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Partial Differential equations I

Matteo Barborini*,[a], Valentin Vassilev Galindo*,[b], Prof. Alexandre Tkatchenko*

Theoretical Chemical Physics group

Faculté des Sciences, des Technologies et de Médecine - Département Physique et sciences des matériaux

*Campus Limpertsberg, Université du Luxembourg - 162 A, avenue de la Faïencerie, L-1511 Luxembourg

[a]matteo.barborini@uni.lu, [b]valentin.vassilev@uni.lu

1. Partial differential equations

In physics the observables usually vary as a function of time and space, and thus are represented by functions of the type $u(x, y, z, t)$ that represent a field. That presence of more than one independent variable, means that the variation of the field will be described by an equation containing the partial derivatives with respect to each variable.
If we consider a field that depends on two variables (x, y) (of which one of the two might be the time) then the general form of a scalar second order partial differential equations (PDE) will be

$$a(x,y)u_{xx} + 2b(x,y)u_{xy} + c(x,y)u_{yy} + \mathcal{F}(x,y,u,u_x,u_y) = 0 \tag{1}$$

where the function $\mathcal{F}(x, y, u, u_x, u_y)$ might be linear

$$\mathcal{F}(x,y,u,u_x,u_y) = d(x,y)u_x + e(x,y)u_y + f(x,y)u + f(x,y) \tag{2}$$

or non-linear, and in which the terms with the second order derivatives represent the **principal part** of the equation.
If we limit ourselves to the linear case, we define the characteristics' equations associated to the two-dimensional linear differential equation as

$$a(x,y)\left(\frac{dy}{dx}\right)^2 + 2b(x,y)\frac{dy}{dx} + c(x,y) = 0 \tag{3}$$

from which we obtain two ordinary differential equations

$$\frac{dy}{dx} = \frac{b(x,y)}{a(x,y)} \pm \frac{\sqrt{b(x,y)^2 - a(x,y)c(x,y)}}{a(x,y)}. \tag{4}$$

The **characteristics** are family of parallel curves (in each point of space only two curves one from each family intersect) on which the partial differential equation reduces to decoupled ordinary differential equations that can be solved analytically.
Here we do not want to enter the details of the transformations defined through the characteristics (for that please look at reference 1), but we want to concentrate on the characterization of the PDE through the discriminant $\Delta = b(x,y)^2 - a(x,y)c(x,y)$.
As a matter of fact, we can distinguish three types of partial differential equations of the second order:

- $\Delta < 0$ elliptic partial differential equation;
- $\Delta = 0$ parabolic partial differential equation;
- $\Delta = 0$ hyperbolic partial differential equation:

each of which characterizes different physical problems. In the following sections we will briefly describe one equation for each of the three types of PDEs.

1.1. Elliptic PDE: Poisson's equation. Poisson's equation characterizes different physical problems. For example it describes the potential field generated by a given charge distribution in space, and in two dimensions it is written as

$$u_{xx} + u_{yy} = -4\pi\rho(x,y) \tag{5}$$

where $u_{xx} + u_{yy}$ is the two-dimensional Laplacian of the electrostatic potential (in this case u)[2]. The characteristics' equations of this elliptic PDE will be imaginary of the form:

$$\frac{dy}{dx} = \pm i \tag{6}$$

so that the characteristic curves will be of the type $y = \pm ix + C$, where C is a constant. There are three types of boundary conditions that are sufficient for the correct definition of this problem:

- Dirichlet boundary conditions: Fix the value of the potential on the boundary;
- Neumann boundary conditions: Fix the value of the derivative of the potential at the boundary (Electric field);
- Mixed boundary conditions: Fix a linear combination of the potential and its derivatives.

