Numerical Methods in Physics and Astrophysics (2022-23)

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Contents

1 | Non-Linear Equations & Systems

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[1] This set of problems for the course developed over the last 12 years with the help of my collaborators:

- Dr. Wolfgang Kastaun (2007-9)
- Dr. Buchart Zink (2010-13)
- Dr. Tanja Bode (2013-15)
- Dr. Daniela Doneva (2015-17)
- Dr. Praveen Manoharan (2021-22)

together with many valuable comments and suggestions from my ex-students.

1.1 | Root Finding: Bisection, Linear Interpolation, $x = g(x)$ & Newton

PROBLEM I

We will consider specifically the following function:

$$f(x) = e^{\sqrt{5}x} - 13.5\cos(0.1x) + 25x^4 \tag{1.1}$$

1. Write a program which uses the **bisection method** to find the positive root of the function above with an accuracy of 10^{-14}.
2. Find this root again, using **linear interpolation**.
3. Implement **Newton's method**.
4. Examine the convergence of the three methods.
5. Explore the robustness of the methods with varying initial guesses and tolerances. What happens when you specify a tolerance below machine precision?

PROBLEM II

Find the eigenvalues λ of the differential equation $y'' + \lambda^2 y = 0$ with the following boundary conditions $y(0) = 0$ and $y(1) = y'(1)$.

Tips, Hints, and Suggestions:

As first step you should try to solve the problem analyticaly by considering the general solution of this wave equation.
Then use the boundary conditions to simplify the solution and the problem will be reduced in finding the roots of a non-linear equation.

1.2 | Nonlinear Systems of Equations

PROBLEM III

We first consider the following nonlinear system of equations

$$f_1(x, y) = xy - 0.1 \tag{1.2}$$
$$f_2(x, y) = x^2 + 3y^2 - 2 \tag{1.3}$$

A1. Solve the nonlinear system of equations using the generalized Newton method. Make sure you find all solutions (there are 4!). Under what conditions would the solver create problems? What checks can you put on/in your solver to avoid diverging from the solution or continuing through with NaNs?

A2. Reformulate the equations and add a function for the "improved" $x = g(x)$ method to the above program. What are the requirements for convergence? How does this affect solving the above system of equations? How is the relative performance for the various roots? How does the program behave if you guess $(x, y) = (2, 1)$?

1.3 | Fractals through Newton - Raphson

PROBLEM IV

Fractals and chaos theory are intricately entwined. In a nutshell, chaos theory amounts to the sensitive, diverging nature of a solution with small changes in the initial conditions. We will go through another chaos problem later in these exercises, but here we delve deeper into the fractal nature of root-finding via the Newton-Raphson method. For these solutions, as 1-dimensional fractals are not as pretty, we will look at solutions to simple functions in the complex plane. The iteration scheme in Newton-Raphson here is the same as for functions in real space:

$$z_{n+1} = z_n - \frac{f(z)}{f'(z)}$$

For each function $f(z)$ we consider in this lab, we create a map of convergence in the (x_0, y_0)-plane where $z_0 = x_0 + iy_0$ is the initial guess to our solver. For which z_0 does the method converge? How fast does it converge? To which root does it converge?

1. Consider first the solution of the function

$$f(z) = z^3 - 1 = 0 \tag{1.4}$$

   - ► Learn how to handle complex numbers in your language of choice.
   - ► Write a function `solve_cnewton` which takes an initial guess and returns the root (if any), the number of iterations need to converge, and the quality of the solution $f(z)$. This should be as simple as grabbing your old newton solver from Lab 1 and upgrading to use complex numbers and interface with the function `get_fdf`.
   - ► Write a program that takes a square $N \times N$ grid in the complex plane and, for each point, uses the above functions to find a root to which the method converges. For a convergence criteria, look for when the change in z is less than ϵ with a certain number of maximum steps M. That is when within M steps $|z_{n+1} - z_n| < \epsilon$. Start with $M = 200$, $\epsilon = 10^{-9}$, and $N = 400$. Define the range of the grid by two gridpoint coordinates (e.g. upper left and lower right). If you know how, take these points as arguments to the main function to ease exploring a given function; otherwise hardcode them initially at $|x_0| < 2$ and $|y_0| < 2$.
   - ► Have the main program print out or save, for every point z_0 of your $N \times N$ grid, a line of format

$$x_0 \quad y_0 \quad k(z) \quad f(z) \quad \log_{10}(n_{\texttt{itns}})$$

     with one blank line after each row of the matrix (if you are working in C in linux). Here $k(z)$ is either the complex root to which the method converges, or zero. n_{itns} is the number of iterations taken to converge, if it does.
   - ▼ Plot $\Im(k(z))$ on the (x, y) plane with a colorscaling in map mode (see hint). Find an interesting region and look at it closer. Repeat. Choose an interesting region and save the plot (with full labels of axes of course!).
   - ▼ Plot $\log(n_{\text{itns}})$ in the (x, y) plane, focusing around a region where the solver does not converge. Comment on what you see.

2. Look at the website http://www.chiark.greenend.org.uk/~sgtatham/newton/ and use your basic code with different functions to explore and understand the convergence and sensitivities of Newton-Raphson. Consider particularly solutions to the function

$$f(z) = 35z^9 - 180z^7 + 378z^5 - 420z^3 + 315z \tag{1.5}$$

   Extra: Choose another function of your choice to present to and discuss with the class.

Tips, Hints, and Suggestions:

- *If you are on a linux machine and you choose to print out the results to stdout, the program* `gnuplot` *can be used to study the results as follows:*

  > gnuplot
  gnuplot> set pm3d map
  gnuplot> splot "<./ComplexRoots" u 1:2:3

  where `ComplexRoots` *is the program name. (If your on another architecture ... perhaps write to a file and read into your favorite visualizer?).*

- *There was no standard for complex numbers in C until the C99 standard. The compiler* `gcc` *(and others) know a data type* `double complex`*, which requires including the extra header "complex.h". A complex number* $z = 3 + 5i$ *is then set by*
  `double complex z = 3.0 + 5*I`.
  The absolute value, real part, imaginary part, and complex phase of a complex number can be calculated by the similarly provided functions `cabs(z)`, `creal(z)`, `cimag(z)`, *and* `carg(z)` *respectively. C++ has <complex> containers, akin to <vector>. Matlab assumes any number could be complex.*

- *The roots of* $f(z) = z^3 - 1$ *are* $\{1, e^{\pm\frac{2}{3}\pi i}\}$*. Or* 1 *and* $(-0.5, \pm 0.8660254040\, i)$.

2 | Linear Systems & Matrices

To be returned by 23.11.2022

PROBLEM I

Should the system of equations be linear but large is size, matrix methods are more useful. Consider the system of equations

$$\begin{aligned} x_1 + 2x_2 + 3x_3 &= 10 \\ 5x_2 + 6x_3 &= 11 \\ 9x_3 &= 12 \end{aligned} \tag{2.1}$$

B1. Write a function which multiplies an N-element vector with a $N \times N$ matrix and prints the resulting vector to screen (even Matlab users). This should be $\lesssim 10$ lines of code. Use this function to calculate the following test case:

$$\begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{pmatrix} \cdot \begin{pmatrix} 10 \\ 11 \\ 12 \end{pmatrix} \tag{2.2}$$

B2. Write a function that solves the system of equations

$$\mathbf{M} \cdot \vec{x} = \vec{b}$$

assuming that $\mathbf{M}$ is an upper-diagonal matrix (back-substitution). Choose a suitable test case. Build in a test to make sure the solution is valid (and/or) test the quality of the solution, then solve the above system of equations. This program will be built upon in the next lab.

