A DIRECT DISCRETE FORMULATION FOR THE WAVE EQUATION

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ABSTRACT. *The paper shows how to give a* direct *discrete formulation of the wave equation starting directly from physical laws, i.e. without passing through differential formulation. Using global variables instead of scalar and vector field functions, a close link between global variables and spatial and temporal elements immediately appears. A preliminary classification of physical variables into three classes, configuration, source and energy variables and the use of two cell complexes, one dual of the other, gives an unambiguous association of global variables to the spatial and temporal elements of the two complexes. Thus one arrives at a discrete formulation of d'Alembert equation on a unstructured mesh.*

1 Introduction

The laws of physical phenomena are usually written in the form of differential equations. This is the case of the equations of d'Alembert, Helmholtz, Fourier, Navier, Navier-Stokes, Maxwell, etc.

In the past decades, with advent of computers and with an increasing demand for a numerical solution of field problems the need arises to convert differential equations into algebraic equations. To perform this conversion many discretization methods have been devised such as Finite Difference, Finite Elements, Finite Volumes, Weight Residual Methods, etc. Even when we use an integral formulation, as in the Finite Volume Method or in Boundary Elements Method, the standard practice is to use integrals of the field functions, the latter being essential ingredients of differential formulation.

Faced with this practice we pose the question: *is it possible to avoid any discretization process of differential equation and to write directly physical laws*

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in a discrete, i.e. algebraic, form? In other words: *is it possible to avoid completely a differential formulation?*

The demand for a discrete formulation, even if motivated by computational purposes, can be raised from a purely theoretical side. In order to see why, we must revise our custom of considering the solution of a differential equation as the "exact" solution. What does "exact" means? Let us take a more realistic approach to the notion of solution. We are well aware that in order to solve something we must input some data: are these data "exact"? The answer is: no. Every measurement is affected, on principle, by a tolerance. Every measuring device belongs to a given class of precision and an infinite precision is neither requested nor attainable. Since the data have a tolerance it follows that also the solution has a tolerance. The results of a calculation need not to be compared with the "exact" solution of a differential equation but with experimental measurements. Notwithstanding that differential equations promise an "exact" solution that is almost never attained! Only in few cases dealing with *linear* equations with *very simple* slab geometry, *very simple* boundary conditions, with a *single* material medium that is *homogeneous* and *isotropic* can a solution in closed form be obtained.

A more realistic viewpoint, that is proper to physicists and engineers, is the one based on the acceptance that the solution of a physical problem must have a prescribed tolerance. Numerical analysis is based on the notion of *error*, measuring apparatus are based on the notion of *precision*, the data have a given *tolerance:* why are we so firmly anchored to the notion of "exact" solution? We see that in order to open the way to a discrete formulation of physical laws the key point is the abandoning of the notion of *exactness* in favour of the notion of *prescribed tolerance*.

In this paper we show that *a direct discrete formulation of acoustic field is possible, it is easy, it is consistent with experiments and it can be immediately used for numerical computation*.

In this formulation the classical procedure of writing physical laws in differential form is inverted. Instead, we start from the direct discrete formalism and deduce the differential formalism whenever it is opportune to do so.

To avoid any possible misunderstanding we point out that what we propose in this paper *is not* a refusal of differential formulation of the laws of physics but *an alternative* to it. We shall then be free to choose one or the other description, as best suits our purposes.

To give a discrete formulation we start with a revision of physical variables: they are directly responsible for the mathematical description of physics.

Differential formulation requires functions of point in order to perform derivatives. Apart from few physical variables that are directly expressed as point functions, such as temperature, electric potential, scalar magnetic potential, displacement, most field functions arise from *global* variables giving the density. Hence pressure is the ratio of a normal force to an area; mass density is the ratio of mass to a volume; strain is the ratio of elongation of a line to its initial length, etc.

The forming of densities is a two step process: the first step is just the ratio

of the global quantity referred to a spatial element endowed with extension (line, surface, volume) to the corresponding extension. This produces *mean* densities. The second step is the limit process of mean densities in order to obtain point functions, i.e. field functions.

A flow is referred to a surface; velocity circulation is referred to a line; momentum content is referred to a volume. We shall call these *global variables*. The commonest name is *integral variables:* we avoid it because it refers to an integration process performed on field functions, be they scalars, vectors, tensors.

It is remarkable that we measure mainly *global* variables: the mean densities are evaluated and easily introduced in digital measuring devices.

One must distinguish between global variables *in space* and global variables *in time*. A global variable in space is one that is not a density; a global variable in time is one that is not a rate.

At this point it seems clear that *a discrete formulation of field laws must be based on global variables.* The forming of mean densities will be requested by the constitutive equations, as we shall show later. The second step of performing the limit will never be performed.

While field variables are functions of points and instants, global variables are *domain functions*. For this reason we put the spatial and temporal domains between square brackets.

To justify the use of global variables we list here their main advantages:

1. *Global variables naturally refer to spatial and temporal elements* such as points (**P**), lines (**L**), surfaces (**S**), volumes (**V**), time instants (**I**) and intervals (**T**), as we shall show. This is implicit when we consider that an integral variable is expressed by an integral over a spatial and temporal region. The process of performing mean densities and the limit process to arrive at field functions is required only by differential formulation. By doing so we hide the association of global variables with extended spatial and temporal elements: this association must be reconstructed later by the discretization process.

2. Since the goal of any numerical simulation is agreement with experimental measurements, and since we measure overall global variables, the use of global variables permits us to maintain a close link between simulation and measurements.

   In particular boundary fluxes can be measured and directly inserted in a discrete formulation. Contrary to this in differential formulation the boundary fluxes must be converted into the normal derivative of the field potentials and a constitutive equation must be involved in order to write Neumann conditions.

3. Balance and circuital laws can be expressed *exactly* in a global form. These laws are valid for whatever closed surface and whatever closed line, even if they enclose different materials. They are valid for homogeneous or

inhomogenous materials, for isotropic or anisotropic ones. This implies *the absence of jump conditions*. It is worthwile remembering that in differential formulation jump conditions are obtained by using small closed surfaces and closed lines across the separation surface of two materials.

4. Using global variables we avoid infinities. The latter arise when we perform a limit of mean densities, a process requires by differential formulation to obtain field functions. The limit process is excluded in a discrete formulation where only mean densities are involved.

5. While differential formulation requires unphysical derivability conditions, using global variables we do not need any derivability conditions.

6. Constitutive laws are experimented and formulated for regions of *uniform* field and *homogeneous* media: this is the case of Fourier's law for heat transfer, of Ohm's law for electrical conduction, of Hooke's law for elastic material. It follows that if we do the approximation that inside every cell the field is *uniform* and the material is *homogeneous* we can implement constitutive laws directly, i.e. without performing the limit process. Once more we have a close link between mathematical modelling and physical facts. Contrary to balance and circuital laws, constitutive equations in a non uniform field region are approximate: this implies that a direct discrete formulation is approximate. We shall take the assumption that *the simplexes are small enough to consider the field uniform and the material homogenous inside every simplex.*

These simple remarks are the premises for a direct discrete formulation of physical laws. In order to carry out such a formulation it is necessary to subdivide the working spatial and temporal region in cells, by means of a *cell complex*. These cells can have, a priori, any shape and any dimension. While squares and cubes can be easily drawn, triangles and tetrahedra are preferable for reasons that will be clearer later. We shall consider only cells in the form of triangles and tetrahedra, i.e. *simplicial complexes*.

2 Direct Dicrete Formulation: the Premises

We call "direct discrete formulation" of physical laws one whose starting point are *physical measurements* and *experimental laws*. Since physical laws are quantitative relations between physical variables, we start with a reexamination of the physical variables themselves. This leads us to highlight the following points:

1. a discrete formulation must use *global variables* instead of *field functions*;
2. global variables are associated with space elements, i.e. *points, lines, surfaces, volumes* and with time elements *instants and intervals*;
3. in this association a pivotal role is played by the two kinds of orientations of spatial and temporal elements, i.e. the notions of *inner* and *outer* orientation;

4. physical variables can be classified in three classes according to the *role* that they play in the physical theory: *configuration*, *source* and *energy* variables;
5. configuration variables are associated with space elements endowed with inner orientation while source variables are associated with space elements endowed with outer orientation;
6. this association suggests *a cell complex and its dual* should be introduced instead of a coordinate system. The cells of the various degrees of the primal complex will be endowed with an inner orientation and those of the dual complex are automatically endowed with an outer orientation.

2.1 Configuration, Source and Energy Variables

The variables of acoustics, as well as those of all classical physical theories, can be divided in three classes.

- *Geometric* and *kinematic* variables that describe the configuration of the field and accordingly will be called *configuration variables*;
- *Static* and *dynamic* variables that describe the sources of the field and accordingly will be called *source variables*;
- *Energy variables* that are obtained doing the product of a configuration for a source variable.

We list here the main physical variables of continuum mechanics:

Configuration variables: displacement $\mathbf{s}$, strain tensor $\boldsymbol{\epsilon}$, velocity $\mathbf{u}$, strain rate tensor $\mathbf{D}$, kinetic potential φ, vorticity $\boldsymbol{\omega}$, vortex flux $\mathbf{W}$, velocity circulation Γ, etc.

Source variables: force $\mathbf{F}$, impulse $\mathbf{I}$, momentum content $\mathbf{P}^c$, momentum flow $\mathbf{P}^{\mathrm{f}}$, momentum density $\mathbf{p}$, mass content m^c, mass flow m^{f}, mass current Q, mass density ρ, mass current density $\mathbf{q}$, stress tensor $\boldsymbol{\sigma}$, pressure p, stream function ψ, etc.

Energy variables: work W, heat Q , potential energy V, kinetic energy T, hentalpy H, entropy $\mathbf{S}$, etc.

This classification is useful in teaching as well as in research. One consequence is that it enables us to define the *constitutive* or *material* equations: *these are the link between the configuration and the source variables of every physical theory and contain material and system parameters*.

2.2 Inner and Outer Orientation

In the association of global variables to a spatial and temporal element there is another essential point that must be considered: the notion of orientation of the element.

Inner orientation. We shall refer to the left part of Fig.(1). An inner orientation of a line means a direction along the line; an inner orientation of a surface means a direction of its bounding line; an inner orientation of a volume means an inner orientation of its bounding surface. An inner orientation of a point means that the point is conceived as a source or as a sink.

Outer orientation. With reference to the right part of Fig.(1), an outer orientation of a volume means a direction across its boundary, this is the usual orientation of inwards or outward normals. An outer orientation of a surface means a direction across the surface usually denoted by a normal unit vector. An outer orientation of a line means a direction of rotation around the line. An outer orientation of a point means that the lines that have an extremum in the point are endowed with outer orientation. Contrary to inner orientation, outer orientation depends on the dimension of the space in which the cell complex is embedded. Thus the outer orientation of a line segment embedded in a three-dimensional space is a sense of rotation *around* the segment; in a two-dimensional space it is an arrow that *crosses* the line and when the segment is embedded in a one-dimensional space, it is represented by two arrows as if the segment were compressed or extended. This is typical orientation used in elasticity to denote compression or traction of a bar.

2.3 Cell Complexes

Dealing with differential formulation it is quite natural to use coordinate systems. On the contrary a discrete formulation deals with global variables that are naturally associated with spatial and temporal elements, i.e. volumes, surfaces, lines, points, time intervals and instants.

Following the practice of algebraic topology, a branch of topology that uses cell complexes, the vertices, edges, faces and cells are considered as "cells" of dimension zero, one, two and three respectively. In short they are denoted as 0-cells, 1-cells, 2-cells and 3-cells. Thus a cell complex is not conceived as a set of small volumes but as a collection of cells of various dimensions.

Given a cell complex, we shall call *primal*, considering a point inside every 3-cell, say its centroid, one can construct another cell complex, called *dual*, taking these points as vertices. If the primal complex is formed of squares (in 2D) or of cubes (in 3D) also the dual one is formed of squares or cubes. The dual complex is simply *staggered* with respect to the primal one as shown in Fig.(3*a*).

In a two dimensional space the primal complex can be made of triangles. In this case considering the circumcenters of the triangles as vertices of the dual complex and connecting the circumcenters of two adjacent triangles one obtains a dual complex. To every 1-cell of the primal complex there corresponds a 2-cell of the dual and the two are orthogonal, as in Fig. (3*b*). The same is true for a three-dimensional complex made of tetrahedra. In this case one can consider the spherocenters: connecting the spherocenters of two adjacent tetrahedra one obtains a dual complex. In this case to every 1-cell of the primal there corresponds a 2-cell of the dual; to every 2-cell of the primal there corresponds a

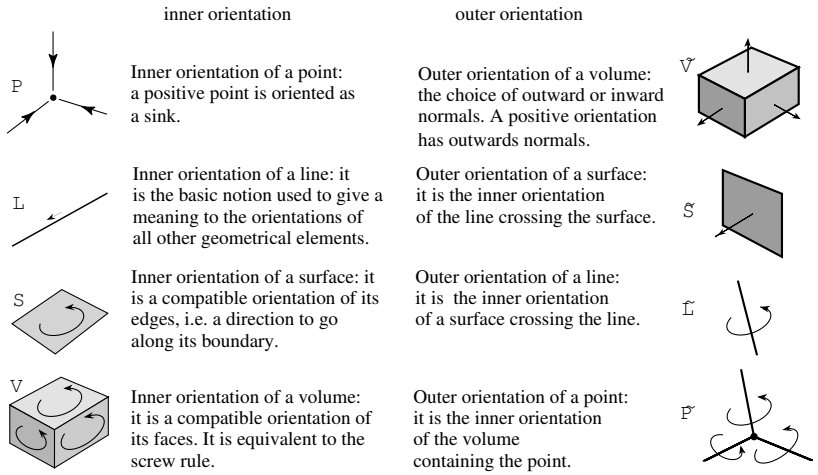

Figure 1: The two notions of inner and outer orientations in three-dimensional space.

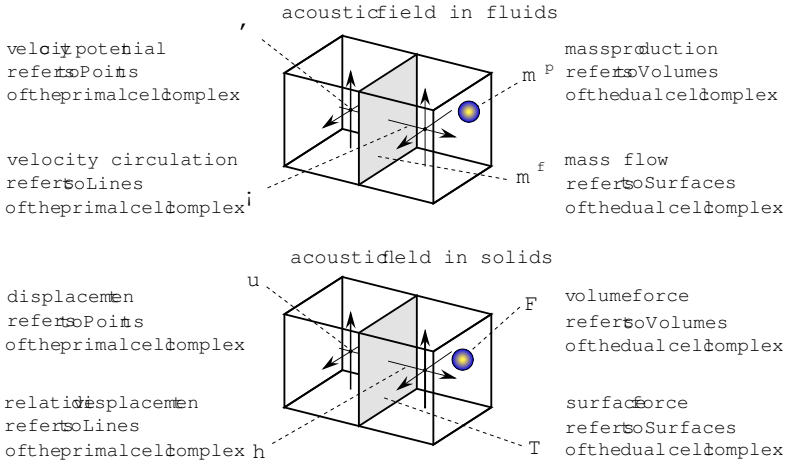

Figure 2: Global physical variables of acoustics and the geometric elements of the primal and dual cell complex with which they are associated.

1-cell of the dual. Moreover, to every 0-cell of the primal it corresponds a 3-cell of the dual. In short: if n denotes the dimension of the space, $(n = 1, 2, 3)$ with every p-cell of the primal it corresponds an $(n-p)$-cell of the dual and viceversa.

The choice of a point inside every n-cell, to be considered as 0-cell of the dual, is arbitrary and can be dictated by computational convenience.

The way of connecting the centers of two adjacent cells is also arbitrary. Hence when one consider the centroids of the n-cells one can connect the adjacent ones by a straigth line or via the centroid of the face, as shown in Fig.($3c$). The last choice is the one considered in algebraic topology and is called *barycentric subdivision.* It has many computational facilities. Doing so the dual of the 1-cell (hi) is the broken line shown as heavy line in Fig.($3c$). With reference to

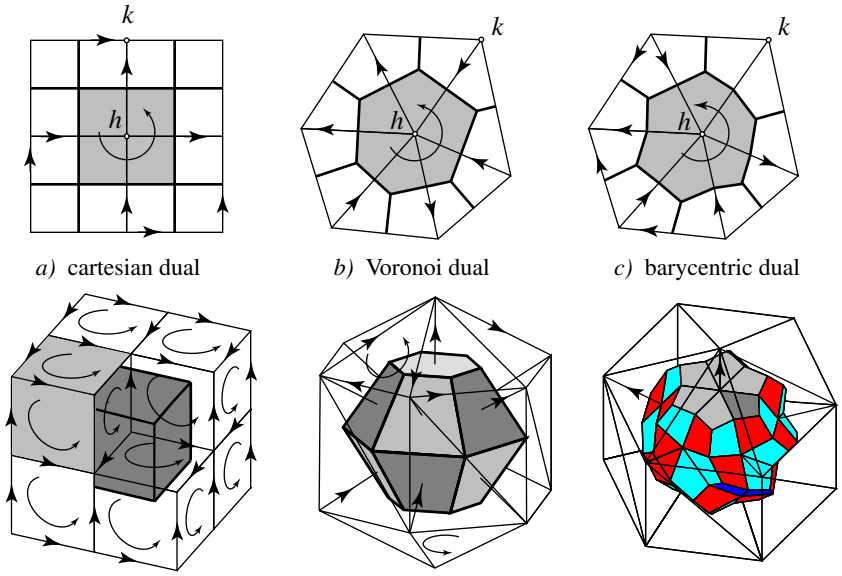

Figure 3: Primal and dual cell complexes.

Fig.(4) one can see that with every 0-cell of the primal complex it corresponds a 3-cell of the dual one. This duality is shown in Fig.(1) in which the elements of the right column are in reverse order to the ones of the left column. All these considerations do not depend on the shape and the dimensions of the cells of the complex. For numerical analysis, however triangular cells in two dimensional spaces and tetrahedral cells in three dimensions are convenient. These simplicial complexes permit a better matching with curved boundaries, can be refined in the regions of strong variation of gradients and fit well with linear interpolation. Furthermore, they are now considered the "de-facto" standard in the numerical analysis and optimization of complex engineering problems. We prefer to use the term "cell-complex" rather than "mesh" because, as we shall show, all space elements forming it are involved in the description.

Given a cell complex we can assign to all its elements an *inner* orientation. This complex will be called *primal*. If we now consider a dual complex, say considering the centroids of the cells as vertices of the dual, automatically all elements of the dual are endowed with *outer* orientation. This is a remarkable geometrical property discovered by Veblen and Whitehead [30, p.55] and intro-

duced in physics by Schouten [23] and Van Dantzig [29]. The notation

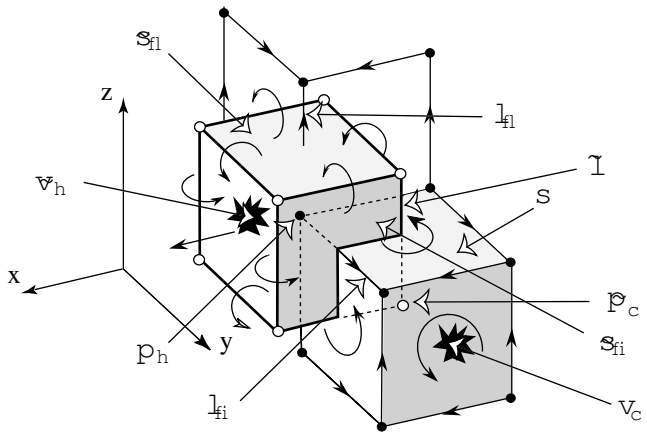

Figure 4: A cell complex in space and its elements. Heavy lines denote the dual complex.

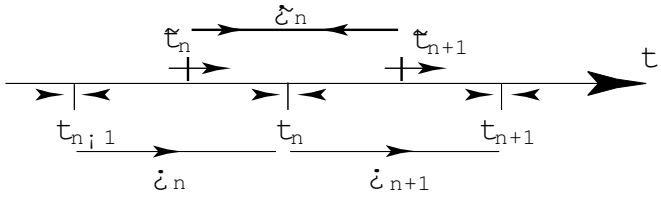

Figure 5: A cell complex in time and its elements. Heavy lines refer to the dual complex.

we use is collected in Fig.(4). One reason of using boldface letters is that the corresponding letters in plain symbol denote the extension of the element. Thus $\tilde{v}_h$ will denote the volume of the 3-cell $\tilde{\mathbf{v}}_h$.

The vertices of the primal cell complex can be numbered following any criterion: it is natural to use the same number to label the dual cell. Thus $\mathbf{p}_h$ will denote a vertex and $\tilde{\mathbf{v}}_h$ its dual cell. An edge of a primal cell can be labeled with two indices, the indices of the vertices connected by the edge. A notational simplification arises if we use a single Greek letter to label the edges of the primal complex, say $\mathbf{l}_\alpha$ instead of $\mathbf{l}_{hi}$. A face of the dual complex will be labeled also with a Greek index, say $\tilde{\mathbf{s}}_\beta$.

2.4 Global Variables and Space Elements

We now show that global variables naturally refer to a space element and to a time element. Table (3.1) lists the main global variables of acoustics and the spatial and temporal elements with which they are associated. In the association between a physical quantity and spatial and temporal elements we must carefully distinguish between field variables (i.e. field functions) and global variables (i.e. domain functions). Velocity is not a global variable but rather the time rate of the displacement and the latter refers to a time interval. For this reason velocity inherited a link with the time interval. This is enforced by the fact that one cannot measure a velocity without introducing a time interval, however small it may be. Pressure is not a global variable but rather the time rate and the surface density of the surface impulse: the latter refers to a surface and a time interval. For this reason pressure inherited a link with surfaces and time intervals.

Having presented the notion of cell complex and its dual and the corresponding notions of inner and outer orientations, we can examine the association of global physical variables to spatial and temporal elements in further detail.

Let us analyze acoustic field in fluids and solids, as shown in Fig.(2). We shall refer also to Figg.(4) and (5).

In the acoustic field in fluids, one can associate mass content to the dual cells $\tilde{\mathbf{v}}_h$ and mass flow to the faces $\tilde{\mathbf{s}}_\alpha$ of the dual cells. Kinetic potential can be associated with the vertices $\mathbf{p}_h$ of the primal cells and velocity circulation with the edges $\mathbf{l}_\beta$ of the primal cells.

In the acoustic field of solids, volume forces are associated with the dual cells $\tilde{\mathbf{v}}_h$ and surface forces across the faces associated with the faces $\tilde{\mathbf{s}}_\alpha$ of the dual cells. The displacements can be associated with the vertices $\mathbf{p}_h$ of the primal cells and the displacement differences will be associated with the edges $\mathbf{l}_\beta$ of the primal cells.

2.5 Global Variables and Temporal Elements

We shall refer to time elements of Fig.(5). A primal cell complex on a time axis exhibits time instants $\mathbf{t}_n$ and time intervals $\boldsymbol{\tau}_n$. Time intervals are endowed with inner orientation orienting them from past towards future. Time instants are endowed with inner orientation conceiving them as *sinks*, i.e. considering positive time intervals when they come to instants. This follows from the custom of considering the time increment of a function as given by

$$\Delta f(t) \stackrel{\text{def}}{=} (+1) f(t + \Delta t) + (-1) f(t). \tag{1}$$

We see from this expression that the "+1" and "-1" can be conceived as *incidence numbers* between time intervals (1-cells) and time instants (0-cells).

Since we have found useful to consider a dual complex in space it will be useful to consider also a dual complex in time. This is formed by the middle instants of the primal time intervals. We shall denote the elements of the dual complex by $\tilde{\mathbf{t}}_n$ and $\tilde{\boldsymbol{\tau}}_n$. The dual time instants inherited an *outer* orientation

from the inner orientation of primal time intervals: this outer orientation is represented by an arrow that crosses the instant. Dual time intervals also inherited an *outer* orientation from the inner orientation of primal time instants: this outer orientation is represented by two arrows that "compress" the segment. The dual time complex has never been considered in physics and, as consequence, neither has the notion of outer orientation.

Using boldface characters for time intervals we have the possibility to use the corresponding normal character for the duration of intervals: so τ_n is the duration of the interval $\boldsymbol{\tau}_n$ and $\tilde{\tau}_n$ is the duration of the dual interval $\tilde{\boldsymbol{\tau}}_n$. Moreover τ_n and $\tilde{\boldsymbol{\tau}}_n$ are positive numbers while $\boldsymbol{\tau}_n$ and $\tilde{\boldsymbol{\tau}}_n$ are time objects endowed with orientation. Then $-\boldsymbol{\tau}_n$ means that we have changed the orientation into its opposite, i.e. we have performed the traditional *time-reversal*. The expression $-\tilde{\boldsymbol{\tau}}_n$ means that the dual time intervals have an opposite sign, i.e. are conceived as bars in traction. Likewise the expression $-\mathbf{t}_n$ means that instants are oriented as sources: this would not be possible if the notation $-t_n$ where used.

When we perform the ratio of a global variable referred a time interval for the duration, the rate becomes a function of the middle instant of the interval. Thus with reference to Fig.(5) and Table (3.8) we have

$$Q_\alpha(t_n) = \frac{m^{\mathrm{f}}[\tilde{\boldsymbol{\tau}}_n, \tilde{\mathbf{s}}_\alpha]}{\tilde{\tau}_n} \qquad \chi_h(\tilde{t}_n) = \frac{X[\boldsymbol{\tau}_n, \mathbf{p}_h]}{\tau_n}. \tag{2}$$

Since rates are no longer global variables in time we use the round brackets for them. We shall use two notations for densities and rates. The first notation $\chi[\boldsymbol{\tau}_n, \mathbf{p}_h]$ using square brackets means that the density or the rate inherited a link with the spatial and temporal elements of its mother variable; the second notation $\chi_h(\tilde{t}_n)$ denotes that the variable is a function of the point and instant.

The association of global variables to spatial and temporal elements is summarized in Table(3.8).

2.6 Physical Variables and Orientation

The fact that physical variables are associated with spatial and temporal elements is only part of the story. It is easy to understand that some physical variables require an inner orientation of the spatial and temporal element and others require their outer orientation. So the vortex strength across a surface can be defined as the velocity circulation along the boundary of the surface. Since the boundary has two possible inner orientations it follows that the vortex strength changes sign when we invert the inner orientation of the surface. (see Fig.6 *left*). On the contrary mass flow across a surface requires an outer orientation of the surface and then changes sign when the outer orientation is reversed (see Fig.6 *right*).

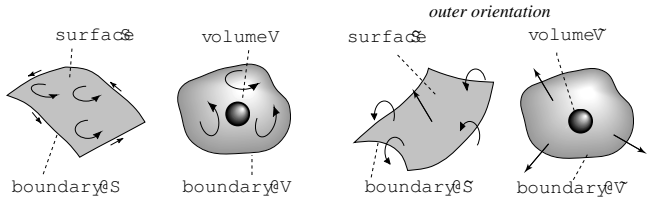

Figure 6: Inner and outer orientation of surfaces, volumes and their boundaries.

2.7 Space and Time Association Rule

These examples show that configuration variables refer to the elements of one cell complex while source variables refer to the elements of the dual complex. Since mass flow and momentum flow need a face endowed with outer orientation, it is natural to apply them to the faces of the dual cell complex.

These examples lead us to formulate the following

ASSOCIATION RULE. *Global configuration variables are associated with spatial and temporal elements of a primal cell complex endowed with inner orientation. Moreover, global source variables and global energy variably are associated with spatial and temporal elements of the dual cell complex endowed with outer orientation.*

In short

configuration variables	source and energy variables
↓	↓
primal complex	dual complex
↓	↓
inner orientation	outer orientation.

This rule [26] offers a rational criterion to associate global variables of every physical theory to spatial and temporal elements and, as such, it is useful in computational physics.

3 Acoustic Waves in Fluids

The discrete formulation of acoustics will be based on the use of global variables; the introduction of mean densities is requested by constitutive equations. Following this line of thought we shall give primary importance not to velocity but to *velocity circulation*. This is a global variable associated with the 1-cells of the primal complex because these are endowed with inner orientation. In doing so we are in agreement with MAC method [10] used in fluid dynamics and with its extension to unstructured meshes [20]; [2]. In fact in these methods one considers the velocity component along every 1-cell: since this component is multiplied by the length of the 1-cell it follows that the true variable is the

circulation. By considering the circulation one avoids the approximation introduced by the scalar product of the velocity in the middle point of every 1-cell for the cell length.

To describe acoustics in fluids it is enough to use a scalar function: this can be pressure, density, kinetic potential or condensation. We shall choose the kinetic potential because it is a kinematical variable.

Since we have a scalar function we need a scalar equation: the natural one is the equation expressing mass conservation.

Acoustics is based on some assumptions: motion is *irrotational* [22, p.251]; velocities are *small* if compared with sound velocity. Introducing the *density excess* ρ^* and the *pressure excess* p^* defined by

$$\begin{cases} p(t,x,y,z) = p_0 + p^*(t,x,y,z) \\ \rho(t,x,y,z) = \rho_0 + \rho^*(t,x,y,z) \end{cases} \tag{3}$$

one assumes that $\rho^* \ll \rho_0$ and $p^* \ll p_0$.

Model assumptions. The discrete formulation will be based on further assumptions: we use a simplicial complex as primal and its barycentric subdivision as dual. We consider that the medium is inhomogeneous, as in layered media, and then ρ_c and the sound velocity c_c can change from one cell to another. The material is homogeneous inside every primal cell $\mathbf{v}_c$ and then density ρ_c and pressure p_c are uniform. Also velocity $\mathbf{u}_c$ is supposed uniform. This is in accordance with the fact that in an irrotational motion the circulation along the boundary of every 2-cell (tetrahedron face) vanishes. In an irrotational motion this hypotesis cannot be accepted.

