Laurette TUCKERMAN
laurette@pmmh.espci.fr

Numerical Methods for
Differential Equations in Physics

Dispersion Relations

Linear time-dependent scalar PDE with constant coefficients on unbounded space domain admits plane wave solutions:

$$u(x,t) = e^{i(kx+\omega t)}$$

PDE $\Longrightarrow$ dispersion relation:

$$\omega = \omega(k)$$

General solution to such a PDE which is first-order in time:

$$u(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i(kx+\omega(k)t)}\hat{u}_0(k)dk$$

where

$$u(x,0) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx}\hat{u}_0(k)dk$$

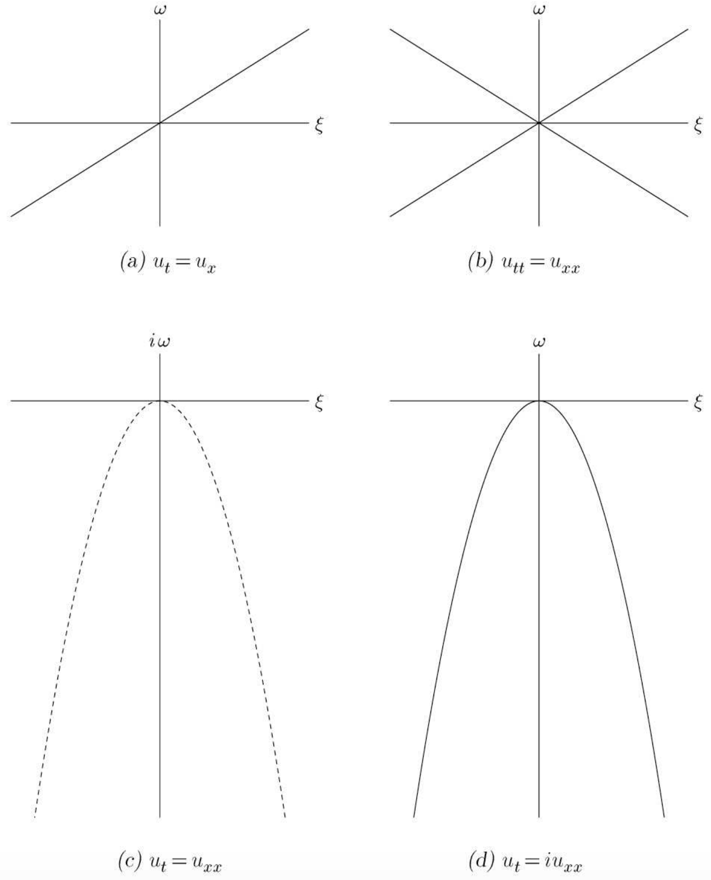
1st-order wave equation

$\omega = k$

2nd-order wave equation

$\omega^2 = k^2$

$\omega = \pm k$



Heat equation

$i\omega = -k^2$

$\sigma = -k^2$

Schrödinger equation

$\omega = -k^2$

Discretize space:

First-order wave equation

$$\begin{aligned} u_t &= u_x \approx \frac{1}{2\Delta x}\left(u(x+\Delta x) - u(x-\Delta x)\right) \\ i\omega e^{i(kx+\omega t)} &= e^{i(kx+\omega t)}\frac{1}{2\Delta x}\left(e^{ik\Delta x} - e^{-ik\Delta x}\right) \\ i\omega &= \frac{1}{2\Delta x} 2i\sin(k\Delta x) \\ \omega &= \frac{1}{\Delta x}\sin(k\Delta x) \to k \;\; \text{for} \;\; \Delta x \to 0 \end{aligned}$$