1.2. Parabolic PDE: Fourier's law and Schrödinger's equation. A typical example of parabolic PDE is Fourier's law of the propagation of heat, that can be expressed in one dimension as :

$$u_t = Du_{xx} \tag{7}$$

where D is the diffusion coefficient that is characteristic of the medium. If the medium is uniform D is a constant and redefining the variable $y = Dt$ we can rewrite the equation as

$$u_{xx} - u_y = 0 \tag{8}$$

with the characteristics define by the equation $\frac{dy}{dx} = 0$ which gives a single family of curves $y = C$, C being a constant.
Also the time dependent Schrödinger's equation is a diffusion equation in imaginary time, in fact in one dimension we can write it as:

$$-i\hbar u_t = -\frac{\hbar^2}{2m}u_{xx} + v(x) \tag{9}$$

and assuming $y = it$ we have that

$$\frac{\hbar^2}{2m}u_{xx} - \hbar u_y = v(x) \tag{10}$$

Since the solution of this kind of problems propagates in an open domain, in order to solve this problem one needs to provide the wave function and its normal derivative (or a linear combination of them) at the initial time of the propagation, in all the domain.

1.3. Hyperbolic PDE: the wave equation. An example of hyperbolic PDE is the wave equation

$$u_{tt} = c^2 u_{xx} \tag{11}$$

that by defining $y = ct$ reduces to

$$u_{yy} = u_{xx} \tag{12}$$

for which the two families of characteristic, obtained by solving the equations $\frac{dy}{dx} = \pm 1$, will be of the form $y = \pm x + C$.
For this type of partial differential equations we need to set boundary conditions and initial conditions, where the former refer to the function u and eventually to its first derivatives (depending on the order of the spatial derivatives) on the frontier of the definition domain (spatial) of u, while the latter are related to the function u and its first derivative u_t at the initial time t_0.

2. Fourier's equation of heat

Let us consider at first Fourier's equation of heat. According to Newton's law, the propagation of heat Q between two surfaces of areas S with temperatures respectively of T_1 and $T_2(> T_1)$ of a material of thickness l in a unit of time Δt can be written as

$$\frac{Q}{S\Delta t} = -\Lambda\frac{T_2 - T_1}{\Delta x} \qquad \left(\text{or } \Lambda\frac{T_1 - T_2}{\Delta x}\right) \tag{13}$$

where Λ is the thermal conductibility of the material. For an infinitesimal element of the surface

$$\frac{dQ}{dSdt}\hat{n} = \Lambda\nabla T \tag{14}$$

If we now consider the infinitesimal volume dV, delimited by the surface dS, of a material with thermal capacity c and density ρ, then the heat necessary to change its temperature dT will be equal to $dQ = \rho c dV dT$, and the quantity of heat per unit of time in a finite Volume will be

$$\frac{dQ}{dt} = \int_V \rho c\frac{dT}{dt}dV. \tag{15}$$

Now, because of the conservation of energy, the heat that enters the infinitesimal volume must all contribute to the increase of temperature, thus substituting $\frac{dQ}{dt}$ in the first equation we have

$$\int_V \rho c\frac{dT}{dt}dV = \Lambda\int_S \nabla T\cdot\hat{n}dS, \tag{16}$$

and for Gauss's theorem we have that the flux through the surface is related to the divergence in the volume

$$\int_V \rho c\frac{dT}{dt}dV = \Lambda\int_V \nabla\cdot\nabla T dV \tag{17}$$

where the divergence of a gradient is the Laplacian so:

$$\int_V \rho c\frac{dT}{dt}dV = \Lambda\int_V \nabla^2 T dV \to \int_V\left[\rho c\frac{dT}{dt} - \Lambda\nabla^2 T\right]dV = 0. \tag{18}$$

This equation holds for any volume V, so the integrand must be null, leaving us with the final differential equation

$$\frac{dT}{dt} = \frac{\Lambda}{\rho c}\nabla^2 T \tag{19}$$

which is Fourier's heat equation.

2.1. Solutions of the one dimensional case. Let us consider Fourier's equation in the one dimensional case, with the diffusion constant $D = \frac{\Lambda}{\rho c}$:

$$u_t = Du_{xx}. \tag{20}$$

In the case of an infinite interval the spatial boundary conditions are the natural ones for which the solution u and its derivatives go to zero at infinite distance. For the time variable we usually assume an initial condition given by a function $u(x, t_0) = F(x)$ where $F(x)$ satisfies the spatial boundary conditions of the solution.
The analytical solution can be given by separating the variables in a form $u(x, t) = \chi(x)\tau(t)$, that substituted in the diffusion equation, leaves us with

$$\frac{1}{D\tau(t)}\frac{d\tau(t)}{dt} = \frac{1}{\chi(x)}\frac{d^2\chi(x)}{dx^2} = -k^2 \tag{21}$$

hat can be set identical to the parameter $-k^2$ that is determined by the boundary conditions. The solution of the equation $\frac{1}{\chi(x)}\frac{d^2\chi(x)}{dx^2} = -k^2$ with the spatial boundary conditions established in the beginning leaves us with solutions of the type $\chi(x) \sim e^{ikx}$, while the equation $\frac{1}{D\tau(t)}\frac{d\tau(t)}{dt} = -k^2$ will give a solution of the form $\tau(t) \sim e^{-Dk^2 t}$, since the global temperature decreases (or increases) exponentially in time.

The solution can be written as the linear combination of the superposition of the two solutions, written in the integral form

$$u(x,t) = \int_k c(k) e^{ikx} e^{-Dk^2 t} dk \tag{22}$$

where the functions $c(k)$ will be determined by the boundary conditions for which

$$u(x,0) = F(x) = \int_k c(k) e^{ikx} dk. \tag{23}$$

From this last equation, we can understand that $F(x)$ is the Fourier transform of $c(k)$, and so this function can be obtained by the inverse transform:

$$c(x) = \frac{1}{2\pi} \int_x F(x) e^{-ikx} dx \tag{24}$$

that substituted in the solution leaves us with

$$u(x,t) = \frac{1}{2\pi} \int \int F(x') e^{-ikx'} e^{ikx} e^{-Dk^2 t} dk dx' = \int G(x-x',t) F(x') dx' \tag{25}$$

where

$$G(x-x',t) = \frac{1}{2\pi} \int e^{ik(x-x')} e^{-Dk^2 t} dk \tag{26}$$

is the Green function for Fourier's diffusion equation. This Green function is the Fourier transform of a Gaussian function, which can be demonstrated to be itself a Gaussian function of the type:

$$G(x-x',t) = \frac{1}{\sqrt{4\pi D t}} e^{-\frac{(x-x')}{4Dt}}. \tag{27}$$

In the particular case in which the initial condition is a Gaussian function

$$F(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{x^2}{2\sigma^2}}, \tag{28}$$

we have that the solution of Fourier's equation has the form

$$u(x,t) = \frac{1}{\sqrt{2\pi(\sigma^2 + 2Dt)}} e^{-\frac{x^2}{2(\sigma^2+2Dt)}} \tag{29}$$

which is still a Gaussian with a variance that increases as a function of time.
Since from an algorithmic point of view we always work with finite intervals, let us now consider the case of the diffusion of heat for a finite interval $x \in [0, L]$. In this case we can write the solution for $\chi(x)$ as the sum of an inifinite number of harmonics

$$\chi(x) = \sum_{n=0}^{\infty} [a_n \sin(k_n x) + b_n \cos(k_n x)] \tag{30}$$

where the parameters of the combination, and the values of k_n will be defined by the boundary, and by the initial conditions. With boundary conditions of the type

$$\chi(0) = \chi(L) = 0. \tag{31}$$

we have that $b_n = 0$ and $\sin(kL = 0)$ (assuming $a_n \neq 0$ otherwise we would have the trivial null solution). From the condition on the $\sin$ we have that $k_n = \frac{n\pi}{L}$, so that the general solution will be of the form

$$u(x,t) = \sum_{n=1}^{\infty} a_n \sin(k_n x) e^{-Dk_n^2 t} \tag{32}$$

In order to obtain the coefficients a_n we can impose an initial condition of the solution, for example we can assume that at time $t_0 = 0$ the temperature is a constant function of space $u(x, t_0) = u_0$ in the whole interval.

