Numerical Methods for PDEs

An introduction

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Outline

Preliminaries

We seek to solve the partial differential equation

$$\mathbb{P}u = f$$

where u is an unknown function on a domain $\Omega \subseteq \mathbb{R}^N$, P is a differential operator, and f is a given function on Ω. Typically u also satisfies some initial and/or boundary conditions. It is seldom possible to find exact solutions analytically.
A numerical method will typically find an approximation to u by making a discretization of the domain or by seeking solutions in a reduced function space.

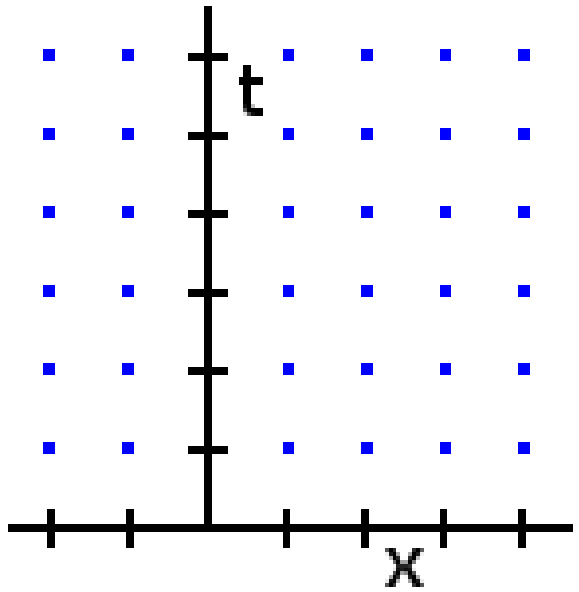
Outline

Finite differences

The basic idea for the finite difference method is to replace derivatives with finite differences. Consider $u = u(x,t)$ and let $h, k > 0$. Then we could use the following approximations:

$$\frac{\partial u}{\partial x} \approx \frac{u(x+h,t) - u(x,t)}{h}$$
$$\frac{\partial u}{\partial t} \approx \frac{u(x,t+k) - u(x,t)}{k}$$

Domain discretization



Let us define a regular grid of points $(x_m, t_n) = (mh, nk)$ for some integers m and n. In general these points need not be equally spaced. The finite difference algorithm will generate approximations to u at each grid point.

Notation

We introduce the notation $u_m^n = u(x_m, t_n)$. Then we can write:

$$\frac{\partial}{\partial x} u_m^n \approx \frac{u_{m+1}^n - u_m^n}{h}$$
$$\frac{\partial}{\partial t} u_m^n \approx \frac{u_m^{n+1} - u_m^n}{k}.$$

These are called *forward differences*; there are many other possible choices.

Example

Consider the one-way wave equation:

$$u_t + a u_x = 0$$

with initial condition

$$u(x, 0) = u_0(x).$$

Here is the forward-time forward-space approximation:

$$\frac{u_m^{n+1} - u_m^n}{k} + a \frac{u_{m+1}^n - u_m^n}{h} = 0,$$

from which we can derive the following *explicit* scheme:

$$u_m^{n+1} = (1 + \tfrac{ak}{h}) u_m^n - \tfrac{ak}{h} u_{m+1}^n.$$

Consistency

Will our finite difference scheme actually generate a solution of the PDE? Consider the one-way wave equation with $a = 1$:

$$\begin{cases} u_t + u_x = 0, \\ u(x,0) = u_0(x). \end{cases}$$

The exact solution is $u(x,t) = u_0(x-t)$, found using the method of characteristics. As time increases, initial data is propagated to the right with speed 1. The forward-time forward-space scheme cannot reproduce this behavior, so the scheme is *inconsistent* with the PDE.