Tips, Hints, and Suggestions:

- Minimize duplicate work – For #A1 start with parts of the last exercise and expand upon it.
- Represent both matrices and vectors as arrays. For matrices, one may define a two-dimensional array $m_{ij} = m[i][j]$. Whether defined as 1- or 2-dimensional, one can access an N^2 array's elements in a 1-dimensional sense as $m_{ij} = m[i * N + j]$. A helper function `get_index(i,j,N)` can be useful.
- Remember that indices in C start at zero.
- The name of an array alone is a pointer to the first element of the array, $m = \&m[0]$.
- Good coding practice does not use single-letter variables except for canonical loop variables i, j, k.

PROBLEM II

1. Write a function with a prototype (in C) [you may use your favourite computer language as well.]
   `int gauss_solve( double * Mij, double * bi, double * x, int n )`
   that solves the linear system of equations $\mathbf{M} \cdot \vec{x} = \vec{b}$ using Gaussian elimination. Initially, assume no pivoting is necessary.

2. Use the above program to solve the system of equations

$$\begin{pmatrix} 2.0 & 0.1 & -0.2 \\ 0.05 & 4.2 & 0.032 \\ 0.12 & -0.07 & 5.0 \end{pmatrix} \cdot \vec{x} = \begin{pmatrix} 10 \\ 11 \\ 12 \end{pmatrix}$$

   and verify the solution.

3. (This question is optional) First use your program as to solve the following system of equations as well.

$$\begin{pmatrix} 1 & 1 & 0 \\ 2 & 2 & -2 \\ 0 & 3 & 15 \end{pmatrix} \cdot \vec{x} = \begin{pmatrix} 1 \\ -2 \\ 33 \end{pmatrix}$$

   Record your result, then add pivoting to the implementation. How does the answer compare between pivoting and no pivoting?

Tips, Hints, and Suggestions:

- For all this exercise, expand on your program for part B of Exercise Set 2.
- *Without* Pivoting, the Gauss method can be described by the following pseudo-code:

---

for $i = 0$ to size-1 **do**
  Divide row i by the diagonal element m_{ii}
  Divide $b[i]$ by the diagonal element m_{ii}
  for $j = i + 1$ to size-1 **do**
    Subtract (row i) * m_{ji} from row j
    Subtract $b[i] * m(j, i)$ from $b[j]$
  end for
end for

  This method creates an upper-diagonal matrix.

- After the matrix and vector has been modified into a system of equations with an upper-diagonal operator and a modified $b[i]$, use (or copy) the back-substitution code from the previous exercise to solve the equation.
- When implementing, attempt to be efficient by setting up the loops so as to avoid multiplying elements that are already guaranteed to vanish. Start with the above pseudo-code and implement this optimization after the above has already been tested (Best Practices in Scientific Coding #6)
- Remember, when passing C-arrays as function arguments, you need the argument to be a pointer to the array. Inside the function, there is no way to test how large the array is, so you will also need to pass integers describing the sizes of the array.

PROBLEM III

1. Find the largest eigenvalue and the corresponding eigenvector of the matrix

$$\begin{pmatrix} 6 & 5 & -5 \\ 2 & 6 & -2 \\ 2 & 5 & -1 \end{pmatrix} \tag{2.3}$$

2. Use Aitken's acceleration to improve the final solution
3. Optional: calculate the other 2 eigenvalues.

Tips, Hints, and Suggestions:

The eigenvalues are (1, 4, 6). The power method gives $r_8 = 6.00000198458$.

PROBLEM IV (optional)

Can you generate using random numbers a real $n \times n$ matrix $\mathbf{A}$ and a random real n-dimension vector $\vec{b}$ and then solve the system $\mathbf{A} \cdot \vec{x} = \vec{b}$ using Gauss-Seidel method or overelaxation? [This exercise can replace any of the first two or come in addition].

3 Interpolation & Extrapolation

3.1 | Interpolation Example – Equation of State (*)

To be returned by 4.12.2021

NOTE: You should try problems I and II. Problem III will be solved later once Praveen discusses the associated physics.

PROBLEM I

Solve one of the following 2.

Problem I-A Prove that the Padé approximations $P[3,4]$ and $P[2,5]$ of the function $f(x) = e^x$ are the following:

$$\begin{aligned} P[7,0] &\approx 1 + x + \frac{1}{2}x^2 + \frac{1}{6}x^3 + \frac{1}{24}x^4 + \frac{1}{120}x^5 + \frac{1}{720}x^6 + \frac{1}{5040}x^7 \quad \text{(Taylor)} \\ P[3,4] &\approx \frac{1 + \frac{3}{7}x + \frac{1}{14}x^2 + \frac{1}{210}x^3}{1 - \frac{4}{7}x + \frac{1}{7}x^2 - \frac{2}{105}x^3 + \frac{1}{840}x^4} \\ P[2,5] &\approx \frac{1 + \frac{2}{7}x + \frac{1}{42}x^2}{1 - \frac{5}{7}x + \frac{5}{21}x^2 - \frac{1}{21}x^3 + \frac{1}{168}x^4 - \frac{1}{2520}x^4} \end{aligned} \tag{3.1}$$

Then test which one of the three is more accurate, compare at $x = 0.5, 1, 2, 5$. What do you observe for the accuracy of the 3 cases. Also, try to plot the 3 approximations as well as the original function.

Problem I-B

Prove that the Padé approximations $P[2,3]$ and $P[4,1]$ of the function $f(x) = e^x$ are the following:

$$\begin{aligned} P[5,0] &\approx 1 + x + \frac{1}{2}x^2 + \frac{1}{6}x^3 + \frac{1}{24}x^4 + \frac{1}{120}x^5 \quad \text{(Taylor)} \\ P[2,3] &\approx \frac{1 + \frac{2}{5}x + \frac{1}{20}x^2}{1 - \frac{3}{5}x + \frac{3}{20}x^2 - \frac{1}{60}x^3} \\ P[1,4] &\approx \frac{1 + \frac{1}{5}x}{1 - \frac{4}{5}x + \frac{3}{10}x^2 - \frac{1}{15}x^3 + \frac{1}{120}x^4} \end{aligned} \tag{3.2}$$

Then test which one of the three is more accurate, compare at $x = 0.5, 1, 2, 5$. What do you observe for the accuracy of the 3 cases Also, try to plot the 3 approximations as well as the original function.

PROBLEM II

Find the polynomial of 3rd degree that takes the 4 values listed in the $f(x_k)$ column below at the corresponding arguments x_k.

k	x_k	$f(x_k)$	$\Delta f(x_k)$	$\Delta^2 f(x_k)$	$\Delta^3 f(x_k)$
0	4	1			
			2		
1	6	3		3	
			5		4
2	8	8		7	
			12		
3	10	20			

Table 3.1: Difference matrix

Hint: After you construct the Newton polynomial if you simply it you will get

$$P(x_k) = \frac{1}{24}\left(2x_k^3 - 27x_k^2 + 142x_k - 240\right)$$

PROBLEM III

NOTE: This will be solved later. Praveen will help you understand what is needed.

