

Lecture Notes for the Course on NUMERICAL MODELS FOR NUCLEAR REACTORS

Prof. WALTER AMBROSINI
University of Pisa, Italy

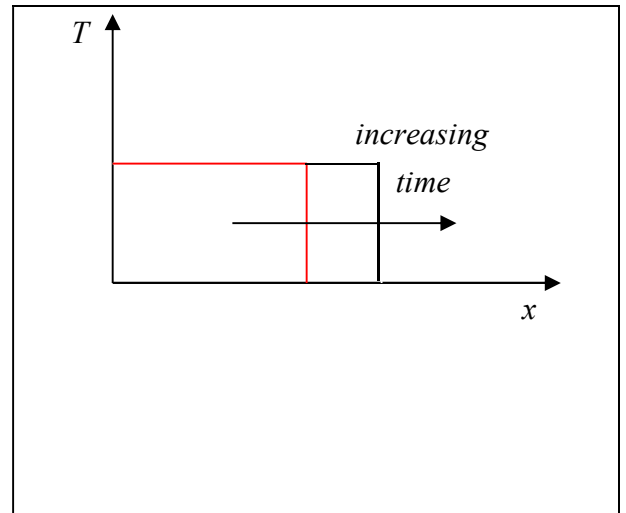
Unit 0 – Introduction

NOTICE: These notes were prepared by Prof. Ambrosini mainly **on the basis of the material adopted by Prof. Bruno Montagnini for the lectures he held up to years ago**, when he left to Prof. Ambrosini the charge of the course held for the Degree in Nuclear Engineering at the University of Pisa. This material is freely distributed to Course attendees or to anyone else requesting it. It has not the worth of a textbook and it is not intended to be an official publication. It was conceived as the notes that the teacher himself would take of his own lectures in the paradoxical case he could be both teacher and student at the same time (sometimes space and time stretch and fold in strange ways). It is also used as slides to be projected during lectures to assure a minimum of uniform, constant quality lecturing, regardless of the teacher's good and bad days. As such, the material contains reference to classical textbooks and material whose direct reading is warmly recommended to students for a more accurate understanding. In the attempt to make these notes as original as feasible and reasonable, considering their purely educational purpose, most of the material has been completely re-interpreted in the teacher's own view and personal preferences about notation. In this effort, errors in details may have been introduced which will be promptly corrected in further versions after discovery. Requests of clarification, suggestions, complaints or even sharp judgements in relation to this material can be directly addressed to Prof. Ambrosini at the e-mail address: walter.ambrosini@ing.unipi.it

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Character of Partial Differential Equation of Mathematical Physics

- The mathematical character of Partial Differential Equations (PDEs) is relevant for their numerical discretization
 - the numerical scheme should reflect, though approximately, *the way in which relevant information is propagated throughout the computational domain*
 - *boundary and initial conditions must be imposed in the numerical method in agreement with the way information is propagated*
- The classification of PDEs envisages three different characters addressing different phenomena; grossly speaking:
 - *hyperbolic*: phenomena involving the propagation of wave fronts progressing along specific space-time paths with finite speed
 - *parabolic*: phenomena involving infinite speed of propagation in space and progressing in time
 - *elliptic*: steady-state distribution of scalars in space
- Examples of *hyperbolic equations*



- the advection of a scalar

$$\frac{\partial T}{\partial t} + w \frac{\partial T}{\partial x} = 0$$

- the “vibrating string”

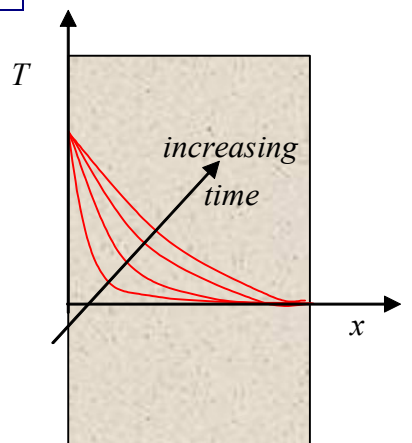
$$\frac{1}{c^2} \frac{\partial^2 T}{\partial t^2} = \frac{\partial^2 T}{\partial x^2} \Rightarrow T(x,t) = f(x-ct) + g(x+ct)$$

