PHYS 410 Project 2

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November 30, 2024

Introduction

In this project, the time-dependent Schrödinger equation is solved numerically in both one dimension and two dimensions. In both cases, solutions account for a time-independent potential term V, which takes the form of a rectangular barrier or well, a double slit (in 2d only), or is zero everywhere. The MATLAB script $sch_1d_cn.m$ implements the Crank-Nicolson discretization approach to solve the Schrödinger equation in 1d, while the script $sch_2d_adi.m$ implements the alternating-direction-implicit (ADI) method to solve the equation in 2d.

The 1d case is tested by conducting convergence testing in the file <code>ctest_1d.m</code> which checks for solution convergence among increasing discretization levels. A similar convergence test is done for two dimensions in the file <code>ctest_2d.m</code>. For the 1d case, the solution "excess fractional probability" is also examined in the files <code>barrier_survey.m</code> and <code>well_survey.m</code>, which provides insights into how much time the quantum particle is spending in a certain location. Lastly, videos of the 2d wave function scattering off a rectangular barrier or well, and producing self-interference through a double slit are created using the scripts <code>video_rec_bar.m</code>, <code>video_rec_well.m</code>, and <code>video_double_slit.m</code>.

Review of Theory

1d Schrödinger Equation

The 1d Schrödinger Equation PDE is given by the following equation:

$$i\psi(x,t)_t = -\psi_{xx} + V(x,t)\psi\tag{1}$$

where the wave function, $\psi(x,t)$, is complex. The equation is to be solved on the domain

$$0 \le x \le 1$$
, $0 \le t \le t_{\text{max}}$

subject to initial and boundary conditions

$$\psi(x,0) = \psi_0(x) \tag{2}$$

$$\psi(0,t) = \psi(1,t) = 0 \tag{3}$$

The family of exact solutions to (1) is

$$\psi(x,t) = e^{-im^2\pi^2t}\sin(m\pi x) \tag{4}$$

where m is a positive integer.

Since the modulus squared of the wave function represents the probability density, $\rho = |\psi|^2 = \psi \psi^*$, the "running integral" of the probability density represents the probability that the particle is to the left of x at any given time t:

$$P(x,t) = \int_0^x \psi(\tilde{x},t)\psi^*(\tilde{x},t)d\tilde{x}$$
 (5)

Note that equation (5) only computes the correct probability if the wave function is properly normalized such that P(1,t) = 1. Even if it is not so normalized, we should have

P(1,t) =conserved to level of solution error

2d Schrödinger Equation

The 2d Schrödinger Equation PDE is given by the following equation:

$$\psi_t = i(\psi_{xx} + \psi_{yy}) - iV(x, y)\psi \tag{6}$$

where the wave function, $\psi(x, y, t)$, is complex. The equation is to be solved on the domain

$$0 \le x \le 1$$
, $0 \le y \le 1$, $0 \le t \le t_{\text{max}}$

subject to initial and boundary conditions

$$\psi(x, y, 0) = \psi_0(x, y) \tag{7}$$

$$\psi(0, y, t) = \psi(1, y, t) = \psi(x, 0, t) = \psi(x, 1, t) = 0 \tag{8}$$

A family of exact solutions to (6) is given by

$$\psi(x, y, t) = e^{-i(m_x^2 + m_y^2)\pi^2 t} \sin(m_x \pi x) \sin(m_y \pi y)$$
(9)

Numerical Approach

$$i\frac{\psi_j^{n+1} - \psi_j^n}{\Delta t} = \frac{1}{2} \left(\frac{\psi_{j+1}^{n+1} - 2\psi_j^{n+1} + \psi_{j-1}^{n+1}}{\Delta x^2} + \frac{\psi_{j+1}^n - 2\psi_j^n + \psi_{j-1}^n}{\Delta x^2} \right) + \frac{1}{2} V_j^{n+\frac{1}{2}} \left(\psi_j^{n+1} + \psi_j^n \right)$$

$$j = 2, 3, \dots, n_x - 1, \ n = 1, 2, \dots, n_t - 1$$

$$(10)$$

$$\psi_1^{n+1} = \psi_{n_x}^{n+1} = 0, \quad n = 1, 2, \dots, n_t - 1$$

 $\psi_j^1 = \psi_0(x_j), \quad j = 1, 2, \dots, n_x$

$$\frac{1}{2\Delta x^2}\psi_{j+1}^{n+1} + \left(\frac{i}{\Delta t} - \frac{1}{\Delta x^2} - \frac{1}{2}V_j\right)\psi_j^{n+1} + \frac{1}{2\Delta x^2}\psi_{j-1}^{n+1}$$
(11)

$$= -\frac{1}{2\Delta x^2} \psi_{j+1}^n + \left(\frac{i}{\Delta t} + \frac{1}{\Delta x^2} + \frac{1}{2} V_j\right) \psi_j^n - \frac{1}{2\Delta x^2} \psi_{j-1}^n \tag{12}$$

$$\begin{split} \partial^{h}_{xx}u^{n}_{i,j} &\equiv \frac{u^{n}_{i+1,j} - 2u^{n}_{i,j} + u^{n}_{i-1,j}}{\Delta x^{2}} \\ \partial^{h}_{yy}u^{n}_{i,j} &\equiv \frac{u^{n}_{i,j+1} - 2u^{n}_{i,j} + u^{n}_{i,j-1}}{\Delta y^{2}} \end{split}$$

$$\left(1 - i\frac{\Delta t}{2}\partial_{xx}^{h}\right)\psi_{i,j}^{n+\frac{1}{2}} = \left(1 + i\frac{\Delta t}{2}\partial_{xx}^{h}\right)\left(1 + i\frac{\Delta t}{2}\partial_{yy}^{h} - i\frac{\Delta t}{2}V_{i,j}\right)\psi_{i,j}^{n},$$

$$i = 2, 3, \dots, n_{x} - 1, \quad j = 2, 3, \dots, n_{y} - 1, \quad n = 1, 2, \dots, n_{t} - 1. \tag{13}$$

$$\left(1 - i\frac{\Delta t}{2}\partial_{yy}^{h} + i\frac{\Delta t}{2}V_{i,j}\right)\psi_{i,j}^{n+1} = \psi_{i,j}^{n+\frac{1}{2}},$$

$$i = 2, 3, \dots, n_x - 1, \quad j = 2, 3, \dots, n_y - 1, \quad n = 1, 2, \dots, n_t - 1.$$
(14)

$$-\frac{i\Delta t}{2\Delta x^2}\psi_{i+1,j}^{n+\frac{1}{2}} + \left(1 + \frac{i\Delta t}{\Delta x^2}\right)\psi_{i,j}^{n+\frac{1}{2}} - \frac{i\Delta t}{2\Delta x^2}\psi_{i-1,j}^{n+\frac{1}{2}}$$
(15)

$$\frac{i\Delta t}{2\Delta y^2}\psi^n_{i,j+1} + \left(1 + \frac{i\Delta t}{\Delta x^2}\right)\psi^{n+\frac{1}{2}}_{i,j} - \frac{i\Delta t}{2\Delta x^2}\psi^{n+\frac{1}{2}}_{i-1,j} \tag{16}$$

Implementation

1d Tridiagonal System

2d Tridiagonal System

Results

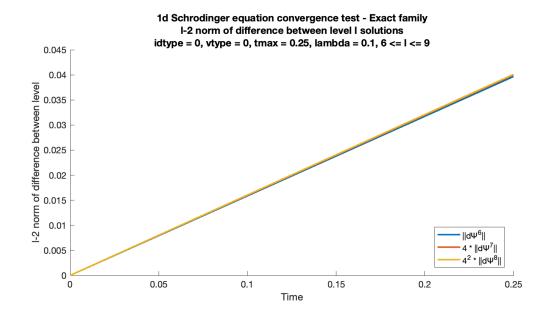


Figure 1: Output 1 of ctest_1d.m - l-2 norm of difference between discretization level solutions for exact family initial conditions.

