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Some experiences on orthogonal grid generation

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Abstract

The present work shows two approaches to the generation of orthogonal or quasi-orthogonal grids applying similar techniques to those implemented by Barrera-Sánchez and Tinoco-Ruiz [Ph.D. Thesis, CIMAT, 1997] on the construction of smooth and convex grids, considering linear combinations of functionals defined over the grid as little perturbations to orthogonality. © 2002 Published by Elsevier Science B.V. on behalf of IMACS.

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1. Basics

1.1. Some history

The development of applications involving the calculus of PDE's numerical solutions over planar regions required previously the generation of a convenient grid on the domain of the equation; in the general case, it is a quite irregular region. This irregularity provokes that certain features needed for the numerical implementation, such as smoothness, convexity and specially orthogonality, are a little hard to get, at least, simultaneously.

Solving the problem of grid generation, Winslow (1966) handled the first presentations of the basic concepts used on this work: area, length, smooth and orthogonality over a grid; later, formal manipulation of these functionals was made by Steinberg and Roaché (1986, see [10]) and Thompson and Warsi (1985, see [10]) by solving Euler–Lagrange differential equations defined over the grid, which are associated to the functionals. They produced good grids on noncomplicated regions, but in general convexity and orthogonality were not achieved.

Castillo (1986–1987) developed the corresponding discrete versions of such functionals, solving a large scale optimization problem associated to the functional. In 1992 Barrera-Sánchez, Castel-

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lanos-Noda and Pérez-Domínguez, see [2] rewrote the discrete version of the problem, improving results and enhancing the control over the geometrical properties of the grid.

Nowadays, the construction of smooth and convex grids over arbitrary irregular planar regions has been solved: the work of Barrera-Sánchez and Tinoco-Ruiz (1997, see [11]) was successful in this direction for very irregular planar regions employing some new area and smoothness functionals.

However, orthogonality of the grid turned out to be difficult to get at the same time, since it implies nonconvexity in many cases. Generation of orthogonal grids, as orthogonal as needed to be useful in some applications, is not a settled issue yet.

1.2. Grids and discrete variational grid generation

1.2.1. Classical functionals

Definition 1. A (continuous) grid $\Psi(\xi,\eta) = (x(\xi,\eta), y(\xi,\eta))$ over a planar region $\Omega \subset \mathbb{R}^2$ is a diffeomorphism $\Psi : I^2 \to \mathbb{R}^2$, where $I = [0, 1]$.

We are interested in those mappings which satisfy $\Psi(\partial I^2) = \partial\Omega$.

Grid generation can be thought as the search of a diffeomorphism extension from a mapping $\psi : \partial I^2 \to \partial\Omega$ to $\Psi : I^2 \to \mathbb{R}^2$.

Historically (meaning the last 30 years), there have been two main different approaches to get that extension; first, algebraic manipulation dealing with interpolation, and second, by solving a PDE associated to the function Ψ. Since Castillo's work, some advances have been made using the so-called variational direct methods.

Definition 2. A planar region is called polygonal if its boundary is a simple (closed) polygon.

Definition 3. An $m \times n$ grid G over a polygonal domain Ω is a set of points in the plane

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

such that $P_{i,1}, P_{i,2}, \dots, P_{i,n}$ is the ith vertical line and $P_{1,j}, P_{2,j}, \dots, P_{m,j}$ is the jth horizontal line.

The sets

$$P_{1,1}, P_{2,1}, \dots, P_{m,1} \quad \text{and} \quad P_{1,n}, P_{2,n}, \dots, P_{m,n},$$

are the upper and lower horizontal boundaries and

$$P_{1,1}, P_{1,2}, \dots, P_{1,n} \quad \text{and} \quad P_{m,1}, P_{m,2}, \dots, P_{m,n}$$

are the left and right vertical boundaries. To our purposes, we must ask that

$$\partial\Omega = \text{polygon}(P_{1,1}, P_{2,1}, \dots, P_{m,1}, P_{m,2}, \dots, P_{m,n}, P_{m-1,n}, \dots, P_{1,n}, P_{1,n-1}, \dots, P_{1,1}).$$

All other points are interior (or inner) to the grid.

Definition 4. A discrete functional over a grid $\{P_{i,j}\}$ is a function

$$I(\{P_{i,j}\}) = \sum_{i,j} f(c_{i,j}),$$

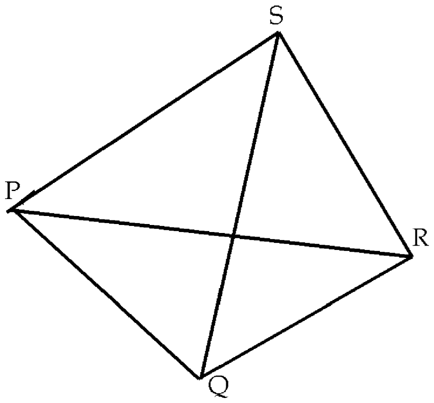

Fig. 1. A typical cell.

where $c_{i,j}$ is the ijth cell of the grid and

$$f(c_{i,j}) = f(P_{i,j}, P_{i+1,j}, P_{i+1,j+1}, P_{i,j+1})$$

is a function measuring some geometrical property over the cell, and in consequence, over the grid.

