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A Direct Discrete Formulation of Field Laws: The Cell Method

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ABSTRACT. *We present a new numerical method for the solution of field equations. The essence of the method is to directly provide a discrete formulation of field laws, without using and requiring a differential formulation. It is proved that, for linear interpolation, the stiffness matrix so obtained coincides with the one of the Finite Element Method. For quadratic interpolation, however, the present stiffness matrix differs from that of FEM; moreover it is unsymmetric. It is shown that by using a parabolic interpolation, a convergence of the fourth order is obtained. This is greater than the one obtained with FEM, using the same interpolation.*

1 Introduction

All existing numerical methods for the solution of field equations have, in one way or another, a differential formulation as their starting point. A discrete formulation is then obtained by means of one of the many discretization methods, such as Finite Difference Method (FDM), Finite Element Method (FEM), or, in general, a weighted residual or weak solution method. Even the Boundary Element Method (BEM) and the Finite Volume Method (FVM), which use an integral formulation, have a differential formulation as their starting point. A differential formulation is easily obtained by considering a finite spatial region, say a control volume or a control surface, and by performing the limit process in order to arrive at densities that are point functions. In this way one obtains the *divergences*, the *curls* and the *gradients* that are typical ingredients of differential formulation. Then one eliminates the geometrical content of physical laws, say balance laws, circuital laws to arrive at pointwise functions. To find a numerical solution, a discrete formulation is required; and then the geometrical content must be, in one way or another, reconstructed: this requires a *discretization* of the differential equations. Many discretization methods have beeen devised, and each of them leads to different sets of algebraic equations for the same mesh (some are symmetric system of equations; while others are not). Faced with this two-way process, a question arises: *Is it really necessary to go from algebraic to differential formulation in order to go back to some other form of finite modelling?* The purpose of this paper is to show that a *direct* discrete formulation of field laws is possible, i.e. it is possible to avoid introducing a differential formulation. Moreover, we shall show that such a discrete formulation is very simple, that it is strictly related to experimental facts, and can be directly used for the numerical solution of field problems.

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2 Physical quantities and equations

The mathematical formulation of physical laws springs from the very existence of physical quantities. Then, if we search for a *direct* finite formulation of physical laws, we must review physical quantities. Three classifications are of use.

Constants and variables. The first classification of physical quantities is into *physical constants* and *physical variables*. *Physical constants* are all quantities that describe the nature of a system or of a material: these are the ones tabulated in books and manuals. They include universal constants, material constants, system parameters, coupling constants, etc. *Physical variables* specify a particular state of a system, the actual configuration of a system, the forces acting on a system, the sources of a field, the many kinds of energy of a system, say its internal energy, its potential or kinetic energy, its enthalpy, etc.

Global and local variables. A second classification of physical variables distinguishes between global and local variables. By *global* variables we mean those that are commonly called *integral variables* such as mass, momentum, energy current, magnetic flux, voltage impulse, etc. On the other hand *local* variables are functions of spatial coordinates and time usually involved in the differential formulations. Among the local variables are: the velocity, stress, temperature, heat current density, electric current density, magnetic induction vector, etc. The above described global variables are naturally associated with spatial and temporal elements such as points (**P**), lines (**L**), surfaces (**S**), volumes (**V**), time instants (**I**) and time intervals (**T**). So a flux is associated with a surface; a voltage with a line; a content, say mass content, with a volume; an impulse with a time interval. This is the same reason why we deals with line, surface, volume densities and rates. Thus global variables are referred not only to points, such as field functions, but often also to lines, surfaces and volumes, i.e. they are *domain* functions instead of point functions. Some variables are associated with points in space and time: they are different from other point functions, because they are not densities or rates. Such variables are displacements in solid

mechanics, kinetic potential in flow mechanics, *gauge* function of electromagnetism, iconal function in optics, ecc. It is worth noting that when carrying out experiments we measure mainly global variables.

Configuration and source variables. A third classification is based on the role of physical variables. Every physical field has its *sources*: they may be electric charges for electrostatics; electric currents for magnetostatics; heat sources for thermal conduction; forces for the solid mechanics and for fluidynamics; masses for the gravitational field (geodesy); etc. On the other hand any physical field has a state variable: so *displacement* describes the geometrical configuration of a deformable solid; the spatial *velocity* field describes the flow of a fluid; *electric potential* describes the configuration of an electric field; *temperature* describes the thermal configuration of a body; etc. Physical variables can be divided in three classes: *configuration variables, source variables, energy variables*. This classification is based on the role that a physical variable plays in a theory (34) [p.155]; (18) [p.1]; [(39)]; [(40)].

$$\textit{physical quantities} \begin{cases} \textit{physical constants} \\ \textit{physical variables} \begin{cases} \textit{configuration variables} \\ \textit{source variables} \\ \textit{energy variables}. \end{cases} \end{cases} \tag{1}$$

We have

- **Configuration variables:** variables that give the configuration of a physical system, and all variables linked to them, by the operations such as sum, integration, difference, division by a length, an area, a volume, an interval, by a limiting process, and then by time and space derivatives. These relations must not contain physical constants. To this class belong the geometrical and kinematical variables of continuous mechanics, generalized coordinates, field potentials, affinities, etc.

- **Source variables:** variables that describe the sources of a field, such as masses, charges and currents; the forces acting on a system, etc, and all variables linked to them, by the operations such as sum, integration, difference, product and division by a length, an area, a volume, an interval, by time and space derivatives. These relations must not contain physical constants. To this class belong the kinetic variable, such as forces, moment of force, momentum, angular momentum, etc, of continuum mechanics.

- **Energy variables:** variables obtained by the product of a configuration variable by a source variable. To this class belong the various forms of energy: kinetic, potential, internal free energy, hentalpy; field energy, work, power, lagrangian, hamiltonian, action, etc.

These criteria give a *functional classification* of physical variables. This is somewhat similar to the classification we make when we divide people in functional classes: workers, office-workers, managers, etc. We list here the main variables of each of the three classes used in physics.

- **Configuration:** displacement, displacement gradient, position vector, relative displacement, strain, strain rate, temperature, temperature gradient, velocity, velocity circulation, velocity potential, vortex strength, vorticity vector, electric field, electric potential, electric tension, electric tension impulse, magnetic flux, magnetic flux density,etc.

- **Source:** force, impulse, mass content, density, mass current, mass current density, mass flow, momentum content, momentum current, stress tensor, pressure, surface force, electric charge content, electric charge flow, electric current, electric flux, heat flux, heat source, magnetic tension, magnetic scalar potential, magnetic field strength, etc.

- **Energy:** work, power, energy, energy current density, energy density, Gibbs free energy, hamiltonian, heat, Hemholtz free energy, enthalpy, kinetic energy, internal energy, lagrangian, magnetic energy, potential energy, etc.

2.1 The two kinds of orientation

Spatial and temporal elements can be endowed with orientation. When we say that a flux is referred to a surface, we are obliged to specify the orientation of the surface, because, the sign of the global variable reverses when the orientation is reversed. There are two kinds of orientations: inner and outer.

- **Inner orientation:** whenever the orientation of a space element lies on the element itself, one says that an inner orientation is established, as shown in Fig. (1*a*). Note that an inner orientation of a point means that the point is conceived as a source or as a sink.

- **Outer orientation:** whenever the orientation of a space element depends on the space in which the element is embedded, an outer orientation is defined, as shown in Fig. (1*b*). Contrary to inner orientation, which is intrinsic, outer orientation depends on the dimension of the space in which the element 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 the typical orientation used in solid mechanics to denote compression or traction of a bar, as in Fig.(2)

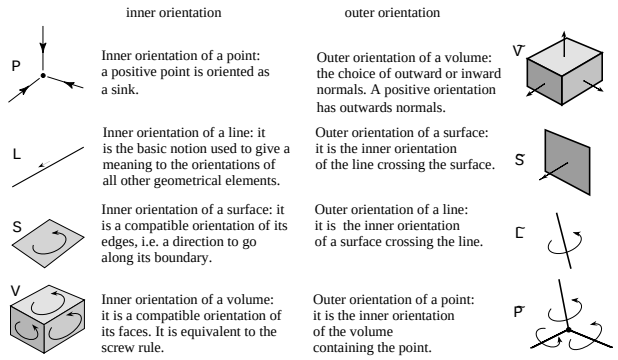

Figure 1 : The two notions of inner and outer orientations in the three-dimensional space.

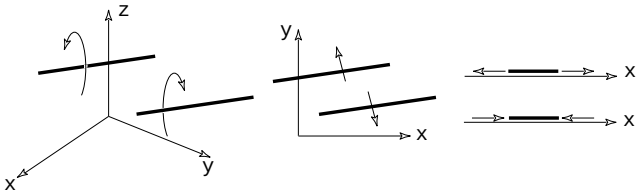

Figure 2 : The outer orientation of a line depends on the dimensions of the embedding space.