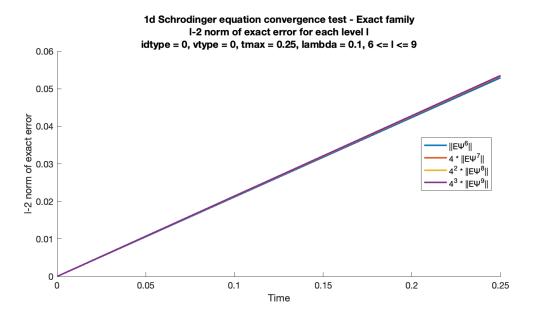


Figure 2: Output 2 of ctest_1d.m - l-2 norm of exact error at each discretization level for exact family initial conditions.

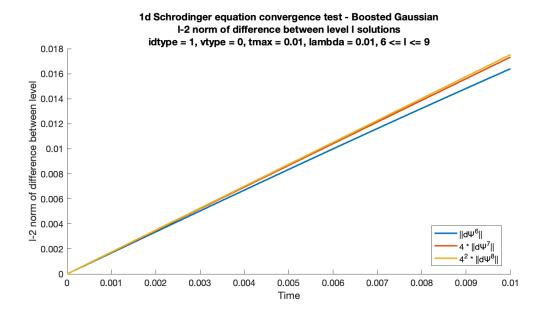


Figure 3: Output 3 of ctest_1d.m - l-2 norm of difference between discretization level solutions for boosted Gaussian initial conditions.

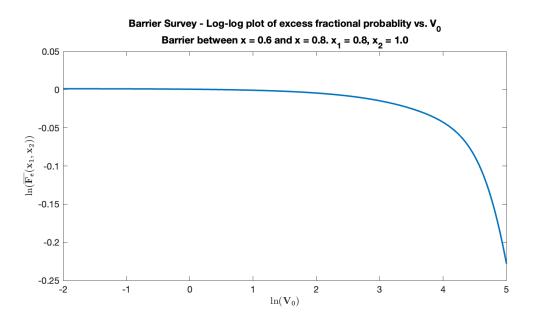


Figure 4: Output of barrier_1d.m - Log-log plot of excess fractional probability vs. V_0 for 1d potential barrier.

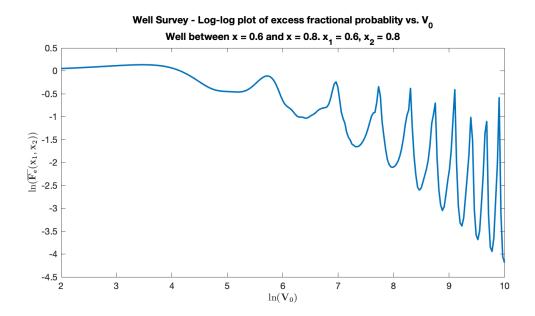


Figure 5: Output of well_ld.m - Log-log plot of excess fractional probability vs. V_0 for 1d potential well

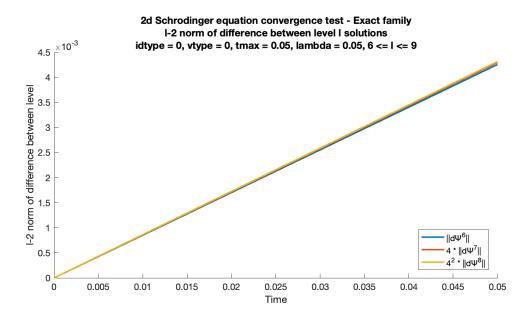


Figure 6: Output 1 of ctest_2d.m - l-2 norm of difference between discretization level solutions.

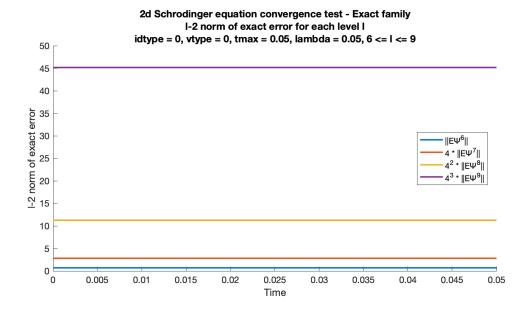


Figure 7: Output 2 of ctest_2d.m - l-2 norm of exact error at each discretization level.

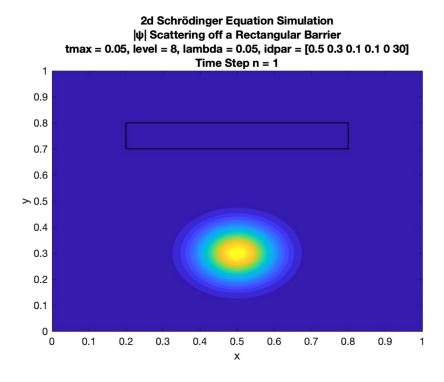


Figure 8: Screenshot of video produced by video_rec_bar.m - Initial conditions.

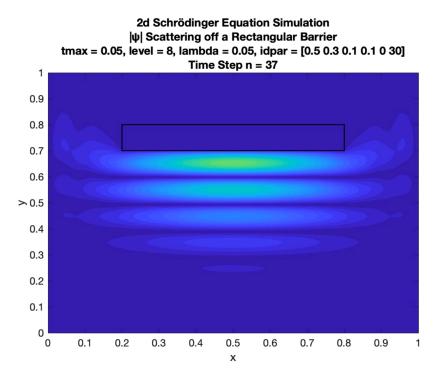


Figure 9: Screenshot of video produced by video_rec_bar.m - Scattering off barrier.

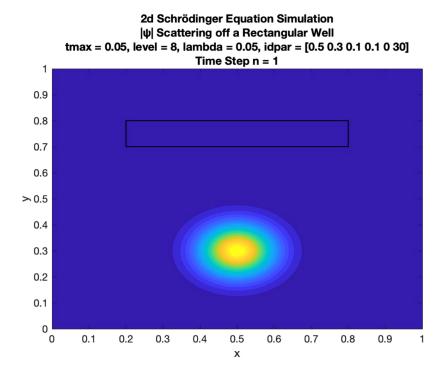


Figure 10: Screenshot of video produced by ${\tt video_rec_well.m}$ - Initial conditions.

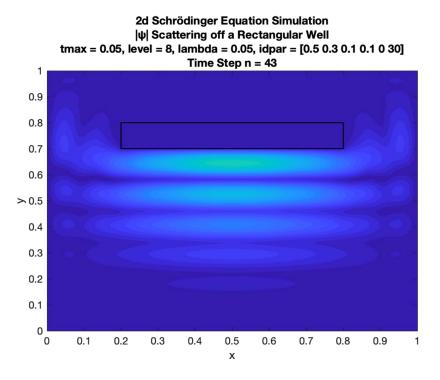


Figure 11: Screenshot of video produced by video_rec_well.m - Scattering off well.

