NENG 685, Class 4, Fall 2017
(Nuclear) Engineering Equations:
October 16, 2017

Introduction

In science and engineering in general, and nuclear engineering in specific, we encounter a wide range of mathematical physics equations. In today's lecture we will introduce some of them.

- Ordinary differential equations (ODEs)
- Partial differential equations (PDEs)
  - Elliptic PDEs
  - Parabolic PDEs
  - Hyperbolic PDEs
- Integro-differential equations
- Integral equations

1 ODEs

The most general form of an n^{th} order linear ordinary differential eqn. is

$$a_n(x)y^{(n)}(x) + a_{n-1}(x)y^{(n-1)}(x) + \cdots + a_2(x)y^{(2)}(x) + a_1(x)y'(x) + a_0(x)y(x) = f(x)$$

where

- a_n are coefficients
- $y^{(n)}$ is the n^{th} derivative of y.

Boundary conditions:

1. Initial Value Problem (**IVP**): if y and its derivatives are given at one end of the domain/interval (e.g. time zero if there's time or spatial starting point if there's only space, etc.)

2. Boundary Value Problem (**BVP**): if y and/or its derivatives are given at each end of the interval

Linear 1st order ODE's

Reminders

- 1st order means that $n = 1$. The coefficients a_1 and a_0 may depend on y or y'.
- Linear means each coefficient only depends on x (i.e., not on y or derivatives of y).

Linear 1st order ODE Example:

$$\frac{dy}{dx} + 3y(x) = \sin(x) \qquad x \in [0, 1]$$

- IVP if boundary conditions are y(0) = 1; y'(0) = 2
- BVP if boundary conditions are y(0)=-1, y(1) = 3

In this case the general solution is obtained through the use of an integrating factor.

Linear 1st order ODE Example:

Point Kinetics analysis of a nuclear reactor is an IVP, linear, 1st order ODE.

$$\begin{aligned}\frac{dn(t)}{dt} &= \frac{\rho(t) - \beta}{l^*} n(t) + \sum_{i=1}^{N} \lambda_i C_i(t) \\ \frac{dC_i(t)}{dt} &= \frac{\beta_i}{l^*} n(t) - \lambda_i C_i(t) \qquad i = 1, \ldots, N\end{aligned}$$

Where (we'll talk more about what these terms mean later)

- n = # neutrons / s
- β = fraction of delayed neutrons
- λ_i = effective decay constant of the ith precursor
- $C_i(t)$ = delayed neutron concentration of the ith precursor
- l^* = mean neutron lifetime
- $\rho = \frac{k-1}{k}$ = reactivity

BCs: $n(0) = n_0$ and $C_i(0) = C_{i,0}$ for $i = 1, \ldots, N$.

Linear 1st order ODE Example:

The number of atoms in a sample during radioactive decay (assuming decay only here) is described by the Bateman equation, which is a linear, 1st order ODE that is in an IVP:

$$\begin{aligned}
\frac{dN_1(t)}{dt} &= -\lambda_1 N_1(t) \\
\frac{dN_i(t)}{dt} &= -\lambda_i N_i(t) + \lambda_{i-1} N_{i-1}(t) \qquad 1 < i < I \\
\frac{dN_I(t)}{dt} &= \lambda_{I-1} N_{I-1}(t) \\
\text{BC: } & N_i(t=0) = N_{i,0}
\end{aligned}$$

note: isotope i decays into $i + 1$. This can be adapted for decay branches, and becomes more complicated if we have neutrons that transmute isotopes.

2nd order ODE Example:

1-D, 1-group, time-independent neutron diffusion equation:

$$\begin{aligned}
-\frac{d}{dx} D(x) \frac{d}{dx}\phi(x) + \Sigma_a(x)\phi(x) &= S(x) \qquad \text{Fixed Source} \\
-\frac{d}{dx} D(x) \frac{d}{dx}\phi(x) + \Sigma_a(x)\phi(x) &= \frac{1}{k}\nu\Sigma_f(x)\phi(x) \qquad \text{Fission / Eigenvalue}
\end{aligned}$$

BCs: (BVP) vacuum, $\phi(\pm a) = 0$

Reminder: eigenpairs

We can formulate systems of equations as matrix-vector systems that look like $\mathbf{A}x = \lambda x$.

