Final Exam (part 2) - Computational Physics 2

10/10
Excellent!

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.

(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.

(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?

(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.

(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.

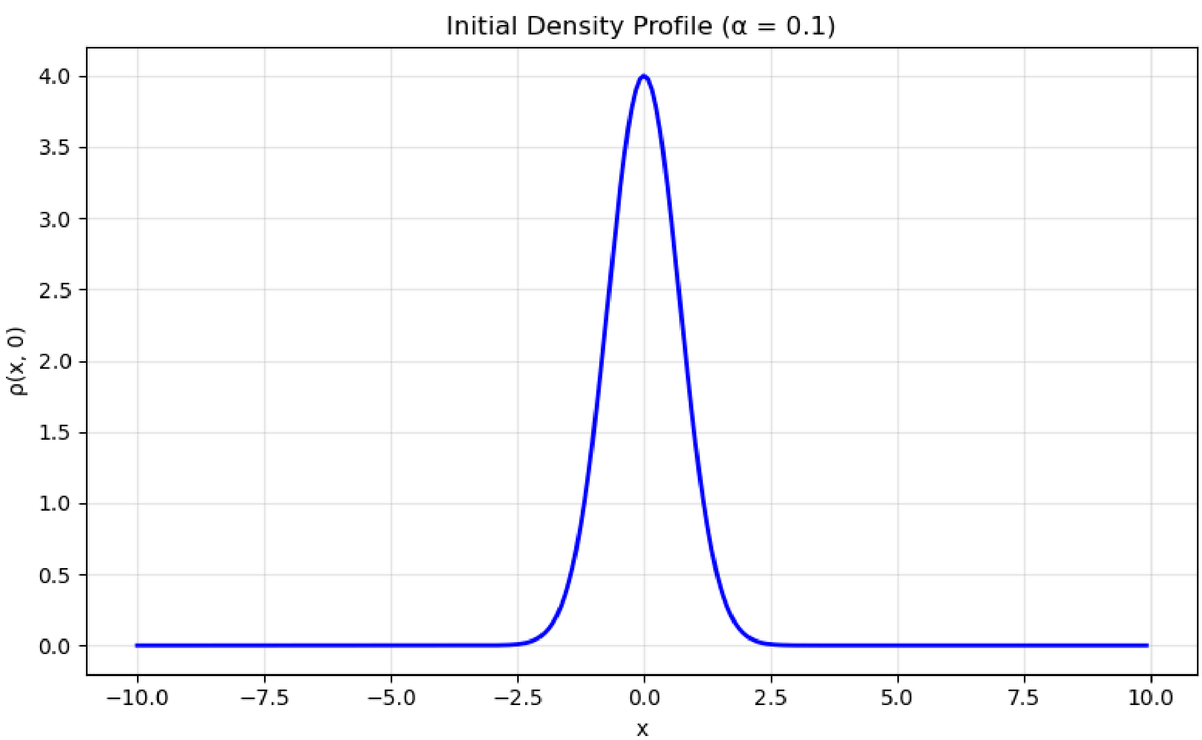
In [1]:

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

class ShockWave1D:
    def __init__(self, N=256, L=20, alpha=0.1):
        """
        Initialize the 1D shock wave simulation.

        Parameters:
        N: Number of grid points
        L: Domain length (centered at 0)
        alpha: Diffusion constant
        """
        self.N = N
        self.L = L
        self.alpha = alpha

        # Spatial grid
        self.x = np.linspace(-L/2, L/2, N, endpoint=False)
        self.dx = self.x[1] - self.x[0]

        # Wavenumbers for FFT
        self.k = 2 * np.pi * np.fft.fftfreq(N, d=self.dx)

        # Initial condition: Gaussian density perturbation
        self.rho0 = 4 * np.exp(-self.x**2)

    def plot_initial_profile(self):
        """Plot the initial density profile."""
        plt.figure(figsize=(8, 5))
        plt.plot(self.x, self.rho0, 'b-', linewidth=2)
        plt.title(f"Initial Density Profile (α = {self.alpha})")
        plt.xlabel("x")
        plt.ylabel("ρ(x, 0)")
        plt.grid(True, alpha=0.3)
        plt.tight_layout()
        plt.show()

