Hexahedral Structured Grid Generation

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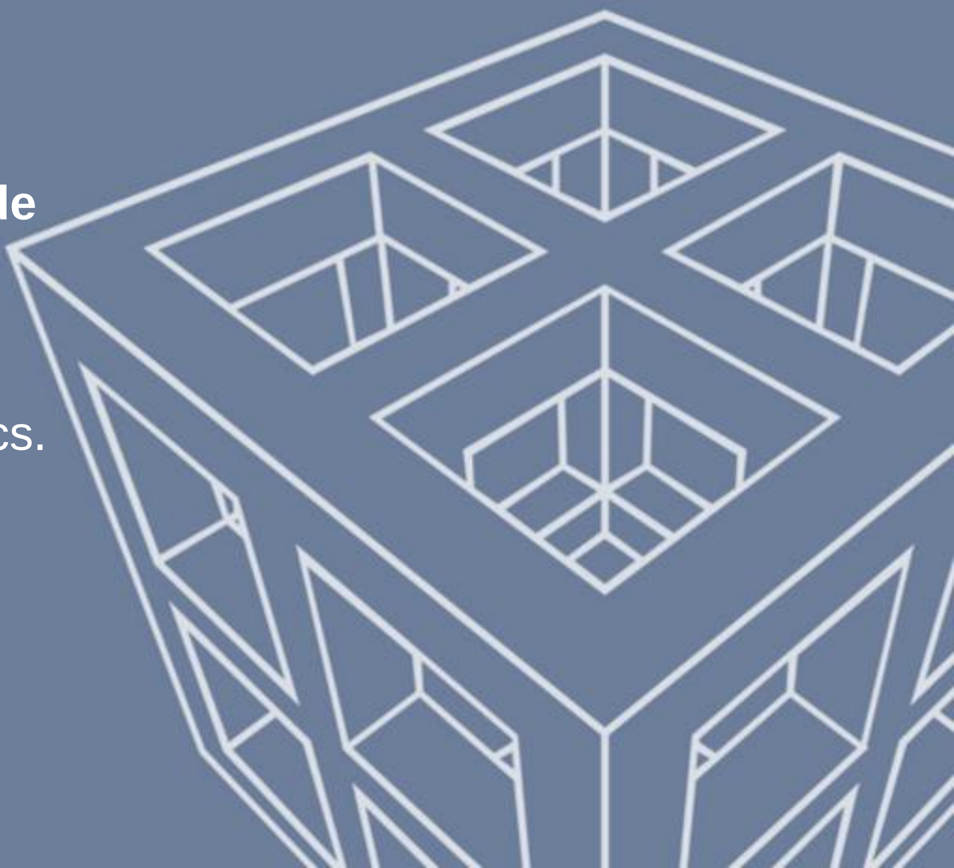


Overview

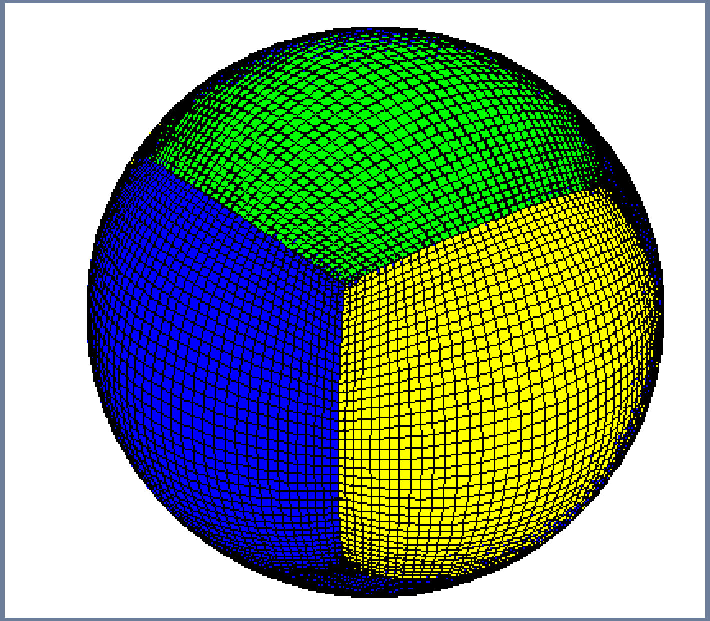
1. The structured grid generation problem.
2. Background.
3. The quasi-harmonic functional Hw.
4. Hexahedral grids.
5. A blast wave problem.
6. Conclusions and future work.
7. References.

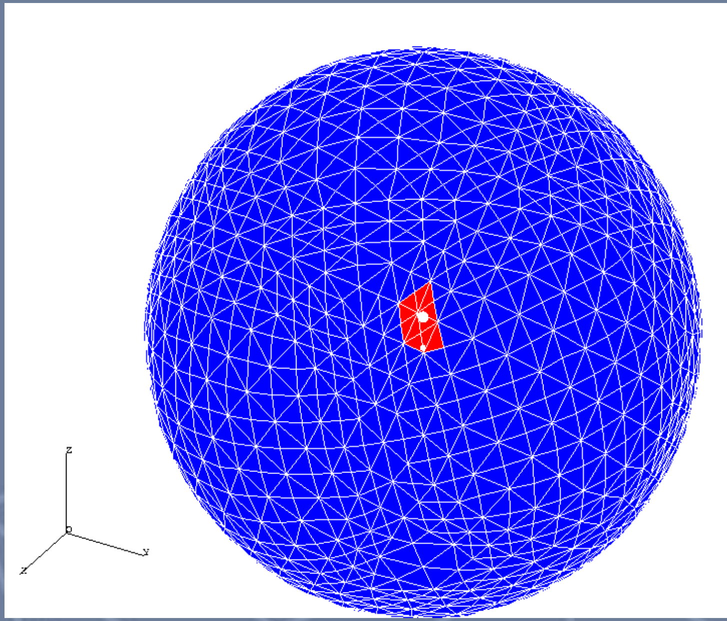
Main problem.

In order to make computational simulations of real life processes it is very useful to have high quality structured grids.

- Structured, convex and hexahedral.
- Geometric properties related to the real process.
- Useful to finite element and finite volume methods.

Structured hexahedral grids. vs. Tetrahedral grids.





- High computational cost.
- Few iterations when using finite element method.
- More precision.

Low computational cost.

More iterations when using finite element method.

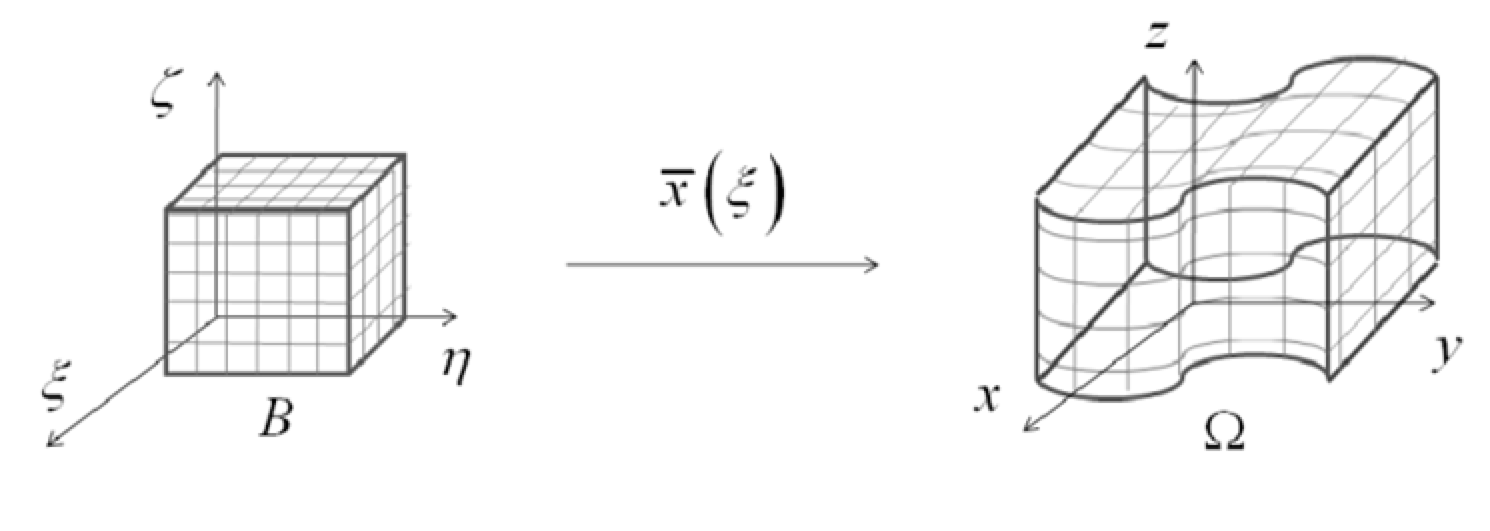
Similar precision with more grid elements

Defining a grid.