2.2 Cell complexes

On dealing with differential formulations, it is quite natural to use coordinate systems. On the contrary, a direct discrete formulation deals with global variables, that are naturally associated with finite sizes of spaces, and finite intervals of time, i.e. volumes, surfaces, lines, time intervals as well as points and instants. We shall denote them as spatial and temporal *elements*. 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. Accordingly 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, which we shall call *primal*, by considering a point inside each 3-cell, say its barycenter, one can construct another cell complex, called *dual*, by taking these points as vertices of dual complex. If the primal complex is formed of squares (in 2D), or of cubes (in 3D), the dual complex is also 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, by considering the circumcenters of the triangles as vertices of the dual complex, and by connecting the circumcenters of two adjacent triangles, one obtains a dual complex. To every 1-cell of the primal complex, there corresponds a 1-cell of the dual; and the two are orthogonal. The same is true of a three-dimensional complex made of tetrahedra as shown in Fig.(3*b*). 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 1-cell of the dual. Moreover to every 0-cell of the primal there corresponds a 3-cell of the dual. In short: if n denotes the dimension of the space, $(n = 1,2,3)$, with each p-cell of the primal there corresponds an $(n-p)$-cell of the dual, and viceversa. The choice of a point inside each n-cell, to be considered as 0-cell of the dual, is arbitrary and can be dictated by computational convenience. How to connect the centers of two adjacent cells is also arbitrary. Thus when one considers the barycenters of the n-cells, one can connect the adjacent ones by a straight line, or via the barycenter of the face, as shown in Fig.(3*c*). The latter choice is the one considered in algebraic topology, and is called the *barycentric subdivision*. It has some computational advantages. Doing so, the dual of the 1-cell (hi) is the broken line shown as heavy line in Fig.(3*c*). With reference to Fig.(4), one can see that to every 0-cell of

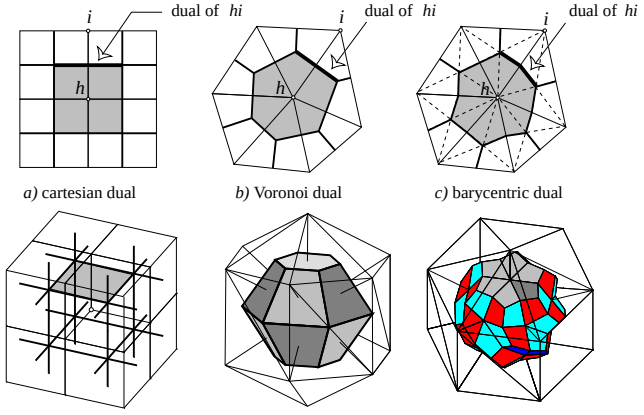

Figure 3 : Primal and dual cell complexes.

the primal complex there 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 those 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 bound-

aries, 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 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 them are involved in the description. Given a cell complex, we can assign to all its elements an *inner* orientation. This complex will be designed as *primal*. If we now consider a dual complex, say considering the barycenters 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 (47) [p.55] and introduced in physics by Schouten (36) and Van Dantzig (46).

2.3 Global variables and cell complexes

Let us examine the link between global variables and space elements of a cell complex.

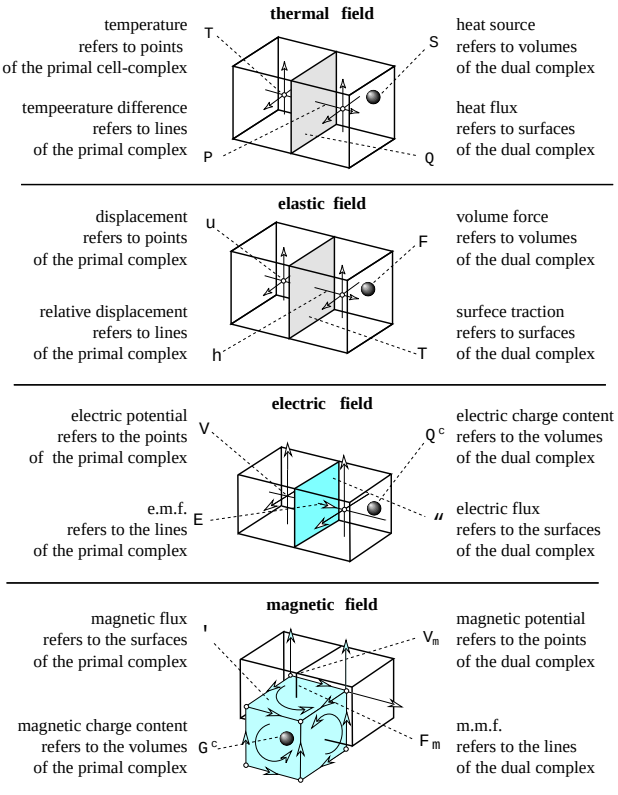

Figure 4 : Physical variables and cell complexes

Thermal field. We shall refer to Fig.(4). Internal energy and heat source are global variables which are associated with the 3-cells of the dual complex; heat fluxes are associated with the 2-cells of the same complex. The temperature of each 3-cell is the one measured in some "central" point of the cell, say its barycenter, i.e. a 0-cell of the primal complex. The temperature difference refers to the line connecting two barycenters, i.e. to a 1-cell of primal complex. Doing so, we see that the configuration variables, i.e. temperature and temperature difference, refer to the elements of the primal complex, while the source variables, i.e. internal energy, heat generation and heat flux, refer to the elements of the dual complex.

Elastic field. A similar analysis can be made for elasticity. Let us consider a cell complex: with each 3-cell there is associated a volume force, and with any face (2-cell) there is associated a surface traction. We can consider the barycenter (0-cell) of any 3-cell: the displacements naturally refer to such 0-cells. The relative displacement is a global variable referred to the line (1-cell) connecting two adjacent barycenters. We see that the source variables refer to the element of a cell complex endowed with an outer orientation (we shall call it dual), while the configuration variables refer to the elements endowed with an inner orientation (we shall call it *primal*).

Electric field. Let us consider a cell complex: with every 3-cell there is associated a charge content, while every 2-cell is associated with the electric flux. The electric potential refers to the barycenter (0-cell) of every 3-cell. The voltage refers to the 1-cell connecting the barycenters. Then source variables, i.e. charge content and electric flux, refer to the elements of a cell complex endowed with an outer orientation (the *dual*), while configuration variables, i.e. electric potential and voltage, refer to the elements endowed with an inner orientation (the *primal*).

Magnetic field. If one considers a cell complex in a spatial region, where a magnetic field is defined, it is easily seen that the magnetic flux Φ is associated with the 2-cells. In order to give a sign to the magnetic flux we need an inner orientation to the 2-cell, i.e. the direction of the current induced in a coil located on the boundary of the 2-cell when the magnetic field is switched off. This shows that the magnetic flux, which is a configuration variable, refers to the 2-cells of the primal complex. The magnetic potential V_{m} is associated with a central point (0-cell) of the 3-cell and then the magnetic tension U_{m} is associated with the 1-cell connecting the centres of two adjacent 3-cells. These four examples show the following important property

> REMARK. *In field theories, the configuration variables are associated with cells endowed with an inner orientation, while the source variables are associated with cells endowed with an outer orientation.*

Even if the reason for this systematic association is not clear, it is remarkable that a *physical* classification of physical variables matches with a *geometrical* classification, based on the

association with oriented space elements. This strong coupling between physical variables and oriented space elements is the key to give a direct discrete formulation to physical laws of fields. The association of physical variables to the elements of a cell complex and its dual has been introduced by Okada (31) and Branin (2).

2.4 The fundamental problem of a physical field

The *fundamental problem* of a physical field can be stated as follows:

- *given the shape and the dimensions of the field domain;*
- *given the spatial and temporal distributions of the field sources;*
- *given the nature of the materials that fill the field domain;*
- *given the boundary conditions that summarize the action of the external sources on the field domain;*

to find the spatial and temporal configuration of the field. The fundamental problem is expressed by the *fundamental equation* i.e. a relation between the source and the potential of the field. Thus the equations of Poisson, Fourier, Navier, Navier-Stokes, are examples of fundamental equations. In any physical field the fundamental equation is the result of the composition of two kinds of "basic" equations: *field equations* and *constitutive equations*. *Field equations* relate configuration variables to each other, and source variables to each other. In differential formulation these equations are described by the operators *grad*, *curl* and *div*. *Constitutive equations*, also called *material equations*, are those that link source variables with configuration variables.

3 A direct discrete formulation

The previous considerations lead us to present a *direct* discrete formulation of field equations. This formulation is based on the use of *global variables* and of a pair of *cell complexes*, a primal and a dual one: it will be called the *Cell Method*. We shall present the method, by considering a static two-dimensional scalar field, such as electrostatics, magnetostatics or a steady two-dimensional scalar field, such as thermal conduction, electrical conduction, irrotational fluid flow, diffusion, percolation, etc. In a differential formulation, all these fields are governed by the Poisson equation. In all these fields, there is a main configuration variable, which is the *potential* of the field; and a main source variable, which is the *source* of the field. To solve the fundamental equation of the field, means finding the potential function once the sources are assigned. While a differential formulation "promises" the knowledge of the potential at *any* point of the domain, a discrete formulation gives the potentials *only* at the 0-cells of a cell complex. The values of the potentials inside any 3-cell can be interpolated using a function, in particular a polynomial. The Poisson equation requires that the domain contains an homogeneous and isotropic material and requires that the potential admits second order partial derivatives. Alternatively if the domain is composed of different materials, it must be subdivided into subdomains, each one containing a homogeneous and isotropic material: the Poisson equation must then be applied to every subdomain and on the separation surfaces *jump conditions* must be satisfied.

All these restrictions are in striking contrast with modern devices formed by different materials; where anisotropy is frequently encountered as in laminated and fiber materials; where concentrated sources, such as laser spots, are present; where physics assures only that the potential is continuous not double differentiable.

The discrete formulation that we shall present, can be applied to fields containing different materials while avoiding jump conditions. The potential is assumed to be continuous and need not be differentiable. The material can be isotropic or anisotropic, homogeneous or non-homogeneous. Each cell can have different constitutive properties: this permits to deals with composite and fiber materials, porous media, damaged materials, inclusions and defects. The sources can be discontinuous and also may be concentrated. The expression "concentrated source" can be understood in two ways: as a source acting on a region that is small but with finite size or as a pointwise source. Since no physical source is really pointwise (laser spots, "pointwise" electric charges and "concentrated" loads are really distribute on small regions), a truly discrete formulation of physical fields must consider only sources distribute on large or small regions *but always of finite size.* The pointwise source is an abstraction that is consequence of the limiting process and, as such, belongs to differential formulations. It follows that in a truly discrete formulation, *infinities do not appear* and then a discrete treatment avoids singularities, in accordance with physics to which infinities are extraneous.

We shall make reference to the field of steady thermal conduction in two dimensions because it can be easily grasped. The discrete formulation requires an interpolation function among the nodal values of the temperature. We shall consider a linear and a quadratic interpolation respectively.[2]

4 Linear interpolation

When we deal with a two-dimensional region, we must not forget that we have to do with a layer of uniform thickness, which we shall denote as t, as shown in Fig. (5d). In this way, any triangle will be considered as the base of a triangular prism whose lateral faces are projected in the sides of the triangle. Our purpose is to write down the fundamental equation for a two dimensional scalar fields. Our goal is to find

[2] We remark that a discrete formulation implies spatial elements of finite size, i.e. avoids the passage to infinitesimal regions. This does not exclude the use of derivatives to perform mathematical operations. It is not our intention to reject the use of infinitesimal calculus in physics (!) but only to avoid that the limit process is applied to volume elements.

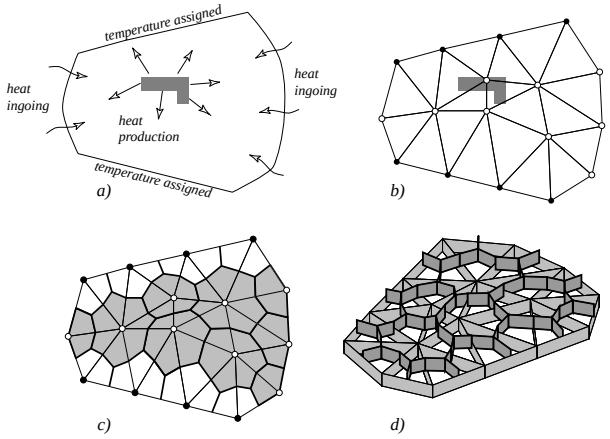

Figure 5 : A primal and dual cell complex for a plane field.

the temperature of all 0-cells, briefly called *nodes*, of the primal complex. As always the boundary conditions are of two kinds: on some parts of the boundary, the temperature can be assigned; while on the remaining parts, the heat flux can be assigned. Our goal then reduces itself to finding the temperature at all the nodes at which it is not assigned: these can be internal as well as boundary nodes. In Fig.(5) the boundary nodes with assigned temperature are noted with filled circles. Since we consider a steady conduction, there is no heat stored inside any 3-cell; and hence the heat produced in any region is equal to the heat outgoing from its boundary. If we impose the heat balance on any dual 3-cell, the tributary region of every node, we obtain as many equations as are the unknown temperatures, see Fig.(5*c*). Let us denote by S_h the heat source rate inside the dual 3-cell h, and by Q_h the rate of heat outgoing from the cell boundary. For boundary nodes, the ones that lie on the part of the boundary in which the incoming heat flux is given, we can add to the heat source rate the heat flux Φ_h entering the dual 3-cell. The energy balance becomes

$$\sum_{c \in \mathcal{J}(h)} Q_h^c = S_h + \Phi_h \tag{2}$$

where $\mathcal{J}(h)$ is the set of primal 3-cells having the node h in common. Equation (2) is valid both for interior and boundary dual 3-cells: in this fashion, one avoids the unnatural separation of differential equations and boundary conditions, which is typical of a differential formulation. The term S_h includes possibly concentrated sources.

4.1 Gradient

In order to evaluate the gradient, we perform a linear interpolation of temperature inside the triangles and express it in terms of the nodal values. We shall describe later the quadratic interpolation in order to obtain approximations of higher order.

With reference to Fig.(6) the linear behaviour of temperature inside the cell c is given by the function

$$T(x,y) = a + g_x x + g_y y. \tag{3}$$

The additive constant a implies that $T(x,y)$ is an *affine* function, not a "linear" one. One can say that an affine function has a linear *behaviour*. The three constants a, g_x, g_y can be obtained by imposing that the function $T(x,y)$ assumes the three values T_h, T_i, T_j in the three nodes h, i, j of the cell c. Then

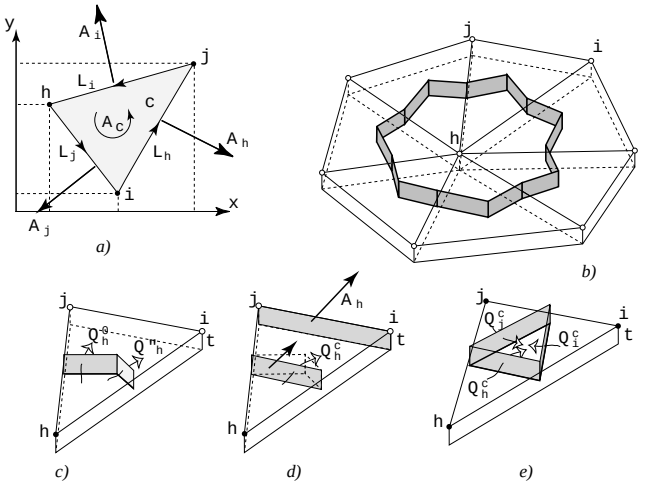

Figure 6 : *a)* The elements of triangle. *b)* The dual polygon conceived as a prism. *c)* the heat flux relative to the node h and *d)* its equivalent; *e)* the three heat fluxes associated with the three vertices.

$$\left\{ \begin{array}{lcl} a + g_x x_h + g_y y_h &=& T_h \\ a + g_x x_i + g_y y_i &=& T_i \\ a + g_x x_j + g_y y_j &=& T_j. \end{array} \right. \tag{4}$$

Subtracting the second equation from the third one, the first from the second one and stating

$$L_{hx} = x_j - x_i \qquad L_{hy} = y_j - y_i \qquad \text{etc.} \tag{5}$$

we obtain

$$\left[\begin{array}{cc} L_{jx} & L_{jy} \\ L_{hx} & L_{hy} \end{array} \right]_c \left\{ \begin{array}{c} g_x \\ g_y \end{array} \right\}_c = \left\{ \begin{array}{c} T_i - T_h \\ T_j - T_i \end{array} \right\}_c . \tag{6}$$

Using Cramer's rule, observing that the determinant of the system is the double of the area A_c of the triangle and since $\mathbf{L}_h + \mathbf{L}_i + \mathbf{L}_j = 0$, as shown in Fig(6*a*), we obtain

$$\left\{ \begin{array}{c} g_x \\ g_y \end{array} \right\}_c = \frac{1}{2A_c} \left[\begin{array}{ccc} -L_{hy} & -L_{iy} & -L_{jy} \\ +L_{hx} & +L_{ix} & +L_{jx} \end{array} \right]_c \left\{ \begin{array}{c} T_h \\ T_i \\ T_j \end{array} \right\}_c . \tag{7}$$

This relation coincides with that of the Finite Element Method, for a linear interpolation over a triangle.

Area. It is convenient to introduce the area-vectors $\mathbf{A}_h, \mathbf{A}_i, \mathbf{A}_j$ of the faces instead of the edge-vectors $\mathbf{L}_h, \mathbf{L}_i, \mathbf{L}_j$. Denoting by t the thickness of the layer, and by $\mathbf{k}$ the unit vector normal to the plane that contains the cell complex, we have:

$$\mathbf{A}_h = t\mathbf{L}_h \times \mathbf{k} \qquad \text{from which} \tag{8}$$

$$A_{hx} = t\,L_{hy} \qquad A_{hy} = -t\,L_{hx}. \tag{9}$$

The same relationship can be obtained for faces i, j. Inserting the last equations in (7) we obtain

$$\left\{ \begin{array}{c} g_x \\ g_y \end{array} \right\}_c = -\frac{1}{2tA_c} \left[\begin{array}{ccc} A_{hx} & A_{ix} & A_{jx} \\ A_{hy} & A_{iy} & A_{jy} \end{array} \right]_c \left\{ \begin{array}{c} T_h \\ T_i \\ T_j \end{array} \right\}_c \tag{10}$$

where $\mathbf{A}_h, \mathbf{A}_i, \mathbf{A}_j$ are the three area-vectors of the prism faces oriented outwards, as shown Fig.(6*c*). We remark that on the denominator we have the volume of the triangular prism as shown Fig(6*c*). Equation (10) can be summarized in a compact notation

$$\mathbf{g}_c = \mathbf{B}_c \mathbf{T}_c \tag{11}$$

where $\mathbf{B}_c$ is a 2×3 matrix. Since we have used a linear approximation, the gradient is uniform inside the triangle.

