One Dimensional Quantum Dynamics Simulator

This application calculates the time-evolution of a one-dimensional quantum system. The user can select from a list of pre-defined potentials and initial wavefunctions or specify his/her own functional forms using IDL syntax. The time-dependent Schrodinger equation is solved based on an algorithm presented in an article by Goldberg, Schey, and Schwartz (Am.J.Phys. 35(5), p. 177-186 (1967)). The flexibility of this application allows the user to explore many different time-dependent quantum phenomena such as tunneling, evolution of mixtures of bound states, dispersive wavepackets, and potential barrier scattering.

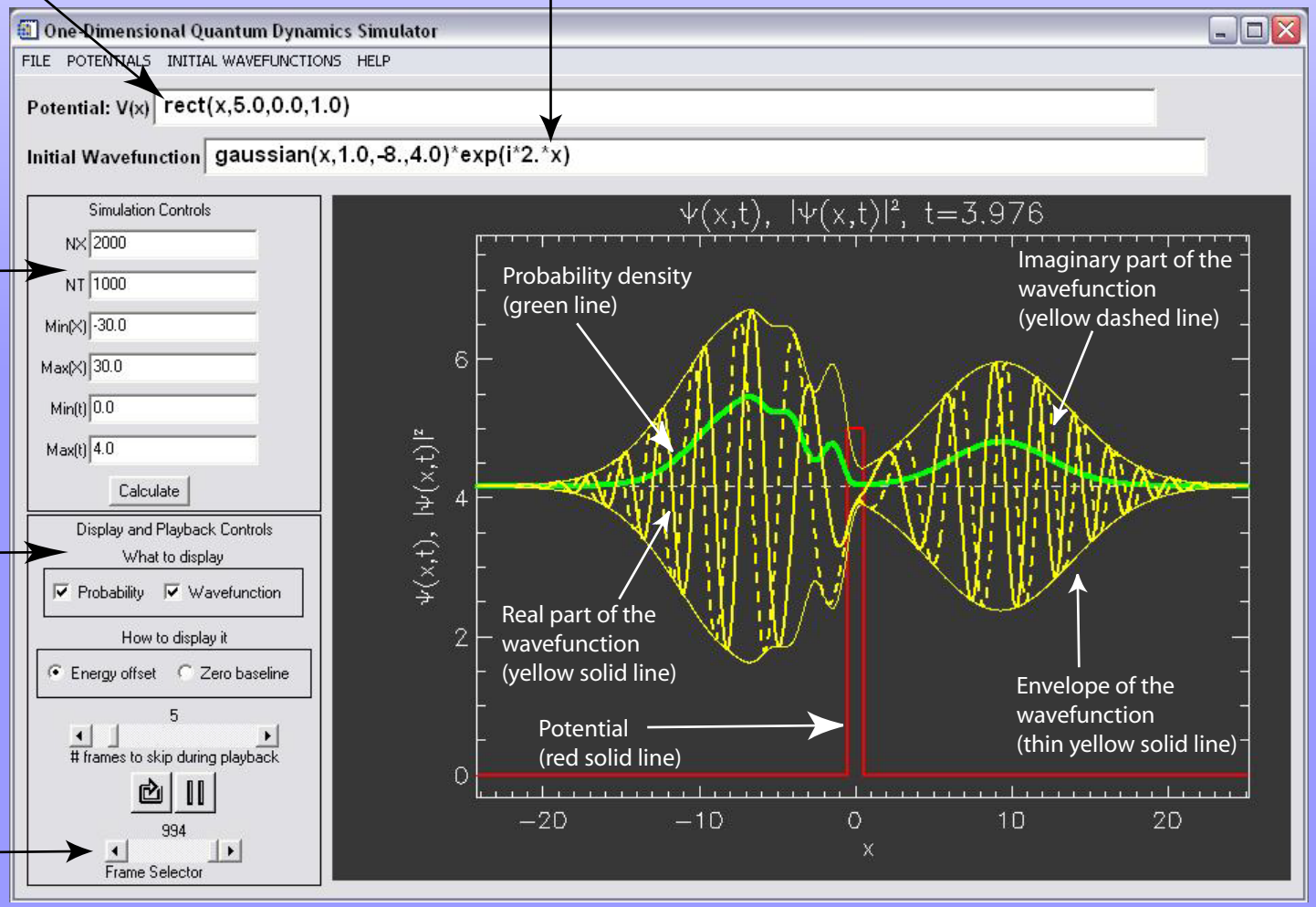
-Application is resizable
-Rubber-band box style dynamic zooming
-Save and restore potential and wavefunction expressions
-Save time-evolution as an animated GIF file
-Write out individual frames in GIF or PNG format

Things to try:

-Suddenly expanding square well (hint: start with an initial wavefunction only defined for half of the barrier width and zero everywhere else)
-Reflectionless potential scattering from a sech^2 potential
-Simple barrier well scattering
-Tunneling between adjacent wells
-Wavepacket propagation into a periodic potential (like an electron in a lattice)

User can specify potential well using IDL functions plus useful built-in functions such as RECT, GAUSSIAN, LORENTZIAN, SECH, and STEP.