3.1 Global Configuration Variables

Continuum mechanics differs from other field theories because it admits a double description, the *material* and the *spatial* one. This implies that in the material description velocity $\mathbf{s}$ is a displacement rate while in the spatial description it is a field vector of which one can perform the circulation Γ along a line. When velocity is considered as displacement rate it is a controvariant vector because the displacement $\mathbf{s}$ is a controvariant vector; when considered as field vector it is a covariant one since it can be the gradient of kinetic potential φ.

From this follows that velocity is not a global variable but a rate in the material description and a line density in the spatial description. Thus in the integral formulation

$$\mathbf{s}_A\,[\mathbf{T}] = \int_{\mathbf{T}} \mathbf{u}_A(t)\,\mathrm{d}t \qquad\qquad \Gamma[\mathbf{I},\mathbf{L}] = \int_{\mathbf{L}} \mathbf{u}(t,\mathbf{P}) \cdot \mathrm{d}\,\mathbf{L}. \tag{4}$$

Acoustics is based on the hypothesis that the velocity field is irrotational. This condition, which is commonly expressed by the differential condition curl $\mathbf{u} = 0$, can be expressed in a discrete formulation stating that the velocity circulation

along any reducible closed path vanishes:

$$\Gamma[\mathbf{I}, \partial\mathbf{S}] = 0. \tag{5}$$

Vortex strength W, that is referred to a surface, can be defined as the velocity circulation along the boundary of the surface. It follows that for an irrotational motion is

$$W[\mathbf{I}, \mathbf{S}] = 0. \tag{6}$$

In this hypothesis one can introduce the kinetic potential φ at every point defined as the velocity circulation from a fixed point to the actual point.

Let us consider a simplicial complex in the working space region and a one-dimensional cell complex in the working time interval, as shown in Fig.(4). To emphasize the association of the kinetic potential with the vertices $\mathbf{p}_h$ of the primal space complex and with the instants $\mathbf{t}_n$ of the primal time complex we write: $\varphi[\mathbf{t}_n, \mathbf{p}_h]$. Since time instants and space points are elements without extension the domain function is reduced to a point function and then we can write simply $\varphi[\mathbf{t}_n, \mathbf{p}_h] \equiv \varphi_h(t_n)$. The space variation of the kinetic potential φ gives the velocity circulation Γ. We will need also the time variations of the kinetic potential we shall call X. The last three variables are global and the spatial and temporal element with which they are associated is shown in Table(3.1). We remark that acceleration is the material derivative of velocity and, for small velocities, in spatial description it can be approximated by the partial time derivative of velocity.

Table 1: Global physical variables of acoustics in fluids and the associated spatial and temporal elements. The suffix "c" means *content*; the suffix "f" means *flow*; the suffix "s" means *surface* and the suffix "v" means *volume*.

global configuration variables	
kinetic potential	$\varphi\,[\mathbf{I}, \mathbf{P}]$
velocity circulation	$\Gamma\,[\mathbf{I}, \mathbf{L}]$
vortex strength	$W[\mathbf{I}, \mathbf{S}]$
(no known name)	$X[\mathbf{T}, \mathbf{P}]$

global source variables	
mass content	$m^{\mathrm{c}}[\tilde{\mathbf{I}}, \tilde{\mathbf{V}}]$
mass flow	$m^{\mathrm{f}}[\tilde{\mathbf{T}}, \tilde{\mathbf{S}}]$
momentum content	$\mathbf{P}^{\mathrm{c}}[\tilde{\mathbf{I}}, \tilde{\mathbf{V}}]$
momentum flow	$\mathbf{P}^{\mathrm{f}}[\tilde{\mathbf{T}}, \tilde{\mathbf{S}}]$
surface impulse	$\mathbf{I}^{\mathrm{s}}[\tilde{\mathbf{T}}, \tilde{\mathbf{S}}]$
volume impulse	$\mathbf{I}^{\mathrm{v}}[\tilde{\mathbf{T}}, \tilde{\mathbf{V}}]$

3.2 Velocity

Once we decide to use the kinetic potential, the fundamental problem of acoustics, in the differential formulation, is to find the kinetic potential φ at *all* space points and at *all* time instants, i.e. $\varphi(t, \mathbf{x})$. In a discrete formulation we can find the kinetic potential only at the 0-cells of the space primal complex and at the 0-cells of the primal time complex: $\varphi[\mathbf{t}_n, \mathbf{p}_h]$. Its value inside every space

3-cell and inside every time 1-cell must be interpolated. The interpolation we carry out is to suppose that the kinetic potential inside every 3-cell $\mathbf{v}_c$ in a time interval $\boldsymbol{\tau}_n$ is an *affine* function of cartesian coordinates and an affine function of time i.e.

$$\varphi(t,x,y,z) = (b + a\,t) + (b_x + a_x\,t)\,x + (b_y + a_y\,t)\,y + (b_z + a_z\,t)\,z \tag{7}$$

This choice implies that the velocity field $\mathbf{u}$ is *uniform* inside every cell and *affine* in every time interval. Since the velocity $\mathbf{u}$ is uniform inside the simplex, for every line segment $\mathbf{L}$ whose boundary points are denoted A and B we can write

$$\mathbf{u}\cdot\mathbf{L} = \varphi_B - \varphi_A \tag{8}$$

or

$$L_x u_x + L_y u_y + L_z u_z = \varphi_B - \varphi_A. \tag{9}$$

This relation permit us to evaluate the velocity components u_x, u_y, u_z at an instant t_n in terms of the kinetic potential at the four vertices of every simplex. Let us call h, i, j, k the four vertices of an 3-cell $\mathbf{v}_c$ ordered so as to form a right-hand helix. Writing equation (7), for the four vertices, subtracting one equation from the preceeding one and denoting by $\mathbf{L}_i$, $\mathbf{L}_j$, $\mathbf{L}_k$ the three vectors that described the oriented edges starting from the vertex h, as shown in Fig.(7), we can write

$$\left[\begin{array}{ccc} L_{ix} & L_{iy} & L_{iz} \\ L_{jx} & L_{jy} & L_{jz} \\ L_{kx} & L_{ky} & L_{kz} \end{array}\right]_c \left\{\begin{array}{c} u_x(t_n) \\ u_y(t_n) \\ u_z(t_n) \end{array}\right\}_c = \left\{\begin{array}{c} \varphi_i(t_n) - \varphi_h(t_n) \\ \varphi_j(t_n) - \varphi_h(t_n) \\ \varphi_k(t_n) - \varphi_h(t_n) \end{array}\right\}_c . \tag{10}$$

Face A_i, opposite to vertex i, is described by the area vector $\mathbf{A}_i = \frac{1}{2}\,\mathbf{L}_k \times \mathbf{L}_j$. With reference to Fig.(7) we obtain

$$\mathbf{A}_i = \tfrac{1}{2}\,\mathbf{L}_k \times \mathbf{L}_j = \tfrac{1}{2}\left|\begin{array}{ccc} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ L_{kx} & L_{ky} & L_{kz} \\ L_{jx} & L_{jy} & L_{jz} \end{array}\right| \tag{11}$$

from which

$$A_{ix} = \tfrac{1}{2}\left|\begin{array}{cc} L_{ky} & L_{kz} \\ L_{jy} & L_{jz} \end{array}\right| , \quad \text{etc.} \tag{12}$$

Similar relations can be obtained for $\mathbf{A}_j, \mathbf{A}_k, \mathbf{A}_h$.

The oriented volume of the tetrahedron is $v_c = 1/6\,(\mathbf{L}_i \times \mathbf{L}_j)\cdot\mathbf{L}_k$. Using Cramer's rule we obtain

$$u_x(t_n) = -\frac{1}{3\,v_c}\Big[A_{ix}\,\varphi_i(t_n) + A_{jx}\,\varphi_j(t_n) + A_{kx}\,\varphi_k(t_n) + A_{hx}\,\varphi_h(t_n)\Big] \tag{13}$$

where we have used the relation $-(A_{ix} + A_{jx} + A_{kx}) = A_{hx}$, as shown in Fig.(7). In conclusion we have:

$$\mathbf{u}_c(t_n) = -\frac{1}{3\,v_c}\sum_{m\in\mathcal{V}(c)} \mathbf{A}_m\,\varphi_m(t_n). \tag{14}$$

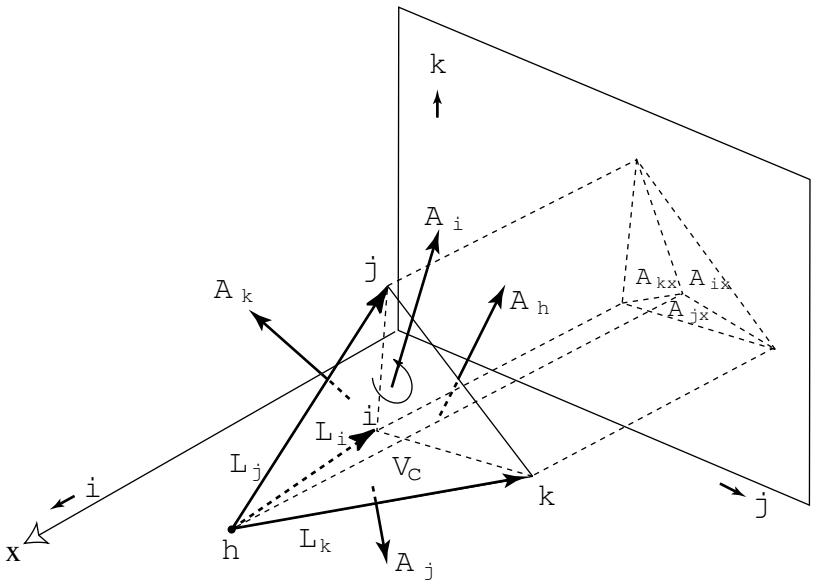

Figure 7: The projection of a tetrahedron face on a coordinate plane.

where $\mathcal{V}(c)$ denotes the set of vertices of the 3-cell $\mathbf{v}_c$.

Then we can evaluate the velocity inside every primal cell (tetrahedron) in terms of the kinetic potential at the vertices of the tetrahedron. These formulae coincide with the classical one used in finite elements[5, p.40], as we show later.

One can see that the notion of affine function fits simplexes perfectly because an affine function has a number of coefficients equal to the number of vertices of a simplex.

3.3 A Short Derivation

Formula (14) is so simple that one might suspect that it can be obtained directly. This is the case. We only need to introduce the discrete analogous of the gradient operator. Let us consider a scalar function $u = f(\mathbf{P})$ defined in a region Ω. Let us consider a point $\mathbf{B}$ in the region and a volume $\mathbf{V}$ that contains the point[1]. Let $\partial\mathbf{V}$ be the boundary of the volume. To deal with a discrete formulation the volume will be chosen as a polyhedron with $\mathbf{B}$ as its centroid. Let us denote by $\mathbf{S}_k$ the k-th face of the polyhedron, with $\mathbf{B}_k$ the centroid of $\mathbf{S}_k$ and with $\mathbf{A}_k$ the area-vector of the face $\mathbf{S}_k$ directed outwards. The vector

$$\mathbf{G}(\mathbf{B}) \stackrel{\text{def}}{=} \frac{\sum_k f(\mathbf{B}_k)\,\mathbf{A}_k}{V} \tag{15}$$

[1] We remark that $\mathbf{V}$ denotes a space region called "volume" and V denotes its extension, also called "volume"!

will be called the *discrete gradient* of the function $f(\mathbf{P})$ at $\mathbf{B}$. It can easily be shown that this formula reduces to the traditional gradient at the limit for $\mathbf{V} \to 0$.

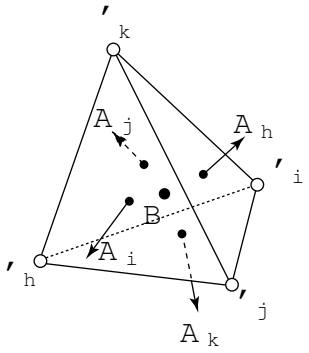

Figure 8: The discrete gradient.

Since the kinetic potential is an affine function, the potentials at the centroids of the faces of the tetrahedron, are given by the aritmetic mean of the potentials at vertices. Then

$$\mathrm{Grad}\,\varphi = \frac{1}{v_c}\left[\frac{\varphi_h+\varphi_i+\varphi_j}{3}\mathbf{A}_k+\frac{\varphi_i+\varphi_k+\varphi_j}{3}\mathbf{A}_h+\ \frac{\varphi_j+\varphi_k+\varphi_h}{3}\mathbf{A}_i+\frac{\varphi_k+\varphi_i+\varphi_h}{3}\mathbf{A}_j\right]. \tag{16}$$

Since $\mathbf{A}_h + \mathbf{A}_i + \mathbf{A}_j + \mathbf{A}_k = 0$ after simplification we obtain

$$\mathbf{u} = -\frac{1}{3\,v_c}(\mathbf{A}_h\,\varphi_h + \mathbf{A}_i\,\varphi_i + \mathbf{A}_j\,\varphi_j + \mathbf{A}_k\,\varphi_k) \tag{17}$$

that coincides with Eq.(14).

3.4 The Function χ

We shall need the variable

$$X[\boldsymbol{\tau}_n, \mathbf{p}_h] \stackrel{\text{def}}{=} \varphi[\mathbf{t}_n, \mathbf{p}_h] - \varphi[\mathbf{t}_{n-1}, \mathbf{p}_h] \tag{18}$$

and the corresponding rate

$$\chi_h(\tilde{t}_n) \stackrel{\text{def}}{=} \frac{X[\boldsymbol{\tau}_n, \mathbf{p}_h]}{\tau_n}. \tag{19}$$

Both variables are unnamed. For small velocities $\chi = \partial_t\varphi$ can be identified with the acceleration potential.

3.5 Global Source Variables

In material description mass is a global variable and it is an attribute of a fluid body. In spatial description mass is split into *mass content* m^{c}, contained in a control volume (a cell), and in *mass flow* m^{f} across a fixed surface (a cell face). The same happens for momentum: there is a *momentum content* $\mathbf{P}^{\mathrm{c}}$ and a *momentum flow* $\mathbf{P}^{\mathrm{f}}$. Lastly, also the impulse can be divided into *volume impulse* and *surface impulse* we shall denote $\mathbf{I}^{\mathrm{v}}, \mathbf{I}^{\mathrm{s}}$.

As we have said, in the spatial description global physical variables naturally refer to space-time elements of a cell complex and of its dual. In particular source variables such as mass, momentum and impulse are associated with dual cells, i.e. with the polyhedra that contain the nodes, because they need spatial elements endowed with outer orientation. The label of a dual cell is the same as that of the vertex of the primal cell contained in it. The amounts of these source variables contained in the dual cell $\tilde{\mathbf{v}}_h$ will be denoted by $m^{\mathrm{c}}_h, \mathbf{P}^{\mathrm{c}}_h, \mathbf{I}^{\mathrm{v}}_h$ respectively. In numerical treatment of continuum mechanics it is natural to start by considering the amount of mass, momentum and volume impulse contained in every primal cell $\mathbf{v}_c$ which will be denoted by $m^{\mathrm{c}}_c, \mathbf{P}^{\mathrm{c}}_c, \mathbf{I}^{\mathrm{v}}_c$ respectively. This implies that we must express the source variables contained in every dual cell $\tilde{\mathbf{v}}_h$ in terms of the amounts that are contained inside every primal cell $\mathbf{v}_c$, as done in Table (3.5).

If one considers simplicial complexes and uses the barycentric subdivision to construct a dual complex, only $1/4$ of a primal cell $\mathbf{v}_c$ is contained in the dual cell $\tilde{\mathbf{v}}_h$. We remark that using Voronoi dual instead of the barycentric one the fraction of the dual cell contained in the primal one is variable from cell to cell.

In fluid dynamics there are six global source variables of interest quoted in Table (3.1). To write balance equations we must use dual cells because they are endowed with outer orientation. This corresponds to the vertex-centered choice of Finite Volume Method (FVM). Balance of mass and of momentum can be written

$$\begin{cases} m^{\mathrm{c}}[\tilde{\mathbf{I}}^{+}, \tilde{\mathbf{V}}] - m^{\mathrm{c}}[\tilde{\mathbf{I}}^{-}, \tilde{\mathbf{V}}] + m^{\mathrm{f}}[\tilde{\mathbf{T}}, \partial\tilde{\mathbf{V}}] = 0 \\ \mathbf{P}^{\mathrm{c}}[\tilde{\mathbf{I}}^{+}, \tilde{\mathbf{V}}] - \mathbf{P}^{\mathrm{c}}[\tilde{\mathbf{I}}^{-}, \tilde{\mathbf{V}}] + \mathbf{P}^{\mathrm{f}}[\tilde{\mathbf{T}}, \partial\tilde{\mathbf{V}}] = \mathbf{I}^{\mathrm{s}}[\tilde{\mathbf{T}}, \partial\tilde{\mathbf{V}}] + \mathbf{I}^{\mathrm{v}}[\tilde{\mathbf{T}}, \tilde{\mathbf{V}}]. \end{cases} \tag{20}$$

In order to introduce configuration variables into balance laws we must use constitutive equations. The latter require the introduction of mean rates and mean densities.

3.6 Mass Current

From mass flow we can define its rate, i.e. mass current Q, and mass current density vector $\mathbf{q}$. Mass flow $m^{\mathrm{f}}[\tilde{\mathbf{T}}, \tilde{\mathbf{S}}]$ is a global variable referred to a time interval and a surface both endowed with outer orientation. Let us consider a small *plane* surface, whose area-vector will be denoted by $\mathbf{A}$, and a small time interval $\tilde{T}$ and its middle instant I. Mass current Q and mass current density

Table 2: A list of useful relations between variables of acoustics in fluids.

$$
\begin{aligned}
\tilde{v}_h &= \frac{1}{4}\sum_{c\in\mathcal{J}(h)} v_c \\
\tilde{v}_h\,\rho_h(\tilde{t}_n) &= \frac{1}{4}\sum_{c\in\mathcal{J}(h)} v_c\,\rho_c(\tilde{t}_n) \\
\mathbf{u}_c(\tilde{t}_n) &= \frac{1}{2}\left[\mathbf{u}_c(t_{n-1}) + \mathbf{u}_c(t_n)\right] \\
\tilde{v}_h\,\rho_h(\tilde{t}_n)\,\mathbf{u}_h(\tilde{t}_n) &= \frac{1}{4}\sum_{c\in\mathcal{J}(h)} v_c\,\rho_c(\tilde{t}_n)\,\mathbf{u}_c(\tilde{t}_n) \\
m^{\mathrm{c}}[\tilde{\mathbf{t}}_n, \tilde{\mathbf{v}}_h] &= \frac{1}{4}\sum_{c\in\mathcal{J}(h)} v_c\,\rho_c(\tilde{t}_n) = \tilde{v}_h\,\rho_h(\tilde{t}_n) \\
\mathbf{P}^{\mathrm{c}}[\tilde{\mathbf{t}}_n, \tilde{\mathbf{v}}_h] &= \frac{1}{4}\sum_{c\in\mathcal{J}(h)} v_c\,\rho_c(\tilde{t}_n)\mathbf{u}_c(\tilde{t}_n) \approx \tilde{v}_h\,\rho_h^0\mathbf{u}_h(\tilde{t}_n) \\
\rho_c(t_n) &= \frac{1}{2}\left[\rho_c(\tilde{t}_n) + \rho_c(\tilde{t}_{n+1})\right] \\
m^{\mathrm{f}}[\tilde{\boldsymbol{\tau}}_n, \partial\tilde{\mathbf{v}}_h] &= \frac{1}{3}\tilde{\tau}_n \sum_{c\in\mathcal{J}(h)} \rho_c(t_n)\,\mathbf{A}_h^c\cdot\mathbf{u}_c(t_n) \approx \frac{1}{3}\tilde{\tau}_n\rho_c^0 \sum_{c\in\mathcal{J}(h)} \mathbf{A}_h^c\cdot\mathbf{u}_c(t_n) \\
\mathbf{P}^{\mathrm{f}}[\tilde{\boldsymbol{\tau}}_n, \partial\tilde{\mathbf{v}}_h] &= \frac{1}{3}\tilde{\tau}_n \sum_{c\in\mathcal{J}(h)} \left[\rho_c(t_n)\mathbf{A}_h^c\cdot\mathbf{u}_c(t_n)\right]\mathbf{u}_c(t_n) \\
&\approx \frac{1}{3}\tilde{\tau}_n\,\rho_c^0 \sum_{c\in\mathcal{J}(h)} \left[\mathbf{A}_h^c\cdot\mathbf{u}_c(t_n)\right]\mathbf{u}_c(t_n) \approx 0 \\
\mathbf{I}^{\mathrm{s}}[\tilde{\boldsymbol{\tau}}_n, \partial\tilde{\mathbf{v}}_h] &= -\frac{1}{3}\tilde{\tau}_n \sum_{c\in\mathcal{J}(h)} p_c(t_n)\,\mathbf{A}_h^c = -\tilde{\tau}_n\,\mathrm{Grad}\,p(t_n)\Big|_h \\
\mathbf{I}^{\mathrm{v}}[\tilde{\boldsymbol{\tau}}_n, \mathbf{v}_h] &= \frac{1}{4}\tilde{\tau}_n\,\mathbf{g} \sum_{c\in\mathcal{J}(h)} v_c\,\rho_c(\tilde{t}_n) = \tilde{\tau}_n\mathbf{g}\,\tilde{v}_h\,\rho_h(\tilde{t}_n) \approx \tilde{\tau}_n\,\mathbf{g}\,\tilde{v}_h\,\rho_h^0
\end{aligned}
$$

