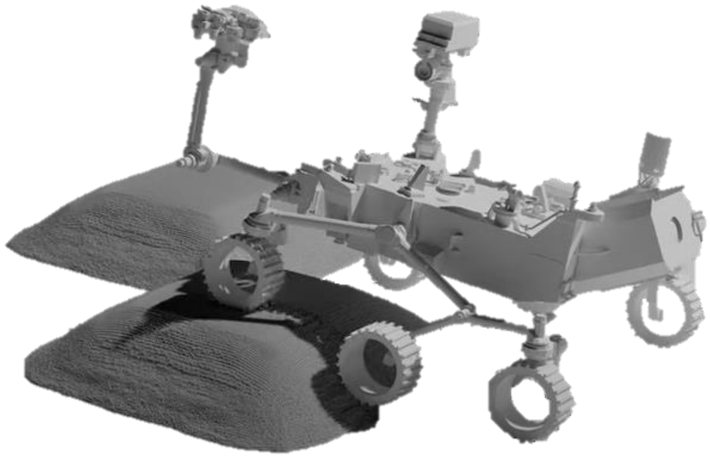
SIMULATING DYNAMIC SYSTEMS

An introduction to using Scipy in Python



UNIVERSITY OF WATERLOO

LEARNING OUTCOMES

- Simulate a system of ordinary differential equations using Scipy
- Plot simulated dynamic trajectories using Matplotlib
- Be familiar with the basic concepts behind ODE integrators

RESOURCES

- APMonitor course
  - https://apmonitor.com/pdc/index.php/Main/SolveDifferentialEquations
- Documentation
  - https://docs.scipy.org/doc/scipy/reference/generated/scipy.integrate.odeint.html
- Many tutorials freely available

SIMULATING DYNAMIC SYSTEMS

- Simulating dynamic systems is vital for enabling engineering applications

Curiosity Rover

Batch Reactor

- Simulate using **numerical methods to approximate dynamics** (e.g., (partial) differential equations)
- Enables us to **computationally experiment** and implement **automation**

ANALYTICAL VS. NUMERICAL METHODS

Analytical Methods

- Separate and integrate

$$g(y)\frac{dy}{dx} = h(x) \Rightarrow \int g(y)dy = \int h(x)dx + C$$

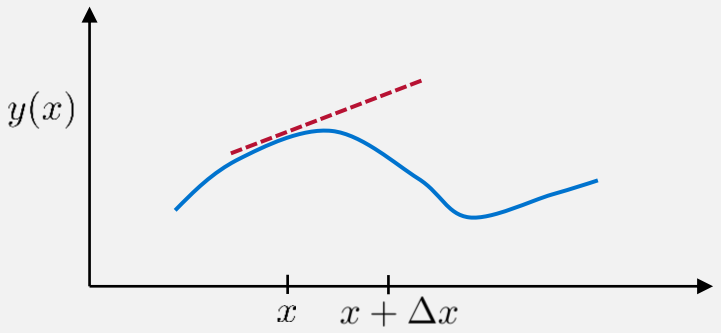
- ODEs of special forms

$$\frac{dy}{dx} = \frac{x+y}{x-y} \Rightarrow \frac{1}{2}\log\left(\frac{y^2}{x^2}+1\right) - \tan^{-1}\left(\frac{y}{x}\right) = C - \log(x)$$

- Solving general ODEs is often difficult or not possible

Numerical Methods

- Seek to numerically approximate the solution
- **Finite difference methods** are common



- **ODE integrators** typically use a range of advanced finite difference techniques

COMMON SIMULATION TOOLS

ODE Integrators

- Common in scripting languages
- Provide numerical solutions to ODE systems

Symbolic Solvers

- Can provide analytic solutions when possible
- Typically, not used for large problems

Optimization Tools

- Can incorporate differential equations when solving optimization problems

Problem Specific

- Simulate dynamics for particular systems

EXPLICIT EULER (FORWARD DIFFERENCE)