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A scheme which *is* consistent with the one-way wave equation for all a is the forward-time center-space scheme:

$$\frac{u_m^{n+1} - u_m^n}{k} + a\frac{u_{m+1}^n - u_{m-1}^n}{2h} = 0.$$

Stability

A poorly-chosen numerical scheme can sometimes result in uncontrolled (and incorrect) growth of the solution. We say that a finite difference scheme for a first-order equation is *stable* if there is an integer J such that for any positive time T, there is a constant C_T such that

$$\|u^n\|_h^2 \leq C_T \sum_{j=0}^{J} \|u^j\|_h^2.$$

This is typically shown using Von Neumann analyis in Fourier space; there is often a strong dependence on the relation between h and k.
The forward-time center-space scheme for the one-way wave equation is unstable.

Implicit schemes

The backward-time center-space scheme is both consistent with the one-way wave equation and unconditionally stable:

$$\frac{u_m^{n+1} - u_m^n}{k} + a\frac{u_{m+1}^{n+1} - u_{m-1}^{n+1}}{2h} = 0$$

This is an *implicit* scheme, since unknown values appear multiple times in the equation. Implicit schemes often allow for much larger grid spacing but require significant additional calculations at each step.

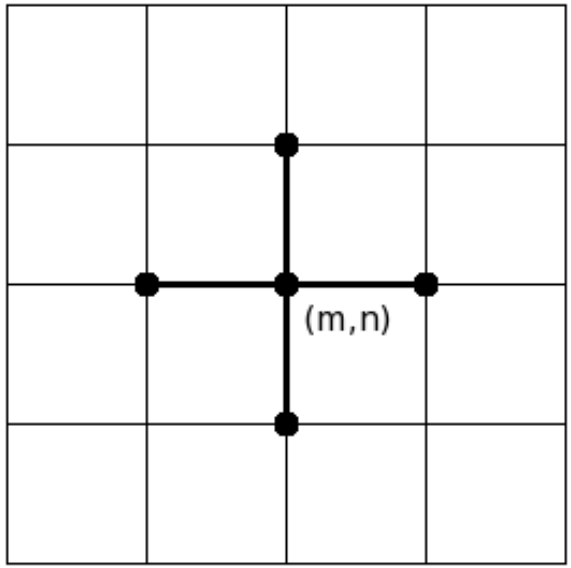
Order of accuracy

Consider Poisson's equation in 2D:

$$u_{xx} + u_{yy} = f.$$

The discrete five-point Laplacian approximation is given by:

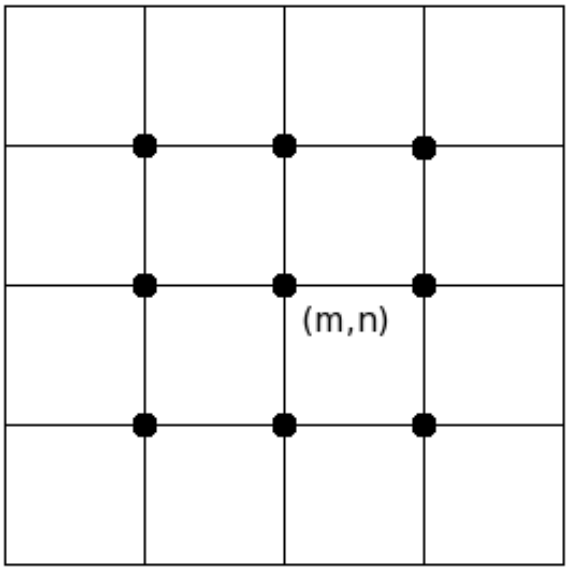
$$u_{m+1,n} + u_{m-1,n} + u_{m,n+1} + u_{m,n-1} - 4u_{m,n} = h^2 f_{m,n}$$



Order of accuracy

The discrete nine-point Laplacian is of higher accuracy: $o(h^4)$ vs. $o(h^2)$. However, it requires more information at each step:

$$\begin{aligned} &\tfrac{1}{6}(u_{m+1,n+1} + u_{m+1,n-1} + u_{m-1,n+1} + u_{m-1,n-1}) + \\ &+\tfrac{2}{3}(u_{m+1,n} + u_{m-1,n} + u_{m,n+1} + u_{m,n-1}) - \tfrac{10}{3}u_{m,n} = \\ &= \tfrac{h^2}{12}(f_{m+1,n} + f_{m-1,n} + f_{m,n+1} + f_{m,n-1}) \end{aligned}$$



