$ and parameter values within $\boldsymbol{f}(\cdot)$ and $\boldsymbol{g}(\cdot)$ that maximizes $\boldsymbol{y}(t)$ at steady-state.

(BATCH) SCHEDULING

Given a fully known $\boldsymbol{f}(\cdot)$ and $\boldsymbol{g}(\cdot)$, *create a schedule for* $\boldsymbol{u}(t)$ that minimizes total time to achieve $\boldsymbol{y}(t)$.

REAL-TIME OPTIMIZATION (RTO)

Given a fully known $\boldsymbol{f}(\cdot)$ and $\boldsymbol{g}(\cdot)$, *find* $\boldsymbol{u}(t)$ that maximizes $\boldsymbol{y}(t)$ over time while satisfying other constraints.

Optimization with DAEs

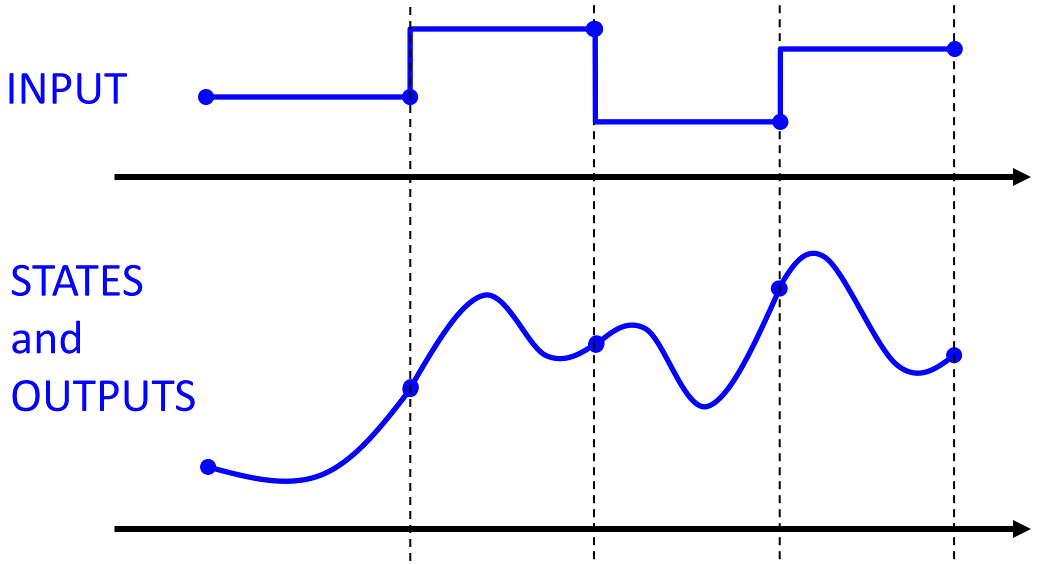
Optimization with DAE

Minimize: $\Psi(t, \boldsymbol{x}(t), \boldsymbol{y}(t), \boldsymbol{u}(t))$

Subject to: $\dot{\boldsymbol{x}} = \boldsymbol{f}\big(t, \boldsymbol{x}(t), \boldsymbol{u}(t)\big)$ States

$\boldsymbol{y} = \boldsymbol{g}(t, \boldsymbol{x}(t), \boldsymbol{u}(t))$ Outputs

and $h_i(t, \boldsymbol{x}, \boldsymbol{u}, \boldsymbol{y}) \leq 0 \qquad i = 1, 2, \ldots, m$



To solve this, we need 2 routines:

DAE SOLVER

Integrate the DAE: Get $\boldsymbol{x}(t)$ and $\boldsymbol{y}(t)$ given $\boldsymbol{u}(t)$ at the next time step, $t + \Delta t$.

NLP SOLVER

Do one iteration: Solve for next updates on the decision variables to minimize $\Psi(t, \boldsymbol{x}(t), \boldsymbol{y}(t), \boldsymbol{u}(t))$

There are three approaches to combine the two:

Single Shooting

DAE SOLVER

$\boldsymbol{u}(t)$ ↑ ↓ $\boldsymbol{x}(t)$, $\boldsymbol{y}(t)$

NLP SOLVER

Multiple Shooting

DAE SOLVER

$\boldsymbol{u}(t)$ $\boldsymbol{x}(0)$ ↑ ↓ $\boldsymbol{y}(t)$

NLP SOLVER

Direct Collocation

NLP SOLVER is also the DAE SOLVER

NLP becomes bigger; results are more accurate

Outline

- Review: Differential Equations
- Optimization with DAEs
- **Orthogonal Collocation**