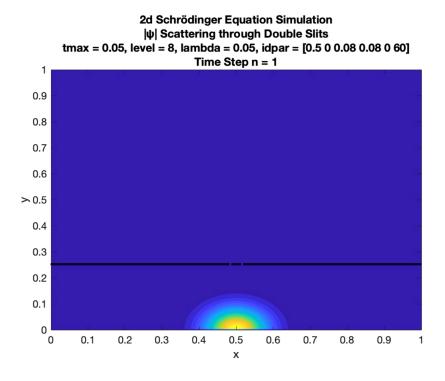


Figure 12: Screenshot of video produced by ${\tt double_slit_well.m-Initial}\ conditions.$

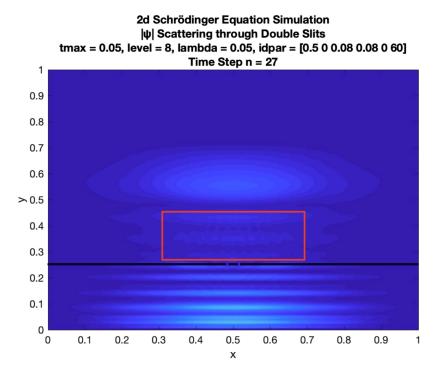


Figure 13: Screenshot of video produced by ${\tt double_slit_well.m}$ - Self interference through slits.

Conclusions

Generative AI was used to help with understanding how to use MATLAB's contourf function for making videos of numerical experiments in 2d. It was also used for help with typesetting this document.

Appendix A - sch_1d_cn.m Code

```
% sch_1d_cn: Solves 1D Schrödinger equation using O(dt^2,dx^2)
  % Crank-Nicolson implicit scheme.
  %
3
  % Inputs:
  %
  %
               Maximum integration time
       tmax:
  %
       level:
               Discretization level
  %
       lambda: dt/dx
  %
       idtype: Selects initial data type
  %
                Vector of initial data parameters
       idpar:
10
  %
                Selects potential type
       vtype:
11
  %
                Vector of potential parameters
       vpar:
  %
13
  %
    Outputs:
14
  %
15
  %
               Column vector of x coordinates [nx]
       \mathbf{x}:
  %
               Column vector of t coordinates [nt]
17
  %
       psi:
               Array of computed psi values [nt x nx]
18
  %
               Array of computed psi_re values [nt x nx]
       psire:
  %
               Array of computed psi_im values [nt x nx]
       psimod: Array of computed sqrt(psi psi*) values [nt x nx]
                Array of computed running integral values [nt x nx]
       prob:
22
  %
       \mathbf{v}:
               Column vector of potential values [nx]
  function [x t psi psire psiim psimod prob v] = ...
24
       sch_ld_cn(tmax, level, lambda, idtype, idpar, vtype, vpar)
25
26
       % Define mesh and derived parameters
       nx = 2^level + 1;
28
       x = linspace(0.0, 1.0, nx);
29
       dx = x(2) - x(1);
30
       dt = lambda * dx;
31
       nt = round(tmax / dt) + 1;
32
       t = (0 : nt-1) * dt;
33
       % Initialize solution, and set initial data
       psi = zeros(nt, nx);
36
       if idtype = 0
37
           % Exact family
           psi(1, :) = sin(idpar(1) * pi * x);
39
       elseif idtype == 1
40
           % Boosted Gaussian
41
           psi(1, :) = exp(1i * idpar(3) * x) .* ...
42
                        \exp(-((x - idpar(1)) ./ idpar(2)) .^{2});
43
       else
44
           fprintf('sch_1d_cn: Invalid idtype=%d\n', idtype);
45
       end
47
       % Set first and last values of initial data to zero
48
       psi(1, 1) = 0;
       psi(1, nx) = 0;
51
       % Initial storage for prob and calculate for initial time
52
       prob = zeros(nt, nx);
53
       for j = 2 : nx
           prob(1, j) = trapz(x(1:j), abs(psi(1, 1:j)).^2);
55
       end
56
```

```
57
        % Initialize potential
58
        v = zeros(1,nx);
59
        if vtype = 0
60
            % No potential - leave unchanged
61
        elseif vtype == 1
            % Rectangular barrier or well
63
            v(x > vpar(1) \& x < vpar(2)) = vpar(3);
64
        else
65
             fprintf('sch_1d_cn: Invalid vtype=%d\n', vtype);
67
        end
68
69
        % Initialize storage for RHS
        f = zeros(nx,1);
71
72
        % Set up tridiagonal system
73
        dl = 0.5/dx^2 * ones(nx, 1);
        d = (1i/dt - 1/dx^2 - 0.5*v.') * ones(nx,1);
75
        du = dl;
76
        % Fix up boundary cases
        d(1) = 1.0;
        du(2) = 0.0;
79
        dl(nx-1) = 0.0;
80
        d(nx) = 1.0;
81
        % Define sparse matrix
82
        A = \operatorname{spdiags}([dl \ d \ du], -1:1, nx, nx);
83
84
        % Compute solution using CN scheme
        \mathbf{for} \quad \mathbf{n} = 1 : \mathbf{nt} - 1
86
            % Define RHS of linear system
87
            f(2:nx-1) = psi(n, 2:nx-1) .* (1i/dt + 1/dx^2 + 0.5*v(2:nx-1)) ...
88
                          + (-0.5/dx^2) * (psi(n, 1:nx-2) + psi(n, 3:nx));
89
             f(1) = 0.0;
90
             f(nx) = 0.0;
91
            % Solve system, thus updating approximation to next time step
92
             psi(n+1, :) = A \setminus f;
            % Set first and last values to zero
94
             psi(n+1, 1) = 0;
95
             psi(n+1, nx) = 0;
96
            % Calculate prob each time step
98
             for j = 2 : nx
99
                 prob(n+1, j) = trapz(x(1:j), abs(psi(n+1, 1:j)).^2);
100
            end
101
        end
102
103
        % Compute real, imaginary, and modulus of each entry in psi
104
        psire = real(psi);
105
        psiim = imag(psi);
106
        psimod = abs(psi);
107
108
        % Convert to column vectors
109
        x = x.;
110
        t = t.;
111
        v = v.;
   end
113
```

