PUC

Série: Monografia em Ciência da Computação

Nº 18/83

AUTOMATIC GENERATION OF TETRAHEDRAL MESHES WITH APPLICATION TO FINITE ELEMENT SOLUTION OF STEFAN PROBLEMS

by

Vitoriano Ruas

Departamento de Informática

PONTIFÍCIA UNIVERSIDADE CATÓLICA DO RIO DE JANEIRO
MARQUÊS DE SÃO VICENTE, 225 — CEP-22453
RIO DE JANEIRO — BRASIL

PUC/RJ - DEPARTAMENTO DE INFORMÁTICA

Série : Monografia em Ciência da Computação, Nº 18/83

Editor : Antônio L. Furtado Setembro, 1983

AUTOMATIC GENERATION OF TETRAHEDRAL MESHES WITH APPLICATION TO FINITE ELEMENT SOLUTION OF STEFAN PROBLEMS

by

Vitoriano Ruas*

* Trabalho parcialmente financiado pela FINEP.

ABSTRACT

A simple and straightforward procedure for the automatic generation of partitions into tetrahedrons of three-dimensional starshaped domains is introduced. The method generalizes the one previously proposed for the two-dimensional case. As in that case, we consider the application of the method to the numerical solution of one-phase Stefan problems.

KEY WORDS

Automatic generation, finite elements, free boundary, heat equation, numerical solution, one-phase problems, spheric coordinates, starshaped domains, Stefan condition, Stefan problem, tetrahedral meshes, three-dimensional problems.

RESUMO

Nesta monografia introduz-se um processo simples e de fácil implementação para a geração automática de partições em tetrahedros de domínios cuja fronteira possa ser expressa em coordenadas esféricas. Esse método generaliza o que fora proposto anteriormente para o caso análogo bidimensional. Como neste último caso, considera-se a aplicação do método a resolução numérica de problemas de Stefan unifásicos.

PALAVRAS - CHAVE

Condição de Stefan, coordenadas esféricas, domínios estrelados, elementos finitos, equação do calor, fronteira livre, geração automática, malhas tetraédricas, problemas unifásicos, problema de Stefan, resolução numérica, tridimensional.

C O N T E N T S

1 - INTRODUCTION

In the framework of the numerical solution of boundary value problems with the finite element method, the generation of the mesh, together with the underlying problems of obtaining optimal numbering of the nodes with respect to the matrix band width, and the coordinates of the vertices of the elements, play a crucial role.

In the case of three-dimensional problems, in general the best approach is the use of tetrahedral elements, due to their flexibility for matching irregular shapes of domains, besides algebraic simplicity, in case curved boundaries are ap - proximated by polyhedrons. However, except for very particular cases such as parallelepipeds or cylinders, the problem of generating automatically the mesh and the associate data above, is a delicate one, if not a challenging problem for finite element method users.

That is why many specialists have devoted themselves to the solution of this problem, attempting to make their methods of generation of finite element meshes as general as possible. In particular the work of A. GEORGE (see e.g. [4]) is significant in this respect. Very good surveys about this question can be found in [12] and [5].

In the latter work HERMELINE came up with a method that provides a very interesting general solution, in the sense that, if one knows the vertices which uniquely describe the boundary of the polyhedron approximating the domain, then the optimal mesh in a given geometrical sense can be generated. Clearly enough , due to its generality, the implementation of his method is not simple, and several parameters describing the mesh must be given by the user.

In any case, it is generally admitted that the best solutions should be those obtained with the sole knowledge of the boundary of the domain, plus, of course, simple data describing the degree of refinement of the mesh. Moreover, as one should point out, a convenient approach is the one based on a first subdivision of the domain into subdomains consisting of macro-sim -

plices , which are next partitioned into smaller simplices by straighforward procedures. This mesh generation process is actually used in many finite element codes or systems, such as MODULEF [8].

In this paper, a method allowing the automatic automatic generation of tetrahedral meshes is proposed, which basically follows both principles above. However it is very simple to implement, as the only necessary input, besides the data which uniquely define the boundary of the domain, is an integer parameter for specification of the desired degree of refinement of the mesh.

The main limitation of the method is the fact that it can only be applied to domains whose boundary can be expressed in spheric coordinates with a suitably chosen origin lying in its interior. As pointed out in [11], this is the case of the very wide subclass of starshaped domains, called nonsigular. Incidentally the method generalizes the one introduced by the author in [9], for the generation of triangular finite element meshes applying to the same kind of domains.

Likewise the two-dimensional case, here again one can easily generate families of partitions arbitrarily fine. Incidentally, the regularity in the usual sense [1] of the family of partitions obtained with the method in two-dimensions was studied in [11]. It appeared in particular that the only condition for satisfying this classical requirement for convergence of the finite element method, was the Lipscnitz continuity of the function which describes the boundary in polar coordinates, with respect to the polar angle. Although we do not treat this question explicitely in this paper, one can quite naturally suppose that the same result applies, if the function describing the boundary of the domain is Lipschitz-continuous with respect to the angular coordinates.

An outline of the paper is as follows: In Section 2 we describe the generation of the mesh; in Section 3 we deal with the problem of calculating the coordinates of a vertex of a certain tetrahedron given its number, assuming that these numbers were obtained in a systematic and optimal way; in Section 4 we briefly consider an application of the mesh generation method to the numerical solution of three-dimensional one-phase Stefan problems. Finally we conclude in Section 5 with some important remarks.

2 - DEFINITION OF THE PARTITION

We first consider a slight modification of the usual partition of a unit cube into tetrahedrons, based on its subdivision into six macrotetrahedros.

Let the origin of the cartesian coordinates x_1, x_2, x_3 be the center of the cube. Taking the coordinate axes parallel to the edges of the cube, the latter is thereby subdivided into eight equal cubes, each one corresponding to an octant.

Let us also number these eights of cubes and octants , respectively by C_μ and $\mathcal{O}_\mu$, where μ is an integer triple subscript $\mu=(\mu_1, \mu_2,\mu_3)$, where:

$$\mu_i = \frac{\text{sign } (x_i)+1}{2} , \quad 1\le i\le 3$$

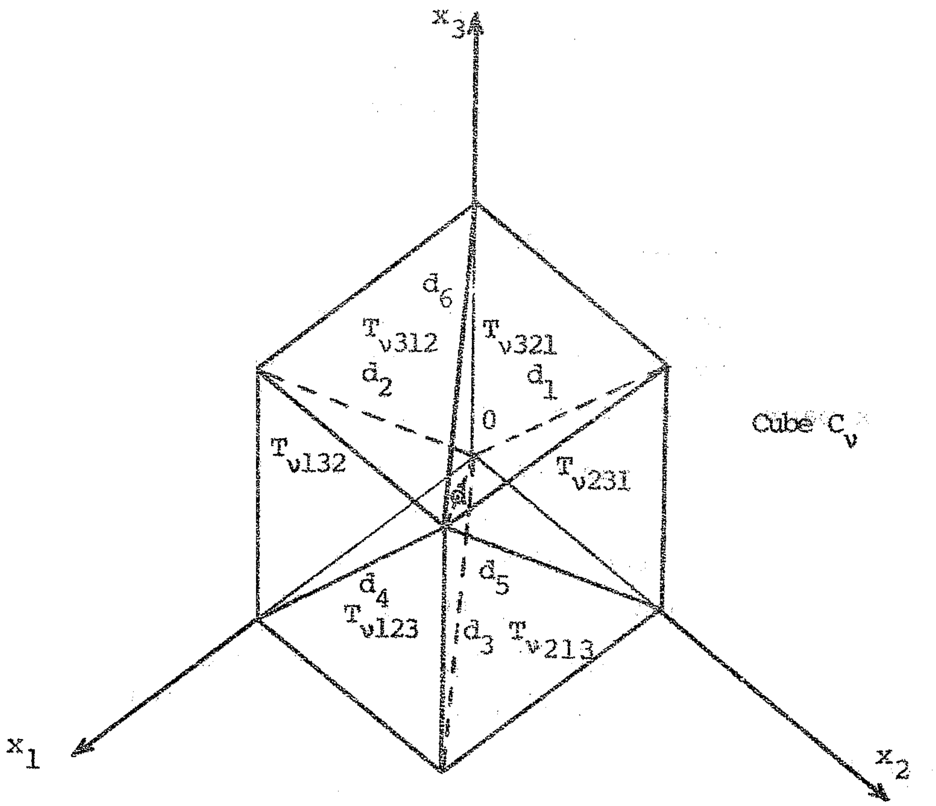
x_i being any nonzero value of the i-th coordinate of a point of $\mathcal{O}_\mu$

Now we refer to Figure 1, and we take as a model octant $\mathcal{O}_\nu$, with $\nu=(1,1,1)$.

Let d be the diagonal of C which is also a diagonal of C_ν, d_1, d_2 and d_3 be the three diagonals of the faces of C_ν intersecting at the origin, and d_4, d_5 and d_6, be the three diagonals of the faces of C_ν intersecting at the order end of d.

As it is well-known, d, $d_1,\ldots,d_6$ subdivide C_ν into six equal tetrahedrons, say, $T_{\nu\alpha}$, where $\alpha=(\alpha_1,\alpha_2,\alpha_3)$ corresponds to a permutation of (1,2,3). The position of each $T_{\nu\alpha}$ is illustrated in self-explanatory Figure 1 . Notice that α is assigned in such a way that, for every point of $T_{\nu\alpha}$, one has $x_{\alpha_1} \ge x_{\alpha_2} \le x_{\alpha_3}$.

Now, given an integer parameter p, $p\ge 1$, we uniformly subdivide C_ν into p^3 equal cubes, and next we join the vertices of these cubes within each tetrahedron $T_{\nu\alpha}$ through segments parallel to its six edges, thereby generating a partition of C_ν into $6p^3$ equal tetrahedrons.



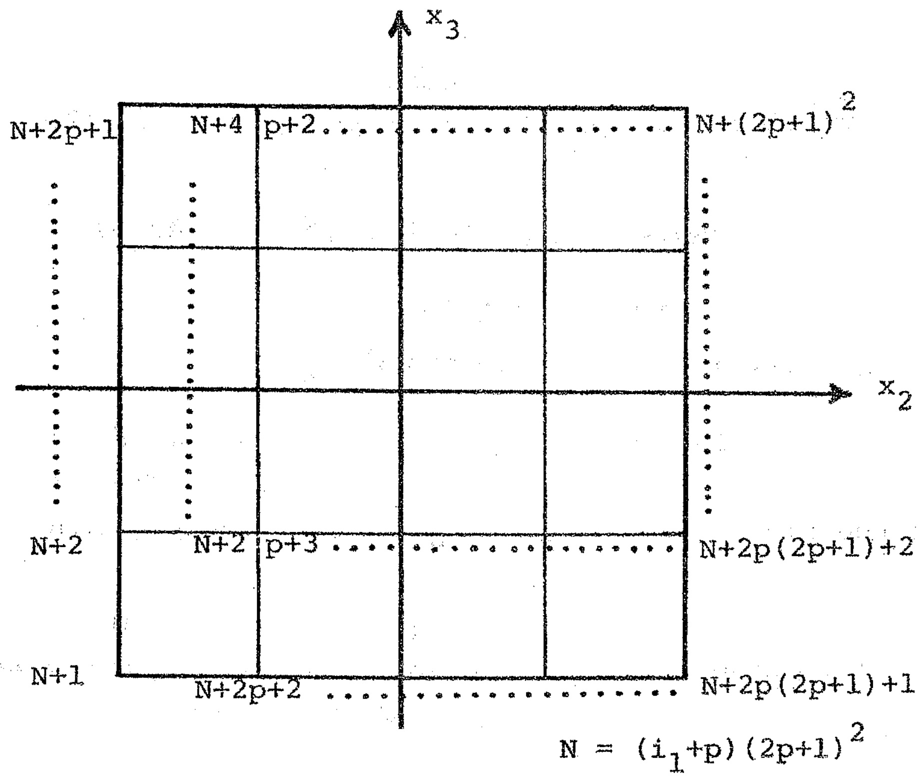
Octant $\mathcal{O}_\nu$ corresponding to the positive values of the co-ordinates Figure 1

Finally, taking the halves of the diagonals of C as a starting point, we proced in the same way for the other seven octants, thus generating a mesh for the whole cube, consisting of $48p^3$ tetrahedrons.

Notice that the coordinates of the vertices of all the tetrahedrons of the partition are of the form

$$\left(\frac{i_1}{2p}, \frac{i_2}{2p}, \frac{i_3}{2p}\right)$$

the i_k's being integers which satisfy $-p \le i_k \le p$. Moreover, it is possible to number the vertices from one to $(2p+1)^3$ in a straight - forward way, by numbering the vertices lying on each face $x_1 = i_1/2p$, one by one for $i_1 = -p$ up to p, in the standard way for squares , as shown in Figure 2 for the i_1-th face.



Numbering of the vertices lying on plane $x_1 = i_1/2p$

Figure 2

For the later convenience, we notice that the coordinates of the vertices lying in tetrahedron $T_{\mu\alpha}$ can be written in the form:

$$
(2.1)\quad \begin{cases} x_{\alpha_1} = (-1)^{\mu_1} \dfrac{-\ell}{2p} , & \ell = 0,1,\ldots,p \\ x_{\alpha_2} = (-1)^{\mu_2} \dfrac{-m}{2p} , & 0 \le m \le \ell \\ x_{\alpha_3} = (-1)^{\mu_3} \dfrac{-n}{2p} , & 0 \le n \le m \end{cases}
$$

Let now Ω be a starshaped domain whose boundary $\partial\Omega$ is given by an equation $\rho = f(\theta,\phi)$ in spheric coordinates, having a suitably chosen origin O in the interior of Ω. For such a domain we will apply a method for generating a partition into tetrahe - drons, which is entirely analogous to the one described above for the cube.

Again we first subdivide Ω into eight octants defined by the three cartesian axes with origin O, associated with the spheric coordinates. Like in the case of the cube, we denote by $\mathcal{C}_\mu$ the part of Ω lying in octant $\mathcal{O}_\mu$, and we take as a model the partition of $\mathcal{C}_\nu$, $\nu=(1,1,1)$ defined in the following way:

First we note that $\mathcal{O}_\nu$ is characterized by

$$0 \le \theta \le \pi/2 \quad \text{and} \quad 0 \le \phi \le \pi/2.$$

Let $\theta_M = \pi/4$ and $\phi_M = \arccos \sqrt{3}/3$.

Now referring to Figure 3, we subdivide $\mathcal{C}_\nu$ into six curved tetrahedrons $\tau_{\nu\alpha}$ with α defined as before. Each tetrahedron is contained in one of the six trihedrons with vertex at the origin and having one edge coinciding with the line given by $(\theta=\theta_M \;, \; \phi=\phi_M)$, while another edge is contained in a coordinate axis. The third edge is the bissector of the quadrant defined by this axis itself and one of the two other axes.

Let now $P_{\nu\alpha 1}$, $P_{\nu\alpha 2}$ and $P_{\nu\alpha 3}$ be the three vertices of $\tau_{\nu\alpha}$ lying on $\partial\Omega$.

Let also $\theta_{\nu\alpha i}$ and $\phi_{\nu\alpha i}$ be the angular coordinates of $P_{\nu\alpha i}$. As a reference we set $\theta_{\nu\alpha 1}=\theta_M$ and $\phi_{\nu\alpha 1}=\phi_M$ $\forall\alpha$, and we let $P_{\nu\alpha 2}$ be the point which lies on the x_{α_1}-axis. An illustration of the location of these points is given in Figure 4 for $\tau_{\nu\alpha}$, $\alpha=(2,3,1)$

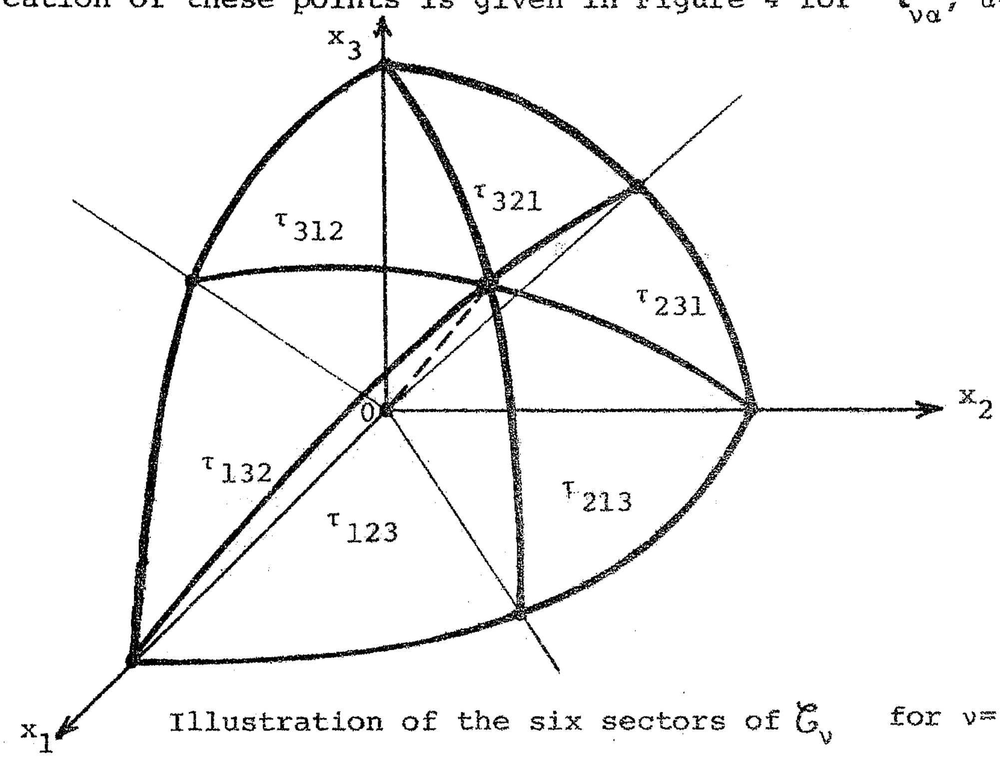
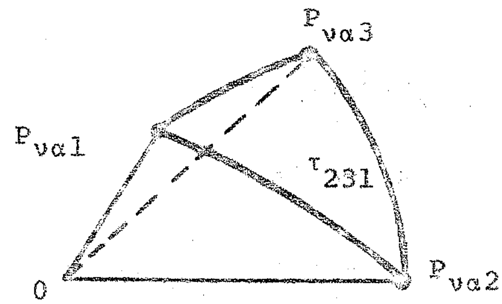


Illustration of the six sectors of $\mathcal{C}_\nu$ for $\nu=(1,1,1)$

Figure 3



$\nu = (1,1,1)$

$\alpha = (2,3,1)$

Location of the $P_{\nu\alpha i}$'s

Figure 4

Now we consider homotetical reductions Ω_ℓ of Ω with origin O and ratii ℓ/p, $\ell=1,2,\dots,p$.

For each sector $\tau_{\nu\alpha}$, the vertices of the partition are the points $P^{\ell mn}_{\nu\alpha}, 0\leq\ell\leq p$, $0\leq m\leq\ell$, $0\leq n\leq m$, defined as follows:

First we have $P^{\ell 00}_{\nu\alpha} = \frac{\ell}{p} P_{\nu\alpha 2} \qquad \forall\ell.$

Next, for fixed ℓ and $m\geq 1$ we have:

Let $\widehat{MON}$ be the angle with vertex at the origin, whose edges pass respectively through points M and N. We call M the left end and N the right end of the angle.

Now, if P is a point of $\partial\Omega$, we further define P^ℓ to be the point $\ell P/p$.

Let then $M^{\ell m}_{\nu\alpha}$ and $N^{\ell m}_{\nu\alpha}$ be the intersections of the polar radii which subdivide $\widehat{P^{\ell}_{\nu\alpha 2}\, O\, P^{\ell}_{\nu\alpha 3}}$ and $\widehat{P^{\ell}_{\nu\alpha 2}\, O\, P^{\ell}_{\nu\alpha 1}}$ into ℓ equal angles, numbered from m=0 up to $m=\ell$, from the left to the right end.

Points $P^{\ell mn}_{\nu\alpha}$ will be the intersections of the polar radii which subdivide $\widehat{M^{\ell m}_{\nu\alpha}\, O\, N^{\ell m}_{\nu\alpha}}$ into m equal angles, numbered from n=0 up to n=m, from the left end to the right end.

Finally we construct the partition of the whole domain by applying the technique just described in an analogous way to the other seven octants. This means that for each octant $_\mu$ we de - fine the associate six sectors $\tau_{\mu\alpha}$, in such a way that x_{α_1} contains one edge of $\tau_{\mu\alpha}$ for each μ, and one face of the same sector lies on the plane $x_{\alpha_3} = 0$. Similarly $P_{\mu\alpha 1}$ $\forall\mu$ and $\forall\alpha$, is taken to be the point of $\partial\Omega$ whose angular coordinates are:

$$\theta_{\mu\alpha 1} = \frac{5\pi}{4} + (\mu_1 - \mu_2 - 2\mu_1\mu_2)\,\frac{\pi}{2} \quad ; \quad \phi_{\mu\alpha 1} = (2\mu_3 - 1)\,\theta_M \quad \forall\alpha$$

and we let $P_{\mu\alpha 2}$ lie on the x_{α_1}-axis.

Next we determine the vertices of the tetrahedrons in the same way as described above for $\tau_{\nu\alpha}$.

Once we know the vertices of the partition, some possibilities remain on how to form the tetrahedrons within each sector $\tau_{\mu\alpha}$. We choose the following way, which yields compatibility at sector interfaces, as seen later.

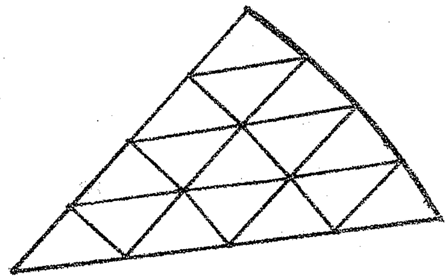
First we refer to the partition of the unit cube.

Now, recalling the expression (2.1) of the coordinates of the vertices of that partition, we can readily establish a one to one correspondence between these and the vertices of the partition of Ω given above. More specifically, this means that point $P_{\mu\alpha}^{\ell mn}$ corresponds to the point of the cube, whose cartesian coordinates are given by (2.1). Hence, if we assign to the $P_{\mu\alpha}^{\ell mn}$'s the same number as the one of the corresponding point of the cube, we can generate the tetrahedrons of the partition of Ω by simply defining their edges to be the segments whose ends have the same pairs of numbers as those for the edges of the tetrahedrons, lying in the unit cube.

Clearly enough, in this way we also obtain for Ω a partition consisting of $48p^3$ tetrahedrons. These can obviously be numbered in the same way as we do for the cube, that is to say, the number of a tetrahedron for Ω is the same as for the cube, if the numbers of their four vertices coincide.

Finally we note that the faces of tetrahedrons, which lie on plane sector interfaces form the same pattern as the triangulation of a sector in the two-dimensional case, as illustrated in Figure 5 for p=4.

p=4



Traces of the tetrahedrons over sector interfaces

Figure 5

3 - CALCULATING THE COORDINATES OF THE VERTICES

With the procedure described in the previous section, we get as a byproduct a straightforward procedure for calculating the coordinates of a vertex of the partition, given its number, say k, $1 \le k \le (2p+1)^3$. Indeed, all that we have to do is to determine μ, α, ℓ, m and n such that $P^{\ell mn}_{\mu\alpha}$ corresponds to the given number, in the following way:

First we can readily determine three integers k_1, k_2 and k_3 such that $1 \le k_i \le 2p+1$, $i=1,2,3$, and:

$$k=k_3+(2p+1)(k_2-1)+(2p+1)^2(k_1-1)$$

In so doing, the values of μ_1, μ_2 and μ_3 are given by:

$$\mu_i = N\left(\frac{k_i}{p+1}\right) \quad , \quad \text{where}$$

$$N(x)=\sup\{n/n\in \mathbb{N}, \ n \le x\}.$$

Next, setting $i_j=|k_j-1-p|$, $1 \le j \le 3$, we determine α by simply ordering the i_j's in such a way that:

$$i_{\alpha_1} \le i_{\alpha_2} \le i_{\alpha_3}.$$

Finally we set $\ell=i_{\alpha_1}$, $m=i_{\alpha_2}$ and $n=i_{\alpha_3}$.

Now all that is left to do is to apply the angle subdivision process described in the previous section, in order to obtain the spheric coordinates of the vertex, and hence its cartesian coordinates, according to the following calculations:

Let M and N be two points whose angular coordinates are (θ_1,ϕ_1) and (θ_2,ϕ_2) respectively. Let β be the angle $\widehat{MON}$ and $\beta_1=\ell\beta/q$, $\beta_2=(q-\ell)\beta/q$, $q\geq\ell\geq 0$.

Now, if x,y and z are the components of the unit vector in the direction of the line lying on the plane of $\widehat{MON}$, which subdivides β into ℓ and $q-\ell$ equal parts, counted from the left and from the right ends respectively, then they satisfy the following equations:

$$\begin{cases} a_1x+b_1y+c_1z=d_1 \\ a_2x+b_2y+c_2z=d_2 \\ x^2+y^2+z^2=1 \end{cases}$$

Where $d_i=\cos\beta_i$, $c_i=\sin\phi_i$, $b_i=\cos\phi_i\sin\theta_i$, $a_i=\cos\phi_i\cos\theta_i$, $i=1,2$.

The first two equations express the fact that point (x,y,z) lies on the surfaces of both cones with vertex at the origin, with axes OM_1 and OM_2, and whose half angles are β_1 and β_2, respectively.

Noticing that there is only one point which lies simultaneously on the surface of the unit ball and on these two surfaces, the system of equations above has only one easy-to-compute solution.

Finally, given x,y,z we compute associate values of θ and ϕ, from which we get $\rho=\ell f(\theta,\phi)/p$, and thus x_1, x_2 and x_3.

4- APPLICATION TO THE SOLUTION OF STEFAN PROBLEMS

In [10] an algorithm for solving two-dimensional one phase Stefan problems using the automatic triangulation process studied in [11], was proposed. We consider in this section an analogous version of that algorithm for the three-dimensional case, using the method for tetrahedral mesh generation described in sections 2 and 3.

As a model we take the following three-dimensional one phase Stefan problem:

We assume that a given medium exists in two phases one and two at time $t=0$, and let $u(x,t)$ be its temperature at point x and time t. We also assume that in one of the phases, say one , the medium is at temperature u_o for $t=0$ and that it occuppies a domain $\Omega_0 = \Omega^* - \bar{\Omega}_1$, where Ω^* and Ω_1 are simply connected open sets whose respective boundaries Γ_0 and Γ_1 can be expressed in spherical coordinates with origin lying in the interior of Ω_1. We assume that in phase two the medium initially occuppies the region $\mathbb{R}^3 - \Omega_0$, and that it is at the temperature of change of phase, namely $u=0$.

Let $\Omega(t)$ be the domain occuppied by phase one at time t and $\Gamma(t)$ be the interface between phases one and two, with $\Gamma(0)=\Gamma_0$. Now, if we apply heat sources on Γ_1, in such a way that the temperature is caused to be equal to a given function $g(x,t)$ $\forall x \in \Gamma_1$ and $\forall t$, u satisfies the heat equation, namely:

(4.1)
$$\begin{cases} \dfrac{\partial u}{\partial t} - \Delta u = 0 \quad \text{in} \quad \Omega(t) \times]0,\infty[\\ u(x,0) = u_o(x) \ \text{in } \Omega_0 \\ u(x,t) = 0 \quad \forall x \in \Gamma(t) \quad \text{and} \quad u(x,t) = g \quad \forall x \in \Gamma_1, \ \forall t \in]0,\infty[\end{cases}$$

Moreover, at the free boundary $\Gamma(t)$, the so-called Stefan condition holds, namely:

(4.2)
$$\nabla\phi \circ \nabla u_{/\phi(x,t)=0} = \frac{\partial \phi}{\partial t}$$

where ϕ is a function such that:

$$\begin{array}{lll} \phi(x,t) = 0 & \text{if} & x \in \Gamma(t) \\ \phi(x,t) < 0 & \text{if} & x \in \Omega(t) \cup \bar{\Omega}_1 \\ \phi(x,t) > 0 & \text{if} & x \notin \overline{\Omega(t) \cup \Omega_1} \end{array}$$

Like in [10] it is convenient to write ϕ in the form

(4.3)
$$\phi = \rho - s(\theta,\phi,t)$$

Notice that, since $u=0$ on $\Gamma(t)$, we can express ∇u only in terms of $\partial u/\partial\rho$ and s for $\rho=s(\theta,\phi,t)$. More specifically we have

$$(4.4)\qquad \frac{\partial u}{\partial\theta}\Big/_{\Gamma(t)} = -\frac{\partial s}{\partial\theta}\,\frac{\partial u}{\partial\rho}\Big/_{\Gamma(t)}$$

$$\frac{\partial u}{\partial\phi}\Big/_{\Gamma(t)} = -\frac{\partial s}{\partial\phi}\,\frac{\partial u}{\partial\rho}\Big/_{\Gamma(t)}$$

Hence, taking (4.3) and (4.4) into (4.2), after simple calculations, the Stefan condition becomes:

$$(4.5)\qquad -\frac{\partial s}{\partial t} = \left[1+\left(\frac{1}{s\sin\phi}\,\frac{\partial s}{\partial\theta}\right)^2+\left(\frac{1}{s}\,\frac{\partial s}{\partial\phi}\right)^2\right]\frac{\partial u}{\partial\rho}\Big/_{\rho=s(\theta,\phi,t)}$$

Now we define the discrete analogue of (4.1)-(4.5) using the automatic tetrahedral mesh generator. In order to avoid nonessential difficulties, we assume that Γ_1 is reduced to a point, namely, the origin of coordinates.

We first approximate $\Omega_0\cup\{0\}$ by a polyhedron Ω_h^0, whose boundary Γ_h^0 has triangular faces. For a given $p\geq 1$, the vertices of Γ_h^0 are precisely the intersections with Γ_0 of the lines defined by $\theta=\theta_{\mu\alpha}^{pmn}$ and $\phi=\phi_{\mu\alpha}^{pmn}$, $\forall\mu,\alpha$ $0\leq m\leq p$, $0\leq n\leq m$.

Let us number the vertices of Γ_h^0 from one to $24p^2+2$, and let s_j^0 be the radial coordinate of the j-th vertex, which we denote by P_j. This vertex is characterized by its angular coordinates θ_j and ϕ_j.

Remark: Each pair of angles $(\theta_{\mu\alpha}^{pmn}, \phi_{\mu\alpha}^{pmn})$ is obviously associated with one value of j. Two or more such pairs will correspond to the same vertex number in case it lies at sector interfaces.

Next we construct the partition of Ω_h^0 using the method of section 2. This construction is obviously possible, since the fact that Ω_0 is starshaped implies that Ω_h^0 is also starshaped. Incidentally, a representation of Γ_h^0 in spheric coordinates $\rho=s_h^0(\theta,\phi)$ can be obtained if we procede as follows:

First we number the faces of $\overset{0}{\Gamma}_h$ from one up to $48p^2$. Next we define a $48p^2\times 3$ array R, whose k-th line contains the number j, $1\le j\le 24p^2+2$ of the vertices of the k-th face of $\overset{0}{\Gamma}_h$. Now we consider that $\overset{0}{s}_h$ varies linearly with x_1, x_2 and x_3 over each face of $\overset{0}{\Gamma}_h$, and that $\overset{0}{s}_h(\theta_j,\phi_j)=\overset{0}{s}_j$, $1\le j\le 24p^2+2$.

Since $s_h^0(\theta,\phi)$ does not have a simple expression, in order to calculate the coordinate of a vertex $P_{\mu\alpha}^{\ell mn}$ of the partition of $\overset{0}{\Omega}_h$, we must determine the number k_o of the face at which the line defined by $\theta=\theta_{\mu\alpha}^{\ell mn}$ and $\phi=\phi_{\mu\alpha}^{\ell mn}$ intersects $\overset{0}{\Gamma}_h$. This face can be determined by means of the following calculations:

Let T_k be the tetrahedron whose vertices are the origin and P_{j_i}, $j_i= R(k,i)$, $1\le i\le 3$ (refer to Figure 6). Taking O to be the fourth vertex of T_k, let λ_i be the volume coordinates of T_k associated with the so-defined local numbering of its vertices, $1\le i\le 4$. Let P be the point (x,y,z) where:

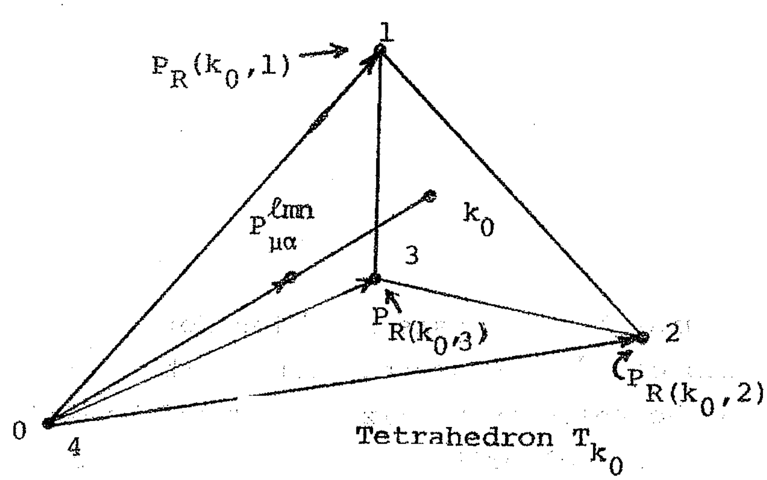
$$x = \sin\phi_{\mu\alpha}^{\ell mn} \cos\theta_{\mu\alpha}^{\ell mn}$$

$$y = \sin\phi_{\mu\alpha}^{\ell mn} \sin\theta_{\mu\alpha}^{\ell mn}$$

$$z = \cos\phi_{\mu\alpha}^{\ell mn} .$$

k_o will be any number such that for tetrahedron T_{k_o} we have

$$\lambda_i(x,y,z)\ge 0 \quad \text{for } i=1,2 \text{ and } 3.$$



k_o-th boundary face associated with vertex $P_{\mu\alpha}^{\ell mn}$

Figure 6

For the later convenience, we store the k_o's in an array S of dimension $(2p+1)^3$. More specifically, S(J) is the number of the boundary face intersected by the line $\theta=\theta_J$, $\phi=\phi_J$, where θ_J and ϕ_J are the angular coordinates of the J-th vertex of the partition. It is also useful to introduce three auxiliary $48p^2 \times 3$ arrays X_s, such that $X_s(k,i)$ is the x_s-coordinate of the i-th vertex of the k-th face, $1\leq s\leq 3$.

Now, given $\Delta t>0$, assume that we know starshaped approximations Ω_h^N and Γ_h^N of $\Omega(N\Delta t)$ and $\Gamma(N\Delta t)$ respectively which are nothing but polyhedrons with triangular faces, whose j-th vertex lies on the same radius as the j-th vertex of Γ_h^0, $\forall N$, $N=1,2,\ldots$ Let s_j^N be the radial coordinate of the j-th vertex of Γ_h^N. In an entirely analogous way as we did for Γ_h^0 and Ω_h^0, we define the equation $\rho=s_h^N(\theta,\phi)$ of Γ_h^N, and we construct the partition of Ω_h^N into $48p^3$ tetrahedrons.

Now we calculate continuous piecewise linear approximations u_h^n of $u(x,N\Delta t)$, associated with the vertices of Ω_h^N by:

$$(M^N + \Delta t\, A^N)u_h^N = M^N u_h^{N-1}$$

with $u_h^N(0) = g(N\Delta t)$,

The generic terms of matrices A and M are respectively given by.

$$a_{ij} = \int_{\Omega_h^N} \nabla\phi_i^N \cdot \nabla\phi_j^N + \int_{\Omega_h^N} \frac{\phi_j^N - \phi_j^{N-1}}{\Delta t} \phi_i^N$$

$$m_{ij} = \int_{\Omega_h^N} \phi_i^N \, \phi_j^N ,$$

where ϕ_i^N is the piecewise linear basis function for the i-th vertex of the partition of Ω_h^N. The second term in the expression of a_{ij} corresponds to the velocity matrix introduced by MORI [6], in the study of an analogous algorithm for one-dimensional problems.

The boundary Γ_h^N can be determined at each time step, if one knows the increment Δs_j^N of the radius s_j^{N-1}, in the fixed direction $(\theta=\theta_j,\ \phi=\phi_j)$. This increment is obtained by means of the following discretization of (4.5):

$$(4.6)\qquad -\frac{\Delta s_j^N}{\Delta t} = \left\{ 1 + \left[\frac{\left(\frac{\partial s_h^N(\theta,\phi)}{\partial\theta}\right)_{j,h}}{(s_h^N(\theta,\phi)\ \sin\phi)_{j,h}} \right]^2 + \left[\frac{\left(\frac{\partial s_h^N(\theta,\phi)}{\partial\phi}\right)_{j,h}}{(s_h^N(\theta,\phi))_{j,h}} \right]^2 \right\} \frac{\partial u_h^N}{\partial\rho}\Big/_{\Gamma_h^N}$$

The notation $(\ .\ )_{j,h}$ stands for an averaging process in the neighborhood of the j-th vertex, defined as follows:

First we let $\mathcal{K}_j$ be the set of faces K of Γ_h^N such that $\bar{K}$ contains vertex P_j. Let M_j denote the cardinal of $\mathcal{K}_j$.

$\left(\frac{\partial s_h}{\partial\theta}\right)_{j,h}$ is the mean value of $\frac{\partial s_h}{\partial\theta}$ given by:

$$\left(\frac{\partial s_h}{\partial\theta}\right)_{j,h} = \frac{1}{M_j} \sum_{K\in\mathcal{K}_j} \int_K \frac{\partial s_h}{\partial\theta}\ ds/\text{area}(K)$$

with an analogous definition for $\left(\frac{\partial s_h}{\partial\phi}\right)_{j,h}$.

Similarly we can evaluate the denominators of (4.6) by

$$(s_h^N \sin\phi)_{j,h} = \frac{1}{M_j} \sum_{K\in\mathcal{K}_j} \int_K s_h^N \sin\phi\ ds\ /\text{area}(K)$$

$$(s_h^N)_{j,h} = \frac{1}{M_j} \sum_{K\in\mathcal{K}_j} \int_K s_h^N\ ds\ /\ \text{area}(K)$$

Remark: The purpose of the latter averaging is to avoid the singularity occurring in the first denominator for $\phi=0$. Except for this restriction, at other vertices one may simply set:

$$(s_h^N)_{j,h} = s_j^N \quad\text{and}\quad (s_h^N \sin\phi)_{j,h} = s_j^N \sin\phi_j. \qquad \Box$$

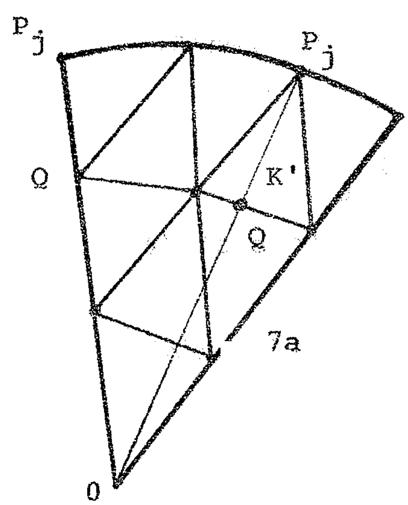
Let us now turn to the problem of calculating the radial derivative of u_h^N at points P_j.

We have three different situations:

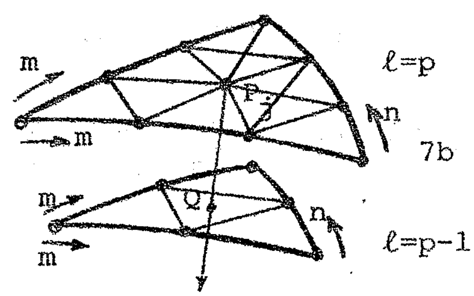
1^{st}) $m=p$, $n=m$, or $n=0$

In this case $\frac{\partial u_h^N}{\partial \rho}$ is obtained like in the two-dimensional version of the algorithm [10], and we have to distinguish two cases:

<u>Case 1</u>: The vertex is not an end of the curved boundary of the plane sector associated with the above values of m and n. We calculate the derivate using triangle of type K shown in Figure 7a below, according to Formula (4.7).



$$(4.7) \quad \frac{\partial u_h^N}{\partial \rho}(P_j) = \frac{u_h^N(P_j) - u_h^N(Q)}{\text{length } (P_jQ)}$$