Methodology

- Consider a 1st order ODE

$$\frac{dy(t)}{dt} = f(y(t), t)$$
$$y(0) = y_0$$

- Define time steps Δt

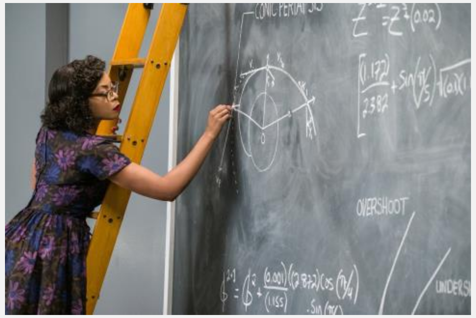
$$t \in [t_0, t_f] \qquad t_k = t_0 + k\Delta t$$

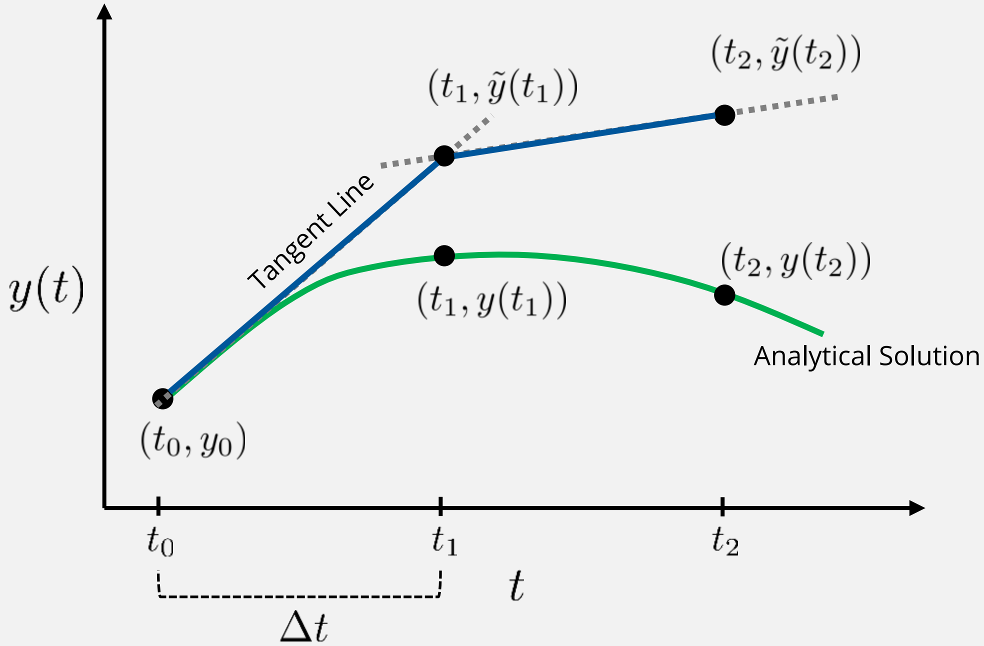
- Approximate derivative as finite difference

$$\left.\frac{dy(t)}{dt}\right|_{t_k} \approx \frac{\tilde{y}(t_{k+1}) - \tilde{y}(t_k)}{\Delta t}$$

- Define update rule

$$\tilde{y}(t_{k+1}) = \tilde{y}(t_k) + f(y(t_k), t_k)\Delta t$$





PROPERTIES: ERROR

Local Truncation Error (LTE)

- Recall update rule

$$\tilde{y}(t_{k+1}) = \tilde{y}(t_k) + f(y(t_k), t_k)\Delta t$$

- Taylor series expansion of analytic solution

$$y(t_k + \Delta t) = y(t_k) + \Delta t \left.\frac{dy(t)}{dt}\right|_{t_k} + O(\Delta t^2)$$

- Difference w/ explicit Euler

$$y(t_k + \Delta t) - \tilde{y}(t_{k+1}) = O(\Delta t^2)$$

- Hence, the error incurred after one step is

$$\boxed{O(\Delta t^2)}$$

Global Truncation Error (GTE)