vector $\mathbf{q}$ are linked by

$$Q(I) = \frac{m^{\mathrm{f}}[\tilde{\mathbf{T}}, \tilde{\mathbf{S}}]}{\tilde{T}} = \mathbf{A} \cdot \mathbf{q}(I). \tag{21}$$

We see that mass current and mass current density vector can be introduced without resorting to the notion of limit simply by considering a small space region in which velocity is uniform in space and affine in time.

Let us consider that part of the boundary of the dual cell that is contained in a primal cell, as shown in Fig.(9*d*). Let us denote as S_1, S_2, S_3 the three faces and $\mathbf{A}_1, \mathbf{A}_2, \mathbf{A}_3$ the corresponding area vectors oriented outward. Let us consider the three lateral faces S_4, S_5, S_6 of the tetrahedron and the relative vectors $\mathbf{A}_4, \mathbf{A}_5, \mathbf{A}_6$ with outward direction as shown in Fig.(9*e*). Since the six faces form the boundary of a volume the sum of their vectors vanishes and then

$$\mathbf{A}_1 + \mathbf{A}_2 + \mathbf{A}_3 = -(\mathbf{A}_4 + \mathbf{A}_5 + \mathbf{A}_6). \tag{22}$$

One can easily see that if one uses the centroids of the edges, faces and

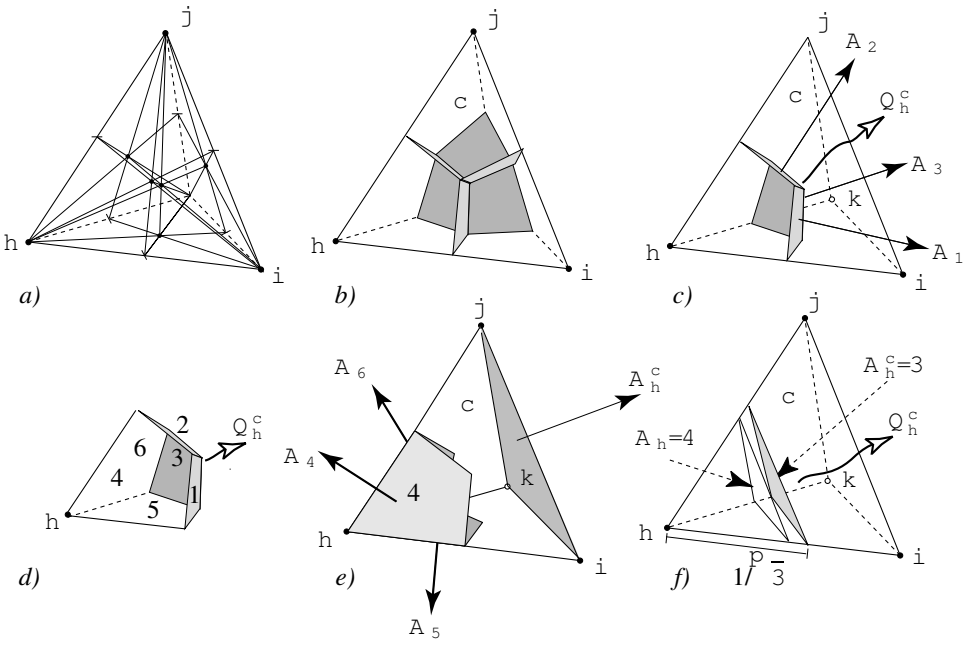

Figure 9: The part of the dual polyhedron contained in the tetrahedron that corresponds to every vertex of the tetrahedron.

volumes the area of every lateral face, like A_4, A_5, A_6, is 1/3 of the area of the corresponding face of the tetrahedron. If we denote by $\mathbf{A}^{\mathrm{c}}_h$ the area-vector of

the face of $\mathbf{v}_c$ opposite to the vertex $\mathbf{p}_h$ and directed outwards, it follows that

$$\mathbf{A}_1 + \mathbf{A}_2 + \mathbf{A}_3 = -\frac{1}{3}(\mathbf{A}_i + \mathbf{A}_j + \mathbf{A}_k) = \frac{\mathbf{A}_h^{\mathrm{c}}}{3} \tag{23}$$

where we have used the property that the sum of the vectors of the four faces of the tetrahedron vanishes. Then the part of the boundary of the dual cell contained in every tetrahedron is equivalent to a triangle parallel to the opposite face h (opposed to the vertex h) and whose area is $1/3$ of the face h. The term "equivalent" means that the area-vector of the equivalent surface is equal to the sum of the three area-vectors, as shown in Fig.$(9f)$.

Hence the mass current Q_h^c crossing the part of the surface of the dual cell contained in the cell $\mathbf{v}_c$ is

$$Q_h^c(t_n) = \frac{1}{3}\mathbf{q}^{\,\mathrm{c}}(t_n). \tag{24}$$

3.7 Constitutive Equations

As we have said, equations that link a source variable with a configuration variable are called *constitutive equations*. We list the constitutive equations of *perfect* fluid dynamics.

- *mass current* $\leftrightarrow$ *velocity:*

$$\mathbf{q}_c(t_n) = \rho_c(t_n)\,\mathbf{u}_c(t_n) \approx \rho_c^0\,\mathbf{u}_c(t_n). \tag{25}$$

  where the suffix "c" refers to a primal 3-cell $\mathbf{v}_c$.

- *momentum content* $\leftrightarrow$ *velocity:*

$$\mathbf{P}^{\,\mathrm{c}}[\tilde{\mathbf{t}}_n, \tilde{\mathbf{v}}_h] = \tilde{v}_h\,\rho_h(\tilde{t}_n)\,\mathbf{u}_h(\tilde{t}_n) \approx \tilde{v}_h\,\rho_h^0\,\mathbf{u}_h(\tilde{t}_n). \tag{26}$$

  We remark that velocity in (25) and in (26) refers to different instants. Then

$$\mathbf{u}_c(\tilde{t}_n) = \frac{\mathbf{u}_c(t_{n-1}) + \mathbf{u}_c(t_n)}{2}. \tag{27}$$

- *momentum flow* $\leftrightarrow$ *velocity:* Denoting by $\mathbf{A}$ the area-vector of a plane surface $\tilde{\mathbf{s}}$ contained in $\mathbf{v}_c$, we have

$$\mathbf{P}^{\,\mathrm{f}}[\tilde{\boldsymbol{\tau}}_n, \tilde{\mathbf{s}}] = \tilde{\tau}_n\,[\mathbf{q}_c(t_n)\cdot\mathbf{A}]\;\mathbf{u}_c(t_n) \approx \tilde{\tau}_n\,\rho_c^0\;(\mathbf{u}_c(t_n)\cdot\mathbf{A})\;\mathbf{u}_c(t_n) \approx 0. \tag{28}$$

- *pressure* $\leftrightarrow$ *volume*; The adiabatic law gives

$$p_c^*(\tilde{t}_n) \approx c_c^2\,\rho_c^*(\tilde{t}_n) \tag{29}$$

  i.e. *pressure excess is proportional to density excess*. We remark that while pressure is referred to dual intervals, and then it is function of the primal instants, density is referred to dual instants, as shown in Table(3.8).

- *mass density* $\leftrightarrow$ χ*:* we shall prove later that the generalized Bernoulli equation leads to the relation

$$\rho_h(\tilde{t}_n) \approx \rho_h^0\,\left[1 - \frac{1}{c_h^2}\,\chi_h(\tilde{t}_n)\right] \tag{30}$$

  where the suffix h refers to a 0-cell $\mathbf{p}_h$ (for χ) and to the dual cell $\tilde{\mathbf{v}}_h$ (for ρ and c).

3.8 Mass Balance

Mass content m^{c} and mass flow m^{f} are global source quantities and, as such, refer to the cells of the dual cell complex both in time and space. Mass content is referred to a volume $\tilde{\mathbf{v}}_h$ and a time instant $\tilde{\mathbf{t}}_n$ while mass flow is referred to a surface $\tilde{\mathbf{s}}_\alpha$ and a time interval $\tilde{\boldsymbol{\tau}}_n$. We can write

$$m^{\mathrm{c}}[\tilde{\mathbf{t}}_n, \tilde{\mathbf{v}}_h] \qquad m^{\mathrm{f}}[\tilde{\boldsymbol{\tau}}_n, \tilde{\mathbf{s}}_\alpha]. \tag{31}$$

With reference to Eq.(20) and to Table (3.8) we can write mass balance in discrete form

$$m^{\mathrm{c}}[\tilde{\mathbf{t}}_{n+1}, \tilde{\mathbf{v}}_h] - m^{\mathrm{c}}[\tilde{\mathbf{t}}_n, \tilde{\mathbf{v}}_h] + m^{\mathrm{f}}[\tilde{\boldsymbol{\tau}}_n, \partial\tilde{\mathbf{v}}_h] = 0. \tag{32}$$

Moreover, mass *going out* from the boundary of the dual 3-cell $\tilde{\mathbf{v}}_h$ is the sum of the masses outflowing across the faces and then

$$m^{\mathrm{f}}[\tilde{\boldsymbol{\tau}}_n, \partial\tilde{\mathbf{v}}_h] = \tilde{\tau}_n \sum_{c \in \mathcal{J}(h)} Q^{\mathrm{c}}_h(t_n) \tag{33}$$

where $\mathcal{J}(h)$ is the set of primal 3-cells that have the 0-cell h in common.