Orthogonal Collocation

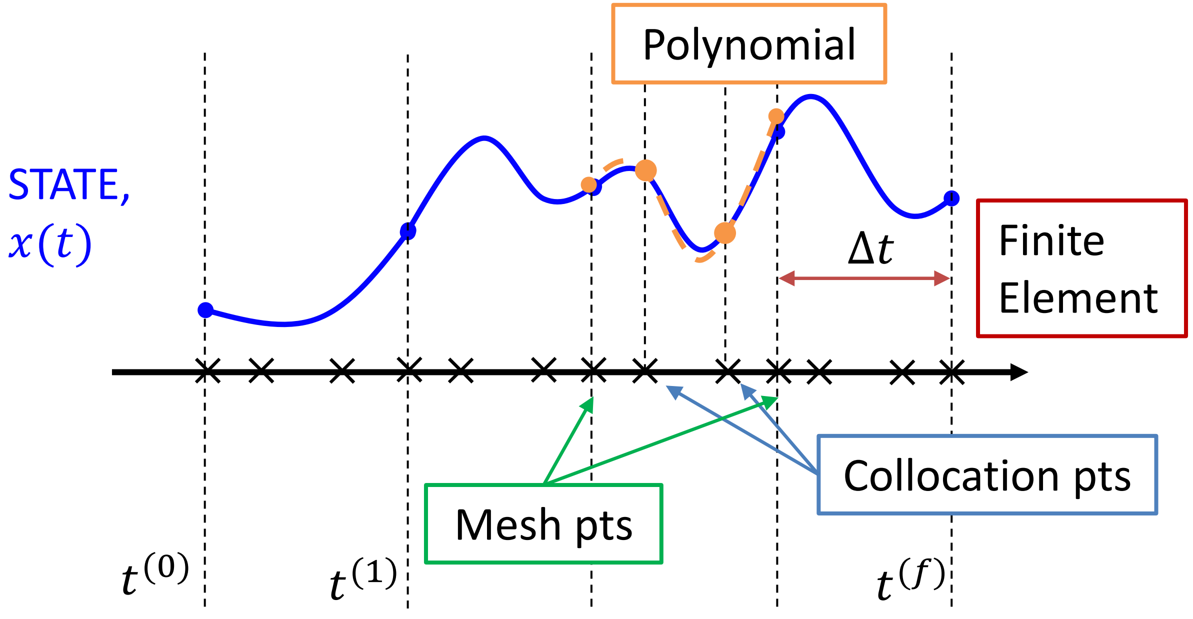
Optimization with DAE

Minimize: $\Psi(t, \boldsymbol{x}(t), \boldsymbol{y}(t), \boldsymbol{u}(t))$

Subject to: $\dot{\boldsymbol{x}} = \boldsymbol{f}\big(t, \boldsymbol{x}(t), \boldsymbol{u}(t)\big)$ States

$\boldsymbol{y} = \boldsymbol{g}(t, \boldsymbol{x}(t), \boldsymbol{u}(t))$ Outputs

and $h_i(t, \boldsymbol{x}, \boldsymbol{u}, \boldsymbol{y}) \leq 0 \qquad i = 1, 2, \ldots, m$



In orthogonal collocation, our goal is to turn the differential equations into a linear system.

$$\boldsymbol{Ax} = \boldsymbol{B}$$

Cubic Polynomial

$$x(t) \approx \sum_{i=0}^{N_c+2} x(\bar{t}_i)\phi_i(\bar{t})$$

A single differential eq'n: $\dfrac{dx(\bar{t})}{d\bar{t}} = f\big(\bar{t}, \boldsymbol{x}(\bar{t}), \boldsymbol{u}(\bar{t})\big)$

becomes $N_{FE} \times N_c + 2$ equalities:

$$\frac{dx(\bar{t})}{d\bar{t}} \cong \frac{1}{\Delta t} \sum_{i=0}^{N_c} \left[\left.\frac{d\phi_i(\bar{t})}{d\bar{t}}\right|_{t=t_j} x(\bar{t}_i) \right] = f\left(\bar{t}_j, \boldsymbol{x}(\bar{t}_j), \boldsymbol{u}(\bar{t}_j)\right)$$

plus $N_{FE} - 1$ continuity constraints:

$$\sum_{m=0}^{N_c} \left[\left.\frac{d\phi_m(\bar{t})}{d\bar{t}}\right|_{\bar{t}_{N_c}^{(i)}} x(\bar{t}_m) \right] = \sum_{m=0}^{N_c} \left[\left.\frac{d\phi_m(\bar{t})}{d\bar{t}}\right|_{\bar{t}_0^{(i+1)}} x(\bar{t}_m) \right]$$

$$\phi_i(\bar{t}) = \prod_{\substack{m=0 \\ m \neq i}}^{N_c+2} \left(\frac{\bar{t} - \bar{t}_m}{\bar{t}_i - \bar{t}_m} \right)$$

Basis functions (polynomials) forced to be 1 at only one collocation point t_m at a time.

Orthogonal Collocation

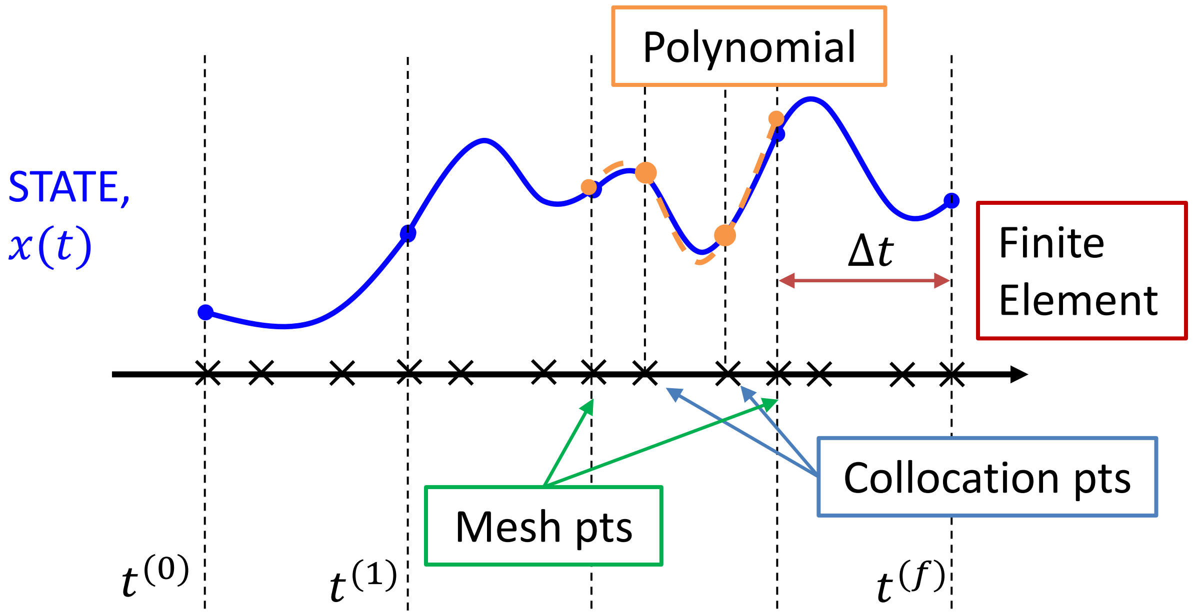
Optimization with DAE

Minimize: $\Psi(t, \boldsymbol{x}(t), \boldsymbol{y}(t), \boldsymbol{u}(t))$

Subject to: $\dot{\boldsymbol{x}} = \boldsymbol{f}\big(t, \boldsymbol{x}(t), \boldsymbol{u}(t)\big)$ States

