Partial differential equations

Matrix formulation and Spectral methods

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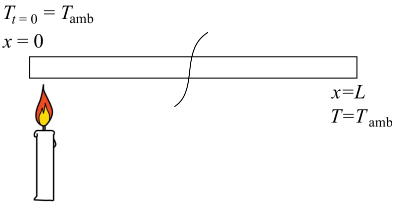
Content

Introduction problem

Problem: Describe the evolution of the temperature distribution of a body (1D rod) being heated in one of its tips



Principle: *Energy conservation*

Consequence: The total variation of the energetic contents within each region in the rod $[x, x + \Delta x]$ equals the net heat flux through the region

Definition of PDE

A partial differential equation (PDE) is an equation establishing a relationship between a function of two or more independent variables and the partial derivatives of this function with respect to these independent variables – i.e., given the multivariate function $f(x_1, x_2, \dots, x_n) : \mathbb{R}^n \longmapsto \mathbb{R}$, the expression

$$F(f, f_{x_1}, f_{x_2}, \dots, fx_n, f_{x_1 x_1}, f_{x_1 x_2}, \dots, f_{x_1 x_2 \cdots x_n}, \dots, f_{x_n \cdots x_{n.}}, x_1, x_2, \dots, x_n) = 0$$

is a PDE where its *order* corresponds to the maximum number of derivatives in the equation

Goal of modeling by PDEs

When approaching to the mathematical modeling of a particular system by PDEs, a major question arises:

Goal of Modeling

Which PDEs are good models for the system?

Scientific method behind

Good models are often the end result of confrontations between experimental data and theory.

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Issues on PDE analysis

1. Does the PDE have any solutions?
2. What kind of "data"do we need to specify in order to solve the PDE?
3. Are the solutions corresponding to the given data unique?
4. What are the basic qualitative properties of the solution?
5. Does the solution contain singularities? If so, what is their nature?
6. What happens if we slightly vary the data? Does the solution then also vary only slightly?
7. What kinds of quantitative estimates can be derived for the solutions?
8. How can we define the size (i.e., "the norm") of a solution in way that is useful for the problem at hand?

Conic section analogy

Conic sections gave name to second-order linear partial differential equation categories because of the analogy of their discriminant, i.e.:

- Conic sections can be written in their general form

$$Ax^2 + Bxy + Cy^2 + Dx + Ey + F = 0$$

- The discriminant $B^2 - 4AC$ permits the classification between hyperbolic, parabolic and elliptic conic sections:

$B^2 - 4AC$	Curve
< 0	Ellipse
$= 0$	Parabola
> 0	Hyperbola

Spatial 2D Second order linear PDE Classification

Spatial 2D Second order linear partial differential equations are of great interest since they are in the base of models in a wide range of Natural Science problems and, then, Engineering applications.

- A general formulation of a 2nd. order linear PDE is as follows:

$$A\partial_{xx}f + B\partial_{xy}f + C\partial_{yy}f + D\partial_{x}f + E\partial_{y}f + Ff = 0$$

so, analogously (just in name!) with conic sections, these equations can be classified as follows:

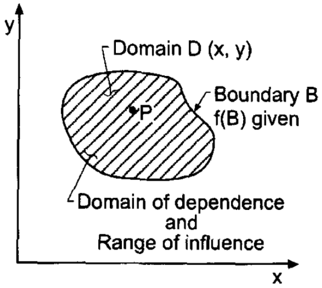
$B^2 - 4AC$	PDE Type	*Characteristic paths*
< 0	Elliptic	Complex
$= 0$	Parabolic	Real and repeated
> 0	Hyperbolic	Real and distinct

Elliptic PDEs

- Elliptic PDE equations are closely related to Equilibrium problems
- Their solution in each point depends on the value of the solution function across the entire domain under consideration. Then, its numerical solution is usually approached by *relaxation algorithms*
- Example: steady heat diffusion (homogeneous Laplacian problem)

$$\nabla^2 T = 0$$

  subject to $aT + bT_n = c$
- Laplacian operator applies as follows: $\nabla^2 T = \Delta T = (\partial_{xx} T + \partial_{yy} T)$

