SF2520 — Applied numerical methods

Lecture 5

Introduction to partial differential equations

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Today's lecture

- Summary of last lecture: high order methods.
- Introduction to partial differential equations
  - Characterization/phenomena modeled
  - Classifications
  - Physical origins

Runge–Kutta methods

- Compute intermediate stages k_j. Make one function evaluation $f(t, y)$ per stage,

$$k_j = f(t_n + hc_j, u_n + h(a_{j,1}k_1 + \cdots + a_{j,j-1}k_{j-1})), \qquad j = 1, \ldots, s.$$

  Take weighted sum of k_j and update as

$$u_{n+1} = u_n + h\left(b_1 k_1 + b_2 k_2 + \cdots + b_s k_s\right).$$

- **Example:** Heun's method (2 stages, 2nd order)

$$\begin{aligned} k_1 &= f(t_n, u_n), \qquad k_2 = f(t_n + h, u_n + hk_1), \\ u_{n+1} &= u_n + h(k_1 + k_2)/2. \end{aligned}$$

- One-step methods. Converges when local truncation error small.
- Absolute stability when

$$|Q(h\lambda)| \leq 1, \qquad Q(z) = \text{an } s\text{-degree polynomial} = e^z + O(z^{p+1}),$$

  for p-th order method with s stages.
- Adaptive Runge–Kutta methods compare two methods with same k_j but different b_j. (`ode45` in Matlab).

Linear multistep methods

- Use several of the previously computed approximations (q steps)

$$\begin{aligned} u_{n+1} = \alpha_0 u_n + \alpha_1 u_{n-1} + \cdots + \alpha_{q-1} u_{n-q+1} \\ + h\left(\beta_{-1} f_{n+1} + \beta_0 f_n + \cdots + \beta_{q-1} f_{n-q+1}\right). \end{aligned}$$

  Just one new function evaluation/step, but old values must be stored.
- Need initial data for $u_0, u_1, \ldots, u_{q-1}$. (Obtained from one-step method.)
- **Example:** Adams–Bashforth 3

$$u_{n+1} = u_n + \frac{h}{12}(23f_n - 16f_{n-1} + 5f_{n-2}), \qquad f_n = f(t_n, u_n).$$

- Converges when local truncation error small and *root condition* satsified: all roots of $\rho(z)$ within unit circle,

$$\rho(z) := \alpha_{q-1} + \alpha_{q-2} z + \cdots + \alpha_0 z^{q-1} - z^q.$$

- Absolute stability when all roots of $\rho(z) + h\lambda\sigma(z)$ within unit circle,

$$\sigma(z) := \beta_{q-1} + \beta_{q-2} z + \cdots + \beta_0 z^{q-1} + \beta_{-1} z^q.$$

- Very high order of accuracy can be reached in a stable way.

Introduction to PDE

Partial differential equation (PDE) =
equation relating an unknown function with its derivatives.

- Unknown function depends on several variables, e.g. $u = u(x, y)$
- Equation includes partial derivatives with respect to those, e.g.

$$u_{xx} + 2u_{xy} + u_{yy} = 0, \qquad (x, y) \in \Omega.$$

- Equation augmented with boundary conditions (BC) , e.g.

$$u = 0, \qquad (x, y) \in \partial\Omega.$$

- Time variable typically plays a special role ("evolution PDE"), e.g. $u = u(x, t)$ and

$$u_t = u_{xx}, \qquad t > 0, \quad x \in \mathbb{R}.$$

- BC called initial condition (IC) for the time boundary $t = 0$,

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

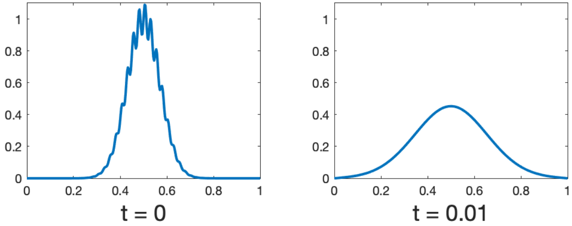
- PDEs very useful modeling tool. Analytical solutions rarely available. Numerical methods needed.

