PHYS 581 Assignment 5 - Capstone Project

100 points total

Due Friday, April 11 (last day of classes!)

Instructions: The simulation of the time dynamics should be done only in C, but feel free to use Mathematica to help set things up and for generating and displaying the movies.

Your job for this assignment is to propagate *either* the one-dimensional Schrödinger wave equation *or* the one-dimensional classical wave equation, assuming that the wave is confined in a box of length ℓ, where $-\ell/2 \leq x \leq \ell/2$, subject to the spatial boundary condition that the amplitude of the wave is zero at $x = \pm\ell/2$ for all times.

The one-dimensional Schrodinger equation is

$$i\hbar \frac{\partial}{\partial t} f(x,t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} f(x,t),$$

where $\hbar$ is Planck's constant, m is the mass of a particle / wave, and $f(x,t)$ is the (complex) wave amplitude. The one-dimensional classical wave equation is

$$\frac{1}{c^2} \frac{\partial^2}{\partial t^2} f(x,t) = \frac{\partial^2}{\partial x^2} f(x,t), \tag{1}$$

where c is the speed of sound in the medium and $f(x,t)$ is the (real) amplitude of the wave. In both cases, set the initial-value condition as

$$f(x,0) = \frac{1}{\sqrt{a}\pi^{1/4}} e^{-x^2/a^2},$$

where $a \in \mathbb{R}$ and $a \ll \ell$, so that $f(x,0)$ is initially normalized to unity, i.e.

$$\int_{-\ell/2}^{\ell/2} f(x,0)dx \approx 1.$$

Obtain the time dynamics of this system for a long enough time that the wave has the opportunity to hit the box's walls and bounce back. For the time propagation, use Runge-Kutta-Fehlberg (i.e. simultaneous fourth-order and fifth-order Runge-Kutta); be sure to code this up yourself and not use a canned routine! For the spatial meshing, use **two** different methods, drawn from this list:

- Finite differencing (beyond lowest order);
- Lagrange interpolating polynomials;
- Gaussian quadrature;
- Fourier series;
- Discrete variable representation;
- Finite-element method.

Output snapshots in time and plot the results as a movie. Discuss the results. Some points to consider: Does the behaviour make sense? Does the amplitude stay normalized? Should it? Does one method work better than the other?