    def rhs(self, t, rho_real):
        """
```

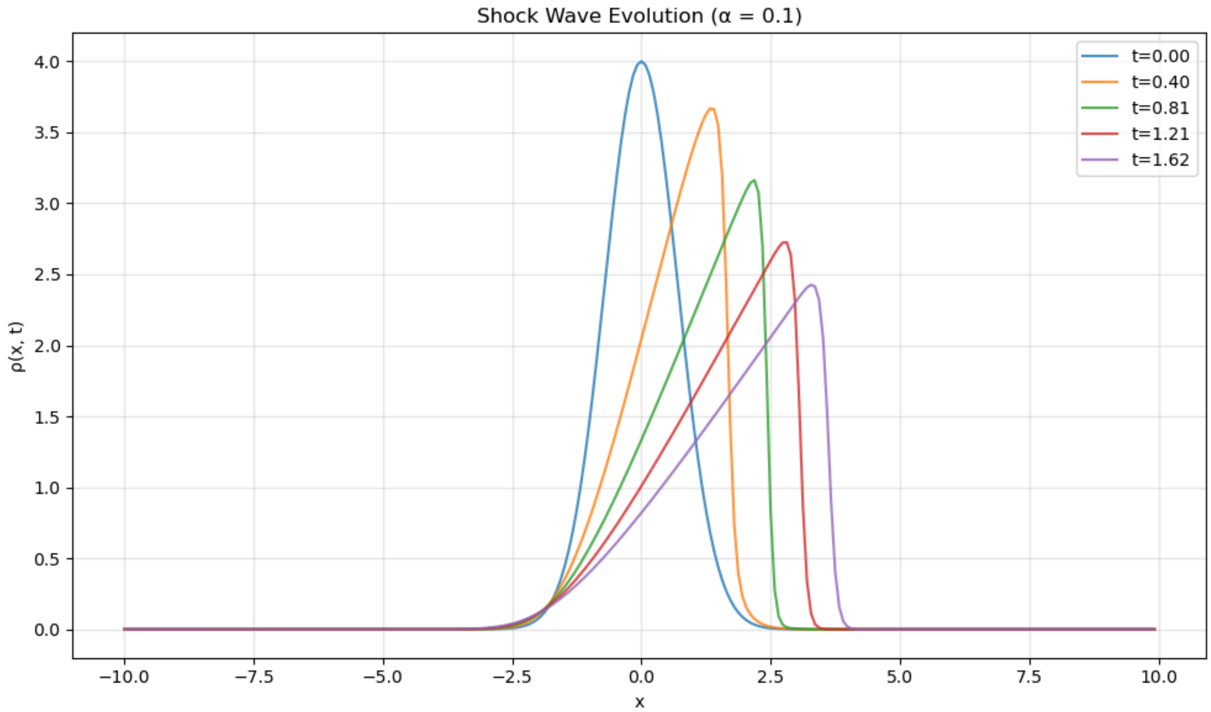
```python
        Right-hand side of the PDE: ∂ρ/∂t = -ρ∂ρ/∂x + α∂²ρ/∂x²

        Returns the RHS in real space for the ODE integrator.
        """
        # Transform to Fourier space
        rho_hat = np.fft.fft(rho_real)

        # Compute spatial derivative ∂ρ/∂x in Fourier space, then transform
        drho_dx = np.fft.ifft(1j * self.k * rho_hat).real

        # Nonlinear convection term: -ρ∂ρ/∂x (computed in real space)
        convection_term = -rho_real * drho_dx

        # Diffusion term: α∂²ρ/∂x² (computed in Fourier space, then transfor
        diffusion_term = np.fft.ifft(-self.alpha * (self.k ** 2) * rho_hat).

        return convection_term + diffusion_term

    def solve(self, t_max=2.0, n_frames=100):
        """
        Solve the PDE using scipy's ODE integrator.

        Returns:
        times: Array of time points
        solutions: Array of density profiles at each time
        """
        t_eval = np.linspace(0, t_max, n_frames)

        sol = solve_ivp(self.rhs, [0, t_max], self.rho0,
                       t_eval=t_eval, method='RK45', rtol=1e-8)

        return sol.t, sol.y.T  # Transpose to get (time, space) shape

    def plot_evolution(self, times, solutions, step=20, alpha_label=None):
        """Plot the evolution of the density field."""
        plt.figure(figsize=(10, 6))

        # Plot every 'step' time frames
        for i in range(0, len(times), step):
            plt.plot(self.x, solutions[i],
                    label=f't={times[i]:.2f}', alpha=0.8)

        title = f'Shock Wave Evolution'
        if alpha_label is not None:
            title += f' (α = {alpha_label})'
        else:
            title += f' (α = {self.alpha})'

        plt.title(title)
        plt.xlabel("x")
        plt.ylabel("ρ(x, t)")
        plt.legend()
        plt.grid(True, alpha=0.3)
        plt.tight_layout()
        plt.show()
```

```python
    def plot_comparison(self, alpha_values, t_max=2.0, n_frames=100):
        """Compare solutions for different alpha values."""
        fig, axes = plt.subplots(1, len(alpha_values), figsize=(15, 5))
        if len(alpha_values) == 1:
            axes = [axes]

        for i, alpha in enumerate(alpha_values):
            # Create new instance with different alpha
            sim_temp = ShockWave1D(N=self.N, L=self.L, alpha=alpha)
            times, solutions = sim_temp.solve(t_max=t_max, n_frames=n_frames

            # Plot final state
            axes[i].plot(self.x, sim_temp.rho0, 'k--', label='Initial', alph
            axes[i].plot(self.x, solutions[-1], 'r-', linewidth=2, label=f'F
            axes[i].set_title(f'α = {alpha}')
            axes[i].set_xlabel('x')
            axes[i].set_ylabel('ρ(x, t)')
            axes[i].grid(True, alpha=0.3)
            axes[i].legend()

        plt.tight_layout()
        plt.show()
```

In [2]:
```python
sim = ShockWave1D(N=256, L=20, alpha=0.1)
sim.plot_initial_profile()
```



In [3]:
```python
alpha = 0.1
times, rhos = sim.solve(t_max=2.0, n_frames=100)
sim.plot_evolution(times, rhos, step=20)
```



Output is in real space

```
In [4]: alphas = [0, 0.1, 9]
        sim.plot_comparison(alphas, t_max=2.0, n_frames=100)
```