$\boldsymbol{y} = \boldsymbol{g}(t, \boldsymbol{x}(t), \boldsymbol{u}(t))$ Outputs

and $h_i(t, \boldsymbol{x}, \boldsymbol{u}, \boldsymbol{y}) \le 0 \qquad i = 1, 2, \ldots, m$

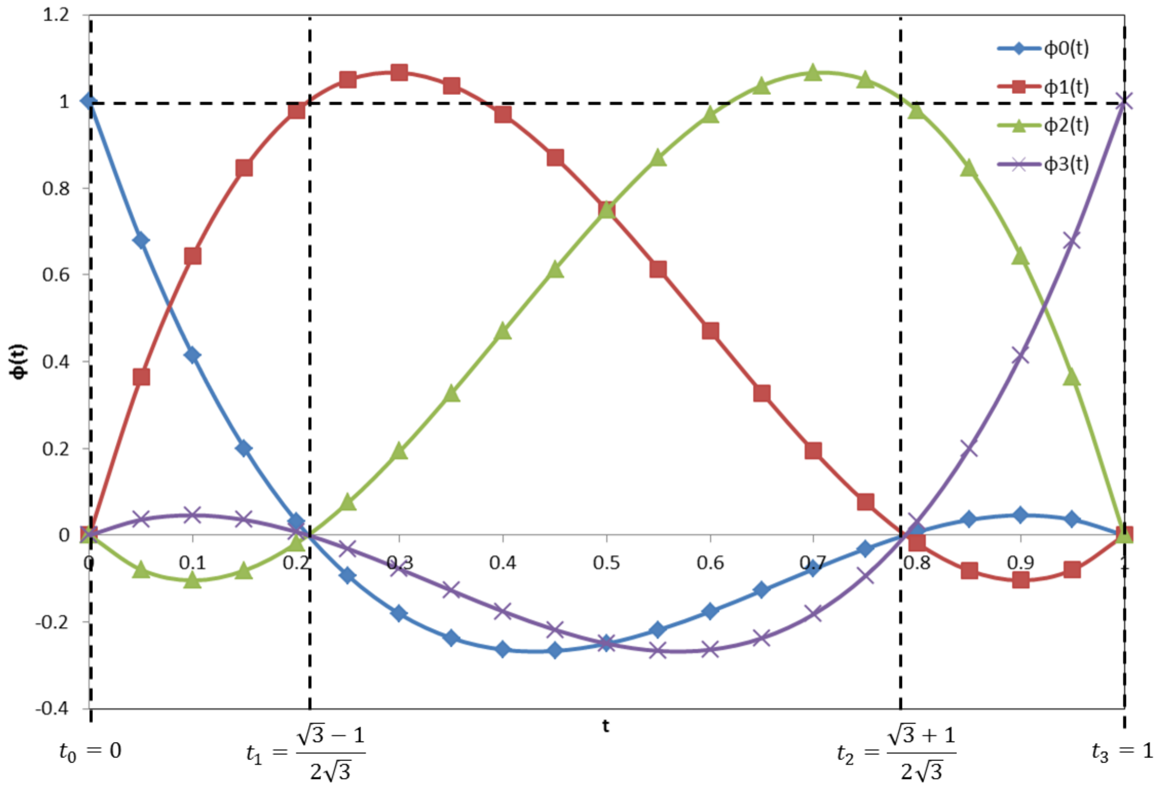


$$\phi_i(\bar{t}) = \prod_{\substack{m=0 \\ m \neq i}}^{N_c+2} \left(\frac{\bar{t} - \bar{t}_m}{\bar{t}_i - \bar{t}_m} \right)$$

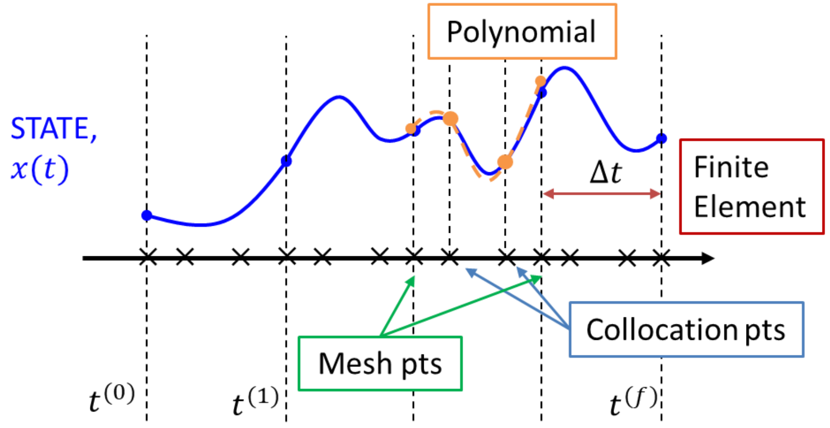
Basis functions (polynomials) forced to be 1 at only one collocation point t_m at a time.

