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Numerical Methods for Differential Equations in Physics

HYPERBOLIC EQUATIONS

Classification of second order linear PDEs

$$a u_{xx} + b u_{xy} + c_{yy} + d u_x + e u_y + f u = g$$

Depends on coefficients a, b, c. Compare to quadratic functions:

$$a x^2 + b x y + c y^2 + d x + e y = g$$

Elliptic: $b^2 - 4ac < 0$

Examples:	**Poisson**	$(\partial_{xx} + \partial_{yy})\, u = g$
	Laplace	$(\partial_{xx} + \partial_{yy})\, u = 0$
	Helmholtz	$\left(\partial_{xx} + \partial_{yy} - k^2 I\right) u = 0$

The domain is closed and the boundary conditions should be any of:

Dirichlet (D):	$u = \gamma$
Neumann (N):	$\partial u / \partial n = \gamma$
Robin (R):	$\alpha u + \beta \partial u / \partial n = \gamma$
Periodic (P):	$u(0) = u(\ell)$ **and** $\partial u / \partial x(0) = \partial u / \partial x(\ell)$

(with additional specification of u at one point for N or P)

Parabolic: $b^2 - 4ac = 0$

Prototype: Heat equation $\partial_t u = \partial_{xx} u$

Note: $y \to t$ time.

Domain of x may be open or closed. D-N-R-P conditions can be used.

Domain of t must be open in forward time. Initial Dirichlet conditions.

Hyperbolic: $b^2 - 4ac > 0$

Prototype: Wave equation (2D) $\partial_{tt} u = \partial_{xx} u$

Note: $y \to t$ time.

Domain of x may be open or closed. D-N-R-P conditions can be used.

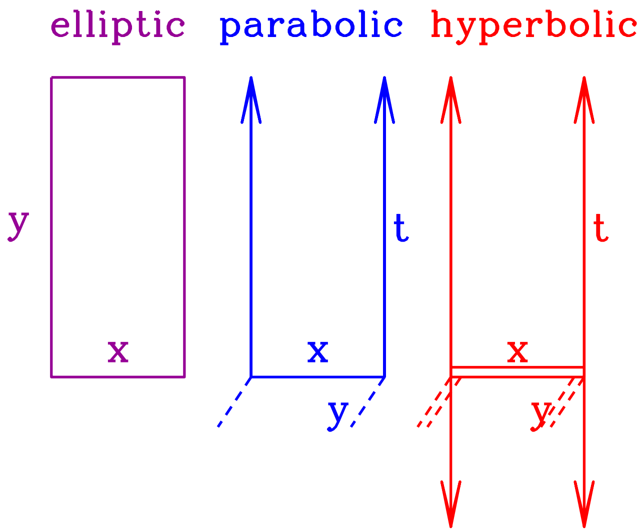
Domain of t must be open in either direction. Initial Cauchy conditions:

Cauchy (C): $u = \gamma$ **and** $\partial u / \partial n = \delta$

Boundary and Initial Conditions

Can generalize to

- **Laplace** $0 = \partial_{xx}u + \partial_{yy}u + \partial_{zz}u$
- **Heat** $\partial_t u = \partial_{xx}u + \partial_{yy}u$
- **Wave** $\partial_{tt} u = \partial_{xx}u + \partial_{yy}u$



Hyperbolic Equations

General definition of hyperbolic equation in one dimension:

$$\partial_t \mathrm{u} = \partial_x \mathrm{f}(\mathrm{u})$$

First order wave equation has $\mathrm{f}(\mathrm{u}) = c\mathrm{u}$.
Can generalize to $\mathrm{x} \in \mathcal{R}^d$, $\mathrm{u} \in \mathcal{R}^s$, $\mathrm{f}^j : \mathcal{R}^s \to \mathcal{R}^s$

$$\partial_t \mathrm{u}(x_1, \ldots x_d) = \sum_{j=1}^{d} \partial_{x_j} \mathrm{f}^j(\mathrm{u}(x_1, \ldots x_d)) = \nabla \cdot \mathrm{f}(\mathrm{u})$$

$d = 1, 2, 3$ is dimensionality of spatial domain. s is number of variables, e.g. (u, v, w) but also temperature, concentration.