Ivanenko [6] gives a variational formulation to generate harmonic and convex grids. He defines a grid $x(\xi)$ over a region $\Omega \subset \Re^3$ simply connected as the homeomorphism

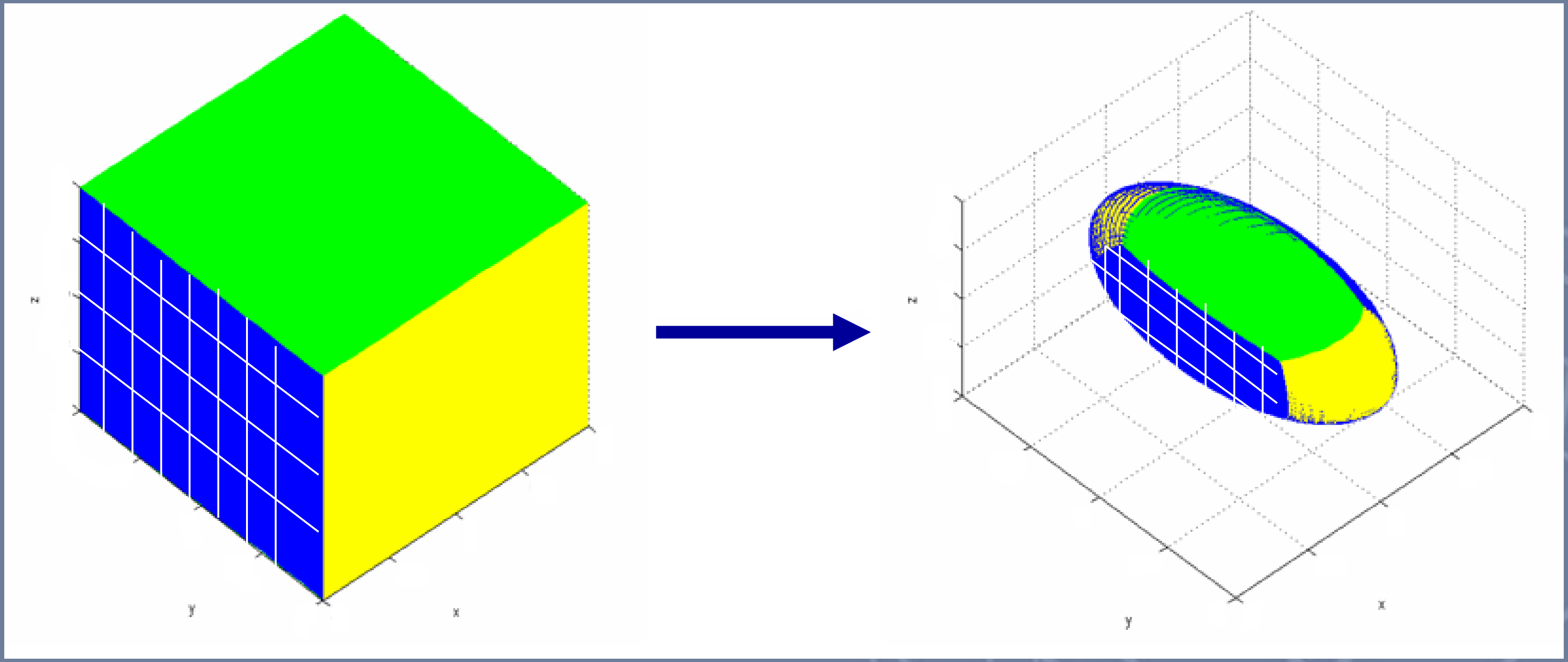
$$\bar{x} : B \rightarrow \Omega$$

where B is the unitary cube [0,1] x [0,1] x [0,1].



Defining a grid.

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



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

The harmonic mapping.

A useful mapping that gives smoothness properties is the harmonic mapping. Let us define the local energy $x(\xi)$ as

$$E(\overline{x}) = \frac{1}{3^{3/2}} \frac{\left(\left\| \overline{x}_{\xi} \right\|^2 + \left\| \overline{x}_{\eta} \right\|^2 + \left\| \overline{x}_{\zeta} \right\|^2 \right)^{3/2}}{\overline{x}_{\xi} \bullet \left(\overline{x}_{\eta} \times \overline{x}_{\zeta} \right)}$$

Ivanenko defines a harmonic mapping as the minimum of the energy functional (or harmonic functional in this case)

$$H(\overline{x}) = \int_B E(\overline{x})\, d\xi\, d\eta\, d\zeta .$$

Liseikin [11] shows that this mapping exists and is an homeomorphism.

Discrete version of the harmonic functional.

Let us consider an uniform grid of dimension *m* x *n* x *p* on the unitary cube

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

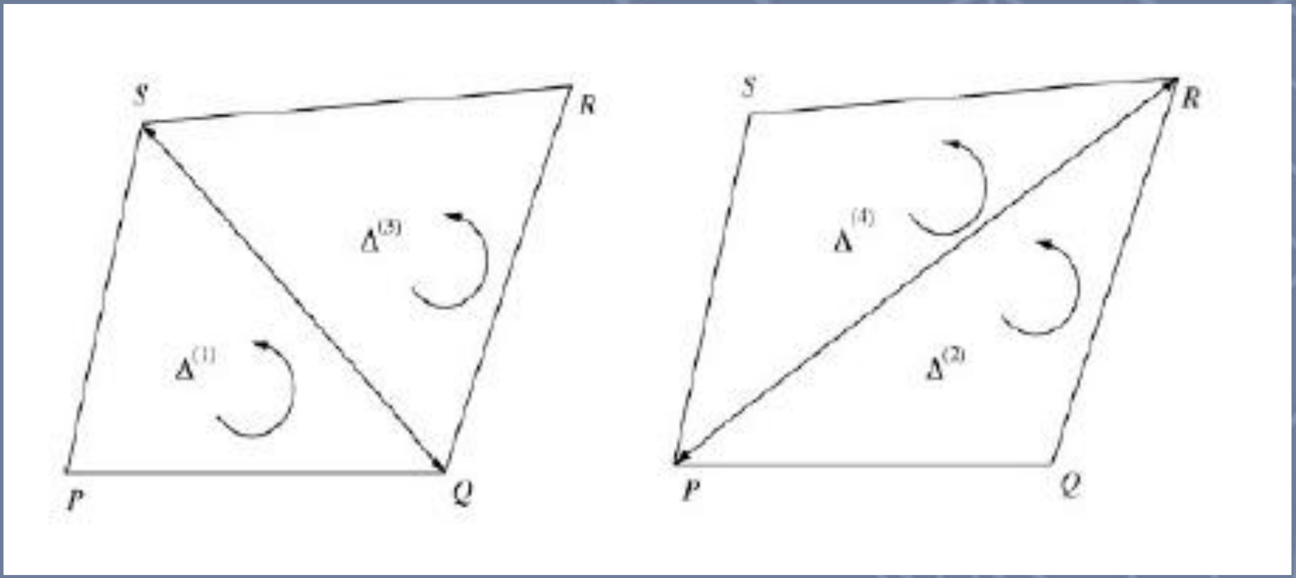
the continuous functional can be approximated by

$$\int_U E(\overline{x})d\xi d\eta d\zeta \approx \sum_{i,j,k}\int_{B_{i,j,k}} E(\overline{x})d\xi d\eta d\zeta$$

Discrete version of the harmonic functional.

In the 2D case the mapping $\bar{x}$ is approximated using a bilinear mapping. 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).

Hence is possible get the positivity of the Jacobian calculating the areas of the oriented triangles:



Discrete version of the harmonic functional.