Pros and cons of finite difference methods

Advantages:

- Fast
- Easy to code

Disadvantages:

- Hard to generalize in complex geometries

Outline

Conservation laws

The finite volume method is used to find numerical solutions to conservation laws. A conservation law is a PDE written generally in the form:

$$\partial_t q(x,t) + \text{div } \mathbf{F}(x,t) = f(x,t),$$

where q is a conserved quantity (i.e. mass, energy), $\mathbf{F}$ is a flux representing a transport mechanism for q, and f is a forcing term. There is an implicit dependence on an unknown $u(x,t)$

Examples of conservation laws

Linear transport equation:

$$\begin{cases} \partial_t u(x,t) + \mathrm{div}(\mathbf{v}u)(x,t) = 0, t > 0, \\ u(x,0) = u_0(x). \end{cases}$$

$$[q = u(x,t), F = \mathbf{v}u(x,t), f = 0]$$

Stationary diffusion equation:

$$\begin{cases} -\Delta u = f, \text{ on } \Omega = (0,1) \times (0,1) \\ u = 0, \text{ on } \delta\Omega \end{cases}$$

$$[q = u(x), F = -\nabla u(x)]$$

Examples of conservation laws

1D Euler equations:

$$\partial_t \begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix} + \partial_x \begin{pmatrix} \rho u \\ \rho u^2 + p \\ u(E+p) \end{pmatrix} = 0.$$

Intro to the Finite Volume method

Let $\Omega \subseteq \mathbb{R}^d$ be our spatial domain, and let $\mathcal{T}$ be a polygonal mesh on Ω. Consider a control volume $K \in \mathcal{T}$. Integrating over K, we have by the divergence theorem:

$$\int_K \partial_t q(x,t)dx + \int_{\partial K} \mathbf{F}(x,t) \cdot \mathbf{n}_K(x) d\sigma = \int_K f(x,t)dx.$$

Let $\mathcal{N}_K \subseteq \mathcal{T}$ be the set of neighbors of K. Then

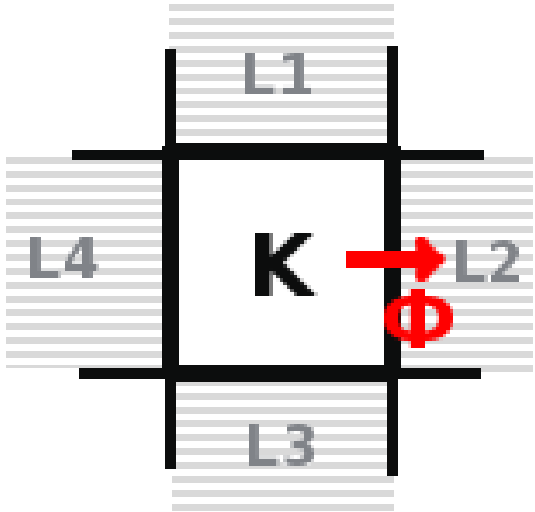
$$\int_K \partial_t q(x,t)dx + \sum_{L \in \mathcal{N}_K} \int_{K \cap L} \mathbf{F}(x,t) \cdot \mathbf{n}_K(x) d\sigma = \int_K f(x,t)dx.$$

Discretization and approximation

Using an explicit forward-time scheme, we can write

$$\int_K \frac{q^{n+1}(x) - q^n(x)}{k} dx + \sum_{L \in \mathcal{N}_K} \Phi^n_{K,L} = \int_K f(x, t_n) dx,$$

where $\Phi^n_{K,L}$ is an approximation to the flux from K to L.



The numerical flux

In a finite volume scheme, we seek an appropriate time discretization as well as numerical flux terms $F^n_{K,L}$ which are

- Conservative, i.e. $F^n_{K,L} = -F^n_{L,K}$.
- Consistent with the PDE.