For the 2nd order shifted **Legendre** polynomial, these are the basis functions:

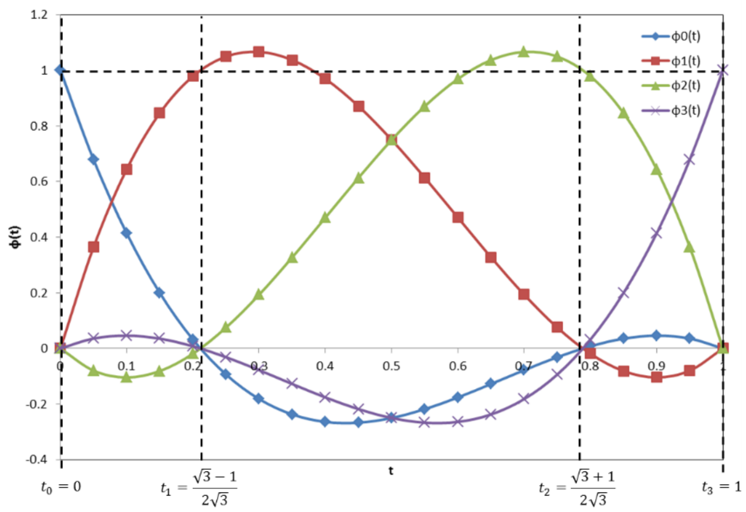
$$\tilde{P}_2(x) = 6x^2 - 6x + 1$$

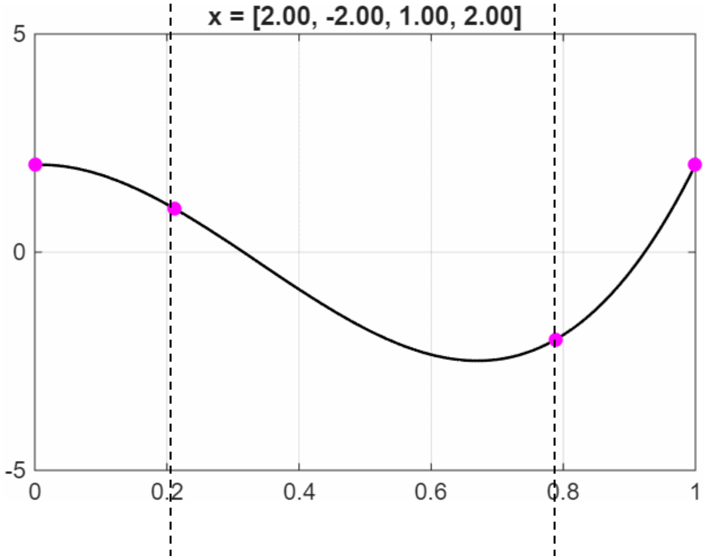


Orthogonal Collocation



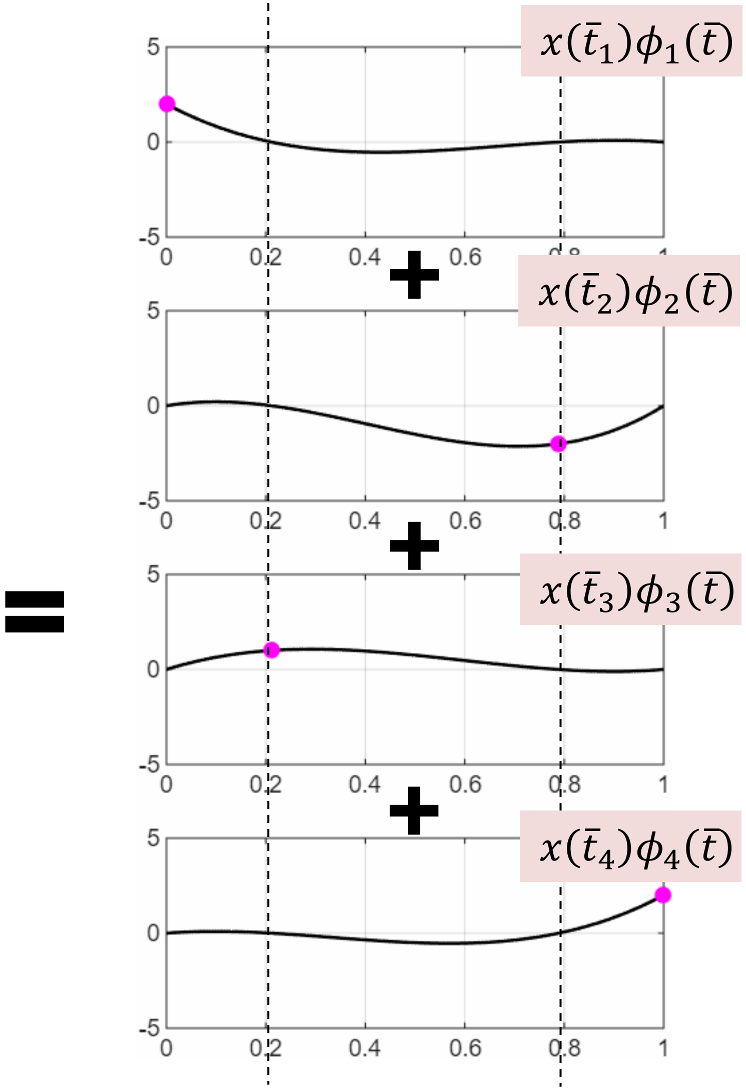
- All we need to fully define the curve within a finite element are 4 values: $x(t_i)$
- Each $x(t_i)$ defines its own cubic polynomial, which is 1 at one collocation point at a time, 0 at the others.
- The sum of 4 cubic polynomials are assumed to approximate the true solution $x(t)$.