Parabolic equations

- Model equation

$$u_t - u_{xx} = 0, \qquad \text{"heat equation", or "diffusion equation".}$$

- Time dependent unknown $u = u(x, t)$, evolution PDE.
- Phenomena: diffusion, "smearing"



- u has a steady state.
- Applications:
  - Heat conduction,
  - Diffusion,
  - Finance: Black & Scholes eq. for option pricing

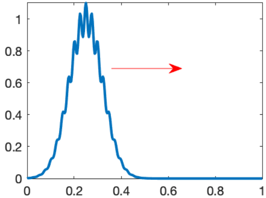
$$u_t + \frac{1}{2}\sigma^2 x^2 u_{xx} + rxu_x - ru = 0.$$

Hyperbolic equations

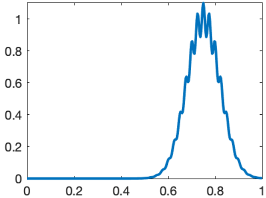
- Model equations ($u = u(x,t)$)

$$u_t + u_x = 0, \qquad \text{"advection equation"},$$
$$u_{tt} - u_{xx} = 0, \qquad \text{"wave equation"}.$$

- Phenomena: transport, wave propagation, advection



t = 0



t = 0.5

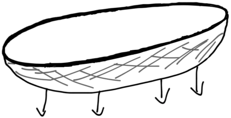
- *u* has a steady no state.
- Applications:
  - Electromagnetic waves (optics, radio, WiFi, ...)
  - Acoustic waves (sound, ultrasound, ...)
  - Elastic waves (earthquakes, ...)
  - Fluid flow (gas dynamics, ...)

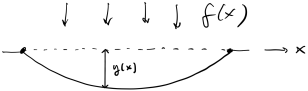
Elliptic equations

- Model equation

$$-(u_{xx} + u_{yy}) = f, \qquad \text{"Poisson equation".}$$

- Time independent unknown $u = u(x, y)$.
- Phenomena: equilibrium, energy minimization





- Steady state as $t \to \infty$ in parabolic eq. $u_t - u_{xx} = f$.
- Applications:
  - Electric potential,
  - Structural mechanics,
  - Potential flow.

Classification of PDEs

- Consider a second order linear PDE in 2D written as

$$Lu := au_{xx} + 2bu_{xy} + cu_{yy} + d_1 u_x + d_2 u_y + eu = 0,$$

 where $a, b, c, \ldots$ are real constants (and a, b, c are not all zeros).

- Introduce the symbol P of the differential operator L by replacing $\partial_x \to x$ and $\partial_y \to y$

$$P(x, y) = ax^2 + 2bxy + cy^2 + d_1 x + d_2 y + e.$$

- If "$P(x, y) =$constant" describes an ellipse, parabola or hyperbola, the PDE is called elliptic, parabolic or hyperbolic, respectively.
  (Cf. conic sections.)
- Governed by the discriminant Δ of the leading quadratic form,

$$\Delta = b^2 - ac, \qquad \begin{cases} \Delta < 0, & \text{elliptic, e.g. } u_{xx} + u_{yy} = 0, \\ \Delta = 0, & \text{parabolic, e.g. } u_x - u_{yy} = 0, \\ \Delta > 0, & \text{hyperbolic, e.g. } u_{xx} - u_{yy} = 0. \end{cases}$$

- PDE type governed by the highest derivatives in L ("principal part of L") i.e. the coefficients a, b, c.

Classification of PDEs

- First order PDEs ($a = b = c = 0$) are classified as hyperbolic if
  - $u_t + au_x = 0$, a real
  - $\boldsymbol{u}_t + A\boldsymbol{u}_x = 0$, A diagonalizable with real eigenvalues
  - $\boldsymbol{u}_t + A\boldsymbol{u}_x + B\boldsymbol{u}_y = 0$, $\alpha_1 A + \alpha_2 B$ ———"——— for all $\alpha_1, \alpha_2 \in \mathbb{R}$
  - $\boldsymbol{u}_t + \boldsymbol{F}(\boldsymbol{u})_x = 0$, $J(\boldsymbol{u})$ ———"——— for all $\boldsymbol{u}(x, t)$

  Typical case is that A, B, J are real symmetric matrices.
- In higher dimensions, $u = u(x_1, \ldots, x_n)$, the second order PDE

$$\sum_{k,\ell=1}^{n} a_{k,\ell} u_{x_k,x_\ell} =: \nabla \cdot (A \nabla u) = 0,$$

  is classified according to the eigenvalues of A:
  - Elliptic: all eigenvalues have same sign, and are non-zero,
  - Parabolic: as elliptic, except one eigenvalue is zero,
  - Hyperbolic: as elliptic, except one eigenvalue has different sign.
- Classifications do not cover all PDEs, e.g. the Schrödinger equation where one parameter is complex, many higher order equations and equations in higher dimensions.

PDE types

Combinations common, e.g.

- Convection–diffusion equation $u = u(x, t)$

$$u_t + u_x - \varepsilon u_{xx} = 0,$$

(weakly parabolic if $\varepsilon \ll 1$).