Appendix B - ctest_1d.m Code

```
% 1.4 − 1d Convergence Testing
 2
      close all;
 3
      clear; clc;
      format long;
 5
     % Convergence Test #1
     - $\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}
10
     % Simulation maximum time
     tmax = 0.25;
     % Discretization levels
13
      minlevel = 6;
      maxlevel = 9;
     % Delta t by Delta x ratio
     lambda = 0.1;
17
     \% \text{ idtype} = 0
                                     -> Exact family (sine wave)
     \% \text{ idtype} = 1
                                        -> Boosted Gaussian
20
     idtype = 0;
21
      idpar = [3]; \% m = 3
22
     \% vtype = 0
                                   -> No potential
     \% vtvpe = 1
                                  -> Rectangular barrier or well
25
      vtype = 0;
26
      vpar = zeros(1,3);
28
     % Perform computation at various levels of discretization, store
29
     % results in cell arrays ...
      for l = minlevel : maxlevel
               % Compute the solution
32
                [x\{1\} \ t\{1\} \ psi\{1\} \ psire\{1\} \ psiim\{1\} \ psimod\{1\} \ prob\{1\} \ v\{1\}] \ \dots
33
                         = sch_ld_cn(tmax, l, lambda, idtype, idpar, vtype, vpar)
34
                [nt\{1\}, nx\{1\}] = size(psi\{1\});
36
37
               \% Since idtype = 0, compute exact solution
                psixct\{1\} = zeros(nt\{1\}, nx\{1\});
39
                for n = 1 : nt\{1\}
40
                          psixct\{l\}(n,:) = exp(-1i * idpar(1)^2 * pi^2 * t\{l\}(n)) \dots
41
                                                            * \sin(idpar(1) * pi * x{1});
42
43
               % Compute exact errors and their rms values for later
44
                Epsi\{1\} = psixct\{1\} - psi\{1\};
45
                rms_Epsi\{1\} = rms(abs(Epsi\{1\}), 2);
46
      end
47
48
     % Calculating the level-to-level differences, taking every second
     % value of the larger length array
      dpsi6 = downsample(downsample(psi\{7\}, 2).', 2).' - psi\{6\};
51
      dpsi7 = downsample(downsample(psi\{8\}, 2).', 2).' - psi\{7\};
52
      dpsi8 = downsample(downsample(psi\{9\}, 2).', 2).' - psi\{8\};
53
     % Compute 1-2 norm of each dpsi, resulting in functions of t
     rms_dpsi6 = rms(abs(dpsi6), 2);
```

```
rms_dpsi7 = rms(abs(dpsi7), 2);
        rms_dpsi8 = rms(abs(dpsi8), 2);
      % Plot scaled errors for different discretization levels
 60
       fig1 = figure;
 61
       rho = 4;
 62
       hold on
        plot(t{6}, rms_dpsi6, 'LineWidth', 2);
       plot(t{7}, rho*rms_dpsi7, 'LineWidth', 2);
        plot(t{8}, rho^2*rms_dpsi8, 'LineWidth', 2);
       xlabel("Time");
       ylabel("1-2 norm of difference between level");
 68
       legend ('|| d\Psi^{\hat{}}6||', '4 * || d\Psi^{\hat{}}7||', '4^2 * || d\Psi^{\hat{}}8||', 'Location', 'best');
 69
        title ({"1d Schrodinger equation convergence test - Exact family"
                        "l-2 norm of difference between level l solutions"
 71
                       "idtype = 0, vtype = 0, tmax = 0.25, lambda = 0.1, 6 \le 1 \le 9"});
 72
       ax = gca;
 73
       ax.FontSize = 12;
 75
      % Plot scaled exact errors for different discretization levels
 76
       fig2 = figure;
       rho = 4;
       hold on
       plot(t\{6\}, rms\_Epsi\{6\}, 'LineWidth', 2);
        plot(t\{7\}, rho*rms\_Epsi\{7\}, 'LineWidth', 2);
        plot(t{8}, rho^2*rms_Epsi{8}, 'LineWidth', 2);
       plot(t{9}, rho^3*rms_Epsi{9}, 'LineWidth', 2);
 83
       xlabel("Time");
 84
       ylabel("1-2 norm of exact error");
       \textbf{legend(', ||E\Psi^{\hat{}}6||', '4 * ||E\Psi^{\hat{}}7||', '4^2 * ||E\Psi^{\hat{}}8||', '4^3 * ||E\Psi^{\hat{}}9||'...}
 86
                         , 'Location', 'best');
 87
        title ({"1d Schrodinger equation convergence test - Exact family"
 88
                       "1-2 norm of exact error for each level 1"
 89
                       "idtype = 0, vtype = 0, tmax = 0.25, lambda = 0.1, 6 \le 1 \le 9"});
 90
       ax = gca;
 91
       ax.FontSize = 12;
 92
 94
       95
       % Convergence Test #2
       \frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\fir}\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\frac{\
 98
       clear;
 99
100
      % Simulation maximum time
       tmax = 0.01;
102
       % Discretization levels
103
       minlevel = 6;
       maxlevel = 9;
       % Delta t by Delta x ratio
106
       lambda = 0.01;
107
      \% idtype = 0
                                     -> Exact family (sine wave)
      \% idtype = 1
                                        -> Boosted Gaussian
110
       idtype = 1;
111
       idpar = [0.50 \ 0.075 \ 0.0];
113
      \% vtype = 0 \rightarrow No potential
```

```
% vtype = 1 -> Rectangular barrier or well
   vtype = 0;
   vpar = zeros(1,3);
118
   % Perform computation at various levels of discretization, store
119
   % results in cell arrays ...
120
   for l = minlevel : maxlevel
121
       % Compute the solution
122
        [x\{1\} \ t\{1\} \ psi\{1\} \ psire\{1\} \ psiim\{1\} \ psimod\{1\} \ prob\{1\} \ v\{1\}] \ \dots
123
            = sch_ld_cn(tmax, l, lambda, idtype, idpar, vtype, vpar);
125
        [nt\{1\}, nx\{1\}] = size(psi\{1\});
126
   end
127
   % Calculating the level-to-level differences, taking every second
129
   % value of the larger length array
130
   dpsi6 = downsample(downsample(psi\{7\}, 2).', 2).' - psi\{6\};
131
   dpsi7 = downsample(downsample(psi\{8\}, 2).', 2).' - psi\{7\};
   dpsi8 = downsample(downsample(psi\{9\}, 2).', 2).' - psi\{8\};
133
134
   % Compute 1-2 norm of each dpsi, resulting in functions of t
135
   rms_dpsi6 = rms(abs(dpsi6), 2);
   rms_dpsi7 = rms(abs(dpsi7), 2);
137
   rms_dpsi8 = rms(abs(dpsi8), 2);
138
139
   % Plot scaled errors for different discretization levels
   fig3 = figure;
141
   rho = 4:
142
   hold on
   plot(t{6}, rms_dpsi6, 'LineWidth', 2);
144
   plot(t{7}, rho*rms_dpsi7, 'LineWidth', 2);
145
   plot(t{8}, rho^2*rms_dpsi8, 'LineWidth', 2);
146
   xlabel("Time");
   ylabel("l-2 norm of difference between level");
148
   legend('||d\P^6||', '4 * ||d\P^7||', '4^2 * ||d\P^8||', 'Location', 'best');
149
   title ({"1d Schrodinger equation convergence test - Boosted Gaussian"
150
           "1-2 norm of difference between level 1 solutions"
           "idtype = 1, vtype = 0, tmax = 0.01, lambda = 0.01, 6 \le 1 \le 9"});
152
   ax = gca;
153
   ax.FontSize = 12;
```