In order to extend the 2D ideas to the 3D case, we need to approximate the mapping $\bar{x}$ by the trilinear mapping

$$r(\xi,\eta,\zeta) = w_1 + w_2\xi + w_4\eta + w_5\zeta + w_3\xi\eta + w_6\xi\zeta + w_8\eta\zeta + w_7\xi\eta\zeta$$

$$with$$

$$w_1 = r_1, \qquad w_2 = r_2 - r_1, \qquad w_3 = r_3 - r_2 - r_4 + r_1,$$

$$w_4 = r_4 - r_1, \qquad w_5 = r_5 - r_1, \qquad w_6 = r_6 - r_2 - r_5 + r_1.$$

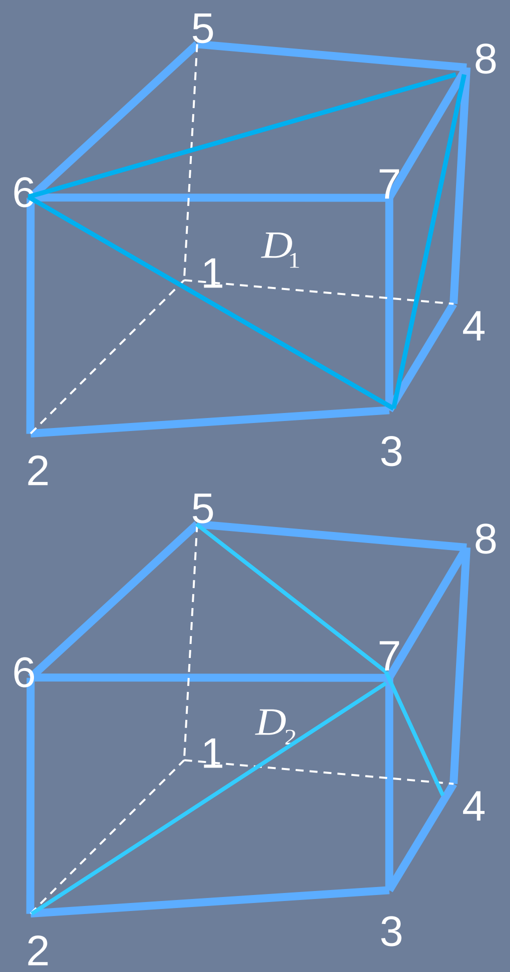
but in this case the Jacobian

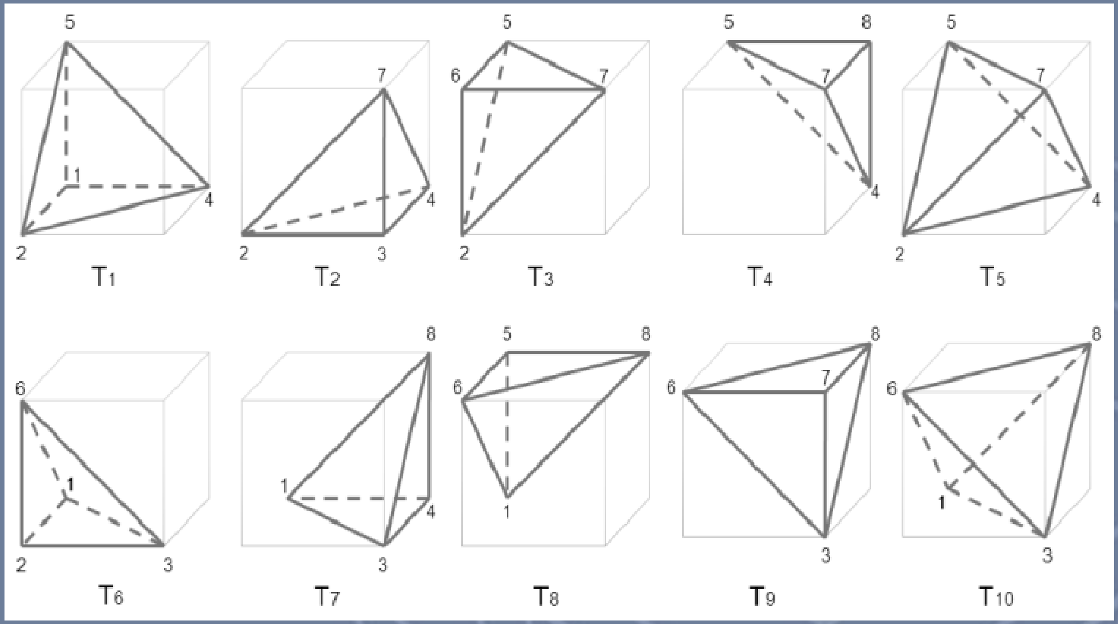
$$J = r_\xi \bullet (r_\eta \times r_\zeta)$$

is a fourth degree polynomial which depends on ξ, η, ζ.

Discrete version of the harmonic functional.

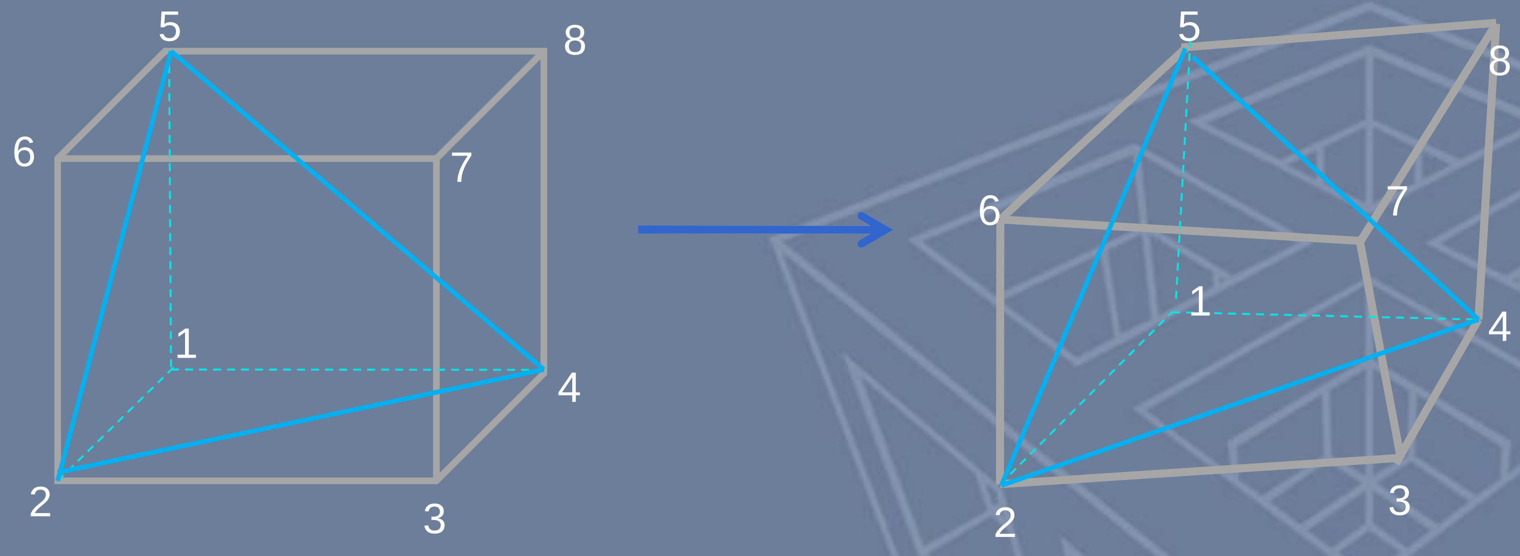
An alternative given by Azarenok [1] considers the two dodecahedra that result when making cuts on the diagonals of the cell.





Discrete version of the harmonic functional.

Instead use the trilinear mapping, we use now 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*.



Discrete version of the harmonic functional.

The Jacobian of the linear transformations is given by

$$J(T_l) = 6 * vol(T_l)$$

hence, if the volume of the tetrahedra is positive then the Jacobian is also positive and the mapping is invertible.

Also the positivity of the volume of the ten tetrahedra generated gives a short condition to verify the convexity of the cells which is reliable in most of the cases (Ushakova [14]).

$$vol(T_l) > 0, \qquad l = 1, 2, \ldots, 10$$

Discrete version of the harmonic functional.

We can discretize the functional by simply averaging over the 10 tetrahedra defined by the two dodecahedrons

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

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

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

hence the large-scale optimization problem to solve is:

$$Compute: \qquad M^* = \arg\min_M H^d(M)$$

Numerical problems in the use of the harmonic functional.

