MATH0024 – Modeling with PDEs

Finite difference and finite element methods for wave and transport equations

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Outline

- Transport equation:
  - Transport operator.
  - Physical examples.
  - Method of characteristics.
- Finite difference method for transport equation:
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  - Consistency, stability, convergence.
  - Courant-Friedrichs-Lewy condition.
  - Dissipation and dispersion errors.
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Transport equation

Transport equation

- The linear first-order partial differential equation
$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = f,$$
where c is a nonvanishing constant, is referred to as the transport equation.

Relationship between wave and transport equations

- In fact, the wave equation
$$\frac{\partial u^2}{\partial t^2} - c^2\frac{\partial u^2}{\partial x^2} = \left(\frac{\partial}{\partial t} + c\frac{\partial}{\partial x}\right)\left(\frac{\partial u}{\partial t} - c\frac{\partial u}{\partial x}\right) = f,$$
can be cast equivalently as the system of two transport equations
$$\begin{cases} \dfrac{\partial w}{\partial t} + c\dfrac{\partial w}{\partial x} = f, \\ \dfrac{\partial u}{\partial t} - c\dfrac{\partial u}{\partial x} = w. \end{cases}$$

Numerical methods for wave and transport equations

- In this lecture, we will primarily consider numerical methods for solving the transport equation.
- Because of the relationship between the wave and transport equations, this is sufficient to illustrate many of the issues that arise in solving both wave and transport equations.

Conservation of mass

- Let us consider a fluid flowing through a region of space. For an open bounded subset $\Omega(t)$ of $\mathbb{R}^m$ with sufficiently smooth boundary $\partial\Omega(t)$ that moves with the flow, conservation of mass reads as

$$\frac{d}{dt}\int_{\Omega(t)} \rho dV_{\boldsymbol{x}} = \int_{\Omega(t)} s dV_{\boldsymbol{x}}, \qquad \begin{cases} \rho\text{: mass density } \left([\rho] = \mathrm{kg\,m^{-3}}\right), \\ s\text{: source } \left([s] = \mathrm{kg\,m^{-3}\,s^{-1}}\right). \end{cases}$$

  Differentiating under the integral sign, we obtain $\int_{\Omega(t)} \left(\frac{\partial \rho}{\partial t} + \mathrm{div}_{\boldsymbol{x}}(\rho \boldsymbol{v})\right) dV_{\boldsymbol{x}} = \int_{\Omega(t)} s dV_{\boldsymbol{x}}$, hence,

$$\frac{\partial \rho}{\partial t} + \mathrm{div}_{\boldsymbol{x}}(\rho \boldsymbol{v}) = s, \qquad \boldsymbol{v}\text{: velocity } \left([\boldsymbol{v}] = \mathrm{m\,s^{-1}}\right).$$

- Thus, in 1D ($m = 1$) and if the velocity v is constant, ρ satisfies the transport equation

$$\frac{\partial \rho}{\partial t} + v\frac{\partial \rho}{\partial x} = s.$$

  As a conclusion, the transport equation can be viewed as modeling the convective transport of a substance carried along with a 1D flow of constant velocity.

Characteristic lines

- Let us consider the transport equation

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = f.$$

  - For a linear coordinate transformation

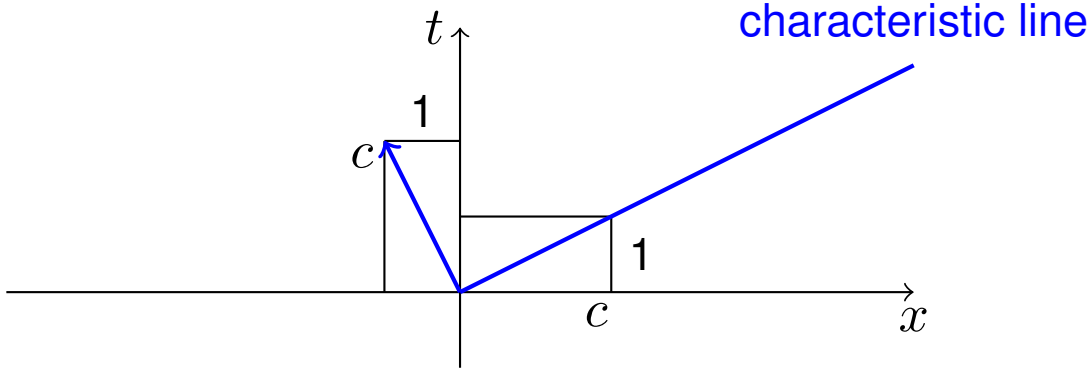
$$\begin{bmatrix} x \\ t \end{bmatrix} \mapsto \begin{bmatrix} \tilde{x} \\ \tilde{t} \end{bmatrix} = \begin{bmatrix} A_{\tilde{x}x} & A_{\tilde{x}t} \\ A_{\tilde{t}x} & A_{\tilde{t}t} \end{bmatrix} \begin{bmatrix} x \\ t \end{bmatrix}.$$