Calculation of the radial derivate of u_h^N

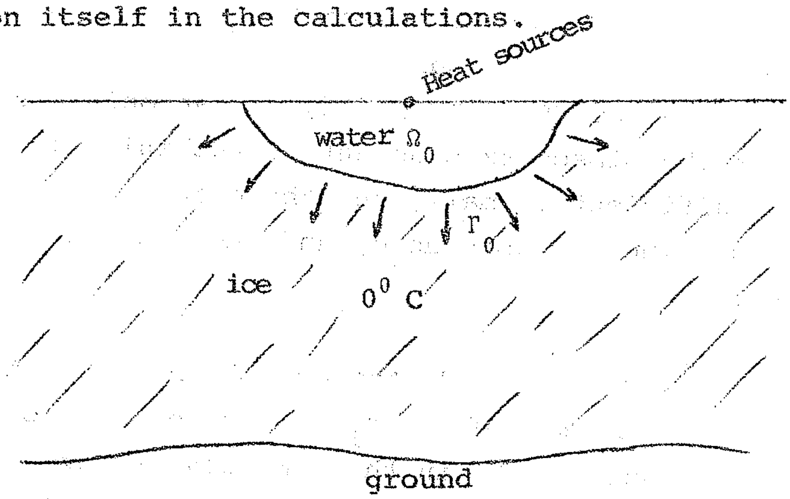
Figure 7

<u>Case 2</u>: The vertex is an end of this curve, in which case we use again (4.7) in connection with triangle K' shown in Figure 7a.

2nd) $0<m<p$ and $n \neq m$

In this case, noticing that the polar radius associated with the boundary vertex intersects the interior of the face whose vertices are $P_{\mu\alpha}^{p-1,m,n}$, $P_{\mu\alpha}^{p-1,m-1,n}$ and $P_{\mu\alpha}^{p-1,m-1,n-1}$, assuming $P_j \equiv P_{\mu\alpha}^{pmn}$, and referring to Figure 7b, the radial derivative can be readily computed by (4.7).

Finally we remark that the above algorithm seems to be particularly suitable for the numerical simulation of ice melting processes above the ground, starting from a small portion of water, where the heat sources are applied, as illustrated in Figure 8. Indeed with simple adaptations one can use our scheme in order to plot the evolution of the water-ice interface through large regions of ice at 0^{o}C, without taking into account the ice region itself in the calculations.



A case where the use of the algorithm is recommended

Figure 8

5 - CONCLUDING REMARKS

1) Some problems may arise when using the mesh generation process described in this paper, if the boundary of the domain has locally large Lipschitz constants with respect to θ and ϕ. In particular in [11] one can find hints on how to remedy an eventual "inside out turning" of the elements.

2) In a forthcoming paper we will deal with the problem of numbering the nodes for any finite element method, in con-

nection with the partition that we consider in this paper. More specifically we will give procedures for optimal and automatic numbering of the nodes.

3) Likewise in the two-dimensional case, the feasability of the algorithm for solving one phase Stefan problems treated in this paper depends on the fact that the domain remains starshaped at every time step. Notice that this will be the case, provided the increment Δs_j^N is positive for every j and N. If g is nonnegative, this will be the consequence of the validity of a discrete maximum principle, in connection with the partition of Ω_h^N (see e.g. [3]). Although in the analagous continuous case (4.1) the fact that the domain remains starshaped for every time t was proved by FRIEDMAN [2], we can only conjecture that if the Lipschitz constant of the initial boundary Γ_0 is sufficiently small, the above mentioned discret maximum principle does hold, and therefore the same result applies.

4) Finally we note that the adaptations of the algorithm of Section 4 to the case where Γ_1 is not reduced to a point, can be carried out in the same way as for the two-dimensional case [10]. This simply means that one reduces and subdivides into equal parts, the segment of each polar radius lying between Γ_1 and Γ_h^N, instead of the polar radius of Γ_h^N itself.

R E F E R E N C E S

[1] CIARLET, P.G.,The finite element method for elliptic problems, North Holland, 1978

[2] FRIEDMAN, A. & KINDERLEHRER, D., A one-phase Stefan pro - blem, Indiana Univ. Math. J. 24(1975)1005-1035.

[3] FUJII, H., Some remarks on finite element analysis of time-dependent field problems, in: Theory and Practice in Finite Element Structural Analysis, Univ. Tokyo Press , Tokyo, 1973, 91-106.

[4] GEORGE, A., Computer implementation of the finite ele - ment method, Stan CS-71-208, Comp. Sci. Dept. Stanford Univ. Calif. 1971.

[5] HERMELINE, Um méthode automatique de maillage en dimen - sion n, Thèse de Doctorat 3^{e} cycle, Univ. Pierre et Marie Curie, Paris, 1980.

[6] MORI, M., Stability and convergence of a finite element method for solving the Stefan problem, Publ. RIMS, Kyoto Univ. 12 (1976) 539-563.

[7] PALMER, J.C. & RUAS, V., Numeração automática de nós para uma família de partições regulares em elementos fi - nitos de tipo simplex, to appear in Revista Brasileira de Computação.

[8] PERRONNET, A., Le module APMEFI, Version 3.2, Club MODU - LEFF, INRIA, France, May 1981.

[9] RUAS, V., Sur l'application de quelques méthodes d'élé - ments finis non conformes à la résolution des problèmes de la flexion et de vibrations de plaques minces, Thèse de 3^{e} cycle, Univ. Pierre et Marie Curie, Paris, 1976.

[10] RUAS, V., A direct method for solving two-dimensional one-phase Stefan problems, Computer Methods in Appl.Mechs. and Engineering, 25(1981)51-64.

[11] RUAS, V., Automatic generation of triangular finite element meshes, Comp. Math. Appl. 5 (1979) 125-140.

[12] SANCHEZ SARMIENTO G., REDEF, um esquema simple para la generación automática de redes de elementos finitos bidimensionales, Tech. Report CNEA-NT 16/80, Centro Atómico Bariloche, Argentina, 1980.