Numerically Solving Partial Differential Equations
— Introduction —

MECH 309 - *Numerical Methods in Mech. Eng.*

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Partial Differential Equations

- Partial differential equations (PDEs) are differential equations involving partial derivatives of an unknown function with respect to more than one independent variable.
  - An ODE has derivatives with respect to one variable, such as time in Newton's second law,
  $$\frac{\mathrm{d}^2 q(t)}{\mathrm{d}t^2} = -\frac{k}{m} q(t) - \frac{b}{m}\frac{\mathrm{d}q(t)}{\mathrm{d}t}, \quad \underbrace{q(0),\ \dot{q}(0) \in \mathbb{R}}_{\text{IVP}} \quad \text{or} \quad \underbrace{q(t_{\text{start}}),\ q(t_{\text{end}})}_{\text{BVP}} \in \mathbb{R}.$$
  - A PDE has partial derivatives with respect to two or more variables, such as x and y in Laplace's equation,
  $$\begin{aligned} \frac{\partial^2 T(x,y)}{\partial x^2} + \frac{\partial^2 T(x,y)}{\partial y^2} &= 0, \\ T(0,y) = 0, \quad 0 < y < b&, \\ T(a,y) = f(y), \quad 0 < y < b&, \\ T(x,0) = 0, \quad 0 < x < a&, \\ T(x,b) = 0, \quad 0 < x < a&. \end{aligned}$$
- PDEs are subject to *boundary conditions*, or even both initial and boundary conditions, meaning PDEs are inherently *boundary-value problems*.

Famous PDEs

- *Navier-Stokes equations* describe the relationship between velocity, density, pressure, and viscosity in a fluid such as air or water.
  - Used in the design of airfoils, wind turbines, propellers, etc.
- *Elasticity equations* describe the relationship between stress and strain in vibrations or structural problems.
  - Used in the design of anything under load, such as bridges, cranes, railway cars, etc.
- *Maxwell's equations* describe the relationship between electric and magnetic field strengths, magnetic flux density, electric charge, current densities in an electromagnetic field.
  - Used to design electric motors, wireless communications hardware, radar, and other electronic technology.
- *Schrödinger's equations of quantum mechanics* describe the relationship between the mass, potential energy, and total energy of the wave function of a particle.
  - Allows a wave interpretation of quantum-mechanical systems that in turn enables solution methods using Fourier series.
- *Einstein's equations of general relativity* describe the relationship between the curvature of spacetime and the energy density of matter in a gravitational field.

Advances in Technology $=$ Solving PDEs *Numerically*

- Although simplified forms of the aforementioned PDEs admit analytical solutions, PDEs describing realistic physical phenomena do NOT admit analytical solutions.
- Not until the digital revolution, and the creation/invention of *numerical solutions* to PDEs, were realistic PDEs solvable.
- Being able to solve realistic PDEs that admit NO analytical solution has *changed the world*.
  - Safer cars, more fuel efficient, cars and aircraft.
  - Clean energy technologies such as wind turbines.
  - Medical technologies.
  - Many more examples.
- Yes . . . numerical methods to solve PDEs has *changed the world* . . . for the better!
  - Actually, ALL numerical methods encountered in this class have *changed the world*.
  - For example, no GPS without nonlinear least squares, no self-driving cars without constrained least squares, no Amazon next-day delivery without optimization, etc.

Notation

- Consider $f : \mathbb{R}^3 \to \mathbb{R}$, $\mathbf{x} = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix}^\mathsf{T} \in \mathbb{R}^3$, and $\mathbf{u} : \mathbb{R}^3 \to \mathbb{R}^3$.
- The gradient of $f(\mathbf{x})$ is

$$\boldsymbol{\nabla} f(\mathbf{x}) = \begin{bmatrix} \frac{\partial}{\partial x_1} \\ \frac{\partial}{\partial x_2} \\ \frac{\partial}{\partial x_3} \end{bmatrix} f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f(\mathbf{x})}{\partial x_1} \\ \frac{\partial f(\mathbf{x})}{\partial x_2} \\ \frac{\partial f(\mathbf{x})}{\partial x_3} \end{bmatrix}. \tag{1}$$

- The divergence of $\mathbf{u}(\mathbf{x})$ is

$$\boldsymbol{\nabla}^\mathsf{T} \mathbf{u}(\mathbf{x}) = \begin{bmatrix} \frac{\partial}{\partial x_1} & \frac{\partial}{\partial x_2} & \frac{\partial}{\partial x_3} \end{bmatrix} \begin{bmatrix} u_1(\mathbf{x}) \\ u_2(\mathbf{x}) \\ u_3(\mathbf{x}) \end{bmatrix} = \frac{\partial u_1(\mathbf{x})}{\partial x_1} + \frac{\partial u_2(\mathbf{x})}{\partial x_2} + \frac{\partial u_3(\mathbf{x})}{\partial x_3} = \sum_{\imath=1}^{3} \frac{\partial u_\imath(\mathbf{x})}{\partial x_\imath}. \tag{2}$$