    we have, by the chain rule,

$$(A_{\tilde{x}t} + cA_{\tilde{x}x})\frac{\partial u}{\partial \tilde{x}} + (A_{\tilde{t}t} + cA_{\tilde{t}x})\frac{\partial u}{\partial \tilde{t}} = f.$$

  - The transport equation is **not elliptic** because a coordinate transformation with $A_{\tilde{x}t} = -c\,A_{\tilde{x}x}$ results in a zero coefficient of $\partial_{\tilde{x}} u$. If the coordinate transformation is orthogonal, the condition $A_{\tilde{x}t} = -c\,A_{\tilde{x}x}$ corresponds to the $\tilde{x}$-axis being along $(x = x, t = -c\,x)$.

    The lines $x = ct +$ constant are **characteristic lines**.



Method of characteristics

- The fact that the transport equation is not genuinely of the first order in the direction $(x = x, t = -c\,x)$ can be exploited to convert this PDE into an equivalent ODE, as we will show below. This procedure is a special case of the **method of characteristics**, a general method for exploiting characteristic surfaces (if they exist) to convert PDEs into equivalent systems of ODEs.
- Let us consider the inhomogeneous problem with general initial datum

$$\begin{cases} \dfrac{\partial u}{\partial t} + c\dfrac{\partial u}{\partial x} = f & \text{in } \mathbb{R}\times]0,+\infty[, \\ u(x,0) = g(x) & \text{on } \mathbb{R}\times\{t=0\}. \end{cases}$$

The transport equation not being genuinely of the first order in direction $(x = x, t = -c\,x)$, we set

$$\begin{cases} x(t) = x_0 + ct, \\ z(t) = u\big(x(t), t\big). \end{cases}$$

This allows the inhomogeneous problem with general initial datum to be converted into the IVP

$$\begin{cases} \dfrac{dz}{dt}(t) = \dfrac{\partial u}{\partial x}\big(x_0+ct,t\big)c + \dfrac{\partial u}{\partial t}\big(x_0+ct,t\big) = f\big(x_0+ct,t\big) & \text{in }]0,+\infty[, \\ z(0) = u(x_0,0) = g(x_0) & \text{at } \{t=0\}. \end{cases}$$

This IVP is solved by $z(t) = u(x_0+ct,t) = g(x_0) + \int_0^t f(x_0+cs,s)ds$ for $t \geq 0$, hence,

$$u(x,t) = g(x-ct) + \int_0^t f\big(x+c(s-t),s\big)ds \qquad \text{for } x \text{ in } \mathbb{R} \text{ and } t \geq 0.$$