Appendix C - barrier_survey.m Code

```
\% 1.5.1 - 1d Barrier Survey
2
  close all;
3
  clear; clc;
  format long;
5
  % Simulation maximum time
  tmax = 0.10;
  % Discretization level
  level = 9;
  % Delta t by Delta x ratio
  lambda = 0.01;
12
13
  \% \text{ idtype} = 0
                 -> Exact family (sine wave)
14
  \% \text{ idtype} = 1
                  -> Boosted Gaussian
  idtype = 1;
  idpar = [0.40, 0.075, 20.0];
17
  \% vtype = 0
                 -> No potential
                 -> Rectangular barrier or well
  \% vtype = 1
20
  vtype = 1;
21
  xmin = 0.6;
  xmax = 0.8;
  lnV0 = linspace(-2, 5, 251);
24
25
  % Survey range
26
  x1 = 0.8;
27
  x2 = 1.0;
28
29
   for idx = 1 : length(lnV0)
30
      % Get this iteration's vpar
31
       vpar = [xmin, xmax, exp(lnV0(idx))];
32
33
      \% Compute the solution
34
       [x{idx} t{idx} psi{idx} psire{idx} psiim{idx} psimod{idx} prob{idx} v{
35
          idx }] ...
          = sch_1d_cn(tmax, level, lambda, idtype, idpar, vtype, vpar);
36
37
      % Compute temporal average of probability matrix
38
       P_{bar} \{ idx \} = mean(prob\{ idx \});
39
      % Normalize the temporal average
40
       P_{bar}\{idx\} = P_{bar}\{idx\} / P_{bar}\{idx\}(end);
42
      % Compute indices of x1 and x2 in the array x
43
      % This only needs to be done once
44
       if idx == 1
45
           46
           47
       end
      % Compute excess fractional probability and its logarithm
50
       Fe_bar\{idx\} = (P_bar\{idx\}(x2\_loc) - P_bar\{idx\}(x1\_loc)) / \dots
51
                        (x{idx}(x2\_loc) - x{idx}(x1\_loc));
52
       lnFe_bar\{idx\} = log(Fe_bar\{idx\})
53
  end
54
55
```

Appendix D - well_survey.m Code

```
\% 1.5.2 - 1d Well Survey
2
  close all;
3
  clear; clc;
  format long;
5
  % Simulation maximum time
  tmax = 0.10;
  % Discretization level
  level = 9;
  % Delta t by Delta x ratio
  lambda = 0.01;
12
13
  \% \text{ idtype} = 0
                 -> Exact family (sine wave)
14
  \% \text{ idtype} = 1
                  -> Boosted Gaussian
  idtype = 1;
  idpar = [0.40, 0.075, 0.0];
17
  \% vtype = 0
                 -> No potential
                 -> Rectangular barrier or well
  \% vtype = 1
20
  vtype = 1;
21
  xmin = 0.6;
  xmax = 0.8;
  lnV0 = linspace(2, 10, 251);
24
25
  % Survey range
26
  x1 = 0.6;
27
  x2 = 0.8;
28
29
   for idx = 1 : length(lnV0)
30
      % Get this iteration's vpar
31
       vpar = [xmin, xmax, -exp(lnV0(idx))];
32
33
      \% Compute the solution
34
       [x{idx} t{idx} psi{idx} psire{idx} psiim{idx} psimod{idx} prob{idx} v{
35
          idx }] ...
          = sch_1d_cn(tmax, level, lambda, idtype, idpar, vtype, vpar);
36
37
      % Compute temporal average of probability matrix
38
       P_{bar} \{ idx \} = mean(prob\{ idx \});
39
      % Normalize the temporal average
40
       P_{bar}\{idx\} = P_{bar}\{idx\} / P_{bar}\{idx\}(end);
42
      % Compute indices of x1 and x2 in the array x
43
      % This only needs to be done once
44
       if idx == 1
45
           46
           47
       end
      % Compute excess fractional probability and its logarithm
50
       Fe_bar\{idx\} = (P_bar\{idx\}(x2\_loc) - P_bar\{idx\}(x1\_loc)) / \dots
51
                        (x{idx}(x2\_loc) - x{idx}(x1\_loc));
52
       lnFe_bar\{idx\} = log(Fe_bar\{idx\})
53
  end
54
55
```

Appendix E - sch_2d_adi.m Code

```
% sch-2d-adi: Solves 2D Schrödinger equation using ADI scheme.
  %
2
  % Inputs:
3
  %
4
  %
                Maximum integration time
       tmax:
  %
       level:
                Discretization level
  %
       lambda: dt/dx
  %
       idtype: Selects initial data type
  %
       idpar:
                Vector of initial data parameters
  %
       vtype:
                Selects potential type
10
  %
                Vector of potential parameters
       vpar:
11
  %
12
  % Outputs:
13
  %
14
  %
                Column vector of x coordinates [nx]
       \mathbf{x}:
15
  %
                Column vector of y coordinates [ny
       y:
  %
                Column vector of t coordinates [nt]
17
       t.:
  %
       psi:
                Array of computed psi values [nt x nx x ny]
18
  %
                Array of computed psi_re values [nt x nx x ny]
       psire:
19
                Array of computed psi_im values [nt x nx x ny]
20
       psimod: Array of computed sqrt(psi psi*) values [nt x nx x ny]
21
                Array of potential values [nx x ny]
       \mathbf{v}:
22
   function [x \ y \ t \ psi \ psire \ psiim \ psimod \ v] = \dots
       sch_2d_adi(tmax, level, lambda, idtype, idpar, vtype, vpar)
24
25
       % Define mesh and derived parameters
26
       nx = 2^level + 1;
                                          ny = nx;
       x = linspace(0.0, 1.0, nx);
                                          y = x;
28
       dx = x(2) - x(1);
                                          dy = dx;
29
       dt = lambda * dx;
30
       nt = round(tmax / dt) + 1;
31
       t = (0 : nt-1) * dt;
32
33
       % Define meshgrid for populating psi(x,y,0) and V(x,y)
34
       [X, Y] = \operatorname{meshgrid}(x, y);
36
       % Initialize solution, and set initial data
37
       psi = zeros(nt, nx, ny);
       if idtype = 0
39
           % Exact family
40
           psi(1, :, :) = sin(idpar(1)*pi*x)' * sin(idpar(2)*pi*y);
41
       elseif idtype = 1
42
           % Boosted Gaussian
43
           % Create variable names for function parameters
44
                                       y0 = idpar(2);
                    = idpar(1);
45
           delta_x = idpar(3); delta_y = idpar(4);
                    = idpar(5);
                                      p_y = idpar(6);
           p_x
47
48
           \% Calculate psi(x, y, 0)
            p si_0 = exp(1 i * p_x * X) .* exp(1 i * p_y * Y) ...
                 * \exp(-(((X - x0).^2)/delta_x^2 + ((Y - y0).^2)/delta_y^2));
51
            psi(1, :, :) = reshape(psi_0, [1, nx, ny]);
52
       else
53
            fprintf('sch_2d_adi: Invalid idtype=%d\n', idtype);
55
       end
56
```

```
% Set boundary conditions of initial data to zero
57
        \% \ t = 0:
                  \psi(0, y, t) = \psi(1, y, t) = \psi(x, 0, t) = \psi(x, 1, t) = 0
58
        psi(1, 1, :) = 0;
59
        psi(1, :, 1) = 0;
60
        psi(1, nx, :) = 0;
61
        psi(1, :, ny) = 0;
62
63
        % Initialize time-independent potential
64
        v = zeros(nx, ny);
65
        if vtype = 0
            % No potential - leave unchanged
67
        elseif vtype = 1
68
            % Rectangular barrier or well
69
            % Create variable names for function parameters
             x_{\min} = vpar(1);
                                  x_{max} = vpar(2);
71
             y_min = vpar(3);
                                  y_max = vpar(4);
72
                   = vpar(5);
             Vc
73
            \% Calculate V(x, y)
75
             v((X >= x_min \& X <= x_max) \& (Y >= y_min \& Y <= y_max)) = Vc;
76
        elseif vtype == 2
            % Double slit
            % Create variable names for function parameters
79
             x1 = vpar(1);
                               x2 = vpar(2);
80
             x3 = vpar(3);
                               x4 = vpar(4);
81
             Vc = vpar(5);
82
             i_{prime} = (ny - 1)/4 + 1;
83
84
            \% Calculate V(x, y)
             Vc_{-indices} = (x \le x1) | (x >= x2 & x <= x3) | (x >= x4);
86
             v(j_prime, Vc_indices) = Vc;
87
             v(j_prime + 1, Vc_indices) = Vc;
88
        else
89
             fprintf('sch_2d_adi: Invalid vtype=%d\n', vtype);
90
             return
91
        end
92
        % Define sparse matrix diagonals for first ADI eqn
94
        dl \, = \, (-1\,i * dt \, / (2 * dx \, \hat{} \, 2) \,) \  \, * \  \, ones \, (nx \, , \  \, 1) \, ;
95
        d = (1 + 1i*dt/(dx^2)) * ones(nx, 1);
96
        du = dl;
97
        % Impose boundary conditions
98
        d(1)
                  = 1.0;
99
        du(2)
                  = 0.0;
100
        dl(nx-1) = 0.0;
101
        d(nx)
                  = 1.0;
102
        % Compute sparse matrix for first ADI eqn
103
        A_half = spdiags([dl d du], -1:1, nx, nx);
104
105
        % Loop that iterates each time step
106
        for n = 1:nt-1
107
            \% reshape \psi to create a 2d matrix at this timestep
             psi_n = reshape(psi(n,:,:), nx, ny);
109
            % Create matrix for \psi^{\hat{}}(n+1/2)
110
             psi_half = zeros(nx, ny);
111
            % Solve tridiagonal system for each j (row)
113
             for j = 2:ny-1
114
```

```
\% Array for holding the RHS of the first ADI eqn
115
                f = zeros(nx,1);
116
                % Compute RHS of first ADI eqn in stages.
118
                f(2:nx-1) = (1i*dt/(2*dy^2)) * (psi_n(2:nx-1, j+1) + psi_n(2:nx
119
                    -1, j-1) ...
                           + (1 - 1i*dt*(1/dy^2 + v(2:nx-1,j)/2)) .* psi_n(2:nx
120
                               -1, j);
                f(2:nx-1) = (1i*dt/(2*dx^2)) * (f(1:nx-2) + f(3:nx)) + ...
121
                              (1 - 1i*dt/dx^2) * f(2:nx-1);
123
                % Impose boundary conditions
124
                f(1) = 0.0;
125
                f(nx) = 0.0;
126
127
                % Solve first ADI system
128
                psi_half(:,j) = A_half \setminus f;
129
                % Impose boundary conditions
130
                 psi_half(1,:) = 0.0;
131
                 psi_half(:,1) = 0.0;
132
                 psi_half(nx,:) = 0.0;
                 psi_half(:,ny) = 0.0;
            end
135
136
            % Define upper and lower sparse matrix diagonals for second ADI eqn
137
            dl = (-1i*dt/(2*dy^2)) * ones(ny, 1);
138
            du = dl;
139
            % Impose boundary conditions
140
                     = 0.0;
            du (2)
            dl(ny-1) = 0.0;
142
143
            % Solve tridiagonal system for each i (column)
144
            for i = 2:nx-1
145
                % Define middle sparse matrix diagonal for second ADI eqn
146
                v_i = reshape(v(i,:), ny, 1);
147
                d = 1 + 1i*dt/dy^2 + (1i*dt/2)*v_i;
148
                % Impose boundary conditions
                d(1) = 1.0;
150
                d(ny) = 1.0;
151
152
                % Compute sparse matrix for second ADI eqn
                A_full = spdiags([dl d du], -1:1, ny, ny);
154
155
                % Compute RHS of second ADI eqn. BCs already imposed previously
156
                f = reshape(psi_half(i,:), ny, 1);
157
158
                \% Solve second ADI system
159
                psi(n+1, i, :) = A_full \setminus f;
160
                % Impose boundary conditions
161
                psi(n+1, 1, :) = 0.0;
162
                psi(n+1, :, 1) = 0.0;
163
                psi(n+1, nx, :) = 0.0;
164
                psi(n+1, :, ny) = 0.0;
165
            end
166
       end
167
       % Compute real, imaginary, and modulus of each entry in psi
169
        psire = real(psi);
170
```

