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6 Shareable Handout Numerical Problem Solving across the Curriculum with Python and MATLAB Using Interactive Coding Templates

# 0 Pre-Workshop Set-Up

This file provides instructions on how to access the workshop's GitHub Repository and how to open and edit .mlx and .ipynb files using MATLAB and Google Colab, respectively.

## 1 Workshop Files Table of Contents

This document.

## 2 Workshop Objectives & Overview

## 3 Numerical Problem Solving Workshop

This file contains the slides presented during the workshop.

## 4 Additional Resources

This file contains a catalog of some existing resources for MATLAB Live Scripts and Jupyter Notebooks.

## 5 Interactive Coding Templates

### 5.0 MATLAB Live Script and Jupyter Notebook Tutorials

#### 5.0.1 M0\_HowToCreate.mlx & J0\_HowToCreate.ipynb

M0\_HowToCreate.mlx covers how to create MATLAB Live Scripts. J0\_HowToCreate.ipynb covers how to use Google Colab to create Jupyter Notebooks.

### 5.1 Linear Equations

#### 5.1.1 M1\_MassBalance.mlx (separate solution file available)

- Intended student use case: This file is designed as a homework problem.
- Numerical technique: Format mass balances as a linear algebraic system in matrix-vector form. Explore the Gauss elimination algorithm implementation.
- ChemE application: Linear mass balances on a reaction/separation system with recycle. Material and energy balances (MEB)

- Workshop activity: Explore a Live Script formatted as a homework assignment. Possibly solve the problem.

## 5.2 Nonlinear Equations

### 5.2.1 M2\_NonlinearSystems.mlx (separate solution file available)

- Intended student use case: This file contains three fully worked examples and a case study that requires students to input a single vector of initial guesses to solve the problem.
- Numerical technique: Newton's method, Picard's method, and Newton-Raphson
- ChemE application: Nonlinear mass balances on a reaction/separation system with recycle. Material and energy balances (MEB), reaction engineering
- Workshop activity: Explore a Live Script formatted as a worked example and complete the Case Study. Reflect on how this might be modified for deployment in a class other than numerical methods.

### 5.2.2 M3\_PipeNetwork.mlx & J3\_PipeNetwork.ipynb

- Intended student use case: This is a template for use in the in-class activity based a previous video lecture. Part a of the problem is done in class and parts b and c are homework.
- Numerical technique: System of Non-linear equations
- ChemE application: Pipe flow networks. How fast does the fluid flow down each pipe segment. Fluids
- Workshop activity: Save a copy of this template and recalculate the flowrates by replacing the constant friction factor with a friction factor that is a function of Reynolds number. Then discuss the difficulties you had in doing this task.

## 5.3 Ordinary Differential Equations (ODEs), Initial Value Problems

### 5.3.1 M4\_NonisothermalPFR.mlx & J4\_NonisothermalPFR.ipynb (separate solution files available)

- Intended student use case: This file is designed to be used by students as a worked example/case study for part a and then as a homework problem or in-class exercise for part b and part c.
- Numerical technique: This case study involves solving a system of first-order ODEs using a given set of initial conditions and the built-in MATLAB/Python ODE solver
- ChemE application: This case study models the behavior of parallel reactions in a nonisothermal plug flow reactor (PFR). Reaction engineering
- Workshop activity: Complete part b and part c of the problem.

### 5.3.2 M5\_ParEstKinetics.mlx & J5\_ParEstKinetics.ipynb (separate solution files available)

- Intended student use case: This file is designed to be used by students as a worked example/case study for the first problem and then as a homework problem for the 2nd problem.
- Numerical technique: parameter estimation using curve fitting built-in functions applied to a dynamic model involving multiple ODEs
- ChemE application: fitting reaction rate constants to data for the kinetics of a fluid catalytic cracker. Reaction engineering, data analysis/lab
- Workshop activity: Explore the worked example/case study for the first problem and then look at the solution file for the 2<sup>nd</sup> problem. How might you adapt this type of case study/worked example and then “your turn” problem for one of your classes?

### 5.3.3 M6\_TankDrainage.mlx & J6\_TankDrainage.ipynb

- Intended student use case: This template is based on an example problem in Felder, Rousseau, and Bullard. Before the class the students watch a video lecture and then in class, they use this template to solve in-class lecture and homework problems.

- Numerical technique: ODE solver with initial conditions
- ChemE application: This is a simple mass balance on an unsteady-state well-mixed tank. Material and energy balances (MEB), controls
- Workshop activity: modify the template to solve the problem in which the mass flowrate out of the tank is  $\dot{m}_{OUT}=4.77*m^{0.5}$  in which  $m$  is the mass in the tank. Discuss the difficulties that you had in modifying this template.

## 5.4 ODEs, Boundary Value Problems

### 5.4.1 M7\_StefanTubeDiffn.mlx & J7\_StefanTubeDiffn.ipynb

- Intended student use case: At Rowan this is the first example of a 2nd order ODE with split boundary values which requires a shooting technique to solve. The students first watch a video out of class and then solve this problem in class activity using this template.
- Numerical technique: ODE solver with both a manual iteration and an automated iteration for determining the split boundary values.
- ChemE application: This is the classic problem of evaporation of a pure liquid and resulting diffusion of a gas down a tube. The device is used to obtain gas-phase diffusion coefficients. Fluids, mass transfer
- Workshop activity: modify this template to solve this problem with a linear temperature profile given at the end. Then discuss the difficulties you had in doing this task.

### 5.4.2 M8\_LaminarPipe.mlx & J8\_LaminarPipe.ipynb

- Intended student use case: This is a template for use with a video lecture in a flipped class. In-class they solve the modified problem by replacing the constant viscosity and density with ones that vary with temperature.
- Numerical technique: ODE solver with an automated iteration for determining the split boundary values.
- ChemE application: Classic modeling of laminar pipe flow. The students compare their numerical solution with the analytical solution and then perform the calculation with a given temperature profile in which there is no analytical solution. Fluids
- Workshop activity: modify this template to solve this problem with a linear temperature profile in which the pipe wall is at 45°C and the centerline ( $r=0$ ) is at 25°C. The

correlations for density and viscosity of water are given in the template. Discuss the difficulties that you had in modifying this template.

## 5.5 Partial Differential Equations

### 5.5.1 M9\_HeatTransfer.mlx (separate solution file available)

- Intended student use case: This is a worked example that students are asked to modify/manipulate to explore the behavior of the system.
- Numerical technique: Method of lines, MATLAB built-in ode solver ode15s
- ChemE application: Heat transfer
- Workshop activity: Explore a fully worked example as an Interactive textbook or in-class activity. Manipulate the requested values (like a student).

## 6 Shareable Handout Numerical Problem Solving across the Curriculum with Python and MATLAB Using Interactive Coding Templates

This document is intended to serve as a shareable handout with all workshop materials directly attached to this file, making it shareable outside of the 2022 ChE Summer School Google Drive.