The discrete version of the harmonic functional

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

is well defined only for grids having positive volume in all the tetrahedra since its integrand is in the form $\frac{\lambda(\overline{x})}{v(\overline{x})}$ *where*

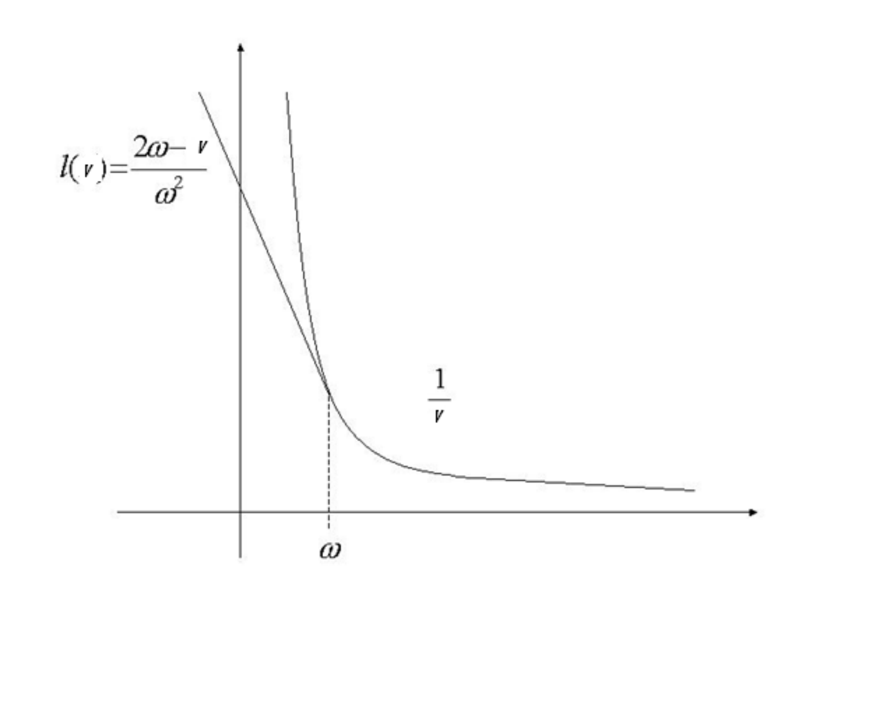
$$v(\overline{x}) = \overline{x}_\xi \bullet \left(\overline{x}_\eta \times \overline{x}_\zeta\right) = vol(T_{ij})$$

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

The quasi-harmonic functional Hw.

The functional uses a control parameter ω which controls the use of negative and small values of *vol*

$$vol(T_{ij}) < \omega$$



$$\varphi_\omega(v) = \begin{cases} \dfrac{(2\omega - v)}{\omega^2}, & v < \omega \\ \dfrac{1}{v}, & v \ge \omega \end{cases},$$

$$\lambda = \frac{\left(\left\| \overline{x}_\xi \right\|^2 + \left\| \overline{x}_\eta \right\|^2 + \left\| \overline{x}_\zeta \right\|^2 \right)^{3/2}}{3^{3/2}},$$

$$H_\omega = \frac{1}{N_c} \sum_{n=1}^{N_c} \sum_{m=1}^{10} \frac{1}{10} \lambda_{n_m} \varphi_{\omega\, n_m}$$

The quasi-harmonic functional Hw.

We get now a quasi-harmonic functional

$$H_{\omega} = \frac{1}{N_c} \sum_{n=1}^{N_c} \sum_{m=1}^{10} \frac{1}{10} \lambda_{n_m} \varphi_{\omega_{n_m}}$$

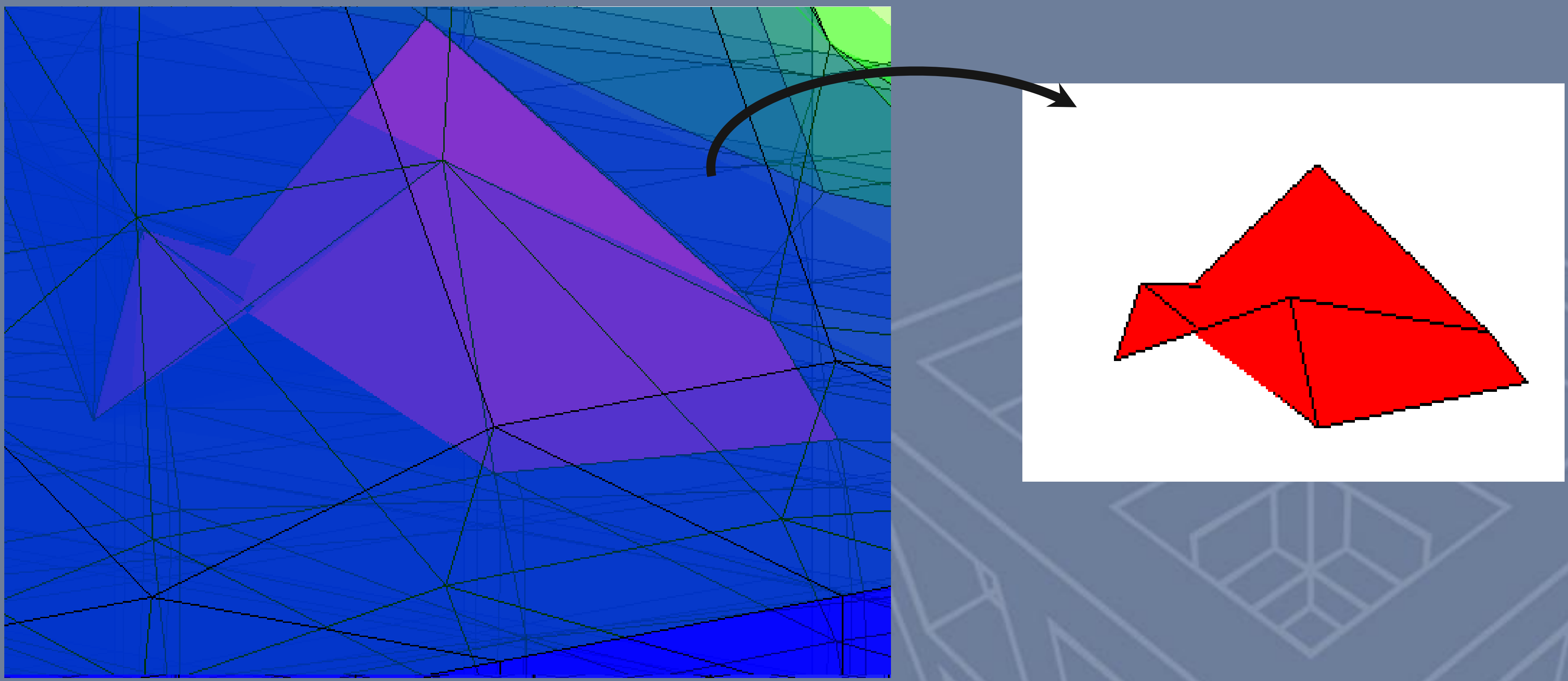
without the numerical problems presented in the harmonic functional.

hence the large-scale optimization problem to solve is:

$$Compute: \qquad M^* = \arg\min_{M} H_{\omega}(M)$$

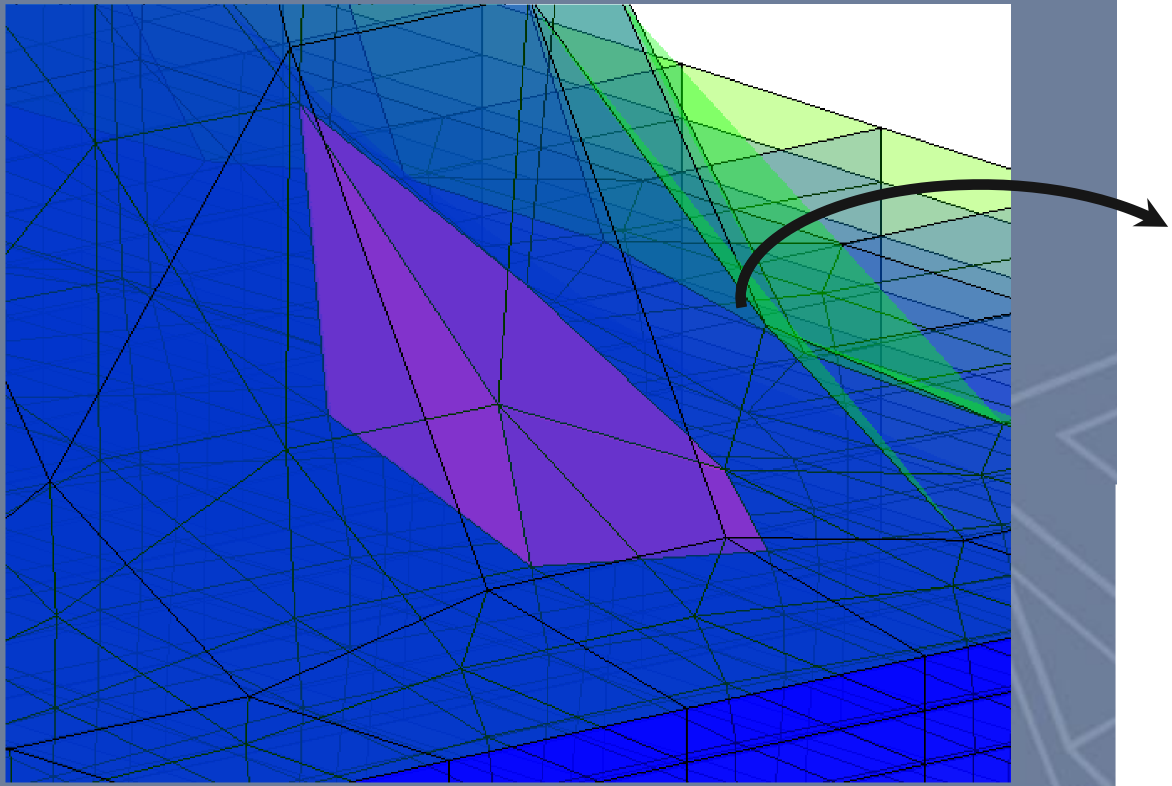
Examples.