Example: traveling wave solution to transport equation

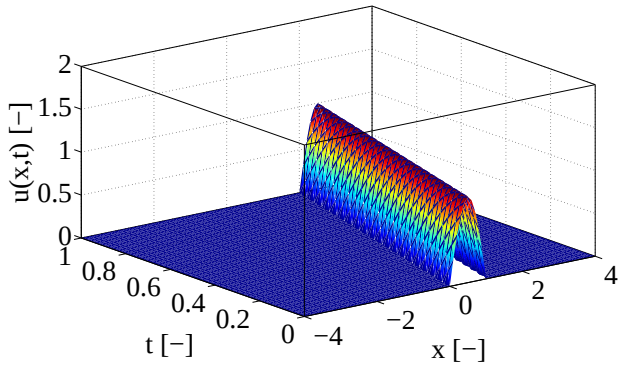
- Let us consider the IVP

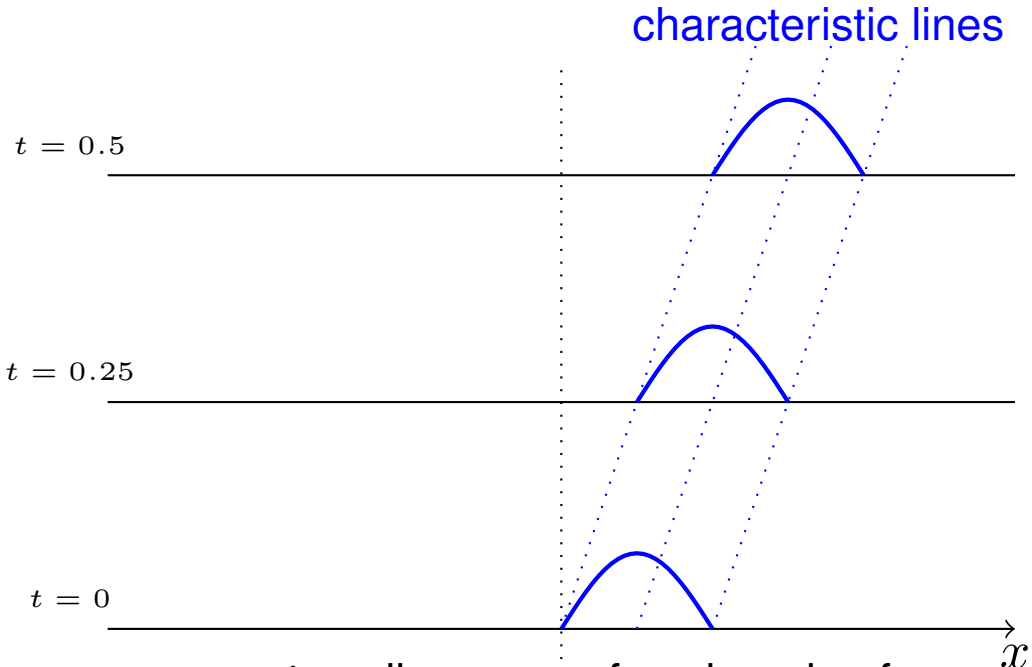
$$\begin{cases} \dfrac{\partial u}{\partial t} + c\dfrac{\partial u}{\partial x} = 0 & \text{in } \mathbb{R}\times]0, +\infty[, \\ u(x,0) = g(x) & \text{on } \mathbb{R} \times \{t = 0\}, \end{cases}$$

  using as initial datum

$$u(x,0) = g(x) = \begin{cases} \sin(\pi x) & \text{if } 0 \le x \le 1, \\ 0 & \text{otherwise.} \end{cases}$$

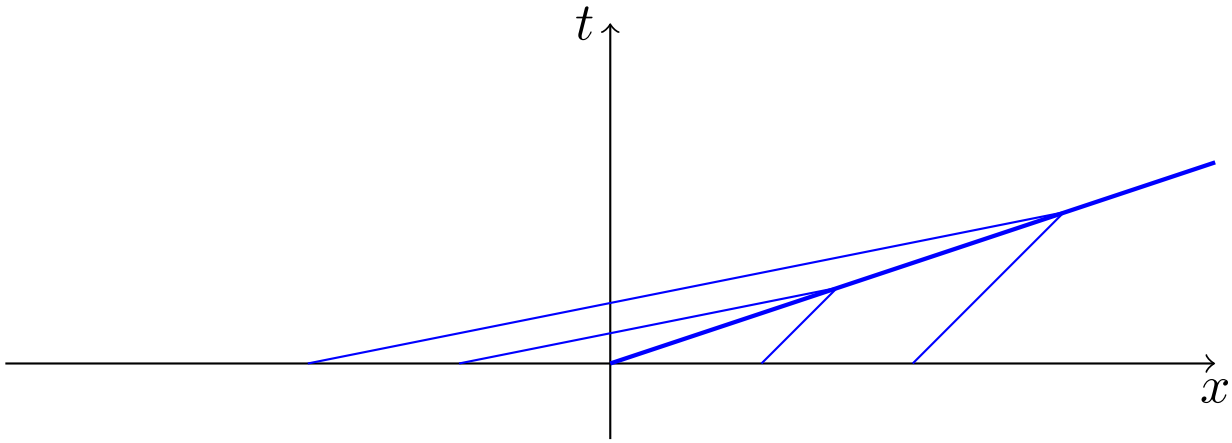
- The following figures show the solution u:





- We can observe that the solution to the IVP appears as a traveling wave of unchanging form moving at a constant velocity of c. If $c > 0$, the wave moves to the right; if $c < 0$, it moves to the left.

Systems of first-order linear and nonlinear conservation laws in less than a nutshell



- Method of characteristics. Nonlinear conservation laws, for example, $\partial_t u + \partial_x f(u) = 0$, can produce a discontinuous response even in the presence of continuous initial data. Classical and distributional solutions. Rankine-Hugoniot shock conditions. Entropy/flux. Boundary conditions. Numerical treatment. Extensions thereof to systems of conservation laws and multiple dimensions.

