Final Exam (part 2) - Computational Physics 2

10/10

Good work!

Deadline: Friday 6 June 2025 (by 23h59)

Credits: 10 points

Please keep the structure provided below and submit an organised notebook with clear answers to each item.

2. FFT method for fluid dynamics: 1D Shock waves

We wish to study the emergence of 1D shock waves in fluids. To do this we will modify our one-way wave equation to account for non-linear convection, i.e. we will consider that the speed of an initial Gaussian density perturbation $\rho(x,0) = 4\,e^{-x^2}$ propagating across a periodic 1D domain is not constant, but a function of the density itself, so that our PDE becomes:

$$\frac{\partial \rho}{\partial t} + \rho \frac{\partial \rho}{\partial x} = 0$$

As we see from the above equation, portions of ρ with larger amplitudes will convect more rapidly, giving rise to wave steepening (i.e. to a discontinuity, which we call a **shock wave**). Without a diffusive term, the shock would become infinitely steep. Therefore, we add a diffusive (parabolic) term to our PDE so that the shock maintains a finite width. Our PDE then becomes:

$$\frac{\partial \rho}{\partial t} + \rho \frac{\partial \rho}{\partial x} = \alpha \frac{\partial^2 \rho}{\partial x^2}$$

where α is a diffusion constant.

Implement the following tasks using **python classes**:

(a) Create an appropriate domain and a reasonable time vector for the problem, and make a plot of the initial density profile.

In [1]:

✓

```python
# Third party libraries

import numpy as np
import matplotlib.pyplot as plt
from scipy.integrate import solve_ivp
import scienceplots
import os
```

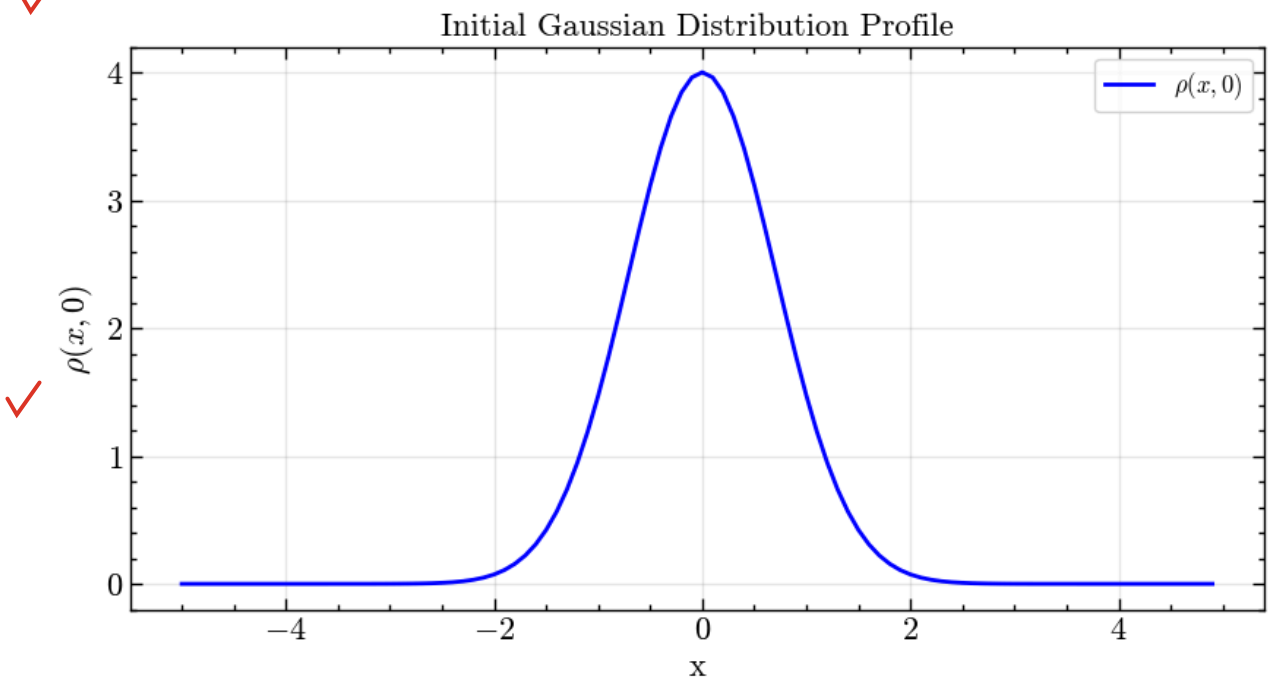
```
import glob
from PIL import Image
import multiprocessing as mp

# Define the style for plotting
plt.style.use(['science', 'notebook', 'no-latex'])
```