- The number of steps

$$\frac{t - t_0}{\Delta t} \propto \frac{1}{\Delta t}$$

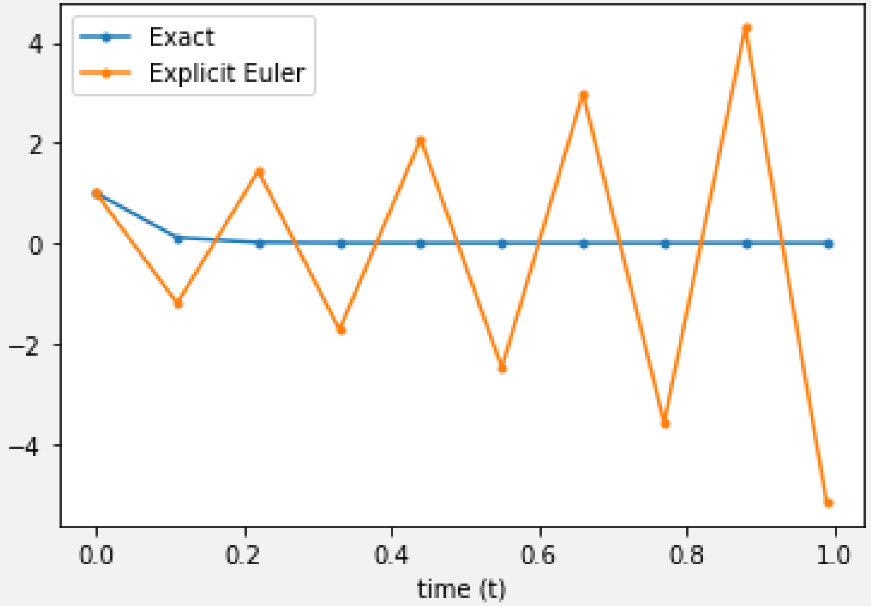
- Multiplying the LTE, we get GTE that is

$$\boxed{O(\Delta t)}$$

- Hence, explicit Euler is a **first order method**
- **Higher order methods are available**

PROPERTIES: STABILITY

Example



Stiff ODEs

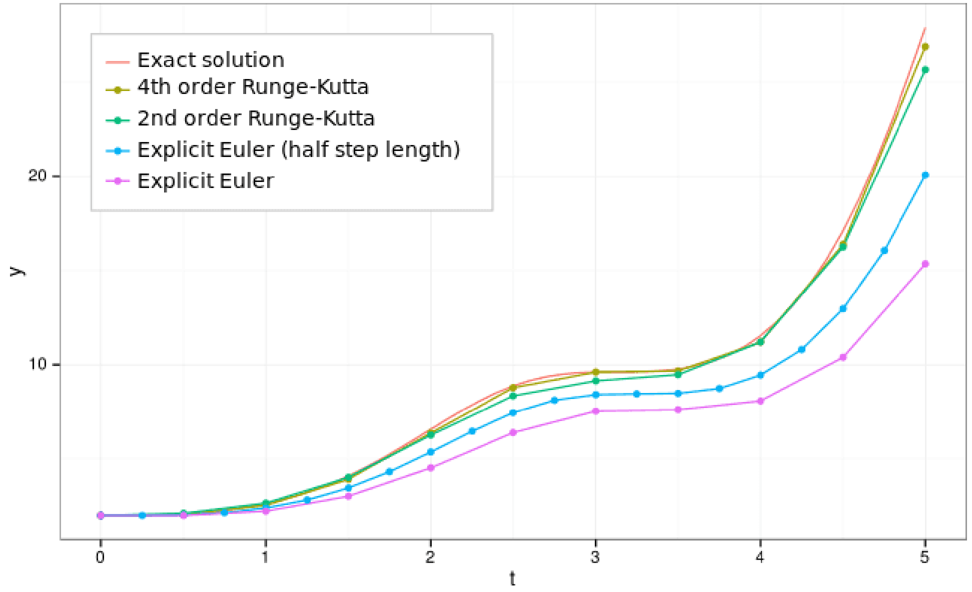
- Systems that exhibit **numerical instability**
- Precise mathematical definition is nontrivial
- Common with **reaction systems**
  - Coexistence of small and large rate constants
- So, what can we do? → Use **implicit methods**

