1 Numerical derivative [6 pts]

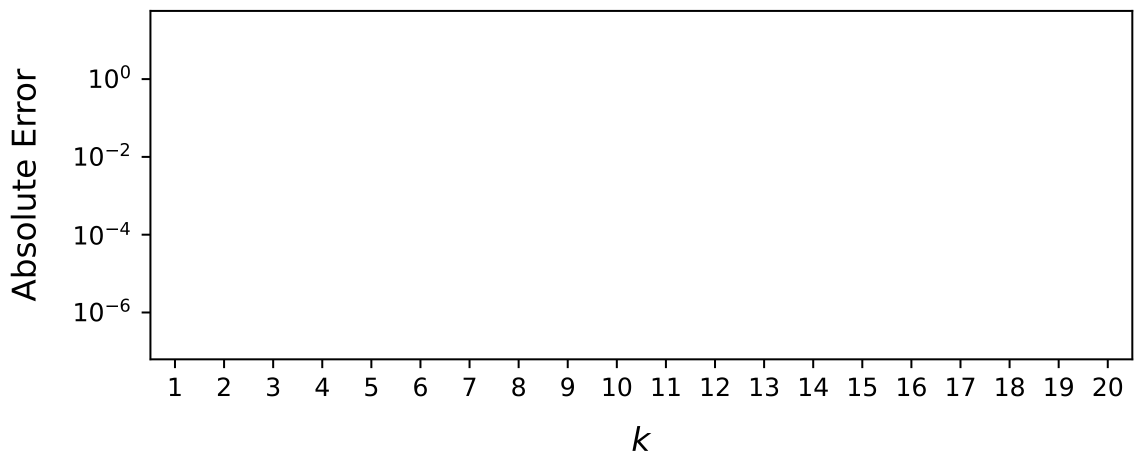
For a function $f(x) = xe^{2x}$, compute the derivative $f'(x)$ at $x = 1$ using the forward difference formula

$$\frac{f(1+h) - f(1)}{h},$$

with $h = 10^{-k}$ for $k = 1, 2, 3, \ldots, 20$.

(a) Plot the absolute error of computed $f'(1)$ compared to its analytic value (i.e. $|f'_{\text{numerical}} - f'_{\text{analytic}}|$), with k along the horizontal axis and the error along the vertical axis. The vertical axis of the plot should be in a logarithmic scale and each axis should be properly labeled. [3 pts]

*Example format below:



(b) For which k, do you get the best precision? [1 pts]

(c) Explain what is happening for the cases with a very small h, for example, $k \gtrsim 18$. [2 pts]

Note : This problem demonstrates *round-off error*, which is a numerical error arising from the finite capacity of digital computers in representing real numbers.

2 Stiff kinetics [12 pts]

Suppose we have three types of particles $\{X, Y, Z\}$ in a box. These particles decay into each other with specific rates. The reaction network is

$$X \to Y$$
$$Y \rightleftarrows Z$$

An X-particle decays into a Y-particle, and a Y particle decays into a Z particle and vice versa. The process $Y \to Z$ is twice slower than the process $Z \to Y$. We can model this reaction network as the following system of first-order ordinary differential equations:

$$\frac{dx}{dt} = -ax \tag{1a}$$

$$\frac{dy}{dt} = ax - by + 2bz \tag{1b}$$

$$\frac{dz}{dt} = by - 2bz \tag{1c}$$

where (x, y, z) are number fractions of each particles, i.e. $x \equiv N_x / N_{\text{total}}$ etc. Initial condition is given as (x_0, y_0, z_0) at $t = 0$.

(a) Find the analytic solution of $x(t)$. [1 pts]

For the following problems, use the forward Euler method for time integration, use a fixed time step size $\Delta t = 0.01$, and integrate up to $t_f = 0.5$.