Equations of states (EoSs) in hydrodynamics are the relation of the pressure locally to the local variables of state of a system (e.g. matter density ρ, specific internal energy ϵ or temperature T). Simulations of hydrodynamic systems generally use an EOS to parameterize the microphysics which cannot be captured in first principle by continuum hydrodynamic equations. Only the simplest regimes have analytic equation EOSs, like an ideal gas law $P = \rho\epsilon(\Gamma - 1)$. In the regime of neutron star interiors, the applicable EoSs are very much a topic of research. Realistic EoSs for neutron star interiors are often generated by physicists using varying degrees of relativity, quantum field theory, and particle physics models.

1. Write a function with a prototype similiar to
   `double interp( double * xs, double * ys, int n, double x )`
   that uses Lagrange-Polynomial interpolation in its generalized form for an unspecified number of known positions (n). Here `xs` are the points where the solution is known, `ys` the evaluated function at these points, `n` the number of known points, and `x` the location at which the value of the function is desired.

2. While the simplest EoS, the barotropic EoS, is of the form $P(\rho) = \kappa\rho^{\Gamma}$, a simple step to add more physics (e.g. by imitating a change in chemistry above a certain density ρ_0) is to create a hybrid-barotropic EoS which we will approximate here as:

   $$P(\rho) = H(\rho_T - \rho)\kappa_1\rho^{\Gamma_1} + H(\rho - \rho_T)\kappa_2\rho^{\Gamma_2} \tag{3.3}$$

   where $\Gamma_1 = 4/3$, $\Gamma_2 = 5/3$, κ_1=20, κ_2=1. For the transition function, $H(\rho)$, use one of the following analytical approximations of the Heaviside function:

   $$H(x) = \frac{1}{1 + e^{-2\alpha x}} \tag{3.4}$$

   $$H(x) = \frac{1}{2}(1 + \tanh(\alpha x)) \tag{3.5}$$

   with the transition density $\rho_T = 5$, and transition speed parameter $\alpha = 5$. Analytically fill the known data arrays, $xs[i] = \rho_i$ and $ys[i] = P(\rho_i)$ over a uniform distribution of n points $x_i = \rho_i$ on the interval $I = [\rho_0, \rho_1]$.

3. *Testing and Analysis:* Create a second set of arrays x_k and y_k for a different set of points x_k uniformly distributed across I with $m = 200$ elements. Fill the y_k array by calling the `interp` function you have just written over the data xs and ys.

   A. Look at the interval $I = [4.5, 5.5]$. Plot the interpolated values for $n = 5, 10, 20$ together with the analytical function. Discuss the errors.

   B. Repeat the above for the interval $I = [0, 10]$. What happens now?

   C. Calculate the chi-square error for the entire function given a number of interpolated points m as

   $$E = \sqrt{\frac{1}{m}\sum_{k=0}^{m-1}(f(x_k) - y_k)^2}. \tag{3.6}$$

Plot $\log(E)$ vs n for a range $n = 3$ to $n = 40$ for the intervals $I = [4.5, 5.5]$, $I = [0, 10]$, and $I = [0 : 30]$.

D. Finally, given a set interval around the transition density ρ_0 of your choosing, explore on your own how different parameters of the above hybrid EoS affect the ability for the interpolator to get the pressure right. Be prepared to discuss this with the class.

Tips, Hints, and Suggestions:

- In order not to need to recompile for each choice of n, make this number a command line argument. To catch commandline arguments,

```
1 int main( int argc, const char **argv) {
2   if ( argc != 2 ) return -1; \\ argc = number of parameters + 1
3   int n = atoi(argv[1]); \\ argv[N] = Nth parameter
4   \\ [...]
5   return 0;
6 }
```

  then the program can be executed with the value of $n = 5$, for example, by executing `./myinterp 5`.

- For those on linux, to plot data graphically, one way to plot this is using the program `gnuplot`:

  >gnuplot
  gnuplot> plot [0:10] 1/(1+exp(-2*a*x)) ... with l
  gnuplot> replot "<./myinterp 5" with p
  gnuplot> replot "<./myinterp 10" with p
  gnuplot> replot "<./myinterp 20" with p

  where `[0:10]` is the desired interval. For others, I would suggest writing a file I/O routine and plot with your favorite visualizer.

- If you're feeling adventurous, make the function `interp` take an array of points to interpolate and an array in which to provide the results. Overhead from function calls can be expensive. This will get you ahead for the next week's exercises.

NOTE:
The suggestion to use specific routines or programs e.g. here "gnuplot" is optional. You may use any other program that serves the purpose.

4 | Numerical Differentiation

4.1 | Numerical Differentiation of Functions

To be returned by 10.12.2021

PROBLEM I

Prove the central difference relation

$$y_0'' = \frac{-y_2 + 16y_1 - 30y_0 + 16y_{-1} - y_{-2}}{12h^2} + O(h^4) \tag{4.1}$$

Try to calculate the explicit form of the error term $O(h^4)$.

PROBLEM II

Consider the function $f(x) = \tan^{-1}(x)$ and calculate the derivative at $x = 0$:
a) using 2 iterations of Richardson extrapolation and compare with the results of the central difference relations.
b) using splines.

5 Numerical Integration

To be returned by 16.12.2022

The problems IV and V will be submitted after the Christmas holidays. Praveen will discuss with you the associated.

PROBLEM I

Find analytically which one of the formulae in Table I we practically implement if we combine Simpson (1/3) with Romberg.

PROBLEM II

Calculate the integral

$$f(x) = \frac{2^x \sin(x)}{x}$$

by using:

1. Simpson (1/3)
2. Romberg with Simpson (1/3)
3. Gauss-Legendre with 4 points (use either data from table 2, or from page 28).

PROBLEM III

Prove **numerically** the following:

$$\int_0^1 \left(\int_0^2 xy^2 dx \right) dy = \frac{2}{3}$$

$$\int_0^1 \left(\int_{2y}^2 xy^2 dx \right) dy = \frac{4}{15}$$

$$\int_0^2 \left(\int_0^{x/2} xy^2 dy \right) dx = ?$$

PROBLEM IV

Quantum Mechanics Application (*)

Besides root-finding, integration is the most ubiquitous fundamental numerical method used in computational physics and astrophysics.

- ► Write a function to fill arrays with the analytical function, to be provided to an integration routine as data. The function should take as arguments the array to be filled, the interval, the number of data points, the *function* to be evaluated, and the stepsize of the data points h.
- ► Write a function for numerical integration using the Newton-Cotes with 2nd order polynomial. Assume half an odd number of data points. The function should return not only the integrated value, but also a measure of its error, E (see tips below).
- ▼ *Application and Testing:*
  (a) Use both above functions to integrate the polynomial $f(x) = x + x^3$ in the interval $[0, 1]$ with $n = 5$ data points. The numerical result should be, up to rounding errors, exact. Why?
  (b) Suppose a particle in a potential well has a wavefunction of the form

$$\Psi(x,t) = \begin{cases} \frac{1}{\sqrt{L}}\left[\sin(\frac{\pi x}{L})e^{-\imath\omega_1 t} + \sin(\frac{2\pi x}{L})e^{-\imath\omega_2 t}\right] & \text{if } 0 < x < L \\ 0 & \text{otherwise} \end{cases} \tag{5.1}$$