- Although we are not studying them in detail in this course this year, systems of first-order linear and nonlinear conservation laws are an important area of the theory of PDEs. For more details, please refer, for example, to AERO0030 Computational fluid dynamics (V. Terrapon).

Finite difference method for transport equation

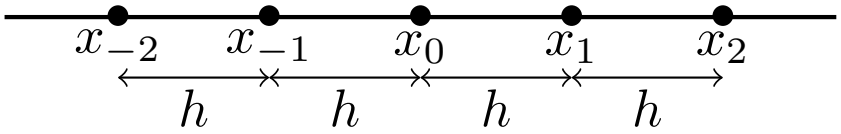
Model problem

- Let us consider the numerical approximation of the solution to the initial-value problem

$$\begin{cases} \dfrac{\partial u}{\partial t} + c\dfrac{\partial u}{\partial x} = 0, & x \in \mathbb{R}, \quad 0 < t < \tau, \\ u(x,0) = g(x), & x \in \mathbb{R}, \end{cases}$$

(initial condition).

- In the spatial domain, let grid points be introduced as follows:



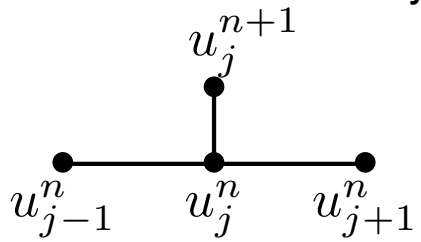
The grid spacing is denoted by h; thus, $x_j = jh$ for $-\infty < j < +\infty$.

- In the time domain, let approximations be computed at successive times $t_0, t_1, t_2, \ldots, t_{\nu_k}$. The time step is denoted by k; thus, $t_n = nk$ for $n = 0, \ldots, \nu_k$ with $\nu_k = \tau/k$.

- System of notation: numerical solution u_j^n approximates exact solution $u(x_j, t_n)$ at (x_j, t_n).

Centered-in-space forward-in-time method

- The centered-in-space forward-in-time method is obtained by requiring that



$$\begin{cases} \dfrac{u_j^{n+1} - u_j^n}{k} + c\dfrac{u_{j+1}^n - u_{j-1}^n}{2h} = 0, & j \in \mathbb{Z}, \quad 0 \leq n \leq \nu_k - 1, \\ u_j^0 = g(x_j), & j \in \mathbb{Z}. \end{cases}$$

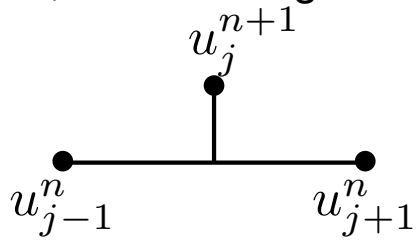
This corresponds to replacing $\frac{\partial u}{\partial x}(x_j, t_n)$ by its centered difference approximation and $\frac{\partial u}{\partial t}(x_j, t_n)$ by its forward difference approximation in the PDE.

- This system of fully discrete equations can be written equivalently as

$$\begin{cases} u_j^{n+1} = u_j^n - \dfrac{1}{2}c\dfrac{k}{h}(u_{j+1}^n - u_{j-1}^n), & j \in \mathbb{Z}, \quad 0 \leq n \leq \nu_k - 1, \\ u_j^0 = g(x_j), & j \in \mathbb{Z}. \end{cases}$$

Lax-Friedrichs method

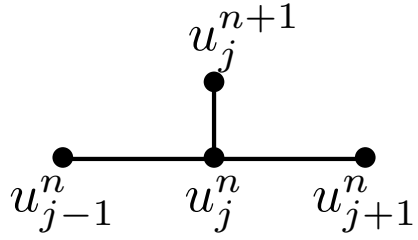
- This Lax-Friedrichs method corresponds to replacing u_j^n by $\frac{1}{2}(u_{j+1}^n + u_{j-1}^n)$ in the centered-in-space forward-in-time method, thus leading to the system of fully discrete equations



$$\begin{cases} u_j^{n+1} = \dfrac{1}{2}(u_{j+1}^n + u_{j-1}^n) - \dfrac{1}{2}c\dfrac{k}{h}(u_{j+1}^n - u_{j-1}^n), & j \in \mathbb{Z}, \quad 0 \leq n \leq \nu_k - 1, \\ u_j^0 = g(x_j), & j \in \mathbb{Z}. \end{cases}$$