In [2]:

```
class ShockWavesInitialProfile:
    """
Docstring missing.
    """
    def __init__(self, dx = 0.1, Lx = 10.0, dt = 0.01, time_tot = 5.0):
        """
        Initialize the ShockWaves class with parameters for simulation.
            Inputs:
                dx (float): Spatial step size.
                Lx (float): Length of the domain.
                dt (float): Time step size.
                time_tot (float): Total simulation time.
        """
        self.dx = dx
        self.Lx = Lx
        self.dt = dt
        self.time_tot = time_tot

        # Time domain
        self.t = np.arange(0, time_tot + dt, dt)

        # Spacial domain
        self.x = np.arange(-Lx/2, Lx/2, dx)

        # Initialize the initial profile
        self.gaussian_init()

    def gaussian_init(self):
        """
        Funtion to initialize a Gaussian function in the spatial domain.
            Input:
                x (array): Spatial points.
            Output:
                rho_0 (array): Save the initial Gaussian distribution.
        """
        rho_0 = 4*np.exp(-self.x**2)

        # Save the intial profile
        self.rho_0 = rho_0

    def plot_initial_profile(self):
        """
        Plot the initial profile of the Gaussian function.
            Output:
                A plot of the initial Gaussian distribution.
        """

        plt.figure(figsize=(10, 5))
```

```
        plt.plot(self.x, self.rho_0, label=r"$\rho(x, 0)$", color="blue")
        plt.title("Initial Gaussian Distribution Profile")

        plt.xlabel("x")
        plt.ylabel(r"$\rho(x, 0)$")

        plt.grid(alpha=0.3)
        plt.legend(frameon=True, fontsize=12)

        plt.show()
```

In [3]:
```
# Instantiate the ShockWaves class
shock_waves = ShockWavesInitialProfile(dx=0.1, Lx=10.0, dt=0.01, time_tot=10

# Plot the initial profile
shock_waves.plot_initial_profile()
```



(b) Write a method for the right-hand-side (RHS) of the PDE that allows you to map in and out of the Fourier domain at each time. Note that this PDE is non-linear, so the function should return the RHS in real space. **Hint:** it may be helpful to write the derivative terms in our PDE in Fourier domain.

$$\frac{\partial \rho}{\partial t} + \rho \frac{\partial \rho}{\partial x} = \alpha \frac{\partial^2 \rho}{\partial x^2}$$

From this equation we ontain the RHS of the PDE:

$$\frac{\partial \rho}{\partial t} = \alpha \frac{\partial^2 \rho}{\partial x^2} - \rho \frac{\partial \rho}{\partial x} = RHS$$

Then, the derivaties are expressed in Fourier $\mathcal{F}$ space:

$$\frac{\partial \rho}{\partial t} \longrightarrow \hat{\rho}_t, \quad \checkmark$$

$$\frac{\partial \rho}{\partial x} \rightarrow ik\hat{\rho}(k,t), \quad \checkmark$$

$$\frac{\partial^2 \rho}{\partial x^2} \longrightarrow -k^2\hat{\rho}(k,t) \quad \checkmark$$

Replacing

Remplazing this in our equation we get:

$$\Rightarrow \quad \hat{\rho}_t(k,t) = -\alpha k^2 \hat{\rho}(k,t) - \rho(x,t) \cdot ik\hat{\rho}(k,t) \quad \checkmark$$

This scheme will help to solve the rhs equation for integrating the PDE.

