

TIME-STEPPING FOR THE SCHROEDINGER EQUATION  
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We'll assume all the constants in the Schroedinger equation are one, so the differential equation is

$$i \frac{\partial \Psi(x, t)}{\partial t} = -\Delta \Psi(x, t) + V(x, t).$$

We write  $\Psi(x, t) = \psi(x, t) + i\phi(x, t)$  and  $V(x, t) = v(x, t) + iw(x, t)$ , with  $\Delta$  the Laplacian operator.

Let's think of

$$\Psi(x, t) = \begin{pmatrix} \psi(x, t) \\ \phi(x, t) \end{pmatrix} \quad \text{and} \quad V(x, t) = \begin{pmatrix} v(x, t) \\ w(x, t) \end{pmatrix}$$

as vectors. Then multiplying by  $i$  in the original formulation is the same as multiplying by the matrix

$$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

in vector form, so we write

$$\frac{\partial}{\partial t} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \Psi(x, t) = \begin{pmatrix} -\Delta & 0 \\ 0 & -\Delta \end{pmatrix} \Psi(x, t) + V(x, t).$$

Let's consider backward differences for now. Let  $t^k = k\Delta t$  for some  $\Delta t > 0$ , then we have

$$\frac{1}{\Delta t} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} [\Psi(x, t^k) - \Psi(x, t^{k-1})] = \begin{pmatrix} -\Delta & 0 \\ 0 & -\Delta \end{pmatrix} \Psi(x, t^k) + V(x, t^k).$$

Multiplying by  $\Delta t$  and collecting all the  $\Psi(x, t^k)$  terms together gives

$$\begin{pmatrix} \Delta t \Delta & -1 \\ 1 & \Delta t \Delta \end{pmatrix} \Psi(x, t^k) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \Psi(x, t^{k-1}) + \Delta t V(x, t^k).$$

Formally, the inverse of the first matrix is

$$(1 + \Delta t^2 \Delta^2)^{-1} \begin{pmatrix} \Delta t \Delta & 1 \\ -1 & \Delta t \Delta \end{pmatrix}$$

So

$$\Psi(x, t^k) = (1 + \Delta t^2 \Delta^2)^{-1} \begin{pmatrix} \Delta t \Delta & 1 \\ -1 & \Delta t \Delta \end{pmatrix} \left[ \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \Psi(x, t^{k-1}) + \Delta t V(x, t^k) \right].$$

Whew!

For a totally discrete problem we replace  $\Psi$  and  $V$  with their finite element approximations and  $\Delta$  with  $\Delta_h$ , the discrete Laplacian associated with this space. Then the only thing that's not immediate is how to solve

$$(1) \quad (I + \Delta t^2 \Delta_h^2)X = Y,$$

where  $X$  and  $Y$  are two-vectors whose components are elements of the finite element space.

But this is straightforward with multigrid.  $(I + \Delta t^2 \Delta_h^2)$  is a positive definite operator, whose condition number is the square of the condition number of the backward difference matrix to be solved for the parabolic problem,  $(I - \Delta t \Delta_h)$ .

If you look at the analysis of the multigrid algorithm, the solution of (1) will take only about twice as many iterations as the solution of

$$(2) \quad (I - \Delta t \Delta_h)X = Y,$$

and each iteration requires two multiplications by  $\Delta_h$  instead of one.

If one takes  $\Delta t \approx h^2$ , then the bound for the conjugate gradient method suggests that conjugate gradient will take roughly the same number of iterations to solve (1) as it takes to solve (2). If, however, we have  $\Delta t \approx h$ , then conjugate gradient applied to (1) will take the *square* of the number of iterations that are needed to solve (2). So that's not feasible.

A similar analysis can be made for the Crank–Nicolson method. Here we have

$$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \frac{[\Psi(x, t^k) - \Psi(x, t^{k-1})]}{\Delta t} = \begin{pmatrix} -\Delta & 0 \\ 0 & -\Delta \end{pmatrix} \frac{[\Psi(x, t^k) + \Psi(x, t^{k-1})]}{2} + V(x, t^{k+1/2}).$$

Multiplying by  $\Delta t$  and collecting all the  $\Psi(x, t^k)$  terms together gives

$$\begin{pmatrix} \frac{\Delta t}{2} \Delta & -1 \\ 1 & \frac{\Delta t}{2} \Delta \end{pmatrix} \Psi(x, t^k) = \begin{pmatrix} -\frac{\Delta t}{2} \Delta & -1 \\ 1 & -\frac{\Delta t}{2} \Delta \end{pmatrix} \Psi(x, t^{k-1}) + \Delta t V(x, t^{k+1/2}).$$

Formally, the inverse of the first matrix is

$$\left(1 + \frac{\Delta t^2}{4} \Delta^2\right)^{-1} \begin{pmatrix} \frac{\Delta t}{2} \Delta & 1 \\ -1 & \frac{\Delta t}{2} \Delta \end{pmatrix}$$

So

$$\Psi(x, t^k) = \left(1 + \frac{\Delta t^2}{4} \Delta^2\right)^{-1} \begin{pmatrix} \frac{\Delta t}{2} \Delta & 1 \\ -1 & \frac{\Delta t}{2} \Delta \end{pmatrix} \left[ \begin{pmatrix} -\frac{\Delta t}{2} \Delta & -1 \\ 1 & -\frac{\Delta t}{2} \Delta \end{pmatrix} \Psi(x, t^{k-1}) + \Delta t V(x, t^{k+1/2}) \right],$$

which is discretized in space in the same way as for backward differences. And we really want to take  $\Delta t \approx h$  for Crank–Nicolson, and hence we should really use multigrid.