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AREA FUNCTIONALS FOR HIGH QUALITY GRID GENERATION

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Abstract. In this paper, to solve the grid generation problem in the context of a large scale optimization process, we describe objective functions having adjustable continuous barriers that can be set in such a way that the variable values in their minimizers are as "non spread out" or "nearly equal" sets as possible. We also present a grid generation method based on those functionals that can be used to generate very high quality structured grids on irregular plane regions by means of a continuation approach. Several numerical examples of grids generated on quite irregular *2D* regions, show the effective performance of the proposed method and its potential in the numerical solution of differential equations.

Keywords: Variational grid generation, grid, quality grids, convex functionals.

1 INTRODUCTION

Variational grid generation has been used quite successfully in the last years. Its beginnings arose in the work of Brackbill and Saltzman[6] in 1982, and in the contributions of Steinberg and Roache[15] in 1986. A major advance in the subject was done in 1988, when Charakhch'yan and Ivanenko[11] introduced a harmonic approach which is very effective in plane irregular regions provided that an initial convex grid is known.

This last requirement was to expensive, in general, for irregular regions. To overcome this problem, some efficient approaches based on convex functionals have been presented in the last years by Barrera, Domínguez-Mota and Tinoco[1,5,8] by making use of adjustable barriers. However, it was observed that for some grids generated for irregular regions, nearly singular grid cells could be obtained.

In this paper, as a solution for the problem describes in the previous paragraph, we introduce a general procedure for the construction of bilateral area functionals that can be used to generate high quality structured grids on irregular regions in a very efficient way.

This paper is organized as follows: Section 1 presents a brief list of some preliminary results. Sections 2 and 3 describe the discrete generation problem we will deal with and sections 4-7 the area functionals to solve it, followed by some implementation details and numerical results in sections 8 and 9. As expected, conclusions about the work end this paper.

2 PROBLEM FORMULATION

The regions to be considered for the grid generation problem of our interest, are simple connected domains Ω in the plane whose boundaries are closed polygonal positively oriented Jordan curves. The grid generation problem can be described as the construction of continuous almost everywhere smooth functions $x(\xi,\eta)$, $y(\xi,\eta)$ that define a one-to-one mapping

$$\mathbf{x} : R \to \Omega$$
$$\mathbf{x} = \mathbf{x}(\xi,\eta)$$

from the unit square

$$R = \{(\xi,\eta) | 0 \le \xi,\eta \le 1\}$$

onto the physical region Ω (Fig. 1).
The mapping $\mathbf{x}(\xi,\eta)$ is required to have a full rank Jacobian matrix of positive determinant to preserve the orientation on R and Ω defined by the boundaries. Thus, the continuous grid generation problem is posed in the following way:
Problem 1 To find a one to one smooth mapping (or continuous grid) $\mathbf{x}(\xi,\eta)$ from the unit square onto the domain Ω that satisfies

$$J = x_\xi y_\eta - x_\eta y_\xi \tag{1}$$

on the whole unit square.

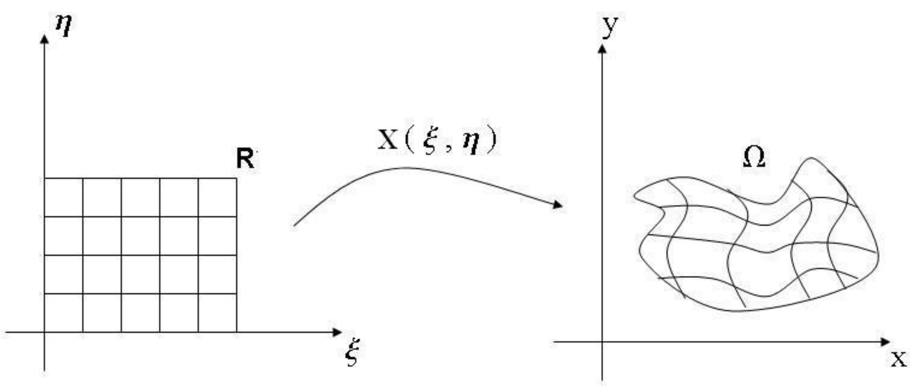

Figure 1 – Mapping between R and Ω

A grid is *admissible* if $\mathbf{x}(\partial R) = \partial\Omega$.
In order to solve this problem, Winslow[14] developed a method based on the calculation of the component functions $\xi(\mathrm{x,y})$, $\eta(\mathrm{x,y})$ of the inverse mapping $\mathbf{x}^{-1}$ defined over Ω and that satisfy the set of Laplace equations

$$\begin{aligned} \xi_{xx} + \xi_{yy} &= 0 \\ \eta_{xx} + \eta_{yy} &= 0 \end{aligned} \qquad (2)$$

with Dirichlet boundary conditions given by $\mathbf{x}^{-1}(\partial\Omega) = \partial R$. However, the direct use of equations (2) for grid generation is not convenient, since grids that might have a non positive Jacobian can be obtained, even on simple regions.
A usual alternative approach is to make a change of variables to transform (2) into a couple of equations for $\mathrm{x}(\xi,\eta)$ and $\mathrm{y}(\xi,\eta)$:

$$\begin{aligned} ux_{\xi\xi} - 2vx_{\xi\eta} + wx_{\eta\eta} &= 0 \\ uy_{\xi\xi} - 2vy_{\xi\eta} + wy_{\eta\eta} &= 0 \end{aligned} \qquad (3)$$

where

$$\begin{aligned} u &= x_\eta^2 + y_\eta^2 \\ u &= x_{\xi\eta} + y_{\xi\eta} \\ w &= x_\xi^2 + y_\xi^2 \end{aligned}$$

