VARIATIONAL GRID GENERATION USING EXPONENTIALS OF AREA.

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ABSTRACT

Some variational methods for grid generation have been successfully developed in the works of Tinoco and Barrera ([8],[9],[10]) by the use of generalizations of Winslow's smoothness functional ([2]) in terms of the so called *k-functionals*, on which a parameter plays an important role in the construction of a sequence of grids which tends to an existing convex one for a given planar region. However, a parameter of this kind is global for a given configuration, and so it doesn't follow in a straightforward way which one is the continuous analog functional from where the discrete k-functional should be coming. This remains as an important issue when we consider the dynamical behavior of these set of expressions.

In this work, in order to construct a convex grid in a given region, we present another discrete functional written in terms of the area of the triangles conforming the cells, which achieves its minimal value when the total area of the region is averaged in the cells, by only asking elementary geometrical requirements.

Keywords: variational, grid, mesh, generation, exponential, convex, Schur-Convex, area.

1. INTRODUCTION.

An arbitrary region in the plane, whose boundary is given by a Jordan piecewise $\mathcal{C}^1$ polygonal curve is the starting point for many methods that build structured grids with quadrilateral elements. A natural identification of four topological sides of such a curve allows the definition of functionals for any grid whose definition domain is the set D of all admissible grids for the region; our aim is that is possible to generate a sequence which tends to a convex grid in D in an intuitive geometrical way if the admissibility conditions guarantee the existence of a mapping between D and the set of the possible values of area for the triangles that conform any cell of the grid.

2. DEFINITION DOMAIN.

Let γ be a polygonal closed simple curve. We denote as P the set of points

$$P = \{p_1, p_2, \cdots, p_n\}$$

on which γ is not $\mathcal{C}^1$; its graph is the set

$$[\gamma] = [p_1, p_2] \cup [p_2, p_3] \cup \cdots [p_n, p_1]$$

where $[a, b]$ stands for the line segment that joins a y b.
This kind of sets will represent the typical boundary of our regions; we refer to $[\gamma]$ together with the interior region it defines as a *polygonal domain* and hereinafter will be denoted as Ω.
On it we can state the following

Definition 1. Let $m, n \in \mathbb{N} \setminus \{1, 2\}$. An $m \times n$ grid (or mesh) G over the polygonal domain Ω is a set

$$G = \{P_{i,j} \mid i = 1, ..., m, j = 1, ..., n\}$$

of points in the plane such that

$$P \subset G. \tag{1}$$

Last condition is essential, since we want to generate admissible grids; we will explain lately what such admissibility means.
In terms of the length of γ, it's easy to define its upper, lower, left and right sides. This gives sense to the use of a double subscript once we have a geometrical meaning for an "horizontal" and a "vertical" directions, going from left to right and upper to lower sides respectively.
So, i^{th} vertical and j^{th} horizontal grid lines are the sets

$$\{P_{i,1}, P_{i,2}, ..., P_{i,n}\}$$

$$\{P_{1,j}, P_{2,j}, ..., P_{m,j}\}.$$

A little bit further, we can identify the corners

$$P_{1,1}, P_{1,n}, P_{m,1}, P_{m,n}$$

and the four sides, constructed for instance by drawing the line segments every point with the next following it in the subscript order for the sets

$$\{P_{1,1}, P_{2,1}, ..., P_{m,1}\}$$

and

$$\{P_{1,n}, P_{2,n}, ..., P_{m,n}\}$$

which give the upper and lower sides; a similar construction is made for the left and right sides.
Each one of the remaining inner points

$$P_{i,j} \quad 1 < i < m; 1 < j <, n$$

has four neighbors

$$P_{i-1,j} \quad P_{i+1,j} \quad P_{i,j+1} \quad P_{i,j-1}$$

to the down, up, right and left, directions respectively; the points in the corners and within the sides have two neighbors each one in the same sense.
This structure is a fundamental step in order to define our functional. Geometrically, it's immediate the identification of G with the $(m-1)\times(n-1)$ quadrilaterals

$$\begin{aligned} &[P_{i,j}, P_{i,j+1}] \cup \\ &[P_{i,j+1}, P_{i+1,j+1}] \cup \\ &[P_{i+1,j+1}, P_{i+1,j}] \cup \\ &[P_{i+1,j}, P_{i,j}] \end{aligned} \tag{2}$$

where $1 \le i < m; 1 \le j < n$. This quadrilateral collection has the same information that G does, so we can without distinction think on G or in the graph generated by joining each point of it with its neighbors in the grid; our structured mesh is given by these quadrilaterals and the relations between points and neighbors.
Condition (1) is necessary for our grid to be admissible: we want it to be built with quadrilateral elements and be logically equivalent to the one with integer coordinates ([11])

$$M = \{(i, j) | 1 \le i \le m; 1 \le j \le m\}.$$

In terms of what we have at hand, our goal is to build a convex admissible mesh within Ω; this can be achieved by using the *k-functionals*([8],[9],[10]), but now we are interested in the definition of a functional in a different way.
From now on we will denote by D the set of all the admissible grids for a given region Ω with boundary γ as stated in the previous paragraphs.

3. DISCRETE FUNCTIONALS.

In each one of the quadrilaterals given by (2), we distinguish the four oriented triangles that conform it and denote them as

$$\begin{aligned}\triangle^1_{i,j} &= \triangle(P_{i,j+1}, P_{i,j}, Pi+1, j)\\ \triangle^2_{i,j} &= \triangle(P_{i,j}, P_{i+1,j}, Pi+1, j+1)\\ \triangle^3_{i,j} &= \triangle(P_{i+1,j}, P_{i+1,j+1}, Pi, j+1)\\ \triangle^4_{i,j} &= \triangle(P_{i+1,j+1}, P_{i,j+1}, Pi, j)\end{aligned}$$

It is easy to see that if the condition

$$\text{area}(\triangle^k_{i,j}) > 0$$

holds for $1 \le i < m; 1 \le j < n; k = 1,2,3,4$, then the grid whose cells are built with such triangles is convex. This is an elementary but very important fact, since if we try to have control over the points on the mesh by controlling the whole cells, convexity can not be guaranteed since a quadrilateral with positive area does not need to be convex ([4],[8]); an easy example can be seen in figure 1. One of the main achievements of the work of Barrera and Pérez ([11]) was to introduce this control, improving the results obtained in quadrilateral elements by Castillo ([1]). In figure 2 we present an example of an actual grid in this context, with the triangles drawn in dotted lines.

The general form of a functional defined over a

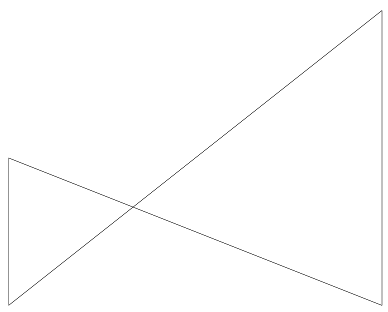

Figure 1. A non convex quadrilateral.

given G is

$$F(G) = \sum_{\triangle \in G} f(\triangle) = \sum_{i=1}^{m}\sum_{j=1}^{n}\sum_{k=1}^{4} f(\triangle^k_{i,j}). \quad (3)$$

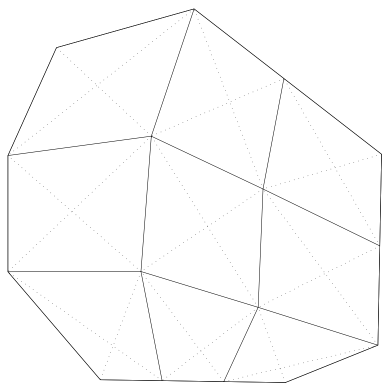

Figure 2. An example of an actual grid.

The positions of the boundary points are fixed meanwhile the unknown and mobile points are the interior ones; this is a Dirichlet-kind problem. The grid we are looking for is the minimum of the large scale optimization problem

$$\min_{G \in D} F(G)$$

and the basis for the success of the k-functionals yields on the fact that the problem is written as an unconstrained one, without explicitely asking the area of the triangles in the cells to be positive, so the approximation to the optimal value is built in a very fast way.
On the other hand, it is important to point out than this is *not* a Delaunay process, since we are always dealing with a structured grid, even if we are handling triangles within it.
Motivation and details for such functionals and for the classical functional forms of (3) in terms or area, length, orthogonality and further developments in terms of them can be found mainly in [2],[9],[10],[3],[5],[1],[11], [6], [7] and some other works; we will just make a brief presentation later.
To our purposes, we will be interested in handle the triangle areas in order to guarantee the existence and uniqueness of an optimal value for the functional in terms of exponential values of such areas.
For the sake of brevity, hereinafter we will denote (3) in the simpler way

$$F(G) = \sum_{q=1}^{N} f(\triangle_q) \quad (4)$$

where $N = 4(m-1)(n-1)$; the summation taken over all the triangles within the cells of the grid as stated above.

4. CLASSICAL FUNCTIONALS.

It is convenient to define the quantity

$$\alpha = a^T J b$$

where

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

for a triangle with sides a and b. The immediate geometrical interpretation of α as twice the oriented area of this triangle allows to write down our functionals in terms of it, looking for conditions to generate grids with positive values of alpha for any triangle.
Within this context, another fundamental quantitie is the average $\overline{\alpha}$ of the values of α over all the triangles in the grid given as

$$\overline{\alpha} = \frac{1}{N}\sum_{q=1}^{N}\alpha_q = \frac{\Omega}{N}$$

where Ω is four times the oriented area defined by the contour $[\gamma]$ and $N = 4(m-1)(n-1)$ as before. So, denoting by $\triangle_q$ the q^{th} oriented triangle with sides a_q and b_q given as 2D column vectors, and using formula (4), we can write the expressions for some of the most classical discrete functionals that appear in the literature. They are the length functional

$$F(G) = \sum_{q=1}^{N}(\|a_q\|^2 + \|b_q\|^2)$$

the area functional

$$F(G) = \sum_{q=1}^{N}(\alpha_q)^2$$

the reciprocal of area functional

$$F(G) = \sum_{q=1}^{N}\frac{1}{\alpha_q} \qquad (5)$$

the orthogonality functional

$$F(G) = \sum_{q=1}^{N}(a_q^T b_q)^2$$

and the smoothness functional

$$F(G) = \sum_{q=1}^{N}\frac{\|a_q\|^2 + \|b_q\|^2}{\alpha_q}. \qquad (6)$$

In general, it is not possible to guarantee that starting from an arbitrary initial grid, the optimization process will produce as result a convex grid; at most for (5) and (6) a simpler result can be shown, taking as initial approximation an already convex grid, so they can not be used for general generation purposes.
However, they motivate a new set of functionals that will be presented in the next section.

5. K-FUNCTIONALS.

If the expression

$$\frac{1}{\alpha_q}$$

is capable of producing a convex grid when already every value of α is positive, then it is natural to seek a "shifting factor" in order to include more arbitrary initial grids; this was the proposal of Tinoco and Barrera ([8]) in the k-area functional

$$F(G) = \sum_{q=1}^{N}\frac{1}{k + \alpha_q}$$

and the k-smoothness functional

$$F(G) = \sum_{q=1}^{N}\frac{\|a_q\|^2 + \|b_q\|^2 - 2\alpha}{k + \alpha_q}$$

for which there are general theorems ([8]) that show that in the case that a convex grid exists within a given boundary, it can be approached by minimizing them; some other results for general k-functionals can be found in [6].
When (4) can be written only in terms of α, it is convenient to use $\alpha/(2\overline{\alpha})$ instead of just α, to guarantee that the functional values and therefore the optimal grids are independent from the scale. The parameter k, calculated in terms of area, is the main key here. But there is not a simple deduction suggesting which one should be the continuous analog of these k-functionals. They can be used with excellent results, but it still remains the question of what is the geometrical continuous meaning of the parameter. It would be desirable to have some other alternatives, at least from a theoretical point of view, showing that starting from any arbitrary initial and often non convex grid we can generate a convex one without the need of a global parameter for it.
An option, which is very interesting from a geometrical point of view for such generation in the subject of the next section.

6. EXPONENTIALS OF AREA.

Tinoco([8]) proposed a result which states that almost every convex functional written in terms of α should be useful for generation; the search for a suitable expression led to the utilization of elementary convex functions as the exponential ones. Considering a single isolated triangle, the following conditions are easy verified as required for a functional on it to generate a convex grid

- we need the functional to have a lower bound,
- its minimum must be achieved when every α is positive and
- it must be convex.

If we relax a little the second requirement, then a good choice (in geometrical sense) for such a functional is the formula

$$f(\triangle) = \exp(-\alpha). \tag{7}$$

So, for the triangle of sides a y b we have

$$\frac{\partial f}{\partial a} = -Jb\exp(-\alpha)$$

$$\frac{\partial f}{\partial b} = Ja\exp(-\alpha)$$

which implies for the critical points

$$a^T Jb = 0$$

$$a^T b = 0$$

that is what we expected. To analyze the behavior of our functional in its critical points, we can consider without lost of generality the triangle with non zero area and vertices (1,0),(0,0) and (l,θ), this last point in polar coordinated and having l fixed (Figure 3). So, the functional (7) can be written as

$$f = \exp(-2l\sin(\theta))$$

and it follows that

$$\frac{\partial f}{\partial \theta} = -2l\cos(\theta)\exp(-2l\sin(\theta))$$

which leads to

$$\theta \equiv \frac{\pi}{2} \pmod{\pi}.$$

Finally, we can conclude from

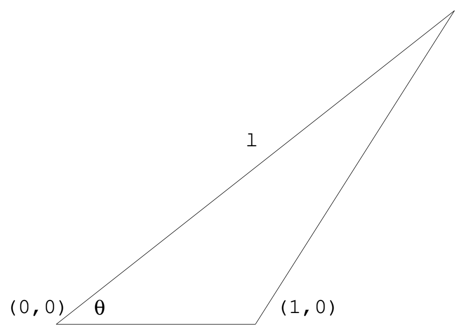

Figure 3. Oriented triangle with a free side.

$$\frac{\partial^2 f}{\partial \theta^2} = \left(2l\sin(\theta) + 4l^2\cos(\theta)^2\right)\exp(-2l\sin(\theta))$$

that

$$\left(\frac{\partial^2 f}{\partial\theta^2}\right)_{\theta=\frac{\pi}{2}} = 2l\exp(-2l) > 0$$

$$\left(\frac{\partial^2 f}{\partial\theta^2}\right)_{\theta=-\frac{\pi}{2}} = -2l\exp(-2l) < 0.$$

This is nothing but what we wanted: our functional for single triangles is minimized by right angle triangles with positive orientation, this is, when ($\theta = \frac{\pi}{2}$); besides it is clearly convex, non negative and $\mathcal{C}^\infty$.
What we need now is to find out a general condition to guarantee that this functions will be useful when we consider the functional for the whole grid.

7. SCHUR-CONVEX FUNCTIONS.

Schur-convex functions were introduced by I. Schur en 1923 [15]; we will show in the next paragraphs that the functional

$$F(G) = \sum_{q=1}^{N} \exp(-\alpha_q) \tag{8}$$

is of this kind and therefore is a suitable choice for the construction we want to do.

Definition 2. An $n \times n$ $S = [s_{ij}]$ matrix is said to be doubly stochastic if $s_{ij} \geq 0$ for $1 \leq i,j \leq n$, and

$$\begin{aligned}\sum_{j=1}^{n} s_{ij} &= 1, \qquad i = 1,2,\cdots,n\\ \sum_{i=1}^{n} s_{ij} &= 1, \qquad j = 1,2,\cdots,n.\end{aligned}$$

Let I be an interval of the real line; we have the following definitions.

Definition 3. A function $f : I^n \to \mathbb{R}$, $n > 1$, is said to be Schur-convex if for every doubly stochastic matrix S

$$f(Sx) \leq f(x)$$

$\forall x \in I^n$. If the inequality is strict whenever $Sx \neq x$, f is called strictly Schur-Convex.

Definition 4. $f : I^n \to \mathbb{R}$, $n > 1$, is said to be symmetric if for every permutation matrix P we have

$$f(Px) = f(x)$$

$\forall x \in I^n$.

Every Schur-convex function is symmetric; the reciprocal does not hold in general([12]).
The next theorem is a classical result known as the Schur test; it gives a sufficient and necessary condition for a function to be Schur-convex. We omit here the also classical proof that can be found in [16], [18] or [17].

Theorem 7.1. *Let $f(x) = f(x_1, x_2, \cdots, x_n) : I^n \to \mathbb{R}$ be symmetrical and $\mathcal{C}^1(I^n)$, where $I \subseteq \mathbb{R}$ is an open interval of the real line. f is Schur convex if and only if*

$$(x_i - x_j)\left(\frac{\partial f}{\partial x_i} - \frac{\partial f}{\partial x_j}\right) \geq 0$$

for $x_i, x_j \in I$, $i,j = 1,...,n$. If in addition, the inequality is strict when $x_i \neq x_j$, $1 \leq i,\ j \leq n$, then f is strictly Schur-Convex.

8. EXP-FUNCTIONALS.

Our goal now is to show that the functional (8) can be used to generate convex grids.
The first step is the following

Theorem 8.1. *The functional (8) is strictly Schur-convex.*

Proof. F is symmetrical, since the mapping $+ : I^n \to \mathbb{R}$ given by $(x_1, x_2, \cdots, x_n) \mapsto x_1 + x_2 + \cdots + x_n$ is; as a straight consequence of 7.1 it is only needed to show that

$$(\alpha_1 - \alpha_2)\left(\frac{\partial f}{\partial \alpha_1} - \frac{\partial f}{\partial \alpha_2}\right) \geq 0$$

So, without lost of generality we can assume that $\alpha_1 > \alpha_2$; then

$$(\alpha_1 - \alpha_2)\left(\frac{\partial f}{\partial \alpha_1} - \frac{\partial f}{\partial \alpha_2}\right) =$$

$$(\alpha_1 - \alpha_2)\left(\exp(-\alpha_2) - \exp(-\alpha_1)\right) > 0$$

since the exponential is a monotonous increasing function, the conclusion of the theorem follows immediately. □

Finally, we have the following result.

Theorem 8.2 (Xin-Min Zhang[12]). *Let $A \in \mathbb{R}$ a positive constant, $I = (-A, A) \subset \mathbb{R}$ be an open interval of the real line, $f : I^n \to \mathbb{R}$ Schur-convex and $C_n = I^n \cap H_n$, where*

$$H_n = \{\Theta = (x_1, \cdots, x_n) \in \mathbb{R}^n \mid \sum_{i=1}^{n} x_i = A\}.$$

Then, f has a minimum value in $\tilde{x} = (\frac{A}{n}, ..., \frac{A}{n}) \in C_n$. Besides, if f is strictly Schur-convex, the minimum value given by $\tilde{x}$ is unique.

Proof. Let us the doubly stochastic $n \times n$ matrix given by $S = [\frac{1}{n}]$. Since f is Schur-convex

$$f(Sx) \leq f(x)$$

$\forall x \in I^n$. Now, $\forall x \in C_n$, we have

$$f(\tilde{x}) = f(Sx) \leq f(x).$$

If f is strictly Schur-convex, then $f(\tilde{x}) < f(x)$, $\forall x \in C_n$, $x \neq \tilde{x}$. □

Very similar results to the one stated above have been widely applied in the theory of majorizations. A very deep, beautiful and interesting insight can be found in the texts of Hardy, Littlewood and Pólya ([17]), and Marshall and Olkin ([18]).
As a straight consequence we have the

Corollary 8.3. *Let $\tilde{D} = \{x = (\alpha_1, \cdots, \alpha_n) | x \in \mathbb{R}^n\}$, where every point in $\tilde{D}$ is such that $\alpha_1, \cdots, \alpha_n$ are the values of α for some $G \in D$; $I = (0, A)$, $\tilde{x}$, and H_n as in 8.2. If $\tilde{x} \in C_n \cap \tilde{D} = [I^n \cap H_n] \cap \tilde{D}$, then the functional (8) has a global minimum when $\alpha_q = \overline{\alpha}$, $q = 1, \cdots, n$.*

This corollary guarantees our functional (8) has the property we require whenever $\tilde{x}$ is admissible for the values of α in a given grid. In the general case for an arbitrary grid, the existence of such a particular solution can not be guaranteed, however, since theorem (8.2) holds for the whole euclidean space, the "average" point works as some kind of "attractor" for points in a neighborhood of it, and working, in consequence, good enough for the generation of convex grids.

9. NUMERICAL IMPLEMENTATION.

For the numerical implementation of (8) once it is written in terms of $\alpha/(2\overline{\alpha})$, one of the main features was the use of a slightly modified version given by

$$F(G) = C_1 \sum_{q=1}^{N} \exp(-C_2 \alpha_q) \tag{9}$$

where C_1 and C_2 are positive constants chosen to sharpen as much as possible the graph of (9); until now they have been selected in an heuristic way as

$$\begin{aligned} C_1 &= 1.0 \\ C_2 &= \begin{cases} \frac{2.0}{\alpha_{-}+1} & \alpha_{-} > -0.5 \\ 2000.0 & \alpha_{-} < -0.5 \end{cases} \end{aligned} \tag{10}$$

where for a grid G,

$$\alpha_{-}(G) = \min_{\triangle \in G} \alpha(\triangle).$$

As it can be seen, the use of these constants has no effect on the previous results, so they can be introduced in the development freely in order to improve the convergence.
To solve the optimization problem, we made use of a Truncated Newton method with a trust region strategy as it is implemented in **UNAMALLA**([13]). The test regions used were polygonal lines approaching the shapes of the Havana bay, South America, Russia and California; their graphics are shown in figure 4.
In every case, starting with an initial non convex grid generated by TFI(Transfinite Interpolation) a convex grid with 21 points by side was achieved in less than 50 iterations being convexity the stop criterion; the graphs of the obtained grids are shown in figures 5,6,7 and 8.