Lax-Wendroff method

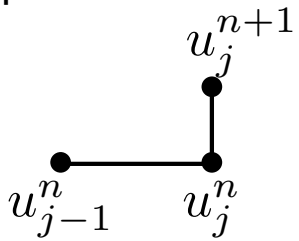
- This Lax-Wendroff method uses the system of fully discrete equations



$$\begin{cases} u_j^{n+1} = u_j^n - \dfrac{1}{2}c\dfrac{k}{h}(u_{j+1}^n - u_{j-1}^n) + \dfrac{1}{2}c^2\dfrac{k^2}{h^2}(u_{j+1}^n - 2u_j^n + u_{j-1}^n), & j \in \mathbb{Z}, \quad 0 \leq n \leq \nu_k - 1, \\ u_j^0 = g(x_j), & j \in \mathbb{Z}. \end{cases}$$

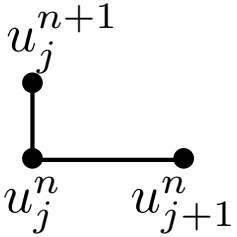
Upwind method

- If $c > 0$ (solution moves to the right), the upwind method uses the system of fully discrete equations



$$\begin{cases} u_j^{n+1} = u_j^n - c\dfrac{k}{h}(u_j^n - u_{j-1}^n), & j \in \mathbb{Z}, \quad 0 \leq n \leq \nu_k - 1, \\ u_j^0 = g(x_j), & j \in \mathbb{Z}. \end{cases}$$

- If $c < 0$ (solution moves to the left), the upwind method uses the system of fully discrete equations



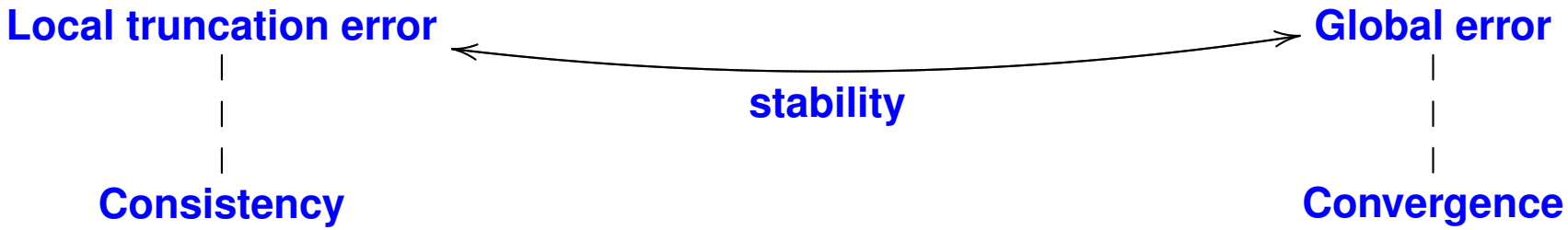
$$\begin{cases} u_j^{n+1} = u_j^n - c\dfrac{k}{h}(u_{j+1}^n - u_j^n), & j \in \mathbb{Z}, \quad 0 \leq n \leq \nu_k - 1, \\ u_j^0 = g(x_j), & j \in \mathbb{Z}. \end{cases}$$

Explicit versus implicit methods

- These methods are all **explicit** methods.

Introduction

- Consistency, stability, and convergence can be analyzed in a manner akin to that of the analyses of time-marching and finite difference methods in Lectures 3 and 7:



- As in Lecture 7, a key aspect of studying consistency, stability, and convergence is in understanding whether some **proper relation must hold between h and k.**
- As in Lecture 7, in addition to a comprehensive analysis of consistency, stability, and convergence, there exist also other approaches that can sometimes give stability restrictions more easily:
  - The **method of lines** provides a bridge with time-marching methods for IVPs, thus allowing stability by using theory for time-marching methods for IVPs.
  - **Von Neumann stability analysis** provides a bridge between finite difference methods and sampling theory, which allows stability to be studied by using Fourier analysis.
- Next, we first describe as an example a Von Neumann stability analysis of the centered-in-space forward-in-time method, and we then summarize the consistency, stability, and convergence properties of all the aforementioned methods.