- the telegraph equation

$$\tau \frac{\partial^2 T}{\partial t^2} + \frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

- the compressible Euler equations

$$\rho \frac{D\vec{w}}{Dt} = -\nabla p + \rho \vec{g}$$



- Examples of *parabolic equations*

- the diffusion of a scalar (heat, concentration)

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

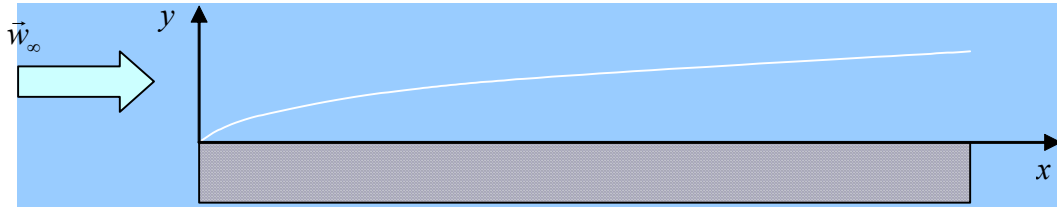
$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2}$$

➤ the laminar boundary layer

$$w_x \frac{\partial w_x}{\partial x} + w_y \frac{\partial w_x}{\partial y} = \nu \frac{\partial^2 w_x}{\partial y^2}$$

$$w_x \frac{\partial T}{\partial x} + w_y \frac{\partial T}{\partial y} = \alpha \frac{\partial^2 T}{\partial y^2}$$

$$w_x \frac{\partial \omega}{\partial x} + w_y \frac{\partial \omega}{\partial y} = D \frac{\partial^2 \omega}{\partial y^2}$$

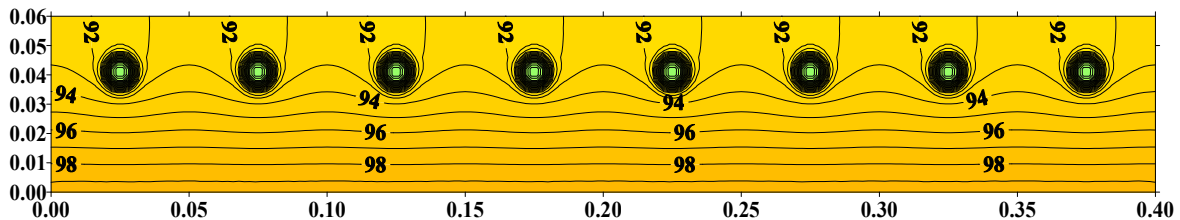


• Examples of *elliptic equations*

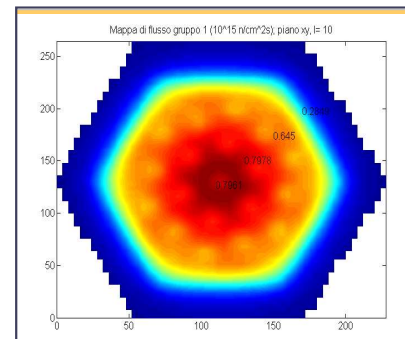
➤ the steady temperature distribution in a solid or the electric potential in a domain

$$\nabla^2 T = 0$$

$$\nabla^2 V = 0$$



➤ the steady neutron flux distribution in a reactor core



$$\text{div} D_g(\vec{r}) \text{grad}_{\vec{r}} \phi_g(\vec{r}) - \Sigma_{r,g}(\vec{r}) \phi_g(\vec{r}) + \sum_{\sigma' < \sigma} \Sigma_{s,g' \rightarrow g}(\vec{r}) \phi_{g'}(\vec{r}) + \frac{\chi_g}{k} \sum_{g'=1}^G \nu \Sigma_{f,g'}(\vec{r}) \phi_{g'}(\vec{r}) = 0 \quad (\vec{r} \in V, g = 1, \dots, G)$$

$$\phi_g(\vec{r}) + d_g \frac{d\phi_g(\vec{r})}{dn} = 0 \quad (\vec{r} \in \partial V, g = 1, \dots, G)$$

- Navier-Stokes equations $\rho \frac{D\vec{w}}{Dt} = \mu \nabla^2 \vec{w} - \nabla p + \rho \vec{g}$ are also elliptic in nature when steady and may be parabolic in transient form

- The sets of partial differential equations as the ones describing fluid-dynamics can be classed into hyperbolic, parabolic or elliptic by evaluating their “characteristic roots”

➤ the system must be written in the form

$$\boxed{\mathbf{A}(x, t, \boldsymbol{\varphi}) \frac{\partial \boldsymbol{\varphi}}{\partial t} + \mathbf{B}(x, t, \boldsymbol{\varphi}) \frac{\partial \boldsymbol{\varphi}}{\partial x} = \mathbf{c}(x, t, \boldsymbol{\varphi})}$$

where $\boldsymbol{\varphi}$ is the vector of unknowns, e.g. $\boldsymbol{\varphi} = \{p, u, w\}$ for single-phase flow and $\boldsymbol{\varphi} = \{p, u_l, u_v, \alpha_v, w_l, w_v\}$ for two-phase flow

➤ then, the “characteristic equation” is solved

$$\boxed{\det(\mathbf{B} - \lambda \mathbf{A}) = 0}$$

- For the scalar advection equation, $\frac{\partial T}{\partial t} + w \frac{\partial T}{\partial x} = 0$, the matrices \mathbf{A} and \mathbf{B} degenerate into 1 and w , giving the characteristic root $\lambda = w$, showing the hyperbolic character of advection.

- Generally speaking,

- when the roots of this equation (*characteristic roots*) are real, the system is said *hyperbolic* and the characteristic roots represent the slope of the *characteristic lines* in the x - t plane, to be interpreted as the lines along which the relevant information is transported; it is:

$$\lambda_i = \frac{dx_i}{dt}$$

- when all the characteristic roots are complex, the system is said *elliptic*;
- in all the other cases, the system is said *parabolic*.
- To better understand the situation, it is worth considering another classification, that can be shown to be equivalent to the above one and applies to second order partial differential equations

$$a(x, t) \frac{\partial^2 \varphi}{\partial t^2} + b(x, t) \frac{\partial^2 \varphi}{\partial t \partial x} + c(x, t) \frac{\partial^2 \varphi}{\partial x^2} + d(x, t) \frac{\partial \varphi}{\partial t} + e(x, t) \frac{\partial \varphi}{\partial x} + f(x, t) \varphi = g(x, t)$$

The classification is based on the value of $\Delta(x, t) = b^2 - 4ac$; for $\Delta(x, t) > 0$ the equation is *hyperbolic*, for $\Delta(x, t) = b^2 - 4ac = 0$ the equation is *parabolic* and for $\Delta(x, t) = b^2 - 4ac < 0$ the equation is *elliptic*.

- The relation between the two classifications can be understood considering that the above second order equation can be converted to a system of first order partial differential equations. In fact, by putting

$$\varphi_1 = \frac{\partial \varphi}{\partial t} \quad \varphi_2 = \frac{\partial \varphi}{\partial x} \quad \varphi_3 = \varphi$$

the second order equation can be rewritten as the system of equations

$$\begin{cases} a(x,t) \frac{\partial \varphi_1}{\partial t} + b(x,t) \frac{\partial \varphi_1}{\partial x} + c(x,t) \frac{\partial \varphi_2}{\partial x} + d(x,t) \varphi_1 + e(x,t) \varphi_2 + f(x,t) \varphi = g(x,t) \\ \frac{\partial \varphi_2}{\partial t} - \frac{\partial \varphi_1}{\partial x} = 0 \\ \frac{\partial \varphi_3}{\partial x} - \varphi_2 = 0 \end{cases}$$

- We have therefore:

$$\mathbf{A} = \begin{bmatrix} a(x,t) & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad \mathbf{B} = \begin{bmatrix} b(x,t) & c(x,t) & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \boldsymbol{\varphi} = \begin{bmatrix} \varphi_1 \\ \varphi_2 \\ \varphi_3 \end{bmatrix}$$

and the characteristic equation becomes

$$\det(\mathbf{B} - \lambda \mathbf{A}) = \begin{vmatrix} b(x,t) - \lambda a(x,t) & c(x,t) & 0 \\ -1 & -\lambda & 0 \\ 0 & 0 & 1 \end{vmatrix} = a(x,t) \lambda^2 - b(x,t) \lambda + c(x,t) = 0$$

- For the vibrating string equation it is

$$\frac{1}{c^2} \frac{\partial^2 T}{\partial t^2} = \frac{\partial^2 T}{\partial x^2}$$

$$\frac{1}{c^2} \lambda^2 - 1 = 0 \quad \Rightarrow \quad \lambda_{1,2} = \pm c$$

The equation is therefore hyperbolic and the two characteristic roots represent the speed of propagation of perturbation (waves) along the x axis in the forward and in the backward directions

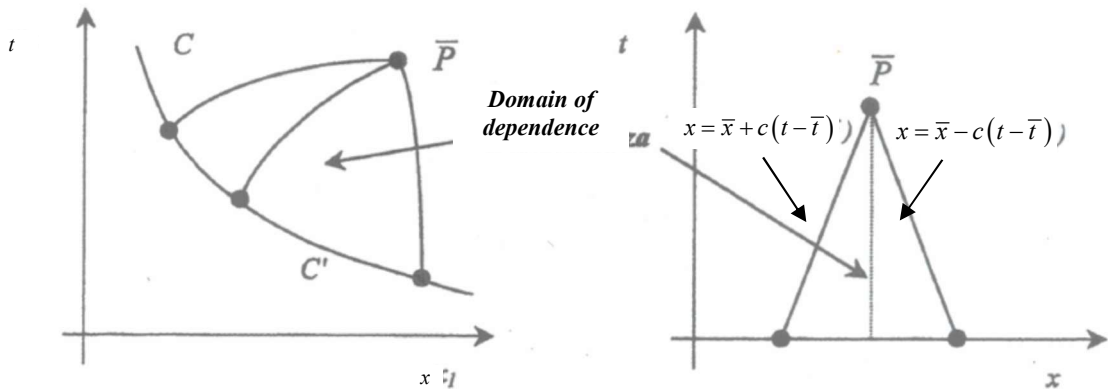
- For the telegraph equation, it is

$$\tau \frac{\partial^2 T}{\partial t^2} + \frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

$$\tau \lambda^2 - \alpha = 0 \quad \Rightarrow \quad \lambda_{1,2} = \pm \sqrt{\alpha/\tau}$$

So, also this equation is hyperbolic and the two characteristic roots depend on the ratio of the two appearing constants. In both cases, the *real characteristic roots*, represent the speed at which information is propagated in space during time for hyperbolic phenomena; the *characteristic lines* represent the paths in the space-time plane along which information is propagated: their local slope is given by the characteristic roots

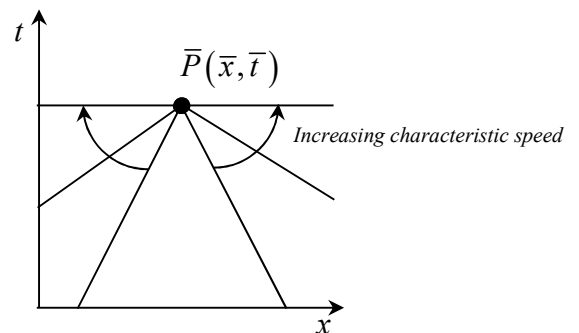
In the figure below, it is clarified that the “*domain of dependence*”, enclosed by the characteristic lines (they may be two and straight, as in the right figure, or more than two and even curved if the characteristic roots are not constant, as in the left one), represents the region from which the state in any given point \bar{P} depends: the relevant information affecting it cannot come from outside the region.



- The telegraph equation helps in understanding that the speed of propagation of information in the heat equation becomes infinite. In fact, for vanishing τ it is

$$\tau \frac{\partial^2 T}{\partial t^2} + \frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \quad \xrightarrow{\tau \rightarrow 0} \quad \frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

and the two characteristic roots $\lambda_{1,2} = \pm \sqrt{\alpha/\tau}$ become infinite. This means that any perturbation travels with infinite speed forth and back along the x axis, and the domain of dependence is all the region below a certain time \bar{t} .



- For the 2D Laplace equation, it is:

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0 \qquad \lambda^2 + 1 = 0$$

and the roots are found to be complex conjugated, showing the elliptic character of the equation.

Some of the above properties can be extended to multidimensional cases and it may happen that equations have a mixed mathematical character, i.e. with hyperbolic (e.g., advection or convection) terms and parabolic (e.g., diffusion) terms.

Sometimes one or the other characteristic dominates, so that we have a clear hyperbolic or parabolic behaviour, but sometimes the behaviour is mixed.

A classical example are the equations of fluid-dynamics that, in similarity with the neutron diffusion equation seen in the module of Reactor Physics, can be derived by an integral, “finite volume” balance, to be reverted to partial differential form as follows.

The general form of multidimensional balance equations to be solved in fluid dynamics is obtained by conservation principles over arbitrary and finite volumes

$$\underbrace{\frac{d}{dt} \int_V \rho \phi dV}_{\text{Rate of change of } \Phi \text{ in } V} = - \underbrace{\int_S \rho \phi \mathbf{w} \cdot \mathbf{n} dS}_S_{\substack{\text{Flux of } \Phi \text{ out of } S \\ \text{due to fluid motion} \\ \text{(advection or convection)}}} + \underbrace{\int_S \Gamma_\phi \nabla \phi \cdot \mathbf{n} dS}_S_{\substack{\text{Flux of } \Phi \text{ out of } S \\ \text{due to molecular motion} \\ \text{(diffusion)}}} + \underbrace{\int_V \rho S_\phi dV}_V_{\text{Volumetric source of } \Phi}$$

where ϕ is the specific value per unit mass of the extensive variable Φ , being the subject of the balance, and Γ_ϕ and S_ϕ are, respectively, the diffusion coefficient and the source per unit mass

By a conventional passage, the balance equation over the arbitrary volume V is firstly transformed by the use of the divergence theorem

$$\underbrace{\int_V \frac{\partial}{\partial t} \rho \phi dV}_{\text{Rate of change of } \Phi \text{ in } V} = - \underbrace{\int_V \nabla \cdot (\rho \phi \mathbf{w}) dV}_V_{\substack{\text{Flux of } \Phi \text{ out of } S \\ \text{due to fluid motion} \\ \text{(advection or convection)}}} + \underbrace{\int_V \nabla \cdot \Gamma_\phi \nabla \phi dV}_V_{\substack{\text{Flux of } \Phi \text{ out of } S \\ \text{due to molecular motion} \\ \text{(diffusion)}}} + \underbrace{\int_V \rho S_\phi dV}_V_{\text{Volumetric source of } \Phi}$$

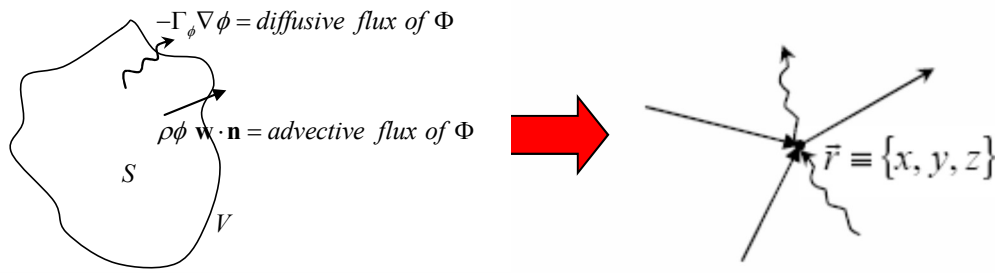
and then the arbitrariness of the selected control volume and the continuity of the functions allows to infer that if

$$\int_V \left[\frac{\partial}{\partial t} (\rho \phi) + \nabla \cdot (\rho \phi \mathbf{w}) - \nabla \cdot (\Gamma_\phi \nabla \phi) - \rho S_\phi \right] dV = 0$$

this implies that the integrand function must be zero everywhere:

$$\boxed{\underbrace{\frac{\partial}{\partial t} (\rho \phi)}_{\text{Transient term}} + \underbrace{\nabla \cdot (\rho \phi \mathbf{w})}_{\substack{\text{Advection} \\ \text{(or convection) term}}} = \underbrace{\nabla \cdot (\Gamma_\phi \nabla \phi)}_{\text{Diffusion term}} + \underbrace{\rho S_\phi}_{\text{Source term}}}$$

In other words, the principle of conservation established for a finite volume is translated to the differential (infinitesimal) form



Since this is the general form of the equations involved in fluid flow, *numerical methods are conceived to deal with the terms appearing in it.*

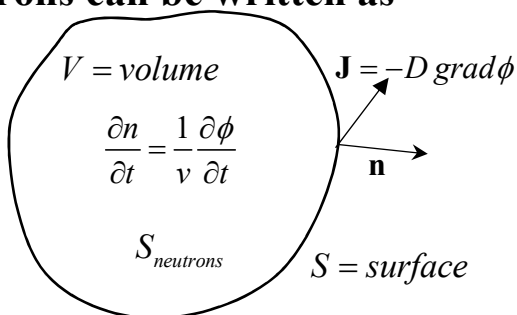
It will be seen that, making use of the “finite volume” technique of discretization, the red arrow in the previous sketch must be inverted: *from the differential equation we must go back to the finite volume conservation principle.*

Please, note the similarity with the combination of the equation of neutron continuity and the Fick’s law, giving the neutron diffusion equation. In this case, neutrons are assumed to have a single energy and $\phi = \left[\frac{\text{neutrons}}{\text{cm}^2 \text{s}} \right]$ has the specific meaning of scalar neutron flux, given by the product of neutron density $n = \left[\frac{\text{neutrons}}{\text{cm}^3} \right]$ by the neutron speed $v = \left[\frac{\text{cm}}{\text{s}} \right]$.

Considering the presence of an absorption rate, given by

$$\Sigma_a \phi = \left[\frac{1}{\text{cm}} \times \frac{\text{neutrons}}{\text{cm}^2 \text{s}} \right] = \left[\frac{\text{neutrons (absorbed)}}{\text{cm}^3 \text{s}} \right]$$

and a volumetric source of neutrons $S_{\text{neutrons}} = \left[\frac{\text{neutrons (emitted)}}{\text{cm}^3 \text{s}} \right]$, the balance of neutrons can be written as



$\int_V \frac{\partial n}{\partial t} dV = - \int_S \mathbf{J} \cdot \mathbf{n} dS - \int_V \Sigma_a \phi dV + \int_V S_{\text{neutrons}} dV$
<div style="display: flex; justify-content: space-around;"> Transient term Diffusion term Absorption term Source term </div>

Now, making use of the divergence theorem and introducing the Fick’s law and the flux in place of the density, we get

$$\underbrace{\int_V \frac{\partial n}{\partial t} dV}_{\text{Transient term}} = - \underbrace{\int_V \text{div } \mathbf{J} dV}_{\text{Diffusion term}} - \underbrace{\int_V \Sigma_a \phi dV}_{\text{Absorption term}} + \underbrace{\int_V S_{\text{neutrons}} dV}_{\text{Source term}}$$

$$\underbrace{\int_V \frac{1}{v} \frac{\partial \phi}{\partial t} dV}_{\text{Transient term}} = \underbrace{\int_V \text{div } D \text{ grad } \phi dV}_{\text{Diffusion term}} - \underbrace{\int_V \Sigma_a \phi dV}_{\text{Absorption term}} + \underbrace{\int_V S_{\text{neutrons}} dV}_{\text{Source term}}$$

Finally, grouping all the terms into a single integral and considering again the arbitrary nature of its selection, we get

$$\int_V \left[\frac{1}{v} \frac{\partial \phi}{\partial t} - \text{div } D \text{ grad } \phi + \Sigma_a \phi - S_{\text{neutrons}} \right] dV = 0$$

and then

$$\frac{1}{v} \frac{\partial \phi}{\partial t} - \text{div } D \text{ grad } \phi + \Sigma_a \phi - S_{\text{neutrons}} = 0$$

$$\boxed{\frac{1}{v} \frac{\partial \phi}{\partial t} = \text{div } D \text{ grad } \phi - \Sigma_a \phi + S_{\text{neutrons}}}$$

There is no surprise in recognising that the same techniques apply for deriving the balance equations (continuity) for the generic “scalar” in a fluid and for the neutron (continuity and) diffusion equation.

It must be in fact remarked that in both cases a basic assumption on the “continuity” of the field is adopted. In other words, we are not looking at the single particles composing the system but to the continuous distribution of their properties, e.g., density, temperature, velocity, etc.

The mathematical character of the transient diffusion equation is clearly parabolic. In particular:

- there is a “marching coordinate” (time) which is “one-sided”, since phenomena evolve along it in a specific direction, requiring an single “initial” information about the system status;
- there is one or more spatial coordinate that, owing to the second order differentiation, are “two-sided”, i.e., require information (i.e., boundary conditions) on both sides for advancing the solution.

PRELIMINARY CONSIDERATIONS ON NUMERICAL DISCRETISATION

Very seldom, partial differential equations for real-life engineering problems admit closed form solutions.

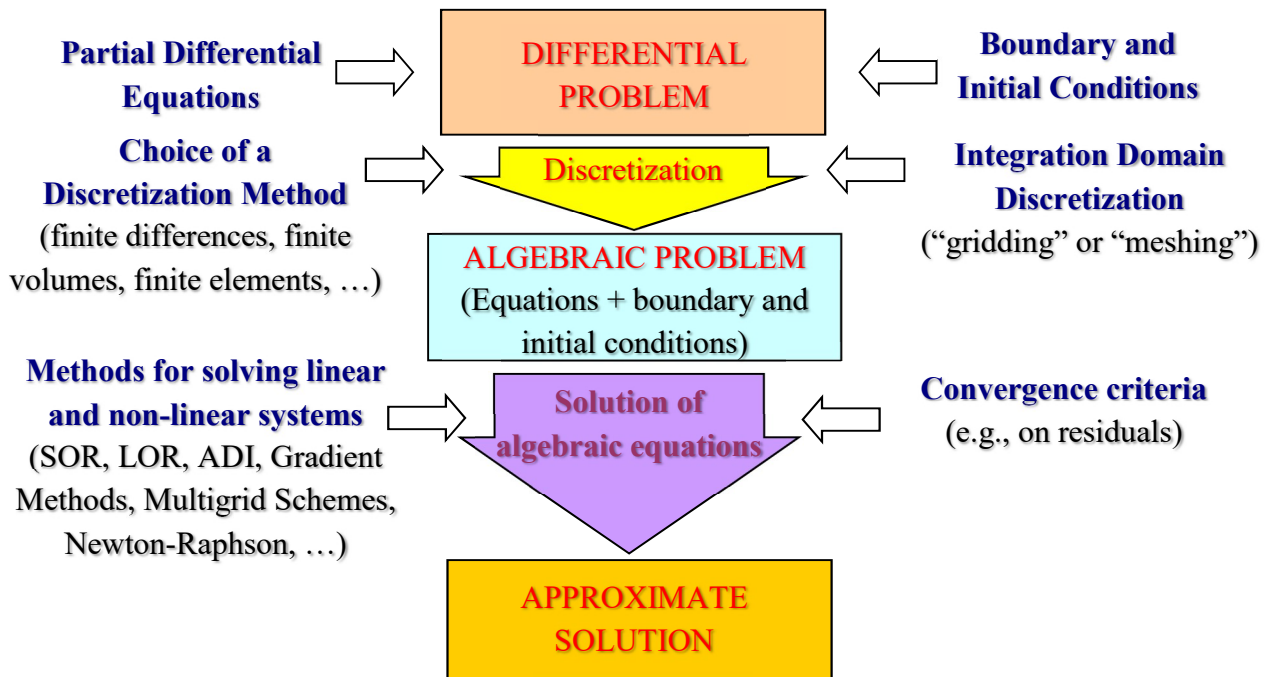
Non-linearity of some terms, complex dependence of basic properties on the solution generally introduce difficulties needing to revert to calculation resources