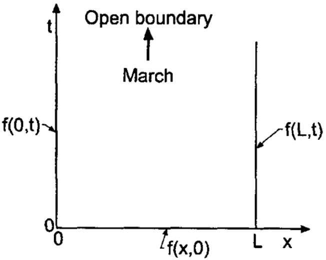


Parabolic PDEs: Heat equation

- Parabolic equations are initial value problems in open domains for at least, one varible.
- They are usually related to Propagation problems (e.g. unsteady diffusion, advection, etc.). Their numerical solution strategy is, then, related to marching algorithms (see finite differences scheme in the Workshop)
- Example: unsteady heat diffusion:

$$T_t = \alpha \nabla^2 T$$

subject to a particular initial temperature distribution $T_0 = f(\mathbf{x}, t)$



Hyperbolic PDEs: Wave equation

- Hyperbolic equations are usually related to Propagation problems (e.g. wave front spreading, oscillatory motion, etc.)
- A classical example of a hyperbolic PDE modeling a propagation problem is the acoustic wave propagation
$$P_{tt} = a^2 \nabla^2 T$$
- Numerical solutions are also based in marching algorithms

Phenomenological classification

The ADR equation (advection -diffusion reaccion) is a second order partial differential equation widely used on the mathematical modeling, has importance because the
The ADR equation (advection - diffusion - reaction) is a second order partial differential equation widely used on the mathematical modeling, has importance the phenomena implied.

$$\frac{\partial \phi}{\partial t} - \vec{\nabla}.k\vec{\nabla}(\phi) + \vec{u}.\vec{\nabla}(\phi) + s\phi = F(\vec{x}) \qquad on \quad \Omega \tag{1}$$

with the boundary conditions **??** y **??**:

$$\phi(\vec{x}) = G(\vec{x}) \qquad sobre \quad \Gamma_\phi \tag{2}$$

$$\vec{\nabla}(\phi) = H(\vec{x}) \qquad sobre \quad \Gamma_\nabla \tag{3}$$

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Boundary Conditions

Establishing the proper boundary conditions is a strong requirement to obtain a good model and, then, a correct, accurate solution to the problem. Among others, there are two main boundary condition types

- Dirichlet boundary conditions
  - Given a function $f : \partial\Omega \to \mathbb{R}$, it is required

$$u(\mathbf{x}) = f(\mathbf{x}), \;\; \mathbf{x} \in \partial\Omega$$

- Von Neumann boundary conditions: Given a function $f : \partial\Omega \to \mathbb{R}$, it is required

$$\frac{\partial u(\mathbf{x})}{\partial n} = f(\mathbf{x}), \;\; \mathbf{x} \in \partial\Omega$$

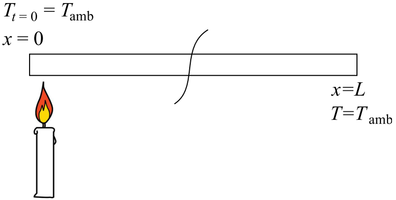
  where n is the unit outward normal of $\partial\Omega$

On PDE Solutions

- There is no general recipe that works for all PDEs.
  - It's needed a particular analysis for each class of PDE.
- Usually, there are no explicit formulas for the solutions to the PDEs. Instead, it's necessary to estimate the solutions without having explicit formulas.
  - A great portion of PDEs, particularly those related to real, complex physical problems, doesn't have an *algebraic/analytic* solution

System Modeling Workshop: Heat Equation

Problem: Describe the evolution of the temperature distribution of a body (1D rod) being heated in one of its tips



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Heat Equation problem statement

- **Fourier's law:** heat flux $\mathbf{q}$ (q_x for 1D) is negatively proportional to the spatial differences for temperature

$$\mathbf{q} = -K\nabla T$$

- The variation on the temperature distribution with time for a specific region is given by the Heat Equation:

$$\frac{\partial T(\vec{x},t)}{\partial t} - \alpha \nabla^2 T(\vec{x},t) = 0$$

- For a unidimensional case, this is written as

$$\frac{\partial T(x,t)}{\partial t} = \alpha \frac{\partial^2 T(x,t)}{\partial x^2}$$

having $T(x,0) = T_{amb}$, $T(L,t) = T_{amb}$, $T(0,t) = T_{flame}$ and $\alpha = \frac{K}{C_\rho}$