- An eigenvector is a non-zero vector x that, when multiplied by the matrix $\mathbf{A}$, yields a constant multiple of x.
- The constant multiple, λ, is the eigenvalue corresponding to the eigenvector.
- There can be (and usually are) more than one eigenvalue, and more than one eigenvector.
- Sometime the equation can be reformulated as as $y\mathbf{A} = \alpha y$ (the left eigenvector). In nuclear, we're used to seeing the right eigenvector formulation.

Aside: Recall

$$\text{gradient is } \nabla T = \vec{i}\frac{\partial T}{\partial x} + \vec{j}\frac{\partial T}{\partial y} + \vec{k}\frac{\partial T}{\partial z}$$
$$\text{divergence is } \nabla \cdot \vec{v} = \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z}$$

2 PDEs

A partial differential equation is an equation containing an unknown function of two or more variables and its derivatives with respect to those variables.

If the PDE is linear in u and all derivatives of u, then we say that the PDE is linear.

$$A\frac{\partial^2 u}{\partial x^2} + B\frac{\partial^2 u}{\partial x \partial y} + C\frac{\partial^2 u}{\partial y^2} + D\frac{\partial u}{\partial x} + E\frac{\partial u}{\partial y} + Fu(x,y) = G$$

This equation is a 2nd order PDE in two variables. It is linear if A through G do not depend on u (they may depend on x and/or y).

Classification of PDEs:

Just as one classifies conic sections and quadratic forms into parabolic, hyperbolic, and elliptic based on the discriminant $B^2 - 4AC$, the same can be done for a second-order PDE at a given point.

[To think about classification, think about replacing ∂x by x and ∂y by y. This converts the PDE into a polynomial of the same degree.]

Note: these classifications only apply to second order PDEs.

The reason we care about this in the context of the Transport Equation:

- For time-dependent 1D transport In a void, the transport equation is like a *hyperbolic* wave equation.
- For highly-scattering regions where Σ_s is close to Σ, the equation becomes *elliptic* for the steady-state case.
- If the scattering is forward-peaked then the equation is *parabolic*.

Let's look at the classifications:

- **Elliptic** if $B^2 - 4AC < 0$.

  Some famous elliptic PDEs:

$$
\begin{gathered}
\nabla^2 u = 0 \qquad \text{Laplace's eqn.} \\
\nabla^2 u = f(x) \qquad \text{Poisson's eqn.} \\
-\frac{\partial}{\partial x} D(x,y) \frac{\partial}{\partial x}\phi(x,y) - \frac{\partial}{\partial y} D(x,y) \frac{\partial}{\partial y}\phi(x,y) + \big(\Sigma_a(x,y) - \frac{1}{k}\nu\Sigma_f(x,y)\big)\phi(x,y) = 0
\end{gathered}
$$

  For each of these there's no B term, so $-4AC < 0$ (in the diffusion equation case since $D(x,y)$ is positive).

  One property of constant coefficient elliptic equations is that their solutions can be studied using the Fourier transform.

- **Parabolic** if $B^2 - 4AC = 0$, e.g.

$$
\begin{gathered}
\frac{\partial u}{\partial t} = k\frac{\partial^2 u}{\partial x^2} \qquad \text{1-D heat eqn.} \\
\frac{1}{v}\frac{\partial \phi(x,t)}{\partial t} = \frac{\partial}{\partial x} D(x,t)\frac{\partial}{\partial x}\phi(x,t) + \big(\nu\Sigma_f(x,t) - \Sigma_a(x,t)\big)\phi(x,t) + S(x,t)
\end{gathered}
$$

  There aren't B or C terms, so $-4AC = 0$

  Equations that are parabolic at every point can be transformed into a form analogous to the heat equation by a change of independent variables. Solutions smooth out as the transformed time variable increases.

A perturbation of the initial (or boundary) data of an *elliptic or parabolic* equation is felt at once by essentially all points in the domain.