Conservation law for scalar u:

$$\int_\Omega d\Omega\, \partial_t u(x, t) = \int_\Omega d\Omega\, \nabla \cdot \mathrm{f}(u)$$

$$\frac{d}{dt} \int_\Omega d\Omega\, u(x, t) = \int_{\partial\Omega} \mathrm{f}(u) \cdot \mathrm{n}$$

i.e. $\mathrm{f}(u)$ is the flux of u and change in quantity of u in domain is only due to flux in or out through boundary $\partial\Omega$ (no source or sink terms in bulk).

Linear constant-coefficient system in one space dimension:

$$\partial_t u = A\partial_x u + Bu + F(x,t)$$

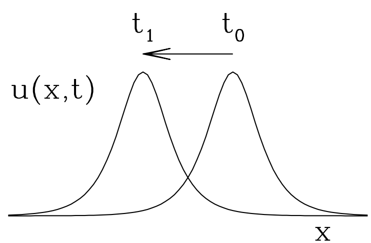
where $\mathrm{x} \in \mathcal{R}$ and u, $F \in \mathcal{R}^s$ and A, B are matrices.
System is hyperbolic if matrix A is diagonalizable with real eigenvalues.

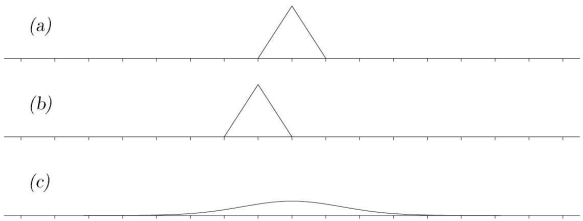
First-order wave equation:

$$\partial_t u = c\partial_x u$$

Analytic solution: traveling wave

$$u(x,t) = u(x+ct, 0)$$





Initial condition

Soln of wave eq: $\partial_t u = \partial_x u$

Soln of heat eq: $\partial_t u = \partial_{xx} u$

Hyperbolic PDE of order n is well-posed initial value problem for first $n-1$ derivatives.

For first order

$$\partial_t u = c\partial_x u$$

must specify $u(x, t = 0)$

For second-order

$$\partial_{tt} u = c^2 \partial_{xx} u$$

must specify initial conditions $u(x, t = 0)$ and $\partial_t u(x, t = 0)$.

Finite difference methods for solving hyperbolic problems

$$\partial_t u = \partial_x u$$

Upwind:

$$u^{\mathrm{UP}}(x, t+\Delta t) = u^{\mathrm{UP}}(x,t) + \frac{\Delta t}{\Delta x}\left(u^{\mathrm{UP}}(x+\Delta x, t) - u^{\mathrm{UP}}(x,t)\right)$$

Leapfrog:

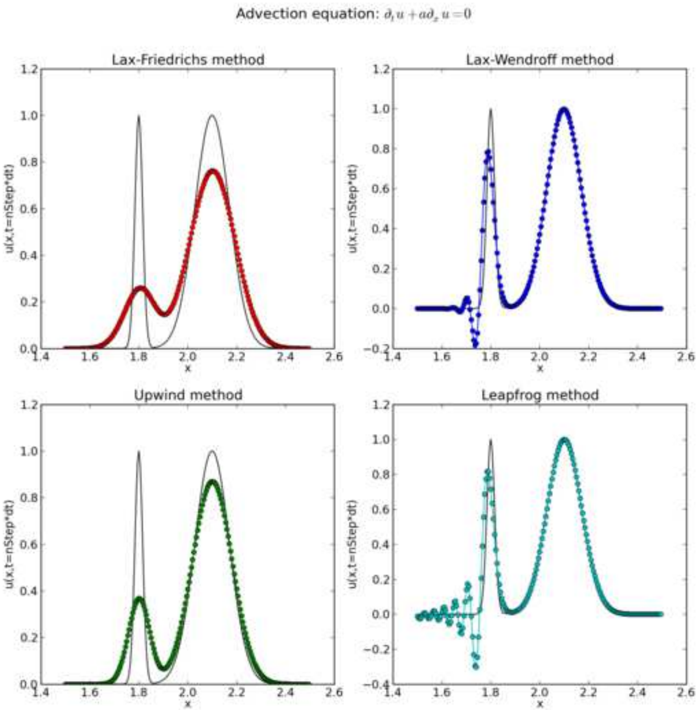
$$u^{\mathrm{LF}}(x, t+\Delta t) = u^{\mathrm{LF}}(x, t-\Delta t) + \frac{\Delta t}{\Delta x}\left(u^{\mathrm{LF}}(x+\Delta x, t) - u^{\mathrm{LF}}(x-\Delta x, t)\right)$$