Among the dual cells there are those that are broken by the boundary of the region Ω. For boundary (broken) dual cells mass flow given by Eq.(33) can be

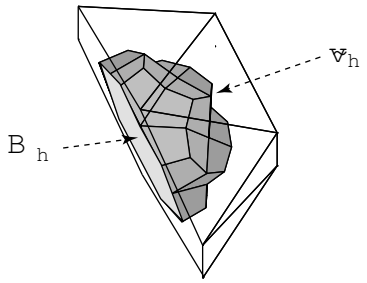

Figure 10: Boundary polyhedra.

written

$$m^{\mathrm{f}}[\tilde{\boldsymbol{\tau}}_n, \partial\tilde{\mathbf{v}}_h] = \sum_{c \in \mathcal{J}(h)} Q^{\mathrm{c}}_h(t_n) - B_h(t_n) \tag{34}$$

where B_h denotes the mass current *entering* the broken dual polyhedron $\tilde{\mathbf{v}}_h$ from the boundary of the region.

We want to express Q^{c}_h in terms of the kinetic potentials at the vertices of the cell $\mathbf{v}_c$. By inserting Eq.(25) and Eq.(14) in Eq.(24) and putting

$$f^{\mathrm{c}}_{hk} \stackrel{\mathrm{def}}{=} -\rho_0 \frac{1}{v_c} \frac{\mathbf{A}^{\mathrm{c}}_h}{3} \cdot \frac{\mathbf{A}^{\mathrm{c}}_k}{3} = f^{\mathrm{c}}_{kh} \tag{35}$$

we obtain

$$Q_h^{\mathrm{c}}(t_n) = \sum_{k \in \mathcal{V}(c)} f_{hk}^{\mathrm{c}}\, \varphi_k(t_n). \tag{36}$$

Remembering Eq.(30), the relation between χ_h and φ_h given by Eq.(19) we obtain

$$m^{\mathrm{c}}[\tilde{\mathbf{t}}_{n+1}, \tilde{\mathbf{v}}_h] - m^{\mathrm{c}}[\tilde{\mathbf{t}}_n, \tilde{\mathbf{v}}_h] = -\frac{\tilde{v}_h}{\tau_n}\, \frac{\rho_h^0}{c_h^2}\, \left[\varphi_h(t_{n+1}) - 2\,\varphi_h(t_n) + \varphi(t_{n-1})\right]. \tag{37}$$

With these results mass balance (32) becomes

$$-\frac{\tilde{v}_h}{\tau_n\, \tilde{\tau}_n}\, \frac{\rho_h^0}{c_h^2}\, \Big[\varphi_h(t_{n+1}) - 2\,\varphi_h(t_n) + \varphi_h(t_{n-1})\Big] + \sum_{c \in \mathcal{J}(h)}\, \sum_{k \in \mathcal{V}(c)} f_{hk}^{\mathrm{c}}\, \varphi_k(t_n) = B_h(t_n). \tag{38}$$

This is the discrete form of d'Alembert equation that can be directly used for computational acoustics. We remark that the same equation is valid for inner and boundary (broken) cells: for inner cells one put $B_h = 0$.

Table 3: Space and time association of acoustical variables: densities and rates in italics.

kinetic potential	$\varphi_h(t_n) = \varphi[\mathbf{t}_n, \mathbf{p}_h]$
velocity circulation	$\mathit{\Gamma}[\mathbf{t}_n, \mathbf{l}_\alpha]$
vortex strength	$W[\mathbf{t}_n, \mathbf{s}_\beta]$
(no known name)	$X[\boldsymbol{\tau}_n, \mathbf{p}_h]$
velocity	$\mathbf{u}_c(t_n) = \mathbf{u}[\mathbf{t}_n, \mathbf{v}_c]$
(no known name)	$\chi_h(\tilde{t}_n) = \chi[\tilde{\mathbf{t}}_n, \mathbf{p}_h]$
mass content	$m^{\mathrm{c}}[\tilde{\mathbf{t}}_n, \tilde{\mathbf{v}}_h]$
mass density	$\rho_h(\tilde{t}_n) = \rho[\tilde{\mathbf{t}}_n, \tilde{\mathbf{v}}_h]$
mass flow	$m^{\mathrm{f}}[\tilde{\boldsymbol{\tau}}_n, \tilde{\mathbf{s}}_\alpha]$
mass current	$Q_\alpha(t_n) = Q[\tilde{\boldsymbol{\tau}}_n, \tilde{\mathbf{s}}_\alpha]$
mass current density	$\mathbf{q}_c(t_n) = \mathbf{q}[\tilde{\boldsymbol{\tau}}_n, \mathbf{v}_c]$
momentum content	$\mathbf{P}^{\mathrm{c}}[\tilde{\mathbf{t}}_n, \tilde{\mathbf{v}}_h]$
momentum flow	$\mathbf{P}^{\mathrm{f}}[\tilde{\boldsymbol{\tau}}_n, \tilde{\mathbf{s}}_\alpha]$
surface impulse	$\mathbf{I}^{\mathrm{s}}[\tilde{\boldsymbol{\tau}}_n, \tilde{\mathbf{s}}_\alpha]$
pressure (stress tensor)	$p_c(t_n) = p[\tilde{\boldsymbol{\tau}}_n, \mathbf{v}_c]$
volume impulse	$\mathbf{I}^{\mathrm{v}}[\tilde{\boldsymbol{\tau}}_n, \tilde{\mathbf{v}}_h]$
body force density	$\mathbf{f}[\tilde{\boldsymbol{\tau}}_n, \tilde{\mathbf{v}}_h]$

3.9 Momentum Balance

Momentum content $\mathbf{P}^{\,\mathrm{c}}$ and momentum flow $\mathbf{P}^{\,\mathrm{f}}$ are global source quantities and, as such, refer to the cells of the dual cell complex both in time and space. Momentum content is referred to a dual cell $\tilde{\mathbf{v}}_h$ and to a dual time instant $\tilde{\mathbf{t}}_n$. With reference to Eq.(20) and Table (3.8) one can write momentum balance in discrete form

$$\mathbf{P}^{\,\mathrm{c}}[\tilde{\mathbf{t}}_{n+1}, \tilde{\mathbf{v}}_h] - \mathbf{P}^{\,\mathrm{c}}[\tilde{\mathbf{t}}_n, \tilde{\mathbf{v}}_h] + \mathbf{P}^{\,\mathrm{f}}[\tilde{\boldsymbol{\tau}}_n, \partial\tilde{\mathbf{v}}_h] = \mathbf{I}^{\,\mathrm{s}}[\tilde{\boldsymbol{\tau}}_n, \partial\tilde{\mathbf{v}}_h] + \mathbf{I}^{\,\mathrm{v}}[\tilde{\boldsymbol{\tau}}_n, \tilde{\mathbf{v}}_h]. \tag{39}$$

In an inviscid fluid the surface forces reduce to the pressure force. Pressure is then the surface density of the surface impulse rate.

With reference to Fig.(9) the sum of the normal forces $\mathbf{N}$ acting on the three surfaces S_1, S_2, S_3 is

$$\mathbf{N}_h^c = -p_c[\mathbf{A}_1 + \mathbf{A}_2 + \mathbf{A}_3] = -p_c\,\frac{\mathbf{A}_h^c}{3}. \tag{40}$$

Then the surface impulse across the boundary of the dual 3-cell is given by

$$\mathbf{I}^{\,\mathrm{s}}[\tilde{\boldsymbol{\tau}}_n, \partial\tilde{\mathbf{v}}_h] = -\tilde{\tau}_n \frac{1}{3} \sum_{c\in\mathcal{J}(h)} p_c(t_n)\,\mathbf{A}_h^c. \tag{41}$$

Since inside every primal 3-cell density and velocity are uniform, momentum flow can be written

$$\mathbf{P}^{\,\mathrm{f}}[\tilde{\boldsymbol{\tau}}_n, \partial\tilde{\mathbf{v}}_h] \approx \tilde{\tau}_n \frac{1}{3} \sum_{c\in\mathcal{J}(h)} \rho_c^0\ (\mathbf{u}_c(t_n)\cdot\ \mathbf{A}_h^c)\ \mathbf{u}_c(t_n). \tag{42}$$

Inserting these expressions in Eq.(39), after division for $\tilde{v}_h\,\tilde{\tau}_n$, and remembering that the discrete gradient of a function $p(t,\mathbf{x})$ can be defined by the expression (15), the momentum balance on the dual cell becomes

$$\mathbf{P}_h^c(\tilde{t}_{n+1}) - \mathbf{P}_h^c(\tilde{t}_n) + \tilde{\tau}_n \frac{1}{3} \sum_{c\in\mathcal{J}(h)} \rho_c^0\,(\mathbf{u}_c(t_n)\cdot\mathbf{A}_h^c)\mathbf{u}_c(t_n) \approx -\tilde{\tau}_n \frac{1}{3} \sum_{c\in\mathcal{J}(h)} p_c(t_n)\,\mathbf{A}_h^c + \tilde{\tau}_n\,\tilde{v}_h \mathbf{f}_h(t_n). \tag{43}$$

Eq.(43) contains the discrete gradient of the pressure with the minus sign, as in the differential case. Neglecting the momentum flow on account of the hypothesis of small velocities, the last equation becomes

$$\frac{\mathbf{u}_h(\tilde{t}_{n+1}) - \mathbf{u}_h(\tilde{t}_n)}{\tilde{\tau}_n} \approx -\frac{\mathrm{Grad}\, p_h^*(t_n)}{\rho_h^0} + \frac{\mathbf{f}_h - \mathrm{Grad}\, p_h^0}{\rho_h^0}. \tag{44}$$

The last terms vanishes because the pressure p_h^0 is in equilibrium with the body force $\mathbf{f}_h$. Remembering Eq.(17) we can write

$$\rho_h^0\,\mathrm{Grad}\,\chi_h(t_n) \approx -\mathrm{Grad}\, p_h^*(t_n). \tag{45}$$

These approximations enable us to obtain the generalized Bernoulli equation in the form

$$\chi_h(t_n) + \frac{p_h^*(t_n)}{\rho_h^0} = C(t_n) \tag{46}$$

where $C(t_n)$ is an arbitrary function of time. Since the kinetic potential is defined modulo an additive function of time we can put $C(t_n) = 0$ (see[12, p.84][11, p.31]). Then we can write the generalized Bernoulli equation as

$$\chi_h(t_n) + \frac{p_h(t_n) - p_h^0}{\rho_h^0} = 0. \tag{47}$$

Since both χ and p must be evaluated at the same instant, we can apply the preceeding relation to the dual instant $\tilde{t}_n$ that is proper for χ. Remembering constitutive equation (29) we can write

$$\rho_h(\tilde{t}_n) \approx \rho_h^0 \left[1 - \frac{1}{c_h^2}\,\chi_h(\tilde{t}_n)\right]. \tag{48}$$

This is the constitutive equation we have assumed, see Eq.(30).

