

# Mat1062: Introductory Numerical Methods for PDE

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April 7, 2009

## 1 Ownership

These notes are the joint property of Rob Almgren and Mary Pugh.

## 2 Nonlinear Schrödinger Equation

This is a classic nonlinear wave equation. It arises physically in a variety of contexts, ranging from nonlinear optics (if the index of refraction depends on light intensity) to dynamics of superfluid helium. It illustrates a lot of interesting behavior,<sup>1</sup> and is a stellar example of spectral methods.

Loosely speaking, the equation comes in two varieties: *defocusing* (or with a *repulsive* potential) and *focusing* (or with an *attractive* potential). The difference between the two cases is just a change of sign, but the behavior of the resulting solutions is very different. We start with the defocusing case.

**Defocusing** The PDE for the complex function  $u(x, t)$  is

$$i u_t = u_{xx} - |u|^2 u \quad \text{or} \quad u_t = -i u_{xx} + i |u|^2 u. \quad (1)$$

In higher dimensions, the equation is the same except the second derivative is replaced by the Laplacian. We'll consider the equation on  $[0, L]$  in one dimension or  $[0, L]^d$  in  $d$  dimensions and will assume periodic boundary

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<sup>1</sup>See Catherine Sulem and Pierre-Louis Sulem, *The Nonlinear Schrödinger Equation: Self-Focusing and Wave Collapse*, Applied Mathematical Sciences Vol. 139, Springer 1999.

conditions. The nonlinearity in (1) is called the *cubic nonlinearity*; another popular choice is  $|u|^{2\sigma}u$  with  $\sigma = 1, 2, \dots$

As always, one way to understand this equation is to look at conserved quantities, two of which are of special importance. The *particle number* is

$$N(t) = \int |u(x, t)|^2 dx$$

(you may normalize it however you like). If the domain were unbounded (no periodicity), then we would impose decay conditions at  $\pm\infty$  so this integral would be finite. To calculate the derivative, we recall that  $|u|^2 = u\bar{u}$ , so

$$\begin{aligned} \frac{dN}{dt} &= \int (u\bar{u}_t + u_t\bar{u}) dx \\ &= \int_0^L \left( u(i\bar{u}_{xx} - i|u|^2\bar{u}) + \bar{u}(-iu_{xx} + i|u|^2u) \right) dx \\ &= \int_0^L \left( i(-u_x\bar{u}_x + u_x\bar{u}_x) + i|u|^2(-u\bar{u} + \bar{u}u) \right) dx \\ &= 0, \end{aligned}$$

where we have integrated by parts once on the derivative terms and used the periodic boundary conditions (or the decay at  $\pm\infty$ ). Thus  $N(t)$  is a constant of the motion.

The other conserved quantity is the energy, or *Hamiltonian*

$$H(t) = \int \left( |\nabla u|^2 + \frac{1}{2}|u|^4 \right) dx$$

(for general  $\sigma$  the second term is  $|u|^{2\sigma+2}/(\sigma+1)$ ). Similar calculations as above show that  $H(t)$  is conserved.

For the 1-D NLS with cubic nonlinearity, there is in fact an infinite family of conserved quantities, which leads to the study of “integrable systems.” In general, though (multi-dimensions or  $\sigma > 1$ ), these are the only two and so we will focus on them.

Existence of the conserved energy  $H$  is of immense importance for understanding the behavior of solutions. Since it is the sum of two positive terms, neither of them can become larger than the initial value of  $H$ . A simple argument then shows that  $u$  must be continuous and bounded and the solution remains well-behaved for all time.

**Focusing** The *focusing* or *attractive* form of the equation is

$$i u_t = u_{xx} + |u|^2 u \quad \text{or} \quad u_t = -i u_{xx} - i |u|^2 u, \quad (2)$$

in which only the sign of the nonlinear term (relative to the derivative) has been changed. The particle number  $N$  is conserved as before. But now the conserved Hamiltonian is

$$H(t) = \int \left( |\nabla u|^2 - \frac{1}{2} |u|^4 \right) dx.$$

Now the conserved energy is the *difference* of two positive terms. Nothing prevents both of them from becoming infinite together: the solution can and does develop very interesting singularities.

## 2.1 Splitting

A standard way to handle equations like NLS, in which  $u_t$  is the sum of two terms, is to look at the PDEs in which only one term appears at a time. Here the structure is particularly simple, because each one is a type of rotation, one in physical and one in Fourier space.