(b) Find the numerical solution of $y(t)$, $z(t)$ for the initial condition $(x_0, y_0, z_0) = (0.6, 0.1, 0.3)$ with $a = 1.0$ and $b = 5.0$. Use the analytic solution of $x(t)$ for discretizing Eq. (1b). Plot the results with proper legends and axis labels. See Figure 1 for an example format. [3 pts]

(c) Suppose that the $Y \rightleftarrows Z$ reaction chain got much faster. Exactly repeat the time integration in **(b)** but with setting $b = 70.0$. How do the solutions $y(t)$ and $z(t)$ behave? (you don't need to attach the plot in the answer sheet) [1 pts]

You can check yourself that if you use a smaller time step size, the solution becomes okay again. But let's continue to use $\Delta t = 0.01$ for the next problem.

(d) When discretizing Eq. (1b) and (1c), we can use a 'future state' of the variables on the right hand side such that the numerical time stepping takes the form

$$\frac{y_{n+1} - y_n}{\Delta t} = a\,x(t_{n+1}) - b y_{n+1} + 2b z_{n+1}\,, \tag{2}$$

$$\frac{z_{n+1} - z_n}{\Delta t} = b y_{n+1} - 2b z_{n+1}. \tag{3}$$

Using a new discretization scheme (2) and (3) for y and z, find the numerical solution with $b = 70.0$. Notice that the future values y_{n+1} and z_{n+1} are on the *both* sides of the discretized equation now, so

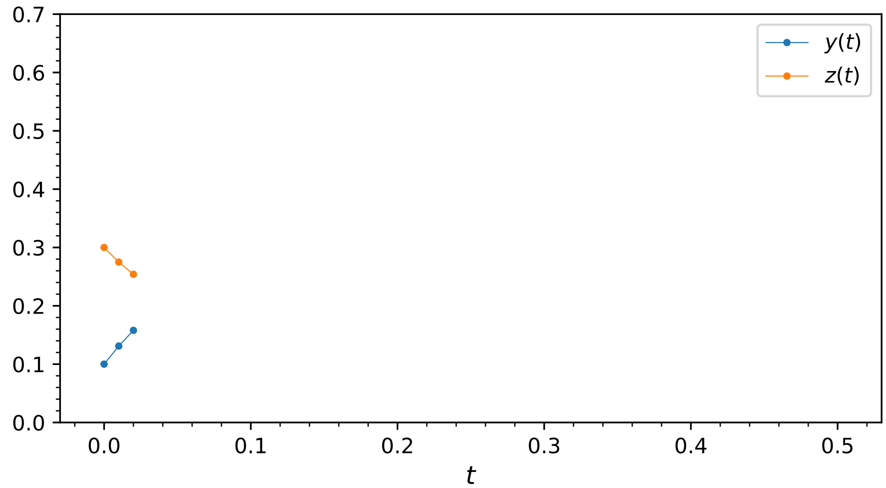


Figure 1: Example answer format for Problem (2b) and (2d).

you may want to somehow find the roots (y_{n+1}, z_{n+1}) for each time step $t_n \to t_n + \Delta t$.

Plot the results in the same format as Figure 1. [7 pts]

Note : Using (unknown) future values (e.g. y_{n+1}) on the right hand side of discretization is called as an *implicit* time stepping method, since that makes the resulting discretized equation implicit (rather than explicit). In particular, the method we used in (2) and (3) is the *backward Euler* method.

There are many cases in astrophysics in which there are multiple physical processes with very different time scales (speeds). Examples include nuclear reactions in stars, photon transfer in astrophysical gas, or neutrino effects in colliding neutron stars.

We are often only interested in a slower process (e.g. focus on the 'slow' evolution of X particles) while neglecting the details of faster ones. In our problem, the reaction between $Y \rightleftarrows Z$ is much faster than $X \to Y$. Implicit steppers are useful in such cases, letting us to avoid using an unacceptably small time step size while we are only interested in the slow part.

3 Kelvin-Helmholtz instability [18 pts]

In this exercise, we will simulate a 2-dimensional shear flow to observe the Kelvin-Helmholtz instability. We will use the `Dedalus` code to solve incompressible hydrodynamics equations. Install the `Dedalus` code on a computer of your choice. Instructions for installing the code can be found here.