Lax-Wendroff:

$$\begin{aligned} u^{\mathrm{LW}}(x, t+\Delta t) = u^{\mathrm{LW}}(x,t) &+ \frac{\Delta t}{2\Delta x}\left(u^{\mathrm{LW}}(x+\Delta x, t) - u^{\mathrm{LW}}(x-\Delta x, t)\right) \\ &+ \frac{\Delta t^2}{2\Delta x^2}\left(u^{\mathrm{LW}}(x+\Delta x, t) - 2u^{\mathrm{LW}}(x,t) + u^{\mathrm{LW}}(x-\Delta x, t)\right) \end{aligned}$$

Lax-Friedrichs:

$$\begin{aligned} u^{\mathrm{LF}}(x, t+\Delta t) = &\frac{1}{2}\left(u^{\mathrm{LF}}(x-\Delta x, t) + u^{\mathrm{LF}}(x+\Delta x, t)\right) \\ &+ \frac{\Delta t}{2\Delta x}\left(u^{\mathrm{LF}}(x+\Delta x, t) - u^{\mathrm{LF}}(x-\Delta x, t)\right) \end{aligned}$$



Leapfrog suffers from spurious high-wavenumber oscillations.
Lax-Wendroff damps these oscillations.

Accuracy of Leapfrog Method

$$u^{\mathrm{LF}}(x, t+\Delta t) = u^{\mathrm{LF}}(x, t-\Delta t) + \tfrac{\Delta t}{\Delta x}\left(u^{\mathrm{LF}}(x+\Delta x, t) - u^{\mathrm{LF}}(x-\Delta x, t)\right)$$

$$\begin{aligned}
u(x, t-\Delta t) &= \left(u - \Delta t u_t + \tfrac{1}{2}(\Delta t)^2 u_{tt} - \tfrac{1}{6}(\Delta t)^3 u_{ttt} + \ldots\right)(x,t) \\
\tfrac{\Delta t}{\Delta x} u(x+\Delta x, t) &= \tfrac{\Delta t}{\Delta x}\left(\cancel{u} + \Delta x u_x + \cancel{\tfrac{1}{2}(\Delta x)^2 u_{xx}} + \tfrac{1}{6}(\Delta x)^3 u_{xxx} + \ldots\right)(x,t) \\
-\tfrac{\Delta t}{\Delta x} u(x-\Delta x, t) &= -\tfrac{\Delta t}{\Delta x}\left(\cancel{u} - \Delta x u_x + \cancel{\tfrac{1}{2}(\Delta x)^2 u_{xx}} - \tfrac{1}{6}(\Delta x)^3 u_{xxx} + \ldots\right)(x,t)
\end{aligned}$$

$$\textbf{Sum} = \left(\cancel{u} - \Delta t u_t + 2\Delta t u_x + \cancel{\tfrac{1}{2}(\Delta t)^2 u_{tt}} - \tfrac{1}{6}(\Delta t)^3 u_{ttt} + \tfrac{1}{3}\Delta t(\Delta x)^2 u_{xxx} \ldots\right)$$

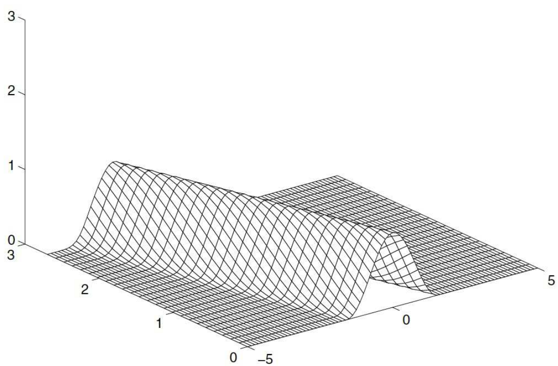
$$u(x, t+\Delta t) = \left(\cancel{u} + \Delta t u_t + \cancel{\tfrac{1}{2}(\Delta t)^2 u_{tt}} + \tfrac{1}{6}(\Delta t)^3 u_{ttt} \ldots\right)(x,t)$$

$$\textbf{Difference} = 2\Delta t\cancel{(u_t - u_x)} + O(\Delta t^3, \Delta t \Delta x^2)$$