Heat flux. With reference to Fig.(6*c*), let us evaluate the heat flux that crosses the shaded faces of the dual 3-cell contained in the triangle c, assuming as positive the outward direction from the node h, as shown in Fig.(6*d*). Since the temperature gradient is uniform, and the material is homogeneous inside any cell, the thermal power across the two faces in Fig.(6*c*) is equal to the one crossing the face connecting the barycenters of two edges as in Fig.(6*d*). Since the last face is parallel to face h and has an area which is one half of A_h, the heat flux going through the face is

$$Q_h^c = \frac{1}{2}(A_{hx}q_x + A_{hy}q_y)_c = \frac{1}{2}(A_{hx} \quad A_{hy})_c \left\{ \begin{array}{c} q_x \\ q_y \end{array} \right\}_c. \tag{12}$$

We remark that the face connecting the barycenters of the edges is the same, if we use the barycentric or the Voronoi subdivision. The three heat fluxes Q_h^c, Q_i^c, Q_j^c shown in Fig.(6*e*) can be gathered in the relation

$$\left\{ \begin{array}{c} Q_h \\ Q_i \\ Q_j \end{array} \right\}_c = \frac{1}{2} \left[\begin{array}{cc} A_{hx} & A_{hy} \\ A_{ix} & A_{iy} \\ A_{jx} & A_{jy} \end{array} \right]_c \left\{ \begin{array}{c} q_x \\ q_y \end{array} \right\}_c. \tag{13}$$

4.2 Constitutive equation

For an anisotropic material, the heat flux density vector $\mathbf{q}_c$ is linked to the gradient $\mathbf{g}_c$ by the constitutive equation

$$\left\{ \begin{array}{c} q_x \\ q_y \end{array} \right\}_c = - \left[\begin{array}{cc} k_{xx} & k_{xy} \\ k_{yx} & k_{yy} \end{array} \right]_c \left\{ \begin{array}{c} g_x \\ g_y \end{array} \right\}_c \tag{14}$$

where $\mathbf{K}_c$ is the 2×2 matrix of thermal conductivity of cell c. We can write the constitutive equation in the form

$$\mathbf{q}_c = -\mathbf{K}_c \mathbf{g}_c. \tag{15}$$

For the common case of isotropic materials, equation (14) becomes the well known Fourier law:

$$q_x = -k\,g_x \qquad q_y = -k\,g_y. \tag{16}$$

or, in vector form

$$\mathbf{q} = -k\,\mathbf{g}. \tag{17}$$

4.3 Fundamental equation

We can now evaluate the heat flux outgoing from every face of the dual polygon and then write the balance on any dual 3-cell. There are two ways to do so: *a)* considering one node at time; *b)* considering one cell at time.

One node at time. Inserting Eq.(10) and (14) into Eq.(12) and introducing the 1×3 vector

$$(f_{hh} \quad f_{hi} \quad f_{hj})_c \stackrel{\text{def}}{=} -\frac{1}{2}(A_{hx} \quad A_{hy})_c \mathbf{K}_c \mathbf{B}_c \tag{18}$$

we can write

$$Q_h^c = (f_{hh} \quad f_{hi} \quad f_{hj})_c \left\{ \begin{array}{c} T_h \\ T_i \\ T_j \end{array} \right\}_c. \tag{19}$$

It follows that the heat outgoing from the dual 3-cell h can be expressed as a scalar product of two vectors: the row vector $(\mathbf{f})_c$ of 1×3 type that depends on the cell geometry and on the material contained, and on the column vector $\mathbf{T}_c$ of the 3×1 type of nodal temperatures of cell c. Considering one node at time, we can write the thermal balance relation by summing all the thermal powers outgoing from the dual 3-cell, as shown in Fig.(6*b*). Considering the dual 3-cell h the heat balance (2) becomes

$$\sum_{c\in\mathcal{J}(h)} (f_{hh} \quad f_{hi} \quad f_{hj})_c \left\{ \begin{array}{c} T_h \\ T_i \\ T_j \end{array} \right\}_c = S_h + \Phi_h. \tag{20}$$

For a numerical treatement, it is convenient to add the boundary inflow Φ_h to the source S_h from the beginning putting $\overline{S}_h \stackrel{\text{def}}{=} S_h + \Phi_h$ as equivalent source. Denoting as N the number of nodes, which coincides with the number of dual 3-cells, and introducing the global vectors

$$\mathbf{T} = (T_1 \ldots T_N)^\mathsf{T} \qquad \overline{\mathbf{S}} = (\overline{S}_1 \ldots \overline{S}_N)^\mathsf{T} \tag{21}$$

we come to a system of the kind

$$\mathbf{F}\mathbf{T} = \overline{\mathbf{S}} \tag{22}$$

where $\mathbf{F}$ is the *global fundamental matrix*. The system so obtained is the discrete equivalent of Poisson differential equations.

One cell at time. For computational purposes it is convenient to proceed with one cell at time, because, in the previous way the calculations on every cell must be repeated three times. Using the notation:

$$\mathbf{Q}_c \stackrel{\text{def}}{=} \left\{ \begin{array}{c} Q_h \\ Q_i \\ Q_j \end{array} \right\}_c \qquad \mathbf{T}_c \stackrel{\text{def}}{=} \left\{ \begin{array}{c} T_h \\ T_i \\ T_j \end{array} \right\}_c \tag{23}$$

and composing Eq. (10) with Eqs.(13) and (14) we obtain

$$Q_c = \frac{1}{4tA_c} \left[\begin{array}{cc} A_{hx} & A_{hy} \\ A_{ix} & A_{iy} \\ A_{jx} & A_{jy} \end{array} \right]_c \mathbf{K}_c \left[\begin{array}{ccc} A_{hx} & A_{ix} & A_{jx} \\ A_{hy} & A_{iy} & A_{jy} \end{array} \right]_c T_c. \tag{24}$$

We remark that the "-" sign that preceeds the matrix $\mathbf{K}_c$ combines with the analogous sign contained in $\mathbf{B}_c$ giving a "+" sign. From this formula, we see that each of the three heat fluxes depends on the nodal temperatures so that we can write

$$\left\{ \begin{array}{c} Q_h \\ Q_i \\ Q_j \end{array} \right\}_c = \left[\begin{array}{ccc} f_{hh} & f_{hi} & f_{hj} \\ f_{ih} & f_{ii} & f_{ij} \\ f_{jh} & f_{ji} & f_{jj} \end{array} \right]_c \left\{ \begin{array}{c} T_h \\ T_i \\ T_j \end{array} \right\}_c . \tag{25}$$

we can write relation (25) as

$$\mathbf{Q}_c = \mathbf{f}_c \mathbf{T}_c. \tag{26}$$

The matrix $\mathbf{f}_c$ will be called the *local fundamental matrix*. We shall show later that it coincides with the local stiffness matrix of the Finite Element Method. For isotropic materials, the relation (24) becomes

$$\left\{ \begin{array}{c} Q_h \\ Q_i \\ Q_j \end{array} \right\}_c = \frac{k_c}{4tA_c} \left[\begin{array}{ccc} \mathbf{A}_h \cdot \mathbf{A}_h & \mathbf{A}_h \cdot \mathbf{A}_i & \mathbf{A}_h \cdot \mathbf{A}_j \\ \mathbf{A}_i \cdot \mathbf{A}_h & \mathbf{A}_i \cdot \mathbf{A}_i & \mathbf{A}_i \cdot \mathbf{A}_j \\ \mathbf{A}_j \cdot \mathbf{A}_h & \mathbf{A}_j \cdot \mathbf{A}_i & \mathbf{A}_j \cdot \mathbf{A}_j \end{array} \right]_c \left\{ \begin{array}{c} T_h \\ T_i \\ T_j \end{array} \right\}_c . \tag{27}$$

We then see that the components of the local fundamental matrix have the form

$$f^c_{pq} = \frac{k_c}{4tA_c} \mathbf{A}_p \cdot \mathbf{A}_q. \tag{28}$$

Let us remark that in Eq.(24), the first matrix is the transposition of $\mathbf{B}_c$, apart from the factor $-2tA_c$. Consequently

$$\mathbf{Q}_c = tA_c \mathbf{B}_c^{\mathsf{T}} \mathbf{K}_c \mathbf{B}_c \mathbf{T}_c \tag{29}$$

and then the local fundamental matrix is symmetric and given by

$$\mathbf{f}_c = tA_c \mathbf{B}_c^{\mathsf{T}} \mathbf{K}_c \mathbf{B}_c. \tag{30}$$

To obtain the global fundamental matrix $\mathbf{F}$ we must assemble all the local fundamental matrices. The process is summarized in the following pseudocode:

```
Let N_c be the number of cells
put F_pq = 0 for all p,q = 1,2,...N_c
for c from 1 to N_c
      let h,i,j be the vertices of the triangle c
      using Eq. (24) evaluate the nine coefficients
      f_1,1   f_1,2   ...   f_3,3
      then the fundamental matrix is
        F_hh  =  F_hh + f_1,1
        F_ih  =  F_ih + f_2,1
        ...   =  ...
        F_jj  =  F_jj + f_3,3
end for
```

(31)

It is easily seen that also the global fundamental matrix is symmetric.

Heat source. The heat source is usually distribuited in a subregion of the domain. To evaluate S_h it is convenient to use a mesh as the one shown in Fig.(7). For the barycentric subdivision, the areas of each quadrilateral in which the triangle is subdivided are $1/3$ of the area of the triangle. If we suppose that the heat source inside every element is uniform, we can write

$$S_h = \frac{1}{3} \sum_{c \in \mathcal{J}(h)} \sigma_c A_c \tag{32}$$

where σ_c is the heat source density.

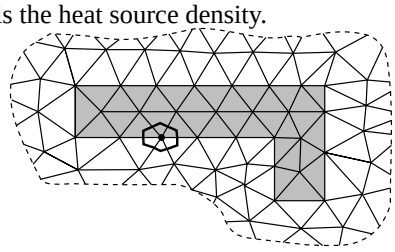

Figure 7 : Thermal generation uniformly distributed in a subregion.

If there are point wise concentrated sources, such as laser's beams, the corresponding amount of source must be added to the dual polygon to which the source belongs.

Heat flux at the boundary. With reference to Fig.(8) let us consider the boundary of the region and g,h,i the adjacent boundary nodes. Let h be the central node and L' and L'' the lengths of the edges preceeding and following h respectively. Let us denote as s the line arc of the boundary with origin in h. Let the heat flux for unit length be a function of the kind $q(s) = a + (b-a)\,s/L$. Denoting as q_g, q_h, q_i the three values

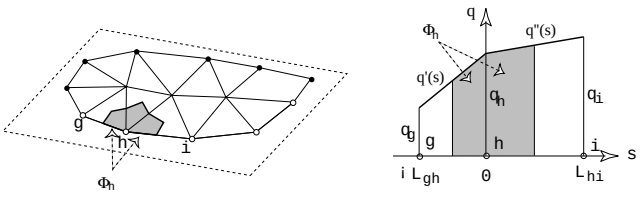

Figure 8 : The boundary nodes in the part of the boundary in which the heat flux is assigned.

of the heat flux density evaluated in the three nodes g,h,i respectively, we can write

$$q'(s) = q_h - \frac{q_g - q_h}{L'}s \qquad q''(s) = q_h + \frac{q_i - q_h}{L''}s. \tag{33}$$

The heat flux entering across the boundary side of the dual polygon will be

$$\left\{ \begin{array}{rcl} \Phi_h & = & \displaystyle\int_{-L'/2}^{0} q'(s)\,\mathrm{d}s + \int_{0}^{L''/2} q''(s)\,\mathrm{d}s \\ & = & \displaystyle\frac{1}{8}L' q_g + \frac{3}{8}(L'+L'')\,q_h + \frac{1}{8}L'' q_i. \end{array} \right. \tag{34}$$

This relation will be useful later for comparison with the analogous relation used in FEM. The procedure described up to now has been applied to fracture in (12), (13), (14), (27), (28), (29), (30); to acoustics (43) and electromagnetism (45), (22).

5 Quadratic interpolation

Up to now we have carried out a linear interpolation inside every primal cell (triangle). Now we show that it is possible to use a quadratic interpolation. To this end we add three nodes p,q,r at the midpoints of the sides, as shown in Fig.(9).

5.1 Local affine coordinates

Let us denote as h,i,j, the three vertices of the triangle c (c stands for *cell*); and let us consider the vertex h as the origin of an affine coordinate system[3], whose axes ξ and η are set along the sides hi and hj respectively. The lengths of the segments hi and hj are assumed as units of measurement along the corresponding axes. As shown in Fig.(9) the relation between local affine coordinates, and the global cartesian ones, is a linear one, given by:

[3] We remember that affine coordinates (35) [p.49], (8) [p.202] are rectilinear coordinates with oblique axes (3) [p.107], strictly related to the *barycentric* (8) [p.216] coordinates, with *areal* (8) [p.218] or *triangular* or *normal* coordinates. They differ from cartesian coordinates because the units on the two axes are fixed indipendently one from the other and then the notion of distance between two points is not defined. This implies the non-metrical nature of affine coordinates. They are the most used coordinates in physics because arise whenever two physical variables of different physical dimensions are represented on rectangular axes, say in the (p,V) diagrams of thermodynamics and in(ε,σ) diagrams of solid mechanics (4) [p.17].

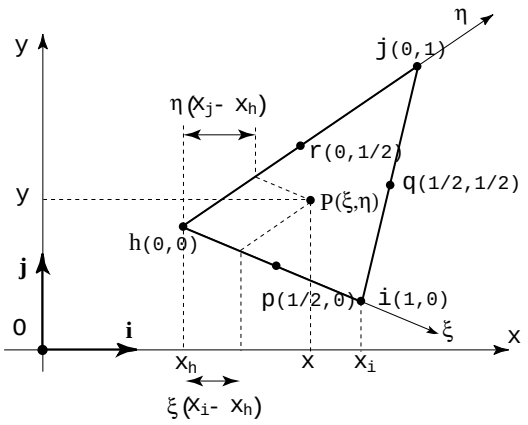

Figure 9 : Relation between the global cartesian coordinates and local affine coordinates.

$$\left\{ \begin{array}{c} x \\ y \end{array} \right\} = \left\{ \begin{array}{c} x_h \\ y_h \end{array} \right\} + \left[\begin{array}{cc} a & b \\ c & d \end{array} \right] \left\{ \begin{array}{c} \xi \\ \eta \end{array} \right\}. \tag{35}$$

The inverse relation is

$$\left\{ \begin{array}{c} \xi \\ \eta \end{array} \right\} = \left\{ \begin{array}{c} p \\ q \end{array} \right\} + \left[\begin{array}{cc} \alpha & \beta \\ \gamma & \delta \end{array} \right] \left\{ \begin{array}{c} x \\ y \end{array} \right\}. \tag{36}$$

We propose to interpolate the temperature inside the triangle c in terms of the six nodal temperatures. Since the relation between the global cartesian coordinates and the affine coordinates is linear, it is immaterial which coordinate system is used to express the quadratic behaviour. It is convenient to use the affine coordinates. We can write

$$T_c(\xi,\eta) = \left(\begin{array}{cccccc} 1 & \xi & \eta & \xi^2 & \xi\eta & \eta^2 \end{array} \right) \left\{ \begin{array}{c} a_h \\ a_i \\ a_j \\ a_p \\ a_q \\ a_r \end{array} \right\}_c. \tag{37}$$

The six coefficients a_k must be determined in terms of the six nodal values of the temperature. One obtains

$$\left\{ \begin{array}{c} a_h \\ a_i \\ a_j \\ a_p \\ a_q \\ a_r \end{array} \right\}_c = \left[\begin{array}{rrrrrr} 1 & 0 & 0 & 0 & 0 & 0 \\ -3 & -1 & 0 & 4 & 0 & 0 \\ -3 & 0 & -1 & 0 & 0 & 4 \\ 2 & 2 & 0 & -4 & 0 & 0 \\ 4 & 0 & 0 & -4 & 4 & -4 \\ 2 & 0 & 2 & 0 & 0 & -4 \end{array} \right] \left\{ \begin{array}{c} T_h \\ T_i \\ T_j \\ T_p \\ T_q \\ T_r \end{array} \right\}_c \tag{38}$$

so that

$$\mathbf{a}_c = \mathbf{C}\mathbf{T}_c. \tag{39}$$

Let us remark that, using affine local coordinates, the matrix coefficients *are the same* for all cells: this fact justifies the use of local affine coordinates. The function (37) can then be written as

$$T_c(\xi,\eta) = \begin{pmatrix} 1 & \xi & \eta & \xi^2 & \xi\eta & \eta^2 \end{pmatrix} \mathbf{CT}_c. \qquad (40)$$

This formula permits to evaluate the function T at every point inside the triangle in terms of its nodal values.

5.2 Gradient

From the relation (40), we obtain

$$\begin{Bmatrix} \partial_\xi T \\ \partial_\eta T \end{Bmatrix} = \begin{bmatrix} 0 & 1 & 0 & 2\xi & \eta & 0 \\ 0 & 0 & 1 & 0 & \xi & 2\eta \end{bmatrix} \mathbf{CT}_c. \qquad (41)$$

The cartesian components of the gradient are

$$\begin{Bmatrix} g_x \\ g_y \end{Bmatrix} = \begin{Bmatrix} \partial_x T \\ \partial_y T \end{Bmatrix} = \begin{bmatrix} \partial_x\xi & \partial_x\eta \\ \partial_y\xi & \partial_y\eta \end{bmatrix} \begin{Bmatrix} \partial_\xi T \\ \partial_\eta T \end{Bmatrix} = \begin{bmatrix} \alpha & \gamma \\ \beta & \delta \end{bmatrix}_c \begin{bmatrix} 0 & 1 & 0 & 2\xi & \eta & 0 \\ 0 & 0 & 1 & 0 & \xi & 2\eta \end{bmatrix} \mathbf{CT}_c \qquad (42)$$

We remark that in a quadratic interpolation the gradient is an *affine* function.