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Numerical solution (1D)

- Differential equation

$$\frac{\partial T(x,t)}{\partial t} = \alpha \frac{\partial^2 T(x,t)}{\partial x^2}$$

- Using finite differences, the model equation results in

$$\frac{T(x,t+h_t) - T(x,t)}{h_t} = \alpha \frac{T(x+h_x,t) - 2T(x,t) + T(x-h_x,t)}{h_x^2}$$

- Replacing and organizing, we obtain

$$T_{x,t+1} = T_{x,t} + \alpha \frac{\Delta t}{(\Delta x)^2} \left(T_{x+1,t} - 2T_{x,t} + T_{x-1,t}\right)$$

having $T(x,0) = T_{amb}$, $T(L,t) = T_{amb}$, $T(0,t) = T_{flame}$ and $\alpha = \frac{K}{C_\rho}$

Algorithm Sketch

- Read L, K, C_ρ, Δx, Δt
- Initialize array $T_{previous}$[0:$L * \Delta x$]
- Initialize array $T_{current}$[0:$L * \Delta x$]
- $\alpha = \frac{K}{C_\rho}$
- while ~stop
  - for i from 0 to $[L * \Delta x]$
    - $T_{current}[i]$=$T_{previous}[i]$+$\alpha \frac{\Delta t}{(\Delta x)^2}$*($T_{previous}[i+1]$-2*$T_{previous}[i]$+$T_{previous}[i-1]$)
    - Write $T_{current}$
  - end for
- end while

Matrix formulation of PDE

If we have a EDP's as above

$$\frac{\partial T}{\partial t} = \frac{K}{C_p}\frac{\partial^2 T}{\partial x^2}$$

We can aproximate the same equation in matrix form

$$\frac{\partial T}{\partial t} = \frac{K}{C_p}[D_N^{(2)}]T_i$$

Where $[D_N^{(2)}]$ is a second derivative matrix and T_i is a vector with the values of T evaluated at x_i points of the domain.

The trick evidently is determine $[D_N^{(2)}]$ and x_i which allow the correct representation of the function T.

The treatment of the time derivatives is like a ODE (Using a Euler or Runge Kutta methods). In the steady state ($\frac{\partial T}{\partial t} = 0$) the problem became in a linear algebra system.

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More general cases

Stady state

$$-k\frac{\partial^2 u}{\partial x^2}+u\frac{\partial u}{\partial x}-g(x)=0$$

$$-k\,[D_N^{(2)}]u_j+v\,[D_N^{(1)}]u_j=g_j$$

$$\left(-k\,[D_N^{(2)}]+v\,[D_N^{(1)}]\right)u_j=g_j$$

$$u_j=\left(-k\,[D_N^{(2)}]+v\,[D_N^{(1)}]\right)\setminus g_j$$

Trasient

$$-\frac{\partial T}{\partial t}-k\frac{\partial^2 u}{\partial x^2}+u\frac{\partial u}{\partial x}-g(x)=0$$

$$\frac{\partial T}{\partial t}=-k\,[D_N^{(2)}]u_j+v\,[D_N^{(1)}]u_j-g_j$$

$$\frac{\partial T}{\partial t}=\left(-k\,[D_N^{(2)}]+v\,[D_N^{(1)}]\right)u_j-g_j$$

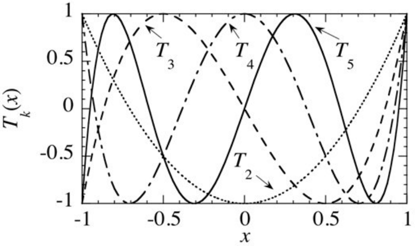
Using Euler method

$$\frac{u_j^{t+1}-u_j^t}{dt}=\left(-k\,[D_N^{(2)}]+v\,[D_N^{(1)}]\right)u_j-g_j$$

$$u_j^{t+1}=\left[\left(-k\,[D_N^{(2)}]+v\,[D_N^{(1)}]\right)u_j-g_j\right]dt+u_j^t$$