The computational domain is $[0, L_x] \times [-L_y/2, L_y/2]$ with $L_x = L_y = 1.0$ with periodic boundaries. At $t = 0$, fluid is moving with $v_x = -0.5$ in the region $|y| < 0.25$, and $v_x = +0.5$ in the region $|y| > 0.25$. More precisely, we assign the initial velocity profile

$$v_x(x, y) = 0.5\left[1 + \tanh\left(\frac{y - 0.25}{\delta_s}\right) + \tanh\left(-\frac{y + 0.25}{\delta_s}\right)\right] \tag{4}$$

with $\delta_s = 5 \times 10^{-4}$. A scalar tracer ("color dye") is added in simulations to visualize the mixing between the two regions.

Instructions:

- Our simulation code can be run with Python within an environment in which `Dedalus` is installed or visible. For example, to run the simulation using 4 processes in parallel, use the following command in the terminal:

  ```
  mpiexec -n 4 python3 kh_instability.py
  ```

  Of course, you can run with a single core with '`-n 1`'. You can also change the grid resolution and final simulation time by editing '`kh_instability.py`'. You can download 'kh_instability.py' file here.
- Running a simulation will create two subdirectories '`/analysis`' and '`/snapshots`'. Once the simulation is complete, you can draw 2D plots of the fluid by running

  ```
  python3 plot_snapshots.py snapshots/*.h5
  ```

  which will automatically generate plots in '`/frames`' subdirectory.
  Here is the 'plot_snapshots.py' file.

Problems:

(a) Edit '`kh_instability.py`' script to add the following form of velocity perturbation to the initial data:

$$v_y(x, y) = A \sin\left(\frac{2\pi m x}{L_x}\right)\left[\exp\left(-\frac{(y - 0.25)^2}{\delta}\right) + \exp\left(-\frac{(y + 0.25)^2}{\delta}\right)\right] \tag{5}$$

with $m = 2$, $A = 5 \times 10^{-3}$ and $\delta = 5 \times 10^{-4}$. This small perturbation triggers the instability which grows over time.

Run the simulation with the grid resolution $(N_x, N_y) = (384, 384)$ and show the simulation snapshot at $t = 2.0$. Use the provided plotting script '`plot_snapshots.py`'. [8 pts]

Since we have excited $m = 2$ perturbation in initial data, you will see two "cat's-eye" vortices per L_x developing along the fluid interface at $y = \pm 0.25$.

(b) Increase the Reynolds number ('`Reynolds`' parameter) to 10^5. Re-run the simulation with $(N_x, N_y) = (384, 384)$ and show the simulation snapshot at $t = 2.0$. Briefly describe how the fluid flow pattern changed. [2 pts]

(c) Theoretical analysis on the growth rate of this instability predicts

$$|v_y(x,y,t)| \sim e^{\alpha t}, \quad \alpha = kU/2 \tag{6}$$

where $k = 2\pi m/L_x$ is the wavenumber of the perturbation and $U = 1.0$ is the magnitude of the velocity shear in our setup. The script '`plot_growth.py`' will load the computed integral

$$I \equiv \int_{x=0}^{L_x} \int_{y=0}^{L_y} |v_y|\, dx dy \tag{7}$$

from the simulation data and draw a plot for you. The perturbation grows exponentially in earlier times, then saturates at a finite value once it becomes fully nonlinear.

Using the same grid resolution and Reynolds number as the problem **(b)**, run the simulation up to $t = 3.0$. Then use a provided python script (e.g. running '`python3 plot_growth.py`') to draw a plot. 'plot_growth.py' file can be found here.

Estimate the exponential growth rate α from the simulation data. You probably want to switch the scale of the vertical axis to a logarithmic scale to ease the analysis. In your numerical experiment, is the growth rate larger or smaller than the theoretical value $\alpha = kU/2$? [8 pts]

Note : The Kelvin-Helmholtz instability can be triggered when two fluid bodies moving with different velocities are in contact. A large number of examples can be found in nature.

