Structured Hexahedral Harmonic Grid Generation.

Barrera Sánchez P., Castellanos L., Cortés J. J., and González Flores G.

Universidad Nacional Autónoma de México, Ciudad Universitaria, México City.
antoniolapetra@gmail.com, jjcaa1@gmail.com, guilmerg@gmail.com

Summary. In this work we present an improved numerical method for structured convex hexahedral grid generation that also produces good quality grids.

1 Introduction.

In $\mathbb{R}^3$ it is difficult to have an efficient algorithm to generate structured hexahedral grids (Knupp [5]). In this paper, we are going to follow the work of Ivanenko [4] and Azarenok [1] in order to build harmonic convex hexahedral grids using an improvement of Azarenok's method through the quasi-harmonic formulation used by Barrera [2] for the 2D problem.

2 Harmonic grids.

A structured grid can be defined as a mapping from the unitary cube onto a simply connected region $\Omega \subset \mathbb{R}^3$ as follows:

A grid $\overline{x}(\bar{\xi})$ on the region $\Omega \subset \mathbb{R}^3$ is a homeomorphism

$$\overline{x} : B \to \Omega \tag{1}$$

where B is the unitary cube $[0,1] \times [0,1] \times [0,1]$.

This mapping induces a natural decomposition of $\partial\Omega$ into six faces, since each face of the cube is mapped to a face of the boundary of Ω

$$\bar{x}(\partial B) = \partial\Omega = \bigcup_{i=1}^{6} \Omega_i \tag{2}$$

with

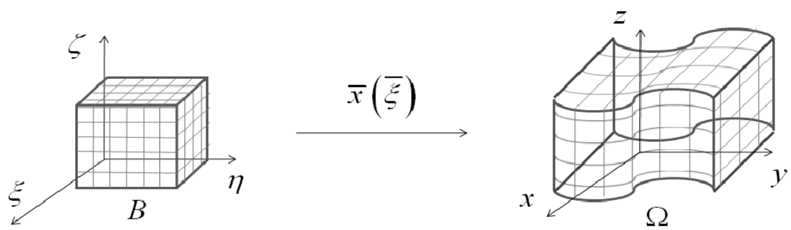


Fig. 1. Grid mapping.

$$\begin{aligned} \Omega_1 &= \bar{x}(B_1)\ , \quad \Omega_2 = \bar{x}(B_2), \\ \Omega_3 &= \bar{x}(B_3)\ , \quad \Omega_4 = \bar{x}(B_4), \\ \Omega_5 &= \bar{x}(B_5)\ , \quad \Omega_6 = \bar{x}(B_6). \end{aligned} \tag{3}$$

where B_i is each face of the untary cube. Hence, each face mapping induces a continuous grid on the surface of Ω_i

$$\bar{x}\big|_{B_i} : B_i \to \Omega_i.$$

A first example of this decomposition is illustrated by the construction of a grid on an ellipsoid, that can be made by using a similar method to that used by LeVeque in [6] to construct a grid on the unitary sphere. Consider an ellipsoid with center at the origin and radius lengths equal to 0.5 along the x, z axes and 1 along the y axis; the method uses a radial mapping of the cube defined in $[-1, 1] \times [-1, 1] \times [-1, 1]$ such that each face of the cube determines a face of the ellipsoid.

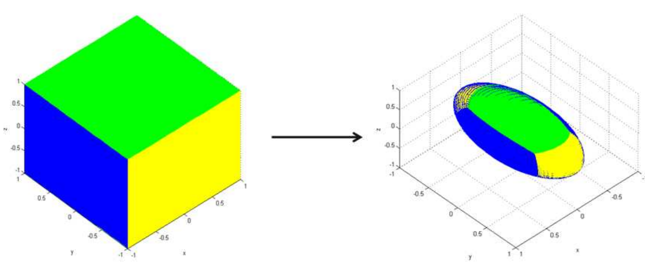


Fig. 2. Radial mapping from the cube to the ellipsoid.

Certainly, this process is more complicated in regions with a more complex geometry, especially in those with irregular boundary (figure 3).