  The probability distribution of the particle $P(x,t) \equiv |\Psi(x,t)|^2$. Find the probability that the particle is in the far right quarter of the potential well

$$P(t \,|\, x \in [3L/4, L]) = \int_{3L/4}^{L} P(x,t)dx \tag{5.2}$$

  for times $t \in \{0, \pi/\Delta\omega\}$ where $\Delta\omega = \omega_2 - \omega_1$. Assume $L = 2, \omega_1 = 3$, and $\omega_2 = 4.5$. Compare the results for all odd data numbers $n \in [5, 501]$. For each n, print n, $\log(E)$, and $\log(h)$ to stdout (or a file). Plot $\log(E)$ vs. $\log(h)$ for both times. Are the plots compatible with the expected convergence rate?
- ▼ *Extra Application*: Consider instead the wavefunction of an electron in the $2s$ state of a hydrogen atom:

$$\Psi_{2s}(r) = \frac{1}{4\sqrt{2\pi a_0^3}}\left[2 - \frac{r}{a_0}\right]e^{-r/(2a_0)} \tag{5.3}$$

  where $a_0 = \frac{\hbar^2}{me^2} = 0.0529$ nm is the first Bohr radius.
  - Calculate the mean radius $\langle r\rangle$ as well as its standard deviation $\sigma^2 = \sqrt{\langle (r - \langle r\rangle)^2\rangle} = \sqrt{\langle r^2\rangle}$ for the $2s$ state knowing

$$\langle r^n\rangle = 4\pi\int_0^\infty \Psi^*(r,t)r^n\Psi(r,t)dr. \tag{5.4}$$

    Find a way to handle the integration endpoints.

Tips, Hints, and Suggestions:

- In practice, it is often necessary to pass a function as a parameter. If you haven't done this yet, in C, an example of this is:

```
1 double wah(double x) { return x*x; }
2
3 double at_zero(double (*fun) (double)) {
4   return fun(0.0);
5 }
6
7 int main() {
8   double a = at_zero(wah);
9 }
```

- To release the assumption of an odd number of data points, one could use the 4-point form for the last section. The reason to choose the 4-point form is that this form has the same convergence order as that used for the rest of the method.

- Remember, the error estimate of the method is proportional the the 4th derivative at the center of the range. Look closely at the central differencing scheme:

$$f_0^{(4)} = \frac{f_2 - 4f_1 + 6f_0 - 4f_{-1} + f_{-2}}{h^4} + O(h^2) \tag{5.5}$$

  and the error for the 2nd order Newton-Cotes integration scheme:

$$E = \frac{1}{90} h^4 f^{(4)}(\chi_1) \tag{5.6}$$

- If you begin with the solution for last time, you'll end up looping over all the n. One way around this is to have a wrapping function which calls what used to be the main function, looping over the number of data points, n. A quick workaround is also to use loops and output redirection in bash (that environment you're typing into when you compile if you aren't using an IDE). At the command line ...

  > for i in (5..501); do
  > rem=$(($i % 2));
  > if [$rem -ne 0]; then
  > ./exe/myIntegration $i >> IntegrationData.txt
  > fi
  > done

  The operation % is the modulo operator. The >> operator takes stdout from your program and appends it to the file following the operator.

PROBLEM V

Mode Decomposition Application (*)

Integration is so integral to computational physics that we will take another week on its basic application. The application this week will be focused on mode decomposition. In many nonlinear physical processes the behavior of a system is considered and understood through an interaction / energy transferral between different modes. Examples of this are neutron star oscillations, gravitational wave content/black hole ringdown, and turbulence.

For an *orthonormal* basis $b_i(\vec{r})$, data which is of the form $\Psi(\vec{r}) = \Sigma_i^\infty A_i b_i(\vec{r})$ can be decomposed through a set of integrals

$$A_i = \int b_i^*(\vec{r})\Psi(\vec{r})dV$$

- Establish functions with a prototype akin to `intg_mymethod(struct integrand)` for numerically integrating a data-based integrand via 2 of the following methods:
  (a) Trapezoidal Rule
  (b) 2nd order Newton-Cotes (from last lab)
  (c) Simpson's 3/8 Rule
  (d) Euler-Maclaurin method (a generalization of integration using splines)
  (e) Gauss-Legendre methods of order 2, 4, and 8
  (f) Splines*

  Make sure to note, and handle accordingly, when the integration method requires a specific integral form and/or boundaries!

- *Testing and Comparison* of your method functions

  - *Basic Comparison:* For each function below, compare the behavior of the *applicable* integration methods over their corresponding intervals, I, rewriting the function to fit a specific form/bounds if straightforwardly possible.

$$f_1(x) = e^x \cos(x), \quad \text{in I=[0,}\pi/2] \tag{5.7}$$

$$f_2(x) = e^x, \quad \text{in I=[-1,3]} \tag{5.8}$$

$$f_3(x) = \begin{cases} e^{2x} & x < 0 \\ x - 2\cos(x) + 4 & x \geq 0 \end{cases}, \quad \text{in I=[-1,1]} \tag{5.9}$$

    For each function and method, calculate the actual error E using the analytical answer for all $n \in [5, 501]$, then plot $\log(E)$ vs $\log(h)$ for all methods (properly labeled – a gnuplot script is useful here to streamline changing functions.). That is, for each function you should have one graph comparing the performance of the methods. Study the convergence rate for the methods and discuss:
    (a) Convergence rates: What was expected? What was observed? Can you give a reason if it these do not match?
    (b) What other integration method could be applied to which integrands to possibly achieve better performance?

- *Application:* [1]Provided on the exercise's website is a sample data set, two resolutions & ascii text format, of $\Psi(\theta)$ from an imaginary π-symmetric experiment/simulation. Find the coefficients A_k

[1]This part of the exrcise leave it aside till we discuss the Partial Differential Equations

for the decomposition of this data of the form

$$\Psi(\theta) = \Sigma_{i=0}^{k_{\max}} A_k P_k^0(\cos(\theta))$$

where $P_l^m(\cos(\theta))$ are the Legendre polynomials ($m = 0$ imposing axisymmetry) whose normalization condition is

$$\int_{-1}^{1} P_n(x) P_k(x) dx = \left(\frac{2}{2n+1}\right) \delta_{nk}$$

You can create a function to provide analytic hard-coded Legendre polynomials up to a reasonable order for applying to an integrand. Make sure you address the normalization properly! The coefficients used in the generation of the data is in the file header.

(a) Which integration method did you choose, and why?

(b) Which modes were you able to recover?

(c) What are the various sources of error in the mode decomposition?

(d) Given the provided data set, which $k_{\max}$ makes sense? Which coefficients are trustworthy?

Tips, Hints, and Suggestions:

- Consider creating your integration method routines to take only a structure, e.g. `struct integral` which contains:
  - `N`, the number of data points to assume
  - `I[2]`: a 2-element array containing the interval of integration
  - `*xdata, *ydata`: pointers to data arrays (declared & allocated elsewhere)
  - `(*get_f)` and/or `(*get_fdf)`: Function handles for the integrand

  This way a simple call to a helper function `fill_integrand(struct integral *)` can fill in the integrand with the current function handle and size n.
- Find a work-around for Simpson's 3/8 Rule where n is not a factor of 3.
- For the Gauss-Legendre method, the roots are given for the specified orders in the lecture notes.
- For spline integration, exploit your matrix libraries from Lab 3. I would suggest developing the lab without this integration method, and then spending time on this.

6 Ordinary Differential Equations

6.1 | Theoretical Exercises

To be returned by 6.1.2023

PROBLEM I

Choose 2 of them.