In [4]:
```python
class ShockWavesSolverV1(ShockWavesInitialProfile):
    """
    """
    def __init__(self, dx=0.1, Lx=10.0, dt=0.01, time_tot=5.0, alpha=0.5):
        """
        Initialize the ShockWavesSolver class with parameters for simulation
            Inputs:
                dx (float): Spatial step size.
                Lx (float): Length of the domain.
                dt (float): Time step size.
                time_tot (float): Total simulation time.
                alpha (float): Diffusion coefficient.
        """
        super().__init__(dx, Lx, dt, time_tot)

        self.alpha = alpha

        # Wavenumber
        self.k = 2 * np.pi * np.fft.fftfreq(len(self.x), d=self.dx)

    def rhs(self, rho):
        """
        Right hand size of the PDE for the shock wave solver.
            Inputs:
                rho (array): Density profile at the current time step.
            Output:
                rhs (array): Right-hand side of the PDE.
        """
        # Compute the Fast Fourier Transform of the density profile
        rho_hat = np.fft.fft(rho)

        # Compute the derivative in Fourier space and
        rho_hat_dx = 1j * self.k * rho_hat

        # Transform back to real space
        rho_dx = np.fft.ifft(rho_hat_dx)

        # Compute the diffusion term in Fourier space
        rho_hat_dx2 = -self.k**2 * rho_hat
```

```
        # Compute the diffusion term in real space
        rho_dx2 = np.fft.ifft(rho_hat_dx2)

        # Compute the right-hand side of the PDE
        rhs = self.alpha * rho_dx2 - rho * rho_dx

        return rhs
```

(c) Choose a reasonable value for the diffusion constant, α, and call your function in (b). What is this function achieving so far and what space (real or Fourier) is the output in?

In [5]:
```
# Define the difusion constant
alpha = 0.1

# Instantiate the ShockWavesSolver class
shock_waves_solver = ShockWavesSolverV1(dx=0.01, Lx=10.0, dt=0.01, time_tot=

# Call the rhs method to compute the right-hand side of the PDE
rhs = shock_waves_solver.rhs(shock_waves_solver.rho_0)
```

In [6]:
```
print(f"The mean imaginary part is: {np.mean(np.abs(rhs.imag))}")
```

```
The mean imaginary part is: 1.0158746510908675e-12
```

In [7]:
```
# plt.figure(figsize=(10, 5))

# plt.plot(shock_waves_solver.x, rhs, label=r"$\rho(x, 0)$", color="blue")
# plt.title("Initial Gaussian Distribution Profile")

# plt.xlabel("x")
# plt.ylabel(r"$\rho(x, 0)$")

# plt.grid(alpha=0.3)
# plt.legend(frameon=True, fontsize=12)

# plt.show()
```

By using the function created in (b) it is seen that the results are in real space. The imaginary part of the output function is zero.

(d) Find and plot the solution, $\rho(x,t)$, **using your FFT method**. For this, you need to feed a scipy ODE integrator with the function you created in (b). **Hint:** make sure you feed the correct wavenumbers to the ODE integrator.