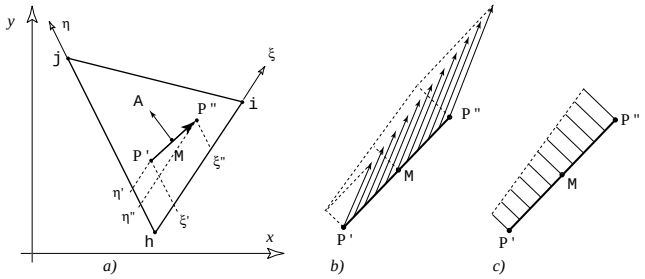

Figure 10 : *a)* The area-vector corresponding to the line segment $P'P$"; *b)* An affine gradient; *c)* The component of the gradient normal to the segment is also an affine function.

Area. We now need a formula to evaluate the area corresponding to a line segment connecting two arbitrary points $P'(\xi',\eta')$ and $P''(\xi'',\eta'')$ contained in the triangle c. With reference to Fig.(10*a*), and using equation (35) we obtain

$$\begin{Bmatrix} x''-x' \\ y''-y' \end{Bmatrix} = \begin{bmatrix} a & b \\ c & d \end{bmatrix}_c \begin{Bmatrix} \xi''-\xi' \\ \eta''-\eta' \end{Bmatrix}_c. \qquad (43)$$

We remark that the area-vector of the face of the triangular prism is obtained by performing a rotation in an anticlockwise direction of 90 degrees and performing the product for the thickness t.

$$\begin{Bmatrix} A_x \\ A_y \end{Bmatrix} = t \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} a & b \\ c & d \end{bmatrix}_c \begin{Bmatrix} \xi''-\xi' \\ \eta''-\eta' \end{Bmatrix}. \qquad (44)$$

It is useful to transpose last relation:

$$\begin{pmatrix} A_x & A_y \end{pmatrix} = t \begin{pmatrix} \xi''-\xi' & \eta''-\eta' \end{pmatrix} \begin{bmatrix} -c & a \\ -d & b \end{bmatrix}_c. \qquad (45)$$

5.3 Constitutive equation

The heat flux vector $\mathbf{q}$ in an anisotropic medium is linked to the temperature gradient by the relation (14), that we now write

$$\begin{Bmatrix} q_x(\xi,\eta) \\ q_y(\xi,\eta) \end{Bmatrix}_c = -\begin{bmatrix} k_{xx} & k_{xy} \\ k_{yx} & k_{yy} \end{bmatrix}_c \begin{Bmatrix} g_x(\xi,\eta) \\ g_y(\xi,\eta) \end{Bmatrix}_c. \qquad (46)$$

that is

$$\mathbf{q}_c = -\mathbf{K}_c\,\mathbf{g}_c\,. \qquad (47)$$

Heat flux. Denoted as M the midpoint of the segment $P'P''$ we have

$$\xi_M = \frac{\xi'+\xi''}{2} \qquad \eta_M = \frac{\eta'+\eta''}{2}. \qquad (48)$$

Since the heat flux $\mathbf{q}$, as the gradient $\mathbf{g}$, is an affine function of the affine coordinates, as shown in Fig.(10*b*, *c*), it follows that, in order to evaluate the flux across the corresponding face, it is not necessary to perform an integration: it is enough to multiply the vector $\mathbf{q}$, evaluated in the midpoint M of the segment, for the area-vector $\mathbf{A}$

$$Q(P',P'') = \begin{pmatrix} A_x & A_y \end{pmatrix} \begin{Bmatrix} q_x(M) \\ q_y(M) \end{Bmatrix}. \qquad (49)$$

This formula replaces Eq.(12) which is valid for linear interpolation. We remark that in Eq.(12) A_{hx}, A_{hy} are the components of the area-vector of the h-face of the triangular prism and this explains the factor $1/2$. Combining equation (49) with the equations (45), (46) and (42), we obtain the flux in the form

$$Q(P',P'') = -t \begin{pmatrix} \xi''-\xi' & \eta''-\eta' \end{pmatrix} \begin{bmatrix} \bar{k}_{xx} & \bar{k}_{xy} \\ \bar{k}_{yx} & \bar{k}_{yy} \end{bmatrix}_c \begin{bmatrix} 0 & 1 & 0 & 2\xi_M & \eta_M & 0 \\ 0 & 0 & 1 & 0 & \xi_M & 2\eta_M \end{bmatrix} \mathbf{CT}_c \qquad (50)$$

where

$$\overline{\mathbf{K}}_c = \begin{bmatrix} \bar{k}_{xx} & \bar{k}_{xy} \\ \bar{k}_{yx} & \bar{k}_{yy} \end{bmatrix}_c = \begin{bmatrix} -c & a \\ -d & b \end{bmatrix}_c \begin{bmatrix} k_{xx} & k_{xy} \\ k_{yx} & k_{yy} \end{bmatrix}_c \begin{bmatrix} \alpha & \gamma \\ \beta & \delta \end{bmatrix}_c \qquad (51)$$

which is a non-symmetric matrix in spite of the symmetry of the matrix $\mathbf{K}_c$. The equation (49) can be written as product of a row vector $\mathbf{R}_c$ times a column vector $\mathbf{T}_c$ i.e.

$$Q(P',P") = \mathbf{R}_c(P',P")\,\mathbf{T}_c. \qquad (52)$$

Putting

$$\mathbf{Z} = \begin{bmatrix} 0 & 1 & 0 & 2\xi_M & \eta_M & 0 \\ 0 & 0 & 1 & 0 & \xi_M & 2\eta_M \end{bmatrix}_c \qquad (53)$$

we can write

$$\mathbf{R}_c(P',P") = -t \begin{pmatrix} \xi''-\xi' & \eta''-\eta' \end{pmatrix} \overline{\mathbf{K}}_c \mathbf{Z}(P',P")\mathbf{C}. \qquad (54)$$

5.4 Fundamental equation

In parabolic interpolation, we have six nodes for each triangle, and we must select a dual complex. This means that we must choose a polygon around each node to be considered as a "tributary region" of the node. A key point is that this dual polygon can be chosen at will. This will permit us to select the polygons that give the maximum order of convergence. Since the three additional nodes p,q,r permit us to divide the triangle h,i,j into four triangles, a first idea is to consider as dual polygons the barycentric ones, as shown in Fig.(13*a*). We shall show that in this way a small increase in the order of convergence, from 2 to 2.3 is obtainable. A much more convenient choice (17) is the one based on Gauss points, as shown in Fig.(11). Let us remember that Gauss' points are symmetrically placed with respect the midpoint of the segment. For two Gauss' points of a segment, of unit length, they have the distance

$$d = \frac{1}{2\sqrt{3}} \tag{55}$$

from the midpoint. With reference to Fig.(11*b*) we consider the heat flux leaving the face $9-10$ contained in cell c and we shall call it $Q_h^c = \mathbf{R}_h^c \mathbf{T_c}$. Similarly the heat flux outgoing from the boundary of the dual polygon of node q contained in cell c will be denoted by $Q_q^c = \mathbf{R}_q^c \mathbf{T_c}$. To each node there corresponds heat flux. Using Eq.(50) to evaluate the heat fluxes we obtain

$$\begin{cases} \mathbf{R}_h^c = +\mathbf{R}(9,8) + \mathbf{R}(8,10) \\ \mathbf{R}_i^c = +\mathbf{R}(14,16) + \mathbf{R}(16,15) \\ \mathbf{R}_j^c = +\mathbf{R}(13,11) + \mathbf{R}(11,12) \\ \mathbf{R}_p^c = -\mathbf{R}(8,10) + \mathbf{R}(8,7) - \mathbf{R}(16,7) - \mathbf{R}(14,16) \\ \mathbf{R}_q^c = -\mathbf{R}(16,15) + \mathbf{R}(16,7) - \mathbf{R}(11,7) - \mathbf{R}(13,11) \\ \mathbf{R}_r^c = -\mathbf{R}(11,12) + \mathbf{R}(11,7) - \mathbf{R}(8,7) - \mathbf{R}(9,8). \end{cases} \tag{56}$$

Every $\mathbf{R}_k^c$ is a six components row-vector that we can write in the form

$$\mathbf{R}_h^c = (\, f_{hh} \quad f_{hi} \quad f_{hj} \quad f_{hp} \quad f_{hq} \quad f_{hr})_c \tag{57}$$

The fundamental equation (2) becomes

$$\sum_{c \in \mathcal{J}(h)} \mathbf{R}_h^c \mathbf{T}_c = \overline{S}_h \tag{58}$$

which is analogous to Eq.(20). In the quadratic interpolation, and with isotropic materials we do not have an explicit formula such as (28), to evaluate the coefficients f_{pq}. Moreover, contrary to what happens in FEM, the matrix thus obtained is not symmetric. This lack of symmetry of the stiffness matrix seems to contrast with the symmetry of the differential operator. We remember that in Finite Element Method one usually chose as weight functions (or test or trial functions) the same shape functions with the purpose of *maintaining* the symmetry (38) [p.430]. The same is done in spectral methods.