1. Derive the 3rd order Runge – Kutta formula

$$y_{n+1} = y_n + \frac{1}{9}(2k_1 + 3k_2 + 4k_3)$$

where

$$\begin{aligned} k_1 &= hf(x, y) \\ k_2 &= hf\left(x + \frac{1}{2}h, y + \frac{1}{2}k_1\right) \\ k_3 &= hf\left(x + \frac{3}{4}h, y + \frac{3}{4}k_2\right) \end{aligned}$$

2. Prove that when the 4th order RK method is applied to an ODE of the form $y' = Ay$ (A is constant) the algorithm will be

$$y_{n+1} = \left(1 + hA + \frac{1}{2}h^2A^2 + \frac{1}{6}h^3A^3 + \frac{1}{24}h^4A^4\right) y_n$$

3. Prove that the 4th order Runge-Kutta formula in the special case that $y' = f(x)$ i.e. the right hand side is independent of y is equivalent to Simpson's rule.

4. Derive the **4th-order Adams-Bashforth** formula

$$y_{n+1} = y_n + \frac{h}{2}(3f_n - f_{n-1})$$

5. Derive the **4th-order Adams-Bashforth** formula

$$y_{n+1} = y_n + \frac{h}{24}(55f_n - 59f_{n-1} + 37f_{n-2} - 9f_{n_3})$$

6. Derive the fourth-order **4th Adams-Moulton** formula

$$y_{n+1} = y_n + \frac{h}{24}(9f_{n+1} + 19f_n + 5f_{n-1} - f_{n_2})$$

PROBLEM II

1st-order ODEs

1. Consider the Initial Value Problems (IVPs) for the 1st order differential equations. Solve them for the interval $x \in [0, 30]$ using the Heun's, 4th order Runge - Kutta and Adams methods.

   You should choose 2 of them to plot the solutions.

   (a)
   $$y' = y\cos(x+y)\,, \quad y(0) = 1\,. \tag{6.1}$$

   (b)
   $$y' = \sin(xy)\cos(x+y)\,, \quad y(0) = 1\,. \tag{6.2}$$

   (c)
   $$y' = xy - x^2\,, \quad y(0) = 1\,. \tag{6.3}$$

   (d) (logistic equation)
   $$y' = y(3-y)\,, \quad y(0) = 1\,. \tag{6.4}$$

   (e) (Riccati equation)
   $$y' = y^2 - x^2\,, \quad y(0) = 1/2\,. \tag{6.5}$$

   (f)
   $$y' = \frac{1}{3x - 2y + 1}\,, \quad y(0) = 0\,. \tag{6.6}$$

PROBLEM III

Try to go as far as you can

In this lab we'll explore first-order non-linear ordinary differential equations. As the coding aspect is straightforward and not challenging, we will apply the subsequent code to several applications.

The form of the equation we'll consider are types of the class of Bernoulli differential equations: an ODE of the form

$$y\prime(x) = b(x)y^{\alpha}(x) + a(x)y(x)$$

where $\alpha > 0$ is some constant. An example you can keep in mind is motion with non-trivial, non-ideal friction forces.

- ► For the heart of your code, write 3 functions to numerical integrate a single first-order ordinary differential equation:
  - 4th order Runge-Kutta
  - Adams-Multon, without corrective step
  - Adams-Multon *with* corrective step

  For the latter two, use the Runge-Kutta method to get the first four function values.
- ▼ *Testing and Comparisons*: Apply this to the following test differential equation.

$$\begin{aligned} y' &= y + x^2 - 2x + \sin(x) \\ y[0] &= 0.1 \end{aligned} \tag{6.7}$$

  on the interval $[0, 2]$.

i. Plot the absolute analytical error, E, at $x = 2$ as a function of the number of steps taken ($N = [10, 5000]$) in a log-log plot and discuss the convergence order.

ii. Plot the error vs the number of function evaluations ($4N$ for RK4, N for Adams without corrections, $2N$ as a minimum for Adams with corrections). Which method is the most efficient?

▼ *Application – Non-ideal Air Resistance*: The evolution of the velocity of a body flowing through a non-ideal fluid can be described by a Bernouilli type differential equation:

$$v'(t) + \mu(t)v(t) - \omega(t)^2 v^3(t) = 0$$

where $\omega(t)$ and $\mu(t)$ are two positive functions. Assume the initial condition $v(0) = 2$

i. Plot the absolute analytical error at $t = 1.5$ with the constant parameters $\omega(t) = \omega_0 = 0.707$, $\mu(t) = \mu_0 = 2$

ii. Keep $\mu_0 = 2$ constant and vary ω_0 in the vicinity of $1/\sqrt{2}$. How does the solution behave? (see note below)

iii. Consider $\omega(t) = \omega_0 \tan(t)$ with $\omega_0 = 1/\sqrt{2}$ and $\mu_0 = 2$ initially. Then slowly decrease μ_0 towards 1.5. Comment on what you see.

Tips, Hints, and Suggestions:

- The exact solution for the primary ODE (6.7) is $y(x) = 0.6e^x - x^2 - \frac{1}{2}(\cos(x) + \sin(x))$
- There are two relevant branches of solution to the 2nd ODE for constant μ and ω, depending on the sign of $\mu - 4\omega^2$:

$$v(t) = \sqrt{\mu}\left[\omega^2 + e^{2\mu t + 2\ln(-\sqrt{\mu/4-\omega^2})}\right]^{-1/2}$$
$$v(t) = \sqrt{\mu}\left[\omega^2 + e^{2\mu t + \ln(\mu/4-\omega^2)}\right]^{-1/2}$$

6.2 | System of ODEs

Do 1 of the 2 i.e., either Problem IV-1 or IV-2.

PROBLEM IV

1. **PROBLEM IV-1 : Lorenz Attractor**

   The Lorenz equation arise from the simplified system describing two-dimensional fluid flow. The system of equations describing the trajectory of a fluid element is

   $$\frac{d\vec{r}}{dt} = \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \sigma(y-x) \\ -xz + \mathcal{R}x - y \\ xy - \beta z \end{pmatrix} \tag{6.8}$$

   with three parameters σ, $\mathcal{R}$, and β. The 1st parameter σ is the Prandtl number, $\sigma \equiv \nu/\kappa$, relating the kinematic viscosity ν to the thermal diffusivity κ. The 2nd parameter $\mathcal{R} \equiv \mathrm{Re}/\mathrm{Re}_{crit}$ is the ratio of the Reynolds number to the critical Reynolds number, where fluid flow changes from laminar to turbulent. The 3rd parameter β is a geometric factor.

   In this problem we consider the specific parameters $\sigma = 10$, $\mathcal{R} = 28$, and $\beta = 8/3$. Once the exercise is complete, you might find it both educational and entertaining to explore the effects of different parameters.