Hence, in order to find suitable grids with that properties, the harmonic mappings are a powerful tool. If we define the local energy of the mapping $\bar{x}$ at $\bar{\xi}$

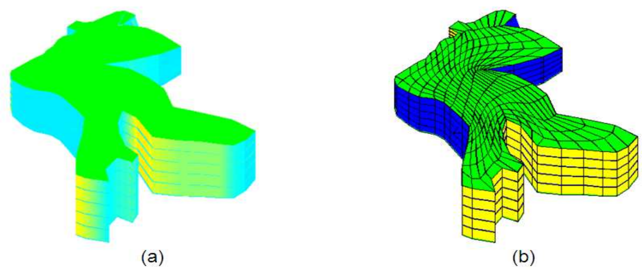


Fig. 3. (a) Habana bay with its six faces. (b) A grid on the Habana bay.

$$E(\bar{x}) = \frac{1}{3^{3/2}} \frac{\left(||\bar{x}_\xi||^2 + ||\bar{x}_\eta||^2 + ||\bar{x}_\zeta||^2\right)^{3/2}}{\bar{x}_\xi \cdot (\bar{x}_\eta \times \bar{x}_\zeta)}. \tag{4}$$

then we can look for the mapping H that minimizes the total energy

$$H(\bar{x}) = \int_B E(\bar{x}) d\xi d\eta d\zeta \tag{5}$$

subject to the given boundary conditions. Liseikin [8] shows that this mapping exists and is an homeomorphism.

The harmonic grid generation problem consist in extending a given homeomorphism $\phi : \partial B \to \partial \Omega$ to a homeomorphism $\bar{x}^* : B \to \Omega$ in such a way that ϕ is a minimizer of H. A possibility to find this extension is to solve the associated Euler-Lagrange equations, however we don't pursue this idea, but that of Ivanenko *et al* [4] based on the discretization of the functional and the calculation of its minimum through a numerical optimization process.

3 Discrete formulation.

Let us consider a uniform grid of dimension $m \times n \times p$ on the unitary cube

$$U = \left((\xi_i, \eta_j, \zeta_k) = \left(\frac{i-1}{m-1}, \frac{j-1}{n-1}, \frac{k-1}{p-1} \right) \middle| 1 \leq i \leq m, 1 \leq j \leq n, 1 \leq k \leq p \right); \tag{6}$$

a discrete grid M of dimension $m \times n \times p$ on Ω can be obtained as the image of U under the homeomorphism $\bar{x}$

$$M = \bar{x}(U).$$

However, we require a specific order on its points, for this reason we introduce the following definition of a **structured discrete grid.**

Let m, n, p natural numbers higher than 2, the set of points of the space that compose a ***structured discrete grid*** *is given by*

$$M = \{P_{i,j,k} | i = 1, ..., m; j = 1, ..., n; k = 1, ..., p\} \tag{7}$$

where the grids on each one of the faces are given by

$$\begin{aligned} M_1 &= \{P_{i,1,k} | i = 1, ..., m, k = 1, ..., p\} \subset \Omega_1 \\ M_2 &= \{P_{1,j,k} | j = 1, ..., n, k = 1, ..., p\} \subset \Omega_2 \\ M_3 &= \{P_{i,n,k} | i = 1, ..., m, k = 1, ..., p\} \subset \Omega_3 \\ M_4 &= \{P_{m,j,k} | j = 1, ..., n, k = 1, ..., p\} \subset \Omega_4 \\ M_5 &= \{P_{i,j,1} | i = 1, ..., m, j = 1, ..., n\} \subset \Omega_5 \\ M_6 &= \{P_{i,j,p} | i = 1, ..., m, j = 1, ..., n\} \subset \Omega_6 \end{aligned} \tag{8}$$

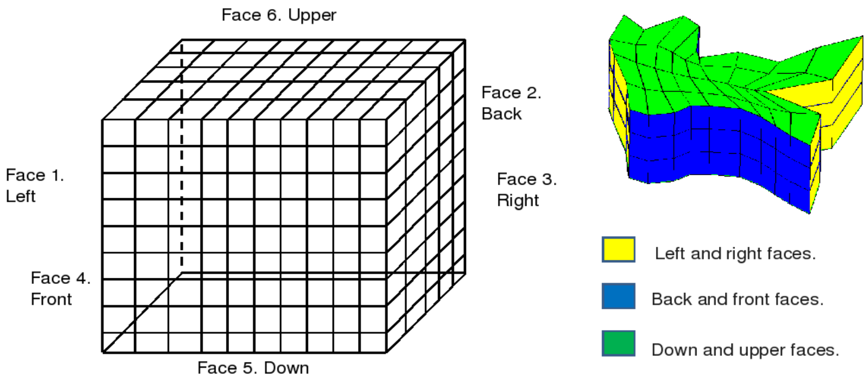


Fig. 4. A structured discrete grid.