Nonetheless, it is important to notice that the numerical solution of equations (3) using a finite difference scheme does not guarantee positiveness of the jacobian (i.e., the convexity) of the transformation $(\xi,\eta) \mapsto (x, y)$ either.
A variational formulation for problem **1**, related to the set of equations (4) for the inverse mapping $\mathbf{x}^{-1}$, was first considered in 1982 by Brackbill and Saltzman[6]. They proposed the functional

$$I_S = \iint_R \frac{x_\xi^2 + x_\eta^2 + y_\xi^2 + y_\eta^2}{J} d\xi d\eta \qquad (4)$$

Equations (3) are the Euler-Lagrange expressions for the functional (4).

3 DISCRETE FORMULATION

Before proceeding any further, some notation must be introduced. Let us consider a region Ω of the plane, defined by a simple, closed and counterclockwise oriented polygonal curve γ of vertexes $V = \{v_1, v_2, \cdots, v_q\}$ (Figure 2).

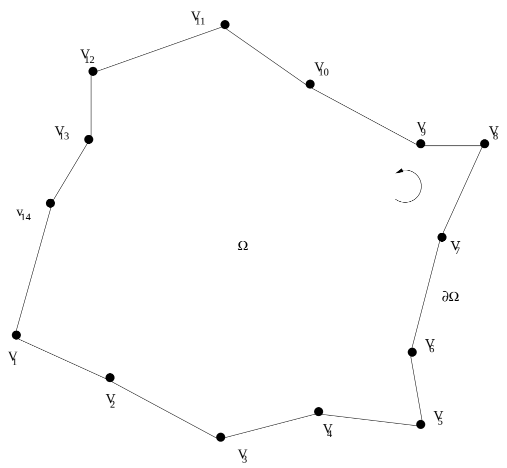

Figure 2 – Example of a region defined by a simple closed polygonal curve

Definition Let m, n be natural numbers with $m, n > 2$. A set G of points of the plane

$$G = \left\{ P_{i,j} \mid i = 1, \ldots, m; \; j = 1, \ldots, n \right\}$$

with boundaries

$$L_1(G) = \{P_{i,1} \mid i = 1, \ldots, m\}$$

$$L_2(G) = \{P_{m,j} \mid j = 1, \ldots, n\}$$

$$L_3(G) = \{P_{i,n} \mid i = 1, \ldots, m\}$$

$$L_4(G) = \{P_{1,j} \mid j = 1, \ldots, n\}$$

is called a structured, admissible and discrete grid* for Ω, of order $m \times n$, if

* With quadrilateral elements.

$$V \subseteq \bigcup_{i=1}^{4} L_i(G).$$

Besides, we will say that G is convex if each one of the $(m-1)(n-1)$ quadrilaterals (or cells) $c_{i,j}$ of vertexes $\{P_{i,j}, P_{i+1,j}, P_{i,j+1}, P_{i+1,j+1}\}$, with $1 \le i < m$ y $1 \le j < n$, is convex.
The sets w $L_1(G)$, $L_2(G)$, $L_3(G)$ y $L_4(G)$ will be considered *the sides of the grid boundary or the grid sides*, and appear in the definition to emphasize our interest in having the same boundary for the region and for the grid.
The unsatisfactory results of the numerical solution of the Euler-Lagrange equation using finite differences led to Ivanenko and Charakhch'yan[9] to propose a different discretization that consists in the minimization of I_S by working with the variational principle itself rather that with the Euler-Lagrange equation.
They approximated the functional (4) by the use of quadrilateral isoperimetric finite elements obtaining the Discrete Harmonic Functional:

$$H(G) = \sum_{i=1}^{m}\sum_{j=1}^{n}\sum_{k=1}^{4} \frac{\lambda(\Delta_{i,j}^{k})}{\alpha(\Delta_{i,j}^{k})} = \sum_{q=1}^{N} \frac{\lambda(\Delta_q)}{\alpha(\Delta_q)} \qquad (5)$$

where m and n are the number of horizontal and vertical points of a discrete grid G respectively, k is used to sequentially denote the four triangles formed with the vertexes of each quadrilateral grid cell, $\lambda(\Delta_q)$ is the length functional and $\alpha(\Delta_q)$ is twice the oriented area for such triangles, as described below. In this formula, the variable N stands for the total number of triangles, equal to four times the number of grid cells.