Spectral methods

Caracteristic	Domain	Spectral methods
Acotado	$[-1, 1]$	Chebyshev o Legendre
Periódico	$[0, 2\pi]$ ó $[-\pi, \pi]$	Fourier
Semi-infinito	$[0, \infty]$	Laguerre
Infinito	$[-\infty, \infty]$	Hermite



Chebyshev polynomials in [-1,1]

Trigonometric form

$$T_k(x) = \cos(k \cos^{-1}(x))$$

Recursive form

$$T_{k+1}(x) = 2xT_k(x) - T_{k-1}(x),$$
con $T_0(x) = 1$ y $T_1(x) = x$.

Chebyshev Collocation

Nodes

$$x_j = \cos(\frac{\pi j}{N}), \quad j = 0, \ldots, N$$

Derivatives matrix

The formulation is like a matrix formulation but using the next matrix:

$$(D_N)^{(1)}_{jl} = \begin{cases} \frac{\bar{c}_j}{\bar{c}_l} \frac{(-1)^{j+l}}{x_j - x_l}, & j \neq l, \\ -\frac{x_l}{2(1-x_l^2)}, & 1 \le j = l \le N-1, \\ \frac{2N^2+1}{6}, & j = l = 0, \\ -\frac{2N^2+1}{6}, & j = l = N. \end{cases}$$

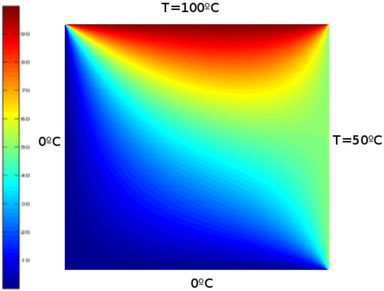
$$(D_N)^{(2)}_{jl} = \begin{cases} \frac{(-1)^{j+l}}{\bar{c}_l} \frac{x_j^2 + x_j x_l - 2}{(1-x_j^2)(x_j - x_l)^2}, & 1 \le j \le N-1, \\ -\frac{(N^2-1)(1-x_j^2)+3}{3(1-x_j^2)^2}, & 1 \le j = l \le N-1 \\ \frac{2}{3} \frac{(-1)^l}{\bar{c}_l} \frac{(2N^2+1)(1-x_l)-6}{(1+x_l)^2}, & j = 0, 1 \le l \le N, \\ \frac{2}{3} \frac{(-1)^{l+N}}{\bar{c}_l} \frac{(2N^2+1)(1+x_l)-6}{(1+x_l)^2}, & j = 0, 1 \le l \le N, \\ \frac{N^4-1}{15}, & j = l = 0, j = l = N. \end{cases}$$

Something about Stabilization

Equation	Stability condition
$\frac{\partial T}{\partial t} = \frac{K}{C_p}\frac{\partial^2 T}{\partial x^2}$	$\frac{K}{C_p}\frac{\Delta t}{\Delta x^2} \leq \frac{1}{2}$
$\frac{\partial T}{\partial t} = \frac{K}{C_p}\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right)$	$\frac{K}{C_p}\frac{\Delta t}{\Delta x^2+\Delta y^2} \leq \frac{1}{8}$
$\frac{\partial T}{\partial t} = c\frac{\partial T}{\partial x}$	$c\frac{\Delta t}{\Delta x} \leq 1$
$\frac{\partial T}{\partial t} = c_x\frac{\partial T}{\partial x} + c_y\frac{\partial T}{\partial x}$	$c_x\frac{\Delta t}{\Delta x} + c_y\frac{\Delta t}{\Delta y} \leq 1$
$\frac{\partial^2 T}{\partial t^2} = c\frac{\partial^2 T}{\partial x^2}$	$c\frac{\Delta t}{\Delta x} \leq 1$

Homework

1. Get the solution of steady state heat transfer (square plate with side equal to 1) , with the shown boundary conditions.



2. Now resolve again but replace the right boundary condition (T=50°C) by the condicions $q_x = \frac{\partial T}{\partial x} = 0$
3. How would be the transient solution for the last 2 cases?
4. Solve the problem proposed on file IdealFlows.pdf.