   - Start by writing a function to numerically integrate a system of N coupled ordinary differential equations in *vector* form using 4th order Runge-Kutta. *It's important to keep the system being solved, including size, separate in this case because we will have an in-class exercise to use these functions in class to solve another example system: the Tolman-Oppenheimer-Volkoff equations for hydrostatic equilibrium in general relativity.*
   - *Single Trajectory Test*

     Use the vectorized 4th order RK4 function function to solve the Lorenz equations as given above in the interval $t = [0 : 50]$ with the initial conditions $\vec{r}(0) = (5, 5, 5)$. After each step, print out $\vec{y}$ and plot the 3-dimensional trajectory (see hint). Use a stepsize $h = 10^{-3}$. You should recognized the Lorenz Attractor.
   - *Double Trajectories and Chaos*

     Integrate the system of ODEs simultaneously for the initial positions $\vec{r}(0) = (5, 5, 5)$ and $\vec{r}(0) = (5, 5, 5 + 10^{-5})$ in the interval $[0, 20]$. For each iteration, print the distance d between the two trajectories. Plot this $\log(d)$ as a function of x.

     i. Plot $\log(d)$ as a function of x.
     ii. Verify that the observed increase in distance is not a numerical artifact caused by too large a stepsize. Compare $\vec{r}(20)$ calculated using $h = 10^{-6}$ and $h = 5 \times 10^{-4}$.
     iii. Estimate, roughly, what order of magnitude a difference of 5×10^{-15} in the initial conditions reaches after an integration time of $t = 50$ (for the exact solution). Then test your estimate using the low resolution.

   Tips, Hints, and Suggestions:

   - 3-dimensional plots are created in `gnuplot` using the following line:
     gnuplot> splot "<./lorenz" u 1:2:3 w l

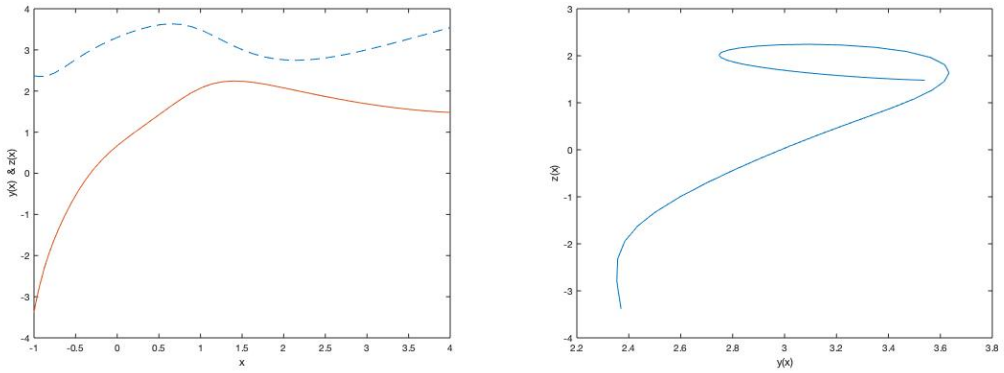
2. **PROBLEM IV-2 : Consider the system of ODEs**

$$\begin{aligned} y' &= \sin(y) + \cos(z\,x) \\ z' &= e^{-yx} + \frac{\sin(z\,x)}{x} \end{aligned} \tag{6.9}$$

with IC $y(-1) = 2.37$ and $z(-1) = -3.48$.

- find the solution in the interval $[-1,\ 4]$ and print it in intervals of $\delta x = 0.25$.
- Plot the numerical solutions of $y(t)$ and $z(t)$ as functions of t .
- Plot of the curve $y(t)$ vs $z(t)$ (parametric plot) .

Figure 6.1: The graphs for question 1 and 2.



PROBLEM V

TOV Equations

OPTIONAL. To be submitted up to 10.2.2023

The Tolman-Oppenheimer-Volkoff (TOV) equations are the relativistic equations of hydrostatic equilibrium with added assumption of spherical symmetry.

The non-relativistic version of these equations can be derived either by addressing a parcel of gas/fluid in a star and balancing the pressure and gravitational forces, or taking the appropriate limit of the Navier-Stokes equation together with the mass continuity equation, both simplified for spherical symmetry:

$$\rho\left(\frac{\partial\vec{u}}{dt}+(\vec{u}\cdot\nabla)\vec{u}\right)=-\vec{\nabla}P+\mu\nabla^2\vec{u}+\vec{F}$$

For a hydrostatic situation, $\vec{u}=0$:

$$\begin{aligned}0&=-\vec{\nabla}P+\vec{F}\\ \vec{\nabla}P&=-\vec{F}\\ \frac{dP}{dr}&=-\vec{F}_{\text{gravity}}=-\frac{Gm\rho}{r^2}\end{aligned}$$

For the relativistic version of the equations, we assume the ideal fluid form of the stress energy tensor

$$T^{\mu\nu}=(\rho+P/c^2)u^\mu u^\nu+Pg^{\mu\nu}$$

where $\rho=\rho_0(1+\epsilon/c^2)$ is the energy density, u^μ is the 4-velocity of the fluid element, ρ_0 is the rest mass density, and ϵ is the specific internal energy of the fluid. We also assume an interior Schwarzschild (static, spherically symmetric) form of the metric:

$$ds^2=-e^{2\nu(r)}c^2dt^2+\left(1-\frac{2Gm(r)}{rc^2}\right)^{-1}dr^2+r^2d\Omega^2$$

where $m(r)$ is the gravitational mass within a coordinate radius r. Using the above stress energy tensor and metric, we reformulate the Einstein Equations

$$G^{\mu\nu}=\frac{8\pi G}{c^4}T^{\mu\nu}.$$

Under *the assumption of a barotropic equation of state* (pressure is a function of density alone, $P=P(\rho)$, we arrive at the coupled system of ordinary differential equations called the TOV equations:

1. Pressure gradient balances gravity	$\frac{dP}{dr}=-G(\rho+P/c^2)\frac{m+4\pi r^3P/c^2}{r(r-2Gm/c^2)}$
2. Mass conservation	$\frac{dm}{dr}=4\pi r^2\rho$
3. Relativistic gravitational potential	$\frac{d\nu}{dr}=\frac{m+4\pi r^3P/c^2}{r(r-2Gm/c^2)}$

For boundary conditions, we can specify the central density of the star, $P(r=0)=P_c(\rho_c)$, $m(r=0)=0$. The metric potential is matched to a true vacuum Schwarzschild spacetime at the surface of the star: $e^{2\nu(r=R)}=1-2GM/rc^2$.

Typical stellar structures are solved using a polytropic equation of state: $P=\kappa\rho_0^\Gamma$ with κ being the polytropic constant and $\Gamma=\frac{d\ln P}{d\ln\rho_0}|_s$ being the adiabatic exponent derived at constant entropy. From

the first law of thermodynamics, $d\epsilon = -Pd(1/\rho_0)$, we can integrate to find the specific internal energy $\epsilon = P/(\rho_0(\Gamma - 1))$.

For $\Gamma = 2$, it is possible to solve this analytically. However, for ideal gases, $\Gamma = 4/3$ (relativistic) or $\Gamma = 5/3$ (unrelativistic) is typical. Realistic equations of state add another layer of complication altogether. Either way, almost all stars require a numerical solution to this set of equations to obtain their stellar structure.

Properties of a solution star

- The *surface* of the star is defined as where the pressure vanishes: $P(R) = 0$.
- The mass function, $m(r)$ is the *gravitational mass* interior to a coordinate radius r. That is, it includes all contributions to the relativistic notion of mass: baryonic mass, internal energy, and the negative gravitational binding energy.
- For the more traditional notion of mass, *baryonic mass*, one must integrate again over the energy density, taking into account the gravitational field. For those with GR experience:

$$m_{baryon}(r) = \int_0^r 4\pi r^2 \rho \sqrt{|g|} dr = \int_0^r \frac{4\pi r^2 \rho}{\sqrt{1 - 2GM/rc^2}}$$

Geometric Units

In general relativity, derivations and solutions are much simplified when in fitting units. For numerical relativity calculations, we then choose geometric (or geometrized) units, defined as $c = G = 1$ (see table). To convert to $M_\odot = 1$ in the last column, we use the geometrized solar mass $M_\odot^* = 1.476 \times 10^5$ cm.