User can specify the initial wavefunction $\Psi(x,t=0)$ using IDL syntax. Application also recognizes "i" as the imaginary unit.



Full control provided over the simulation conditions including number of spatial and time discretization steps.

Full control provided over the playback including skipping frames, pause/resume animation, plotting the probability and/or the real & imaginary components of the wavefunction.

Manually select the frame to display.

Functions available in SE_SIM.PRO *in addition* to the built-in IDL functions:

1. $$\mathrm{STEP}(x) = \begin{cases} 1, x > 0 \\ \tfrac{1}{2}, x = 0 \\ 0, x < 0 \end{cases}$$

2. $$\mathrm{RECT}(x, R_o, x_o, W) = R_o \bullet \left[\mathrm{STEP}\left(x - \left(x_o - W/2\right)\right) - \mathrm{STEP}\left(x - \left(x_o + W/2\right)\right)\right]$$

3. $$\mathrm{GAUSSIAN}(x, A, x_o, \mathrm{FWHM}) = \frac{A}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{x - x_o}{\sigma}\right)^2\right), \sigma = \mathrm{FWHM}/2.354$$

4. $$\mathrm{LORENTZIAN}(x, A, x_o, \mathrm{FWHM}) = \frac{A\Gamma}{\pi} \frac{1}{(x - x_o)^2 + \Gamma^2}, \Gamma = \mathrm{FWHM}/2$$

5. $$\mathrm{SECH}(x) = \frac{1}{\mathrm{COSH}(x)}$$

Quick-start:

1. Press the *calculate* button when the application starts to see the first example. You will see the animated sequence play through once.
2. Press the *play* button to replay the sequence, possibly changing the playback rate with the slider to skip frames.
3. Use the frame selection slider to examine an individual frame from the animated sequence. Use the mouse to zoom into particular regions of interest.
4. Enter your own potential and/or initial wavefunction…or try one of the examples below.

Examples to explore:

Wavepacket in a simple-harmonic oscillator potential:
NX = 1000, NT = 2000, T=5
Initial wavefunction: GAUSSIAN(x,1.0,-2.0,2.0)*exp(i*7.0*x)
Potential: 2.0*x^2.

Suddenly expanding square well:
NX = 1000, NT = 2000, T = 2.0
Initial wavefunction: SIN(!PI*x)*RECT(x,1.0,-0.5,2.0)+0.0*i
Potential: RECT(X,-1000.0,0.0,2.0)

Wavepacket scattering from step discontinuity:
NX = 1000, NT = 1000, T = 3.0
Initial wavefunction: GAUSSIAN(x,1.0,-5.0,2.0)*exp(i*3.0*x)
Potential: 5.0*STEP(x)

Reflectionless potential scattering:
NX = 1000, NT = 1000, T = 2.0
Initial wavefunction: GAUSSIAN(x,1.0,-7.0,2.0)*exp(i*6.0*x)
Potential: (-18.0*(1.0+18.0)/(0.8^2))*(SECH(x/0.8))^2

Tunneling through a square barrier:
NX = 1000, NT = 1000, T = 1.0
Initial wavefunction: GAUSSIAN(x,1.0,-5.0,2.0)*exp(i*7.0*x)
Potential: RECT(x,20.0,0.0,1.0)

Wavepacket propagation in a periodic lattice:
NX = 3500, NT=1500, T = 3.0
Initial wavefunction: GAUSSIAN(x,1.0,-8.0,5.0)*exp(i*0.35*7.0*x)
Potential: 6.2*RECT(x,1.0,12.5,25.0)*sin(7.0*x)

Wavepacket non-propagation in a periodic lattice:
NX = 3500, NT=1500, T = 3.0
Initial wavefunction: GAUSSIAN(x,1.0,-8.0,5.0)*exp(i*0.5*7.0*x)
Potential: 12.5*RECT(x,1.0,12.5,25.0)*sin(7.0*x)