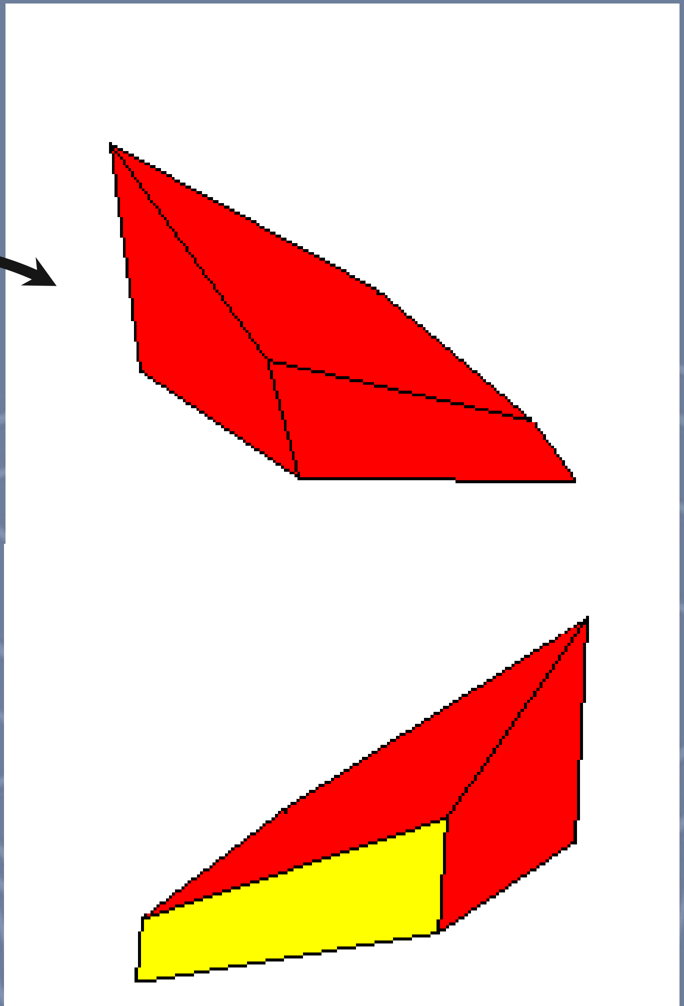
We can take an initial non convex grid:



Examples.

And get an optimal grid:

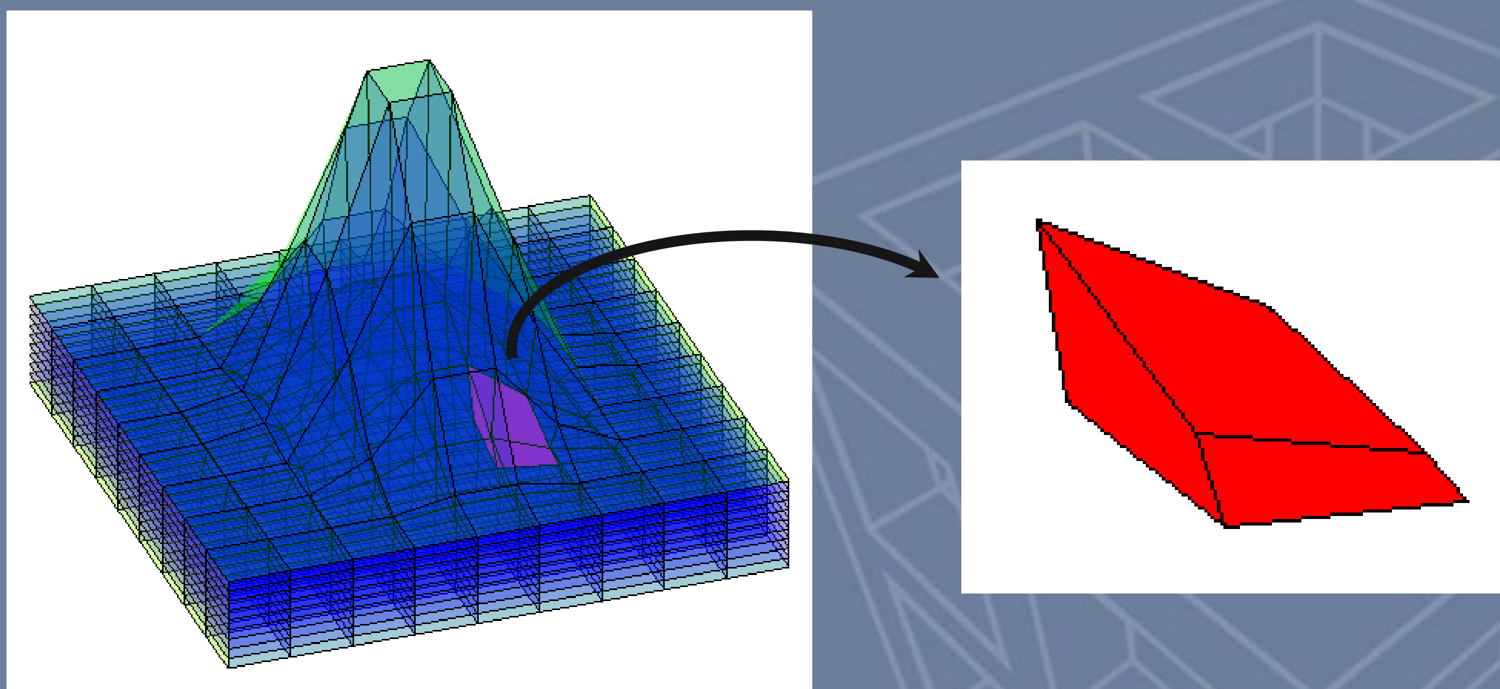




The red faces are not plane.

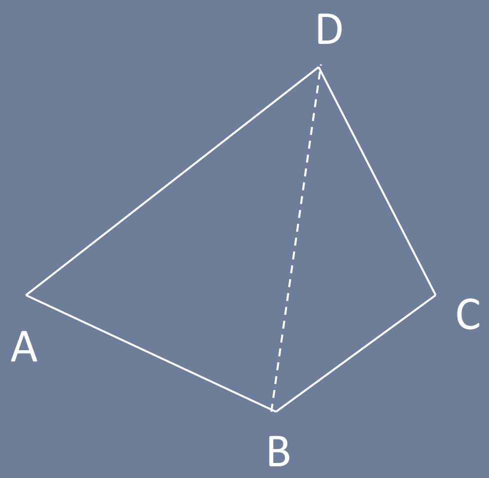
Hexahedral grids.

A **problem** arises when generating convex grids using the quasi-harmonic functional. The problem is, that not all the cells in the optimal grid are hexahedral since not all the cell faces are plane.



Coplanarity conditions.

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



$$k = \left| Volume(\,face(C_{i,j,k}))\right| < tol$$

However, to include this coplanarity conditions explicitly in the optimization problem produces a large scale problem with restrictions.

The modified quasi-harmonic functional.

