CS 450: Numerical Anlaysis[1]

Partial Differential Equations

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[1] *These slides have been drafted by Edgar Solomonik as lecture templates and supplementary material for the book "Scientific Computing: An Introductory Survey" by Michael T. Heath (slides).*

Partial Differential Equations

- *Partial differential equations (PDEs)* describe physical laws and other continuous phenomena:

- The *advection PDE* describes basic phenomena in fluid flow,

$$u_t = -a(t,x)u_x$$

where $u_t = \partial u/\partial t$ and $u_x = \partial u/\partial x$.

Types of PDEs

- Some of the most important PDEs are *second order*:
- The *discriminant* determines the canonical form of second-order PDEs:

Characteristic Curves

- A *characteristic* of a PDE is a level curve in the solution:

- More generally, characteristic curves describe curves in the solution field $u(t, x)$ that correspond to solutions of ODEs, e.g. for $u_t = -a(t, x)u_x$ with $u(0, x) = u_0(x)$,

Method of Lines

- *Semidiscrete methods* obtain an approximation to the PDE by solving a system of ODEs. Consider the heat equation,

$$u_t = cu_{xx} \text{ on } 0 \leq x \leq 1, \quad u(0,x) = f(x), u(t,0) = u(t,1) = 0.$$

- This *method of lines* often yields a stiff ODE:

Semidiscrete Collocation

- Instead of finite-differences, we can express $u(t, x)$ in a spatial basis $\phi_1(x), \dots, \phi_n(x)$ with time-dependent coefficients $\alpha_1(t), \dots, \alpha_n(t)$:

- For the heat equation $u_t = cu_{xx}$, we obtain a linear constant-coefficient vector ODE:

Fully Discrete Methods

- Generally, both time and space dimensions are discretized, either by applying an ODE solver to a semidiscrete method or using finite differences.
  - *Again consider the heat equation* $u_t = cu_{xx}$ *and discretize so* $u_i^{(k)} \approx u(t_k, x_i)$,
  - *This iterative scheme corresponds to a 3-point stencil,*

Implicit Fully Discrete Methods

- Using Euler's method for the heat equation, stability requirement is
- This step-size restriction on stability can be circumvented by use of implicit time-stepper, such as backward Euler,
- Using the trapezoid method to solve the ODE we obtain the second-order *Crank-Nicolson method*,

Convergence and Stability

- *Lax Equivalence Theorem*: consistency + stability = convergence
  - *Consistency means that the local truncation error goes to zero, and is easy to verify by Taylor expansions.*
  - *Stability implies that the approximate solution at any time t must remain bounded.*
  - *Together these conditions are necessary and sufficient for convergence.*
- Stability can be ascertained by spectral or Fourier analysis:
  - *In the method of lines, we saw that the eigenvalues of the resulting ODE define the stability region.*
  - *Fourier analysis decomposes the solution into a sum of harmonic functions and bounds their amplitudes.*

CFL Condition

- The domain of dependence of a PDE for a given point (t, x) is the portion of the problem domain influencing this point through the PDE:

- *The Courant, Friedrichs, and Lewy (CFL) condition* states that for an explicit finite-differencing scheme to be stable for a hyperbolic PDE, it is necessary that the domain of the dependence of the PDE must be contained in the domain of dependence of the scheme:

Time-Independent PDEs

- We now turn our focus to time-independent PDEs as exemplified by the *Helmholtz equation*:

$$u_{xx} + u_{yy} + \lambda u = f(x, y)$$

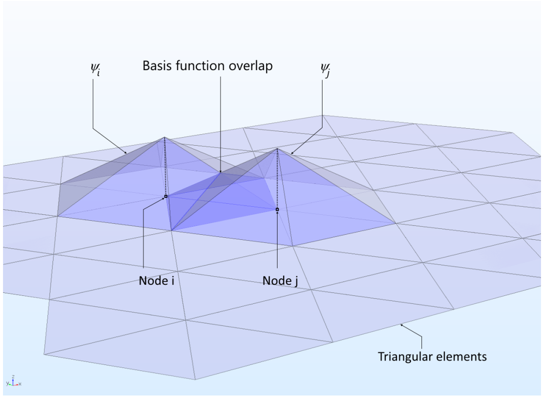
- We discretize as before, but no longer perform time stepping:

Finite-Differencing for Poisson

- Consider the Poisson equation with equispaced mesh-points on $[0, 1]$:

Multidimensional Finite Elements

- There are many ways to define localized basis functions, for example in the 2D FEM method[2]:



Sparse Linear Systems

- Finite-difference and finite-element methods for time-independent PDEs give rise to sparse linear systems:
  - *typified by the 2D Laplace equation, where for both finite differences and FEM,*

- *Direct methods* apply LU or other factorization to $\boldsymbol{A}$, while *iterative methods* refine $\boldsymbol{x}$ by minimizing $\boldsymbol{r} = \boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}$, e.g. via Krylov subspace methods.

Direct Methods for Sparse Linear Systems

- It helps to think of $\boldsymbol{A}$ as the adjacency matrix of graph $G = (V, E)$ where $V = \{1, \dots n\}$ and $a_{ij} \neq 0$ if and only if $(i, j) \in E$:

- Factorizing the lth row/column in Gaussian elimination corresponds to removing node i, with nonzeros (new edges) introduces for each k, l such that (i, k) and (i, l) are in the graph.

***Demo:** Sparse Matrix Factorizations and Fill-In*

Vertex Orderings for Direct Methods

- Select the node of minimum degree at each step of factorization:
- Graph partitioning also serves to bound fill, remove vertex separator $S \subset V$ so that $V \setminus S = V_1 \cup \cdots \cup V_k$ become disconnected, then order $V_1, \ldots, V_k, S$:
- *Nested dissection* ordering partitions graph into halves recursively, ordering each separator last.

Sparse Iterative Methods

- Sparse iterative methods avoid overhead of fill in sparse direct factorization. *Matrix splitting* methods provide the most basic iterative methods:

Sparse Iterative Methods

- The *Jacobi method* is the simplest iterative solver:
- The Jacobi method converges if A is strictly row-diagonally-dominant:

Gauss-Seidel Method

- The Jacobi method takes weighted sums of $\boldsymbol{x}^{(k)}$ to produce each entry of $\boldsymbol{x}^{(k+1)}$, while Gauss-Seidel uses the latest available values, i.e. to compute $x_i^{(k+1)}$ it uses a weighted sum of

$$x_1^{(k+1)}, \dots x_{i-1}^{(k+1)}, x_i^{(k)}, \dots, x_n^{(k)}.$$

- Gauss-Seidel provides somewhat better convergence than Jacobi:

Successive Over-Relaxation

- The *successive over-relaxation* (SOR) method seeks to improve the spectral radius achieved by Gauss-Seidel, by choosing

$$\boldsymbol{M} = \frac{1}{\omega}\boldsymbol{D} + \boldsymbol{L}, \quad \boldsymbol{N} = \Big(\frac{1}{\omega} - 1\Big)\boldsymbol{D} - \boldsymbol{U}$$

- The parameter ω in SOR controls the 'step-size' of the iterative method:

__Demo:__ Jacobi vs Conjugate Gradient

Conjugate Gradient

- The solution to $\boldsymbol{Ax} = \boldsymbol{b}$ when $\boldsymbol{A}$ is symmetric positive definite is the minima of the quadratic optimization problem,

$$\min_{\boldsymbol{x}} \boldsymbol{x}^T \boldsymbol{Ax} - \boldsymbol{x}^T \boldsymbol{b}$$

- Conjugate gradient works by picking $\boldsymbol{A}$-orthogonal descent directions

- The convergence rate of CG is linear with coefficient $\frac{\sqrt{\kappa(\boldsymbol{A})}-1}{\sqrt{\kappa(\boldsymbol{A})}+1}$:

Preconditioning

- Preconditioning techniques choose matrix $\boldsymbol{M} \approx \boldsymbol{A}$ that is easy to invert and solve a modified linear system with an equivalent solution to $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$,

$$\boldsymbol{M}^{-1}\boldsymbol{A}\boldsymbol{x} = \boldsymbol{M}^{-1}\boldsymbol{b}$$

- $\boldsymbol{M}$ is chosen to be an effective approximation to $\boldsymbol{A}$ with a simple structure: