Introduction to Numerical Solution of Partial Differential Equations

Hugo Franco, PhD

UNIVERSIDAD CENTRAL

April 26, 2014

Encuesta Estudiantes de la SED

https://es.surveymonkey.com/s/7S3VNVK

Notation

Partial derivatives –and their presence in partial differential equations– are noted in several ways according to the author (and the context in each specific field). For example, these three expressions denote the same:

$$\begin{aligned}\frac{\partial f(x,t)}{\partial t} &= \kappa\frac{\partial^2 f(x,t)}{\partial x^2}\\ \partial_t f &= \kappa\partial_{xx} f\\ f_t &= \kappa f_{xx}\end{aligned}$$

where simplicity and clarity (and often space) are the criteria to choose a particular notation

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 $f(x_1, x_2, \ldots, x_n) : \mathbb{R}^n \longmapsto \mathbb{R}$, the expression

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

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

Examples and *linearity*

Being $f = f(x, t)$

$$
\begin{aligned}
\partial_t^2 f + \cos f \partial_x f &= 0 \\
\partial_t^2 f + 2\partial_x^3 f &= t \\
-\partial_t f + (1 + x)\partial_x^2 f &= f
\end{aligned}
$$

Which are linear and nonlinear? Which are their order?

$$
\begin{aligned}
\partial_t^2 f + \partial_x f &= \sin x^2 \\
-\partial_t g + 2\partial_x^2 g &= t
\end{aligned}
$$

is a second-order linear system of PDEs in the unknowns f and g

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.

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

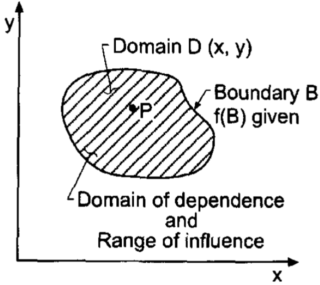
Elliptic PDEs

- 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: $\nabla^2 T = \Delta T = (\partial_{xx} T + \partial_{yy} T)$

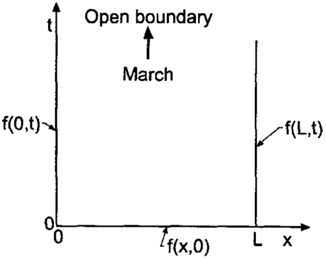


Parabolic PDEs: Heat equation

- 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

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

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

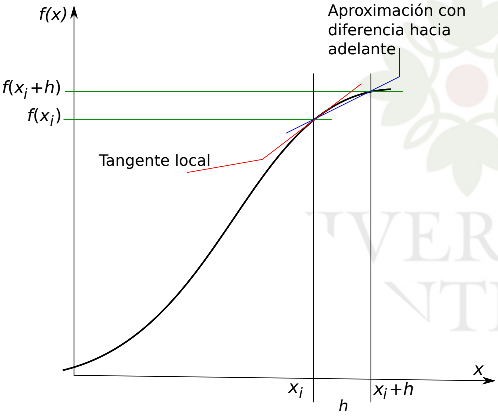
  where n is the unit outward normal of $\partial\Omega$

On PDE Solutions

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

Numerical derivative interpretation



be $f(x)$ a continuous 1-differentiable function. Then

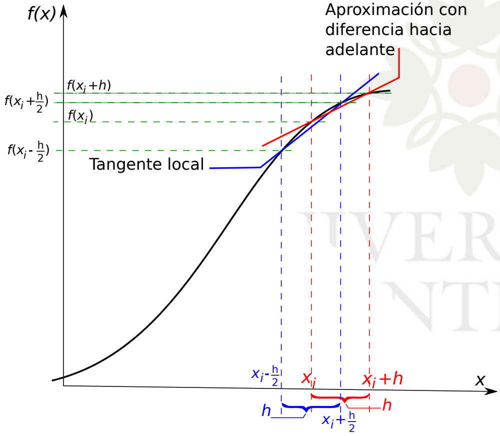
$$f'(x_i) = \lim_{h \to 0} \frac{f(x_i + h) - f(x_i)}{h}$$

Numerically approximating, having $0 < h \ll 1$, it holds that

$$f'(x_i) \simeq \frac{f(x_{i+1}) - f(x_i)}{h}$$

Problem: slope approximation is different to actual slope of the tangent hyperplane at x_i

Centered finite differences



Solution: keep the approximation step in a value of h but adapt the evaluation interval of the derivative approximation around x_i

$$f'(x_i) = \lim_{h\to 0} \frac{f(x_i+\frac{h}{2}) - f(x_i-\frac{h}{2})}{h}$$

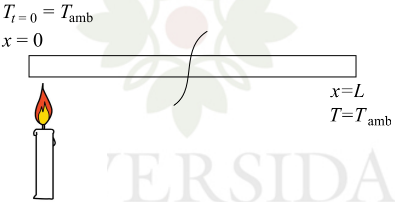
numerically approximating, given $0 < h \ll 1$,this yields

$$f'(x_i) \simeq \frac{f(x_{i+1}) - f(x_{i-1})}{h}$$

Numerical approximation of $f'(x_i)$ is usually closer to its real value using centered differences than using forward or backwards differences

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



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

Previous knowledge on the problem

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

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

  - Using conservation laws and applying the Fourie's law, the heat equation arises:

$$\frac{T(x,t+\Delta t)-T(x,t)}{\Delta t} = \frac{1}{C_\rho}\frac{q_x(x)-q_x(x+\Delta x)}{\Delta x}$$

$$\frac{T(x,t+\Delta t)-T(x,t)}{\Delta t} = \frac{K}{C_\rho}\frac{\frac{\partial T(x+\Delta x,t)}{\partial x}-\frac{\partial T(x,t)}{\partial x}}{\Delta x}$$

for $\Delta t \to 0$ and $\Delta x \to 0$

$$\frac{\partial T}{\partial t} = \frac{K}{C_\rho}\nabla^2 T$$

Heat Equation problem statement

- La variación de la distribución de temperaturas a lo largo del tiempo para una región está dada por la Ecuación del Calor:

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

- La aproximación a un caso unidimensional se convierte en

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

having $T(x,0) = T_{amb}$, $T(L,t) = T_{amb}$ and $T(0,t) = T_{flame}$

Numerical solution (1D)

- The second derivative can be approximated as

$$f''(x) = \frac{f'(x+\frac{h}{2}) - f'(x-\frac{h}{2})}{h}$$

where

$$f'(x+\frac{h}{2}) \simeq \frac{f(x+h)-f(x)}{h}$$
$$f'(x-\frac{h}{2}) \simeq \frac{f(x)-f(x-h)}{h}$$

- replacing, it becomes

$$f''(x) = \frac{f(x+h)-2f(x)+f(x-h)}{h^2}$$

- Then, 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

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

Algorithm Sketch

- Read L, K, C_ρ, Δx, Δt
- Initialize array $T_{previous}$[0:$L * \Delta x$]
- Initialize array $T_{current}$[0:$L * \Delta x$]
- $\alpha = {}^{K}/_{C_\rho}$
- 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

Further methods

- Finite Element Methods: complex geometries
- Finite Volume Methods: complex geometries and relationships
- Spectral Methods: better accuracy for smooth problems
- Mesh–free methods: reduce artifacts due to discretization