$$x(t) \approx \sum_{i=0}^{N_c+2} x(\bar{t}_i)\phi_i(\bar{t})$$

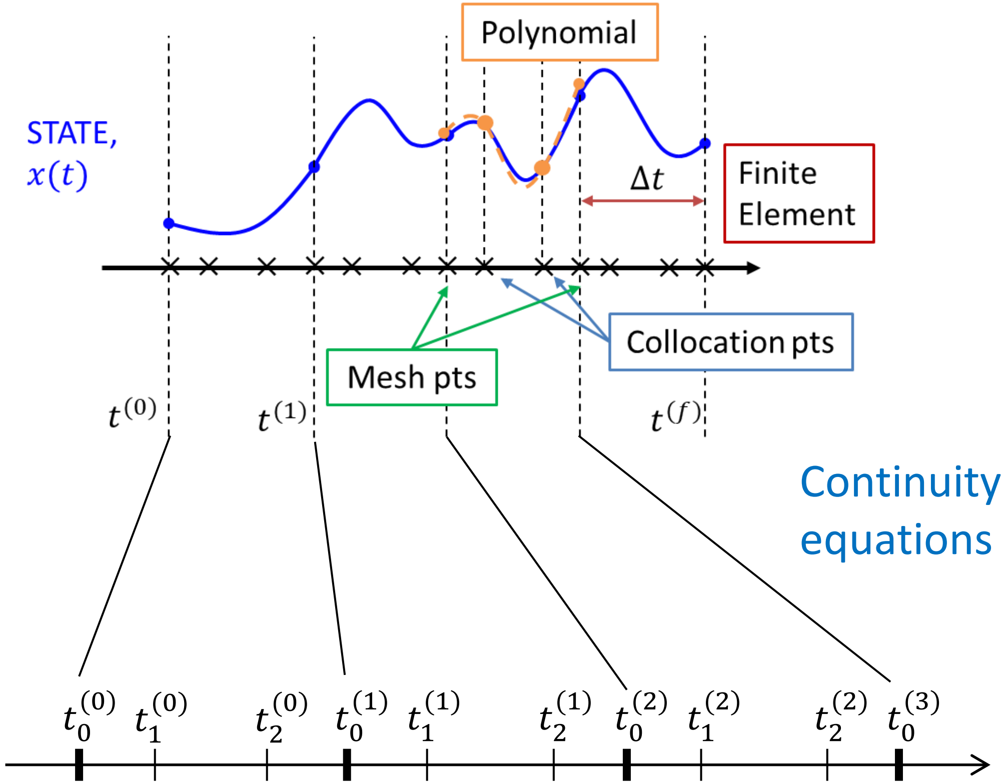
These are the 4 basis functions, one for each collocation point:



Orthogonal Collocation

In orthogonal collocation, our goal is to turn the differential equations into a linear system.

$$\dot{\boldsymbol{x}} = \boldsymbol{f}\big(t, \boldsymbol{x}(t), \boldsymbol{u}(t)\big)$$
$$\boldsymbol{y} = \boldsymbol{g}\big(t, \boldsymbol{x}(t), \boldsymbol{u}(t)\big) \quad \Rightarrow \quad \boldsymbol{Ax} = \boldsymbol{B}$$



Here is an example of the resulting linear system for 2 states (or 2 differential equations), 2 collocation points, and 3 finite elements:
Legend: X = non-zero

States, $\boldsymbol{x}$

x_1										x_2										Inputs, $\boldsymbol{u}$							
$t_0^{(0)}$	$t_1^{(0)}$	$t_2^{(0)}$	$t_0^{(1)}$	$t_1^{(1)}$	$t_2^{(1)}$	$t_0^{(2)}$	$t_1^{(2)}$	$t_2^{(2)}$	$t_0^{(3)}$	$t_0^{(0)}$	$t_1^{(0)}$	$t_2^{(0)}$	$t_0^{(1)}$	$t_1^{(1)}$	$t_2^{(1)}$	$t_0^{(2)}$	$t_1^{(2)}$	$t_2^{(2)}$	$t_0^{(3)}$	$A_0^{(0)}$	$A_0^{(1)}$	$A_0^{(2)}$	$A_0^{(3)}$	$T_0^{(0)}$	$T_0^{(1)}$	$T_0^{(2)}$	$T_0^{(3)}$
X	X	X	X							X										X							
X	X	X	X								X									X							
X	X	X	X									X								X							
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									X							X	X	X	X								X

Continuity equations

Collocation matrix

Outline

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- **Pyomo DAE**

Pyomo DAE

Simulate the following ODE in the domain $t \in [0, 2]$:

$$\frac{dz}{dt} = z^2 - 2z + 1$$

with the initial condition $z(0) = -3$. Compare the result with the analytical solution:

$$z(t) = \frac{4t - 3}{4t + 1}$$

and also with scipy's RK45 solver.

```
model = m = ConcreteModel()

m.t = ContinuousSet(bounds=(0,2))

m.z = Var(m.t)
m.dzdt = DerivativeVar(m.z)

m.obj = Objective(expr=1) # Dummy Objective

def _zdot(m, i):
    return m.dzdt[i] == m.z[i]**2 - 2*m.z[i] + 1

m.zdot = Constraint(m.t,rule=_zdot)


def _init_con(m):
    return m.z[0] == -3

m.init_con = Constraint(rule=_init_con)

# Discretize using collocation
discretizer = TransformationFactory('dae.collocation')
discretizer.apply_to(m, nfe=4, ncp=3,
                     scheme='LAGRANGE-RADAU')

# Solve using Pyomo IPOPT
solver = SolverFactory('cyipopt')
solver.solve(m, tee=True)

colloc_t = list(m.t)
colloc_z = [value(m.z[i]) for i in m.t]

plt.plot(colloc_t,colloc_z,'ro--’)
plt.xlabel('t')
plt.grid()
plt.show()
```

Pyomo DAE

Simulate the following ODE in the domain $t \in [0, 2]$:

$$\frac{dz}{dt} = z^2 - 2z + 1$$

with the initial condition $z(0) = -3$. Compare the result with the analytical solution:

$$z(t) = \frac{4t - 3}{4t + 1}$$

and also with scipy's RK45 solver.