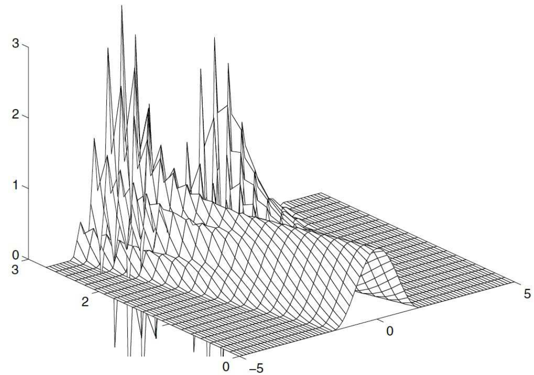
Stability of Leapfrog Method

Leapfrog method used to solve $\partial_t u = U\partial_x u$

with initial condition: $u(x,t=0) = \begin{cases} \cos^2 x & |x| \leq \frac{\pi}{2} \\ 0 & |x| \leq \frac{\pi}{2} \end{cases}$



$$\frac{U\Delta t}{\Delta x} = 0.9$$



$$\frac{U\Delta t}{\Delta x} = 1.1$$

Fourier or von Neumann stability analysis: insert $e^{i\xi x}$

$$u(j\Delta x, n\Delta t) = z^n e^{i\xi x_j} \qquad \lambda \equiv U\Delta t/\Delta x$$

Leapfrog:

$$z^{n+1}e^{i\xi x_j} = z^{n-1}e^{i\xi x_j} + \lambda\left(z^n e^{i\xi x_{j+1}} - z^n e^{i\xi x_{j-1}}\right)$$

$$z = z^{-1} + \lambda\left(e^{i\xi\Delta x} - e^{-i\xi\Delta x}\right)$$

$$z - z^{-1} = 2i\lambda\sin(\xi\Delta x)$$

$$u^{\mathrm{LF}}(x, t+\Delta t) = u^{\mathrm{LF}}(x, t-\Delta t) + \tfrac{\Delta t}{\Delta x}(u^{\mathrm{LF}}(x+\Delta x, t) - u^{\mathrm{LF}}(x-\Delta x, t))$$

Upwind:

$$z^{n+1}e^{i\xi x_j} = z^n e^{i\xi x_j} + \lambda\left(z^n e^{i\xi x_{j+1}} - z^n e^{i\xi x_j}\right)$$

$$z = 1 + \lambda\left(e^{i\xi\Delta x} - 1\right)$$

Lax-Wendroff:

$$z^{n+1}e^{i\xi x_j} = z^{n-1}e^{i\xi x_j} + \tfrac{1}{2}z^n\lambda\left(e^{i\xi x_{j+1}} - e^{i\xi x_{j-1}}\right) + \tfrac{1}{2}\lambda^2 z^n\left(e^{i\xi x_{j+1}} - 2e^{i\xi x_j} + e^{i\xi x_{j-1}}\right)$$

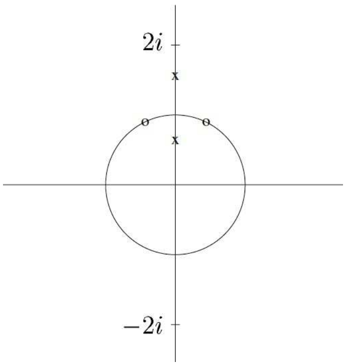
$$z = z^{-1} + \tfrac{1}{2}\lambda\left(e^{i\xi\Delta x} - e^{-i\xi\Delta x}\right) + \tfrac{1}{2}\lambda^2\left(e^{i\xi\Delta x} - 2 + e^{-i\xi\Delta x}\right)$$