$$\tilde{y}(t_{k+1}) = \tilde{y}(t_k) + f(y(t_{k+1}), t_{k+1})\Delta t$$

ODE INTEGRATION

- Numerically approximate system of ODEs by taking a series of steps
- Higher order methods are typical
- Runge-Kutta (RK) methods are common

$$y_{n+1} = y_n + h \sum_{i=1}^{s} b_i k_i, \qquad \begin{aligned} k_1 &= f(t_n, y_n), \\ k_2 &= f(t_n + c_2 h, y_n + (a_{21} k_1) h), \\ k_3 &= f(t_n + c_3 h, y_n + (a_{31} k_1 + a_{32} k_2) h), \\ &\ \vdots \\ k_s &= f(t_n + c_s h, y_n + (a_{s1} k_1 + a_{s2} k_2 + \cdots + a_{s,s-1} k_{s-1}) h) \end{aligned}$$



- Linear multistep methods are also popular
  - Utilizes linear combination of previous steps

USING SCIPY

scipy.integrate.odeint

```
scipy.integrate.odeint(func, y0, t, args=(), Dfun=None, col_deriv=0, full_output=0,
ml=None, mu=None, rtol=None, atol=None, tcrit=None, h0=0.0, hmax=0.0, hmin=0.0, ixpr=0,
mxstep=0, mxhnil=0, mxordn=12, mxords=5, printmessg=0, tfirst=False)
```
[source]

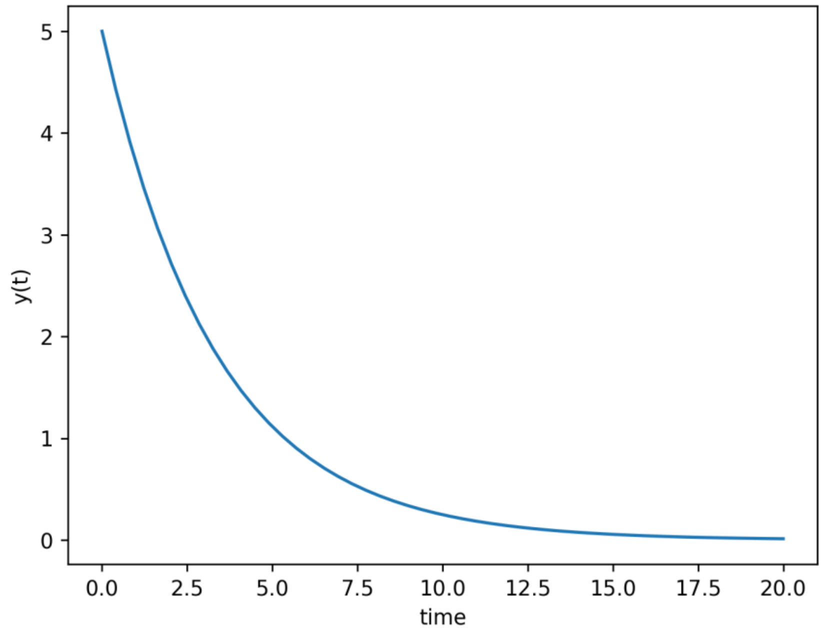
Integrate a system of ordinary differential equations.