Dimension	**cgs**	**Geometrized**	$c = G = M_\odot = 1$ **Units**
Length	$d = d(\text{cm})$	$d^*(\text{cm}) = d$	$d_*(-) = d/M_\odot^*$
Time	$t = t(\text{s})$	$t^*(\text{cm}) = ct$	$t_*(-) = ct/M_\odot^*$
Mass	$M = M(\text{g})$	$M^*(\text{cm}) = (G/c^2)M$	$M_*(-) = (G/M_\odot^* c^2)M$
Mass Density	$\rho_0 = \rho_0(\text{g cm}^{-3})$	$\rho_0^*(\text{cm}^{-2}) = (G/c^2)\rho_0$	$\rho_{0,*}(-) = (GM_\odot^{*,2}/c^2)\rho_0$
Energy	$E = E(\text{erg})$	$E^*(\text{cm}) = (G/c^4)E$	$E_*(-) = (G/M_\odot^* c^4)E$
Energy Density	$e = e(\text{erg cm}^{-3})$	$e^*(\text{cm}^{-2}) = (G/c^4)e$	$e_*(-) = (GM_\odot^{*,2}/c^4)e$
Pressure	$P = P(\text{dyne cm}^{-2})$	$P^*(\text{cm}^{-2}) = (G/c^4)P$	$P_*(-) = (GM_\odot^{*,2}/c^4)P$
Specific Internal Energy	$\epsilon = \epsilon(\text{erg g}^{-1})$	$\epsilon^*(-) = (1/c^2)\epsilon$	$\epsilon_*(-) = (1/c^2)\epsilon$

The trickier quantity for the TOV equations is the polytropic equation. Given conversion factors α_p and α_{ρ_0} for the pressure and energy density respectively between units A and B, the conversions are (regardless of which)

$$\begin{aligned} P(B) &= \alpha_p P(A) \\ \rho_0(B) &= \alpha_{\rho_0} \rho(A) \\ \kappa(B)(\rho_0(B))^\Gamma &= \alpha_p\, \kappa(A)(\rho_0(A))^\Gamma \end{aligned}$$

Solving for $\kappa(B)$, we see that the conversion depends on the adiabatic exponent:

$$\kappa(B) = \alpha_p \alpha_{\rho_0}^{-\Gamma} \kappa(A)$$

A Stellar Structure Solver

You should already have a working RK4 solver for an n-dimensional coupled set of ODEs.

- ► Implement the hydro TOV equations (only P, m required), assuming a polytropic equation of state. You can choose to code in either cgs or $G = c = M_\odot = 1$ units as long as you are consistent. While P and m have boundary conditions at $r = 0$, ν has an outer boundary condition which must be applied at the end of the solve. Notice also that the equations for dP/dr and $d\nu/dr$ misbehave at $r = 0$ and thus require a hack for small r.
- ► Write a wrapper function, e.g. `make_star`, which takes the central density of the star ρ_0, as well as the EoS parameters Γ and κ to solve the equations. Print out the location of the surface of the star, R, and the gravitational mass of the star, $M = m(R)$. You might want to dig out an interpolator for this, or go for the nearest gridpoint if your grid is at a high enough resolution.
- ▼ Consider a basic star with $\rho_{0,c} = 5 \times 10^{14}\,\mathrm{g\,cm^{-3}}$, $\kappa = 3000$ (in $G = c = M_\odot = 1$ units), and $\Gamma = 2.5$. Verify its gravitational mass and radius, which should be $M = 0.8657$ and $R = 8.27$ in $G = c = M_\odot = 1$ units. Then vary the central density and make a plot of $M(\rho_c)$. What is the maximum mass for this equation of state? If time permits, vary κ and Γ as well and plot $M(\kappa)$ and $M(\Gamma)$.

7 | Boundary & Characteristic Value Problems

To be returned by 16.1.2023

PROBLEM I

A general 1-D BVP is given by, e.g.,

$$u''(x) = g(u, x) \tag{7.1}$$
$$u(x_1) = u_1, u(x_2) = u_2$$

To solve via the shooting method, reformulate the problem as a (2d) root finding problem of the function $f(v) : v \to u_v(x_2) - u_2$ where u_v is a solution to 7.1 with the initial conditions $u_v(x_1) = u_1$, $u'_v(x_1) = v$.

- ► Develop a function akin to `solve_by_shooting` which takes a function handle and boundary conditions. The function must be formulated as a root-finding problem system of equations. Then use your Runge-Kutta 4 routine from earlier labs to find $u_v(x_2)$. Use linear interpolation to approach the correct value of v.
- ▼ Solve the boundary value problem

$$u'' = \left(1 - \frac{x}{5}\right) u + x \tag{7.2}$$
$$u(1) = 2 \tag{7.3}$$
$$u(3) = -1 \tag{7.4}$$

  using the Shooting Method. To solve the initial value problem, use the 4th order Runge-Kutta method with a stepsize of 10^{-4}.

  - How quickly does the Linear Interpolation method converge? Why?
  - Plot the solutions for each iteration of the root finder on top of each other.

- ▼ Now solve the nonlinear boundary value problem

$$u'' = \left(1 - \frac{x}{5}\right) uu' + x \tag{7.5}$$
$$u(1) = 2 \tag{7.6}$$
$$u(3) = -1 \tag{7.7}$$

  - How many iterations are now necessary to achieve the accuracy of 10^{-4}?
  - Plot the solutions for each iteration of the root finder on top of each other.

Tips, Hints, and Suggestions:

- To use RK4, first rewrite Eqn(1) into a system of first order differential equations:

$$u' = v \tag{7.8}$$
$$v' = x + \left(1 - \frac{x}{5}\right) u \tag{7.9}$$

- The solutions for the linear boundary value problem is given through $u'(1) = -3.4950$, while the solution of the nonlinear BVP through $u'(1) = -2.0161$.

PROBLEM II
Solve the linear BVP (use shooting method)

$$\frac{d^2y}{dx^2} - 2y = 0 \quad \text{with} \quad y(0) = 1.2\,, \quad y(1) = 0.9$$

PROBLEM II
Solve the linear BVP (use **matrix method**, and comment on the accuracy if your compare with the previous problem.)

$$\frac{d^2y}{dx^2} - 2y = 0 \quad \text{with} \quad y(0) = 1.2\,, \quad y(1) = 0.9$$

PROBLEM IV (use shooting method) Solve the non-linear BVP (use shooting method)

$$\frac{d^2y}{dx^2} + \frac{(2+y^2)y}{1+y^2} = 1 \quad \text{with} \quad y(0) = 0\,, \quad y(2) = 3$$

8 Partial Differential Equations

8.1 | ELLIPTIC PDEs

To be returned by 6.2.2023

Successive Over Relaxation – Laplace Equation

PROBLEM I
Consider the example for S.O.R. in the lecture, the 2-dimensional Cartesian Laplace Equation

$$\nabla^2 \psi(x, y) = 0 \tag{8.1}$$

in the region $x \in [0, 4]$ and $y \in [0, 4]$ with the Dirichlet boundary conditions $\psi(x, 0) = 20$, $\psi(0, y) = 80$, $\psi(x, 4) = 180$, and $\psi(4, y) = 0$

1. Solve the Laplace equation above using S.O.R. (Successive Over Relaxation) on a numerical grid with resolution of 5×5 points, where the outermost points lie on the edge and only the value of the innermost points need to be solved. As a convergence criteria, the maximum change of all the points between iterations should be smaller than $\varepsilon = 10^{-5}$. Use $\omega = 1$. Check your numerical solution against the solution in the lecture notes.
2. Use the "optimal" ω from the lecture notes. Compare the number of iterations.
3. Vary both ω and ε to verify the above optimal ω is truly optimal. Plot log(# of iterations) vs ω simultaneously for several orders of magnitude of ε (e.g. 10^{-5}, 10^{-10}, 10^{-15}).