If one choose weight functions different form shape functions the symmetry is destroyed.

From a computational point of view the advantage of symmetric algebraic system is sensible when direct methods of solution are used; but it is immaterial when using iterative methods.

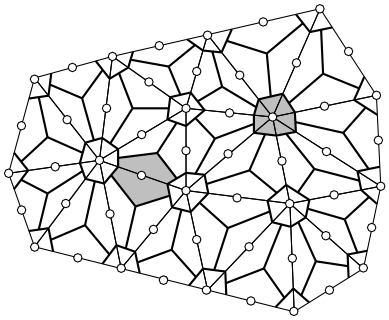

Figure 12 : The dual complex (heavy lines) using two Gauss points for each edge.

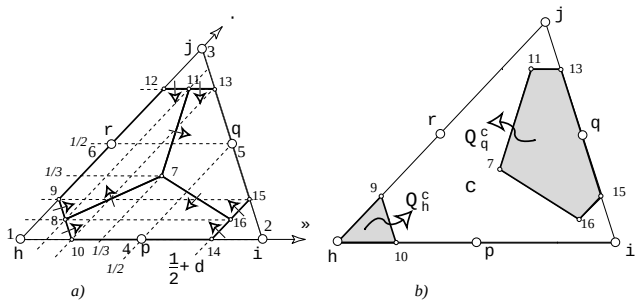

Figure 11 : *a)* The subdivision of the triangle into dual polygons using two Gauss points on each edge; *b)* the part of the dual polygons of nodes h and q contained in triangle c.

5.5 Example

The cell method is similar to the *direct* or *physical* approach used at the early stages of FEM (19) [p.22]; (21) [p.35]; (11). This method has not been developed to obtain a convergence order greater than the second one. Accordingly Fenner wrote: "*the direct equilibium formulations described before are not applicable to variable strain elements*" (11) [p.153]. It is highly likely that this fact has caused the demise of the physical approach. On the other hand, the cell method starts from a different philosophy, which allows the use of interpolation functions that are the great advantage of the Finite Element Method over that of the Finite Volume Method. This allows the physical approach to be revived.

We quote here an example. Consider a two dimensional scalar field described by a potential u without distributed sources whose solution is the harmonic function $u(x,y) = \exp(x)\cos(y)$.[4]. In the square $0 \le x \le 1, 0 \le y \le 1$, given the Dirichlet boundary conditions, we construct the system of algebraic equations by means of the cell method using a quadratic interpolation function in each triangle. The square domain is divided into squares; each square is subdivided in two triangles using one diagonal. For each triangle the nodes are its three vertices and the three midpoints. We interpolate the potential $u(x,y)$ with a quadratic function. A first root-means-square value of the errors at nodes. This error decreases with the length of the side of the triangles according to the power 2.3, as shown in Fig. (14). As a second choice we consider the subdivision made using two Gauss points for each edge, as shown in Fig.(13*b*): in this case the order of convergence is 4.0. The result has beeb compared with Abaqus using quadratic interpolation and superconvergence points (library DC2D6): the errors agree up to the fourteen digit.

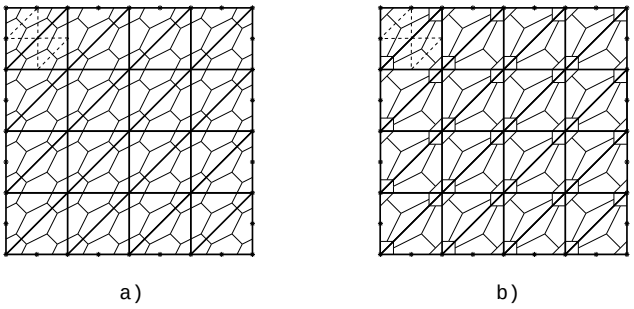

Figure 13 : *a)* The barycentric subdivision; *b)* the subdivision using two Gauss points for each edge.

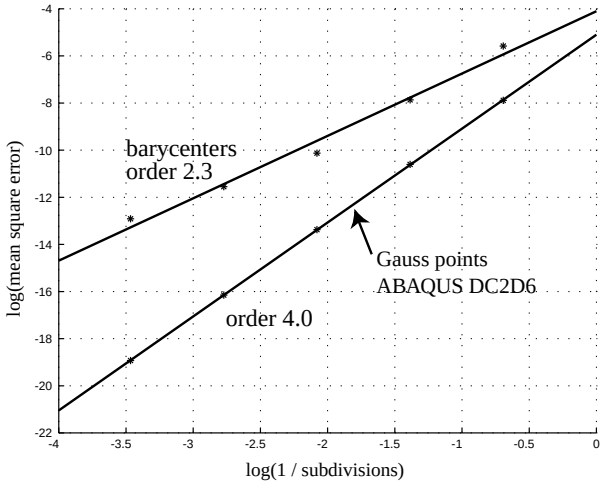

Figure 14 : The order of convergence of the two subdivisions.

choice is the barycentric subdivision: in this case, the dual polygon of each node is the one bounded by the lines connecting the barycenters, as shown in Fig.(13*a*). To compare the approximate values with the exact ones we evaluate the

[4] In the differential formulation such a field is described by the Laplace equation $\Delta u(x,y) = 0$

6 Comparison with finite element method

Let us show that the fundamental matrix obtained through the cell method, in the case of a *linear* interpolation, is the same as FEM. We shall limit our comparison to the Poisson equation. The latter can be written in weak form, using a test function ψ:

$$\int_\Omega \psi\,[-k\nabla\cdot\nabla T(\mathbf{x}) - \sigma(\mathbf{x})]\;\mathrm{d}\Omega = 0 \qquad \textit{for every } \psi \quad (59)$$

We want to introduce integration by parts, and use ψ here, to lower the order of derivatives on T. Doing so, we come near to the physical fact: in fact the differentiability conditions imposed by differential formulation are greater than those imposed by the physical phenomenon. After division of the domain Ω in triangular finite elements, in every element c we interpolate the temperature $T(\mathbf{x})$ with a function $T^c(\mathbf{x})$ which is a linear combination of its nodal values. The coefficients of this linear combination are the element shape functions $N_k^c(\mathbf{x})$:

$$T^c(\mathbf{x}) = \sum_{h\in\mathcal{N}(c)} T_h N_h^c(\mathbf{x}) \quad (60)$$

where $\mathcal{N}(c)$ is the set of nodes of the element c. After this, we express the function $T(\mathbf{x})$ in all the domain as a sum of the functions $T^c(\mathbf{x})$

$$T(\mathbf{x}) = \sum_{e=1}^{m} T^c(\mathbf{x}) = \sum_{c=1}^{m}\sum_{h\in\mathcal{N}(c)} T_h N_h^c(\mathbf{x}) = \sum_{h=1}^{N} T_h N_h(\mathbf{x}) \quad (61)$$

where we have introduced the *nodal* shape functions $N_h(\mathbf{x})$, shown in Fig.(15*a*). FEM chooses shape functions as test

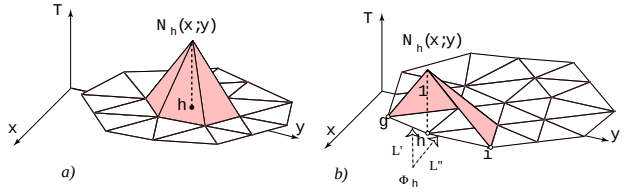

Figure 15 : The nodal shape functions: *a)* for an internal node; *b)* for a boundary node.

functions: $\psi_h(\mathbf{x}) = N_h(\mathbf{x})$. In this way the following system of

equations is obtained

$$\int_\Omega N_h(\mathbf{x}) \left[-k\nabla\cdot\nabla \left\{ \sum_{k=1}^{N} T_k N_k(\mathbf{x}) \right\} - \sigma(\mathbf{x}) \right] \mathrm{d}\Omega = 0. \quad (62)$$

Performing an integration by parts we obtain

$$\sum_{k=1}^{N} \Big[\int_\Omega k\nabla N_h(\mathbf{x})\cdot\nabla N_k(\mathbf{x})\,\mathrm{d}\Omega \Big] T_k = \int_\Omega N_h(\mathbf{x})\,\sigma(\mathbf{x})\,\mathrm{d}\Omega + k\int_{\partial\Omega} N_h(\mathbf{x}) \frac{\partial T(\mathbf{x})}{\partial n}\,\mathrm{d}S. \quad (63)$$

Since the shape functions have a linear behaviour their gradients are uniform and can be moved out of the integration symbol. In such a way we obtain the fundamental matrix of FEM

$$\begin{cases} \text{in 2D:} & f_{pq} = kt A_c \nabla N_p(\mathbf{x})\cdot\nabla N_q(\mathbf{x}) \\ \text{in 3D:} & f_{pq} = kV_c \nabla N_p(\mathbf{x})\cdot\nabla N_q(\mathbf{x}). \end{cases} \quad (64)$$

We shall now show that, by using simplicial complexes the system is the same as the one obtained with the cell method. To show this we shall refer to Fig.(16).