- We will use odient instead of solve_ivp
  - For control simulations, we need to control the time steps
- Reformulate ODEs into standard form
- Make a function that returns the LHS
- Requires the LHS function, initial values, and time steps
- Automatically detects stiffness and chooses numerical method

BASIC EXAMPLE

- Simulate the following with Scipy and plot with Matplotlib
  - Let $k = 0.3$

$$\frac{dy(t)}{dt} = -k\, y(t) \qquad y(0) = 5$$

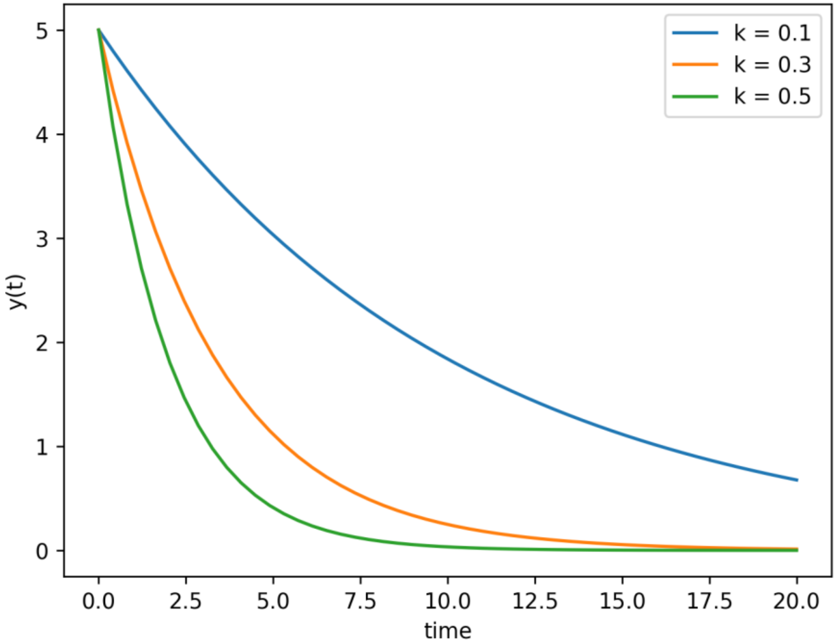



```python
from scipy.integrate import odeint
import numpy as np
import matplotlib.pyplot as plt

# function that returns dy/dt
def model(y, t):
    k = 0.3
    dydt = -k * y
    return dydt

# set the parameters
y0 = 5
ts = np.linspace(0, 20)

# solve ODE
ys = odeint(model, y0, ts)

# plot results
plt.plot(ts, ys)
plt.xlabel('time')
plt.ylabel('y(t)')
plt.show()
```

USING PARAMETER ARGUMENTS

- Simulate the following with Scipy and plot with Matplotlib
  - Plot $k \in \{0.1, 0.3, 0.5\}$

$$\frac{dy(t)}{dt} = -k\,y(t) \qquad y(0) = 5$$



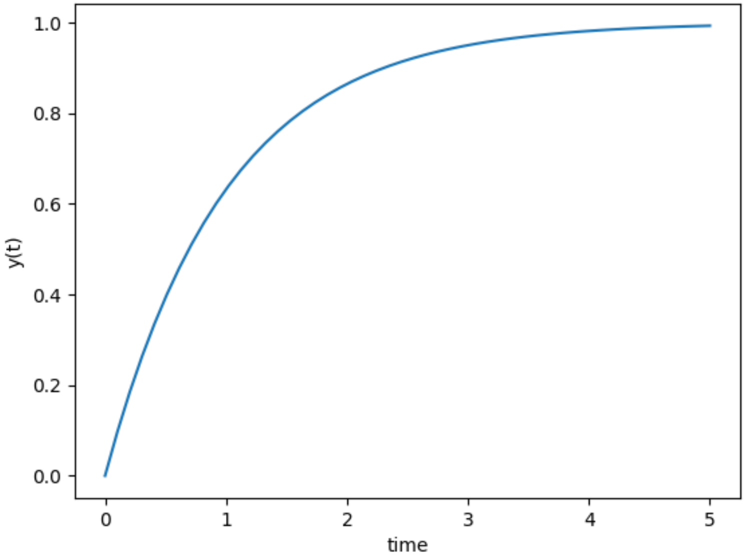

```python
from scipy.integrate import odeint
import numpy as np
import matplotlib.pyplot as plt

# function that returns dy/dt
def model(y, t, k):
    dydt = -k * y
    return dydt

# set the parameters
y0 = 5
ts = np.linspace(0, 20)
ks = [0.1, 0.3, 0.5]

# solve ODEs and plot
plt.figure()
for k in ks:
    ys = odeint(model, y0, ts, args=(k,))
    plt.plot(ts, ys, label='k = '+str(k))

# Show the finalized plot
plt.legend(loc='best')
plt.xlabel('time')
plt.ylabel('y(t)')
plt.show()
```