In [8]:
```
# Add the solution method to the class

class ShockWavesSolver(ShockWavesInitialProfile):
    """
    """
    def __init__(self, dx=0.1, Lx=10.0, dt=0.01, time_tot=5.0, alpha=0.5):
        """
        Initialize the ShockWavesSolver class with parameters for simulatior
```

```
            Inputs:
                dx (float): Spatial step size.
                Lx (float): Length of the domain.
                dt (float): Time step size.
                time_tot (float): Total simulation time.
                alpha (float): Diffusion coefficient.
        """
        super().__init__(dx, Lx, dt, time_tot)

        self.alpha = alpha

        # Wavenumber
        self.k = 2 * np.pi * np.fft.fftfreq(len(self.x), d=self.dx)

    def rhs(self, t, rho):
        """
        Right hand size of the PDE for the shock wave solver.
            Inputs:
                rho (array): Density profile at the current time step.
            Output:
                rhs (array): Right-hand side of the PDE.
        """
        # Compute the Fast Fourier Transform of the density profile
        rho_hat = np.fft.fft(rho)

        # Compute the derivative in Fourier space and
        rho_hat_dx = 1j * self.k * rho_hat

        # Transform back to real space
        rho_dx = np.fft.ifft(rho_hat_dx)

        # Compute the diffusion term in Fourier space
        rho_hat_dx2 = - self.k**2 * rho_hat

        # Compute the diffusion term in real space
        rho_dx2 = np.fft.ifft(rho_hat_dx2)

        # Compute the right-hand side of the PDE
        rhs = self.alpha * rho_dx2 - rho * rho_dx

        return rhs.real # Return only the real part

    def solve(self):
        """
        Solver for the shock wave PDE using the scipy library.
            Output:
                sol (array): The solution object containing the time evoluti
        """

        # Solve the PDE using scipy
        sol = solve_ivp(fun = self.rhs, t_span = (0., self.t[-1]),
                        y0 = self.rho_0, method = 'RK45', t_eval = self.t, t

        # Pritn the message of success
        print(sol.message)
```

```
        # Extract the solution
        self.sol = sol.y

        return sol
```

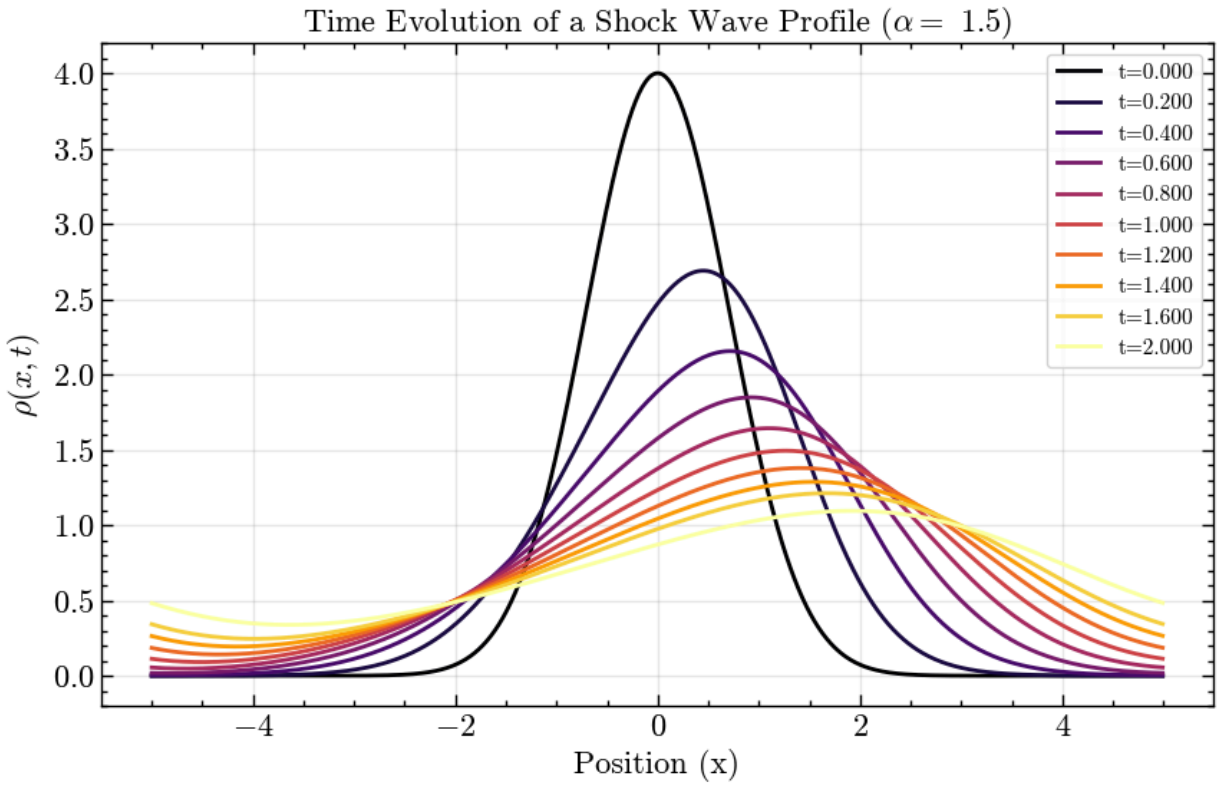
In [9]:
```
# Define the difusion constant
alpha = 1.5

# Instantiate the ShockWavesSolver class
shock_waves_solver = ShockWavesSolver(dx = 0.01, Lx = 10.0, dt = 0.01, time_

# Solve the PDE
solution = shock_waves_solver.solve()
```

```
/home/alanp/.local/lib/python3.10/site-packages/scipy/integrate/_ivp/common.
py:39: UserWarning: The following arguments have no effect for a chosen solv
er: `tol`.
  warn("The following arguments have no effect for a chosen solver: {}."
The solver successfully reached the end of the integration interval.
```