Von Neumann stability analysis of the centered-in-space forward-in-time method

- For the centered-in-space forward-in-time method, we have $u_j^{n+1} = u_j^n - \frac{1}{2}c\frac{k}{h}(u_{j+1}^n - u_{j-1}^n)$.
- Provided that the values $\{u_j^n\}_{j=-\infty}^{+\infty}$ can be considered to be a "meaningful" sampling of a function u^n (specifically, provided that they can be considered as the sampling of a smooth band-limited function at a rate higher than the Nyquist rate), we can use the Poisson formula to obtain

$$u_j^{n+1} = \frac{1}{2\pi}\int_{-\pi/h}^{\pi/h} \hat{u}^n(\xi)\Big(\underbrace{1 - \frac{1}{2}c\frac{k}{h}\big(\exp(i\xi h) - \exp(-i\xi h)\big)}_{=\gamma(\xi)=1-ic\frac{k}{h}\sin(\xi h)}\Big)\exp(i\xi hj)d\xi.$$

- We can observe that the amplitude of the amplification factor is such that

$$|\gamma(\xi)|^2 = 1 + \left(c\frac{k}{h}\sin(\xi h)\right)^2 > 1 \quad \text{if } c \neq 0 \text{ and } \xi \neq \frac{m\pi}{h},\ m \in \mathbb{Z}.$$

- Hence, by the Parseval inequality (if it applies), we obtain

$$\|u^{n+1}\|^2 = \frac{1}{2\pi}\int_{-\pi/h}^{\pi/h} |\hat{u}^n(\xi)|^2|\gamma(\xi)|^2 d\xi > \|u^n\|^2,$$

  thus indicating that the numerical solution diverges as time tends to infinity.

- We can conclude that the centered-in-space forward-in-time method is **unconditionally unstable** (and hence should not be used in practice).

Consistency, stability, and convergence of aforementioned finite difference methods

- For each of the aforementioned finite difference methods, we provide the "Big-oh" characterization of the local truncation error, and we indicate whether (checkmark) or not (cross) stability and convergence properties can be proven:

	Local truncation error	Stability	Convergence
Centered-in-space forward-in-time	$O(h^2 + k)$	✗	✗
Lax-Friedrichs	$O(h + k + h^2/k)$	✓	✓
Lax-Wendroff	$O(h^2 + k^2)$	✓	✓
Upwind	$O(h + k)$	✓	✓

- As in the case of the analysis of centered-in-space forward-in-time method for the heat equation, the analysis of stability and convergence of the Lax-Friedrichs, Lax-Wendroff, and upwind methods leads to a requirement for some proper relation to hold between h and k. Specifically, in the literature, their stability and convergence properties are typically obtained under the restriction $\left|c\frac{k}{h}\right| \leq 1$.

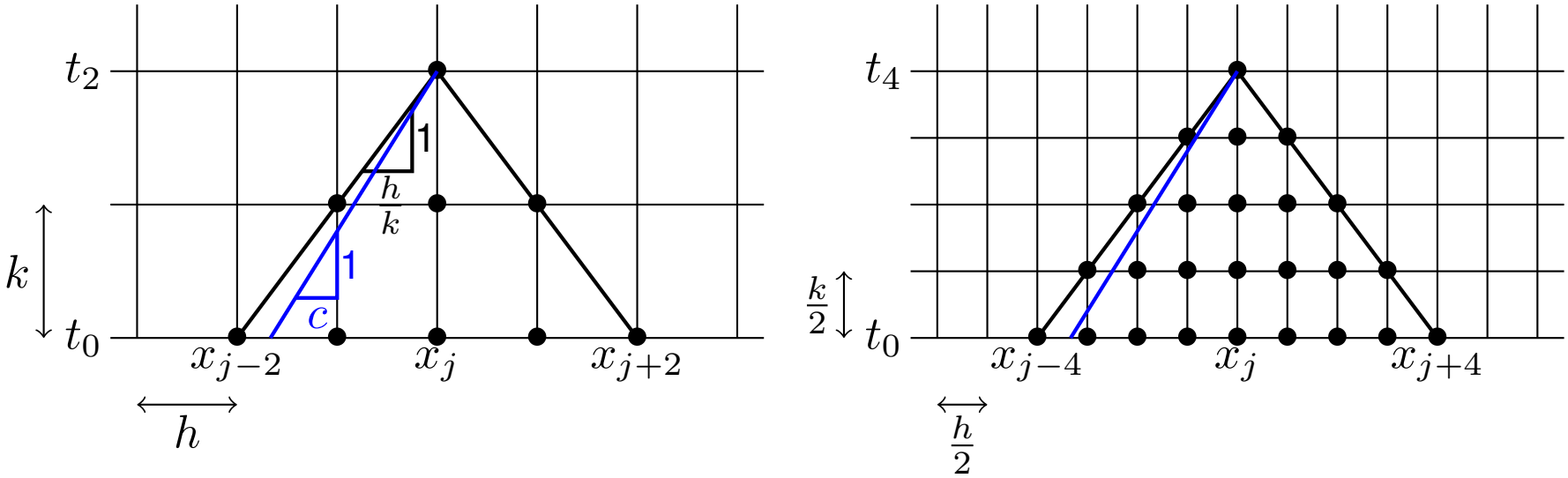
- Please refer to the literature for further details.