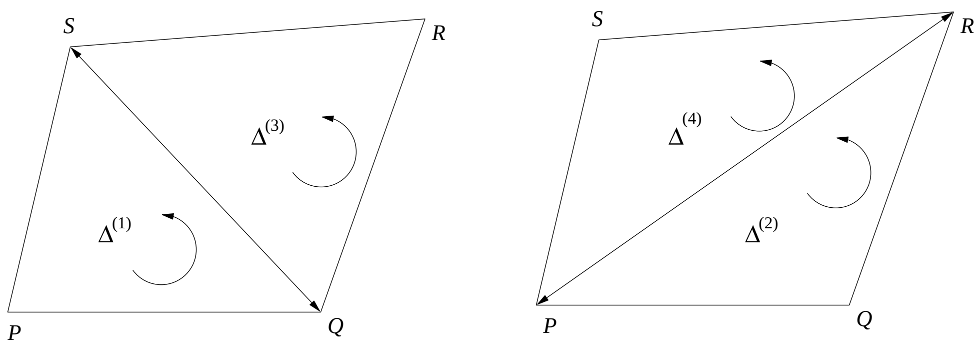

Figure 3 – Example The four oriented triangles defined by a quadrilateral grid cell

In order to define α and λ, we consider every grid cell as divided into four oriented triangles in order to control the convexity of the cells (Fig. 3). Thus, for the oriented triangle with vertexes Q, P, R, the functions λ and α are defined as

$$\begin{aligned}\lambda(\Delta(Q,P,R)) &= \|P-Q\|^2+\|P-R\|^2\\ \alpha(\Delta(Q,P,R)) &= (P-Q)^t\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}(P-R)\end{aligned} \tag{6}$$

where $\|\cdot\|$ denotes the Euclidean norm. Clearly, a grid G is *convex* if $\min\{\alpha(\Delta_q)>0 \mid q=1,\ldots,N\}$.
In what follows we will use α and $\alpha(\Delta_q)$ indistinctly, as well as the average value $\overline{\alpha}(G)$ of the N values of α for a grid G. The set $M(\Omega)$ will denote the whole set of admissible grids for a region Ω.

In this context, the discrete grid generation problem can be posed, in general, as a large scale optimization one:
Problem 2 To solve

$$G^* = \arg\min_G \sum_{q=1}^{N} f(\Delta_q)$$

over the set $M(\Omega)$ of admissible grids for a region.
Therefore, a numerical grid is a minimizer of some discrete functional and will be also referred to as an optimal grid.
The adequate selection of f is the keystone to get some important properties on those minimizers, such as convexity and smoothness. It is even possible to assert that for numerical purposes, the main goal is to propose functions f for which such minimizers are convex grids.
A simple and efficient functional that can be used to solve problem **2** will be described in the next section.

4 THE FUNCTIONAL S_3

Barrera and Domínguez-Mota[8] proposed a solutions for convex grid generation problem **2** using area functionals (i.e., with no explicit dependence on λ) and proved the following theorem:
Theorem 1. *If f is a C^2 strictly decreasing convex and bounded below function such that $f(\alpha)\to 0$ as $\alpha\to\infty$, then the functional*

$$S(G)=\sum_{q=1}^{N} f(t\alpha(\Delta_q)) \tag{7}$$

is minimized by convex grids for $t>0$ large enough[1].
Theorem **1** shows that the number of functions useful to generate convex grids is quite large, but, for numerical purposes, it is convenient to use some very economical choices for f like

$$s_3(\alpha)=\begin{cases}1/\alpha, & \alpha\ge 1\\ (\alpha-1)(\alpha-2)+1, & \alpha<1\end{cases}$$

can be used, for which the functional for a grid G, whose values of α are $(\alpha_1,\ldots,\alpha_N)^T$, is given by

$$S_3(G) = \sum_{i=1}^{N} s_3(t\alpha_i). \qquad (8)$$

5 ε_c-CONVEXITY

Minimization of S_3 can be successfully used to generate convex grids, as it has been reported in several previous papers[1,2,8]. However, an important issue observed in experimentation must be addressed: Since the last iterations in the optimization process required to generate the final convex grid have to deal with few non convex cells whose area is very close to zero, for some quite irregular regions, these last iterations must be performed with a large value of t, and are slower that the first ones in term of the number of function evaluations.
This is caused mainly for the presence of cells with a relatively large positive area because the function s_3 decreases quite fast as t and α increase. Naturally, from a numerical view, it is quite convenient to find a strategy to improve the ratio between the maximum and minimum values of α in the generated grids.
This latter task can be approached from two different but complementary angles. The first one is related with the original definition of convexity, related with the bounds for the domain Ω: It must be noted that the condition $\min\{\alpha(\Delta_q) > 0 \mid q = 1,\ldots,N\}$, when evaluated numerically, can give rise to an ill-posed scale-depending definition of convexity.
Therefore, *it is of the greatest relevancy to select an adequate framework for a practical numerical definition*. To do so, we propose in a first step to scale the region Ω to satisfy the condition

$$\overline{\alpha}(G) = 1,$$

since this average depends only on the region scale, not on a particular grid, and then to choose an $\varepsilon_c << 1$ value. Thus, we will say that a grid G is ε_c-convex if

$$\min\{\alpha(\Delta_q) > \varepsilon_c \mid q = 1,\ldots,N\}$$

It is important to emphasize that one measure of the grid generation problem is the greatest value ε_c for which ε_c-convex grids exist.

6 THE FUNCTIONAL $S_{3,\tau}$

Once a practical definition of convexity has been proposed, we are in position to discuss the second approach and propose improvements for last iterations in the optimization process that deal with few non convex cells with nearly zero areas.
The theoretical foundations for theorem **1** show that for $\tau > 0$ the functional

$$S_{3,\tau}(G) = \sum_{i=1}^{N} s_3(t(\alpha_i - \tau)) \qquad (8b)$$

can actually be minimized for grids G satisfying

$$\min\{\alpha(\Delta_q) > \tau \mid q = 1,\ldots,N\}$$

for $t > 0$ if the set $\left\{G \in M(\Omega) \middle| \alpha_{-}(G) > \tau\right\}$ is non empty.

This functional is clearly an improvement of S_3. However, within the same context it is even possible to design and amazing new functional, as we will see in the next section.

7 THE BILATERAL FUNCTIONAL B_3

It has been observed that the presence of cells with a large normalized positive area because the function s_3 decreases quite fast as t and α increase.

To overcome this problem, Tinoco[4] proposed the use of an area functional with two poles acting as barriers. In a similar way, the same strategy proposed for (8) and (8b) can be applied again, recalling that the functional was designed to increase the lower α values in a grid by means of the parameter t. This is exemplified in Figure 4, where the typical level sets for S_3 are shown: The sketched surfaces contain the point $(1,1,1)^T$, but for the largest value $t = 1$ the set is completely contained the first octant. Thus, as theorem **1** states, if there exists convex grids for a region, the minimum values of S_3, when evaluated in admissible grids, are attained for convex grids for t large enough.

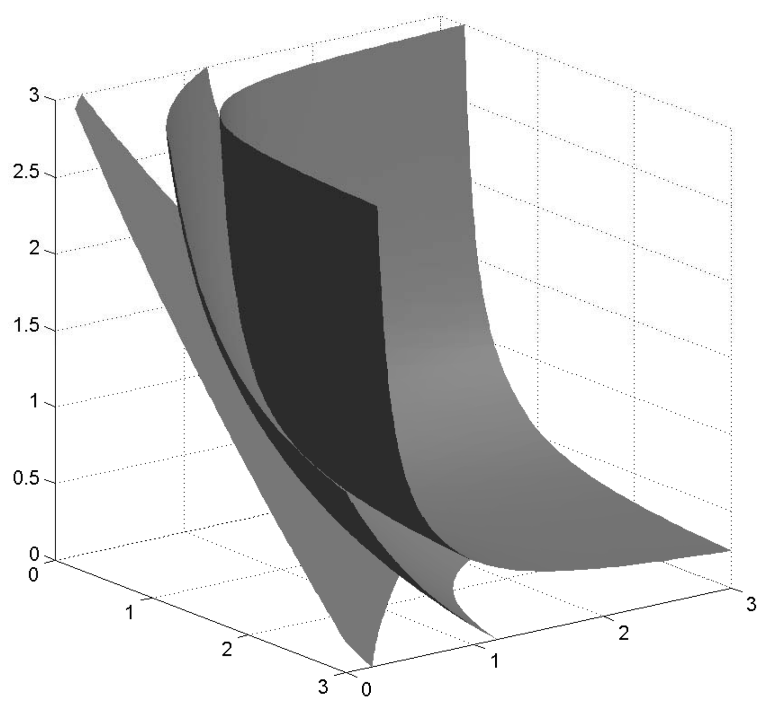

Figure 4 – Typical level sets for S_3

Thus, to avoid very large cell areas, it is straightforward to consider a "reflection" of S_3 to create a second control barrier that decreases the higher α values as much as possible. Consequently, we define the new functional B_3 as

$$B_3(G) = \sum_{i=1}^{N} (s_3(t(\alpha_i - \tau)) + s_3(\frac{t}{c}(\alpha_0 - \alpha_i))) \qquad (9)$$

where $t > 0$, and $c > 0$ is a fixed parameter to control the relative rigidity between the two barriers in (9) and $\alpha_0 > \overline{G}$ is another fixed parameter to control large cell areas.

The typical level sets for B_3 are shown in figure 5. It can be seen that as t increases, as in the case of S_3, the level set for $(1,1,1)^T$ is eventually contained inside the first octant, but now, for this new functional is a *bounded set*.