Pros and cons of finite volume methods

Advantages:

- Robust and cheap for conservation laws
- Can handle complex geometries

Disadvantages:

- High precision difficult (see: Discontinuous Galerkin)

Outline

Intro to spectral methods

Spectral methods are global methods. We seek to approximate u with a linear combination of smooth basis functions:

$$u(x) \approx \sum_{k=0}^{N} a_k \phi_k(x).$$

The basis functions ϕ_k are, for example, trigonometric functions or Chebyshev polynomials.

Basis functions

The choice of basis functions should meet three requirements:

1. Approximation $\sum_{k=0}^{N} a_k \phi_k(x)$ must converge rapidly.
2. Given a_k, it should be easy to determine b_k such that $\frac{d}{dx}\left(\sum_{k=0}^{N} a_k \phi_k(x)\right) = \sum_{k=0}^{N} b_k \phi_k(x)$.
3. It should be fast to convert between coefficients a_k, for $k = 0, \ldots, N$, and values $v(x_i)$ at some set of nodes x_i, for $i = 0, \ldots, N$.

Basis functions

Periodic problems: Trigonometric functions satisfy (1) and (2) immediately. Thanks to the FFT (1965), they also satisfy (3).

Non-periodic problems: Legendre and Chebyshev polynomials are the preferred choice.

Determining coefficients

To determine the expansion coefficients, we consider the residual $R(x,t)$ when the expansion is substituted in the governing equation. There are three main techniques:

- *Tau.* Select a_k to satisfy BCs, make the residual orthogonal to as many basis functions as possible.
- *Galerkin.* Combine basis functions into a new set in which all functions satisfy the BCs, then make residual orthogonal to as many of the new basis functions as possible.
- *Collocation (PS).* Select a_k to satisfy BCs, make residual *zero* at as many spatial points as possible.

Pros and cons of spectral methods

Advantages:

- Error decays rapidly with N
- Small dissipative and dispersive errors
- Can handle coarse grids

Disadvantages:

- Complex geometries
- Shock handling

Outline

Intro to the finite element method

We seek to solve a PDE of the form

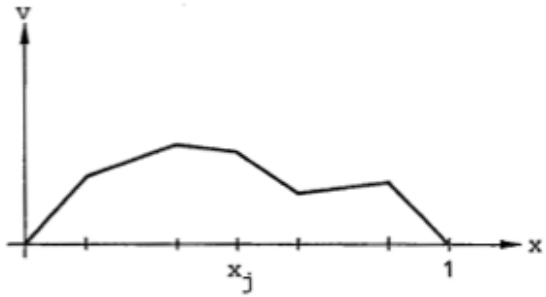
$$\mathbb{P}u = f$$

by finding an approximation $\tilde{u} \in \mathcal{V}$, for some function space $\mathcal{V}$. We wish to minimize the residual $R(x)$:

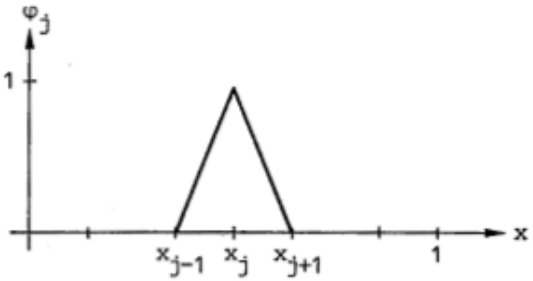
$$\mathbb{P}\tilde{u} - f = R(x).$$

Choosing a basis

We choose $\mathcal{V}$ usually to be the set of continuous or C^1 functions which are piecewise polynomial of degree p.



Let $\mathcal{T}$ be a mesh. Then we choose basis functions $\phi_k(x) \in V$ with compact support over grid cells.



$$\text{So: } \tilde{u}(x) = \sum_{k=0}^{N} a_k \phi_k(x).$$

Weak formulation

Instead of solving the PDE directly, we solve instead an *integral* or *weak* formulation:

$$\int_\Omega (\mathbb{P}u - f)v_j dx = 0,$$

where v_j are *test functions*.