Courant-Friedrichs-Lewy condition

Notion of Courant-Friedrichs-Lewy condition

- A numerical method can be convergent only if its **numerical domain of dependence contains the exact domain of dependence** of the PDE, at least in the limit as h and k tend to zero. This condition for convergence is referred to as the Courant-Friedrichs-Lewy condition (**CFL condition**).
- The CFL condition is necessary but not sufficient for convergence. If it is violated, then the numerical method cannot be convergent; if it is satisfied, then the numerical method might be convergent, but a proper analysis of consistency, stability, and convergence is still required to prove this.
- Next, we show as an example that the Lax-Wendroff method satisfies the CFL condition when h and k are refined while keeping their ratio equal to a constant value that satisfies the aforementioned stability restriction $\left|c\frac{k}{h}\right| \leq 1$.

Proof of Lax-Wendroff method satisfying Courant-Friedrichs-Lewy condition



Courant-Friedrichs-Lewy condition

Proof of Lax-Wendroff method satisfying Courant-Friedrichs-Lewy condition (continued)

- In the Lax-Wendroff method, the value u_j^{n+1} depends on u_{j-1}^n, u_j^n, and u_{j+1}^n. These values depend in turn on $u_{j-1}^n, \ldots, u_{j+2}^{n-1}$. Tracing back to the initial time, we obtain a triangular grid.

- If we decrease h and k while keeping their ratio equal to a constant value, the numerical solution at (x, t) becomes dependent on more values of the initial data, but these values all remain located within the same interval $[x - t\frac{h}{k}, x + t\frac{h}{k}]$ and become merely denser. The numerical domain of dependence of the point (x, t) is the interval $[x - t\frac{h}{k}, x + t\frac{h}{k}]$.

- For the transport equation, the exact solution at the point (x, t) depends on the initial data only at a single point, namely, $x - ct$. The exact domain of dependence of the point (x, t) is the point $x - ct$.

- Thus, if we decrease h and k while keeping their ratio equal to a constant value that satisfies $\left|c\frac{k}{h}\right| \leq 1$, we have $x - t\frac{h}{k} \leq x - ct \leq x - t\frac{h}{k}$, so that the numerical domain of dependence indeed contains the exact domain of dependence, as asserted.

Dissipation and dispersion errors

Notions of dissipation and dispersion errors

- We have seen that the exact solution to an IVP involving the transport equation appears as a traveling wave of unchanging form that moves at a constant velocity of c.

- Numerical methods can introduce a **dissipation error**, that is, they can introduce a form of damping that results in the numerical solution being reduced in amplitude with respect to the exact solution.

- In addition, numerical methods can introduce a **dispersion error**, that is, they can introduce a form of dispersion that results in certain components of the numerical solution moving slower or faster than the corresponding components of the exact solution.

- Dissipation and dispersion errors can be analyzed mathematically, for example, by using Fourier analysis; please refer to the literature for further details. In the frame of this course, we limit ourselves to a numerical study of dissipation and dispersion errors as part of a homework exercise.

Finite element method for wave equation

Finite element method for wave equation

Model problem

- Let us consider the numerical approximation of the solution to the initial-boundary value problem

$$\begin{cases} \dfrac{\partial^2 u}{\partial t^2} - c^2 \dfrac{\partial^2 u}{\partial x^2} = 0, & 0 < x < 1, \quad < t < \tau, \\ u(0,t) = u(1,t) = 0, & < t < \tau, \quad \text{(boundary conditions)}, \\ u(x,0) = g(x) \text{ and } \dfrac{\partial u}{\partial t}(x,t) = w(x), & 0 < x < 1, \quad \text{(initial condition)}. \end{cases}$$

Variational formulation

- A variational formulation of this initial-boundary value problem:

Given sufficiently regular space-dependent functions g and w, find a sufficiently regular space- and time-dependent function u with $u(0,t) = u(1,t) = 0$ for $0 < t < \tau$ such that

$$\int_0^1 \frac{\partial^2 u}{\partial t^2}(x,t) v(x) dx + c^2 \int_0^1 \frac{\partial u}{\partial x}(x,t) \frac{dv}{dx}(x) dx = 0, \qquad 0 < t < \tau,$$

for all sufficiently regular space-dependent functions v with $v(0) = 0$ and $v(1) = 0$

and the initial conditions $u(x,0) = g(x)$ and $\frac{\partial u}{\partial t}(x,0) = w(x)$ for $0 < x < 1$ are fulfilled.