By imposing this condition we have that:

$$\sum_{n=1}^{\infty} a_n \sin(k_n x) = u_0 \tag{33}$$

and by multiplying both sides of the equation by $\sin(k_m x)$ and integrating in the interval $x \in (0, L)$ we have that

$$\sum_{n=1}^{\infty} a_n \int_0^L \sin(k_n x)\sin(k_m x)dx = u_0 \int_0^L \sin(k_m x)dx. \tag{34}$$

We can now apply a change of variable considering that $k_m x = \frac{m\pi x}{L}$ and $k_n x = \frac{n\pi x}{L}$, thus setting $y = \frac{x\pi}{L}$ we have $dx = \frac{L}{\pi}dy$ and the equation reduces to

$$\sum_{n=1}^{\infty} a_n \frac{L}{\pi} \int_0^{\pi} \sin(ny)\sin(my)dy = u_0 \frac{L}{\pi} \int_0^{\pi} \sin(my)dy \tag{35}$$

the leaves us with

$$a_n \frac{L}{\pi}\frac{\pi}{2}\delta_{mn} = \frac{u_0 L}{m\pi}[1-(-1)^m] \to a_m = \frac{2u_0}{m\pi}[1-(-1)^m] \to a_n = \frac{4u_0}{n\pi} \qquad n = 1, 3, 5, \ldots \tag{36}$$

The coefficients are non zero only for odd numbers so we finally have that the full solution will have the form

$$u(x,t) = \sum_{n=1,3,5,\ldots}^{\infty} \frac{4u_0}{n\pi} \sin(\frac{n\pi}{L}x)e^{-D(\frac{n\pi}{L})^2 t}. \tag{37}$$

2.2. Euler discretization for the diffusion equation. In order to find the algorithmic solution of the the diffusion equation $u_t = Du_{xx}$ we must discretize the spatial and temporal dimensions introducing a time step Δt and a spacial step Δx. By applying the explicit Euler discretization scheme, the derivatives that appear in the equation can be approximated at the first order in their intervals, so that we have:

$$\frac{u(x_m, t_{n+1}) - u(x_m, t_n)}{\Delta t} = D\frac{u(x_{m+1}, t_n) - 2u(x_m, t_n) + u(x_{m-1}, t_n)}{\Delta x^2}. \tag{38}$$

From this equation we can obtain the time evolution of the solution at a chosen position x_m as

$$u(x_m, t_{n+1}) = u(x_m, t_n) + \frac{D\Delta t}{\Delta x^2}\left[u(x_{m+1}, t_n) - 2u(x_m, t_n) + u(x_{m-1}, t_n)\right]. \tag{39}$$

In order to study the stability of this algorithm, we use the von Neumann analysis. We consider a single mode k of the solution written in the form:

$$u(x,t) = \tau(t)e^{ikx}. \tag{40}$$

By substituting this equation in the algorithmic solution we obtain:

$$\tau(t+\Delta t)e^{ikx} = \tau(t)e^{ikx} + \frac{D\Delta t}{\Delta x^2}\left[\tau(t)e^{ik(x+\Delta x)} - 2\tau(t)e^{ikx} + \tau(t)e^{ik(x-\Delta x)}\right], \tag{41}$$

that reduces to:

$$\begin{aligned}\tau(t+\Delta t) = \tau(t)\left[1 + \frac{D\Delta t}{\Delta x^2}\left(e^{ik\Delta x} + e^{ik\Delta x} - 2\right)\right] = \\ = \tau(t)\left[1 - \frac{2D\Delta t}{\Delta x^2}\left(1 - \cos(k\Delta x)\right)\right] = \tau(t)\left[1 - \frac{4D\Delta t}{\Delta x^2}\sin^2\left(\frac{k\Delta x}{2}\right)\right].\end{aligned} \tag{42}$$

The Fourier mode is amplified at each step by the factor in the square brackets, and in order for the solution not to diverge, we must have that:

$$\left|\frac{\tau(t+\Delta t)}{\tau(t)}\right| = \left|1 - \frac{4D\Delta t}{\Delta x^2}\sin^2\left(\frac{k\Delta x}{2}\right)\right| \leq 1 \tag{43}$$

that is

$$-1 \leq 1 - \frac{4D\Delta t}{\Delta x^2} \sin^2\left(\frac{k\Delta x}{2}\right) \leq 1 \to -2 \leq -\frac{4D\Delta t}{\Delta x^2} \sin^2\left(\frac{k\Delta x}{2}\right) \leq 0 \to \frac{4D\Delta t}{\Delta x^2} \sin^2\left(\frac{k\Delta x}{2}\right) \leq 2 \tag{44}$$

and since $0 \leq \sin^2\left(\frac{k\Delta x}{2}\right) \leq 1$ for different values of k, we finally have that:

$$\frac{4D\Delta t}{\Delta x^2} \sin^2\left(\frac{k\Delta x}{2}\right) \leq \frac{4D\Delta t}{\Delta x^2} \leq 2 \to \Delta t \leq \frac{\Delta x^2}{2D} \tag{45}$$

This last condition means that in order for the integration to be stable, if the space discretization is halved the time discretization step has to become four times smaller.

2.3. Crank-Nicolson scheme for the diffusion equation. Another, more stable, well known method for solving the diffusion equation is the implicit Crank-Nicolson scheme, which consists in writing the second order spatial derivative as a combination of the second order derivatives at different time steps, that is

$$\begin{aligned}\frac{u(x_m,t_{n+1}) - u(x_m,t_n)}{\Delta t} &= D\frac{u(x_{m+1},t_{n+1}) - 2u(x_m,t_{n+1}) + u(x_{m-1},t_{n+1})}{2\Delta x^2} + \\ &+ D\frac{u(x_{m+1},t_n) - 2u(x_m,t_n) + u(x_{m-1},t_n)}{2\Delta x^2}.\end{aligned} \tag{46}$$

If we separate the terms corresponding to an identical time in the evolution; t_{n+1} on the left side and t_n on the right, we have that

$$\begin{aligned}u(x_m,t_{n+1}) - \frac{D\Delta t}{\Delta x^2}\left[u(x_{m+1},t_{n+1}) - 2u(x_m,t_{n+1}) + u(x_{m-1},t_{n+1})\right] = \\ = u(x_m,t_n) + \frac{D\Delta t}{\Delta x^2}\left[u(x_{m+1},t_n) - 2u(x_m,t_n) + u(x_{m-1},t_n)\right].\end{aligned} \tag{47}$$

The right side of this equation is known through the initial conditions at time t_0:

$$d(x_m,t_0) = u(x_m,t_0) + \frac{D\Delta t}{\Delta x^2}\left[u(x_{m+1},t_0) - 2u(x_m,t_0) + u(x_{m-1},t_0)\right],$$

with $d(0,t_0) = 0$ and $d(L,t_0) = 0$. The terms on the left side represent a full set of coupled equations that can be written in matrix form as

$$\mathbf{A}\bar{u}(t_{n+1}) = \bar{d}(t_n)$$

where the two column vectors are defined as

$$\bar{d}(t_n)^\top = \begin{pmatrix} d(x_0,t_n) & d(x_1,t_n) & \cdots & d(x_{n-1},t_n) & d(x_n,t_n) \end{pmatrix}$$

and

$$\bar{u}(t_{n+1})^\top = \begin{pmatrix} u(x_0,t_{n+1}) & u(x_1,t_{n+1}) & \cdots & u(x_{n-1},t_{n+1}) & u(x_n,t_{n+1}) \end{pmatrix}$$

and the matrix is defined (setting $C = \frac{D\Delta t}{\Delta x^2}$) as:

$$\mathbf{A} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ -C & (1+2C) & -C & \cdots & 0 & 0 & 0 \\ 0 & -C & (1+2C) & \cdots & 0 & 0 & 0 \\ \vdots & & & & & & \\ 0 & 0 & 0 & \cdots & -C & (1+2C) & -C \\ 0 & 0 & 0 & \cdots & 0 & 0 & 1 \end{pmatrix}.$$