- $v_j = \frac{\partial R}{\partial a_j}$: Least-squares method.
- $v_j = \mathbf{1}_{\Omega_j}$: Finite Volume method.
- $v_j = \phi_j$: Galerkin's method.

Pros and cons of finite element methods

Advantages:

- Can be very accurate
- Handles complex geometries

Disadvantages:

- ???

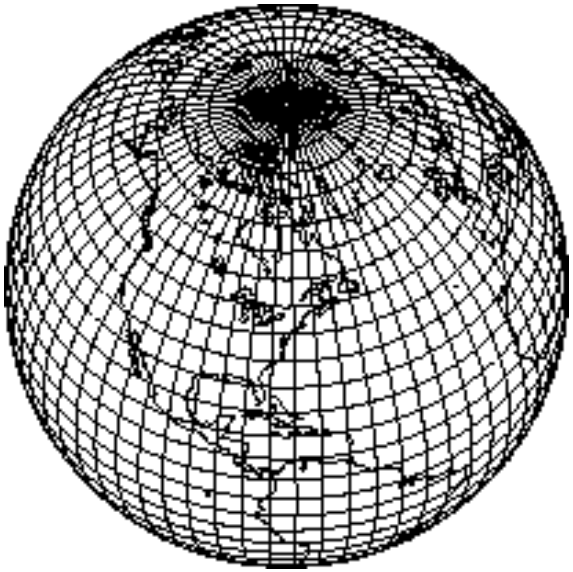
Outline

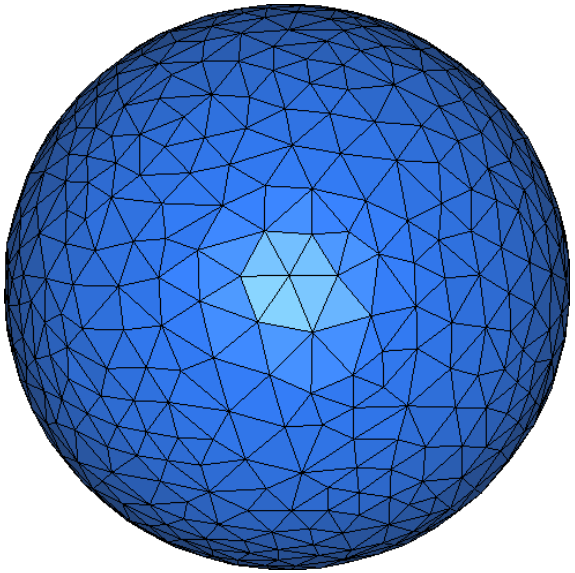
Boundary Conditions

Boundary Conditions!!

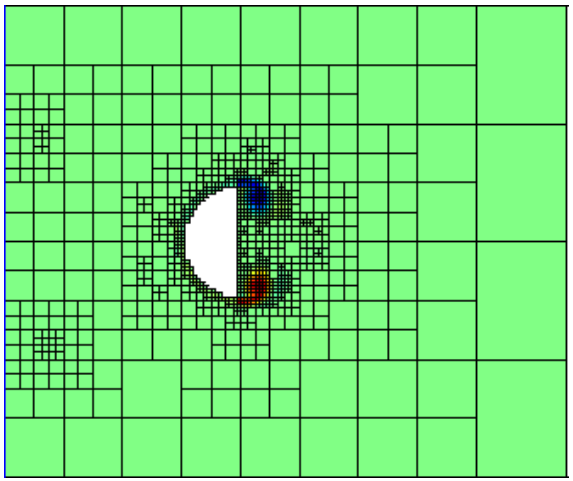
Grids

Choice of grid:





Adaptive mesh refinement:



Computational concerns

- Accuracy vs. speed
- Parallelizability

Other topics of interest

- Continuous Galerkin methods
- Discontinuous Galerkin methods
- Level set methods (Stan Osher, et al)
- Spectral/hp element methods

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