- Vlasov–Poison equation $u = u(x, y, v, w, t)$, $\phi = \phi(x, y, t)$

$$u_t + vu_x + wu_y + \phi_x u_v + \phi_y u_w = 0,$$
$$-(\phi_{xx} + \phi_{yy}) = \int udvdw.$$

Here u is the density of charged particles at (x, y) with velocity (v, w) and ϕ is the electric potential.

Alternative form, if $u = u(\boldsymbol{x}, \boldsymbol{v}, t)$, $\phi = \phi(\boldsymbol{x}, t)$,

$$u_t + \boldsymbol{v} \cdot \nabla_x u + \nabla_x \phi \cdot \nabla_v u = 0, \qquad -\Delta\phi = \int ud\boldsymbol{v}.$$

Adding realism

PDEs above model idealized and simplified situations. Reality more complicated, although most important features and numerical difficulties captured by model equations.

Examples of additional issues:

- Higher dimensions

$$u_t - u_{xx} = 0 \quad \Rightarrow \quad u_t - \Delta u = 0.$$

- Systems of equations

$$u_t + u_x = 0 \quad \Rightarrow \quad \boldsymbol{u}_t + A\boldsymbol{u}_x = 0.$$

  Ex.: Maxwell equations $\boldsymbol{u} = (\boldsymbol{B}, \boldsymbol{H})^T$.
- Variable coefficients

$$u_t + u_x = 0 \quad \Rightarrow \quad u_t + (a(x)u)_x = 0,$$
$$u_t - \Delta u = 0 \quad \Rightarrow \quad u_t + \nabla \cdot (\kappa(x)\nabla u) = 0.$$

  Ex.: Material properties that vary in space.

Adding realism

- Source terms

$$u_t + u_x = 0 \quad \Rightarrow \quad u_t + u_x = f(x,t).$$

- Nonlinearities

$$u_t + u_x = 0 \quad \Rightarrow \quad u_t + f(u)_x = 0.$$

Ex.: Isentropic flow: $(m = \rho u)$

$$\boldsymbol{u}_t + \boldsymbol{F}(\boldsymbol{u})_x = 0, \qquad \boldsymbol{u} = \begin{pmatrix} \rho \\ m \end{pmatrix}, \quad \boldsymbol{F}(u) = \begin{pmatrix} \rho u \\ \frac{m^2}{\rho} + \kappa \rho^\gamma \end{pmatrix}.$$

- Combinations of the above (see Chapter 5 in Edsberg).
Ex. Incompressible Navier–Stokes equations:

$$\underbrace{\boldsymbol{u}_t + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u}}_{\text{nonlinear advection}} = \underbrace{\boldsymbol{g}}_{\text{source (gravity)}} - \nabla p + \underbrace{\mu \Delta \boldsymbol{u}}_{\text{parabolic term}},$$

$$\underbrace{\nabla \cdot \boldsymbol{u} = 0.}_{\text{elliptic equation (in disguise)}}$$

Physical origins of some PDEs

Two examples of physics principles that leads to PDE models are:

- Conservation.

  Conservation of mass, momentum, energy, . . . in time plus constitutive relation for flux lead to parabolic and hyperbolic equations, called conservation laws.

- Energy minimization.

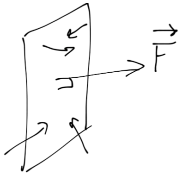
  Equilibrium obtained from energy minimization leads to elliptic equations.

Conservation laws

Many classical PDEs are based on conservation principles and derived as follows.

- Let $u(t, x)$ be the unknown, e.g. the number of particles per volume moving around in a fluid.
- Define the flux $\boldsymbol{F}(t, x)$ such that

$$\begin{aligned} |\boldsymbol{F}| := &\text{ net number of particles flowing in} \\ &\text{ direction } \boldsymbol{F} \text{ per area and time} \end{aligned}$$



(i.e. net number of particles flowing through a m^2 surface orthogonal to $\boldsymbol{F}$ per second)

- Then the net total number of particles passing through a surface S per second is

$$Q(t) = \int_S \boldsymbol{F} \cdot \vec{n} \, dS,$$

where $\vec{n}$ is the surface normal.

Conservation laws, cont.