The cell method. A numerical method that uses global variables as a starting point, referring configuration variables to corresponding cells of a primal complex and source variables to corresponding cells of the dual, avoiding both the differential formulation and the integral formulation will be called the *cell method*.

4 Comparison with Finite Element Method

We now prove that the matrix that we obtained *coincides* with that of FEM when the cells are simplexes and linear shape functions are used. In FEM the weak formulation of the differential equation leads to

$$f_{hk}^c = -\rho_0 \int_{v_c} \nabla N_h(\mathbf{x}) \cdot \nabla N_k(\mathbf{x})\, \mathrm{d}V. \tag{49}$$

Using linear shape functions we have

$$f_{hk}^c = -\rho_0\, v_c\, \nabla N_h(\mathbf{x}) \cdot \nabla N_k(\mathbf{x}). \tag{50}$$

With reference to Fig.(11) we have[13, p.43;p.50].

$$\nabla N_h^{\mathbf{c}}(\mathbf{x}) = -\frac{\mathbf{n}_h^{\mathbf{c}}}{d_h} = -\frac{A_h \mathbf{n}_h^{\mathbf{c}}}{A_h\, d_h} = \frac{\mathbf{A}_h^{\mathbf{c}}}{3\, v_c} \tag{51}$$

We then have

$$f_{hk}^{\mathbf{c}} = -\rho_0\, v_c\, \nabla N_h^{\mathbf{c}} \cdot \nabla N_k^{\mathbf{c}} = -\rho_0\, \frac{1}{v_c}\, \frac{\mathbf{A}_h^{\mathbf{c}}}{3} \cdot \frac{\mathbf{A}_k^{\mathbf{c}}}{3} \tag{52}$$

that coincides with the one given in our approach, see Eq.(35). We remark that FEM distributes the currents to the nodes while in the cell method they are associated with the faces of the dual cells and are not transferred to the nodes.

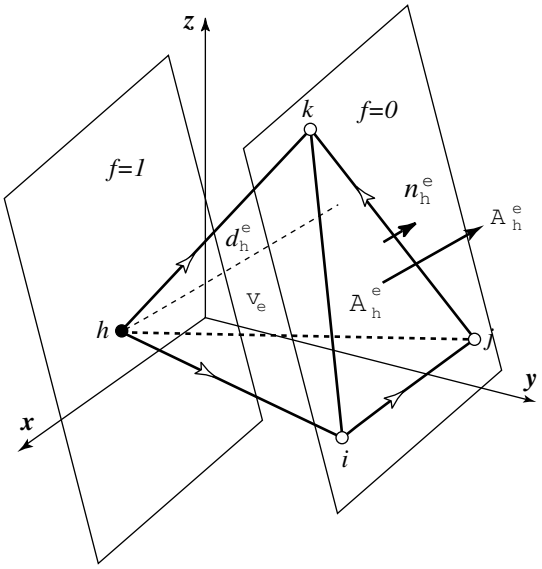

Figure 11: Since a linear shape function $N_h^c(x)$ assumes the value 1 in the vertex h and 0 on the remaining vertices, its gradient is uniform inside the tetrahedron; it is directed from the opposite edge (or face) towards the vertex h and its modulus is $1/d_h$.

5 Comparison with the Finite Volume Method

The Cell Method (CM) is very similar to the Finite Volume Method (FVM). The main differences are listed below.

- FVM uses the integral form of the conservation equations as the starting point [6, p.67]. Though in principle it does not require the availability of the differential formulation, in practice one uses *field variables*, that are the natural ingredients of differential formulation, and evaluate global variables by integration. "*To obtain the algebraic equation for each control volume, the surface and volume integrals need to be approximated using quadrature formulae.*" [6, p.68]

  CM, on the contrary, directly uses *global variables* and take experimental laws (balance laws, circuital laws, constitutive laws, etc) in their discrete

form.

- in FVM the control volumes are chosen according to three schemes: the *node centered* or *vertex-based*, the *cell centered* and the *cell vertex* schemes. "*For cell-centered schemes, the control volumes are taken as the triangles themselves, whereas for a vertex-based scheme the control volumes are taken as the cells defined by the dual mesh.*" [15, p.22]

  CM starts with a *pair* of dual complexes. Physical variables have a well defined reference to the spatial elements of a cell complex and its dual. The conservation law is enforced on the dual polygon of every primal vertex: in this respect (and only in this respect) it corresponds to the vertex=based (or node-centered) scheme of FVM.

- FVM usually do not use interpolating functions inside every primal cell.

  CM, on the contrary, permits us to use *interpolating functions* on the primal cells in order to obtain higher order of convergence, as in FEM. Thus a fourth order convergence on a structured mesh made of triangles has been obtained considering the parabolic interpolating functions inside the triangles: see [28].

5.1 Conclusions

It is customary to obtain a discrete (or finite) formulation of the equations of acoustics and other physical fields passing through differential formulation. The paper has shown that it is possible to obtain a discrete formulation starting directly from experimental laws. This is accomplished using global variables and realizing their natural association with spatial and temporal elements. In such an association an important role is played by the notions of inner and outer orientations of a spatial and temporal element. This leads us to use a cell complex and its dual instead of a coordinate system. Once the variable of acoustics are classified in one of the three classes, configuration, source and energy variables, it is seen that configuration variables are naturally referred to the cells of a primal complex while source variables are referred to those of the dual complex.

Constitutive equations, that link configuration with source variables, require the introduction of mean densities and mean rates. The approximation of considering the field inside every cell of the primal complex as uniform permits us to avoid the limit process.

The procedure presented is not peculiar to acoustics in fluids but can be applied to every field. It has been applied to elasticity [4]; mechanics of fracture [7], [8], [9], [16]; mechanics of masonry [17], [18]; mechanics of sintered alloys [3]; elasto-plasticity [19]; electromagnetism [27],[14].

The scheme here presented gives a second order accuracy on a structured mesh. It has been proved that using parabolic interpolation functions inside every triangle one can obtain a fourth order accuracy on structured meshes [28], [31].

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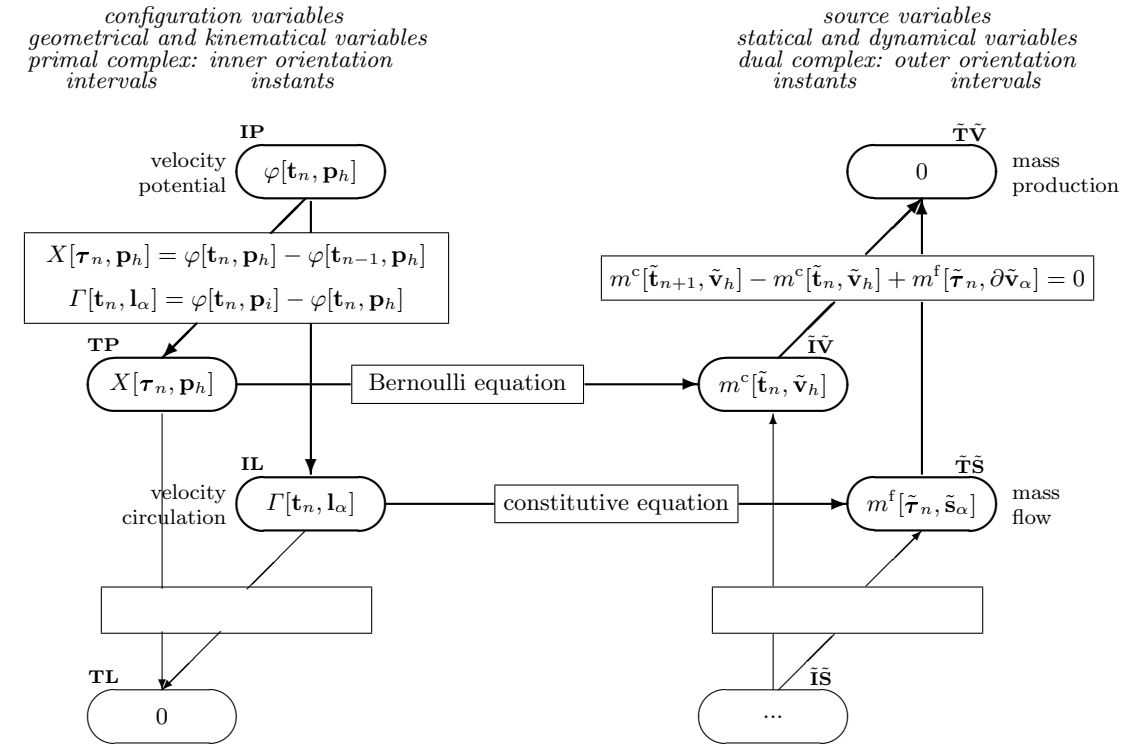
Table 4: *above:* The discrete structure of acoustics in fluids; *below:* The differential structure of acoustics in fluids.



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