We include the coplanarity conditions inside the functional as the regularization

$$C\sum_{i=1}^{6} k_i^2$$

hence the actual optimization problem is to solve

$$Compute: \qquad M^* = \arg\min_{M}\left(H_\omega(M) + C\sum_{l=1}^{N_{CF}}\sum_{i=1}^{6} k_{(li)}^2 \right)$$

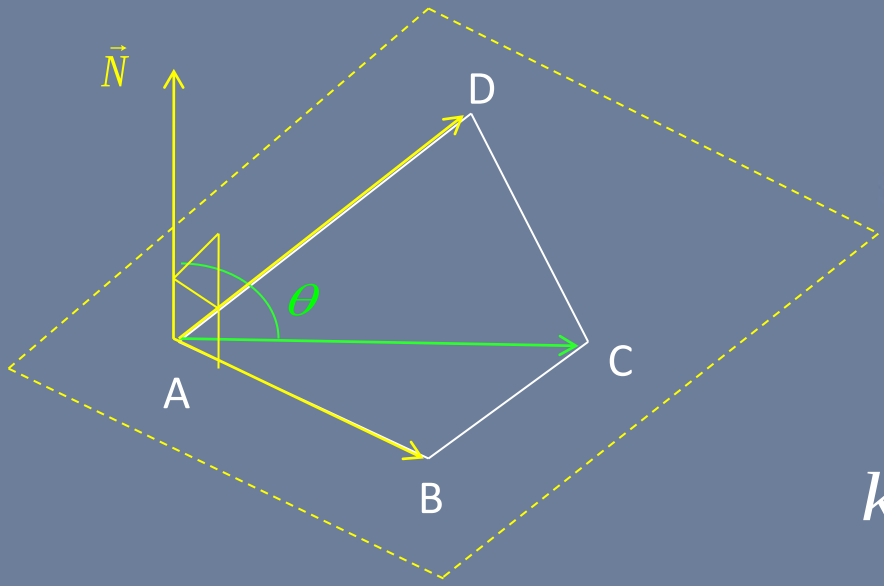
which is well defined over the set of interior cells.

Numerical limitations.

Grid	Can we get coplanarity?
Cos 5-5-10	No. Vol max =0.0243004. 100% non hexahedral cells.
Swan 7-7-5	No. Vol max =4.96*10^{-5}. 97% non hexahedral cells.
Peak 10-10-10	No. Vol max =0.00036997. 77% non hexahedral cells.

A new coplanarity condition.

To overcome the numerical limitations we use the next coplanarity condition



$$\vec{N} = \overline{AB} \times \overline{AD}$$

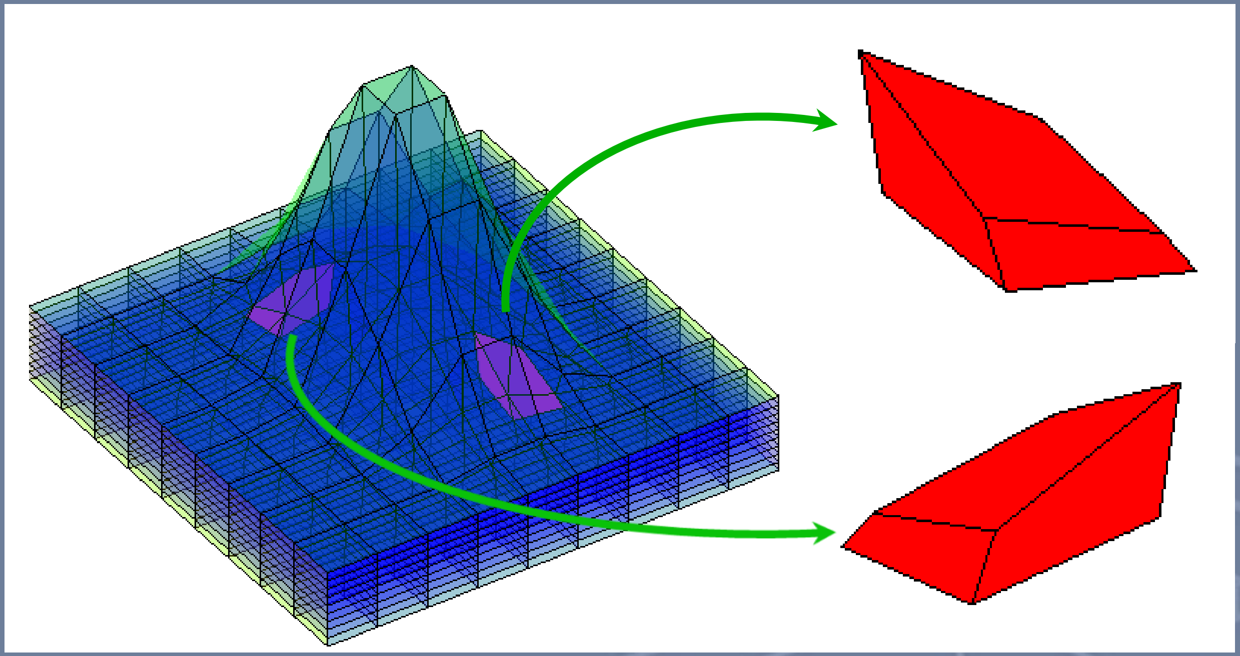
$$we\ need\ \ \theta \approx 90^{\circ}$$

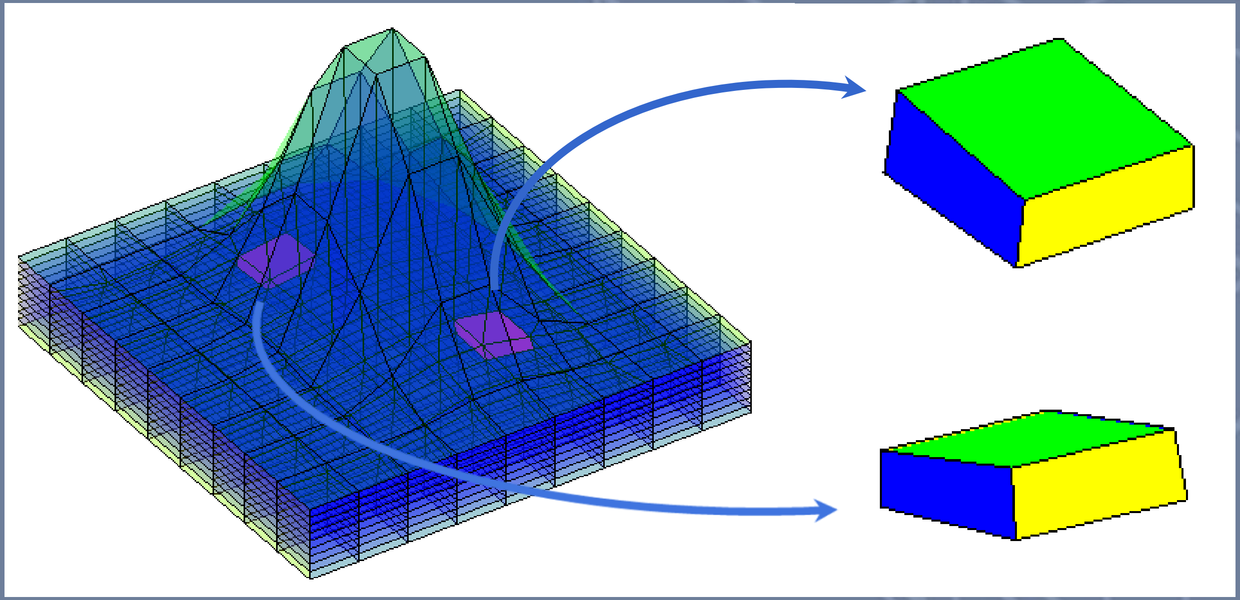
$$k\ = \cos(\theta) = \frac{\vec{N}^{t}\,\overline{AC}}{\left\|\vec{N}\right\|\left\|\overline{AC}\right\|} < tol$$

Numerical experiments.

