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 embedded in this file, making it shareable outside of the 2022 ChE Summer School Google Drive and avoiding potentially broken links in the future.

To access the .mlx and .ipynb files, right click on the paperclip icon and chose “Save Embedded File to Disk…” option. Other embedded files can be accessed in the same way or by clicking the paperclip icon and proceeding through the security prompts.

We have also recorded a video summarizing several key aspects of interactive coding templates using MATLAB Live Scripts and Jupyter Notebooks. The video is available here.

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0 Pre-Workshop Set-Up

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

1 Workshop Files Table of Contents

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 2nd 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 mdotOUT=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 the 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.