Applying the strategy of theorem **1**, it is true that in the general case, if there is at least a convex grid G_0 for a region, the level set for G_0 defined by B_3 will be contained in the first "hyper-octant" of the Euclidean space for t large enough.

Then, the minimizers of B_3 will be attained in points inside the bounded region by the level set, *id est*, in convex grids. The left barrier in B_3 will take care of convexity, and the right one will improve the quality.

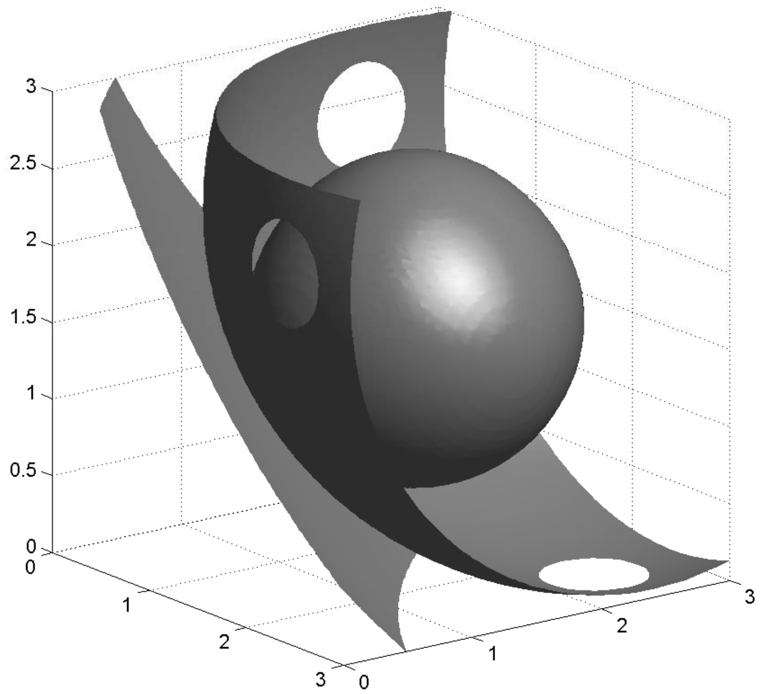

Figure 5 – Typical level sets for B_3

8 IMPLEMENTATION DETAILS

In order to design an algorithm based on theorem **1** and the functionals introduced on the previous sections to generate a grid sequence that converges to a convex one, since the value of t is unknown *a priori* and therefore must be updated after starting from an initial guess, the following considerations have to be taken into account:

1. $\overline{\varepsilon_c}$ **-convexity.** For the practical implementation the definition of convexity we will use a tolerance value ε_c. We set $\overline{\varepsilon_c} = \varepsilon_c \cdot \overline{\alpha}(G)$. Thus, an $\overline{\varepsilon_c}$-convex grid satisfies that $\alpha\_(G_n^*) > \varepsilon_c \cdot \overline{\alpha}(G) = \overline{\varepsilon_c}$.
2. **Initial value for** t. For an initial non convex grid, a reasonable choice for this value is half the average area: $t_1 = \overline{\alpha}(G)/2$. If the initial grid is already convex, it is convenient to set a larger value, for instance $t_1 = 20\overline{\alpha}(G)$.
3. **Optimization loop**. In order to optimize the grid for each value of t_n, the tolerances for the stopping criteria, `tolf` for the relative error between successive function values and `tolg` for the gradient norm, should be set with care. In the implementation presented below we write the values we proved in our codes.

Thus, the algorithm for the generation of convex grids using our functionals is the following:
Algorithm. Convex grid generation.

0. Given $\varepsilon_c, t_{\max}, \tau$, $\mu > 1$ and an initial grid G_1. Set $\overline{\varepsilon_c} = \varepsilon_c \cdot \overline{\alpha}(G)$, $n = 1$

    if $(\alpha\_(G_n^*) < \overline{\varepsilon_c})$ then *(non-convex)*

        Set $t_1 = \overline{\alpha}(G)/2$, tolf$=10^{-4}$, tolg$=10^{-2}$

    else (*convex*)

        Set $t_1 = t_{\max}$, tolf$=(epsmach)^{1/2}$, tolg$=10^{-5}$

    end

1. Solve

$$G_n^* = \arg\min_{G \in M(\Omega)} \{S_{3,\tau}(G)\} \qquad or \qquad G_n^* = \arg\min_{G \in M(\Omega)} \{B_3(G)\}$$

2.

