Computational Physics

Partial Differential Equations: Time-dependent Schrödinger Equation

Lectures based on course notes by Pablo Laguna and Kostas Kokkotas

revamped by Deirdre Shoemaker

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1-dim Schrödinger Equation

Consider the Schrödinger equation describing the evolution of a quantum state Ψ:

$$i\,\hbar\frac{\partial\Psi}{\partial t} = H\,\Psi \quad \text{where} \quad H = -\frac{\hbar^2}{2\,m}\nabla^2 + V(\vec{x})$$

The wave function Ψ must satisfy the unitary condition

$$\int_{-\infty}^{+\infty} |\Psi|^2 d^3\vec{x} = 1$$

and boundary conditions

$$\Psi(\vec{x} \to \infty, t) = 0$$

For simplicity, we will consider the 1-dim case, where

$$H = -\frac{\hbar^2}{2\,m}\frac{\partial^2}{\partial x^2} + V(x)$$

we will also set $\hbar = 1$ and $m = 1/2$

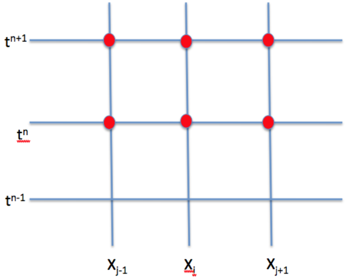
What type of discretization is

$$\Psi^{n+1} = \left(I + \frac{1}{2} i \Delta t H\right)^{-1} \left(I - \frac{1}{2} i \Delta t H\right) \Psi^n$$

Re-write is as

$$i \left[\frac{\Psi_j^{n+1} - \Psi_j^n}{\Delta t}\right] = H \left[\frac{\Psi_j^{n+1} + \Psi_j^n}{2}\right]$$

Crank-Nicolson



Iterative Crank-Nicolson

Recall that the approximation to $\partial_t \Psi = \rho[\Psi]$

$$\frac{\Psi^{n+1} - \Psi^n}{\Delta t} = \rho \left[\frac{\Psi^{n+1} - \Psi^n}{2} \right]$$

will require a matrix inversion because of Ψ^{n+1} in the r.h.s. of the equation. Is there a way to avoid this?

Yes, we will obtain Ψ^{n+1} from a series of intermediate steps similar to the Runge-Kuta method.

Let's make this simpler for a moment

$$\partial_t u = \partial_x u$$

explicit $\dfrac{u_j^{n+1} - u_j^n}{\Delta t} = \dfrac{u_{j+1}^n - u_{j-1}^n}{2\Delta x}$ unstable

$$\xi = 1 + i\alpha \sin k\Delta x$$

$|\xi|^2 > 1$ for all α

implicit $\dfrac{u_j^{n+1} - u_j^n}{\Delta t} = \dfrac{u_{j+1}^{n+1} - u_{j-1}^{n+1}}{2\Delta x}$

$\xi = \dfrac{1}{1 + i\alpha \sin k\Delta x}$ stable

$|\xi|^2 > 1$ all α

crank-nicholson : average both

$$\xi = \frac{1 + \frac{1}{2} i\alpha \sin k\Delta x}{1 - \frac{1}{2} i\alpha \sin k\Delta x}$$

$|\xi|^2 = 1$ marginally stable

iterative CN

calculate an intermediate variable ${}^{(1)}\tilde{u}$
using EXPLICIT scheme

#1 — $$\frac{{}^{(1)}\tilde{u}_j^{n+1} - u_j^n}{\Delta t} = \frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x}$$

— now form a new variable ${}^{(1)}\bar{u}$ by averaging in time

$$ {}^{(1)}\bar{u}_j^{n+1/2} = \frac{1}{2}\left({}^{(1)}\tilde{u}_j^{n+1} + u_j^n \right)$$

— complete timestep using explicit again

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{{}^{(1)}\bar{u}_{j+1}^{n+1/2} - {}^{(1)}\bar{u}_{j-1}^{n+1/2}}{2\Delta x}$$

#2 — $$\frac{{}^{(2)}\tilde{u}_j^{n+1} - u_j^n}{\Delta t} = \frac{{}^{(1)}\bar{u}_{j+1}^{n+\frac{1}{2}} - {}^{(1)}\bar{u}_{j-1}^{n+1/2}}{2\Delta x}$$

— $$ {}^{(2)}\bar{u}_j^{n+1/2} = \frac{1}{2}\left({}^{(2)}\tilde{u}_j^{n+1} + u_j^n \right)$$

— $$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{{}^{(2)}\bar{u}_{j+1}^{n+1/2} - {}^{(2)}\bar{u}_{j-1}^{n+1/2}}{2\Delta x}$$

... as many iterations as needed

Stability?