SIMPLE EXERCISES: WHAT IS THE LONG-TERM STEADY STATE?

- Problem 1

$$\frac{dy(t)}{dt} = -y(t) + 1$$

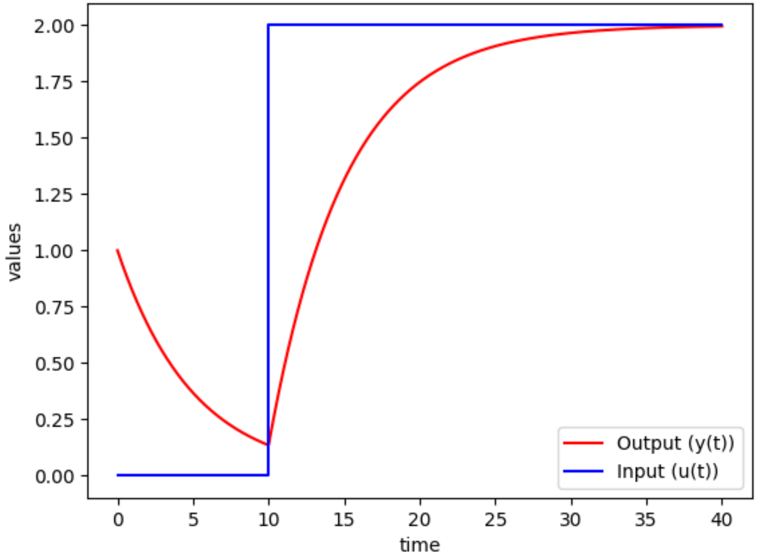
$$y(0) = 0$$



- Problem 2

$$5\,\frac{dy(t)}{dt} = -y(t) + u(t) \qquad u(t) = \begin{cases} 0 & t < 10 \\ 2 & t \geq 10 \end{cases}$$