- Let Ω be a volume with surface area $\partial\Omega$. Because of conservation of particles (no new are created or destroyed),

$$\underbrace{\frac{d}{dt}\underbrace{\int_{\Omega} u\,dx}_{\text{\# particles in }\Omega}}_{\text{change in \# particles}} = \underbrace{-Q(t)}_{\substack{\text{\# particles flowing}\\ \text{out through }\partial\Omega}} = -\int_{\partial\Omega} \boldsymbol{F}\cdot\vec{n}\,dS.$$

- This gives the conservation law for u in integral (weak) form

$$\int_{\Omega} u_t\,dx + \int_{\partial\Omega} \boldsymbol{F}\cdot\vec{n}\,dS = 0, \qquad \forall\Omega.$$

- Applying the divergence theorem to second integral gives

$$\int_{\Omega} u_t\,dx + \int_{\Omega} \nabla\cdot\boldsymbol{F}\,dx = 0, \qquad \forall\Omega.$$

- True for any Ω. If u and $\boldsymbol{F}$ are smooth enough it will also hold pointwise

$$u_t + \nabla\cdot\boldsymbol{F} = 0.$$

  This is the conservation law for u in differential (strong) form.

Remarks

- The conservation law
$$u_t + \nabla \cdot \boldsymbol{F} = 0,$$
is the mathematical encoding of the conservation property.
- Precisely the same arguments can be made for anything that is conserved, such as mass, momentum, energy, heat, etc.
- The dynamics of such quantities will therefore all satisfy conservation laws with *some* flux $\boldsymbol{F}$.
- If $f(x, t)$ particles are created/destroyed per volume · time, then
$$\frac{d}{dt}\int_\Omega u\,dx = \underbrace{-Q(t)}_{\substack{\text{\# particles flowing}\\ \text{out through } \partial\Omega}} + \underbrace{\int_\Omega f\,dx}_{\substack{\text{\# particles created or}\\ \text{destroyed}}} = \int_\Omega -\nabla \cdot \boldsymbol{F} + f\,dx,$$
which gives the conservation law with a source term,
$$u_t + \nabla \cdot \boldsymbol{F} = f.$$

Conservation laws, fluxes

- The conservation law,

$$u_t + \nabla \cdot \boldsymbol{F} = 0, \qquad \text{is not closed.}$$

  Only one equation, but $n+1$ unknowns in n dimensions $(u, \boldsymbol{F})$.
- Need to express $\boldsymbol{F}$ in terms of u. Use constitutive relations based on more precise physics.
- Example 1: Particles moving passively with constant (known) velocity $\boldsymbol{v}$. Then

$$\boldsymbol{F} = u\boldsymbol{v},$$

  particles per unit area and time, and the PDE becomes

$$u_t + \nabla \cdot (u\boldsymbol{v}) = u_t + \boldsymbol{v} \cdot \nabla u = 0,$$

  which is the advection equation.

Conservation laws, flux examples

- Example 2: For large number of particles moving randomly the flux follows Fick's law,

$$\boldsymbol{F} = -d\nabla u, \qquad d = \text{diffusion coefficient.}$$

  This gives the diffusion equation

$$u_t - \nabla \cdot (d\nabla u) = 0.$$

  Note: Net flux of particles in the direction of the negative gradient of the concentration means net flow from regions with many particles to regions with fewer particles, pushing the particles to be more evenly distributed.

- Example 3: Heat conduction, where u is the temperature. The (heat) flux satisfies Fourier's law

$$\boldsymbol{F} = -\kappa\nabla u, \qquad \kappa = \text{thermal conductivity.}$$

  This gives the heat equation

$$u_t - \nabla \cdot (\kappa\nabla u) = 0.$$

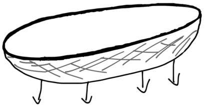
- In general, if $\boldsymbol{F}$ depends locally on u, the PDE is hyperbolic, if it depends on ∇u, it is parabolic. PDE is linear/nonlinear if $\boldsymbol{F}$ is.

Energy minimization principle

Equilibrium states resulting from energy minimization are described by elliptic equations.

Example: The membrane problem.

Let $f(x)$ be the load distribution and $u(x)$ the resulting displacement of the membrane.



- The potential energy of this system for a given u is

$$W[u] = \int_\Omega \underbrace{\frac{|\nabla u(x)|^2}{2}}_{\text{elastic energy}} - \underbrace{f(x)u(x)}_{\text{work by } f}\, dx.$$

- The physical solution u^* is the function which minimizes $W[u]$ over all functions which are zero on $\partial\Omega$.