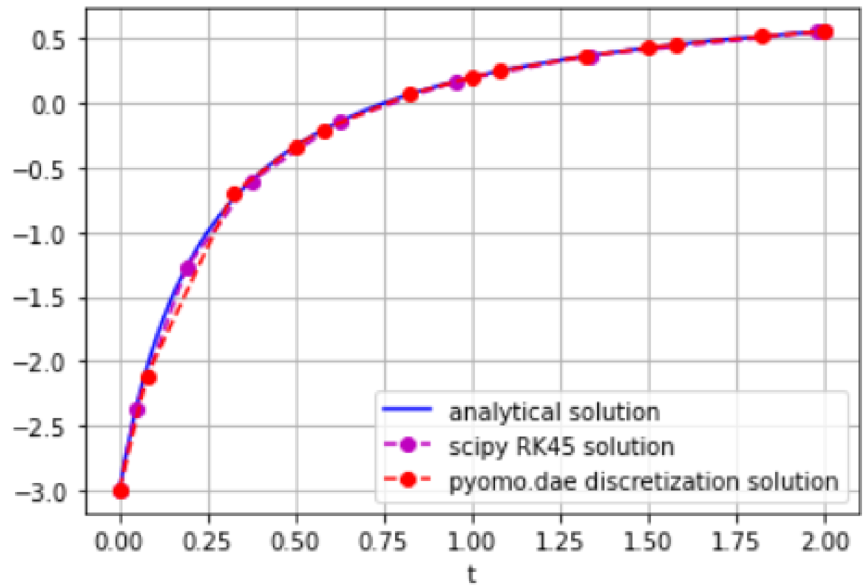
```
Number of nonzeros in equality constraint Jacobian...:       87
Number of nonzeros in inequality constraint Jacobian.:        0
Number of nonzeros in Lagrangian Hessian.............:       13

Total number of variables............................:       26
                     variables with only lower bounds:        0
                variables with lower and upper bounds:        0
                     variables with only upper bounds:        0
Total number of equality constraints.................:       26
Total number of inequality constraints...............:        0
        inequality constraints with only lower bounds:        0
   inequality constraints with lower and upper bounds:        0
        inequality constraints with only upper bounds:        0

iter    objective    inf_pr   inf_du lg(mu)  ||d||  lg(rg) alpha_du alpha_pr  ls
   0  1.0000000e+00 3.00e+00 0.00e+00  -1.0 0.00e+00    -  0.00e+00 0.00e+00   0
   1  1.0000000e+00 2.29e+00 0.00e+00  -1.0 7.00e+00    -  1.00e+00 1.00e+00H  1
   2  1.0000000e+00 1.92e-01 0.00e+00  -1.0 1.53e+00    -  1.00e+00 1.00e+00h  1
   3  1.0000000e+00 2.37e-03 0.00e+00  -2.5 1.02e-01    -  1.00e+00 1.00e+00h  1
   4  1.0000000e+00 7.92e-07 0.00e+00  -3.8 1.37e-03    -  1.00e+00 1.00e+00h  1
   5  1.0000000e+00 2.09e-13 0.00e+00  -8.6 4.86e-07    -  1.00e+00 1.00e+00h  1

Number of Iterations....: 5

EXIT: Optimal Solution Found.
```



Pyomo DAE

Solve the following BVP within $x \in [0, 10]$ then compare Pyomo DAE with scipy BVP:

$$y'' - y'(\sin x) + xy = \cos x$$

$$\text{B.C. } y(0) = 0.5, \quad y(10) = -1$$

```
m = ConcreteModel()
m.xf = Param(initialize=10)
m.x = ContinuousSet(bounds=(0,m.xf))
m.y1 = Var(m.x)  # This is dy/dx
m.y2 = Var(m.x)  # This is the original y

m.dy1dt = DerivativeVar(m.y1)  # This is dy^2/dx^2
m.dy2dt = DerivativeVar(m.y2)  # This is dy/dx

m.obj = Objective(expr=1)  # Dummy Objective

def _zdot1(m, i):
    return m.dy1dt[i] == m.y1[i]*np.sin(i) - i*m.y2[i] + np.cos(i)
m.zdot1 = Constraint(m.x, rule=_zdot1)

def _zdot2(m, i):
    return m.dy2dt[i] == m.y1[i]
m.zdot2 = Constraint(m.x, rule=_zdot2)

def _boundary_con(m):
    yield m.y2[0] == 0.5
    yield m.y2[m.xf] == -1

m.boundary_con = ConstraintList(rule=_boundary_con)

# Discretize using collocation
discretizer = TransformationFactory('dae.collocation')
discretizer.apply_to(m, nfe=20, ncp=3, scheme='LAGRANGE-RADAU')

# Solve using Pyomo IPOPT
solver = SolverFactory('cyipopt')
solver.solve(m, tee=True)

colloc_x = list(m.x)
colloc_y = [value(m.y2[i]) for i in m.x]

plt.plot(colloc_x,colloc_y,'ro--')
plt.xlabel('x')
plt.grid()
plt.show()
```

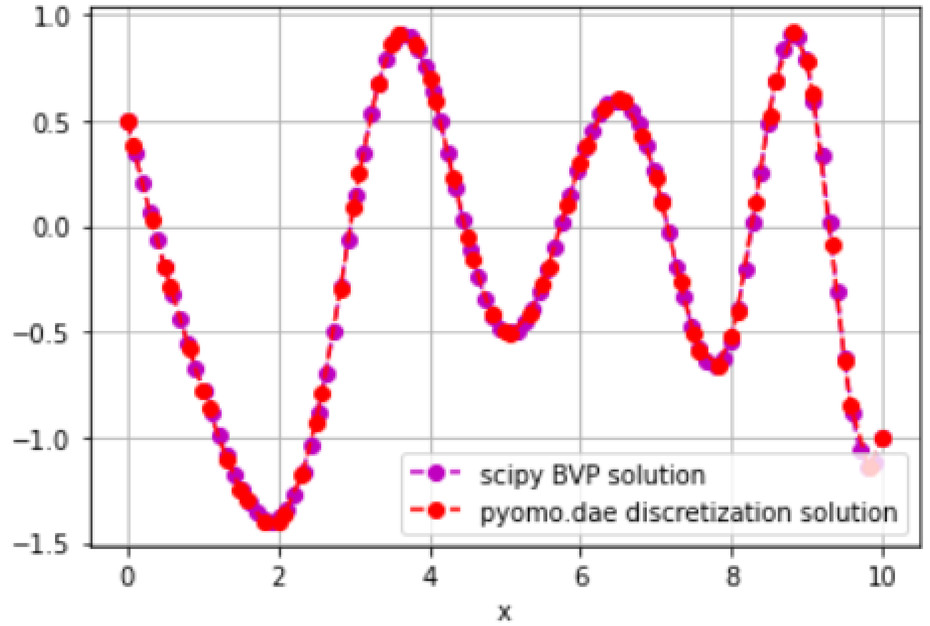
Pyomo DAE

Solve the following BVP within $x \in [0, 10]$ then compare Pyomo DAE with scipy BVP:

$$y'' - y'(\sin x) + xy = \cos x$$

$$\text{B.C.}\ y(0) = 0.5,$$
$$y(10) = -1$$

```
EXIT: Optimal Solution Found.
   Iteration    Max residual  Max BC residual  Total nodes    Nodes added
       1          1.18e-03       5.55e-16          100             1
       2          7.07e-04       0.00e+00          101             0
Solved in 2 iterations, number of nodes 101.
Maximum relative residual: 7.07e-04
Maximum boundary residual: 0.00e+00
```




```
Number of nonzeros in equality constraint Jacobian...:      905
Number of nonzeros in inequality constraint Jacobian.:        0
Number of nonzeros in Lagrangian Hessian.............:        0

Total number of variables............................:      244
                     variables with only lower bounds:        0
                variables with lower and upper bounds:        0
                     variables with only upper bounds:        0
Total number of equality constraints.................:      244
Total number of inequality constraints...............:        0
        inequality constraints with only lower bounds:        0
   inequality constraints with lower and upper bounds:        0
        inequality constraints with only upper bounds:        0

iter    objective    inf_pr   inf_du lg(mu)  ||d||  lg(rg) alpha_du alpha_pr  ls
   0  1.0000000e+00 1.00e+00 0.00e+00  -1.0 0.00e+00    -  0.00e+00 0.00e+00   0
   1  1.0000000e+00 7.11e-15 0.00e+00  -1.7 1.03e+01    -  1.00e+00 1.00e+00h  1

Number of Iterations....: 1

                                   (scaled)                 (unscaled)
Objective...............:   1.0000000000000000e+00    1.0000000000000000e+00
Dual infeasibility......:   0.0000000000000000e+00    0.0000000000000000e+00
Constraint violation....:   7.1054273576010019e-15    7.1054273576010019e-15
Complementarity.........:   0.0000000000000000e+00    0.0000000000000000e+00
Overall NLP error.......:   7.1054273576010019e-15    7.1054273576010019e-15
```

Pyomo DAE

Simulate the following SIR model for $t \in [0,200]$ days, with $\beta = 0.1, \gamma = 0.04$, and a population of $N = 100$:

$$\frac{dS}{dt} = -\frac{\beta IS}{N}$$

$$\frac{dI}{dt} = \frac{\beta IS}{N} - \gamma I$$

$$\frac{dR}{dt} = \gamma I$$

Use initial conditions $S(0) = 95, I(0) = 3, R(0) = 2$. Redo the simulation with $\beta = 0.08$ then compare.

```python
m = ConcreteModel()
m.t = ContinuousSet(bounds=(0,200))

m.S = Var(m.t, initialize=95)
m.I = Var(m.t, initialize=3)
m.R = Var(m.t, initialize=2)
m.beta = Param(initialize=0.1, mutable=True)
m.gamma = Param(initialize=0.04)
m.N = Param(initialize=100)
m.dSdt = DerivativeVar(m.S)
m.dIdt = DerivativeVar(m.I)
m.dRdt = DerivativeVar(m.R)

m.obj = Objective(expr=1)  # Dummy Objective
m.zdot1 = Constraint(m.t, rule=lambda m, i: \
                    m.dSdt[i] == -m.beta*m.I[i]*m.S[i]/m.N)
m.zdot2 = Constraint(m.t, rule=lambda m, i: \
                    m.dIdt[i] == m.beta*m.I[i]*m.S[i]/m.N - m.gamma*m.I[i])
m.zdot3 = Constraint(m.t, rule=lambda m, i: \
                    m.dRdt[i] == m.gamma*m.I[i])
def _init_con(m):
    yield m.S[0] == 95
    yield m.I[0] == 3
    yield m.R[0] == 2
m.init_con = ConstraintList(rule=_init_con)

# Discretize using collocation
discretizer = TransformationFactory('dae.collocation')
discretizer.apply_to(m, nfe=20, ncp=3, scheme='LAGRANGE-RADAU')

# Solve using Pyomo IPOPT
solver = SolverFactory('cyipopt')
solver.solve(m, tee=True)
colloc_t = list(m.t)
colloc_S = [value(m.S[i]) for i in m.t]
colloc_I = [value(m.I[i]) for i in m.t]
colloc_R = [value(m.R[i]) for i in m.t]
plt.plot(colloc_t,colloc_S,'mo--', label='Susceptible (S)')
plt.plot(colloc_t,colloc_I,'ro--', label='Infected (I)')
plt.plot(colloc_t,colloc_R,'bo--', label='Removed (R)')
plt.legend(loc='best')
plt.xlabel('Days')
plt.grid()
```

Pyomo DAE

Simulate the following SIR model for $t \in [0,200]$ days, with $\beta = 0.1, \gamma = 0.04$, and a population of $N = 100$:

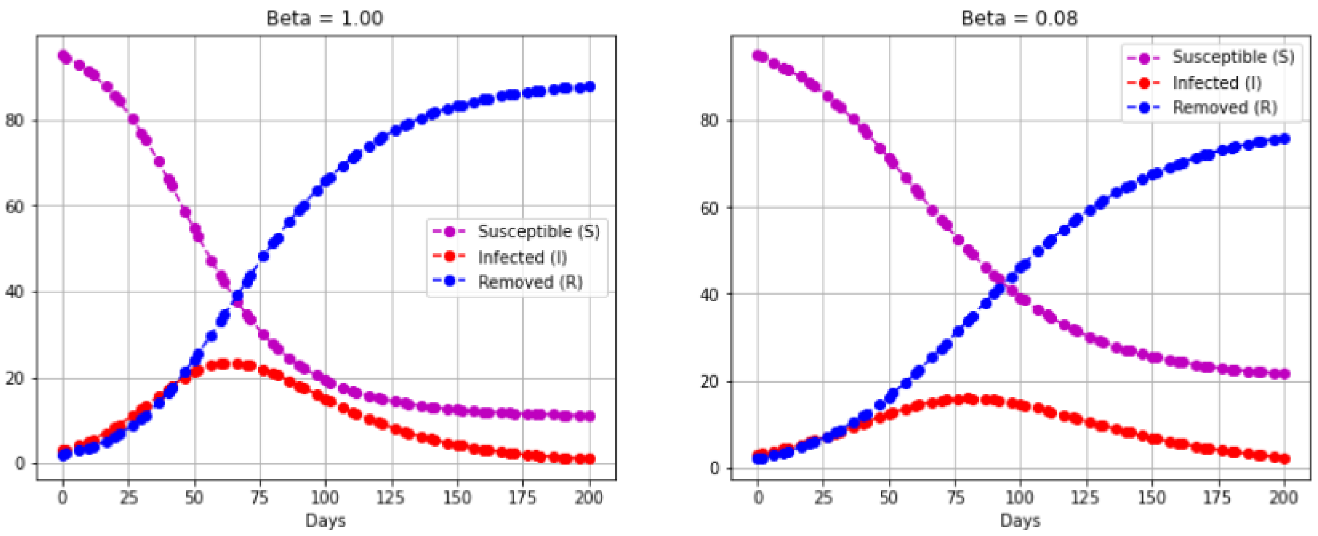
$$\frac{dS}{dt} = -\frac{\beta IS}{N}$$

$$\frac{dI}{dt} = \frac{\beta IS}{N} - \gamma I$$

$$\frac{dR}{dt} = \gamma I$$

Use initial conditions $S(0) = 95, I(0) = 3, R(0) = 2$. Redo the simulation with $\beta = 0.08$ then compare.

```
EXIT: Optimal Solution Found.
```




```
Number of nonzeros in equality constraint Jacobian...:     1391
Number of nonzeros in inequality constraint Jacobian.:        0
Number of nonzeros in Lagrangian Hessian.............:       61

Total number of variables............................:      366
                     variables with only lower bounds:        0
                variables with lower and upper bounds:        0
                     variables with only upper bounds:        0
Total number of equality constraints.................:      366
Total number of inequality constraints...............:        0
        inequality constraints with only lower bounds:        0
   inequality constraints with lower and upper bounds:        0
        inequality constraints with only upper bounds:        0

iter    objective    inf_pr   inf_du lg(mu)  ||d||  lg(rg) alpha_du alpha_pr  ls
   0  1.0000000e+00 2.85e-01 0.00e+00  -1.0 0.00e+00    -  0.00e+00 0.00e+00   0
   1  1.0000000e+00 3.29e-01 0.00e+00  -1.7 1.22e+05    -  1.00e+00 2.44e-04h 13
   2  1.0000000e+00 5.24e-01 0.00e+00  -1.7 4.77e+04    -  1.00e+00 4.88e-04h 12
   3  1.0000000e+00 5.31e-01 0.00e+00  -1.7 1.82e+04    -  1.00e+00 9.77e-04h 11
   4  1.0000000e+00 4.12e-01 0.00e+00  -1.7 8.15e+03    -  1.00e+00 3.91e-03h  9
   5  1.0000000e+00 3.92e-01 0.00e+00  -1.7 2.41e+03    -  1.00e+00 7.81e-03h  8
   6  1.0000000e+00 3.60e-01 0.00e+00  -1.7 1.05e+03    -  1.00e+00 3.13e-02h  6
   7  1.0000000e+00 5.49e-01 0.00e+00  -1.7 3.08e+02    -  1.00e+00 1.25e-01h  4
   8  1.0000000e+00 5.58e-01 0.00e+00  -1.7 7.61e+01    -  1.00e+00 5.00e-01h  2
   9  1.0000000e+00 8.21e-02 0.00e+00  -1.7 1.02e+01    -  1.00e+00 1.00e+00h  1
iter    objective    inf_pr   inf_du lg(mu)  ||d||  lg(rg) alpha_du alpha_pr  ls
  10  1.0000000e+00 1.83e-03 0.00e+00  -2.5 2.51e+00    -  1.00e+00 1.00e+00h  1
  11  1.0000000e+00 1.67e-06 0.00e+00  -3.8 7.90e-02    -  1.00e+00 1.00e+00h  1
  12  1.0000000e+00 2.16e-12 0.00e+00  -8.6 8.72e-05    -  1.00e+00 1.00e+00h  1
```

Outline

- Review: Differential Equations
- Optimization with DAEs
- Orthogonal Collocation
- **Pyomo DAE**
  - Optimal Control
  - Parameter Estimation
  - Data Reconciliation

OPTIMAL CONTROL

Given a fully known $\boldsymbol{f}(\cdot)$ and $\boldsymbol{g}(\cdot)$, *find* $\boldsymbol{u}(t)$ that achieves *a desired trajectory* in $\boldsymbol{y}(t)$ while satisfying other constraints.

PARAMETER ESTIMATION

Given a real data set of $\boldsymbol{u}(t)$ and $\boldsymbol{y}(t)$, *find all parameter values* within $\boldsymbol{f}(\cdot)$ and $\boldsymbol{g}(\cdot)$ that fits the data.

DATA RECONCILIATION

Given a real data set of $\boldsymbol{u}(t)$ and $\boldsymbol{y}(t)$, and fully known $\boldsymbol{f}(\cdot)$ and $\boldsymbol{g}(\cdot)$, *reconcile* the *actual* $\boldsymbol{y}(t)$ with the *simulated* $\boldsymbol{y}(t)$.