A grid cell $C_{i,j,k}$ is formed by the vertices

$$\begin{aligned} r_1 &= P_{i,j,k}, & r_2 &= P_{i+1,j,k}, \\ r_3 &= P_{i+1,j+1,k}, & r_4 &= P_{i,j+1,k}, \\ r_5 &= P_{i,j,k+1}, & r_6 &= P_{i+1,j,k+1}, \\ r_7 &= P_{i+1,j+1,k+1}, & r_8 &= P_{i,j+1,k+1}. \end{aligned}$$

where $1 \leq i \leq m-1$, $1 \leq j \leq n-1$ and $1 \leq k \leq p-1$. Note that if $1 < i < m-1, 1 < j < n-1, 1 < k < p-1$, $C_{i,j,k}$ is an interior cell.

Consider two dodecahedrons with the same vertices, each one of them with five tetrahedra, four at the corners and one in the interior. Then, each grid cell will be divided into ten tetrahedra, eight at the corners and two interior ones.

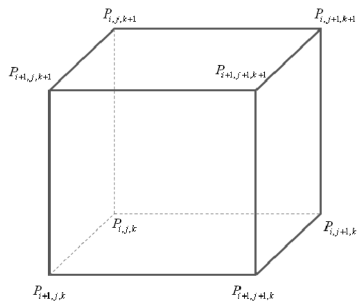


Fig. 5. The cell $C_{i,j,k}$ of the grid.

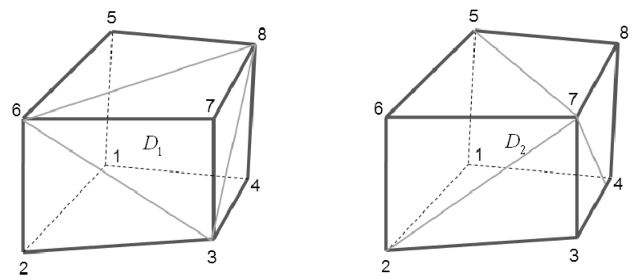


Fig. 6. The two dodecahedrons obtained from the cell.

This tetrahedral partition is very important since it will be used to define the convexity conditions.

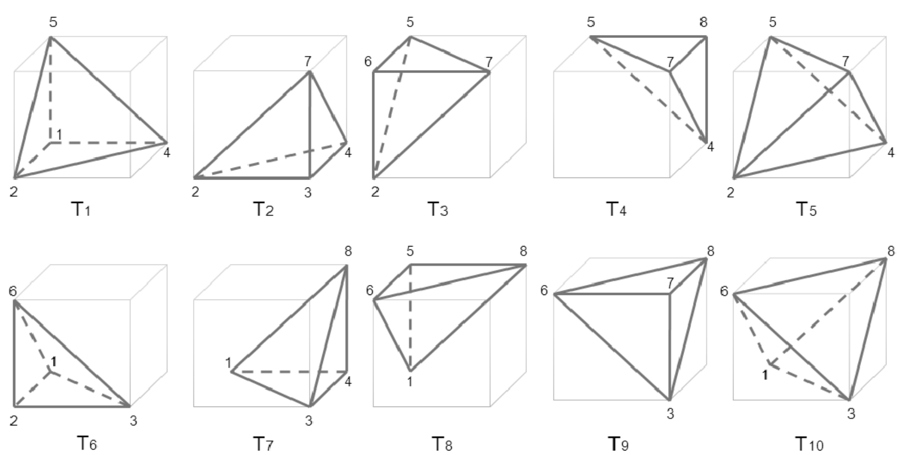


Fig. 7. The 10 tetrahedra in the cell.

In the discrete formulation, we need to define what we understand for a convex and hexahedral grid. Since a given M induces an approximation Ω_h of Ω called **hexahedral approximation** of Ω, it is straightforward to make the following definition.

Convex hexahedral grid. *Let Ω be a region in $\mathbb{R}^3$ whose discrete representation is given by the hexahedral approximation Ω_h, we say that a grid M on Ω_h is convex and hexahedral if all its cells are convex and hexahedral.*

Thus, the main problem to solve is as follows:

Let Ω be a region in $\mathbb{R}^3$ whose discrete representation is given by the hexaedral aproximation Ω_h, we want generate a discrete structured grid M on Ω_h such that the grid be convex and hexaedral.