In [10]:
```
class Plotter():
    """
    Class to plot the solution of the PDE.

    """
    def __init__(self, object):
        """
        Initialize the Plotter class with parameters for plotting.
            Inputs:
                x (array): Spatial points.
                t (array): Time points.
                solution (array): Solution of the PDE.
        """
        self.x = object.x
        self.t = object.t
        self.sol = object.sol
        self.alpha = object.alpha

        # Create a meshgrid for 2D plotting
        self.X, self.T = np.meshgrid(self.x, self.t)

    def plot_snapshots(self, frames = 10):
        """
        Plot snapshots of probability density at specified times.
            Input:
                frames(int): Number of frames to plot selected within the ti
            Output:
                A plot showing the evolution of the wavefunction over time.
        """

        # Create time indices
        t_step = self.t.shape[0] // frames
        time_indices = [(t_step*i) for i in range(0, frames - 1)]
        time_indices.append(- 1)  # Ensure the last index is included
```

```
        # Figure environment
        plt.figure(figsize = (10, 6))


        # Plot snapshots
        colors = plt.cm.inferno(np.linspace(0, 1, len(time_indices)))
        for i, t_idx in enumerate(time_indices):

            plt.plot(self.x, self.sol[:, t_idx], color=colors[i], label=f"t=

        plt.xlabel("Position (x)")
        plt.ylabel(r"$\rho(x,t)$")
        plt.title(r"Time Evolution of a Shock Wave Profile ($\alpha =$ " + f

        plt.legend(frameon = True, fontsize = 11)
        plt.grid(True, alpha = 0.3)
        plt.show()
```

In [11]:
```
plotter = Plotter(shock_waves_solver)
plotter.plot_snapshots(frames=10)
```



(e) Repeat the above calculations for two additional α values (one of them should be 0). Then, make a figure (or movie) with three panels comparing the results for different α values and briefly discuss the role of this parameter in regulating the morphology of the shock wave.

In [12]:
```
# Define the difusion constant
alpha_2 = 0.5

# Instantiate the ShockWavesSolver class
```

```
shock_waves_solver_2 = ShockWavesSolver(dx = 0.01, Lx = 10.0, dt = 0.01, tim

# Solve the PDE
solution_2 = shock_waves_solver_2.solve()
```

```
The solver successfully reached the end of the integration interval.
```

In [13]:
```
# plotter2 = Plotter(shock_waves_solver_2)
# plotter2.plot_snapshots(frames=10)
```

In [14]:
```
# Define the difusion constant
alpha_3 = 1.e-1

# Instantiate the ShockWavesSolver class
shock_waves_solver_3 = ShockWavesSolver(dx = 0.1, Lx = 10.0, dt = 0.01, time

# Solve the PDE
solution_3 = shock_waves_solver_3.solve()
```

```
The solver successfully reached the end of the integration interval.
```

In [15]:
```
# plotter3 = Plotter(shock_waves_solver_3)
# plotter3.plot_snapshots(frames=10)
```