    if $(\alpha\_(G_n^*) > \overline{\varepsilon_c})$ then

        (finish) ``an $\overline{\varepsilon_c}$-convex grid has been obtained for the current value of $\overline{\varepsilon_c}$"

    else

        Set $t_{n+1} = \min\{\mu \cdot t_n, t_{\max}\}$

        if$(t_{n+1} = t_{\max})$ then

            (finish)``NO $\overline{\varepsilon_c}$-convex grid has been obtained , Try with a lower value for $\overline{\varepsilon_c}$"

        end

        Set tolf$= \max\{(epsmach)^{1/2}, \text{tolf} \cdot 10^{-1}\}$,

        tolg$= \max\{10^{-5}, \text{tolf} \cdot 10^{-1}\}$, $n = n + 1$

        go back to step 1

    end

9 NUMERICAL TESTS

For the numerical tests, four test regions with complex boundaries representing Havana Bay, Peru, Ucha Lake in Russia and Great Britain were selected.
After selecting the four sides on each boundary, initial grids with 40 points by side were generated algebraically using Transfinite Interpolation and scaled to satisfy $\overline{\alpha} = 1$.
The parameters for the initial grids are shown in table 1: α_- and α_+ represent the minimum and maximum values of α for every grid respectively, and **Inocon** is the corresponding number of non convex grid cells.

Region	α_-	α_+	**Inocon**
Havana	-3.61660	13.75990	395
Peru	-4.12686	3.649765	182
Ucha	-7.63817	8.854598	464
Great Britain	-6.28183	9.393747	604

Table 1: Area values before optimization

Using the algorithm described in the preceding section with parameters

$$
\begin{aligned}
t_1 &= 1 \\
\mu &= 2 \\
\varepsilon_c &= 10^{-2} \\
n &= 1, \ldots, 5
\end{aligned}
$$

and minimizing by means of a Trust Region Newton Method (TRON) that solves bound constrained nonlinear optimization problems[13], the minimization of the functional $S_{3,\tau}$ produced the convex grids included in figure 6; the corresponding parameters are in table 2.
The ratio in the last column of table 2 is a measure of the difficulty of meshing each region. Clearly, the regions called Havana, Ucha and Great Britain have a great inherent complexity.

Region	α_-	α_+	α_- / α_+
Havana	0.0162	5.1828	319.5102
Peru	0.0523	3.1881	61.0145
Ucha	0.0153	7.3674	480.9168
Great Britain	0.0101	7.9512	784.6574

Table 2: Area values obtained using the functional S_3

Next, choosing $\tau = 10^{-1}$, we tested the functional $S_{3,\tau}$ with the same parameters and initial grids. The final numbers are in table 3 and the generated grids in figure 7.

Region	α_-	α_+	α_-/α_+
Havana	0.1029	5.2060	50.5928086
Peru	0.2500	2.5090	10.036
Ucha	0.1012	5.6109	55.4436759
Great Britain	0.1132	6.5731	58.0662544

Table 3: Area values obtained using the functional $S_{3,\tau}$

Finally, we set $\varepsilon_c = 10^{-1}$ and applied the algorithm to minimize B_3 (See table 4 and figure 8).