We start by solving the problem of generating convex harmonic grids, later on we discuss the hexahedral part. Then, we need to analyze the possible convexity conditions on the cells.

3.1 Convexity conditions.

In 2D, the condition to guarantee that the mapping is a homeomorphism and every cell is convex is that the Jacobian of the bilinear mapping to be positive in all the points of the cell (particularly at the corners).

In 3D, the trilinear mapping from each cell of the unitary cube $C = \{(\xi, \eta, \zeta) : 0 \leq \xi, \eta, \zeta \leq 1\}$ onto a cell in the space x, y, z is given by

$$r(\xi, \eta, \zeta) = w_1 + w_2\xi + w_4\eta + w_5\zeta + w_3\xi\eta + w_6\xi\zeta + w_7\xi\eta\zeta \tag{9}$$

with

$$w_1 = r_1,\, w_2 = r_2 - r_1,\, w_3 = r_3 - r_2 - r_4 + r_1$$
$$w_4 = r_4 - r_1,\, w_5 = r_5 - r_1,\, w_6 = r_6 - r_2 - r_5 + r_1$$

$$w_7 = r_7 - r_3 - r_6 - r_8 + r_2 + r_4 + r_5 - r_1, \quad w_8 = r_8 - r_4 - r_2 + r_1$$

and r_i the coordinates of the vertex i of the cell (fig 5).

However, a similar condition to that in 2D can not be easily obtained since the Jacobian of the trilinear mapping is given by the mixed product

$$J(\xi, \eta, \zeta) = r_\xi \cdot (r_\eta \times r_\zeta) \tag{10}$$

with

$$r_\xi = w_2 + w_3\eta + w_6\zeta + w_7\eta\zeta,\ r_\eta = w_4 + w_3\xi + w_8\zeta + w_7\xi\zeta,$$
$$r_\zeta = w_5 + w_6\xi + w_8\eta + w_7\xi\eta \qquad (11)$$

In this case, the Jacobian is a fourth degree polynomial that depends on the variables ξ, η, ζ, hence we can't have a necessary and sufficient convexity condition based only on the Jacobian of the trilinear mapping evaluated at the tetrahedrals. Up to the present date, such conditions remains unknown.

Using the analysis made by Azarenok [1] and Ushakova [9] it is possible to give a short condition to verify the convexity of the cells which is reliable in most of the cases. To do this, we use the dodecahedrical cells and the tetrahedra illustrated in the figures 6 and 7. First, we need to consider an orientation of the cells grid in such a way that a convex cell has all its tetrahedra with positive volume.

Therefore, a convexity condition for a cell can be:

$$volume(T_l) > 0, \quad l = 1, 2, ..., 10 \qquad (12)$$

with T_l the volume of the tetrahedron l of the cell $C_{i,j,k}$.

3.2 The harmonic functional (discrete version).

It is possible to approximate the discrete functional is by means of the trilinear mapping (9), however, for this approximation the mapping $\bar{x}$ might not be a homeomorphism. Then using a set of linear transformations of the basic tetrahedron in the space ξ, η, ζ on its correspondent tetrahedron in the space x, y, z, we can get a discretization of the harmonic functional in function of that ones.

Since

$$\int_B E(\bar{x})d\xi d\eta d\zeta = \sum_{i,j,k} \int_{B_{i,j,k}} E(\bar{x})d\xi d\eta d\zeta,$$

and there is a set of linear transformations that define the tetrahedra in the physical space, we can discretize the functional by simply averaging over the 10 tetrahedra defined by the two dodecahedrons in fig. 6

$$\int_{B_{i,j,k}} E(\bar{x})d\xi d\eta d\zeta \approx \sum_{i=1}^{10} \frac{1}{10}[E_i];$$

hence we can approximate the total sum in a similar form and get the discrete version of the harmonic functional

$$H^d(M) = \frac{1}{N_c} \sum_{j=1}^{N_c} \sum_{i=1}^{10} \frac{1}{10}[E_i]_j \qquad (13)$$

with M a discrete structured grid, $[E_i]_j$ the value of the integrand in each tetrahedron i of the cell j, and N_c the total number of grid cells.

The discretization is well defined only for grids having positive volume in all the tetrahedra. Working with that kind of grids we can solve the problem

$$Compute: \quad M^* = arg\min_M H^d(M) \tag{14}$$

and get an harmonic grid through a large-scale optimization problem with $3(m-2)(n-2)(p-2)$ variables.

However, the construction of an initial grid with this property can be very expensive and in the optimization process we could obtain tetrahedra with negative volume.

To overcome this pitfall we propose a variant of the discrete harmonic functional, namely the H_ω functional, using the main ideas developed by Barrera and Domínguez in [3] for the 2D problem.

3.3 The quasi-harmonic functional H_ω.

Let us write the function (4) in the form $\frac{\lambda(\bar{x})}{V(\bar{x})}$ where

$$\begin{aligned} \lambda(\bar{x}) &= \frac{1}{3^{3/2}}\left(||\bar{x}_\xi||^2 + ||\bar{x}_\eta||^2 + ||\bar{x}_\zeta||^2\right)^{3/2} \\ V(\bar{x}) &= \bar{x}_\xi \cdot (\bar{x}_\eta \times \bar{x}_\zeta). \end{aligned}$$

For the latter formula one can see that if for a tetrahedron T_i the value of $V(T_i) = volume(T_i)$ is very small or negative the optimization process can fail.

The idea in H_ω functional consist in choosing a suitable parameter value $\omega > 0$, next to define a positive, convex and strictly decreasing real function $\varphi_\omega(V) \in C^1$, and use it to “fix” the functional H^d. Due to numerical purposes, an effective election is

$$\varphi_\omega(V) = \begin{cases} \frac{2\omega - V}{\omega^2}, & V < \omega \\ \frac{1}{V}, & V \geq \omega \end{cases} \tag{15}$$

since if V takes a value smaller than ω then the functional takes a “safe” value instead of the natural value of the functional (see the figure 8) . Thus we get a functional with a numerical performance which is close similar to that of H^d but without its numerical complications.

Hence, the functional H_w is defined as

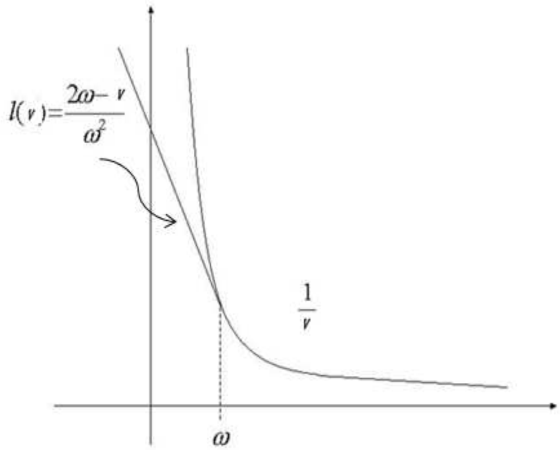


Fig. 8. Graphic visualization of the funcion $\varphi_\omega(V)$.

$$H_w = \frac{1}{N_c}\sum_{j=1}^{N_c}\sum_{i=1}^{10}\frac{1}{10}\lambda_{i,j}\varphi_{\omega_{i,j}}, \tag{16}$$

where $\lambda_{i,j}$ and $\varphi_{\omega_{i,j}}$ represent the evaluations of λ and $\varphi_\omega(V)$ in the tetrahedron i of the cell j, and N_c is the total number of cells.

4 Optimization procedure (convex harmonic grids).

Once the discrete functional H_w has been defined, the next step is to compute the minimum of a large scale optimization problem without restrictions.

The process starts with a possibly non-convex initial generated by algebraic methods. Note that not all the grid points have to be taken into account in the optimization process since only the interior points are variable, therefore, before the optimization process we need determinate those tetrahedra in the grid cells having all its vertices in the boundary and verify wether its volumes is positive. Other important condition is the convexity of the boundary grids.

Hence, the optimization problem to be solved is:

$$Compute: \quad M^* = arg\min_M H_w(M) \tag{17}$$

over the set of grids for the hexaedral aproximation Ω_h.

To solve this problem a Newton truncated method with a trust region strategy is used [7]. The main requirements for the method are:

a) Function evaluations.
b) Value of the function gradients.
c) Sparsity patron of the hessian matrix.

The formulas used for the function and gradients evaluations are the same ones used by Azarenok in [1].