Appendix F - ctest_2d.m Code

```
% 2.4 − 2d Convergence Testing
2
   close all;
3
   clear; clc;
   format long;
5
  % Simulation maximum time
  tmax = 0.05;
  % Discretization levels
  minlevel = 6;
   maxlevel = 9;
  % Delta t by Delta x ratio
12
   lambda = 0.05;
13
14
  \% \text{ idtype} = 0
                  -> Exact family (sine wave)
  \% idtype = 1
                  -> Boosted Gaussian
  idtype = 0;
17
   idpar = [2, 3];
18
  mx = idpar(1); my = idpar(2);
20
  \% vtype = 0 \rightarrow No potential
21
  \% vtype = 1
                -> Rectangular barrier or well
22
  vtype = 0;
   vpar = zeros(1,5);
24
25
  % Perform computation at various levels of discretization, store
26
  % results in cell arrays ...
   for l = minlevel : maxlevel
28
       % Compute the solution
29
       [x\{1\} y\{1\} t\{1\} psi\{1\} psire\{1\} psiim\{1\} psimod\{1\} v\{1\}] = ...
30
            sch_2d_adi(tmax, 1, lambda, idtype, idpar, vtype, vpar)
31
32
       [nt\{1\}, nx\{1\}, ny\{1\}] = size(psi\{1\});
33
34
       % Define meshgrid for computing exact psi(x,y,t)
       [X\{1\}, Y\{1\}] = meshgrid(x\{1\}, ', y\{1\}, ');
36
37
       % Compute exact solution
38
       psixct\{1\} = zeros(nt\{1\}, nx\{1\}, ny\{1\});
39
       for n = 1 : nt\{l\}
40
            psixct_n\{1\} = exp(-1i*(mx^2 + my^2)*pi^2*t\{1\}(n)) * ...
41
                            \sin(\max \pi X\{1\}) .* \sin(\max \pi Y\{1\});
            % Enforce boundary conditions
43
            psixct_n\{1\}(1, :)
                                     = 0.0;
44
            psixct_n\{l\}(:, 1)
                                     = 0.0;
45
            psixct_n\{1\}(nx\{1\}, :) = 0.0;
            psixct_n\{1\}(:, ny\{1\}) = 0.0;
47
            psixct\{1\}(n, :, :) = reshape(psixct_n\{1\}, [1, nx\{1\}, ny\{1\}]);
48
       end
49
       % Compute exact errors and their rms values for later
51
       Epsi\{1\} = psixct\{1\} - psi\{1\};
52
       Epsi_2d\{1\} = reshape(Epsi\{1\}, nt\{1\}, nx\{1\}*ny\{1\});
53
       rms_Epsi\{1\} = rms(abs(Epsi_2d\{1\}), 2);
55
       % Downsample each psi for differencing
56
```

```
psi_ds\{1\} = psi\{1\}(1:2:end, 1:2:end, 1:2:end);
57
58
        % Flatten each 3d array into a 2d array
59
        psi_2d\{1\} = reshape(psi\{1\}, nt\{1\}, nx\{1\}*ny\{1\});
60
        psi_ds_2d\{1\} = reshape(psi_ds\{1\}, (nt\{1\}-1)/2+1, ...
61
                                  ((nx{1}-1)/2+1)*((ny{1}-1)/2+1));
62
   end
63
64
   % Calculating the level-to-level differences, taking every second
65
   % value of the larger length array
   dpsi6 = psi_ds_2d\{7\} - psi_2d\{6\};
   dpsi7 = psi_ds_2d\{8\} - psi_2d\{7\};
68
   dpsi8 = psi_ds_2d\{9\} - psi_2d\{8\};
69
   % Compute 1-2 norm of each dpsi, resulting in functions of t
71
   rms_dpsi6 = rms(abs(dpsi6), 2);
72
   rms_dpsi7 = rms(abs(dpsi7), 2);
   rms_dpsi8 = rms(abs(dpsi8), 2);
75
   % Plot scaled errors for different discretization levels
76
   fig1 = figure;
   rho = 4;
   hold on
79
   plot(t{6}, rms_dpsi6, 'LineWidth', 2);
80
   plot(t{7}, rho*rms_dpsi7, 'LineWidth', 2);
   plot(t{8}, rho^2*rms_dpsi8, 'LineWidth', 2);
   xlabel("Time");
83
   ylabel ("1-2 norm of difference between level");
84
   legend ('||d\P^6||', '4 * ||d\P^7||', '4^2 * ||d\P^8||', 'Location', 'best'); title ({"2d Schrodinger equation convergence test – Exact family"
86
            "l-2 norm of difference between level 1 solutions"
87
           "idtype = 0, vtype = 0, tmax = 0.05, lambda = 0.05, 6 \le 1 \le 9"});
88
   ax = gca;
89
   ax.FontSize = 12;
90
91
   % Plot scaled exact errors for different discretization levels
92
   fig2 = figure;
   rho = 4;
94
   hold on
95
   plot(t{6}, rms_Epsi{6}, 'LineWidth', 2);
   plot(t{7}, rho*rms\_Epsi{7}, 'LineWidth', 2);
   plot(t\{8\}, rho^2*rms\_Epsi\{8\}, 'LineWidth', 2);
   {\tt plot}\left(\,t\,\{9\}\,,\ {\tt rho\,\^3*rms\_Epsi}\,\{9\}\,,\ {\tt 'LineWidth\,'}\,,\ 2\right);
99
   xlabel("Time");
100
   ylabel("l-2 norm of exact error");
101
   {\tt legend('||E\Psi^{\hat{}}6||', '4 * ||E\Psi^{\hat{}}7||', '4^2 * ||E\Psi^{\hat{}}8||', '4^3 * ||E\Psi^{\hat{}}9||' \dots}
102
            , 'Location', 'best');
103
    title ({"2d Schrodinger equation convergence test - Exact family"
104
           "1-2 norm of exact error for each level 1"
105
           "idtype = 0, vtype = 0, tmax = 0.05, lambda = 0.05, 6 \le 1 \le 9"});
106
   ax = gca;
107
   ax.FontSize = 12;
108
```