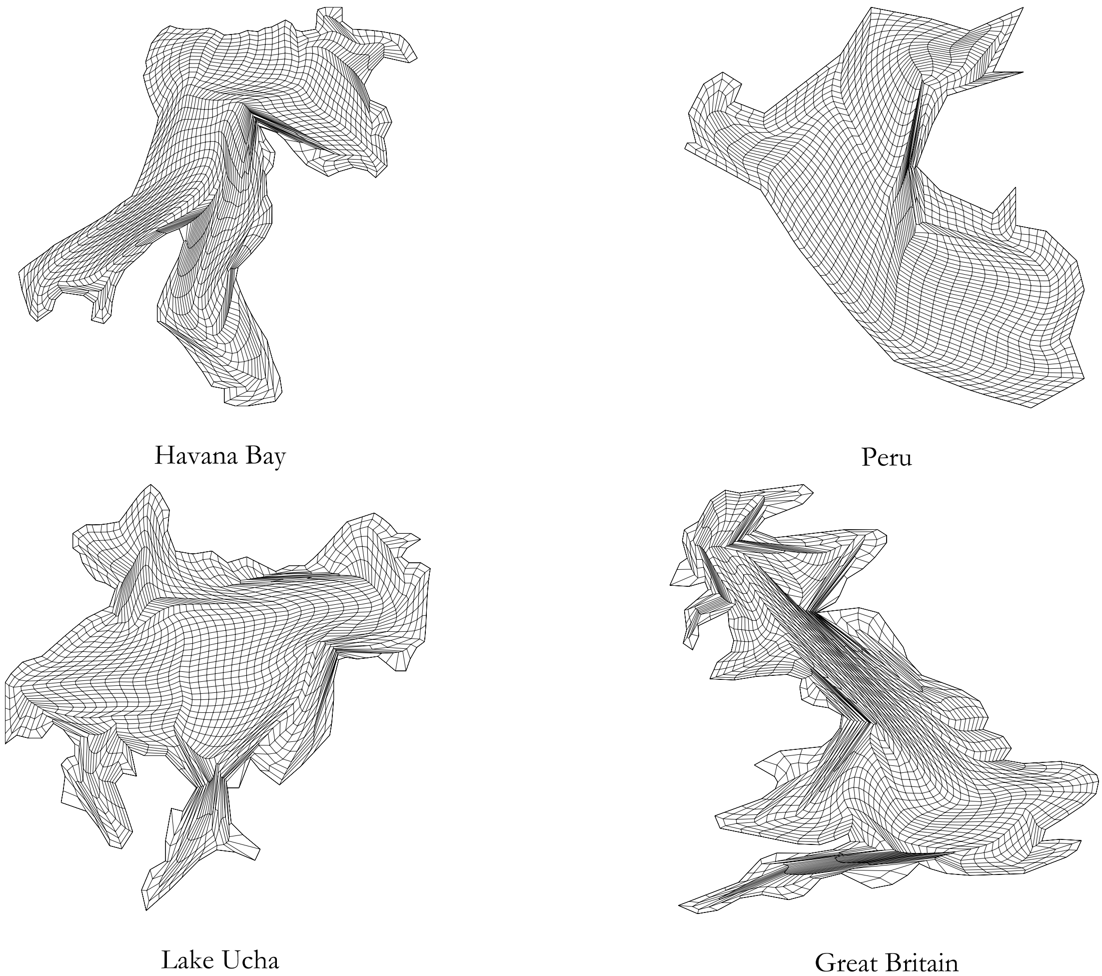

Figure 6 – Grids generated with S_3

It is straightforward to see that the minimum value of α has been notably improved causing a very significant decrease of the ratio α_{-}/α_{+} as expected. In this sense, it can be said that the quality of the grids generated with $S_{3,\tau}$ and B_3 is much greater.

Region	α_{-}	α_{+}	α_{-}/α_{+}
Havana	0.1029	4.1454	40.2918
Peru	0.1733	1.5255	8.8048
Ucha	0.1704	5.8632	34.4096
Great Britain	0.1426	5.0716	35.5529

Table 4: Area values obtained using the functional B_3

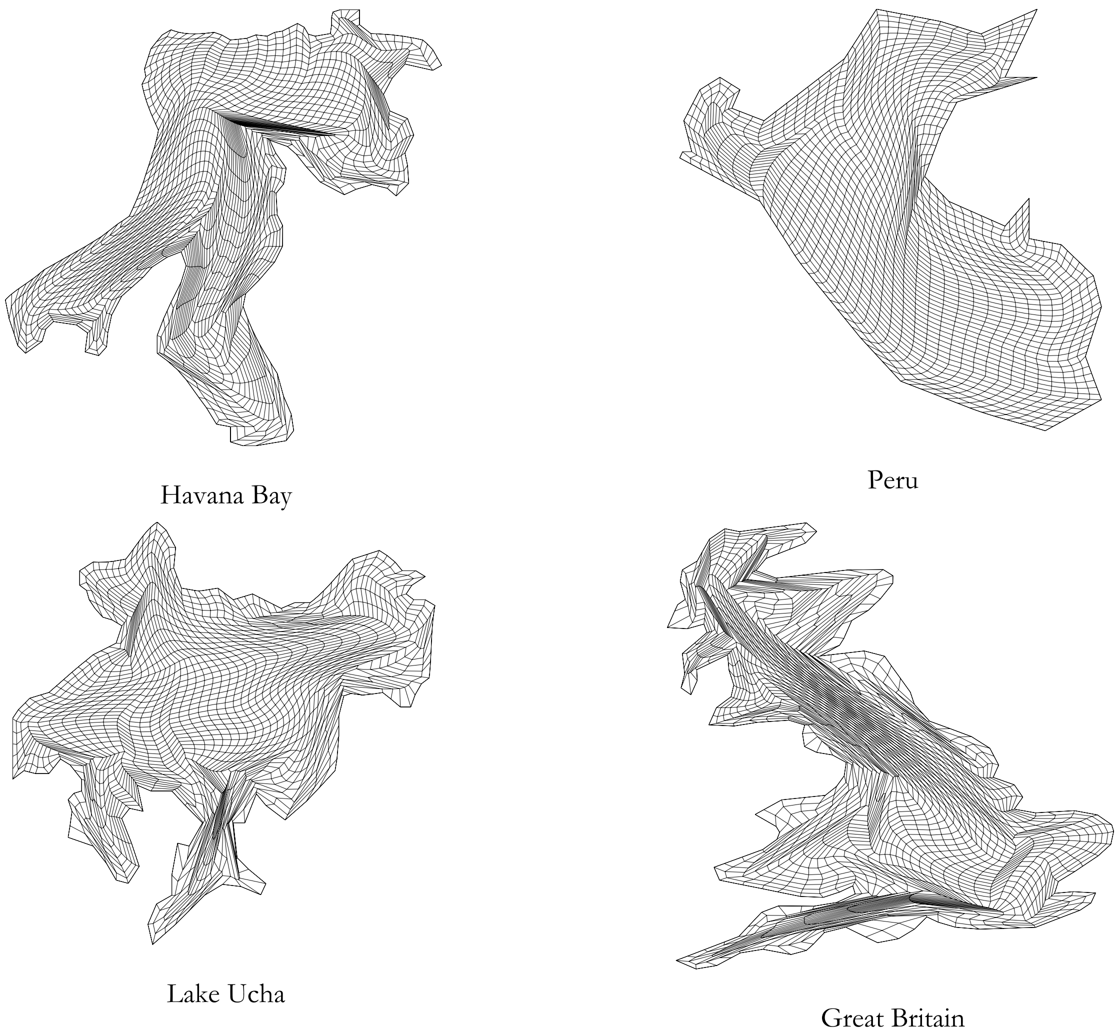

Figure 7 – Grids generated with $S_{3,\tau}$

The effect τ and the second barrier in the functionals is quite evident. The values of α of the grids obtained with $S_{3,\tau}$ and B_3 are less spread out that the corresponding values for the grids generated with S_3.

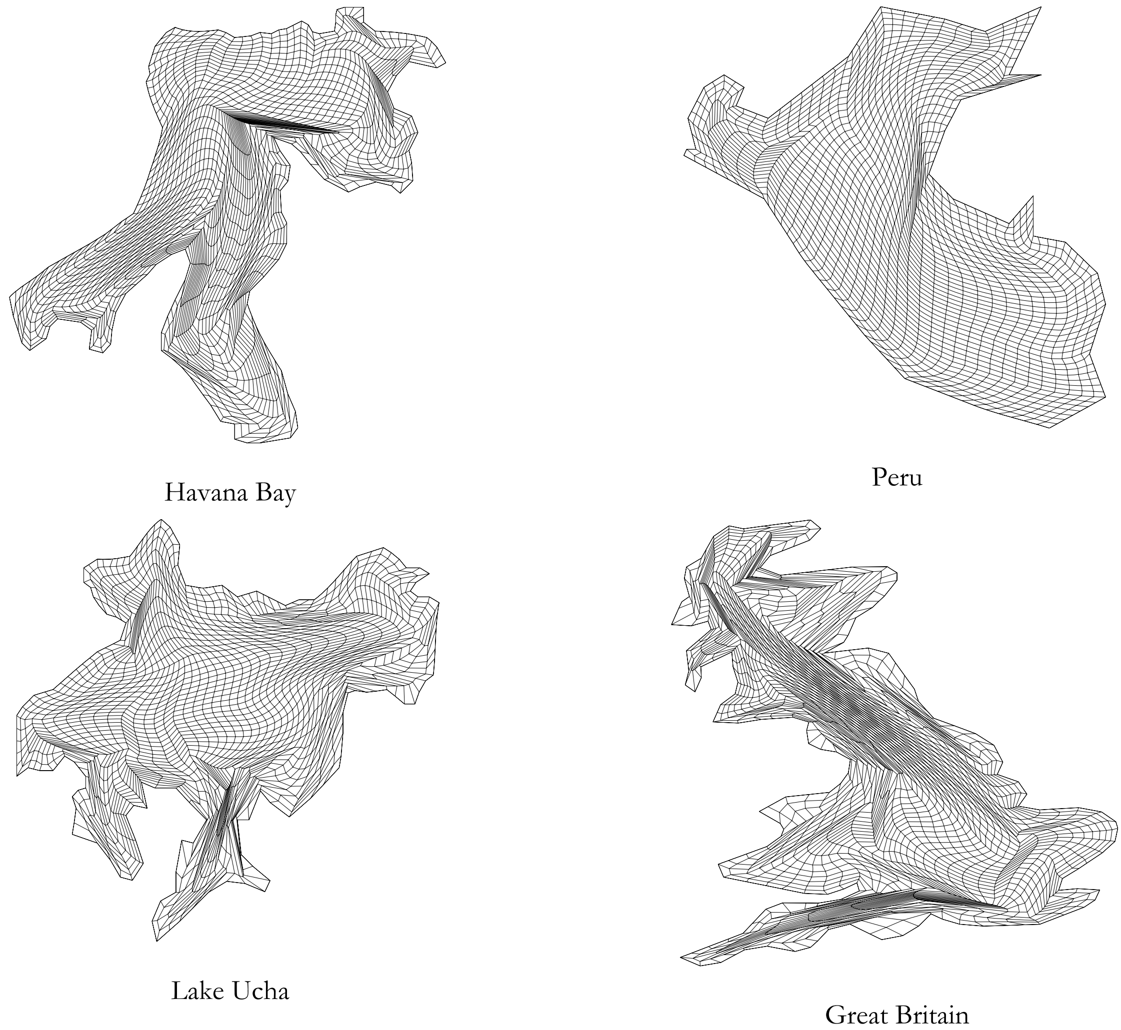

Figure 8 – Grids generated with B_3

10 CONCLUSIONS

An efficient and robust algorithm to generate high quality structured convex grids was presented in this paper. Since very few methods are useful to generate structured convex grids in irregular plane regions, the proposed algorithm can be very useful for a number of modeling systems.

Current researches deal with the use of the grid generated in the implementation of high order numerical schemes for the solution of differential equations defined over irregular plane domains.

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