- The curl of $\mathbf{u}(\mathbf{x})$ is

$$\boldsymbol{\nabla}^{\times}\mathbf{u}(\mathbf{x}) = \begin{bmatrix} 0 & -\frac{\partial}{\partial x_3} & \frac{\partial}{\partial x_2} \\ \frac{\partial}{\partial x_3} & 0 & -\frac{\partial}{\partial x_1} \\ -\frac{\partial}{\partial x_2} & \frac{\partial}{\partial x_1} & 0 \end{bmatrix} \begin{bmatrix} u_1(\mathbf{x}) \\ u_2(\mathbf{x}) \\ u_3(\mathbf{x}) \end{bmatrix} = \begin{bmatrix} \frac{\partial u_3(\mathbf{x})}{\partial x_2} - \frac{\partial u_2(\mathbf{x})}{\partial x_3} \\ \frac{\partial u_1(\mathbf{x})}{\partial x_3} - \frac{\partial u_3(\mathbf{x})}{\partial x_1} \\ \frac{\partial u_2(\mathbf{x})}{\partial x_1} - \frac{\partial u_1(\mathbf{x})}{\partial x_2} \end{bmatrix}, \tag{3}$$

where the “cross matrix” is

$$\mathbf{x}^{\times} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}^{\times} = \begin{bmatrix} 0 & -x_3 & x_2 \\ x_3 & 0 & -x_1 \\ -x_2 & x_1 & 0 \end{bmatrix}. \tag{4}$$

- The Laplacian of $f(\mathbf{x})$ is

$$\boldsymbol{\nabla}^2 f(\mathbf{x}) = \boldsymbol{\nabla}^{\mathsf{T}}\boldsymbol{\nabla} f(\mathbf{x}) = \begin{bmatrix} \frac{\partial}{\partial x_1} & \frac{\partial}{\partial x_2} & \frac{\partial}{\partial x_3} \end{bmatrix} \begin{bmatrix} \frac{\partial f(\mathbf{x})}{\partial x_1} \\ \frac{\partial f(\mathbf{x})}{\partial x_2} \\ \frac{\partial f(\mathbf{x})}{\partial x_3} \end{bmatrix} = \frac{\partial^2 f(\mathbf{x})}{\partial x_1^2} + \frac{\partial^2 f(\mathbf{x})}{\partial x_2^2} + \frac{\partial^2 f(\mathbf{x})}{\partial x_3^2} = \sum_{\imath=1}^{3} \frac{\partial^2 f(\mathbf{x})}{\partial x_\imath^2}. \tag{5}$$

- It’s standard to use the notation

$$u_x = \frac{\partial u(x,y,z)}{\partial x}, \quad u_y = \frac{\partial u(x,y,z)}{\partial y}, \quad u_{xy} = \frac{\partial^2 u(x,y,z)}{\partial x \partial y}, \quad \text{etc.,} \tag{6}$$

for partial derivatives within PDEs.

Order

- The *order* of a PDE is the order of the highest derivative.
- For example,

$$u_{xx} + 3u_y - u_z = xyz$$

  is a second-order PDE, where $u(x, y, z)$.

Linear versus Nonlinear

- Consider $u : \mathbb{R}^n \to \mathbb{R}$ where $n = 2$ or $n = 3$. For simplicity, think of $u(x, y)$ or $u(x, y, z)$.
- The PDE

$$u_{xx} + 3u_y - u_z = xyz$$

  is a second-order, linear, nonhomogenous, PDE.
- The PDE

$$(u_{xx})^2 - u_{xy} = 0$$

  is a second-order, nonlinear, homogenous, PDE.

Linearity in More Detail

- The word *linear* means superposition and scaling must hold.
- In the context of a PDE, what must be linear?
- A PDE such as

  $$u_{xx} + 3u_y - u_z = xyz$$

  can be written in *operator form*

  $$\mathcal{L}u(x, y, z) = f(z, y, z).$$

- In particular,

$$\begin{aligned} u_{xx} + 3u_y - u_z &= xyz, \\ \frac{\partial^2 u(x,y,z)}{\partial x^2} + 3\frac{\partial u(x,y,z)}{\partial y} - \frac{\partial u(x,y,z)}{\partial z} &= xyz, \\ \underbrace{\left(\frac{\partial^2}{\partial x^2} + 3\frac{\partial}{\partial y} - \frac{\partial}{\partial z}\right) u(x,y,z)}_{\mathcal{L}u(x,y,z)} &= \underbrace{xyz}_{f(x,y,z)}. \end{aligned}$$