Figure 2: Examples

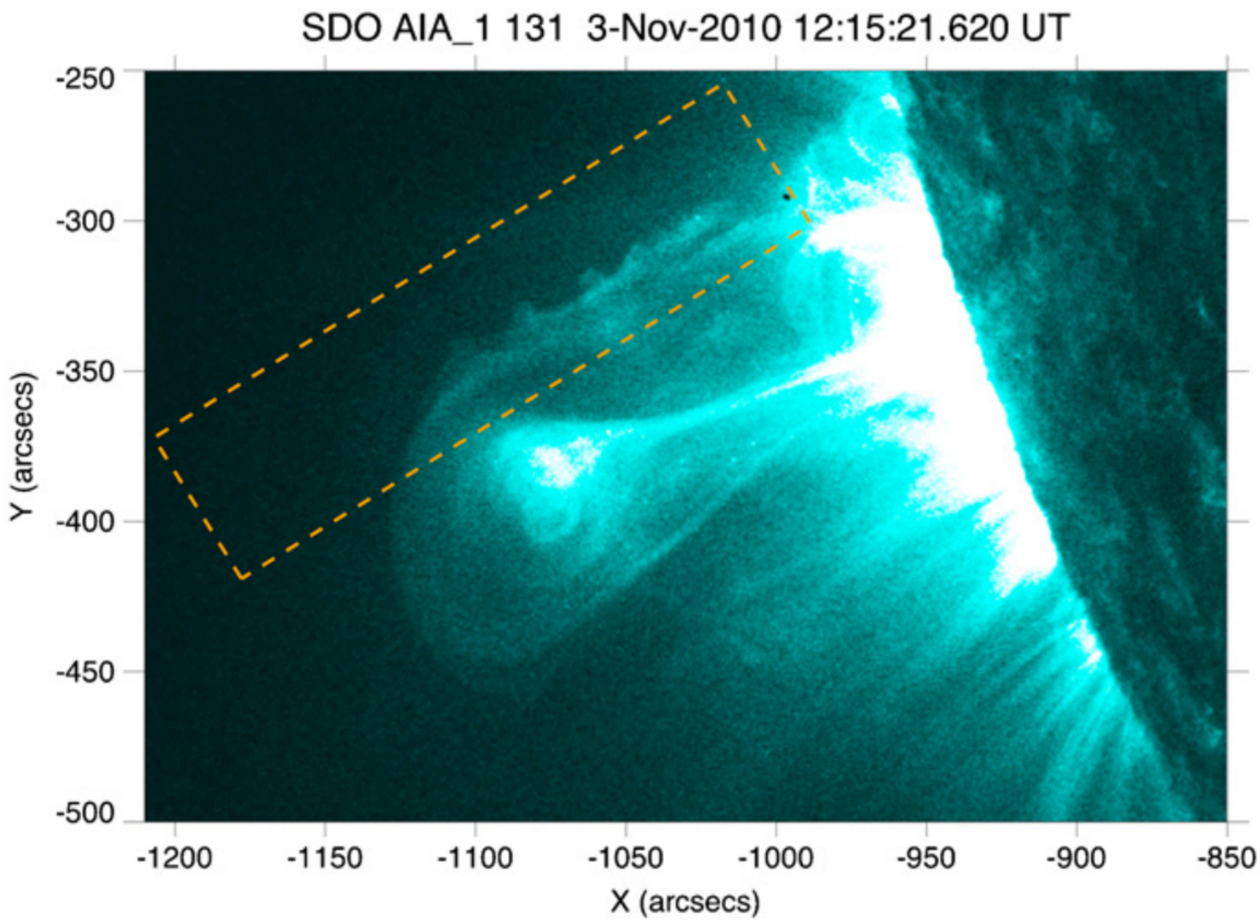


Figure 3: Magnetic Kelvin-Helmholtz instability in the solar corona (Foullon+2011, ApJL 729 L8)

4 Integration Bee [tie breaker]

Evaluate the following integral

$$I = \int_0^{\infty} e^{-(x \sin x)^2} \, dx \tag{8}$$