**Rotation in Fourier space** First, let us consider the linear wave equation

$$i u_t = u_{xx}.$$

Since this is a linear equation with constant coefficients, its solutions are described by looking at individual Fourier modes. With  $u(x, t) = U(t) \exp(i\xi x)$ , we immediately see that  $iU'(t) = -\xi^2 U(t)$ , so we can write the solution as

$$u(x, t) = U_0 e^{i\xi^2 t} e^{i\xi x} = U_0 e^{i\xi(x+\xi t)}.$$

Of course, in a periodic box of length  $L$ ,  $\xi$  is restricted to the discrete values  $2\pi\ell/L$  for  $\ell$  an integer.

The phase speed  $c = -\xi$  of the mode depends on  $\xi$ . Thus this wave equation is *dispersive*: different wavelengths propagate at different speeds. This is in contrast to hyperbolic systems like  $u_{tt} = c^2 u_{xx}$ , in which each different wavelength propagates at the *same* speed  $c$  (except for errors introduced by the discretization). For a dispersive system any initial “shape” inevitably breaks up into a combination of many waves.

To compute this solution via the Fourier representation we take

$$u(x, 0) = \sum_{\ell} \hat{u}_{\ell}(0) e^{i2\pi\ell x/L},$$

(whether the sum is finite or not), then the solution at later times is

$$u(x, t) = \sum_{\ell} \hat{u}_{\ell}(t) e^{i2\pi\ell x/L}, \quad \hat{u}_{\ell}(t) = e^{i(2\pi\ell/L)^2 t} \hat{u}_{\ell}(0).$$

Each mode just sits there and spins independently of all the others. Note that the rotation rate increases quadratically with  $\ell$ . On a discrete grid of size  $n$ , the highest mode is  $n/2$ , so the fastest rotation rate is  $(\pi n/L)^2$ . The rotation period of the  $\ell$ th mode is  $T_{\ell} = 2\pi/(2\pi\ell/L)^2 = L^2/2\pi\ell^2$ , so the shortest period is  $T_{n/2} = 2L^2/\pi n^2$ .

If you wanted to do an explicit method, without using the special rotation structure, then you would need to take the time step  $\tau$  smaller than this intrinsic time. It is just as for the diffusion equation, where we needed to resolve the decay time of the highest modes.

**Rotation in physical space** The other half of the problem is

$$i u_t = -|u|^2 u.$$

Since this equation has no space derivatives, it is just an ODE at each point, and the solution is immediately seen to be

$$u(x, t) = e^{i|u|^2 t} u(x, 0).$$

Again, this is just a rotation, that keeps constant the value of  $|u(x, t)|^2$ . Each separate spatial point just sits and spins independently.

## 2.2 Pseudo-spectral algorithm

Now we can put all this together into a numerical algorithm. The idea is that we do each effect in alternation (use a “Splitting Method”). But since one is easiest to do in physical space, the other in Fourier, we have to keep transforming back and forth. That is why it is called “pseudo-spectral:” a fully spectral algorithm would do all operations in Fourier space, but that works for very few problems since almost everything has nonlinearity.

Such algorithms only became possible with the invention of the fast Fourier transform.

Here is the outline of how to get to from time level  $n$  to time level  $n + 1$  with time step  $k$ . Start with a list  $(u_0^n, \dots, u_{N-1}^n)$  representing the solution at time level  $n$ . Here,  $N$  is the number of intervals in space.

1. *Forward transform.* Do an FFT on  $u^n$  to compute the Fourier coefficients  $\hat{u}_\ell^n$ .
2. *Fourier rotation.* Spin each mode as follows:

$$\hat{u}_\ell^* = \exp(i\xi_\ell^2 k/2) \hat{u}_\ell^n, \quad \xi_\ell = \frac{2\pi}{L} \min\{\ell, N - \ell\}$$

(it should be  $\ell - N$  rather than  $N - \ell$ , but we square it anyway).

3. *Backward transform.* Do an inverse FFT on  $\hat{u}^*$  to compute the elements  $u_j^*$  in the physical-space representation.
4. *Physical rotation.* Rotate each grid point in place:

$$u_j^{n+1} = \exp(i|u_j^*|^2 k/2) u_j^*$$