$$y(0) = 1$$

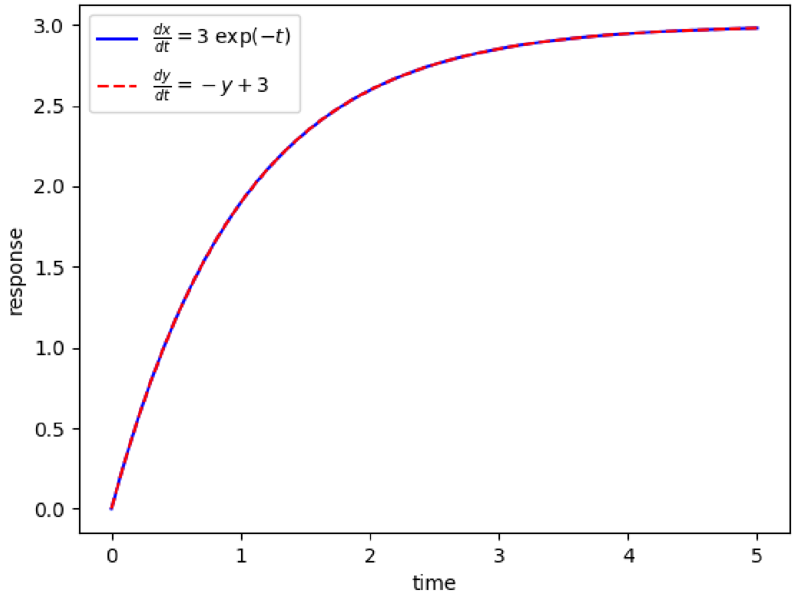


SIMPLE EXERCISES

- Problem 3

$$\frac{dx(t)}{dt} = 3\ exp(-t) \qquad \frac{dy(t)}{dt} = 3 - y(t)$$

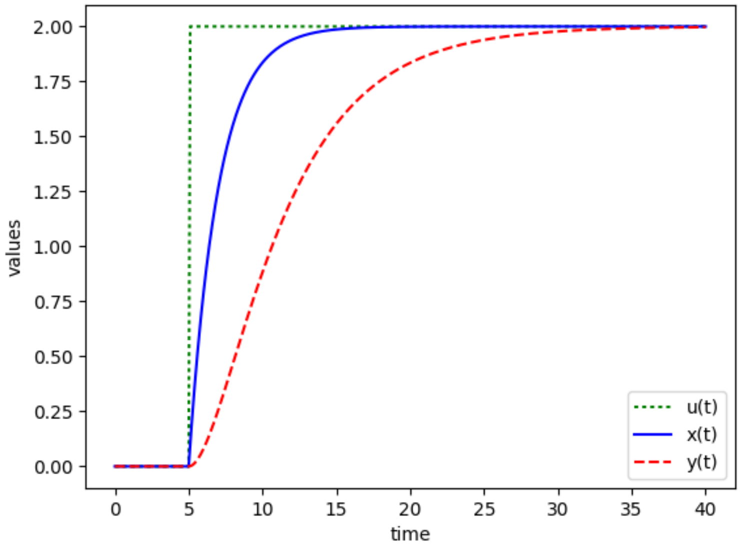
$$x(0) = y(0) = 0$$



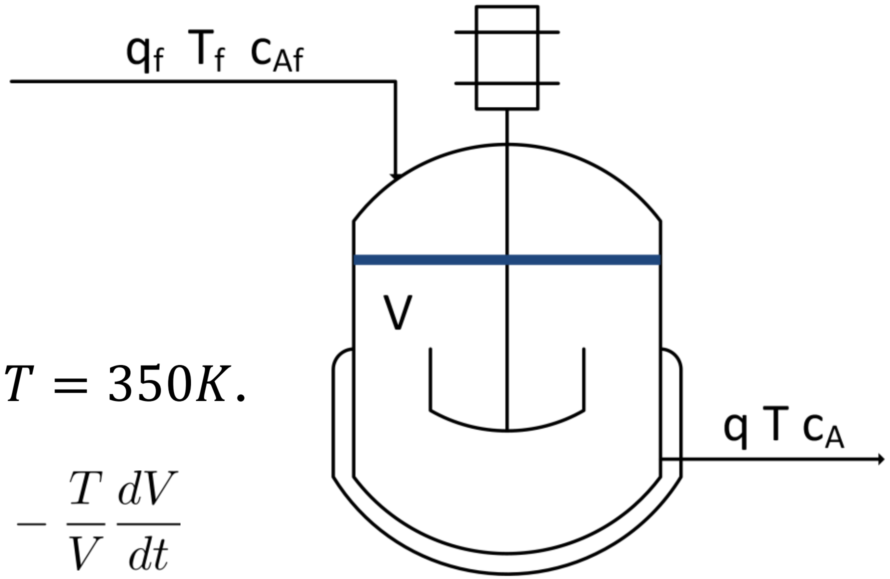
- Problem 4

$$2\ \frac{dx(t)}{dt} = -x(t) + u(t) \qquad u(t) = \begin{cases} 0 & t < 5 \\ 2 & t \geq 5 \end{cases}$$