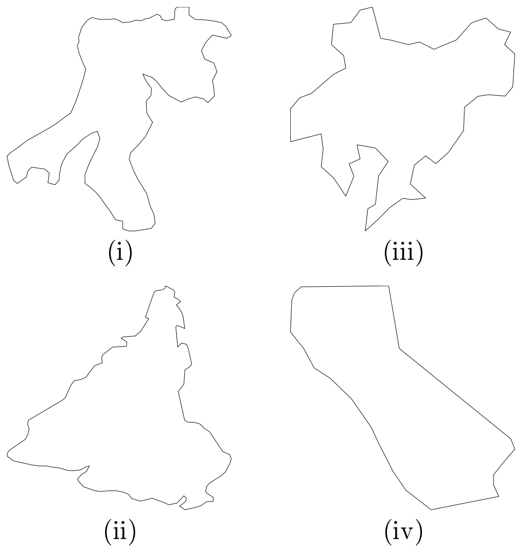

Figure 4. Boundaries used.

10. CONCLUSIONS.

A geometrically intuitive functional for the construction of convex structured grid is indeed given by (8), and it's straightforward to see that its continuous analog is given by a expression of the kind

$$\int_{\Omega} e^{-J(\xi,\theta)} d\xi d\eta$$

where ξ, η, are the variables of the physical domain and $J(\xi, \theta)$ is the Jacobian. In terms of this formula, we can investigate the behavior of the associated Euler-Lagrange equations, to find out in which way they imply the convexity of a grid using such equations as a generating system; this goal is one of the parts of our present work, since the full comprehension of the properties of this functional is expected to motivate some ideas leading to the formulation of a complete dynamical theory including the k-functionals.
The main value of this development is theoretical, further considerations need to be done from a practical point of view regarding the constants C_1 and C_2, to control the sometimes "explosive" values of the exponentials of α; however, it is very important to see that we have finally "designed" a functional which works without the need of a special parameter within the theory.

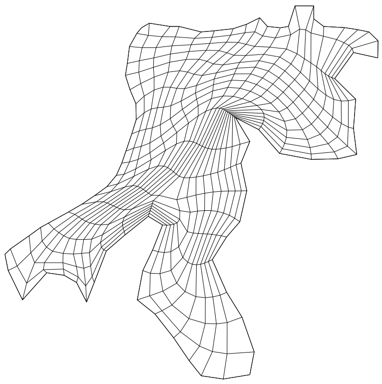

Figure 5. Havana bay grid.

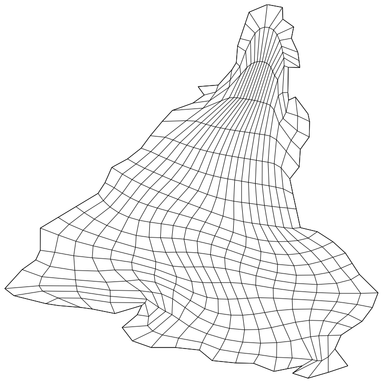

Figure 6. South America grid.

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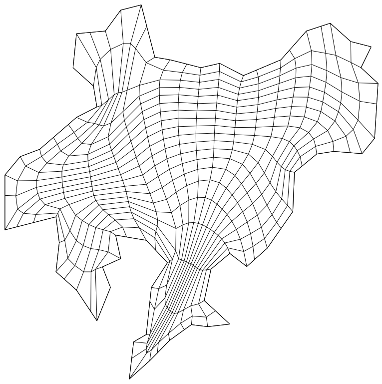

Figure 7. Russia grid.

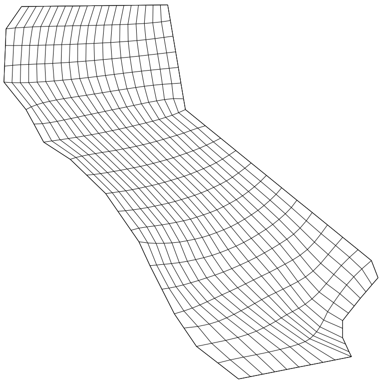

Figure 8. California grid.

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