- **Hyperbolic** if $B^2 - 4AC > 0$, e.g.

$$
\frac{\partial^2 u}{\partial t^2} - c^2\frac{\partial^2 u}{\partial x^2} = 0 \qquad \text{1-D wave eqn.}
$$

  There's no B term, and the C term is negative so $-4AC > 0$

  - if u and its first t derivative are arbitrarily specified with initial data on the initial line $t = 0$ (with sufficient smoothness properties), then there exists a solution for all of t.

  - The solutions of hyperbolic equations are "wave-like." If a disturbance is made in the initial data of a hyperbolic differential equation, then not every point of space feels the disturbance at once.

– Relative to a fixed time coordinate, disturbances have a finite propagation speed. They travel along the characteristics of the equation.

higher order PDE classification

If there are n independent variables $x_1, x_2, \ldots, x_n$, a general linear partial differential equation of second order has the form

$$Lu = \sum_{i=1}^{n}\sum_{j=1}^{n} a_{i,j} \frac{\partial^2 u}{\partial x_i x_j} + \text{ Lower Order Terms } = 0$$

The classification depends upon the signature of the eigenvalues of the coefficient matrix $a_{i,j}$.

1. Elliptic: The eigenvalues are all positive or all negative.
2. Parabolic: The eigenvalues are all positive or all negative, save one that is zero.
3. Hyperbolic: There is only one negative eigenvalue and all the rest are positive, or there is only one positive eigenvalue and all the rest are negative.
4. Ultrahyperbolic: There is more than one positive eigenvalue and more than one negative eigenvalue, and there are no zero eigenvalues. There is only limited theory for ultrahyperbolic equations (Courant and Hilbert, 1962).

3 Integro-Differential Equations

...are equations that involves both integrals and derivatives of a function. The general first-order, linear (only with respect to the term involving the derivative) integro-differential equation is of the form

$$\frac{d}{dx}u(x) + \int_{x_0}^{x} f(t, u(t))dt = g(x, u(x)) \; , \qquad u(x_0) = u_0 \; , \qquad x_0 \geq 0 \; .$$

This is the equation type we will likely deal with the most.

Nuclear Example:

One-dimensional in space, one-dimensional in angle, time-independent, monoenergetic neutron transport equation:

$$\mu\frac{\partial\psi(x,\mu)}{\partial x} + \Sigma_t\psi(x,\mu) = \frac{\Sigma_s}{2}\int_{-1}^{1} d\mu'\psi(x,\mu') + S(x,\mu)$$

where the angular neutron flux is a function of one spatial variable (x) and one angular variable ($\mu = \cos(\theta)$).

4 Integral Equations

...are equations in which an unknown function appears under an integral sign. Integral equations are classified according to three different dichotomies, creating eight different kinds:

1. Limits of integration

   (a) both fixed: Fredholm equation

   $$f(x) = \int_a^b K(x,t)\,\varphi(t)\,dt$$

   (b) one variable: Volterra equation

   $$f(x) = \int_a^x K(x,t)\,\varphi(t)\,dt$$

2. Placement of unknown function

   (a) only inside integral: first kind (both above examples)

   (b) both inside and outside integral: second kind

   $$\varphi(x) = f(x) + \lambda\int_a^x K(x,t)\,\varphi(t)\,dt$$

3. Nature of known function, f

   (a) identically zero: homogeneous

   (b) not identically zero: inhomogeneous

Both Fredholm and Volterra equations are linear integral equations, due to the linear behaviour of $\phi(x)$ under the integral. A nonlinear Volterra integral equation has the general form:

$$\varphi(x) = f(x) + \lambda \int_a^x K(x,t)\, F(x,t,\varphi(t))\, dt$$

where F is a known function.

The integral form of the Neutron Transport Equation is

$$\psi(\vec{r},\hat{\Omega},E) = \int_0^\infty d\rho' \; \exp[-\int_0^{\rho'} d\rho'' \, \Sigma_t(\vec{r}-\rho''\hat{\Omega},E)]q(\vec{r}-\rho'\hat{\Omega},\hat{\Omega},E)$$

where q contains fixed, inscattering, and fission sources. That is, $q = f(\psi)$.