Appendix G - video_rec_bar.m Code

```
% 2.5 - 2d Video of Scattering off Rectangular Barrier
2
  close all;
3
  clear; clc;
  format long;
  % Simulation maximum time
  tmax = 0.05;
  % Discretization level
  level = 8;
  % Delta t by Delta x ratio
  lambda \,=\, 0.05;
12
13
  % idtype = 0 -> Exact family (sine wave)
14
  \% \text{ idtype} = 1
                -> Boosted Gaussian
  idtype = 1;
            = idpar(1);
                             v0 = idpar(2);
17
  \%delta_x = idpar(3); delta_y = idpar(4);
         = idpar(5); p_y = idpar(6);
  idpar = [0.5, 0.3, 0.1, 0.1, 0.0, 30];
20
21
  \% vtype = 0
                -> No potential
  \% vtype = 1
                     Rectangular barrier or well
                 ->
  \% vtype = 2
                 -> Double Slit
  vtvpe = 1:
25
  x_{\min} = 0.2;
                 x_{max} = 0.8;
  y_{min} = 0.7;
                  y_{max} = 0.8;
  %Vc
       = \operatorname{vpar}(5);
28
  vpar = [x_min, x_max, y_min, y_max, 1e8];
29
30
  % Compute solution
  [x \ y \ t \ psi \ psire \ psiim \ psimod \ v] = \dots
32
       sch_2d_adi(tmax, level, lambda, idtype, idpar, vtype, vpar);
33
34
  % Dimensions of matrix
  [nt, nx, ny] = size(psimod);
36
37
  % Create a VideoWriter object
  video = VideoWriter('../../output/problem2/rec_bar.avi');
  video.FrameRate = 30;
40
  open (video);
41
  % Create a figure and define where the rectangle indicating where
  % the potential barrier is will be drawn
44
  figure;
  rect_xmin = x_min * (nx - 1) + 1;
  rect_ymin = y_min * (ny - 1) + 1;
47
  rect\_xlen = (x\_max - x\_min) * (nx - 1);
48
  rect_ylen = (y_max - y_min) * (ny - 1);
49
  % Loop over time steps
51
  for n = 1:nt
52
       \% reshape \psi to create a 2d matrix at this timestep
53
       psi_n = reshape(psimod(n,:,:), nx, ny);
55
      % Create filled contour plot
56
```

```
contourf(psi_n, 20, 'LineStyle', 'none');
57
        colormap(" default");
58
        xlabel('x');
59
        ylabel('y');
60
        title ({ '2d Schrödinger Equation Simulation'
61
                 |\psi| Scattering off a Rectangular Barrier'
                  t_{tmax} = t_{tmax}, num2str(tmax), t_{tmax} = t_{tmax}, num2str(level), \dots
63
                  'tmax = ', num2str(vmax), ', idpar = [', ...
64
                  num2str(idpar(1)), ', num2str(idpar(2)), ', ', ...
num2str(idpar(3)), ', num2str(idpar(4)), ', ...
num2str(idpar(5)), ', num2str(idpar(6)), ']']
65
67
                ['Time Step n = ', num2str(n)]});
68
        ax = gca;
69
        ax.FontSize = 12;
71
        % Set axis limits for consistency
72
        axis ([1 nx 1 ny]);
73
        % Set color axis limits to match data range
74
        \operatorname{clim}([\min(\operatorname{psimod}(:)) \max(\operatorname{psimod}(:))]);
75
76
        % Scale the axes tick labels to range from 0 to 1
        xticks(linspace(1, nx, 11));
        yticks(linspace(1, ny, 11));
79
        xticklabels(linspace(0, 1, 11));
80
        yticklabels(linspace(0, 1, 11));
81
82
        % Draw rectangle where the potential is
83
        rectangle ('Position', [rect_xmin, rect_ymin, rect_xlen, rect_ylen], ...
84
                     'EdgeColor', 'black', 'LineWidth', 1);
86
        % Write to video file
87
        frame = getframe(gcf);
88
        writeVideo (video, frame);
89
   end
90
91
  % Close the video file and figure
   close (video);
```