Most of the adopted numerical discretisation techniques refer to three categories, though more sophisticated schemes (e.g., spectral, pseudo-spectral, etc.) are also introduced. The three main techniques are:

- **finite difference methods**: the partial derivatives in the equations are substituted with appropriate expressions in terms of “finite differences” of the functions and of the independent variables (e.g., a derivative may be substituted by an incremental ratio), *leading to systems of algebraic equations* in the unknown variables
- **finite volume methods**: in this case the partial differential equations (PDEs) are reverted back to the integral form they were drawn from (see previous pages) and the volume and surface integrals appearing in them are expressed in algebraic form, *leading to systems of algebraic equations* in the unknown variables
- **finite element methods**: these techniques make use of the “method of weighted residuals” (to be discussed later on) in which the solution of the equation is expressed in approximate form (generally, in terms of low degree polynomials) and the resulting discrepancy obtained in the PDE by substituting it (the “residual”) is dealt with by integrating after multiplying by a weighting function; also this process *leads to systems of algebraic equations* in the unknown variables

In this course, it is chosen to illustrate examples of applications of the three techniques, discussing in the end their relevant features. So, we will start with “intuitive” discretisations of the problems we will be facing and then we will reflect on the generalisation of the adopted techniques

The figure in the next page provides anyway the general sketch of the problems faced when passing from a partial differential equation problem to its approximate numerical solution.



Later on we will discuss the basic mathematical properties of *consistency*, *stability* and *convergence* that numerical schemes need to satisfy to be sound tools in our hands

In addition to these properties we must consider *another relevant property of numerical schemes adopted for engineering applications* that can be stated as follows:

while solving by numerical means a conservation equation, care must be taken that no spurious sources or sinks of the conserved quantity will appear even while working with finite space and time increments

In other words, we can afford having an approximate solution of our equations, because of the use of a coarse time or space grid, but we can never afford that the discretization process will not preserve exactly the conserved quantity: this **“conservative”** character of the numerical schemes is therefore a fundamental requirement

THE EQUATIONS CONSIDERED IN THIS COURSE

With respect to the program of the course held in past years (up to Academic Year 2015-2016), this course reconsiders the previous material having the ambition to cover a wider range of problems, at the price of simplifying or discarding some treatment

In particular, though the attention is still focused on the numerical models for Reactor Physics, elements regarding the treatment of fluid-dynamic problems are introduced

This choice is coherent with the need to provide learners with knowledge and skills that will allow them to tackle the multi-physics coupled problems that is necessary to solve for nuclear reactor core analysis in normal and accident conditions

So, the problems to be coped with will involve the numerical modelling aspects of:

- reactor criticality problems, by steady-state neutron diffusion equations;
- reactor kinetics problems, by the transient neutron diffusion equation;
- neutron transport, by the integral and the integro-differential equation;
- thermal-hydraulic and Computational Fluid Dynamic (CFD) equations, together with some of their solution techniques

The result is intended to be an overall global picture of numerical solution techniques that the learner will possibly integrate in his/her understanding of the reactor cores and their behaviour