Second-order wave equation

$$\begin{aligned} u_{tt} &= u_{xx} \approx \frac{1}{\Delta x^2}\left(u(x+\Delta x) - 2u(x) + u(x-\Delta k)\right) \\ -\omega^2 e^{i(kx+\omega t)} &= e^{i(kx+\omega t)}\frac{1}{\Delta x^2}\left(e^{ik\Delta x} - 2 + e^{-ik\Delta x}\right) \\ -\omega^2 &= \frac{1}{\Delta x^2}\left(e^{ik\Delta x/2} - e^{-ik\Delta x/2}\right)^2 \\ -\omega^2 &= \frac{1}{\Delta x^2}\left(2i\sin\left(\frac{k\Delta x}{2}\right)\right)^2 \\ \omega^2 &= \left(\frac{2}{\Delta x}(\sin\left(\frac{k\Delta x}{2}\right)\right)^2 \to k^2 \;\; \text{for} \;\; \Delta x \to 0 \\ \omega &= \pm\frac{2}{\Delta x}(\sin\left(\frac{k\Delta x}{2}\right) \to \pm k \;\; \text{for} \;\; \Delta x \to 0 \end{aligned}$$

Heat equation

$$u_t = u_{xx} \approx \frac{1}{\Delta x^2}\left(u(x+\Delta x) - 2u(x) + u(x-\Delta x)\right)$$

$$i\omega = -\left(\frac{2}{\Delta x}\sin\left(\frac{k\Delta x}{2}\right)\right)^2 \to -k^2 \;\text{ for }\; \Delta x \to 0$$

Schrödinger Equation

$$u_t = i\, u_{xx} \approx \frac{1}{\Delta x^2}\left(u(x+\Delta x) - 2u(x) + u(x-\Delta x)\right)$$

$$i\omega = -i\left(\frac{2}{\Delta x}\sin\left(\frac{k\Delta x}{2}\right)\right)^2$$

$$\omega = -\left(\frac{2}{\Delta x}\sin\left(\frac{k\Delta x}{2}\right)\right)^2 \to -k^2 \;\text{ for }\; \Delta x \to 0$$

The spatially-discretized and exact dispersion relations agree if

$$k\Delta x \ll 2\pi \iff \Delta x \ll 2\pi/k = \lambda$$

Many gridpoints per wavelength

1st-order wave equation

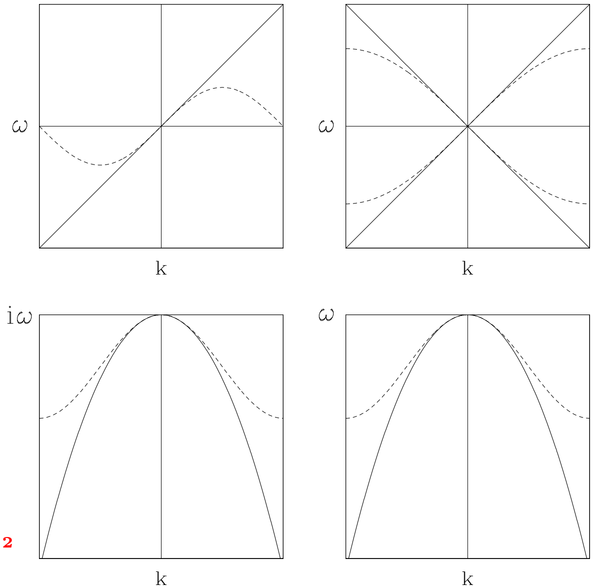
$$\omega_{\text{exact}} = k$$

$$\omega_{\text{num}} = \frac{1}{\Delta x}\sin(k\Delta x)$$

2nd-order wave equation

$$\omega_{\text{exact}} = \pm k$$

$$\omega_{\text{num}} = \pm\frac{2}{\Delta x}(\sin\left(\frac{k\Delta x}{2}\right)$$



Heat equation

$$i\omega_{\text{exact}} = -k^2$$

$$i\omega_{\text{num}} = -\left(\frac{2}{\Delta x}\sin\left(\frac{k\Delta x}{2}\right)\right)^2$$

Schrödinger equation

$$\omega_{\text{exact}} = -k^2$$

$$\omega_{\text{num}} = -\left(\frac{2}{\Delta x}\sin\left(\frac{k\Delta x}{2}\right)\right)^2$$