$$z = z^{-1} + \lambda i\sin(\xi\Delta x) + \lambda^2(\cosh(\xi\Delta x) - 1)$$

$$z - z^{-1} = 2i\lambda \sin(\xi \Delta x)$$
$$0 = z^2 - 1 - z2i\lambda \sin(\xi \Delta x)$$
$$z = i\lambda \sin(\xi \Delta x) \pm \sqrt{1 - \lambda^2 \sin^2(\xi \Delta x)}$$

$$\lambda < 1 \Longrightarrow 1 - \lambda^2 \sin^2(\xi \Delta x) > 0 \Longrightarrow a = \sqrt{1 - \lambda^2 \sin^2(\xi \Delta x)} \quad \text{real}$$
$$|z|^2 = \lambda^2 \sin^2(\xi \Delta x) + 1 - \lambda^2 \sin^2(\xi \Delta x) = 1$$

$$\lambda > 1 \Longrightarrow 1 - \lambda^2 \sin^2(\xi \Delta x) < 0 \Longrightarrow a = \sqrt{1 - \lambda^2 \sin^2(\xi \Delta x)} \quad \text{imag}$$
$$|z|^2 = (i\lambda \sin(\xi \Delta x) + a)^2 > 1 \text{ for values of } \xi \Delta x \text{ surrounding } \pi/2$$



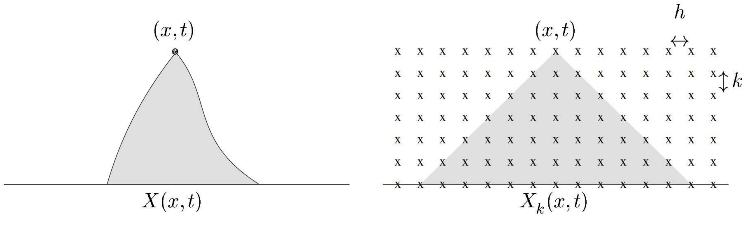
$|z| > 1 \Longrightarrow$ **growth in time**

○ $\lambda = 0.9$

× $\lambda = 1.1$

CFL condition: $|U|\Delta t/\Delta x \leq 1$

Domain of Dependence (Courant, Friedrichs, Lewy = CFL)



continuous system **discretized system**

$X(x,t)$ is the set of all points x where the initial data $u(x,t=0)$ may have some effect on the solution $u(x,t)$.

In parabolic systems such as $u_t = u_{xx}$, information travels infinitely fast. Magnitude of influence of faraway data may decay exponentially with distance but influence will still be present. $X(x,t)$ is the entire real line.

In hyperbolic systems such as $u_t = u_x$ or $u_{tt} = u_{xx}$, perturbations travel at finite speed and so $X(x,t)$ is finite for each x and t. Curves which bound $X(x,t)$ are the characteristic curves.

For convergence of a numerical approximation of a PDE, the continuous domain of dependence must be contained in the limiting numerical domain of dependence as $\Delta t \to 0$.

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

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

Four equations

1st order wave equation:

$$\partial_t u = \partial_x u$$

2nd order wave equation:

$$\partial_{tt} u = \partial_{xx} u$$

Heat equation:

$$\partial_t u = \partial_{xx} u$$

Schrödinger equation:

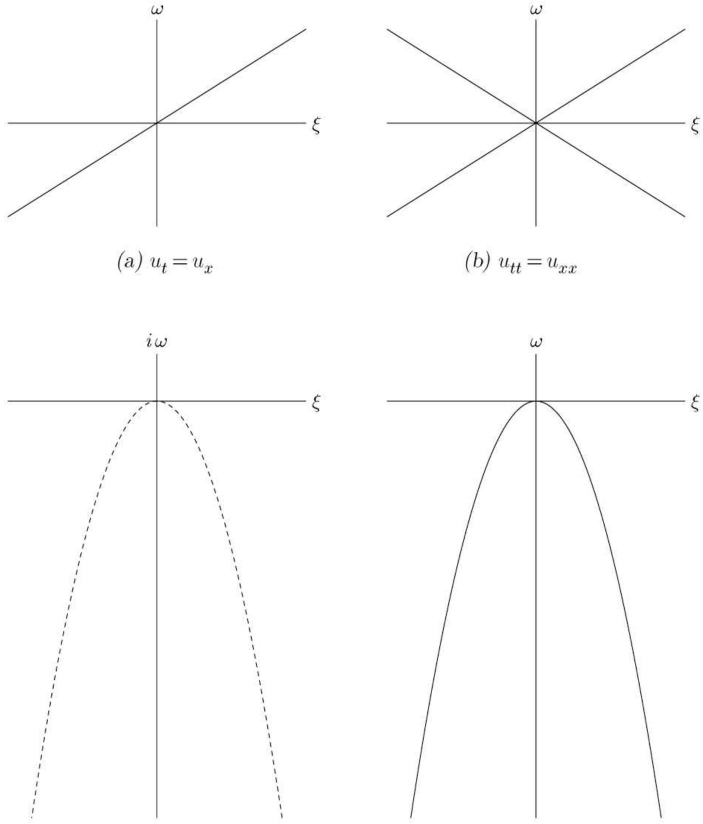
$$\partial_t u = i\partial_{xx} u$$

1st-order wave equation

$$\partial_t u = \partial_x u$$
$$\omega = k$$

2nd-order wave equation

$$\partial u_{tt} = \partial_{xx} u$$
$$\omega^2 = k^2$$
$$\omega = \pm k$$



(a) $u_t = u_x$

(b) $u_{tt} = u_{xx}$

(c) $u_t = u_{xx}$

(d) $u_t = iu_{xx}$

Heat equation

$$\partial_t u = \partial_{xx} u$$
$$i\omega = -k^2$$
$$\sigma = -k^2$$

Schrödinger equation

$$\partial u_{tt} = i\partial_{xx} u$$
$$\omega = -k^2$$

Discretize space via centered first or second order finite differences

First-order wave equation

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

Second-order wave equation

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

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

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

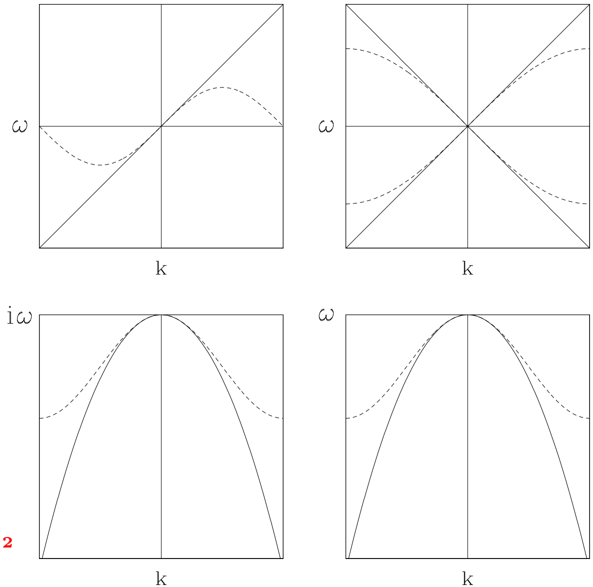
Many gridpoints per wavelength

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)

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

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

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

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

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

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:

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

Numerical group velocity obtained via implicit differentiation: d/dk

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

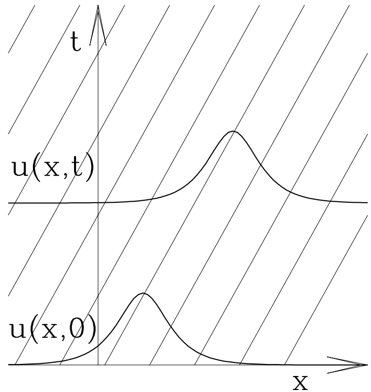
Hyperbolic Equations: Characteristics

First-order wave equation:

$$u_t = c u_x$$

Analytic solution: traveling wave

$$u(x,t) = u(x+ct, 0)$$



The wave equation <u>carries</u> the initial condition through time.

Generalization: $0 = u_t + g(x,t,u) u_x$

$$0 = u_t + \frac{dx}{dt} u_x$$

u **is constant along curve** $x(t)$ **such that** $\frac{dx}{dt} = g(x,t,u)$**:**

$$\frac{du}{dt} = \frac{\partial u}{\partial t} + \frac{\partial u}{\partial x}\frac{dx}{dt} = 0$$

Burger's equation: $u_t + uu_x = 0$