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Summary

Numerical methods in aerothermodynamics MECA-H-407

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Appel à contribution

Synthèse Open Source

Ce document est grandement inspiré de l'excellent cours donné par Gérard DEGREZ à l'EPB (École Polytechnique de Bruxelles), faculté de l'ULB (Université Libre de Bruxelles). Il est écrit par les auteurs susnommés avec l'aide de tous les autres étudiants et votre aide est la bienvenue ! En effet, il y a toujours moyen de l'améliorer surtout que si le cours change, la synthèse doit être changée en conséquence. On peut retrouver le code source à l'adresse suivante

```
https://github.com/nenglebert/Syntheses
```

Pour contribuer à cette synthèse, il vous suffira de créer un compte sur *Github.com*. De légères modifications (petites coquilles, orthographe, ...) peuvent directement être faites sur le site ! Vous avez vu une petite faute ? Si oui, la corriger de cette façon ne prendra que quelques secondes, une bonne raison de le faire !

Pour de plus longues modifications, il est intéressant de disposer des fichiers : il vous faudra pour cela installer LaTeX, mais aussi *git*. Si cela pose problème, nous sommes évidemment ouverts à des contributeurs envoyant leur changement par mail ou n'importe quel autre moyen.

Le lien donné ci-dessus contient aussi un README contenant de plus amples informations, vous êtes invités à le lire si vous voulez faire avancer ce projet !

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Contents

Introduction

Fluid dynamics is based on continuity hypothesis, all quantities can be expressed as a continuous function of time and space coordinates. The governing equations are partial differential equations. Because of the geometrical complexity of the domain and of the equations, we need strategies. The first one is to forget about the equations and to rely on experiments. The second is to consider simplified cases, and approximate theoretical analytic solutions (aerodynamics). The third approach is numerical approach. Disadvantages and advantages of the different methods can be listed as:

- **Experimental:** the advantage is that it is the most realistic, but requires equipment, there are scale problems (similarity), interferences (tests in finite space), measurement difficulties and operating costs.
- **Theoretical**: the advantage is that we have a mathematical expression and we don't have to repeat calculus, but it is restricted to simple geometries and linear problems.
- **Numerical**: the advantages are that we can dead with complex geometries, non linear problems and unsteady problems, but there are truncation errors, problems with boundary conditions like the finite space in experiment and the computation cost.

In reality these approaches are complementary. We can use the second method to simplify the numerical computations, crucial for example for costly operations like computations on turbulence. The evolution of numerical cost over the past 40 years has been particularly impressive, cost decreased dramatically. In the other hand, the experimental cost tends to increase (technical personal, material,...). Nowadays we can measure many things impossible to measure before. This explains why the numerical computations have spread incredibly.

The design relies mainly on the numerical methods and less on the experimental testing, but it is still needed to confirm the data. We can use the numerical methods in many fields and we could call this « numerical physics ». We should deal with this in a single course of computational method and then to specialize it to the specific disciplines. An approximate solution to a problem is some kind of mathematical entity, an object, which depends on a finite number of real parameters, and which constitutes a representation of the continuous field under study. The numerical solution belongs to a finite dimension space whereas the theoretical to an infinite.

There are different types of numerical representation:
- **Discrete:** collection of either point values (samples of the solutions) or subdomain averages. We are not able to give an exact solution on basis of these points, but rather an estimation.
- **Functional:** the solution is expressed as a function $u*(x) = f(x, a_i)$, depending on a set of variables. Most of the time the dependence is linear: $u* = \sum_{i=1} n a_i v_i(x)$ where $v_i(x)$ are a priori specified functions.

Ones we have chosen the numerical representation method, we have to generate a system of algebraic equations linking the parameters from the representation and the governing equations. The last step is to solve the system. The step of generating the equations system is called **discretization**. For one problem, several discretizations are possible. Some examples are given, consult the syllabus for more details.

Chapter 1

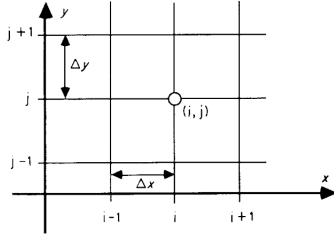# Discretization methods

1.1 Finite difference method

Figure 1.1

It is based on discrete representation of numerical solution consisting in values of the solution at the nodes of a Cartesian mesh of uniform spacing (Figure 1.1). The discretization will consist in estimating the partial derivatives appearing in the governing equations by some algebraic relations at the nodes. Because of the limitation of the mesh we cannot deal with curved geometries. To do so we need coordinate changes. In this type of mesh, each grid point can be identified by a set of indexes i, j, (k), this type of mesh is called **structured mesh**. The neighbors are implicitly given by the index identification.

1.1.1 Evaluation of derivatives by finite differences

Difference formulas for the derivative $\partial u/\partial x$

The value of a function $u(x)$ on a point of indexes i,j on the mesh is noted u_{ij}, for time dependent functions we use u_i^n where n denotes the time index and i the space index. Let's estimate $(\partial u/\partial x)_{ij}$, by definition:

$$\left.\frac{\partial u}{\partial x}\right|_{ij} = \left.\frac{\partial u}{\partial x}\right|_{x_0,y_0} = \lim_{\xi \to 0} \frac{u(x_0 + \xi, y_0) - u(x_0, y_0)}{\xi} \tag{1.1}$$

By taking $\xi = \Delta x$ to fit our grid points we get:

$$\left.\frac{\partial u}{\partial x}\right|_{ij} \approx \lim_{\Delta x \to 0} \frac{u(x_0 + \Delta x, y_0) - u(x_0, y_0)}{\Delta x} = \frac{u_{i+1\,j} - u_{ij}}{\Delta x} \tag{1.2}$$

In order to find a systematic way of deriving the equations, let's build the Taylor expansion of $u(x, y)$ around the mesh point ij:

$$u_{i+1\,j} = u_{ij} + \Delta x \left.\frac{\partial u}{\partial x}\right|_{ij} + \frac{\Delta x^2}{2} \left.\frac{\partial^2 u}{\partial x^2}\right|_{ij} + \frac{\Delta x^3}{6} \left.\frac{\partial^3 u}{\partial x^3}\right|_{\xi} \qquad x_0 \leq \xi \leq x_0 + \Delta x$$

$$\Leftrightarrow \left.\frac{\partial u}{\partial x}\right|_{ij} = \frac{u_{i+1\,j} - u_{ij}}{\Delta x} - \underbrace{\frac{\Delta x}{2} \left.\frac{\partial^2 u}{\partial x^2}\right|_{ij} - \frac{\Delta x^2}{6} \left.\frac{\partial^3 u}{\partial x^3}\right|_{\xi}}_{\text{truncation error}} = \frac{u_{i+1\,j} - u_{ij}}{\Delta x} + \mathcal{O}(\Delta x) \tag{1.3}$$

3

Giving the **forward difference formula**. We have then a truncation error which behavior is dominated by the first term when $\Delta x \to 0$, so that $TE = \mathcal{O}(\Delta x)$, meaning that there exists a bounded number K such that $\Delta x < \epsilon \to |TE| < K\Delta x$. The truncation error is always in the form $TE = \mathcal{O}(\Delta x^q)$ where q is the order of accuracy. The forward finite difference approximation of $\frac{\partial u}{\partial x}$ is first order accurate since $q = 1$. I

If the order of the method is larger, for example second order, it means that if $\Delta x \to 0$, after a certain Δx_{crit} the truncation error goes to 0 faster than the truncation error of a lower order method. If the mesh is not finer than a critical value, this is not true. When we go higher than a second order it is not clear in practice if we have something better because increasing the order allows the use of larger mesh, but is computationally expensive too.

The definition for the derivative is not unique, for instance the **backward difference formula**:

$$u_{i-1\,j} = u_{ij} - \Delta x \left.\frac{\partial u}{\partial x}\right|_{ij} + \frac{\Delta x^2}{2}\left.\frac{\partial^2 u}{\partial x^2}\right|_{ij} + H.O.T \Leftrightarrow \left.\frac{\partial u}{\partial x}\right|_{ij} = \frac{u_{ij} - u_{i-1\,j}}{\Delta x} + \mathcal{O}(\Delta x) \qquad (1.4)$$

We have an infinity of finite difference formula if make the linear combination of the two last expressions. For example if we sum half of the two we get the **central finite difference formula**:

$$\left.\frac{\partial u}{\partial x}\right|_{ij} = \frac{u_{i+1\,j} - u_{i-1\,j}}{2\Delta x} + \mathcal{O}(\Delta x2) \qquad (1.5)$$

We see that the central difference formula is more accurate than the others and involves the same mesh distance. We could thus get as high order as desired, but at the cost of increasing the number of neighboring grid points in the equation and thus the computational cost.

General method to obtain finite difference formulas

- Choose the stencil (set of points involved in the expression);
- write Taylor series expansion of all the points in the stencil around the point where the derivative is to be evaluated;
- write the finite difference formula as a linear combination of stencil point values and adjust the coefficients such that it approximates the derivative to be evaluated with the desired order of accuracy.

EXAMPLE: Let's compute the finite difference formula for $\partial^2 u/\partial x^2$ using $i-1\,j, ij$ and $i+1\,j$ (first step). The second step gives:

$$u_{i+1\,j} = u_{ij} + \Delta x \left.\frac{\partial u}{\partial x}\right|_{ij} + \frac{\Delta x^2}{2}\left.\frac{\partial^2 u}{\partial x^2}\right|_{ij} + \frac{\Delta x^3}{6}\left.\frac{\partial^3 u}{\partial x^3}\right|_{ij} + \frac{\Delta x^4}{24}\left.\frac{\partial^4 u}{\partial x^4}\right|_{ij} + H.O.T$$

$$u_{ij} = u_{ij} \qquad (1.6)$$

$$u_{i-1\,j} = u_{ij} - \Delta x \left.\frac{\partial u}{\partial x}\right|_{ij} + \frac{\Delta x^2}{2}\left.\frac{\partial^2 u}{\partial x^2}\right|_{ij} - \frac{\Delta x^3}{6}\left.\frac{\partial^3 u}{\partial x^3}\right|_{ij} + \frac{\Delta x^4}{24}\left.\frac{\partial^4 u}{\partial x^4}\right|_{ij} + H.O.T$$

The third step gives:

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_{ij} = au_{i+1\,j} + bu_{ij} + cu_{i-1\,j} = (a+b+c)u_{ij} + (a-c)\Delta x \left.\frac{\partial u}{\partial x}\right|_{ij} + (a+c)\left.\frac{\partial^2 u}{\partial x^2}\right|_{ij} + H.O.T \quad (1.7)$$

Depending on the accuracy needed, establish a system of 3 equations of 3 variables and solve by imposing the value for the different terms. For example if we want to approximate exactly we should cancel all the terms except the second order derivative term.

We can repeat this method again and again to obtain various finite difference formulas. You can consult pages 14 and 15 of the syllabus to see the list, not useful, just know that we can express the mixed second derivatives like $\partial^2 u/\partial x \partial y$ too.

Derivation of finite difference formulas using operators

In order to make the writing more compact, let's introduce some operators:

$$
\begin{array}{llll}
E_x^{+1} u_{ij} = u_{i+1\,j} & \text{Forward shift} & E_x^{-1} u_{ij} = u_{i-1\,j} & \text{Backward shift} \\
\delta_x^+ u_{ij} = u_{i+1\,j} - u_{ij} & \text{Forward difference} & \delta_x^- u_{ij} = u_{ij} - u_{i-1\,j} & \text{Backward difference} \\
\mu_x u_{ij} = \frac{1}{2}\left(u_{i+\frac{1}{2}\,j} + u_{i-\frac{1}{2}\,j}\right) & \text{Averaging} & \delta_x u_{ij} = u_{i+\frac{1}{2}\,j} - u_{i-\frac{1}{2}\,j} & \text{Centered difference}
\end{array}
$$

Another operator for the centered difference can be used:

$$
\bar{\delta}_x = \frac{1}{2}\left(\delta_x^+ + \delta_x^-\right) \qquad \Rightarrow \bar{\delta}_x u_{ij} = \frac{1}{2}\left(u_{i+1\,j} - u_{i-1\,j}\right) \tag{1.8}
$$

All these operators are also valid for y coordinate. The following relations are verified:

$$
\delta^+ = E^{+1} - 1 \qquad \delta^- = 1 - E^{-1} \qquad \bar{\delta} = \mu\delta = \delta\mu \tag{1.9}
$$

It is easy to derive finite difference formulas with these operator. For example, the Taylor series expansion of $u(x)$ is:

$$
\begin{gathered}
u(x + \Delta x) = u(x) + \Delta x \frac{\partial u}{\partial x}(x) + \frac{\Delta x^2}{2}\frac{\partial^2 u}{\partial x^2}(x) + \dots \\
\Leftrightarrow Eu(x) = \left(1 + \Delta x D + \frac{(\Delta x D)^2}{2} + \dots\right)u(x) \qquad \Leftrightarrow Eu(x) = \exp(\Delta x D)u(x)
\end{gathered} \tag{1.10}
$$

where we clearly see the Taylor expansion of $\exp(\Delta x D)$ and where $D_x = \frac{\partial u}{\partial x}$. We can then make the following manipulation:

$$
E = \exp(\Delta x \partial) \leftrightarrow \ln(E + \mathbf{1} - \mathbf{1}) = \ln(1 + \delta^+) = \Delta x D \qquad \Rightarrow D = \frac{\ln(1 + \delta^+)}{\Delta x} \tag{1.11}
$$

And finally if we make the Mac Laurin expansion:

$$
D = \frac{\delta^+}{\Delta x} - \frac{\delta^{+2}}{2\Delta x} + \frac{\delta^{+3}}{3\Delta x} + \dots \tag{1.12}
$$

By keeping the first term we find the first order forward difference formula, by keeping the second term we find the second order one, and so on.

1.1.2 Finite difference formulas for partial differential equations

There is two strategy to express equations:
- **Strategy 1**: simply assemble the finite difference formula for each individual derivative;
- **Strategy 2**: same strategy used to find the finite difference in many steps, select the stencil, Taylor expansion on each point of the stencil, write the FD formula as a linear combination of the stencil points values and select the coefficients.

The first method is the most used. For the Laplace equation $\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$ we have:

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_{ij} = \frac{\delta_x{}^2 u_{ij}}{\Delta x^2} + \mathcal{O}(\Delta x^2) \qquad \left.\frac{\partial^2 u}{\partial y^2}\right|_{ij} = \frac{\delta_y{}^2 u_{ij}}{\Delta y^2} + \mathcal{O}(\Delta y^2) \qquad (1.13)$$

If we sum this up we get:

$$\frac{\delta_x{}^2 u_{ij}}{\Delta x^2} + \frac{\delta_y{}^2 u_{ij}}{\Delta y^2} = 0 \qquad \Rightarrow \frac{u_{i+1\,j} - 2u_{ij} + u_{i-1\,j}}{\Delta x^2} + \frac{u_{i\,j+1} - 2u_{ij} + u_{i\,j-1}}{\Delta y^2} = 0 \qquad (1.14)$$

The equation can contain a first order derivative and there can thus exists several discretization (forward, backward, ...).

1.1.3   Arbitrary geometries - irregular meshes

The method we have seen is very simple, we love it. But the expressions rapidly become very difficult when dealing with irregular meshes. In addition, the order of accuracy is lower when irregular meshes compared to the regular one with same size mesh. The formulas become intractable for more than 3 points. We cannot only use uniform meshes for at least two reasons:

- **Computational domain geometry:** when the boundary is curved, it is quasi impossible to use uniform rectangular mesh. On the aerofoil example below, one can see that the grid points not always intersect the nodes on the geometry.
- **Presence of regions where the solution varies rapidly:** for example, in fluid mechanics, there are regions such as the boundary layer where the fluid properties vary more rapidly than anywhere else. It is thus interesting to have finer mesh there and larger mesh somewhere where we don't care.
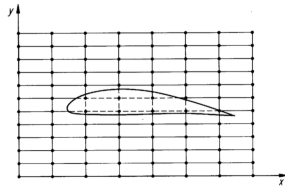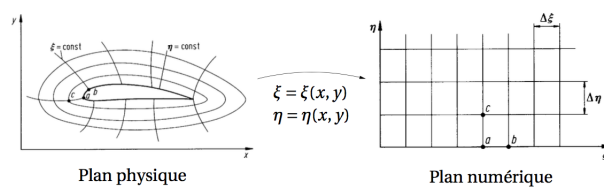
Figure 1.2   Figure 1.3

To tackle these problems, one can use coordinate transformation as suggests Figure 1.3. One can thus first fit a certain geometry, but also achieve a local concentration of mesh points. There are two disadvantages to this: we transform the geometrical complexity into equation complexity, and it is very difficult to find these transformation (numerical methods needed). The good news are that in the numerical plane, the mesh is regular and numerical algorithms have high efficiency, the transformation will be discussed later.

1.2   Finite volume method

The main idea is to take advantage of conservation equations whose fundamental form is the **integral form**, we discretize the integral. The principle consist in the application of the control volume method (macroscopic balances) in a large scale. The classical example is to have a bent tube, the flow exerts a force on the elbow and we can easily estimate it by momentum balance. We just take several small volumes where to apply this.

The great advantage of this method is to use arbitrary polygons (2D) or polyhedra (3D) as control volume so that it offers great **flexibility**. Unlike the finite difference method, the finite volume method can accommodate arbitrary control volume shapes, this eases mesh generation dramatically. There are some independent variables (time and space) that does not need flexibility it is the time variable, this is why wee still use finite differences for time discretization. In addition, since the integral form is discretized, it allows the computation of **weak solutions** of the flow.

1.2.1 Fundamental principles and variants of the method

Let's consider the integral form of a general system of conservation equations:

$$U = \begin{pmatrix} \rho \\ \rho\vec{u} \\ \rho E \end{pmatrix} \qquad \Rightarrow \frac{\partial U}{\partial t} + \nabla.\vec{F} = Q, \tag{1.15}$$

where $\vec{F}$ is the **flux vector** and Q the **source term**. If we take the momentum equation and the conservation equation, we can see that there is a part independent of the derivative of U (convective term) and a diffusive term dependent of $\nabla U \rightarrow \vec{F} = \vec{F}(U, \nabla U)$:

$$\frac{\partial \rho\vec{u}}{\partial t} + \nabla(\underbrace{\rho\vec{u} \otimes \vec{u} + p\bar{\bar{1}}}_{\text{convective}} - \underbrace{\bar{\bar{\tau}}}_{\text{diffusive}}) = \rho\vec{g} \tag{1.16}$$

The corresponding integral form is the basic original form obtained by integration of the equation over a control volume Ω:

$$\frac{d}{dt} \int_\Omega U \, d\Omega + \oint_{\partial\Omega} \vec{F}.\vec{n} \, dS = \int_\Omega Q \, d\Omega \tag{1.17}$$

Remark that discontinuities are allowed in this integral form since we do not have to verify the differentiation everywhere in the domain. If we subdivide the domain in elementary volumes and use the average value of U on that volumes $\int_{\Omega_k} U \, d\Omega = U_k \Omega_k$ these are chosen as the parameters of the discrete representation, and assume the control volume to be a polygon (Γ_m the faces), we have:

$$\frac{d}{dt}(\Omega_k U_k) + \sum_{\Gamma_m \in \partial\Omega_k} \int_{\Gamma_m} \vec{F}.\vec{n} \, dS = \int_{\Omega_k} Q \, d\Omega \tag{1.18}$$

To make the discretization, we need to evaluate the remaining surface and volume integrals in terms of neighboring control volume averages. How to build the control volumes? First a mesh of non-overlapping elementary surfaces/volumes is generated, these are called cells. The design of control volumes must respect a certain number of conditions:

- the union of CVs must cover the whole domain of interest;
- the CVs may overlap but the boundaries of a CV should be either lying on the domain boundary or belong to the boundary of another CV. Each CV boundary must be shared by two CVs;
- the expression of the flux integral on a common edge should be the same for the two CVs it belongs to.

Consider two CVs K and L with a common face Γ_c and make the sum:

$$\frac{d}{dt}(\Omega_K U_K) + \sum_{\Gamma_m \in \partial\Omega_K} \int_{\Gamma_m} \vec{F}.\vec{n}\, dS = \int_{\Omega_K} Q\, d\Omega$$

$$\frac{d}{dt}(\Omega_L U_L) + \sum_{\Gamma_m \in \partial\Omega_L} \int_{\Gamma_m} \vec{F}.\vec{n}\, dS = \int_{\Omega_L} Q\, d\Omega \tag{1.19}$$

$$\Rightarrow \frac{d}{dt}(\Omega_K U_K + \Omega_L U_L) + \sum_{\Gamma_m \in \partial\Omega_K \cup \partial\Omega_L \setminus \Gamma_c} \int_{\Gamma_m} \vec{F}.\vec{n}\, dS = \int_{\Omega_K \cup \Omega_L} Q\, d\Omega$$

where we can observe that the common boundary integral disappears since the flux should be the same but the normals are opposite to each others. This last property is called **telescopic property** that ensures the conservation at the discrete level and the capture of discontinuities. Indeed, if the flux was different on K and L, the term would remain.
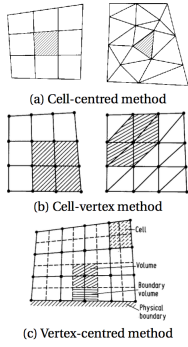

(a) Cell-centred method

(b) Cell-vertex method

(c) Vertex-centred method

Figure 1.4

Several arrangement methods exists:
- the CV coincide with the mesh cell → cell-centered method;
- the CV is made out of mesh cells having a common vertex → cell-vertex method;
- the CV is made out of part of mesh cells sharing a common vertex → vertex centered method.

In the two last ones, it is common to associate the volume average to the corresponding vertex as done in finite difference. Only these will be considered. Let's mention that it is not compulsory to use the same CVs for different equations of a system of equations.

1.2.2 Evaluation of fluxes through faces

In general we will approximate the integral over a length/surface $Gamma_i$ by a one point quadrature integration formula:

$$\int_{\Gamma_m} \vec{F}.\vec{n}\, dS \approx \vec{F}_m.\vec{n}_m S_m \tag{1.20}$$

This is sufficient for first order and second order methods, for higher order you have to use more points quadrature. Moreover, higher order are not easy to construct, this is why we have finite element methods. Let's discuss about aerothermodynamic problems ($\vec{F} = \vec{F}(U, \nabla U)$) in 1D for simplicity. We will consider a vertex-centered 1D FV method and the CVs are segments. The discretization becomes:

$$\frac{d}{dt}(\Delta x_i U_i) + F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}} = 0 \tag{1.21}$$

How to express the $F_{i+1/2}$ and the other in function of cell averages? One needs to specify a **numerical flux formula** which plays the same role as finite difference formulas in finite difference method. We will say that:

$$F_{i+\frac{1}{2}} \approx \Phi(U_{i-k+1}, \ldots, U_{i+k}) \tag{1.22}$$

For the method to be at least of order one, the approximation should be exact for a uniform field $\Phi(U, \ldots, U) = F(U)$. The simplest choice is to take an arithmetic average of the fluxes or of the variables:

$$\Phi(U_i, U_{i+1}) = (F_i + F_{i+1})/2 \qquad \Phi(U_i, U_{i+1}) = F\left(\frac{U_i + U_{i+1}}{2}\right) \tag{1.23}$$

This applied to (1.21) gives:

$$\frac{d}{dt}(\Delta x_i U_i) + \frac{F_i + F_{i+1}}{2} - \frac{F_{i-1} + F_i}{2} = 0 \qquad \Rightarrow \frac{dU_i}{dt} + \frac{F_{i+1} - F_{i-1}}{2\Delta x_i} = 0 \tag{1.24}$$

which is the same expression as obtained by central finite difference formula. One can retrieve the first order forward and backward finite difference formula by choosing $\Phi(U_i, U_{i+1}) = F(U_{i+1})$ and $\Phi(U_i, U_{i+1}) = F(U_i)$.

Let's come back to the nature of the finite volume numerical representation. It consists of a set of average values over subdomains and is thus clearly a discrete representation. For cell-centered or vertex-centered methods (not overlapping) it is easy to reconstruct a functional representation out of the averages. A piecewise constant reconstruction and a linear reconstruction are illustrated below.
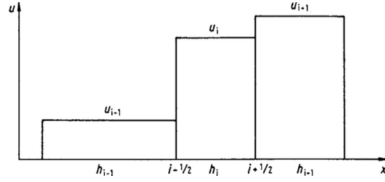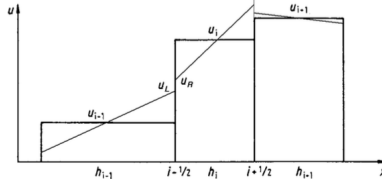

Figure 1.5   Figure 1.6

In the second, the solution gradient is estimated in each CV but the reconstruction remains discontinuous at the boundaries so that it does not eliminate the need for a numerical flux function to compute the flux across the boundaries. But it allows to easily construct more accurate flux functions, starting from a two variable flux function:

$$F_{i+\frac{1}{2}} \approx \Phi(U_i, U_{i+1}) \tag{1.25}$$

associated with the constant reconstruction, one obtains more accuracy by replacing U_i and U_{i+1} by U_L and U_R. For instance using the backward flux formula $\Phi(U_L, U_R) = F(U_L)$ and a gradient estimation in CV i based on the back point:

$$\left(\frac{\partial U}{\partial x}\right)_i \approx \frac{U_i - U_{i-1}}{\Delta x} \qquad \Rightarrow U_{L,i+\frac{1}{2}} = \frac{3}{2}U_i - \frac{1}{2}U_{i-1}, \tag{1.26}$$

One can obtain the following space discretization:

$$\frac{dU_i}{dt} + \frac{1}{\Delta x}\left(F\left(\frac{3U_i - U_{i-1}}{2}\right) - F\left(\frac{3U_{i-1} - U_{i-2}}{2}\right)\right) = 0 \tag{1.27}$$

and for a particular $F(U) = au$, we have:

$$\frac{dU_i}{dt} + a\frac{3U_i - 4U_{i-1} + U_{i-2}}{2\Delta x} \tag{1.28}$$

which is the one we found in previous section. Generally, for a polynomial reconstruction of order k we shall obtain a discretization of order at least $k + 1$. For the diffusive fluxes we have to estimate the gradient of variables on the faces which can be done directly or by averaging the estimated gradients in the two neighboring CVs. This is done by Green-Gauss theorem:

$$\int_\Omega \nabla U \, d\Omega = \oint_\Gamma U \vec{n} \, dS \tag{1.29}$$

by choosing an auxiliary control volume Ω centered on the point where one wishes to estimate the gradient.

1.2.3 Vertex-centered finite volumes in two dimensions and comparison with finite differences in transformed coordinates
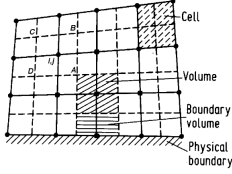

Figure 1.7

Here we will show that the FV method is equivalent to the FD in transformed coordinates. We consider first a vertex centered FV method on a structured mesh and then FD method in transformed coordinates. The advantage of structured mesh is the explicit connectivity, but its generation is more complex. We take the finite volume around the point i, j. Let's write the Euler equation:

$$\frac{\partial U}{\partial t} + \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} = \frac{\partial U}{\partial t} + \nabla . \vec{F} = 0 \tag{1.30}$$

The finite volume discretization over the 4 points can be written as:

$$\Omega_{ABCD} \frac{dU_{ij}}{dt} + \sum_{m=1}^{4} \vec{F}_m \vec{n}_m l_m = 0 \tag{1.31}$$

where $\vec{F}_m$ can be chosen as the average value (middle of sides) and $n_x l = \Delta y, n_y l = -\Delta x$ since if we consider the angle θ made by AB we have that $\vec{n} = \cos\theta \vec{e}_1 + \sin\theta \vec{e}_2$ with $\cos\theta = \frac{\Delta y_{AB}}{AB}$ and $\sin\theta = -\frac{\Delta x_{AB}}{AB}$. Ω_{ABCD} can be computed as the vector product of diagonals:

$$\Omega_{ABCD} = \frac{1}{2} |\Delta \vec{x}_{AC} \times \Delta \vec{x}_{BD}| = \frac{1}{2} (\Delta x_{AC} \Delta y_{BD} - \Delta x_{BD} \Delta y_{AC}) \tag{1.32}$$

We see that the remaining work to discretize is to express $\frac{dU_{ij}}{dt}$ by a finite difference formula. We could do in other way.

Let's now examine the transformed coordinates FD, let's do the chain rule and replace the expressions in Euler equation to get the transformed coordinates equation:

$$\frac{\partial F_x}{\partial x} = \xi_x \frac{\partial F_x}{\partial \xi} + \eta_x \frac{\partial F_x}{\partial \eta} \qquad \frac{\partial F_y}{\partial y} = \xi_y \frac{\partial F_y}{\partial \xi} + \eta_y \frac{\partial F_y}{\partial \eta} \tag{1.33}$$

$\xi_x, \xi_y, \eta_x \eta_y$ are the **metric terms**. We have the relation $\frac{dx}{d\xi} \frac{d\xi}{dx} = 1$ that can be generalized into matrix as follows:

$$\begin{pmatrix} x_\xi & x_\eta \\ y_\xi & y_\eta \end{pmatrix} \begin{pmatrix} \xi_x & \xi_y \\ \eta_x & \eta_y \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{1.34}$$

We can express the following relations:

$$\xi_x = \frac{\begin{vmatrix} 1 & x_\eta \\ 0 & y_\eta \end{vmatrix}}{\begin{vmatrix} x_\xi & x_\eta \\ y_\xi & y_\eta \end{vmatrix}} \qquad \Rightarrow J\xi_x = y_\eta \quad J\xi_y = -x_\eta \quad J\eta_x = -y_\xi \quad J\eta_y = x_\xi$$

$$\Rightarrow \frac{\partial(J\xi_x)}{\partial \xi} + \frac{\partial(J\eta_x)}{\partial \eta} = 0 \qquad \frac{\partial(J\xi_y)}{\partial \xi} + \frac{\partial(J\eta_y)}{\partial \eta} = 0 \tag{1.35}$$

We can multiply by J (1.33) and find:

$$J\frac{\partial F_x}{\partial x} = J\xi_x\frac{\partial F_x}{\partial \xi} + J\eta_x\frac{\partial F_x}{\partial \eta} = \frac{\partial(J\xi_x F_x)}{\partial \xi} + \frac{\partial(J\eta_x F_x)}{\partial \eta} - F_x\underbrace{\left(\frac{\partial(J\xi_x)}{\partial \xi} + \frac{\partial(J\eta_x)}{\partial \eta}\right)}_{=0}$$

$$J\frac{\partial F_y}{\partial y} = J\xi_y\frac{\partial F_y}{\partial \xi} + J\eta_y\frac{\partial F_y}{\partial \eta} = \frac{\partial(J\xi_y F_y)}{\partial \xi} + \frac{\partial(J\eta_y F_y)}{\partial \eta} - F_y\underbrace{\left(\frac{\partial(J\xi_y)}{\partial \xi} + \frac{\partial(J\eta_y)}{\partial \eta}\right)}_{=0}$$

(1.36)

So that by multiplying the transformed Euler equation (conservative) by J and replacing we get:

$$J\frac{\partial U}{\partial t} + \frac{\partial(J\xi_x F_x + J\xi_y F_y)}{\partial \xi} + \frac{\partial(J\eta_x F_x + J\eta_y F_y)}{\partial \eta} = 0 \tag{1.37}$$

We can now discretize this equation using centered finite differences:

$$J\frac{\partial U_{ij}}{\partial t} + \frac{(J\xi_x F_x + J\xi_y F_y)_{i+\frac{1}{2}\,j} - (J\xi_x F_x + J\xi_y F_y)_{i-\frac{1}{2}\,j}}{\Delta\xi}$$

$$+ \frac{(J\eta_x F_x + J\eta_y F_y)_{i\,j+\frac{1}{2}} - (J\eta_x F_x + J\eta_y F_y)_{i\,j-\frac{1}{2}}}{\Delta\eta} = 0$$

(1.38)

where $\Delta\xi = \Delta\eta = 1$. We can easily rewrite this by defining the middle point as average:

$$J\frac{\partial U_{ij}}{\partial t} + (J\nabla\xi)_{i+\frac{1}{2}\,j}\frac{\vec{F}_{ij} + \vec{F}_{i+1\,j}}{2} - (J\nabla\xi)_{i-\frac{1}{2}\,j}\frac{\vec{F}_{i-1\,j} + \vec{F}_{ij}}{2}$$

$$+ (J\nabla\eta)_{i\,j+\frac{1}{2}}\frac{\vec{F}_{ij} + \vec{F}_{i\,j+1}}{2} - (J\nabla\eta)_{i\,j-\frac{1}{2}}\frac{\vec{F}_{i\,j-1} + \vec{F}_{ij}}{2} = 0$$

(1.39)

We can express the derivatives of the metric terms easily, for example for:

$$(J\xi_x)_{i+\frac{1}{2}\,j} = (y_\eta)_{i+\frac{1}{2}\,j} = \frac{y_B - y_A}{\Delta\eta} = \Delta y_{AB}$$

$$(J\xi_y)_{i+\frac{1}{2}\,j} = (-x_\eta)_{i+\frac{1}{2}\,j} = \frac{-x_B + x_A}{\Delta\eta} = -\Delta x_{AB}$$

(1.40)

We found out that $(J\nabla\xi)_{i+\frac{1}{2}\,j} = (\vec{n}l)_{AB}$ and we can do the same for the others. To conclude, we have to proof that $J = \Omega_{ij}$ but this is obvious by computing the determinant and we know the expression of $\vec{x}_\xi$ and $\vec{x}_\eta$ at point $i\pm\frac{1}{2}\,j$ and $i\,j\pm\frac{1}{2}$ so we just have to make the average to have ij:

$$J_{ij} = |\vec{x}_\xi \times \vec{x}_\eta|_{ij} = \frac{1}{2}(\Delta\vec{x}_{DA} - \Delta\vec{x}_{BC} \times \Delta\vec{x}_{AB} - \Delta\vec{x}_{CD}) \tag{1.41}$$

We can conclude that FV is the generalization of FD in changed coordinate. The advantage of the finite volume is that we can now deal with any quadrilateral.

1.3 Finite element method

It is based on a functional representation, a linear combination of basis or **shape functions** $u*(x) = \sum_{i=1}^{n} a_i v_i(x)$ and the parameters are the **coefficients** of the basis functions, that are determine such that we get the best approximation of the exact solution. It differs from Galerkin and Ritz method by the selection of a **piecewise polynomial interpolation function** as

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shape functions. It is a method to construct generalized finite difference formulas. For example, the numerical solution parameters are values of the solution at particular points (nodes) and the discretized equations have a local character as in FD.

The convergence of the method is primordial, the numerical solution must tend to the exact solution when the number of parameters tends to infinity.

1.3.1 Various form of a differential equation

We already saw that the conservation laws can be put under an integral form. But other forms exist, for example the **weak form** and the **variational form**.

The **differential form**, also called strong form (needs to be satisfied on all points of the domain and thus the derivatives too). Then we have the **integral form** developed by physicians and that does not require to be differentiable everywhere and thus allows the existence of discontinuities: **weak solutions**.

To illustrate the weak form, consider the elastic deformation of a bar fixed at his upper end and submitted to its own weight and a traction force at the other end. Taking x-axis pointing downward, the strong form is:

$$\frac{d}{dx}\left(k\frac{du}{dx}\right) + \mu g = 0 \qquad u(0) = 0 \quad k\frac{du}{dx}(L) - F = 0 \tag{1.42}$$

where u is the displacement, k the rigidity (can be discontinuous) and μ the mass per unit length. As the equation must be satisfied everywhere, we can integrate the equation after having multiplied by a test function and add a null term due to the boundary condition:

$$-\int_0^L \nu(x)\left[\frac{d}{dx}\left(k\frac{du}{dx}\right) + \mu g\right]\,dx + \nu(L)\left[k\frac{du}{dx}(L) - F\right] = 0 \tag{1.43}$$

And by integrating by parts $f = \nu(x)$ and $g' = \frac{d}{dx}(k\frac{du}{dx})$:

$$\int_0^L \left[\frac{d\nu}{dx}k\frac{du}{dx} - \mu g\nu\right]\,dx - \underbrace{\nu(0)k\frac{du}{dx}(0)}_{=0} - \nu(L)F = 0 \tag{1.44}$$

where we make the underbraced term $= 0$ by choosing $\nu(0) = 0$ in order to satisfy the boundary condition at the fixation. This is the weak form of the equation and is also found by application of the virtual work theorem. The highest differentiation order is here reduced from two to one and allows the first order derivative to be discontinuous. This example does not contain that unless the material property is discontinuous.

In fluid mechanics, shocks are discontinuities and consider the following equation in conservation form of a quasi-one dimensional nozzle flow:

$$\frac{d}{dx}\left(\frac{u^2}{2}\right) - xu = 0 \qquad u(-1) = 1; \quad u(1) = -0.5$$

$$u\frac{du}{dx} = xu \Leftrightarrow u = \frac{x^2}{2} + c \tag{1.45}$$

By considering the two boundary conditions the discontinuity appears:

$$U_L = \frac{x^2+1}{L} \qquad U_R = -1 + \frac{x^2}{2} \tag{1.46}$$

The weak form of the previous equation is again obtained using the weighting function $\nu(x)$ that must now vanish at 1 and -1:

$$\int_{-1}^{1} \nu(x) \left[\frac{d}{dx}\left(\frac{u^2}{2}\right) - xu \right] dx = \int_{-1}^{1} \left[\frac{d\nu}{dx}\frac{u^2}{2} - ux \right] dx = 0a \tag{1.47}$$

where there is no longer the derivative of u. Come back to the bar, an extremum case can be to choose a variation for $\nu(x) = \delta u(x)$ such that:

$$\int_{0}^{L} \left[\frac{d\delta u}{dx} k \frac{du}{dx} - \mu g\delta u \right] dx - \delta u(L)F = 0 = \delta \left[\int_{0}^{L} \left[\frac{k}{2}\left(\frac{du}{dx}\right)^2 - \mu gu \right] dx - u(L)F \right] \tag{1.48}$$

This can be interpreted as the variation of the total energy and the solution is the one that gives stationary energy.

1.3.2 Shape functions - finite element interpolation

As explained, shape functions are piecewise polynomial interpolation functions and its parameters are values of the numerical solution in certain points. Here are the principles to construct these shape functions:

- The domain is divided into a set of non-overlapping simple polygons or polyhedra (the edges are not forced to be straight);
- To each domain we associate some points called **nodes** and we get an **element**. In almost all cases, the nodes include the vertices but could also be on the edges or inside the element.;
- To each node N is associated a function $\nu_n(x)$ which is defined locally within the element as a polynomial interpolation function. It must vanish at other nodes:

$$\forall P \in \Omega_e : \nu_n(xp) = \delta_{np} \tag{1.49}$$

This definition of the interpolation function has several consequences:
— The order of the polynomial is directly linked to the number of nodes. For example for a triangular 3 nodes element we will use a linear interpolation in 2 space variables (P1), while for quadratic polynomials 6 nodes are required since we have 6 coefficients in the interpolation (P2).

— The shape function is defined locally for each element. The global basis function associated to a node is thus simply the function equal to the local basis function on each element. If the node belongs to one element the global basis function is the local basis function of the element, if it belongs to several, the global basis function is made of all the local shape function of all the elements it belongs to. A consequence is that the global function associated to node N vanish on all other nodes (called compact support).

Also since the basis functions are uniquely defined on each element and since they coincide on a mesh belonging to several element, these are continuous functions.

— The coefficients of the interpolations are values of the numerical solution at the corresponding node:

$$u^*(x_i) = \sum_{j=1}^{n} a_j \nu_j(x_i) = a_i \qquad (1.50)$$

We shall call them $a_i = u_i$.

We are going to consider some example in 1D, where we have to divide the the domain into set of intervals and associate nodes. The attribution of nodes differs from polynomial order.
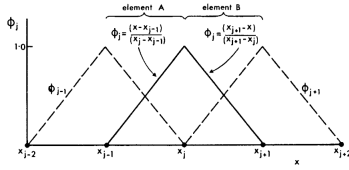
Figure 1.8

P1 element First order polynomial has two coefficients ($a + bx$) thus we need two nodes per element to determine them all, we take them on vertices. If we call the local shape functions on element A and B, the global shape function around node j is made of the two.

$$\phi_i^A = \frac{x - x_{j-1}}{x_j - x_{j-1}} \qquad \phi_i^B = \frac{x_{j+1} - x}{x_{j+1} - x_j} \qquad (1.51)$$

P2 element We have now a 2nd order polynomial ($a + bx + cx^2$) with 3 coefficients and thus 3 nodes are needed. In general the third node is placed at the middle of the element. The shape functions can be simply chosen via the Lagrange interpolation, for example:

$$\phi_j^A = \frac{(x_{j+2}-x)(x_{j+1}-x)}{(x_{j+2}-x_j)(x_{j+1}-x_j)} \qquad \phi_{j+1}^A = \frac{(x_{j+2}-x)(x-x_j)}{(x_{j+2}-x_{j+1})(x_{j+1}-x_j)}$$
$$\phi_{j+2}^A = \frac{(x_{j+1}-x)(x-x_j)}{(x_{j+1}-x_{j+2})(x_{j+2}-x_j)} \qquad (1.52)$$

or for higher dimensions, using a parent element. The parent element is defined in ξ, η for the higher dimension case and in ξ coordinate for 1D where for P2 element the nodes are placed at 0, 1/2 and 1. The shape functions in the normalized coordinates are:

$$\phi_1 = (2\xi - 1)(\xi - 1) \qquad \phi_2 = 4\xi(1 - \xi) \qquad \phi_3 = \xi(2\xi - 1) \qquad (1.53)$$

The same shape functions can be used for the transformation, in higher dimension we have:

$$x(\xi, \eta) = \sum x_i \phi_i(x, y) \qquad y(\xi, \eta) = \sum y_i \phi_i(x, y) \qquad (1.54)$$

We speak about **isoparametric mapping** in this case since the polynomial order is equal to the number of nodes. If lower order polynomials are used we speak of subparametric mapping.

Figure 1.9
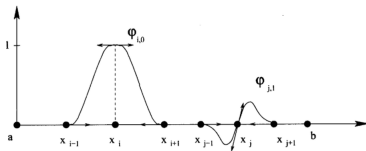
P3 Hermite element We have $a + bx + cx^2 + dx^3$, we need thus 4 nodes per element. We could just do as before so use Lagrange interpolation with the 2 vertices and two internal nodes, but it is also possible to use Hermite element: we only use the vertices and the numerical parameters are not only solution at nodes but also of its derivative. We have 2 dof at each node so that the shape functions in the normalized element are:

$$\phi_{0,0} = (2\xi + 1)(\xi - 1) \quad \phi_{0,1} = \xi(\xi - 1)^2 \quad \phi_{1,0} = (3 - 2\xi)\xi^2 \quad \phi_{1,1} = (\xi - 1)\xi^2 \qquad (1.55)$$

In P1 and P2 the basis functions have discontinuous derivatives. The advantage of Hermite is to ensure also the continuity of the derivatives at the nodes. The other advantage is counting

the number of dof. Suppose an interval from 0 to L and n elements in the interval, how many unknowns with Lagrange? $\#dof = n + 1 + 2internals = n + 1 + 2n = 3n + 1 = \mathcal{O}(3n)$ while it is $\mathcal{O}(2n)$ for Hermite. We have the same accuracy at a lower cost.

1.3.3 Discretization - extremum form: Ritz method

In some cases we do have a variational form, we can find the numerical solution by imposing it to make the variation stationary within the set of numerical solutions of the chosen form:

$$\frac{\partial E(u^h)}{\partial u_i} = 0 \qquad i = 1, \ldots, n \tag{1.56}$$

We have thus n equations and n unknowns and the solution will be the best in the energy sense. Generally we have something of the form:

$$
\begin{aligned}
E(u) &= \int_\Omega F(u, \nabla u)\, d\Omega + \int_{\partial\Omega} g(u)\, d\Gamma \\
\Rightarrow \frac{\partial E(u^h)}{\partial u_i} &= \int_\Omega \left[\frac{\partial F}{\partial u}\frac{\partial u^h}{\partial u_i} + \frac{\partial F}{\partial u_{x_p}}\frac{\partial}{\partial u_i}\left(\frac{\partial u^h}{\partial x_p}\right) \right] d\Omega + \int_{\partial\Omega} \frac{\partial g(u)}{\partial u}\frac{\partial u^h}{\partial u_i}\, d\Gamma = 0 \\
&= \int_\Omega \left[\frac{\partial F}{\partial u}v_i + \frac{\partial F}{\partial u_{x_p}}\frac{\partial v_i}{\partial x_p} \right] d\Omega + \int_{\partial\Omega} \frac{\partial g(u)}{\partial u}v_i\, d\Gamma = 0
\end{aligned} \tag{1.57}
$$

The last line of the equation is obtained by remembering $u^h(x) = \sum_{i=1}^n u_i v_i(x)$. Remark that the last line is the weak form of the equation with v_i as test function.

1.3.4 Discretization - weak form: weighted residual method

All the differential equations cannot be put under variational form and the previous case is not always applicable. In contrast weak form exists in all case and can be used as basis for discretization. Symbolically if we have $D(u) = 0$, for a numerical solution u^h the equation will not vanish. We will have a residual $D(u^h) = r^h$. It is thus logical to determine the coefficients u_i so that the residual is minimized. The **least-square** definition consists in minimizing the residual quadratic nom:

$$J(u^h) = \int_\Omega (r^h)^2\, d\Omega \tag{1.58}$$

where for simplicity we considered prescribed solution at the boundary but in general case the boundary condition terms should be added. The minimization consists in:

$$\frac{\partial J(u^h)}{\partial u_i} = \int_\Omega 2\frac{\partial r^h}{\partial u_i}r^h\, d\Omega = 0 \qquad i = 1, \ldots, n \tag{1.59}$$

the weighting functions are $w_i^{LS} = 2(\partial r^h/\partial u_i)$, and after integration we find the weak form of the differential equation:

$$\int_\Omega [vF(u, \nabla u) + \nabla v.\vec{g}(u, \nabla u)]\, d\Omega + \int_{\Gamma=\partial\Omega} vH(u)\, d\Gamma = 0 \tag{1.60}$$

were we choose $v_i = w_i(x)$. You take as many weighting functions as parameters. Let's enumerate a certain number of requirements the w_i should satisfy:
- They should be in the same number of the numerical parameters/shape functions to provide closed algebraic system;

- They should form a complete set: if you have a domain Ω the weighting functions should fill the whole domain, no empty space.

Discretization is not unique it depends on the choice of weight.

Galerkin method

The shape functions satisfy the two criteria. If we do that we refind the Ritz method. When a problem can be cast in extremum form, Galerkin method is similar to the Ritz method and is optimal in energy sense. Since the weighting functions belongs to the same functional space than the numerical solution, it requires continuity of the shape functions only up to one order less than that of the highest derivative in the weak form.

Least squares method

Has been seen at the beginning of the section. It has the advantage to be tackled by classical minimization methods and to solve the instability problems of the Galerkin method for convection problems. But in contrast it requires C^1 continuities for second order derivatives, costly.

Point collocation method

One of the drawbacks of previous methods is to perform computation of comlpex integrals. This can be avoided by using Dirac distributions as weighting functions $w_i(x) = \delta(x - x_i)$ so that the discrete equations become $r^h(x) = 0$. The main disadvantages are that to require a high order approximation and to be less accurate.

Subdomain collocation method

This is a finite volume-like method whereas the previous is a finite element-like method. We choose piecewise constant functions equal to one on a subdomain Ω_i and zero elsewhere:

$$\int_{\Omega_i} r^h \, d\Omega = 0 \tag{1.61}$$

This approach offers advantage when the equation to be solved is a conservation law so that the integral can be transformed into surface integral through Gauss theorem. This is known as control-volume based finite element method. The number of subdomains must be equal to the number of nodes. The method is similar to cell vertex centered or vertex centered method since the subdomain is chosen as the set of nodes like them.

Petrov-Galerkin method

When it is not one of the previous method and we use several weighting we speak of that.

1.4 Spectral methods

1.4.1 Representation

Just like finite element, it is based on a functional representation of the solution $u^*(x) = \sum_{i=1}^n a_i v_i(x)$. The difference is that instead of choosing a piecewise polynomial as shape function, we choose trigonometric functions or families of orthogonal functions. For example in lifting line theory it was logical to express $\Gamma(\theta) = \sum m = 1^N a_m \sin mx$ with $\Gamma(0) = \Gamma(\pi) = 0$, use

of truncated Fourrier serie. As long as the solution is smooth it provides accurate values for few terms in the serie. There are 2 fundamental differences, basic functions are infinitely differentiable, we don't have to worry about the continuity. In finite elements we had C^0 continuity. The convergence is much faster for spectral methods when number of elements increases: FE: $\epsilon \propto h^{k+1}$, spectral: $\epsilon \propto \exp(-1/h)$. The approximation can be noted as:

$$u^*(x) = \sum_{k=-\frac{n}{2}+1}^{\frac{n}{2}} \hat{u}_k \exp\left(\frac{2\pi I k x}{L}\right) \tag{1.62}$$

For periodic problems, v_i are trigonometric functions. For non periodic problems we use families of orthogonal polynomials such as Chebyskev, Legendre, Laguerre. Spectral methods is very limited to some problems, it is used for numerical computations around the atmosphere (forecasting).

But there is a price to pay for that, the shape functions are not defined locally but globally and the shape functions do not represent the solution value in some certain point. They are non zero over the whole domain, so the system of equations is not sparse, all the parameters are coupled. Basis functions are not of compact support!

Discretization

Same as FE. Since the basis functions are infinitely differentiable we don't have problems with collocations.

Chapter 2

Elements of PDE's

Convergence was an interesting issue but the type of the equation we have to solve is also important. This is why we study the elements of the theory of PDE's

2.1   Quasi-linear equations – Conservative form

A quasi-linear equation is an equation that is linear in the highest derivatives. We start with a first order equation.

General form of a first order quasi-linear equation in two variables

For example for a two space variables, it means that we look for a function of $u(x, y)$ involving only first derivatives. And typically we have a linear combination of x and y derivatives and the coefficients may depend on u too:

$$P(x, y, u)\frac{\partial u}{\partial x} + Q(x, y, u)\frac{\partial u}{\partial y} = R(x, y, u) \tag{2.1}$$

This doesn't mean that the equation is linear, for example $\frac{\partial u}{\partial x} + u\frac{\partial u}{\partial y} = S(x, y, u)$ non linear Burger's equation.

General form of a second order quasi-linear equation in two variables

The second order equation in 2 space variables:

$$
\begin{aligned}
P\left(x, y, u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}\right)\frac{\partial u^2}{\partial x^2} + 2S\left(x, y, u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}\right)\frac{\partial u^2}{\partial x \partial y} \\
+ T\left(x, y, u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}\right)\frac{\partial u^2}{\partial y^2} = H\left(x, y, u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}\right)
\end{aligned}
\tag{2.2}
$$

In most applications in fluid mechanics, the factors multiplying the higher order derivatives do not depend explicitly on the independent variables x, y. But they will depend implicitly since u is a function of x, y. Let's give an example of this, 2D potential equation for compressible flows:

$$(a^2 - u^2)\frac{\partial^2 \varphi}{\partial x^2} - 2uv\frac{\partial^2 \varphi}{\partial x \partial y} + (a^2 - v^2)\frac{\partial^2 \varphi}{\partial y^2} = 0 \tag{2.3}$$

Quasi-linear equations can appears under the conservative/divergence form would be in the form

$$\frac{\partial g_x}{\partial x} + \frac{\partial g_y}{\partial y} (= \nabla.\vec{g}) = S(x, y, u) \tag{2.4}$$

where $g_x, g_y = \vec{g}(x, y, u) = \vec{g}\left(x, y, u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}\right)$ for respectively a first order and a second order equation. Notice that it is possible to recover from here the quasi-linear form. Let's call $\tilde{g}_x(x, y) = g_x(x, y, u(x, y))$ first order equation then we have that by chain rule that:

$$\frac{\partial \tilde{g}_x}{\partial x} = \frac{\partial g_x}{\partial x} + \frac{\partial g_x}{\partial u}\frac{\partial u}{\partial x} \qquad \frac{\partial \tilde{g}_y}{\partial y} = \frac{\partial g_y}{\partial y} + \frac{\partial g_y}{\partial u}\frac{\partial u}{\partial y} \tag{2.5}$$

Then the sum of the two gives:

$$\frac{\partial \tilde{g}_x}{\partial x} + \frac{\partial \tilde{g}_y}{\partial y} = \frac{\partial g_x}{\partial x} + \frac{\partial g_y}{\partial y} + \frac{\partial g_x}{\partial u}\frac{\partial u}{\partial x} + \frac{\partial g_y}{\partial u}\frac{\partial u}{\partial y}$$
$$\frac{\partial \tilde{g}_x}{\partial u}\frac{\partial u}{\partial x} + \frac{\partial \tilde{g}_y}{\partial u}\frac{\partial u}{\partial y} = S - \frac{\partial g_x}{\partial x} - \frac{\partial g_y}{\partial y} \tag{2.6}$$

where we refined our coefficients P and Q. For a first order equation in 2 space variables the converse is true as well. Indeed, defining $P = \frac{\partial \hat{P}}{\partial u}$ and $Q = \frac{\partial \hat{Q}}{\partial u}$, the chain rule is:

$$\frac{\partial \tilde{P}}{\partial x} = \frac{\partial \hat{P}}{\partial x} + \frac{\partial \hat{P}}{\partial u}\frac{\partial u}{\partial x} = \frac{\partial \hat{P}}{\partial x} + P\frac{\partial u}{\partial x} \qquad \Rightarrow P\frac{\partial u}{\partial x} = \frac{\partial \tilde{P}}{\partial x} - \frac{\partial \tilde{P}}{\partial x} \tag{2.7}$$

Replacing these in the general first order equation form, we find back the conservative form:

$$\frac{\partial \tilde{P}}{\partial x} + \frac{\partial \tilde{Q}}{\partial y} = S + \frac{\partial \hat{P}}{\partial x} + \frac{\partial \hat{Q}}{\partial y} \tag{2.8}$$

For a second order equation, this is not always possible.

2.2 Characteristic surfaces and wave-like solutions

2.2.1 First order scalar equation in m independent variables

It means that we have a linear combination such as:

$$a_i \frac{\partial u}{\partial x_i} = 0 \tag{2.9}$$

For simplicity we take the source term $= 0$. We suppose to solve an initial value problem (Cauchy problem). We imagine that the solution is known on some hyper-surface S^* (in 2D a curve) of equation $F(x_i) = 0$. Does this problem have one and only one solution?

The value of u on the surface is called the **trace** of the solution on the hyper surface and it is specified. Imagine that we can construct a function $\varphi(x, y)$ such that it is equal to u on the surface. Typically if we think in 2D, we specify u on a curve and we elongate it arbitrarily. Because the function $\varphi = u$ on the surface, then the tangential derivative of φ and u are the same. If we construct the function $\varphi - \lambda F$ is also equal to u on the surface whatever the value of λ. In other words, I know u on the curve, I construct a function φ and then I say that all the function $\varphi - \lambda F$ are the same as u, so we have an infinite number of solution on the surface. But there exists one λ for which the normal derivative will be the same as the normal derivative of u:

$$\nabla\varphi - \lambda\nabla F = \nabla u \qquad \Leftrightarrow \frac{\partial \varphi}{\partial x_i} - \lambda\frac{\partial F}{\partial x_i} = \frac{\partial u}{\partial x_i} \quad i = 1, \dots, m \tag{2.10}$$

The unknowns in this equation are the partial derivatives of u but are given by $a_i \frac{\partial u}{\partial x_i} = 0$. We have thus a system of $m+1$ equations and $m+1$ unknowns. The system can be put under matrix form as:

$$\begin{pmatrix} 1 & \cdots & & & \frac{\partial F}{\partial x_1} \\ & 1 & & & \frac{\partial F}{\partial x_2} \\ \vdots & & & & \vdots \\ a_1 & a_2 & \cdots & a_m & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial u}{\partial x_1} \\ \vdots \\ \frac{\partial u}{\partial x_m} \\ \lambda \end{pmatrix} = \begin{pmatrix} \frac{\partial \varphi}{\partial x_1} \\ \vdots \\ \frac{\partial \varphi}{\partial x_m} \\ 0 \end{pmatrix} \tag{2.11}$$

The system has only one and only one solution unless if the determinant is equal to 0, unless the surface S is such that $a_i \frac{\partial F}{\partial x_i} = 0 = \vec{a}.\nabla F$. In fact ∇F is parallel to the normal to the surface because all the tangential derivatives are 0 and the only component that cannot be 0 is the normal derivative, so $\nabla F \propto \vec{n}$. And if we say $\vec{a}.\vec{n} = 0$, this means that the surface is tangent to $\vec{a}$. These are called **characteristic lines** of a **characteristic surface**. The response to the question is thus that yes the solution is unique unless if the surface is a characteristic surface. In 2D this is a characteristic curve.

The original equation admits solutions of the form: $u = \hat{u}\exp(IF(x_i))$ where $F(x_i) = 0$ are equations of characteristic surfaces. Because if we compute $\frac{\partial u}{\partial x_i} = Iu\exp(IF(x_i))\frac{\partial F}{\partial x_i} = Iu\frac{\partial F}{\partial x_i}$ and thus

$$a_i \frac{\partial u}{\partial x_i} = IU \underbrace{a_i \frac{\partial F}{\partial x_i}}_{=0} \tag{2.12}$$

Lines of constant F are wave fronts of wave-like solutions since we have $\exp(IF(x_i))$ similar to $\exp(kx - \omega t)$. A special case is when $a_i = cst \to \frac{\partial F}{\partial x_i = n_i}$ where we have planar wave that propagates without dilatation or damping.

2.2.2   Second order equations in one unknown in two dimension

Consider the second order equation in two variables. That is the equation in the form:

$$R\frac{\partial^2 u}{\partial x^2} + 2S\frac{\partial^2 u}{\partial x \partial y} + T\frac{\partial^2 u}{\partial y^2} = 0 \tag{2.13}$$

In this case we have to provide u and ∇u but if we know the surface we can compute ∇u. Let's call $p = \frac{\partial u}{\partial x}$ and $q = \frac{\partial u}{\partial y}$ on the curve. Let's call φ a function equal to p on C. It results that $\varphi = p + \lambda F$ on C and therefore there exists a value of λ such that $\nabla \varphi = \nabla p + \lambda \nabla F$. So we have also for the second variable:

$$\psi = q + \mu F \qquad \Rightarrow \nabla \psi = \nabla q + \mu \nabla F \tag{2.14}$$

The unknowns are λ, μ, the components of the gradients p and q. But we know that

$$\nabla p = \frac{\partial^2 u}{\partial x^2}\vec{e}_x + \frac{\partial^2 u}{\partial x \partial y}\vec{e}_y \qquad \nabla q = \frac{\partial^2 u}{\partial y^2}\vec{e}_y + \frac{\partial^2 u}{\partial x \partial y}\vec{e}_x \tag{2.15}$$

Again we have a system of equation

$$
\begin{pmatrix}
1 & 0 & 0 & \frac{\partial F}{\partial x} & 0 \\
0 & 1 & 0 & \frac{\partial F}{\partial y} & 0 \\
0 & 1 & 0 & 0 & \frac{\partial F}{\partial x} \\
0 & 0 & 1 & 0 & \frac{\partial F}{\partial y} \\
R & 2S & T & 0 & 0
\end{pmatrix}
\begin{pmatrix}
\frac{\partial p}{\partial x} \\
\frac{\partial p}{\partial y} = \frac{\partial q}{\partial x} \\
\frac{\partial q}{\partial y} \\
\lambda \\
\mu
\end{pmatrix}
=
\begin{pmatrix}
\frac{\partial \varphi}{\partial x} \\
\frac{\partial \varphi}{\partial y} \\
\frac{\partial \psi}{\partial x} \\
0 \\
0
\end{pmatrix}
\tag{2.16}
$$

If we try to compute the determinant we will get

$$
\det = R\frac{\partial F}{\partial x}\left(-\frac{\partial F}{\partial x}\right) - 2S\frac{\partial F}{\partial x}\frac{\partial F}{\partial y} + T\left(-\frac{\partial F}{\partial y}\right)\frac{\partial F}{\partial y} = -\left(\frac{\partial F}{\partial y}\right)^2\left[Rz^2 + 2Sz + T\right] \tag{2.17}
$$

where $Z = \frac{\frac{\partial F}{\partial x}}{\frac{\partial F}{\partial y}} = \frac{n_x}{n_y}$. The line $F(x,y) = 0$ is a characteristic line when $Rz^2 + 2Sz + T = 0$. If $S^2 - RT > 0$ so we have 2 roots and thus 2 characteristic directions at each point. In the case $S^2 - RT < 0$ we have no real root no characteristic line for this equation. And if $S^2 - RT = 0$ we have 2 identical roots so 1 characteristic direction. If now we have a quadratic term like

$$
Rx^2 + 2Sxy + Tx^2 = 0 \tag{2.18}
$$

The first case would give a hyperbole, the second an elliptic equation and the last we have a parabolic equation.

Applicaition: potential flow equation

$$
\begin{aligned}
R = a^2 - u^2 \qquad S = -uv \qquad T = a^2 - v^2 \\
\Rightarrow S^2 - RT = u^2v^2 - (a^2 - u^2)(a^2 - v^2) = a^2[u^2 + v^2 - a^2] = a^4\left[M^2 - 1\right]
\end{aligned}
\tag{2.19}
$$

We can see that when $M > 1$ hyperbolic, $M = 1$ parabolic, $M < 1$ elliptic.

2.2.3 System of first order equations in two dimensions

We can write it in the form of a system of n equations and n unknowns:

$$
A_x\frac{\partial U}{\partial x} + A_y\frac{\partial U}{\partial y} = 0 \tag{2.20}
$$

It is now U that is provided on the curve C of equation $F(x,y) = 0$. We call V a vector function which is identical to U on C. We are going to have a vector of Lagrange multipliers Θ:

$$
V = U + \Theta F \text{ on C} \qquad \Rightarrow \frac{\partial V}{\partial x} = \frac{\partial U}{\partial x} + \Theta\frac{\partial F}{\partial x} \qquad \frac{\partial V}{\partial y} = \frac{\partial U}{\partial y} + \Theta\frac{\partial F}{\partial y} \tag{2.21}
$$

We will again have the matrices:

$$
\begin{pmatrix}
I & 0 & \frac{\partial F}{\partial x}I \\
0 & I & \frac{\partial F}{\partial y}I \\
A_x & A_y & 0
\end{pmatrix}
\begin{pmatrix}
\frac{\partial U}{\partial x} \\
\frac{\partial U}{\partial y} \\
\Theta
\end{pmatrix}
=
\begin{pmatrix}
\frac{\partial V}{\partial x} \\
\frac{\partial V}{\partial y} \\
0
\end{pmatrix}
\tag{2.22}
$$

Again we have to compute the determinant. The characteristic directions are $|A_xn_x + A_yn_y| = 0$ and if we make the evidences:

$$
n_x|A_x + \lambda A_y| = 0 \qquad n_y\left|-A_x\frac{-n_x}{n_y} + A_y\right| = 0 \tag{2.23}
$$

where $\frac{-n_x}{n_y}$ is the slope of the tangent to the characteristic lines. We end up with an eigenvalue problem

$$|A_y - \lambda A_x| = 0 \tag{2.24}$$

if $\det(A_x) \neq 0$ so $|A_y - \lambda A_x| = |A_x||A_x^{-1}A_y - \lambda I| = 0$. We have n real roots, n lin indep real eigenvectors (hyperbolic) or n real roots, m<n lin indep real eigenvectors (parabolic).

$$R\frac{\partial^2 u}{\partial x^2} + 2S\frac{\partial^2 u}{\partial x \partial y} + T\frac{\partial^2 u}{\partial y^2} = 0 \quad \Leftrightarrow \quad R\frac{Dp}{\partial x} + S\left(\frac{\partial p}{\partial y} + \frac{\partial q}{\partial x}\right) + T\frac{\partial q}{\partial y} = 0$$

$$\begin{bmatrix} R & S \\ 0 & 1 \end{bmatrix} \frac{\partial}{\partial x} \begin{pmatrix} p \\ q \end{pmatrix} + \begin{pmatrix} S & T \\ 1 & 0 \end{pmatrix} \frac{\partial q}{\partial x} - \frac{\partial p}{\partial y} = 0 \tag{2.25}$$

we also have the case elliptic problem with n complex roots, other possibilities = hybrid.

2.2.4 Systems of n equations in m independant variables

In that case the generalization is:

$$A_i \frac{\partial U}{\partial x_i} = 0 \tag{2.26}$$

where A is n by n matrix and U a n by 1 vector. The equations for the characteristic surfaces is now:

$$|1_i n_i| = 0 \tag{2.27}$$

Here because the n are components of the unit normal, but in x, y they are associated to one vector. If now we devide by n_1 we would have $|A_i n_i/n_1| = 0$ meaning that we would have $m-1$ variables. To illustrate suppose that we have:

$$|A_x n_x + A_y n_y + A_z n_z| = 0 \tag{2.28}$$

We can write this in the following way:

$$\left|\frac{A_x n_x + A_y n_y}{n_z} + A_z\right| = 0 \quad \Rightarrow \quad \left|\frac{A_x n_x + A_y n_y}{\sqrt{n_x^2 + n_y^2}} - \frac{\sqrt{n_x^2 + n_y^2}}{n_z} + A_z\right| = 0 \tag{2.29}$$

where in fact the first term is the direction of n and the second term plays the role of the previous λ. If it is in 4D, we would have 2 angular directions defining the n direction. $m-2$ variables can be chosen arbitrarily and the last is given by the eigenvalue problem. The system is hyperbolic wrt to A_z if the eigenvalues all real and we have a complete set of eigenvectors for all directions whatever the direction. If in contrast if they are all complex whatever the direction, it is indetermined. The Euler equations will be:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = 0 \quad U = \begin{pmatrix} \rho \\ \rho u \\ \rho E \end{pmatrix} \quad F = \begin{pmatrix} \rho u \\ p + \rho u2 \\ \rho u H \end{pmatrix} \tag{2.30}$$

in 1D unsteady z is an independent variable. We also know that $p = \rho R T = \rho(c_p - c_v)T$ and $z = c_v T = \rho(\gamma - 1)c_v T$ and $p = \rho(\gamma - 1)e, E = e + \frac{u^2}{2}, H = E + \frac{p}{\rho}$, so that we have:

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$$\frac{\partial F}{\partial U} = \begin{pmatrix} 0 & 1 & 0 \\ \frac{\partial p}{\partial e} - u^2 & 2u + \frac{\partial p}{\partial \rho u} & \frac{\partial p}{\partial \rho E} \\ \times & \times & \times \end{pmatrix} \tag{2.31}$$

And we see that the eigenvalues are real: $u + a, u, u - a$. In 2D the U and F vectors are 4 and thus the matrix will be 4×4 :

$$2D: \quad \frac{\partial U}{\partial t} + \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} = 0$$

$$3D: \quad \frac{\partial U}{\partial t} + \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z} = 0 \tag{2.32}$$

They are both unsteady with 3 and 4 independant variables. We see that these are hyperbolic wrt the time variable!

Conclusion

If the system has real eigenvalues and a complete set of real eigenvalues for all values of the arbitrary parameters (m-2) $\rightarrow$ the system is hyperbolic wrt the variable of interest $\rightarrow$ this variable plays a special role, it is the evolution or time-like variable.

If the system has only complex eigenvalues the equation is elliptic. In that case, it is generally elliptic wrt all variables.

2.2.5 Notion of well posed problem

Problem that has one and only one solution, depending continuously on the prescribed initial/boundary data. And they give the example of Laplace's equation:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \tag{2.33}$$

and we compute the solution on the domain Ω which is the right half plane where $x > 0$. The boundary of the domain is $u(0, y) = 0$ and $\frac{\partial u}{\partial x}(0, y) = h(y)$. Since it is elliptic equation it has not real characteristic curve so we know that the curves are not characteristic and so that we have one and only one solution. If we take $h(y) = 0$ we have $u = 0$, if we take $h(y) = \frac{\sin ny}{n}$ then $u = \frac{1}{n^2} \sinh nx \sin ny$. As $n \rightarrow \infty, h \rightarrow 0$ if we perturb the boundary data infinitesimally the solution will vary a lot. When we are never sure that the solution depends continuously on the boundary condition and when we have uncertainties on the boundary conditions we can never be sure of the solution. This is why if we have 2 boundary we have to impose one condition on each boundary.

2.3 Properties of hyperbolic equations

2.3.1 Nature of the solution - Riemann invariants

For simplicity, consider a system of n equations in 2 independent variables $|A_x n_x + A_y n_y| = 0 \Leftrightarrow |A_y - \lambda A_x| = 0$ where $\lambda = -n_x/n_y$. If A_x is positive definite regular matrix:

$$|A_x(A_x^{-1} A_y - \lambda I)| = 0 \qquad \Rightarrow |A_x| |\underbrace{A_x^{-1} A_y}_{A} - \lambda I| = 0 \tag{2.34}$$

The λ_s are the eigenvalues of A. Calling $|A - \lambda I|$ $\quad Av = \lambda v$ where v are the right eigenvectors and l the line eigenvectors: $lA = \lambda l \Leftrightarrow (lA)^t = \lambda l^t$. We have the following algebraic identities:

$$Av_1 = \lambda_1 v_1 \quad Av_2 = \lambda_2 v_2 \dots \qquad \Rightarrow AR = R\Lambda \Leftarrow R^{-1}AR = \Lambda \Leftarrow R^{-1}A = \Lambda R^{-1} \qquad (2.35)$$

The same can be done for the left eigenvalues and we can find the relation $L = R^{-1}$. Let's imagine that the initial problem to solve was (as in aerodynamics course - Riemann):

$$A_x \frac{\partial U}{\partial x} + A_y \frac{\partial U}{\partial y} = S \qquad \Leftrightarrow \frac{\partial U}{\partial x} + A\frac{\partial U}{\partial y} = \underbrace{A_x^{-1}S}_{G} \Leftrightarrow L\frac{\partial U}{\partial x} + \Lambda L\frac{\partial U}{\partial y} = LG \qquad (2.36)$$

If now we consider the first eigenvalue:

$$l_{11}\frac{\partial u_1}{\partial x} + l_{12}\frac{\partial u_2}{\partial x} + \dots + l_{1n}\frac{\partial u_n}{\partial x} + \lambda \left[l_{11}\frac{\partial u_1}{\partial y} + \dots \right] = (LG)_1$$

$$l_{11}\frac{\partial u_1}{\partial x} + \lambda l_{11}\frac{\partial u_1}{\partial y} = l_{11}\left(\frac{\partial u_1}{\partial x} + \lambda \frac{\partial u_1}{\partial y} \right) = l_{11}\left(\frac{\partial u_1}{\partial x} + \tan\theta \frac{\partial u_1}{\partial y} \right) \qquad (2.37)$$

$$= \frac{l_{11}}{\cos\theta}\left(\cos\theta \frac{\partial u_1}{\partial x} + \sin\theta \frac{\partial u_1}{\partial y} \right)$$

where $\frac{1}{\cos\theta} = \sqrt{1 + \lambda^2}, \vec{e}_\theta . \nabla u = \frac{du_1}{dS_1}$. This can be done for every indexes and we get:

$$\frac{1}{\cos\theta}\left(l_{11}\frac{du_1}{dS_1} + \dots + l_{1n}\frac{du_n}{dS_n} \right) = h_1 \qquad (2.38)$$

For a system of n equations, the system transforms into a system of n ordinary differential equations:

$$l_{ij}\frac{du_j}{dS_i} = h_i \cos\theta_i = \frac{h_i}{\sqrt{1 + \lambda_i^2}} \qquad (2.39)$$

Can we simplify further? If l_{ij} do not depend explicitly on the independent variables x, y (they depend only on u_j), there may exist a function $f(u_j)$ such that

$$fl_{ij}\frac{du_j}{dS_i} = \frac{dR_i}{dS_i} \qquad (2.40)$$

with the conditions:

$$fl_{ij} = \frac{\partial R_i}{\partial u_j} \Rightarrow \frac{\partial fl_{ij}}{\partial u_k} = \frac{\partial fl_{ij}}{\partial u_j} \qquad fl_{ik} = \frac{\partial R_i}{\partial u_k} \qquad (2.41)$$

f is called an integrating factor. If $n \ll 2 \to f$ always exists, if l_{ij} are constant $\forall n, R_i = l_{ij}u_j$. We finally have

$$\frac{dR_i}{ds_i} = \frac{h_i}{\sqrt{1 + \lambda_i^2}} \qquad \Rightarrow R_i = cst \qquad (2.42)$$

R_i are the Riemann invariants. The summary is given on the figure p55. Second figure, let's try to think about the properties of the solution. Imagine that the solution here for 2 unknowns, so 2 characteristics. Let's think that the solution is prescribed on the curve Γ, the solution at point P has to depend on all the values in the dark region since we have an integration. The rest of the region is the region of silence.

Consider 1D inviscid flow in a tube. Continuity, x-momentum and energy equations tells that:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0 \qquad \rho \frac{\partial u}{\partial t} + \rho u \frac{\partial u}{\partial x} = -\frac{\partial p}{\partial x} = -a^2 \frac{\partial \rho}{\partial x} \qquad \dot{s} = 0 \qquad (2.43)$$

If initial data are homentropic (uniform initial entropy): $s = cst$. We can rewrite:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0 \qquad \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + \frac{a^2}{\rho} \frac{\partial \rho}{\partial x} = 0$$

$$\Rightarrow \frac{\partial}{\partial t} \begin{pmatrix} \rho \\ u \end{pmatrix} + \begin{pmatrix} u & \rho \\ \frac{a^2}{\rho} & u \end{pmatrix} \frac{\partial}{\partial x} \begin{pmatrix} \rho \\ u \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \qquad (2.44)$$

After computing the eigenvectors we found that they are: $\lambda = u \pm a$. If we make the drawing, we have the graph of x in function of t and since the length is limited on top at L due to energy, we have to specify the upper and lower boundary to be able to compute in all the domain. We have to supply as many information as the number of characteristic curves entering the domain.

DO THE NON-LINEAR HE READS THE SYLLABUS he stoped at the graphs.
We see on the right that we can find a continuous function to define the transition region. But in the right hand side we could have 2 solutions, not unically defined solution so we need to look for a weak solution. This is done by weightening the function in a certain way:

$$\int_0^\infty dt \int_{-\infty}^\infty \nu \left[\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} \right] dx = 0 \qquad (2.45)$$

Then we can integrate by part and find that:

$$\int \int \nu \left[\frac{\partial u}{\partial t} + \frac{\partial u^2/2}{\partial x} \right] dx\, dt = \int \int \left[\frac{\partial uv}{\partial t} + \frac{\partial}{\partial x} \frac{u^2}{2} \nu \right] dx\, dt - \int \int \left[u \frac{\partial \nu}{\partial t} + \frac{\partial \nu}{\partial x} \frac{u^2}{2} \nu \right] dx\, dt = 0 = \int_0^\infty \int_{-\infty}^\infty \left[u \frac{\partial \nu}{\partial t} + \right.$$

$$(2.46)$$

Integral:

$$\frac{d}{dt} \int_{x_e}^{x_r} u\, dx + \left[\frac{u^2}{2} \right]_{x_e}^{x_r} = 0 \qquad (2.47)$$

Do all the text alone mohofokor.

2.4 Properties of elliptical equations

2.4.1 Nature of the solution

We want to discuss the nature of the solutions and we consider the Laplace equation as example:

$$\Delta u = \nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \qquad (2.48)$$

We consider the similar problem as previously $u(0, y) = g_1(y)$ and $\frac{\partial u}{\partial x}(0, y) = g_2(y)$. We will use a Fourrier transform:

$$u(x, y) = \frac{1}{2\pi} \int_{-\infty}^\infty \hat{u}(x, \omega) e^{i\omega y}\, d\omega \qquad \frac{\partial u}{\partial y} = \frac{1}{2\pi} \int_\infty^\infty i\omega \hat{u}(x, \omega) e^{i\omega y}\, dy \qquad \frac{\partial^2 u}{\partial y^2} = \frac{1}{2\pi} \int_\infty^\infty -\omega^2 \hat{u}(x, \omega) e^{i\omega y}\, dy$$

$$(2.49)$$

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So that the equation becomes:

$$\frac{\partial^2 \hat{u}}{\partial x^2} - \omega^2 \hat{u} = 0 \qquad \hat{u} = A(\omega)e^{\omega x} + B(\omega)e^{-\omega x} \tag{2.50}$$

and thus

$$u(x,y) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \left[A(\omega)e^{\omega x} + B(\omega)e^{-\omega x}\right]e^{i\omega y}\, d\omega \tag{2.51}$$

where

$$A(\omega)+B(\omega) = \int_{-\infty}^{\infty} g_1(y)e^{-i\omega y}\, dy \qquad \Rightarrow u(0,y) = g_1(y) = \frac{1}{2\pi}\int_{-\infty}^{\infty}[A(\omega)+B(\omega)]e^{i\omega y}\, d\omega \qquad \frac{\partial u}{\partial x}(0,y) = g_2(y) =$$

$$\tag{2.52}$$

to have finally

$$\frac{\partial u}{\partial x} = \frac{1}{2}\int_{-\infty}^{\infty}\omega[A(\omega)e^{\omega x} - B(\omega)e^{\omega x}]e^{i\omega y}\, dy \tag{2.53}$$

If we introduce a perturbation into the domain it will be felt in the whole domain, the region of dependance is the entire domain. This is a completely different behavior than the previous case. We have some examples: if we inject a heating resistor in a pool, we will have a temperature increase in the whole pool, but since it increases exponentially from the source we don't feel it far away.

2.4.2   Well posed problem for an elliptic system

For this we have to impose the second condition so that the expansion due to the exponent is canceled.

Existence of the solution

If we know the solution on the boundary we can compute everywhere.

Solution uniqueness

Continuity in the sense of Hadamard

2.5   Parabolic equations

2.6   ●

Consider the following equation, 2D small disturbance potential equation:

$$(1 - M_\infty^2)\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0 \qquad S^2 - RT = M_\infty^2 - 1 \tag{2.54}$$

> 0 (hyperbolic) $M_\infty^2 > 1$, < 0 (elliptic) $M_\infty^2 < 1$. Consider a mesh and we discretize by central differences on a coarse 4x4 mesh. Normally we have 2 indexes but here we consider the points by full number, and we don't need the corners. If I consider a generic point O, I will neighbour the points by N W E S and the expression will be:

$$(1-M_\infty^2)\frac{\phi_W + \phi_E - 2\phi_O}{\Delta x^2} + \frac{\phi_N + \phi_S - 2\phi_O}{\Delta y^2} = 0 \qquad \Delta x = \Delta y = h \qquad \rightarrow (1-M_\infty^2)[\phi_W + \phi_E - 2\phi_O][\phi_N + \phi_S - 2\phi$$

$$(2.55)$$

If the equation is elliptic we just have to consider the sides and we know the ϕ on the sides. We can build a matrix, since we know the values on the sides we can just put 1 on diagonals for 3 first and then we go into internal points and we make the equation:
put the equation in figure.