- If the operator $\mathcal{L}$ satisfies superposition and scaling in $u(x, y, z)$ on the domain of interest, the operator is linear, and the PDE is linear.
- To be extra clear, if superposition

$$\mathcal{L}(u(x,y,z)+v(x,y,z)) = f(z,y,z)+g(x,y,z)$$
$$\Updownarrow$$
$$\mathcal{L}u(x,y,z)+\mathcal{L}v(x,y,z) = f(z,y,z)+g(z,y,z)$$

  and scaling

$$\mathcal{L}(\alpha u(x,y,z)) = \alpha f(z,y,z),$$
$$\Updownarrow$$
$$\alpha\left(\mathcal{L}u(x,y,z)\right) = \alpha f(z,y,z)$$

  both hold on the domain of interest, the PDE is linear.

- Is the PDE

$$u_{xx} + 3u_y - u_z = xyz$$

  linear?
- Check superposition. To this end,

$$\begin{aligned}
\mathcal{L}(u(x,y,z) + v(x,y,z)) &= f(z,y,z) + g(x,y,z), \\
\left(\frac{\partial^2}{\partial x^2} + 3\frac{\partial}{\partial y} - \frac{\partial}{\partial z}\right)(u(x,y,z) + v(x,y,z)) &= (xyz + xyz) \\
\left(\frac{\partial^2 u(x,y,z)}{\partial x^2} + 3\frac{\partial u(x,y,z)}{\partial y} - \frac{\partial u(x,y,z)}{\partial z}\right) + & \\
\left(\frac{\partial^2 v(x,y,z)}{\partial x^2} + 3\frac{\partial v(x,y,z)}{\partial y} - \frac{\partial v(x,y,z)}{\partial z}\right) &= (xyz) + (xyz), \\
\mathcal{L}u(x,y,z) + \mathcal{L}v(x,y,z) = f(z,y,z) + g(z,y,z).
\end{aligned}$$

- Superposition holds!

- Check scaling. It follows that

$$
\begin{aligned}
\mathcal{L}(\alpha u(x,y,z)) &= \alpha f(z,y,z),\\
\left(\frac{\partial^2}{\partial x^2} + 3\frac{\partial}{\partial y} - \frac{\partial}{\partial z}\right)(\alpha u(x,y,z)) &= \alpha(xyz)\\
\alpha\left(\frac{\partial^2 u(x,y,z)}{\partial x^2} + 3\frac{\partial u(x,y,z)}{\partial y} - \frac{\partial u(x,y,z)}{\partial z}\right) &= \alpha(xyz),\\
\alpha\left(\mathcal{L}u(x,y,z)\right) &= \alpha f(z,y,z).
\end{aligned}
$$

- Scaling holds!
- Because the operator satisfies superposition and scaling, the PDE is linear!

Second-Order PDEs

- A second-order PDE is of the form

$$a u_{xx} + 2b u_{xy} + c u_{yy} + d u_x + e u_y + \phi u = f, \tag{7}$$

  where the coefficients a, b, c, d, e, ϕ could be constant or a function of x, y, and $f = f(x, y)$ in general.
- The PDE (7) is
  - **elliptic** if $b^2 - ac < 0$.
  - **parabolic** if $b^2 - ac = 0$,
  - **hyperbolic** if $b^2 - ac > 0$,
- This terminology is analogous to a conic section,

$$a x^2 + 2bxy + c y^2 + dx + ey + \phi = 0,$$

  which describes an ellipse, parabola, or hyperbola according to the sign of the discriminant $b^2 - ac$.

Examples of Elliptic, Parabolic, and Hyperbolic PDEs

- The *Laplace equation* is
$$u_{xx} + u_{yy} = 0,$$
is elliptic because $b^2 - ac = 0^2 - (1)(1) = -1 < 0$.
  - The Laplace equation describes the velocity potential of irrotational incompressible flows, steady-state heat distribution, a voltage field, etc.
- The *diffusion equation*, also called the *heat equation*, is
$$u_t = \alpha^2 u_{xx},$$
where $y = t$ and α^2 is constant is parabolic because $b^2 - ac = 0^2 - (\alpha^2)(0) = 0$.
  - The diffusion equation describes the diffusion of heat via condition, or the diffusion of a anti-cancer drugs in an organ, or the diffusion of a chemical in water.
- The *wave equation* is
$$u_{tt} = c^2 u_{xx},$$
where $y = t$ and c^2 is constant is hyperbolic because $b^2 - ac = 0^2 - (c^2)(-1) = c^2 > 0$.
  - The wave equation describes any wave phenomena: acoustics, vibrations, water waves, electromagnetic waves, etc.