Appendix H - video_rec_well.m Code

```
% 2.5 - 2d Video of Scattering off Rectangular Well
2
  close all;
3
  clear; clc;
  format long;
5
  % Simulation maximum time
  tmax = 0.05;
  % Discretization level
  level = 8;
  % Delta t by Delta x ratio
  lambda \,=\, 0.05;
12
13
  % idtype = 0 -> Exact family (sine wave)
14
  \% \text{ idtype} = 1
                -> Boosted Gaussian
  idtype = 1;
            = idpar(1);
                             v0 = idpar(2);
17
  \%delta_x = idpar(3); delta_y = idpar(4);
         = idpar(5); p_y = idpar(6);
  idpar = [0.5, 0.3, 0.1, 0.1, 0.0, 30];
20
21
  \% vtype = 0
                -> No potential
  \% vtype = 1
                     Rectangular barrier or well
                 ->
  \% vtype = 2
                 -> Double Slit
  vtvpe = 1:
25
  x_{\min} = 0.2;
                  x_{max} = 0.8;
  y_{min} = 0.7;
                  y_{max} = 0.8;
  %Vc
       = \operatorname{vpar}(5);
28
  vpar = [x_min, x_max, y_min, y_max, -1e8];
29
30
  % Compute solution
  [x \ y \ t \ psi \ psire \ psiim \ psimod \ v] = \dots
32
       sch_2d_adi(tmax, level, lambda, idtype, idpar, vtype, vpar);
33
34
  % Dimensions of matrix
  [nt, nx, ny] = size(psimod);
36
37
  % Create a VideoWriter object
  video = VideoWriter('../../output/problem2/well_bar.avi');
  video.FrameRate = 30;
40
  open (video);
41
  % Create a figure and define where the rectangle indicating where
  % the potential barrier is will be drawn
44
  figure;
  rect_xmin = x_min * (nx - 1) + 1;
  rect_ymin = y_min * (ny - 1) + 1;
47
  rect\_xlen = (x\_max - x\_min) * (nx - 1);
48
  rect_ylen = (y_max - y_min) * (ny - 1);
49
  % Loop over time steps
51
  for n = 1:nt
52
       \% reshape \psi to create a 2d matrix at this timestep
53
       psi_n = reshape(psimod(n,:,:), nx, ny);
55
      % Create filled contour plot
56
```

```
contourf(psi_n, 20, 'LineStyle', 'none');
57
        colormap(" default");
58
        xlabel('x');
59
        ylabel('y');
60
        title ({ '2d Schrödinger Equation Simulation'
61
                 |\psi| Scattering off a Rectangular Well'
                  t_{tmax} = t_{tmax}, num2str(tmax), t_{tmax} = t_{tmax}, num2str(level), \dots
63
                  ', lambda = ', num2str(lambda), ', idpar = [', ...
64
                  num2str(idpar(1)), '', num2str(idpar(2)), '', ...
num2str(idpar(3)), '', num2str(idpar(4)), '', ...
num2str(idpar(5)), '', num2str(idpar(6)), ']']
65
67
                ['Time Step n = ', num2str(n)]});
68
        ax = gca;
69
        ax.FontSize = 12;
71
        % Set axis limits for consistency
72
        axis ([1 nx 1 ny]);
73
        % Set color axis limits to match data range
74
        \operatorname{clim}([\min(\operatorname{psimod}(:)) \max(\operatorname{psimod}(:))]);
75
76
        % Scale the axes tick labels to range from 0 to 1
        xticks(linspace(1, nx, 11));
        yticks(linspace(1, ny, 11));
79
        xticklabels(linspace(0, 1, 11));
80
        yticklabels(linspace(0, 1, 11));
81
82
        % Draw rectangle where the potential is
83
        rectangle ('Position', [rect_xmin, rect_ymin, rect_xlen, rect_ylen], ...
84
                     'EdgeColor', 'black', 'LineWidth', 1);
86
        % Write to video file
87
        frame = getframe(gcf);
88
        writeVideo (video, frame);
89
   end
90
91
  % Close the video file and figure
   close (video);
```

Appendix I - video_double_slit.m Code

```
% 2.5 - 2d Video of Scattering through a Double Slit
2
  close all;
3
  clear; clc;
  format long;
5
  % Simulation maximum time
  tmax = 0.05;
  % Discretization level
  level = 8;
  % Delta t by Delta x ratio
  lambda \,=\, 0.05;
12
13
  \% \text{ idtype} = 0
                 -> Exact family (sine wave)
14
  \% \text{ idtype} = 1
                 -> Boosted Gaussian
  idtype = 1;
            = idpar(1);
                             v0 = idpar(2);
17
  \%delta_x = idpar(3); delta_y = idpar(4);
         = idpar(5); p_-y = idpar(6);
  idpar = [0.5, 0.0, 0.08, 0.08, 0.0, 60];
20
21
  \% vtype = 0
                -> No potential
  \% vtype = 1
                      Rectangular barrier or well
                 ->
  \% vtype = 2
                -> Double Slit
  vtvpe = 2:
25
  x1 = 0.48;
                x2 = 0.49;
  x3 = 0.51;
                x4 = 0.52;
  %Vc
        = \operatorname{vpar}(5);
28
  vpar = [x1, x2, x3, x4, 1e8];
29
30
  % Compute solution
  [x \ y \ t \ psi \ psire \ psiim \ psimod \ v] = \dots
32
       sch_2d_adi(tmax, level, lambda, idtype, idpar, vtype, vpar);
33
34
  % Dimensions of matrix
   [nt, nx, ny] = size(psimod);
36
37
  % Create a VideoWriter object
   video = VideoWriter('../../output/problem2/double_slit.avi');
   video.FrameRate = 30;
40
  open (video);
41
42
  % Create a figure
43
  figure;
44
45
  % Loop over time steps
   for n = 1:nt
47
       % reshape \psi to create a 2d matrix at this timestep
48
       psi_n = reshape(psimod(n,:,:), nx, ny);
49
       % Create filled contour plot
51
       contourf(psi_n, 20, 'LineStyle', 'none');
52
       colormap(" default");
53
       xlabel('x');
       ylabel('y');
55
       title ({ '2d Schrödinger Equation Simulation'
56
```

```
|\psi| Scattering through Double Slits'
57
                 ['tmax = ', num2str(tmax), ', level = ', num2str(level), ...
58
                  ', lambda = ', num2str(lambda), ', idpar = [', ...
59
                  num2str(idpar(1)), ', num2str(idpar(2)), ', ',
num2str(idpar(3)), ', num2str(idpar(4)), ', ',
num2str(idpar(5)), ', num2str(idpar(6)), ']']
60
61
62
                ['Time Step n = ', num2str(n)]});
63
        ax = gca;
64
        ax.FontSize = 12;
65
        % Set axis limits for consistency
67
        axis([1 nx 1 ny]);
68
        % Set color axis limits to match data range
69
        \operatorname{clim}([\min(\operatorname{psimod}(:)) \max(\operatorname{psimod}(:))]);
70
71
        % Scale the axes tick labels to range from 0 to 1
72
        xticks(linspace(1, nx, 11));
73
        yticks(linspace(1, ny, 11));
74
        xticklabels(linspace(0, 1, 11));
75
        yticklabels(linspace(0, 1, 11));
76
        % Draw rectangles where the double slit potential is
        hold on
79
        rectangle ('Position', [1, (ny - 1)/4 + 1, floor(x1*nx), 1], ...'EdgeColor', 'black', 'LineWidth', 1);
80
81
        rectangle ('Position', [ceil(x2*nx), (ny-1)/4+1, ceil((x3-x2)*nx),
82
                     'EdgeColor', 'black', 'LineWidth', 1);
83
        rectangle ('Position', [ceil(x4*nx), (ny - 1)/4 + 1, floor((1 - x4)*nx),
                    'EdgeColor', 'black', 'LineWidth', 1);
85
        hold off
86
87
        % Write to video file
88
        frame = getframe(gcf);
89
        writeVideo (video, frame);
90
   end
92
   % Close the video file and figure
93
   close (video);
```