For supersonic case, we know $\frac{\partial \phi}{\partial x}$ on point 1:

$$\phi_2 + \phi_c - \phi_4 - \phi_a = 0 \qquad \left.\frac{\partial \phi}{\partial x}\right|_1 = \frac{\phi_4 - \phi_a}{2h} = u_1 \text{ (specified)} \qquad\qquad (2.56)$$

He showed some slides

Chapter 3

Numerical methods for evolution problems

We are going to consider model equations for hyperbolic and parabolic equations which will be respectively:

$$\frac{\partial u}{\partial t} + \underbrace{a}_{\text{or } u} \frac{\partial u}{\partial x} = 0 \qquad \frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} \tag{3.1}$$

3.1 Consistency - stability - convergence

Convergence is a concept we have introduced before, the numerical method is convergent if $\lim_{h \to 0} ||u^h - u|| = 0$ where u^h is the approximate numerical solution and u the exact solution and h is representative of the mesh size. In such method the h is inversely prop to the number of degrees of freedom. For methods based on a functional representation (finite elements, spectral methods), convergence can be proven directly using functional analysis, see literature. The evolution variable is special, here time. When it is time dependent problem, we use finite differences for time integration, we don't need flexibility for time it is uniform. For Finite differences convergence cannot be proven directly, but in contrasts is proven indirectly using the concept of consistency and stability.

3.1.1 Consistency

We say that a numerical method is consistent if $\lim_{h \to 0} ||D^h(u^h) - D(u)||$, where $D(u)$ is the differential operator applied to exact solution and the other discrete approximation of the differential operator. That's nothing else but the truncation error. For example if the problem was:

$$\frac{\partial u}{\partial x} = f \qquad \frac{u_{i+1} - u_{i-1}}{2h} = f_i \qquad \to \frac{u_{i+1} - u_{i-1}}{2h} - \left(\frac{\partial u}{\partial x}\right)_i + f_i - f_i = TE = \mathcal{O}(\Delta x^2) \tag{3.2}$$

We know that the truncation error was of the form $\mathcal{O}(h^2)$. So we need that to be consistent the polynomial is at least first order accurate $p \leq 1$. Sometimes, this implies a condition on discretization steps. Example:

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0 \tag{3.3}$$

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The Lax method gives:

$$\frac{u_i^{n+1} - \frac{1}{2}(u_{i-1}^n + u_{i+1}^n)}{\Delta t} + a\frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} = 0 \qquad \Rightarrow \begin{cases} u_{i+1}^n = u_i^n + \Delta x\left(\frac{\partial u}{\partial x}\right)_i^n + \frac{\Delta x^2}{2}\left.\frac{\partial^2 u}{\partial x^2}\right|_i^n + \frac{\Delta x^3}{6}\left.\frac{\partial^3 u}{\partial x^3}\right|_i^n \quad \Delta t\left(\frac{\partial u}{\partial t}\right. \\ u_i^{n+1} = u_i^n + \Delta t\left(\frac{\partial u}{\partial t}\right)_i^n + \frac{\Delta t^2}{2}\left.\frac{\partial^2 u}{\partial t^2}\right|_i^n \end{cases}$$

$$(3.4)$$

ODE: Compute the solution at time T with $\Delta t \to a$. A method is stable id $u^h, h(\Delta t) \to 0, nh \gg T$ is bounded (does not grow unboundedly).

Lax's equivalence theorem

For a large class of well posed initial value problems, consistency and stability are necessary and sufficient condition for convergence.

3.2 Spectrum of the space discretization - Fourrier analysis

If we start from a PDE and we discretize all the variables except the evolution variables, we get a system of ODS:

$$\frac{dU}{dt} = F(U) \tag{3.5}$$

If the PDE is linear, and if the discretization formula is linear, then this system becomes a system of ODE:

$$\frac{dU}{dt} = SU + Q \tag{3.6}$$

where U is an n vector and S is an $n \times n$ matrix. So far all the discretization methods we discussed, have been linear, for example:

$$\frac{\partial u}{\partial x} \approx \frac{u_{i+1}u_{i-1}}{2\Delta x} \tag{3.7}$$

because if we replace u by a combination of u and v we will have a linear combination. It turns out that for hyperbolic problems and in particular for non-linear ones, linear discretization will produce purely oscillatory solutions, except first order. It has been discovered that it was possible to go beyond first order discretization without oscillatory solution but this is not viewed in the frame of this course.

If we assume that the matrix S has a complete set of eigenvalues and eigenvectors (real or complex) then we know that the matrix can be diagonalized such that $LS = \Lambda L$. By multiplying the equation by L we have:

$$L\frac{dU}{dt} - LSU = LQ \Leftrightarrow L\frac{dU}{dt} - \Lambda LU = LQ \qquad \Rightarrow \frac{dw_i}{dt} - \lambda^{(i)}w_i = (LQ)_i \tag{3.8}$$

which gives a set of uncoupled equations. We call that the model equations. The set of eigenvalues is the spectrum of the space discretization of the PDE. It will depend on the PDE and the discretization. Sometimes, the search for the eigenvalues is as difficult than solving the problem, this is why we make also an approximation of the spectrum.

3.2.1 Spectrum of the central space discretization of the diffusion equation

The equation we want to look at is the model of parabolic equations:

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} \tag{3.9}$$

where α is the diffusivity coefficient $[L^2 T^{-1}]$. The evolution parameter is t, imagine we want to solve it for going from 0 to L in N intervals so that $\Delta t = L/N$. We have thus $N+1$ points. If we look to the discretization of an internal point:

$$\frac{du_i}{dt} = \alpha \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} \tag{3.10}$$

We will consider 3 problems varying from boundary conditions. We have to impose an initial condition on one boundary at left and right boundary.

- Dirichlet BCs: u_0, u_N specified

$$\frac{d}{dt} \begin{pmatrix} u_1 \\ \vdots \\ u_{N-1} \end{pmatrix} = \frac{\alpha}{\Delta x^2} \begin{pmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ \vdots & & & \\ & & 1 & -2 \end{pmatrix} \begin{pmatrix} u_1 \\ \vdots \\ u_{N-1} \end{pmatrix} + \begin{pmatrix} \frac{\alpha u_0}{\Delta x^2} \\ \vdots \\ \frac{\alpha u_N}{\Delta x^2} \end{pmatrix} \tag{3.11}$$

The eigenvalues are:

$$\lambda^j = \frac{-4\alpha}{\Delta x^2} \sin^2 \left(\frac{\pi j}{2N} \right) \qquad j = 1 \dots N-1 \tag{3.12}$$

We can solve now:

$$\lambda^1 = -\frac{4\alpha}{\Delta x^2} \sin^2 \frac{\pi}{2N} \approx -\frac{4\alpha}{\Delta x^2} \left(\frac{\pi}{2N} \right)^2 = -\frac{\alpha}{L^2} \pi^2$$

$$\lambda^{(N-1)} = -\frac{4\alpha}{\Delta x^2} \sin^2 \frac{\pi(N-1)}{2N} \approx \frac{-4\alpha}{\Delta x^2} \tag{3.13}$$

- Neumann/Dirichlet: $\frac{\partial u}{\partial x}\big|_0, u_N$ specified

$$\frac{du_0}{dt} = \frac{\alpha}{\Delta x^2}(u_1 - 2u_0 + u_{-1}) = \frac{\alpha}{\Delta x^2}(2u_1 - 2u_0) - \frac{2\alpha q_0}{\Delta x}$$

$$\frac{\partial u}{\partial x}\Big|_0 = \frac{u_1 - u_{-1}}{2\Delta x} = q_0 \Rightarrow u_{-1} = u_1 - 2q_0 \Delta x \tag{3.14}$$

So that here we have:

$$\frac{d}{dt} \begin{pmatrix} u_0 \\ \vdots \\ u_{N-1} \end{pmatrix} = \frac{\alpha}{\Delta x^2} \begin{pmatrix} -2 & 2 & & \\ 1 & -2 & 1 & \\ \vdots & & & \\ & & 1 & -2 \end{pmatrix} \begin{pmatrix} u_0 \\ \vdots \\ u_{N-1} \end{pmatrix} + \begin{pmatrix} -\frac{2\alpha q_0}{\Delta x^2} \\ \vdots \\ \frac{\alpha u_N}{\Delta x^2} \end{pmatrix} \tag{3.15}$$

The eigenvalues are:

$$\lambda^j = \frac{-4\alpha}{\Delta x^2} \sin^2 \left(\frac{(2j-1)\pi j}{4N} \right) \qquad j = 1 \dots N \tag{3.16}$$

We can solve now:

$$\lambda^1 = -\frac{4\alpha}{\Delta x^2}\sin^2\frac{\pi}{4N} \approx -\frac{4\alpha}{\Delta x^2}\left(\frac{\pi}{4N}\right)^2 = -\frac{\alpha}{4L^2}\pi^2$$

$$\lambda^{(N)} = -\frac{4\alpha}{\Delta x^2}\sin^2\frac{\pi(2N-1)}{4N} \approx \frac{-4\alpha}{\Delta x^2} \tag{3.17}$$

- Periodic BC: $u_0 = u_N$

$$\frac{d}{dt}\begin{pmatrix} u_1 \\ \vdots \\ u_N \end{pmatrix} = \frac{\alpha}{\Delta x^2}\begin{pmatrix} -2 & 1 & & & 1 \\ 1 & -2 & 1 & & \\ \vdots & & & & \\ 1 & & & 1 & -2 \end{pmatrix}\begin{pmatrix} u_1 \\ \vdots \\ u_N \end{pmatrix} \tag{3.18}$$

The eigenvalues are:

$$\lambda^j = \frac{-4\alpha}{\Delta x^2}\sin^2\left(\frac{\pi j}{N}\right) \qquad j = 0\ldots N-1 \tag{3.19}$$

We can solve now:

$$\lambda^0 = 0$$
$$\lambda^{(1)} = -\frac{4\alpha}{\Delta x^2}\sin^2\frac{\pi}{N} = \frac{-4\alpha}{L^2}\pi^2 \tag{3.20}$$
$$\lambda^{\frac{N-1}{2}} \approx -\frac{4\alpha}{\Delta x^2}$$

The diffusion equation becomes:

$$\frac{\partial u}{\partial t} = \alpha\frac{\partial^2 u}{\partial x^2} \quad u = \hat{u}(t)g(x) \quad g(x)\frac{d\hat{u}}{dt} = \alpha\hat{u}(t)g"(x) \Rightarrow \frac{d\hat{u}}{\hat{u}dt} = \alpha\frac{g"}{g} = cst - \alpha k^2 g" + k^2 g = 0 \quad \Leftrightarrow \frac{d\hat{u}}{dt} + alpha$$
$$\tag{3.21}$$

where

$$g = A\cos kx / B\sin kx \qquad g(0) = g(L) = 0 \Rightarrow A = 0 \Rightarrow B\sin kL = 0 \, la\, suite\, j'ai\, pas \tag{3.22}$$

Approximation of the spectrum by Fourrier analysis

Remember that a running discrete equation at inner point was given by:

$$\frac{du_i}{dt} = \alpha\frac{u_{i+1} - 2u_i + u_{i+1}}{\Delta x^2} \tag{3.23}$$

The Fourrier analyis is to assume a preiodic solution in space:

$$u(x,t) = \hat{u}(t)e^{ikx} \qquad u_i(t) = u(x_i,t) = \hat{u}(t)e^{ikx_i} \qquad u_{i\pm1}(t) = u(x_{i\pm1},t) = \hat{u}(t)e^{ikx_{i\pm1}} = \hat{u}(t)e^{ik(x_i\pm\Delta x)} = u_i e^{\pm ik}$$
$$\tag{3.24}$$

where η is the reduced wave number. We have thus that:

$$\frac{du_i}{dt} = \alpha\frac{e^{i\eta} - 2 + u^{-i\eta}}{\Delta x^2}u_i = \frac{2\alpha}{\Delta x^2}\underbrace{(\cos\eta - 1)}_{1-2\sin\frac{\eta}{2}}u_i = \underbrace{-\frac{4\alpha}{\Delta x^2}\sin^2\frac{\eta}{2}}_{\text{Fourrier footprint }\lambda}u_i \tag{3.25}$$

Since λ is negative it is on the negative Figure for this.