One way to solve this problem is by inverting the **A** matrix obtaining the equation

$$\mathbf{A}^{-1}\bar{d}(t_n) = \bar{v}(t_{n+1})$$

Yet, since the matrix inversion requires $O(n^3)$ multiplications, it is best to use another approach through the tridiagonal matrix algorithm (or Thomas algorithm) which requires only $O(n)$ multiplications. A brief description of the algorithm can be found in the next section (without being demonstrated).
Here, let us study the stability of the algorithm. In order to do so, we can apply again the von Neumann stability conditions, substituting the trial solution of the form $u(x,t) = \tau(t)e^{ikx}$ in the algorithm's equation, for which we obtain

$$\begin{aligned}\tau(t+\Delta t)e^{ikx} - \frac{D\Delta t}{\Delta x^2}\left[\tau(t+\Delta t)e^{ik(x+\Delta x)} - 2\tau(t+\Delta t)e^{ikx} + \tau(t+\Delta t)e^{ik(x+\Delta x)}\right] = \\ = \tau(t)e^{ikx} + \frac{D\Delta t}{\Delta x^2}\left[\tau(t)e^{ik(x+\Delta x)} - 2\tau(t)e^{ikx} + \tau(t)e^{ik(x-\Delta x)}\right] . \end{aligned} \tag{48}$$

Following the same considerations used before for Euler's algorithm, we have

$$\tau(t+\Delta t)\left[1 + \frac{4D\Delta t}{\Delta x^2}\sin^2\left(\frac{k\Delta x}{2}\right)\right] = \tau(t)\left[1 - \frac{4D\Delta t}{\Delta x^2}\sin^2\left(\frac{k\Delta x}{2}\right)\right], \tag{49}$$

so that $|\tau(t+\Delta t)/\tau(t)| < 1$ for all values of k, that is: the Crank-Nicolson algorithm is unconditionally stable.

2.4. Tridigonal matrix algorithm (or Thomas algorithm). We consider the system of equations in matrix format

$$\mathbf{A}\bar{u} = \bar{v}$$

where $\bar{u}$ and $\bar{v}$ are two vectors of length n of which $\bar{v}$ is known, and **A** is a square matrix of $n \times n$ elements defined as:

$$\mathbf{A} = \begin{pmatrix} b_1 & c_1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ a_2 & b_2 & c_2 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & a_3 & b_3 & c_3 & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & a_{n-1} & b_{n-1} & c_{n-1} \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & a_n & b_n \end{pmatrix}$$

To solve this problem we first define a forward sweep from $i = 1$ to $i = n$ to compute the parameters α_i and β_i defined as:

$$\alpha_i = \begin{cases} \frac{c_i}{b_i} & i = 1 \\ \frac{c_i}{b_i - a_i\alpha_{i-1}} & i = 2, 3, \ldots, n-1 \end{cases}$$

and

$$\beta_i = \begin{cases} \frac{v_i}{b_i} & i = 1 \\ \frac{v_i - a_i\beta_{i-1}}{b_i - a_i\alpha_{i-1}} & i = 2, 3, \ldots, n \end{cases}$$

and afterwards we construct the solution $\vec{u}$ as:

$$u_n = \beta_n \qquad u_i = \beta_i - \alpha_i u_{i+1} \quad i = n-1, n-2, \ldots, 1.$$

References

(1) Courant, R.; Hilbert, D. *Methods of Mathematical Physics*; John Wiley & Sons, Ltd, 2008; Chapter 3, pp 154–239.
(2) Jackson, J. D. *Classical electrodynamics; 3rd ed.*; Wiley: New York, NY, 1975.