General Classification

- Second order, liner, constant coefficient, nonhomogenous PDEs are always of the form
$$\sum_{\imath=1}^{n}\sum_{\jmath=1}^{n} a_{\imath\jmath}\frac{\partial^2 u(\mathbf{x})}{\partial x_\imath \partial x_\jmath} + \sum_{\imath=1}^{n} b_\imath \frac{\partial u(\mathbf{x})}{\partial x_\imath} + cu(\mathbf{x}) = f(\mathbf{x}), \tag{8}$$
where $u(\mathbf{x}) = u(x_1, x_2, \cdots, x_{n-1}, x_n)$.
- Let $\boldsymbol{\nabla} = \begin{bmatrix} \frac{\partial}{\partial x_1} & \frac{\partial}{\partial x_2} & \cdots & \frac{\partial}{\partial x_{n-1}} & \frac{\partial}{\partial x_n} \end{bmatrix}^\mathsf{T}$.
- Equation (8) can then be written in operator form,
$$\left(\boldsymbol{\nabla}^\mathsf{T}\mathbf{A}\boldsymbol{\nabla} + \boldsymbol{\nabla}^\mathsf{T}\mathbf{b} + c\right) u(\mathbf{x}) = f(\mathbf{x}),$$
where $\mathbf{A}$ is symmetric.
- The type of PDE is dictated by the definiteness of $\mathbf{A}$.
  - If $\mathbf{A} > 0$ or $\mathbf{A} < 0$ the PDE is **elliptic**.
  - If $\mathbf{A} \geq 0$ or $\mathbf{A} \leq 0$ the PDE is **parabolic**.
  - If $\mathbf{A}$ has just one eigenvalue a different sign from the rest the PDE is **hyperbolic**.
    - For instance, when the eigenvalues are $1, 2, -1$.
  - If none of the above are satisfied the PDE is **ultra-hyperbolic**.

- The *Laplace equation*

$$u_{xx} + u_{yy} = 0,$$

can be written as

$$\left(\boldsymbol{\nabla}^{\mathsf{T}}\mathbf{A}\boldsymbol{\nabla}\right) u(x,y) = 0, \qquad \mathbf{A} = \mathbf{1} > 0,$$

indicating the PDE is elliptic.

- The *diffusion equation*

$$\alpha^2 u_{xx} = u_t,$$

can be written as

$$\left(\nabla^{\mathsf{T}} \mathbf{A} \nabla + \nabla^{\mathsf{T}} \mathbf{b}\right) u(x,t) = 0, \qquad \mathbf{A} = \begin{bmatrix} \alpha^2 & 0 \\ 0 & 0 \end{bmatrix} \geq 0, \quad \mathbf{b} = \begin{bmatrix} 0 \\ -1 \end{bmatrix},$$

indicating the PDE is parabolic.

  - Note, $\nabla = \begin{bmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial t} \end{bmatrix}$.

- The *wave equation*

$$c^2 u_{xx} = u_{tt},$$

can be written as

$$\left(\boldsymbol{\nabla}^{\mathsf{T}} \mathbf{A} \boldsymbol{\nabla}\right) u(x,t) = 0, \qquad \mathbf{A} = \begin{bmatrix} c^2 & 0 \\ 0 & -1 \end{bmatrix},$$

where the eigenvalues of $\mathbf{A}$ are c^2 and -1. The PDE is hyperpolic.

  - Again, note that $\boldsymbol{\nabla} = \begin{bmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial t} \end{bmatrix}$.

Boundary Conditions

- Just like an ODE is not complete with either initial conditions (as in an IVP) or boundary conditions (as in a BVP), a PDE is not complete without initial conditions (ICs) or boundary conditions (BCs), or sometimes both.
- There are three types of BCs that can be specified on $\partial\Omega$, the boundary of the problem domain Ω.
  - **Dirichlet** BCs specify $u(\mathbf{x})$ for all $\mathbf{x} \in \partial\Omega$.
  - **Neumann** BCs specify the derivative of $u(\mathbf{x})$ for all $\mathbf{x} \in \partial\Omega$.
  - **Robin** BCs specify a mix of $u(\mathbf{x})$ and the derivative of $u(\mathbf{x})$ for all $\mathbf{x} \in \partial\Omega$.

Existence, Uniqueness, Conditioning (Stability)

- This is complicated.
- We will just assume when given a PDE with BCs a solutions exists and the solution is unique, and the problem is well conditioned (asymptotically stable).

References

Slides based on [1, Ch. 18, 19, 20], [2, Ch. 12, 15], [3, Ch. 16], [4, Ch. 11].

Additional inspiration taken from ME 303 - Engineering Mathematics (2004 version) taught by Prof. Davidson (U. Waterloo).

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