Animate the 3-panel figures

In [16]:
```
class Animation():
    """
    Class to create an animation of the shock wave evolution with different
    """
    def __init__(self, solutions):
        """
        Initialize the Animation class with parameters for animation.
            Input:
                Solutions (list): List of solution objects for different dif
        """

        self.solutions = solutions
        self.x = solutions[0].x
        self.t = solutions[0].t

        # Define the colors for plotting each snapshot
        self.colors = plt.cm.inferno(np.linspace(0, 1, len(self.t)))

        # Define the name of the output file
        self.file_name = "shock_wave"

    def plot_shock_waves(self, j):
        """
        Function to save a figure of the shock wave solutions.
            Input:
                j (int): Index of the time step to plot.
            Output:
                A plot showing the shock wave evolution at time step j for
                each diffusion coefficient in the solutions list.
        """
```

```
        # Create a figure with subplots
        fig, axs = plt.subplots(1, 3, figsize=(20, 5), sharey=True)

        for i in range(len(axs)):

            axs[i].plot(self.solutions[i].x, self.solutions[i].sol[:, j], cc

            axs[i].set_title(r"$\alpha =$" + f"{self.solutions[i].alpha}")
            axs[i].set_xlabel("Position (x)")
            #axs[i].set_ylabel(r"$\rho(x,t)$")

            axs[i].grid(True, alpha=0.3)
            axs[i].legend(frameon=True, fontsize=11)
            axs[i].set_xlim(-5, 5)
            axs[i].set_ylim(0, 5)

        # Set common labels
        axs[0].set_ylabel(r"$\rho(x,t)$")
        fig.suptitle("Shock Wave Evolution with Different Diffusion Coeffici

        plt.tight_layout()

        # Save the figure frame
        plt.savefig(self.output_dir + f"/{self.file_name}" + ".{:03d}.png".f
        plt.close()

    def animate(self):
        """
        Generate an animated GIF from the evolution of the wavefunction.
            Outputs:
                GIF saved in the output folder.
        """
        # Create a directory to save the figures
        if os.path.isdir("outputfolder_P2"):
            print(f"Directory 'outputfolder' already exists.")
        else:
            print(f"Directory 'outputfolder_P2' has been created.")
            os.mkdir("outputfolder_P2")

        # Define the directory name for saving the figures
        name_dir = "outputfolder_P2"

        # Create all images
        n_cpu = mp.cpu_count() // 2
        print(f"The image generation is distributed among {n_cpu} cores")
        self.output_dir = name_dir # Define output folder

        # Paralelize image generation
        pool = mp.Pool(processes = n_cpu)
        pool.map(self.plot_shock_waves, range(0, self.t.shape[0]))

        #Read all the generated figures to create the movie

        #Define the input directory
        images_input = name_dir + f"/{self.file_name}.***.png"
```

```
        # Collect the images
        imgs = (Image.open(f) for f in sorted(glob.glob(images_input)))

        img = next(imgs)

        #Define the output directory
        imgif_output = name_dir + f"/{self.file_name}.gif"

        # Save the GIF
        img.save(fp = imgif_output, format="GIF", append_images=imgs,\
                save_all=True, duration = 100, loop = 0)

        return print(f"The movie was generated correctly in '{name_dir}/' as
```

In [17]:
```
# Define the list of solutions to be animated
solutions = [shock_waves_solver, shock_waves_solver_2, shock_waves_solver_3]

# Instantiate the Animation class
animation = Animation(solutions)

# Generate the animation
animation.animate()
```

```
Directory 'outputfolder_P2' has been created.
The image generation is distributed among 4 cores
The movie was generated correctly in 'outputfolder_P2/' as: shock_wave.gif
```

In [18]:
```
# Show the animation (uncomment this)
from IPython.display import Image, display

# display(Image(filename="outputfolder_P2/shock_wave.gif"))
```

As expected, the diffusivity factor affects the contribution of the parabolic term included to avoid a discontinuity or shock wave. When the diffusivity factor α is higher, the evolution of the density profile is smoother and maintains a finite width. However, when α is close to zero, a discontinuity starts to form over time, making the shock wave evident. The smaller the value of α, the steeper the shock becomes.