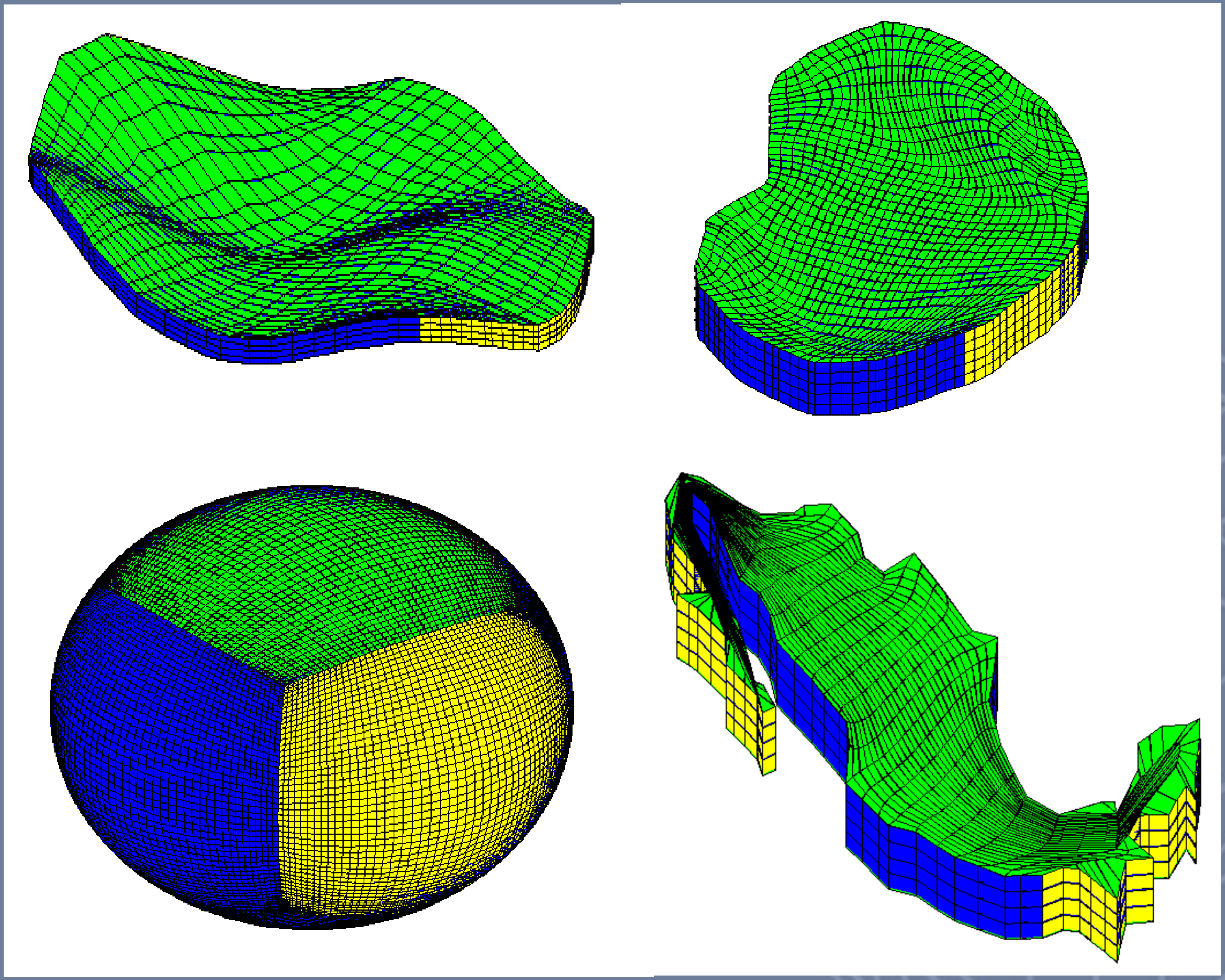
Grid	Can we get coplanarity by the first condition?	Can we get coplanarity by the second condition?
Cos 5-5-10	No. Vol max =0.0243004. 100% non hexahedral cells.	Yes. Cos max = $3.64 \cdot 10^{-8}$ Vol max = $4.53 \cdot 10^{-6}$
Swan 7-7-5	No. Vol max =$4.96 \cdot 10^{-5.}$ 97% non hexahedral cells.	Yes. Cos max = $3.52 \cdot 10^{-8}$ Vol max = $6.97 \cdot 10^{-6}$
Peak 10-10-10	No. Vol max =0.00036997. 77% non hexahedral cells.	Yes. Cos max = $1.88 \cdot 10^{-8}$ Vol max = $1.47 \cdot 10^{-9}$
Bottle 15-15-10	Yes. Vol max = $7.38 \cdot 10^{-10}$	Yes. Cos max = $1.22 \cdot 10^{-8}$ Vol max = $2.6 \cdot 10^{-10}$

Examples.





Examples.



A blast wave problem.

We apply our grids in a blast wave problem studied in [10] by Randall Leveque. The problem is simulated on an unitary sphere solving a system of hyperbolic PDE’s using CLAWPACK. The grid used by Leveque is generated by a radial mapping of the cube [-1,1] x [-1,1] x [-1,1].

A blast wave problem.

The Euler equations for a compressible polytropic gas are given in standard conservation form

$$\partial t\, q + \nabla \cdot f\,(q) = 0,$$

with

$$\mathbf{q} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ E \end{pmatrix}, \quad \mathbf{f}(\mathbf{q}) = \begin{pmatrix} \rho u & \rho v & \rho w \\ \rho u^2 + p & \rho v u & \rho w u \\ \rho u v & \rho v^2 + p & \rho w v \\ \rho u w & \rho v w & \rho w^2 + p \\ u(E+p) & v(E+p) & w(E+p) \end{pmatrix}$$

A blast wave problem.

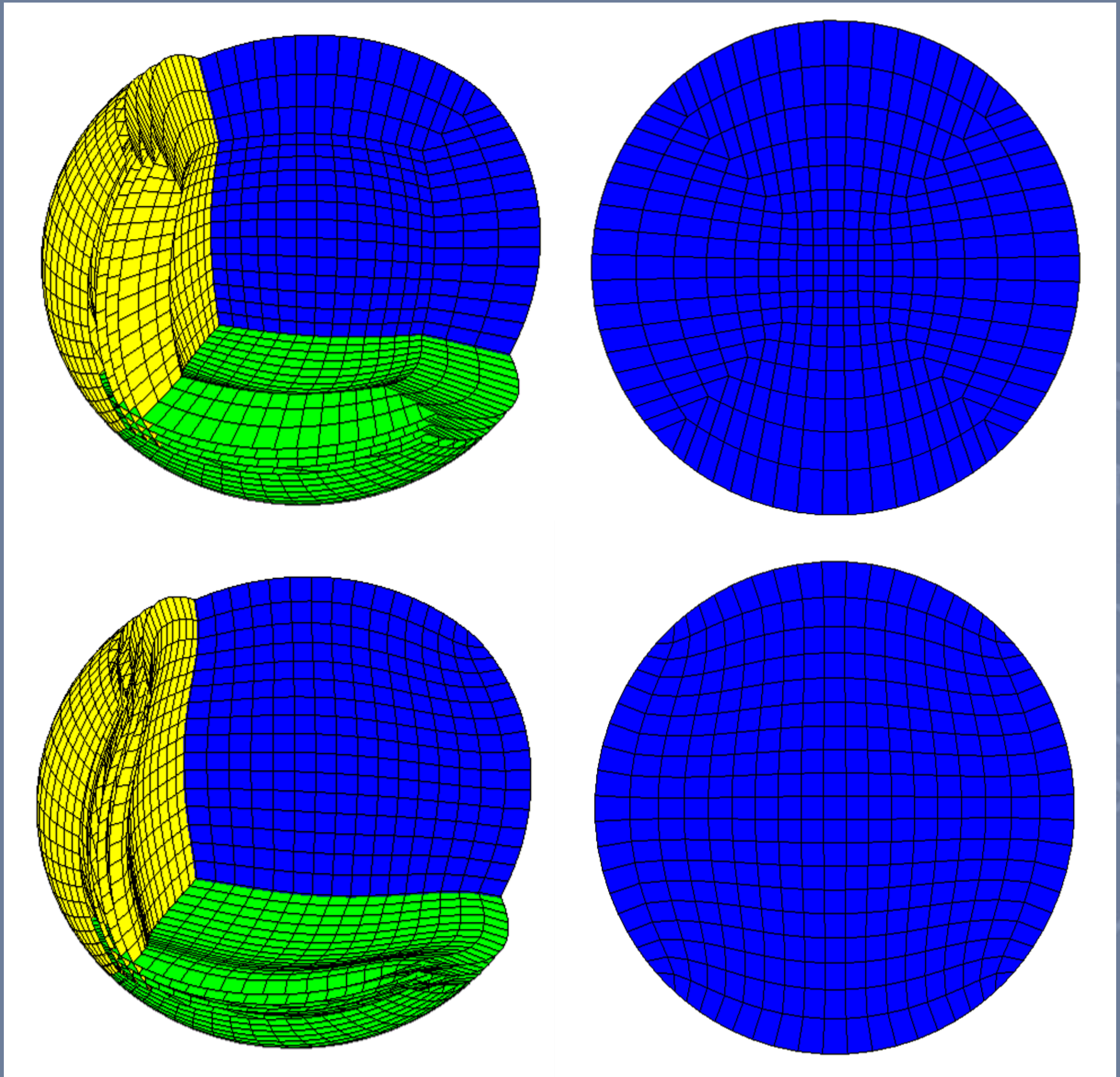
The conserved quantities are the density *ρ*, momentum ρ ▪ u = (ρu, ρv, ρw), and total energy *E*. In addition to these equations, we must supply an equation of state that relates the pressure *p* to the conserved quantities.