Membrane problem

- Mathematically, we need to solve the minimization problem:

  Find $u^* \in \mathcal{V}$ such that

  $$W[u^*] \leq W[u], \qquad \forall u \in \mathcal{V},$$

  where $\mathcal{V}$ is a function space of all *admissible functions*.
- A good choice for $\mathcal{V}$ in this context is the Sobolev space $H_0^1(\Omega)$, which contains functions u such that

  $$\begin{aligned} u &\in L^2(\Omega), \qquad \text{i.e. } \int_\Omega u^2 dx < \infty, \\ \nabla u &\in L^2(\Omega), \qquad \text{i.e. } \int_\Omega |\nabla u|^2 dx < \infty, \\ u &= 0 \text{ on } \partial\Omega. \end{aligned}$$

- Note: The first two conditions ensure that the potential energy $W[u]$ is bounded when $f \in L^2(\Omega)$.

Variational calculus

Variational calculus can now be used to characterize the solution u^*.

- For any $\varepsilon \in \mathbb{R}$ and $v \in \mathcal{V}$ we should have

$$J_v(\varepsilon) \equiv W[u^* + \varepsilon v] \geq W[u^*],$$

  since $u + \varepsilon v \in \mathcal{V}$ if $u, v \in \mathcal{V}$.
- Therefore $J_v(\varepsilon)$ has a global minimum at $\varepsilon = 0$ for all $v \in \mathcal{V}$.
- Hence,

$$0 = \frac{dJ_v(0)}{d\varepsilon} = \frac{d}{d\varepsilon} W[u^* + \varepsilon v]\Big|_{\varepsilon=0}.$$

- But,

$$W[u^*+\varepsilon v] = \int_\Omega \frac{|\nabla u^*|^2}{2} - fudx + \varepsilon \int_\Omega \nabla u^* \cdot \nabla v - fvdx + \varepsilon^2 \int_\Omega \frac{|\nabla v|^2}{2} dx.$$

- Consequently,

$$\int_\Omega \nabla u^* \cdot \nabla v - fvdx = 0, \qquad \forall v \in \mathcal{V}.$$

Conclusions

We showed u^* is a solution to the weak form of the Poisson equation:

$$\text{Find } u \in \mathcal{V} \text{ such that:} \qquad \int_\Omega \nabla u \cdot \nabla v - fv dx = 0, \qquad \forall v \in \mathcal{V}. \tag{1}$$

- If u^* is smooth enough, i.e. $u^* \in C^2(\Omega)$, then we can integrate by parts in (1) to get
$$\int_\Omega (-\Delta u^* - f) v dx = 0, \qquad \forall v \in \mathcal{V},$$
which is enough to conclude that u^* satsfies the usual strong form of the Poisson equation

$$\text{Find } u \in \mathcal{V} \text{ such that:} \quad -\Delta u = f \quad \text{in } \Omega \qquad \text{and } u = 0 \text{ on } \partial\Omega.$$

Generalizations

- In general the energy W would have the form

$$W[u] = \int_\Omega L(x, u, \nabla u) dx,$$

for some nonlinear function $L = L(x, u, q)$.

- The procedure above would then lead to the weak form: Find $u \in \mathcal{V}$ such that

$$\int_\Omega \nabla_q L(x, u, \nabla u) \cdot \nabla v + L_u(x, u, \nabla u) v dx = 0, \qquad \forall v \in \mathcal{V}.$$

- The strong form is the Euler–Lagrange equation

$$\begin{aligned} \nabla_x \cdot \nabla_q L(x, u, \nabla u) - L_u(x, u, \nabla u) &= 0, && \text{in } \Omega. \\ u &= 0, && \text{on } \partial\Omega, \end{aligned}$$

which is elliptic if the solution represents a *strict* local minimum of the energy.

Weak and strong forms of PDE

Compare weak forms

$$\int_\Omega u_t\,dx + \int_{\partial\Omega} \boldsymbol{F}\cdot\vec{n}\,dS = 0, \qquad \int_\Omega \nabla u\cdot\nabla v - fv dx = 0,$$

(for all Ω, v) and strong forms

$$u_t + \nabla\cdot\boldsymbol{F} = 0, \qquad -\Delta u = f.$$

- Strong form compact and more intuitive. Basis for finite difference methods. Weak form used in finite elements and finite volumes.
- Strong form requires functions. Not well-defined for instance when $\boldsymbol{F}$ is discontinuous (common in hyperbolic problems) and f is not differentiable (e.g. point load in membrane problem).
- Weak form more general. Solutions well-defined for a larger class of problems. (A strong solution is also a weak solution.)
- Weak forms typically closer to the "truth". Most conservation laws and elliptic PDEs models an underlying problem of the types described above. The weak form then gives the physically relevant solutions when the strong form imposes too strong regularity conditions.
- For rigorous mathemathical analysis the weak form is preferred.