$$5\ \frac{dy(t)}{dt} = -y(t) + x(t) \qquad x(0) = y(0) = 0$$

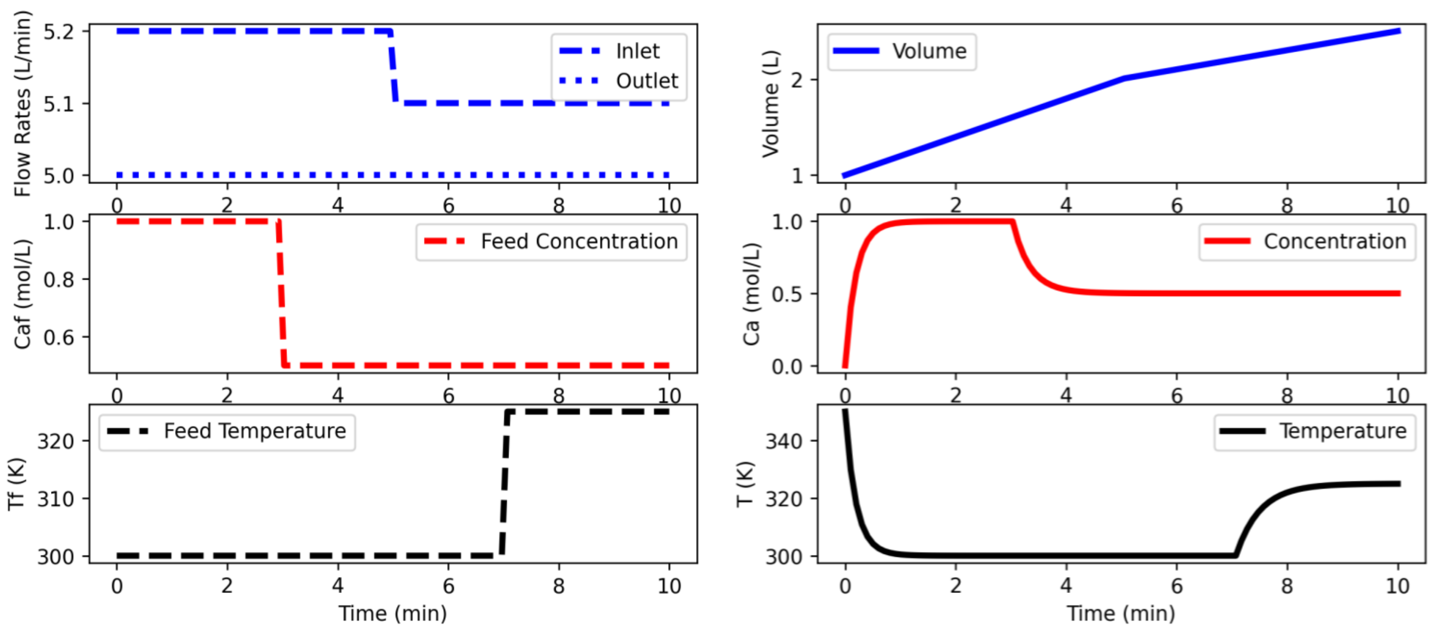


CASE STUDY: MIXER



- Recall the mixer model we developed
  - Initial conditions for the vessel are $V = 1.0L,\ c_A = 0.0\frac{mol}{L}, T = 350K$.

$$\frac{dV}{dt} = q_f - q \qquad \frac{dc_A}{dt} = \frac{q_f c_{Af} - q c_A}{V} - \frac{C_A}{V}\frac{dV}{dt} \qquad \frac{dT}{dt} = \frac{q_f T_f - qT}{V} - \frac{T}{V}\frac{dV}{dt}$$



BEFORE NEXT TIME

- Quiz 2: Due at 11:59 pm via Learn
- Assignment 1: Due Monday at 1:30 pm via Learn
- Prepare for lecture (~1 hr)
  - https://apmonitor.com/pdc/index.php/Main/ModelLinearization
  - https://apmonitor.com/pdc/index.php/Main/FirstOrderSystems
  - https://apmonitor.com/pdc/index.php/Main/FirstOrderGraphical
  - https://apmonitor.com/pdc/index.php/Main/FirstOrderPlusDeadTime