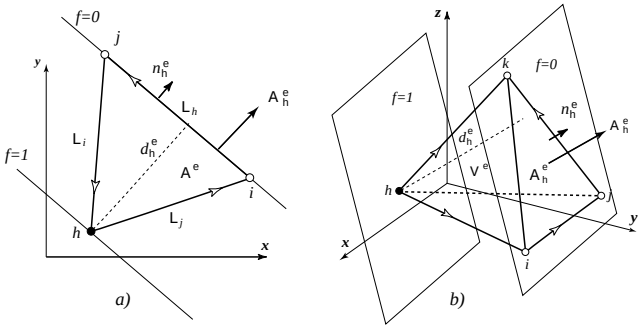

Figure 16 : Since the shape function is equal to one in one vertex and zero in the other vertices, the modulus of its gradient is the inverse of the distance between the corresponding vertex and it opposite side (or its opposite face in 3D).

In two dimensions. Let us observe that the shape functions $N_h^c(x,y)$ can be obtained easily considering that the remaining vertices i, j belong to an equipotential straight line corresponding to the value zero of a function i.e. $f(x,y) = 0$, and that node h belongs to the straight line parallel to the preceeding and corresponds to the value one: $f(x,y) = 1$. The gradient vector will be orthogonal to the two parallel straight lines and will have as modulus the ratio $1/d_h^c$ where d_h^c is the distance of the vertex h from side L_h. Hence we have

$$\nabla N_h^c(x,y) = -\frac{\mathbf{n}_h^c}{d_h^c} = -\frac{L_h t\,\mathbf{n}_h^c}{L_h t\, d_h^c} = -\frac{\mathbf{A}_h^c}{2tA_c}. \quad (65)$$

Let us remark that the "minus" sign is a consequence of the fact that we have chosen the outgoing normal: in fact the gradient has the direction of increasing values of $f(x,y)$ and hence it goes in the opposite direction. In FEM it is common to choose the inward normal to avoid this minus sign.

In three dimensions. As is shown in Fig.(16*b*) one considers the three vertices i, j, k in which the shape function vanishes as belonging to a plane equipotential surface. On this plane the function will be zero and on the parallel plane passing from vertex h will be equal to 1. We shall obtain (21) [p.50]

$$\nabla N_h^c(x,y,z) = -\frac{\mathbf{n}_h^c}{d_h^c} = -\frac{A_h \mathbf{n}_h^c}{A_h d_h^c} = -\frac{1}{3V_c}\mathbf{A}_h^c. \quad (66)$$

It follows that the elements of the local fundamental matrix are

$$\begin{aligned} f_{pq}^c &= kt A_c \nabla N_p^c\cdot\nabla N_q^c = \frac{k}{4tA_c}\mathbf{A}_p^c\cdot\mathbf{A}_q^c \\ f_{pq}^c &= kV_c \nabla N_p^c\cdot\nabla N_q^c = \frac{k}{9V_c}\mathbf{A}_p^c\cdot\mathbf{A}_q^c \end{aligned} \quad (67)$$

that coincides with that of cell method (28) (48) [p.56], (21) [p.43, 50]. Hence we can say that *the cell method, for linear shape functions on simplicial complex, gives a simple way to obtain the same stiffness matrix as the FEM*.

Source term S_h. In FEM with a source which is *uniformly* distribuited over the whole domain, the source term is given by

$$\begin{aligned} S_h &= \sum_{c\in\mathcal{J}(h)} \int_{A_c} \sigma N_h^c(x,y)\,\mathrm{d}A = \sigma \sum_{c\in\mathcal{J}(h)} \frac{A_h^c}{3} = \sigma A_h \\ S_h &= \sum_{c\in\mathcal{J}(h)} \int_{V_c} \sigma N_h^c(x,y,z)\,\mathrm{d}V = \sigma \sum_{c\in\mathcal{J}(h)} \frac{V_h^c}{4} = \sigma V_h \end{aligned} \quad (68)$$

and in the cell method we have

$$\text{in 2D} \quad S_h = \sigma A_h \qquad \text{in 3D} \quad S_h = \sigma V_h. \quad (69)$$

Then: *for a source which is uniformly distribuited on the whole domain the source terms of FEM coincide with those of the cell method.* Matters are different when sources are not uniformly distributed and hence for *mass matrix* in dynamical problems. In FEM a concentrated source is distributed to the vertices according to the "lever rule": this follows from the fact that the right side of the balance equation (63) contains the form functions $N_h(x)$. On the contrary in the cell method a concentrated source is entirely charged to the dual polygon in which it is located, as in FVM. This implies a difference in the second members of the fundamental equations of CM when compared with FEM (21) [p.45].

Boundary flux Φ_h. With reference to Fig.(15*b*) let us consider three adjacent boundary nodes g,h,i. Let L' and L'' be the lengths of the edges preceeding and following the central node h. Proceeding as in Fig.(17*b*) the shape functions will be

$$N'(s) = 1 + \frac{s}{L'} \qquad N''(s) = 1 - \frac{s}{L''}. \tag{70}$$

The quantities Φ_h of FEM will be given by

$$\begin{cases} \Phi_h &= \displaystyle\int_{-L'}^{0} N'(s)\, q'(s)\, \mathrm{d}s + \int_{0}^{L''} N''(s)\, q''(s)\, \mathrm{d}s \\ &= \dfrac{1}{6} L' q_g + \dfrac{1}{3}(L' + L'')\, q_h + \dfrac{1}{6} L'' q_i. \end{cases} \tag{71}$$

This result is slightly different from the one of cells given by

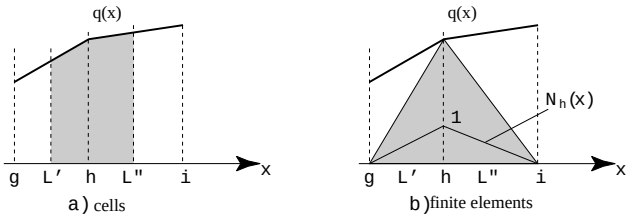

Figure 17 : The boundary heat fluxes evaluated: *a)* by cell method; *b)* by FEM.

Eq. (34). The difference between the two Q_h vanishes for a uniform boundary distribution, i.e. when $q_g = q_h = q_i$.

7 Comparison with finite volume method

The Cell Method (**CM**) is very similar to the Finite Volume Method (**FVM**)(15)(33). The main differences are listed below.

- **FVM** uses the integral forms of the conservation equations as the starting point (15) [p.67]. Though in principle it does not require the availability of the differential formulation, in practice one uses *field variables*, which are the natural ingredients of differential formulation, and evaluates 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.*" (15) [p.68]. **CM**, on the contrary, uses directly *global variables* and takes 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*, 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.*" (25) [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 any primal vertex: in this respect (and only in this respect) it corresponds to the vertex=based (or node-centered) scheme of FVM.

- **FVM** does not use interpolating functions inside any primal cell, there is no particular reason that would limit this approach, at least theoretically. **CM**, on the contrary, as FEM, uses *interpolating functions* on the primal cells.

- in **FVM** and in the vertex-based scheme, the control volume is formed by the polygons of the baricentric subdivision or by Voronoi polygons. In **CM** the control volume is free and can be chosen at will, in particular it can be chosen to give the maximum order of convergence.

- **FVM**, which evolved from Finite Difference Method in the early seventies (32) [p.93], starts considering rectangular (or cubical) grids: unstructured grids, in particular simplicial grids, are an exception (15) [p.233], (9). However, in recent years, FVM has re-gained popularity also for complex geometries (where once FEM had no competitors). **CM** on the contrary, starts directly with simplicial complexes i.e. *unstructured* grids.

- **FVM**. Convergence up to fourth order is obtained by interpolating the field potential using *cartesian* grids only, as in FDM (20). On unstructured meshes, in particular on non-orthogonal meshes, "*the interpolation is usually performed treating linear lines piecewise as if they where straight; if the lines changes direction at the cell face an additional error is introduced.*" (15) [p.221] "*Any higher order FVM schemes requires interpolation of higher order at more than one cell face locations. This is manageable on structured grids, but rather difficult on unstructured grids.*" (15) [p.229] FVM "*compared with alternative methods has a limited order of accuracy, usually no more than second order ...*" (26) [p.19]. It is without doubt, however, that high order FVM has not received particular attention. This is due, essentially, to the fact that one of the first application of FVM has been in CFD (Computational Fluid Dynamics), where the field function is, generally, "not smooth" and therefore higher order methods do not provide an increase in accuracy which counter-balances the augmented computational cost. **CM** the use of interpolating functions in any primal cell permits us to obtain a higher order of convergence, as in FEM. Thus a fourth order convergence is obtained considering the field functions quadratic inside the simplex, i.e. the heat flux *affine* inside any simplex. In this case the heat flux is evaluated exactly by the midpoint rule.

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