Tips, Hints, and Suggestions:

- Use helper functions from previous matrix manipulation labs.
- Remember to poison the initial grid to make bookkeeping mistakes obvious.
- Several useful helper functions for a clean code:
  - Initialize a matrix to a certain value everywhere
  - Calculate the maximum of the absolute value of the interior of a matrix
  - Check interior for NaNs (return an iteration count of -1 for these ω choices)

8.2 | HYPERBOLIC PDEs

Problems II and III to be returned by 10.2.2023

PROBLEM II :
Solve numerical the hyperbolic PDE

$$\frac{\partial^2 y}{\partial t^2} - (1+2x)\frac{\partial^2 y}{\partial x^2} = 0 \quad \text{where} \quad 0 \le x \le 1$$

Assume that the boundaries are fixed and the initial conditions

$$y(x,0) = 0 \quad \text{and} \quad \left(\frac{\partial y}{\partial t}\right)_{(x,0)} = x(1-x)\,.$$

PROBLEM III :
Solve numerical the hyperbolic PDE

$$\frac{\partial^2 y}{\partial t^2} - x(1-x)\frac{\partial^2 y}{\partial x^2} + (1-x^2) = 0 \quad \text{where} \quad 0 \le x \le 1$$

where the initial conditions are:

$$y(x,0) = x(1-x)\,, \quad y_t(x,0) = 0\,,$$

and the boundary conditions

$$y(0,t) = 0\,, \quad y(1,t) = 0\,.$$

8.2.1 PDEs – The Advection Equation

The advection equation can be derived from, e.g., the continuity equation for the one-dimensional drift of an incompressible fluid:

$$u(x, t+\Delta t) = u(x - v\Delta t, t)$$

which can be expanded for sufficiently small Δt by a Taylor expansion of both sides to bring, to first order, the advection equation:

$$\partial_t u + v\partial_x u = 0 \tag{8.2}$$

where we assume a constant velocity v. This is a hyperbolic PDE which, given $u(x, t = 0)$ gives a unique solution at some later time t. The analytic method of choice to solve this would be the method of characteristics, but we will look at various explicit numerical approaches:

PROBLEM III:
Solve the advection equation given an initial Gaussian pulse:

$$u(x,0) = e^{-(x-2)^2}$$

in the range $x \in [-4, 15]$, with $v = 0.03$, $\Delta t = 0.05$, $\Delta x = 0.1$, from $t = 0$ to $t = 200$.

- Discuss the effectiveness of the methods.
- For each method, evolve using two other resolutions and show convergence.
- What happens when you evolve the above methods outside their stability regime?

PROBLEM IV – Traffic Simulation - Optional:
The simple generalization of the advection equation is to have the speed of the advection be related to the function being advected itself:

$$\partial_t \rho(x,t) + f(\rho, x)\partial_x \rho(x,t) = 0 \tag{8.3}$$

When $\rho(x,t)$ is chosen to represent the number density of cars on a road, this form of equation is used by engineers as the basis for managing traffic.

▼ Now solve the nonlinear Burger Equation

$$\partial_t u(x,t) + u\partial_x u(x,t) = 0 \tag{8.4}$$

for $u(x,t)$.

- How many iterations are now necessary to achieve the accuracy of 10^{-4}?
- Plot the solutions for each iteration of the root finder on top of each other.

PROBLEM V- Optional:
The generalization of the advection equation can function-dependent velocities:

$$\partial_t \rho(x,t) + v(\rho)\partial_x \rho(x,t) = 0 \tag{8.5}$$

When ρ is the number density of cars, this equation is used to start modeling traffic flows. Take the simplest case,

$$v(\rho) = v_{\text{max}}\left(1 - \frac{2\rho}{\rho_{\text{max}}}\right)$$

where v_{max} is, say, the speed limit while ρ_{max} is the maximum density (bumper-to-bumper traffic). We can always rescale our ρ to units such that $\rho_{\text{max}} = 1$ and $v_{\text{max}} = 1$.

Re-derive the Lax-Wendroff and Upwind Schemes to account for the variable velocity and include 2nd order (in space) corrections. Implement these new versions. You might set up the code to print out the solution often enough to generate a surface plot $\rho(x,t)$ of the solution.

PROBLEM VI - Optional:
Consider then an initially Gaussian distribution, modeling the region around a traffic jam: $\rho(x,0) = e^{-x^2/2}$. Start with a base resolution of $\Delta x = 0.05$ and $\Delta t = 0.01$ and pay attention to what happens after $t = 0.8$.

1. Plot a comparison between Upwind and Lax-Wendroff at several choice times.
2. For each method, evolve using two other resolutions and show convergence.
3. Looking at your results, which method would you choose for solving a PDE where discontinuities can result?

PROBLEM VII - Optional:
Create a function which evolves a grid-based function of space, $u_i = u(x_i)$, with options for all of the following methods, neglecting terms of the order specified:

1. **FTCS** – Forward in time, 1^{st}-order (2-pt stencil) centered in space
2. **FTFS** – Forward in time, 1^{st}-order forward in space
3. **Lax-Wendroff** – Multi-step (see lecture notes), $\mathcal{O}(\Delta x^2), \mathcal{O}(\Delta t^3)$

Have the function spit out 5 equally-spaced snapshots of the evolution, including the initial and final state. Remember to create a scratch array to avoid using updated values in the updates of neighboring points, and think carefully on how to handle the edges of the spatial array.

Tips, Hints, and Suggestions:

- The relevant stencils for methods 1a-d are:

$$\begin{cases} \text{FTCS} & u_i^{j+1} = u_i^j - \frac{v\Delta t}{2\Delta x}\left(u_{i+1}^j - u_{i-1}^j\right) \\ \text{FTFS} & u_i^{j+1} = u_i^j - \frac{v\Delta t}{\Delta x}\left(u_{i+1}^j - u_i^j\right) \\ \text{Lex-Wendroff} & u_i^{j+1} = u_i^j - \frac{v\Delta t}{\Delta x}\left(u_{i+1}^j - u_{i-1}^j\right) + \frac{v^2\Delta t^2}{2\Delta x^2}\left(u_{i+1}^j - 2u_i^j + u_{i-1}^j\right) \end{cases}$$

- The advection form of the traffic equation above can be rewritten in the form of a conservation/continuity equation

$$\partial_t \rho + \partial_x F(\rho) = 0$$
$$F(\rho) = u(\rho) \cdot \rho = v_{\max}(1 - \frac{\rho}{\rho_{\max}})$$

  which can simplify your derivation of the Lax-Wendroff scheme for variable velocity advection. Careful consider what you are conserving also in deriving the 2nd order non-linear Upwind scheme for non-uniform velocity.