Discretize space and time (leapfrog scheme)

$$
\begin{aligned}
u_t &= u_x \\
u(x, t+\Delta t) &= u(x, t-\Delta t) + \tfrac{\Delta t}{\Delta x}\left(u(x+\Delta x, t) - u(x-\Delta x, t)\right) \\
e^{i(kx+\omega(t+\Delta t))} &= e^{i(kx+\omega(t-\Delta t))} + \tfrac{\Delta t}{\Delta x}\left(e^{i(k(x+\Delta x)+\omega t)} - e^{i(k(x-\Delta x)+\omega t)}\right) \\
e^{i\omega\Delta t} &= e^{-i\omega\Delta t} + \tfrac{\Delta t}{\Delta x}\left(e^{ik\Delta x} - e^{-ik\Delta x}\right) \\
2i\sin(\omega\Delta t) &= \tfrac{\Delta t}{\Delta x} 2i\sin(k\Delta x) \\
\sin(\omega\Delta t) &= \tfrac{\Delta t}{\Delta x}\sin(k\Delta x)
\end{aligned}
$$

Phase velocity:

$$c(k,\omega) = -\frac{\omega}{k}$$

$$f(x,t) = \exp(i(kx + \omega(k)t)) = \exp\left(ik\left(x + \frac{\omega(k)}{k}t\right)\right)$$

Group velocity: velocity of wavepackets and energy

$$c_g = -\frac{d\omega}{dk}$$

$$f(x,t) = \exp(i(k_1 x + \omega(k_1)t)) + \exp(i(k_2 x + \omega(k_2)t))$$

$$\begin{aligned} f(x,t) &= \exp\left(i\left(\frac{k_1+k_2}{2}x + \frac{\omega(k_1)+\omega(k_2)}{2}t\right)\right) \\ &\times \left[\exp\left(i\left(\frac{k_1-k_2}{2}x + \frac{\omega(k_1)-\omega(k_2)}{2}t\right)\right)\exp\left(-i\left(\frac{k_1-k_2}{2}x + \frac{\omega(k_1)-\omega(k_2)}{2}t\right)\right)\right] \\ &= \exp\left(i\left(\frac{k_1+k_2}{2}x + \frac{\omega(k_1)+\omega(k_2)}{2}t\right)\right) 2\cos\left(\frac{k_1-k_2}{2}x + \frac{\omega(k_1)-\omega(k_2)}{2}t\right) \\ &= \exp\left(i\left(\bar{k}x + \omega(\bar{k})t\right)\right) 2\cos\left(\frac{\Delta k}{2}\left(x + \frac{\Delta\omega}{\Delta k}t\right)\right) \\ &\to \underbrace{\exp\left(i\left(\bar{k}x + \omega(\bar{k})t\right)\right)}_{\text{carrier wave}} \underbrace{2\cos\left(\frac{\Delta k}{2}(x + c_g t)\right)}_{\text{envelope}} \end{aligned}$$

For first-order wave equation

$$\omega_{\text{exact}} = k \Longrightarrow \frac{\omega}{k} = 1 \text{ and } \frac{d\omega}{dk} = 1$$

Temporal leapfrog, spatial centered differences:

$$\sin(\omega_{\text{num}}\Delta t) = \frac{\Delta t}{\Delta x}\sin(k\Delta x)$$

Numerical group velocity obtained via implicit differentiation: d/dk

$$\begin{aligned}\cos(\omega_{\text{num}}\Delta t)\,\Delta t\,\frac{d\omega_{\text{num}}}{dk} &= \frac{\Delta t}{\Delta x}\,\cos(k\Delta x)\,\Delta x \\ \frac{d\omega_{\text{num}}}{dk} &= \frac{\cos(k\Delta x)}{\cos(\omega_{\text{num}}\Delta t)} \\ &\rightarrow 1 \text{ for } \Delta x, \Delta t \rightarrow 0\end{aligned}$$