For the polytropic gas, the equation of state is given by

$$E = \frac{p}{\gamma - 1} + \frac{1}{2}\rho(u^2 + v^2 + w^2),$$

where ϒ is the adiabatic gas constant. We use the value for air and set
ϒ = 1.4.

The two used grids.



Initial conditions.

- p = 5 inside a sphere of radius 0.2 and center (0,0,−0.4).

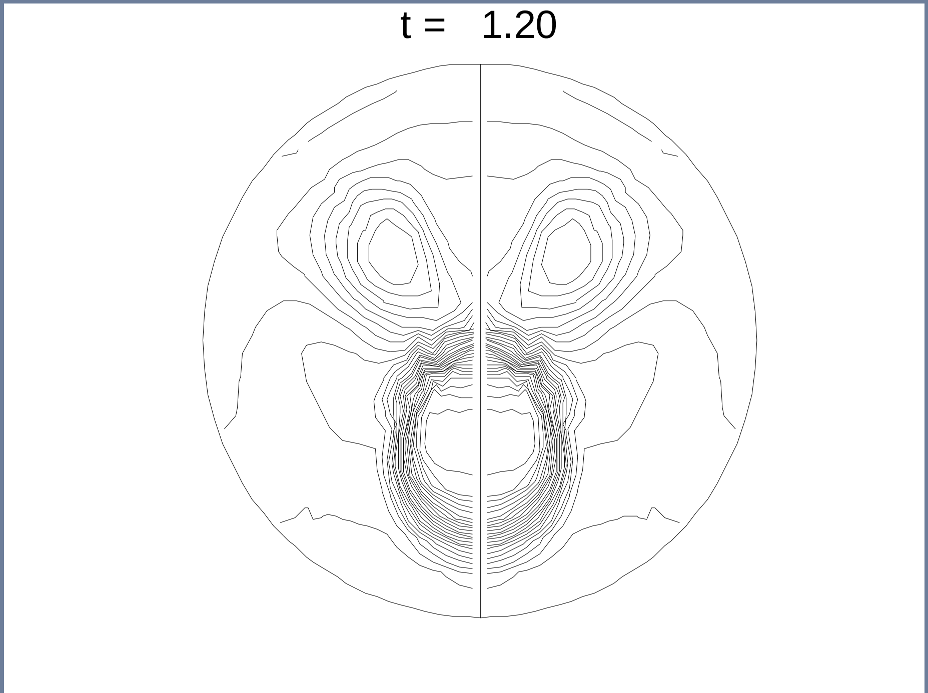
•Outside this sphere p = 1.

- Density equals to 1 inside the sphere of radius 0.2 and 0 outside the sphere.

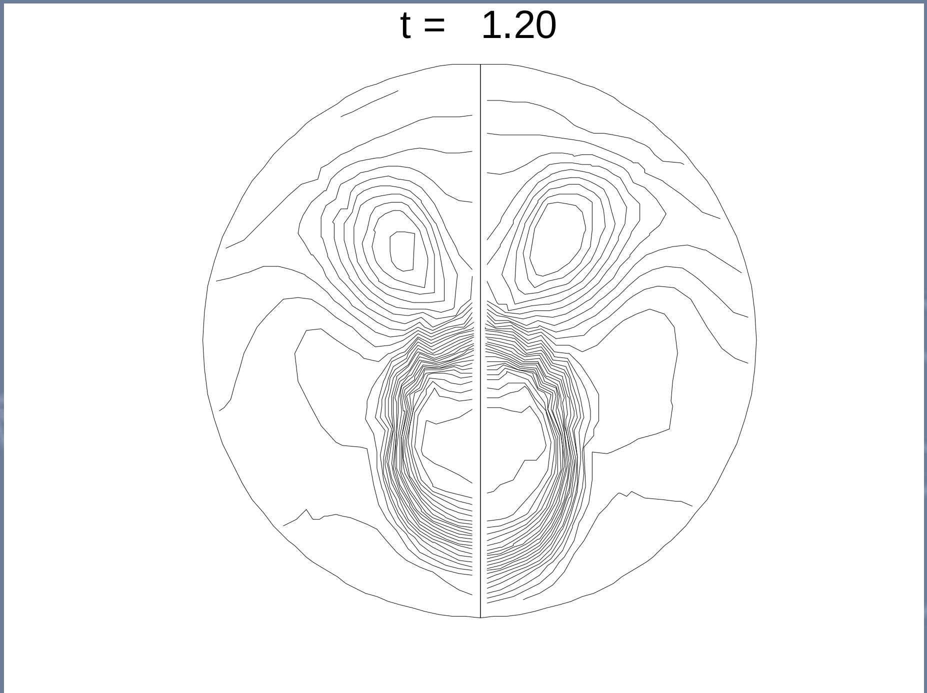
- Solid wall boundary condition.

Blast wave simulations.

Radial grid.

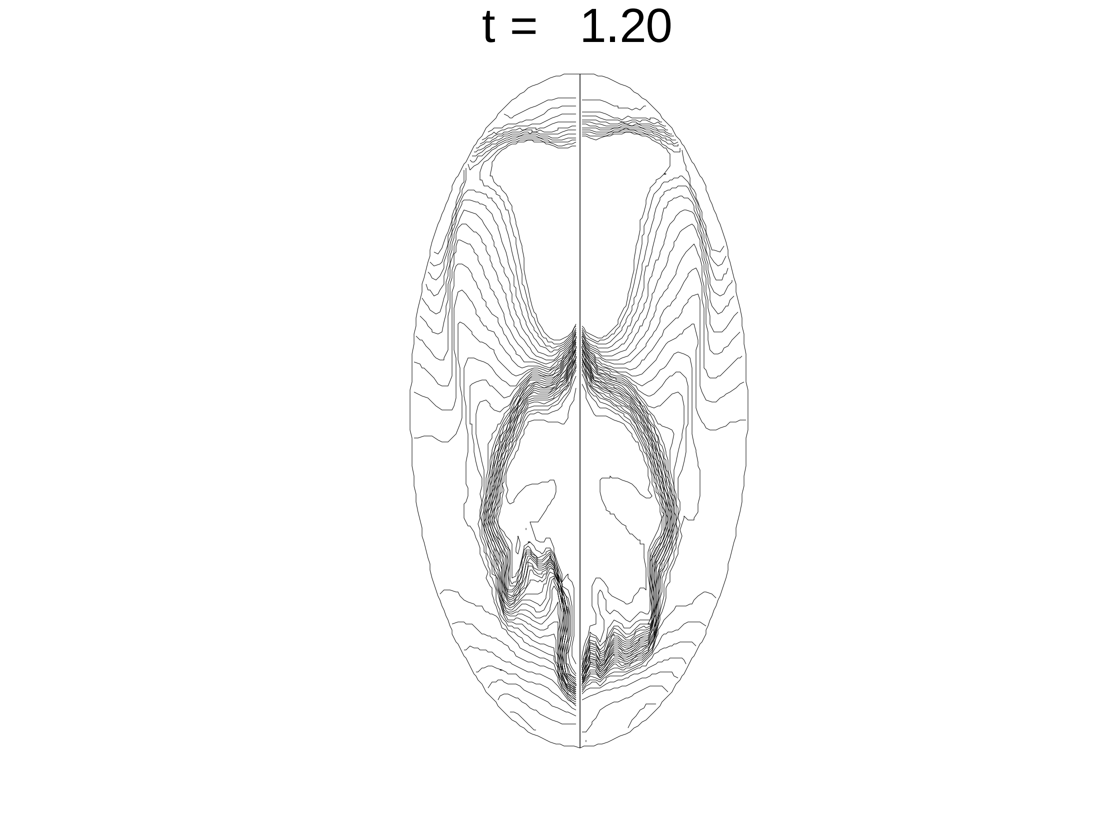


Structured convex and hexahedral grid.



Blast wave simulations.

A simulation on an ellipsoid.



Conclusions and future work.

Conclusions:

- The generation of structured and convex grids using a quasi- harmonic functional starting with a non convex grid is possible.

- The generation of hexahedral grids over the set of interior cells improving the quality of the cells it is also possible.

- The grids generated can be useful to simulate PDE's problems.

Future work:

- Generate grids on more complex regions.

- Calibrate the internal parameters in the grid generator.

- Work other PDE's problems.

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Thanks!!