Finite element method for wave equation

Galerkin approximation

- Let a finite number μ_h of basis functions $\varphi_1, \ldots, \varphi_{\mu_h}$ be given. Let each basis function φ_j be a sufficiently regular space-dependent function such that $\varphi_j(0) = \varphi_j(1) = 0$.
- Then, the Galerkin approximation leads to the construction of an approximate solution u^h of the form of a linear combination of the basis functions, that is, $u^h(x,t) = \sum_{j=1}^{\mu_h} u_j(t)\varphi_j(x)$.
- The coefficients $u_1(t), \ldots, u_{\mu_h}(t)$ are determined by requiring the equation in the variational formulation to hold for all test functions that are linear combinations of the basis functions.
- Written compactly, the Galerkin approximate problem thus obtained takes the following form:

$$\begin{cases} [M]\dfrac{d^2\boldsymbol{u}}{dt^2}(t) + [K]\boldsymbol{u}(t) = 0 & \text{for } 0 < t < \tau, \\ \boldsymbol{u}(0) = \boldsymbol{g} \quad \text{and} \quad \dfrac{d\boldsymbol{u}}{dt}(0) = \boldsymbol{w} & \text{at } t = 0, \end{cases}$$

  where $[M]$ and $[K]$ are square μ_h-dimensional matrices with $M_{ij} = \int_0^1 \varphi_i\varphi_j dxdx$ and $K_{ij} = \int_0^1 \frac{d\varphi_i}{dx}\frac{d\varphi_j}{dx}dx$ and $\boldsymbol{g}$ and $\boldsymbol{w}$ are μ_h-dimensional vectors such that $u^h(x,0) = \sum_{j=1}^{\mu_h} g_j\varphi_j(x)$ and $\frac{du^h}{dt}(x,0) = \sum_{j=1}^{\mu_h} w_j\varphi_j(x)$ are appropriate approximations of $g(x)$ and $w(x)$ for $0 < x < 1$.
- This initial-value problem can be discretized in time by using any appropriate time-marching method.

Finite element method

- A finite element method is obtained when the basis functions in the Galerkin approximation are constructed, after meshing the domain, as elementwise low-degree polynomials.

Summary and conclusion

- The numerical approximation of the solution to an initial-boundary value problem requires the discretization of space and time. The discretization of space and time are not independent of each other. Often, a proper relation must hold between them to ensure convergence as they are refined.
- Key properties of a numerical method:
  - Convergence.
  - It may also be desirable that certain properties of the exact solution are preserved in the numerical solution. This leads to analyses of absolute stability, Von Neumann stability, Courant-Friedrichs-Lewy condition, dispersion and dissipation errors, and so forth.
- Consistency, stability, and convergence are analyzed to evaluate how good finite difference methods are in approximating solutions to IBVPs. As an alternative to such analyses, there exist also other approaches that can sometimes provide guidance more easily:
  - The method of lines bridges finite difference methods for IBVPs with time-marching methods for IVPs, thus allowing stability of the former to be studied by using theory for the latter.
  - Von Neumann stability analysis provides a bridge between finite difference methods and sampling theory, which allows stability to be studied by using Fourier analysis.
  - Courant-Friedrichs-Lewy condition.
- Variational formulation. Galerkin approximation. Finite element method.
- Working through numerical examples is very helpful towards understanding this material. Please do not hesitate to come up with examples yourself to try things out using small Matlab codes.

References

Suggested reading material

- P. Olver. Introduction to Partial Differential Equations. Springer, 2014. Sections 5.3, 5.4, and 8.4.

Additional references also consulted to prepare this lecture

- C. Gasquet and P. Witomski. Analyse de Fourier et applications. Masson, 1990.
- R. LeVeque. Finite difference methods for ordinary and partial differential equations. SIAM, 2007.
- P.-A. Raviart and J.-M. Thomas. Introduction à l'analyse numérique des équations aux dérivées partielles. Dunod, 1993.
- C. Soize. Méthodes mathématiques en analyse du signal. Masson, 1993.