4.1 Practical algorithm.

The basic structure of the algorithm is as follows:

a) Choose an initial and admisible grid M_0 (usually non convex).
b) Choose $\omega_0 > 0$ such that the functional H_ω is well defined for M_0.
c) Solve a large scale optimization problem to find an optimal grid M^* of $H_\omega(M)$.
d) Update

$$
\begin{aligned}
M_0 &\leftarrow M^* \\
\omega_0 &\leftarrow \frac{1}{2}\omega_0
\end{aligned}
$$

e) Repeat the process until a convex harmonic grid has been found.

Next we show some examples of three dimensional harmonic convex grids generated by this algorithm.

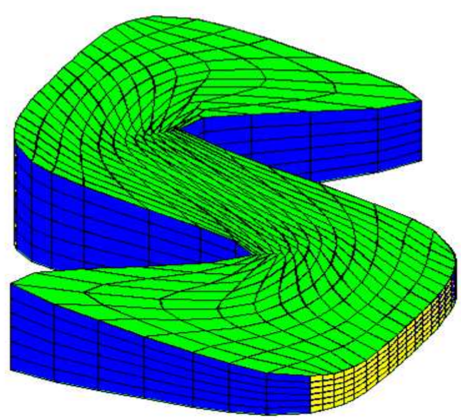


Fig. 9. A Grid of the swan of dimension $20 \times 20 \times 7$.

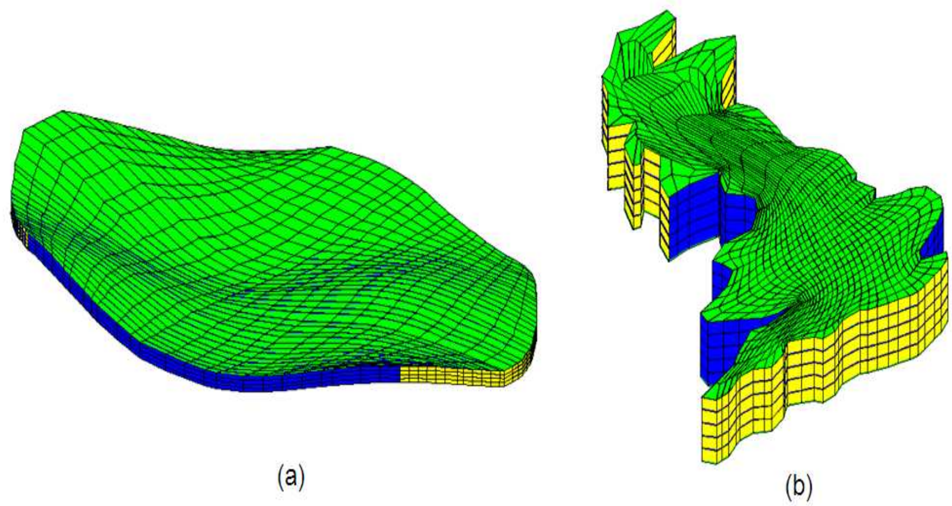


Fig. 10. (a) Grid of an oil reservoir (1) of dimension $35 \times 25 \times 5$. (b) Grid of the Great Britain of dimension $30 \times 30 \times 6$.

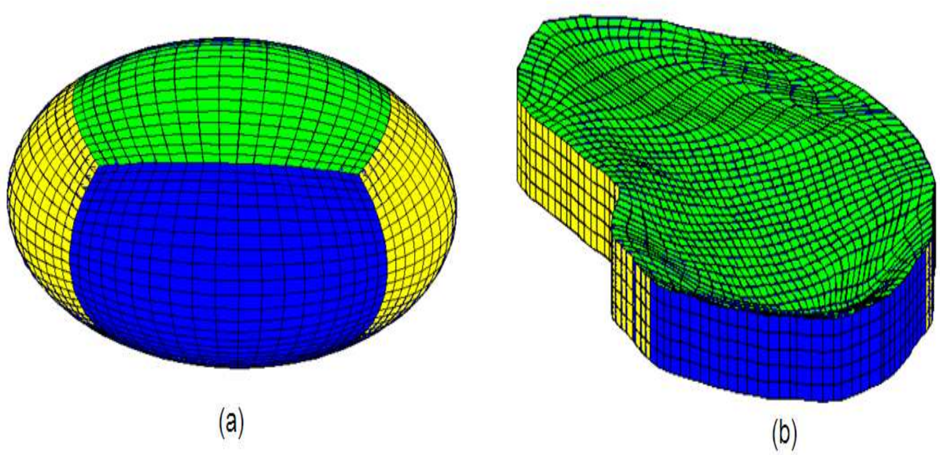
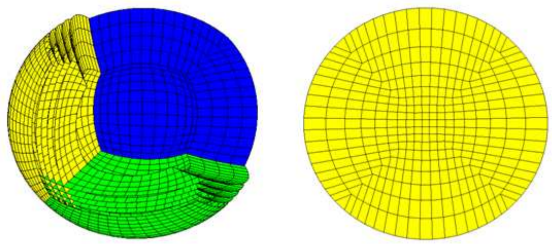
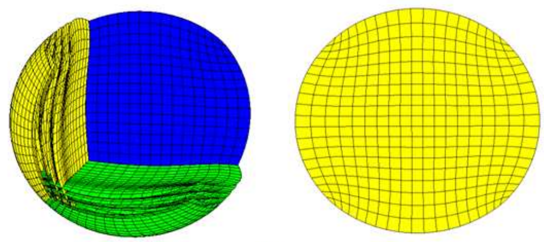


Fig. 11. (a) Grid of a ellipsoid of dimension $20 \times 20 \times 20$. (b) Grid of an oil reservoir (2) of dimension $35 \times 35 \times 6$.

The next example shows a comparison between a grid for a sphere generated by LeVeque in [6] using a radial mapping of the unitary cube and a grid generated with our algorithm. We can appreciate the discontinuities in the first grid and their lack in the second grid, also the smoothness caused by the functional H_ω is clearly illustrated.



(a)



(b)

Fig. 12. (a) Grid of a sphere of dimension $20 \times 20 \times 20$ generated by Leveque in [6] and some layers. (b) Grid of a sphere of dimension $20 \times 20 \times 20$ and some layers generated by our algorithm.

In the process of generating a convex harmonic grid using the quasi-harmonic functional not all the cells in the optimal grid are hexahedral in the sense that all the cell faces are plane, the next table shows the number of interior non-hexahedral cells in the examples.

Grid	Dimension	Interior cells	No hexahedral cells in the optimal grid
Ellipsoid	$20 \times 20 \times 20$	4913	4909
Great Britain	$30 \times 30 \times 6$	2187	2007
Oil reservoir (1)	$35 \times 25 \times 5$	1408	1384
Oil reservoir (2)	$35 \times 35 \times 6$	3072	3015
Sphere	$20 \times 20 \times 20$	4913	4905
Swan	$20 \times 20 \times 7$	1156	1154

Table 1. Optimal grids and its no hexahedral cells.

5 Convex hexahedral harmonic grid generation.

If a face of a cell is not plane this can be seen as a tetrahedron, then if we use all the tetrahedra associated to the grid cell faces without repetitions we can include a measure of coplanarity calculating the volume V_f of the tetrahedron that corresponds at each face, hence given $\epsilon > 0$ sufficiently small we say that a face is ϵ-plane if

$$V_f = \left|volume(face(C_{i,j,k}))\right| < \epsilon$$

so, for each cell the condition is given by

$$\alpha \sum_{f=1}^{6} V_f^2 \tag{18}$$

is small, where α is a positive constant.

However, to include this coplanarity restrictions explicitly in the optimization problem produces a large scale problem with restrictions which is more complicated. So we include the coplanarity conditions inside the functional as a regularization, hence the actual optimization problem to solve is

$$Calculate: \quad M^* = arg \min_{(M,\alpha)} H_w(M) + \alpha \sum_{f=1}^{N_F} V_f^2 \tag{19}$$

over the set of grids for the hexaedral aproximation Ω_h and the total number of faces in the grid without repetitions N_F.

An important aspect is the number of variables and restrictions in the optimization problem in order to determine if it is well defined. The amount of variables is given by the the interior points of the grid and the variables by the planar faces desired on the grid.

Until this moment we have studied two cases:

a) The coplanarity only in the interior cells.
b) The coplanarity in all the interior faces (including the interior faces on cells of the boundary).

In order to find a **hexahedral grid**, *i.e.* a grid with all the interior cells hexahedral, is easy to prove that the case (a) is well defined. The case (b) is in general not well defined and we need add some variables or eliminate some restrictions. We present the analysis for the first case and a few examples of hexahedral grids.