Back to our toy $\partial_t u = \partial_x u$

define $\beta = \frac{\alpha}{2} \sin k\Delta x$

(0) $\xi = 1 + 2i\beta$

(1) $\xi = 1 + 2i\beta - 2\beta^2$

unstable

(2) $\xi = 1 + 2i\beta - 2\beta^2 - 2i\beta^3$

(3) $\xi = 1 + 2i\beta - 2\beta^2 - 2i\beta^3 + 2\beta^4$

stable $\beta^2 \leq 1$

. . .

unstable

stable . . .

gr-qc/9909026 Teukolsky

iCN of Schrödinger

Schrödinger $\quad i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi$

$V = 0$ "free particle"

iCN uses explicit as 1st guess & then iterates corrections

$$\frac{\partial \psi}{\partial t} = \rho \frac{\partial^2}{\partial x^2} \psi$$

iterative CN

calculate an intermediate variable ${}^{(1)}\tilde{\psi}$
using EXPICIT scheme

#1 — $$\frac{{}^{(1)}\tilde{\psi}^{n+1}_j - \psi^n_j}{\Delta t} = \rho \frac{\psi^n_{j+1} + \psi^n_{j-1} - 2\psi^n_j}{\Delta x^2}$$

— now form a new variable ${}^{(1)}\bar{u}$ by averaging in time

$$ {}^{(1)}\bar{\psi}^{n+1/2}_j = \frac{1}{2}\left({}^{(1)}\tilde{\psi}^{n+1}_j + \psi^n_j\right)$$

— complete timestep using explicit again

$$\frac{\psi^{n+1}_j - \psi^n_j}{\Delta t} = \rho \frac{{}^{(1)}\bar{\psi}^{n+1/2}_{j+1} + {}^{(1)}\bar{\psi}^{n+1/2}_{j-1} - 2\,{}^{(1)}\bar{\psi}^{n+1/2}_j}{\Delta x^2}$$

#2 — $\dfrac{{}^{(2)}\tilde{\psi}_j^{n+1} - \psi_j^n}{\Delta t} = \rho \dfrac{{}^{(1)}\bar{\psi}_{j+1}^{n+\frac{1}{2}} + {}^{(1)}\bar{\psi}_{j-1}^{n+1/2} - 2\,{}^{(1)}\bar{\psi}_j^{n+1/2}}{\Delta x^2}$

— ${}^{(2)}\bar{\psi}_j^{n+1/2} = \frac{1}{2}\left({}^{(2)}\tilde{\psi}_j^{n+1} + \psi_j^n\right)$

— $\dfrac{\psi_j^{n+1} - \psi_j^n}{\Delta t} = \rho \dfrac{{}^{(2)}\bar{\psi}_{j+1}^{n+1/2} + {}^{(2)}\bar{\psi}_{j-1}^{n+1/2} - 2\,{}^{(2)}\bar{\psi}_j^{n+1/2}}{\Delta x^2}$

... as many iterations as needed

Psuedo Code

Same setup as CN except no dCN matrix

. . .

LOOP OVER TIME

LOOP OVER iCN iteration

compute new ${}^{(iter)}\bar{\psi}_j^{n+1}$ using explicit

compute average ${}^{(iter)}\bar{\psi}_j^{n+1/2}$

compute right hand side using ${}^{(iter)}\bar{\psi}_j^{n+1}$

Calculate ψ_j^{n+1} using right-hand side

repeat

END

PLOT

END

ham here is equivalent to H and holds both $\frac{\partial^2}{\partial x^2}$ and several constants

```
%* Loop over desired number of steps (wave circles system once)

for iter=1:max_iter

 %* Current becomes old
  psi_o = psi;

  %* ICN loop
  for icn_step = 0:2

      %* take an Euler/explicit step
      rhs_psi = -i_imag*ham*psi;
      psi = psi_o + tau*rhs_psi;

      %* Calculate average
      psi_h = 0.5*(psi + psi_o);

      %* calculate RHS of equation
      rhs_psi = -i_imag*ham*psi_h;

      %* Take a step
      psi = psi + tau*rhs_psi;

      %* End ICN loop
  end


  %* Periodically record values for plotting
  if( rem(iter,plot_iter) < 1 )
    iplot = iplot+1;
    p_plot(:,iplot) = psi.*conj(psi);
    plot(x,p_plot(:,iplot));     % Display snap-shot of P(x)
    xlabel('x'); ylabel('P(x,t)');
    title(sprintf('Finished %g of %g iterations',iter,max_iter));
    axis(axisV); drawnow;
  end

end
```

Euler step

average

update

psi is an array of $x, 1^{Nx}$

and h is a matrix $Nx \times Nx$