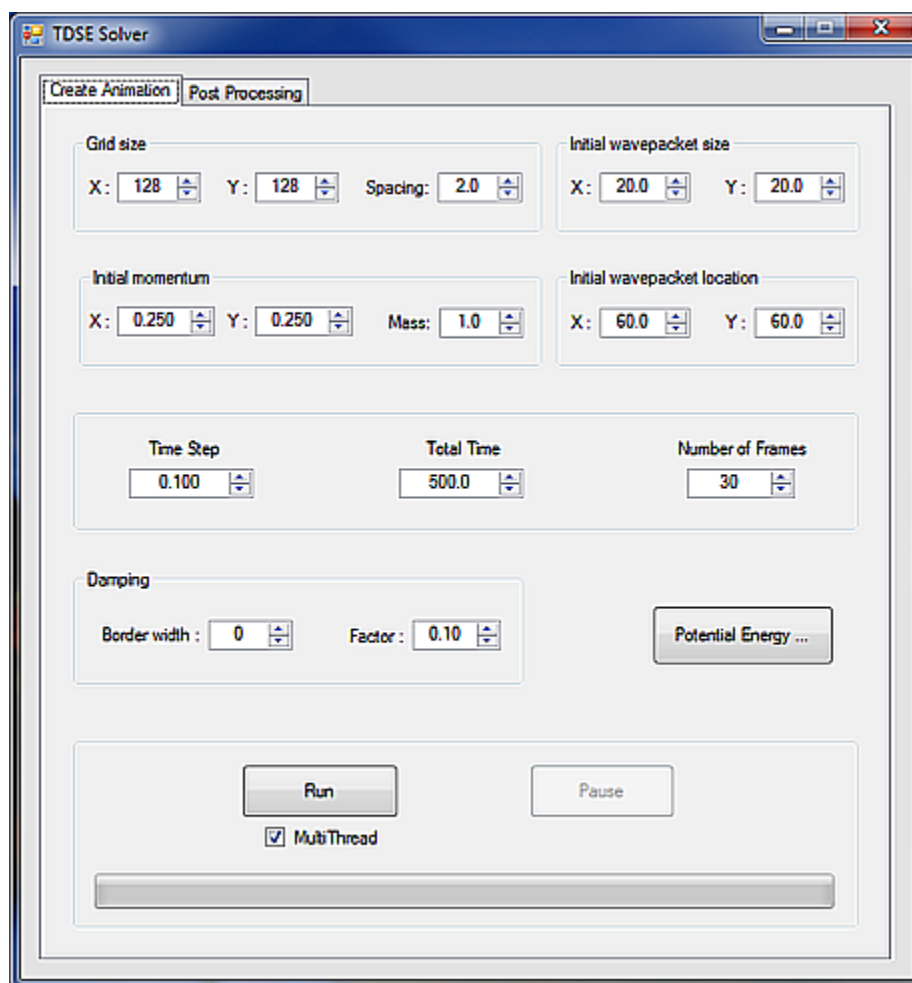


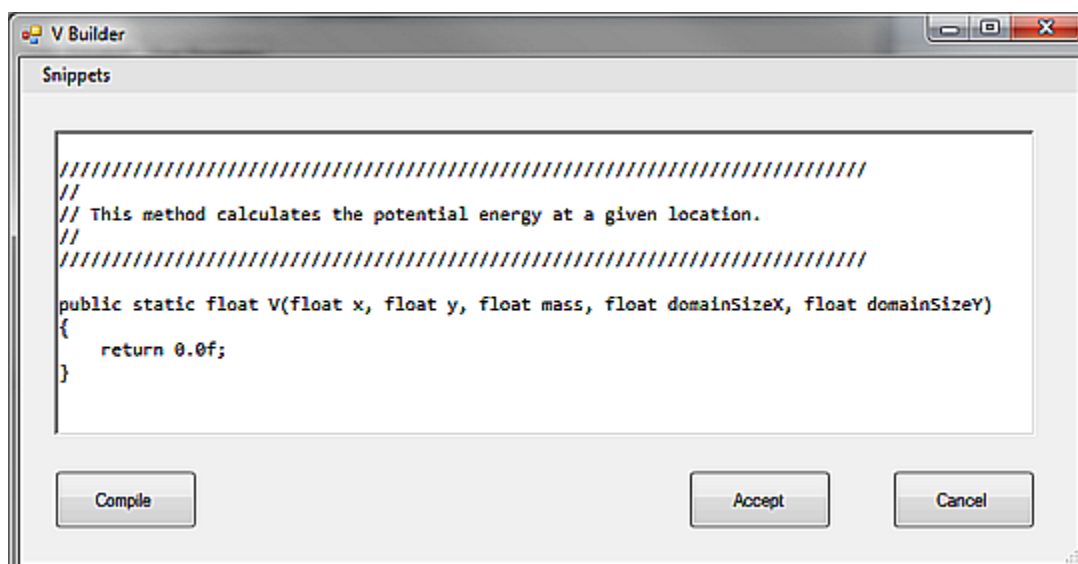
User Guide for TDSE Solver

Here is a brief example of a typical session:

1. Run the 2-dimensional, 1-particle solver (TdseSolver_2D1P.exe). The main window will be shown:

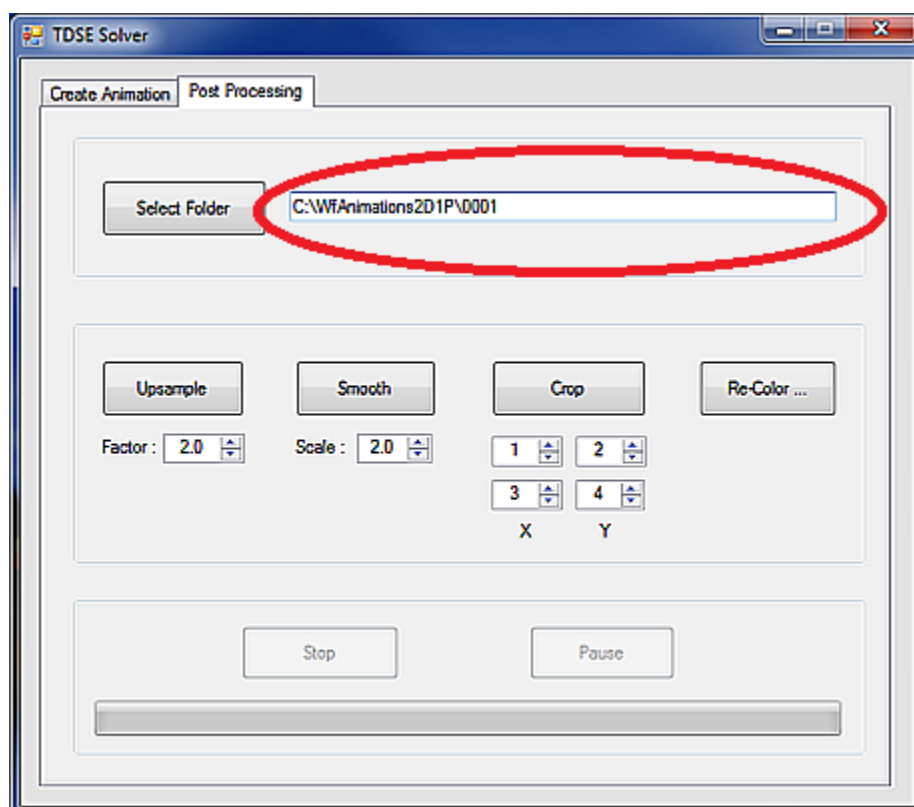


2. Click on the **Potential Energy** button. This brings up an editor window where you can type in code to compute the potential energy as a function of the spatial coordinates x and y:

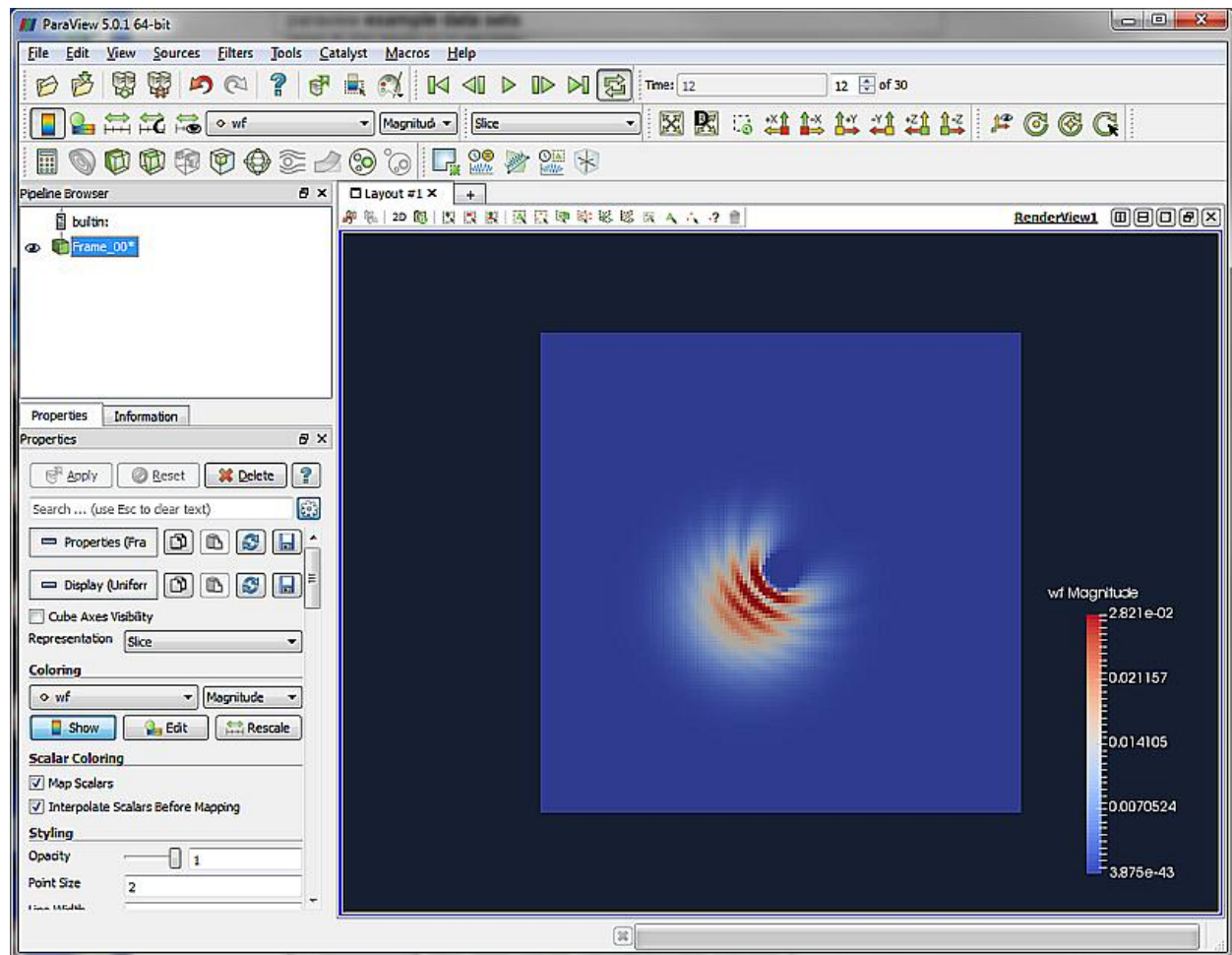


A quick way to get started is to choose one of the pre-defined potentials from the **Snippets** menu, for example the “Cylinder” snippet. Click the **Accept** button when done.

Adjust the other parameters as desired. Then click the **Run** button on the main form. The progress bar will increment and after a few seconds the UI will be re-enabled. At this point the frames of the wavefunction animation have been computed and saved to disk as .vtk files. Their location will be shown on the **Post Processing** tab:



You can now load these files into [ParaView](#) and render them any way you like. (Please see the ParaView documentation for more details.)



You can also return to the **Post Processing** tab on the TDSE Solver app, and perform any of the following operations on the “raw” output files:

- Upsample: Increases the number of grid points in the numerical wave functions by performing bi-cubic interpolation on the existing points.
- Smooth: Applies a smoothing filter to the wavefunctions.
- Crop: Crops the borders of the wavefunction grid. (This seems to be the best way to eliminate reflected waves from an animation: Perform the calculation on a grid that is larger than you need, then crop the borders where the unwanted reflections are visible. It is computationally expensive, but seems to work better than damping or imposing absorbing boundary conditions.)
- Re-color: Allows custom coloring of the animations by letting you specify an arbitrary mapping from complex wave function values to RGB color values.