5.1 Analysis of variables and restrictions.

We have already seen that the number of variables is

$$N_{var} = 3(m-2)(n-2)(p-2),$$

and taking the layers in the direction x, y, z we can get the faces for the block of interior cells as

$$F_{C_{int}} = (m-2)(n-3)(p-3) + (n-2)(m-3)(p-3) + (p-2)(m-3)(n-3).$$

To guarantee a well-posed optimization problem we need

$$F_{C_{int}} < N_{var}$$

which is easy to prove. Hence the coplanarity in the block of interior cells defines a well-posed problem and we can find a harmonic grid with hexahedral interior cells by minimization.

5.2 Optimization procedure (convex hexaedral harmonic grids).

For the implementation of the coplanarity condition we add the regularization in the functional H_ω and apply the optimization process until we find a hexahedral grid without losing the convex cells. The proposed algorithm is as follows:

a) Choose an initial convex grid M_0.
b) Choose $\omega_0 = 10^{-8}$ (the limit value since the initial grid is convex), and $\alpha = 1/(2\mu)$ with μ starting in 0.1.
c) Solve $H_w(M) + \alpha \sum_{f=1}^{N_F} V_f^2$ to find the optimal grid M^*, here the face volume tolerance is $\epsilon = 10^{-6}$.
d) Update

$$M_0 \leftarrow M^*$$
$$\mu \leftarrow 0.1\mu$$

e) Repeat the process until find a convex hexahedral harmonic grid.

In the figures 13 and 14 we illustrate some examples of hexahedral grids generated by this algorithm.

6 Final remarks and future work.

In this work we illustrate a quasi-harmonic functional to generate convex harmonic grids in 3D. The process usually starts with a non convex initial grid and solving a large scale optimization we get a convex harmonic grid,

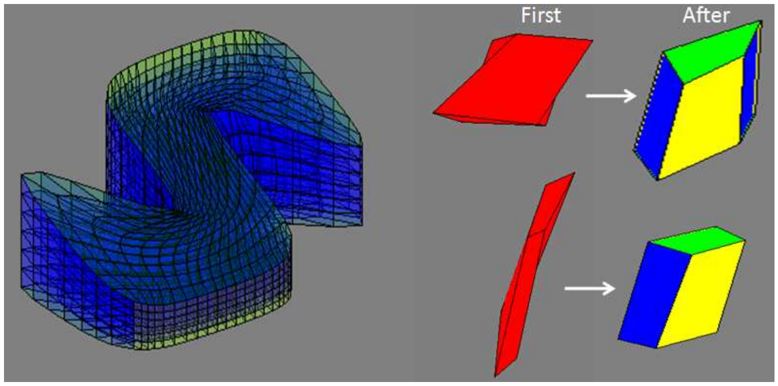


Fig. 13. Swan grid of dimension $20 \times 20 \times 7$ and some cells before and after the coplanarity algorithm.

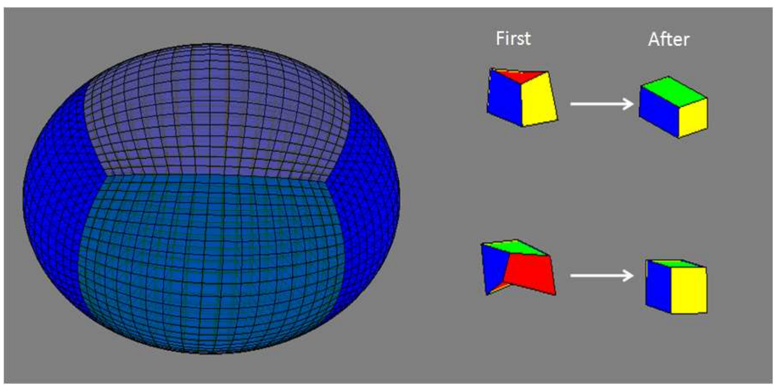


Fig. 14. Elipsoid grid of dimension $20 \times 20 \times 20$ and some cells before and after the coplanarity algorithm.

however this process not guarantee that the grid have hexahedral cells. We proof that it is possible, in general, to generate grids with all the interior cells hexahedra and propose an algorithm to solve this problem based in a regularization applied to the quasi-harmonic functional. An interesting point to be worked is the application of our grids in simulations of real problems, especially in those solved by partial differential equations, taking advantage of the good quality of the grids in the performance of that problems.

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