Since $I(\{P_{i,j}\})$ is a function in several variables, generally two plane variables (its coordinates) for every inner point of the grid for a non symmetric region, the problem of finding an optimal grid must be solved using a unrestricted large-scale optimization method, so this implementation is very fast. Further information on the strategies employed can be found in [2].

Now, we will consider a "typical" cell as shown in Fig. 1. Over this cell, we can state the definitions of our basic direct functionals.

We start introducing the bilinear mapping proposed by Barrera-Sánchez and Pérez-Domínguez, considering the simplest mapping r from I^2 to our cell given by

$$r(\xi, \eta) = A + B\xi + C\eta + D\xi\eta,$$

where A, B, C, and D are chosen in order to satisfy

$$r(0,0) = P, \qquad r(1,0) = Q, \qquad r(0,1) = S, \qquad r(1,1) = R.$$

These conditions lead to

$$r(\xi, \eta) = P + (Q - P)\xi + (S - P)\eta + (R - Q + P - S)\xi\eta$$

and therefore

$$r_\xi(\xi, \eta) = Q - P + (R - Q + P - S)\eta,$$
$$r_\eta(\xi, \eta) = S - P + (R - Q + P - S)\xi.$$

Hence,

$$r_\xi(0,0) = Q - P, \qquad r_\xi(1,0) = Q - P, \qquad r_\xi(0,1) = R - S, \qquad r_\xi(1,1) = R - S,$$
$$r_\eta(0,0) = S - P, \qquad r_\eta(1,0) = R - Q, \qquad r_\eta(0,1) = S - P, \qquad r_\eta(1,1) = R - Q.$$

It must be noted that $r_\xi(0,0)$ and $r_\eta(0,0)$ depend only on S, P, Q, in other words, it depends on $\triangle SPQ$; similarly, $r_\xi(1,0)$ and $r_\eta(1,0)$ depend only on $\triangle PQR$, $r_\xi(0,1)$ and $r_\eta(0,1)$ depend exclusively on $\triangle RSP$, $r_\xi(1,1)$ and $r_\eta(1,1)$ depend only on $\triangle QRS$. The Jacobian of r is given by

$$J = r_\xi^{\mathrm{T}} J_2 r_\eta, \quad \text{where } J_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

From this we can write

$$J(0,0) = (Q-P)^{\mathrm{T}} J_2 (S-P) = 2\,\mathrm{area}(\triangle SPQ)$$

and similar expressions for $J(1,0)$, $J(0,1)$ and $J(1,1)$.

By defining

$$\alpha(\triangle ABC) = (C-B)^{\mathrm{T}} J_2 (A-B)$$

we can write $J(0,0) = \alpha(\triangle SPQ)$ and similar expressions for the remaining three triangles of the cell; these expressions represent the area functional on each of the four triangles of our cell.

The length functional for an individual triangle can be written as

$$\lambda = \|r_\xi\|^2 + \|r_\eta\|^2$$

so

$$\lambda(0,0) = \|Q-P\|^2 + \|S-P\|^2,$$
$$\lambda(1,0) = \|Q-P\|^2 + \|R-Q\|^2,$$
$$\lambda(0,1) = \|R-S\|^2 + \|S-P\|^2,$$
$$\lambda(1,1) = \|R-S\|^2 + \|R-Q\|^2$$

and again, defining

$$\lambda(\triangle ABC) = \|A-B\|^2 + \|C-B\|^2$$

we can write

$$\lambda(0,0) = \lambda(\triangle SPQ), \quad \lambda(1,0) = \lambda(\triangle PQR), \quad \lambda(0,1) = \lambda(\triangle RSP), \quad \lambda(1,1) = \lambda(\triangle QRS).$$

One of the functionals we are more interested in, the orthogonality functional, is written as

$$O = r_\xi^{\mathrm{T}} r_\eta.$$

Now we define

$$o(\triangle ABC) = (A-B)^{\mathrm{T}}(C-B)$$

and write, as before,

$$O(0,0) = o(\triangle SPQ), \qquad O(1,0) = o(\triangle PQR),$$
$$O(0,1) = o(\triangle RSP), \qquad O(1,1) = o(\triangle QRS).$$

If we name the ijth cell as $P_{i,j}Q_{i,j}R_{i,j}S_{i,j}$, and the four triangles on it as

$$\triangle S_{i,j}P_{i,j}Q_{i,j} = \triangle_{i,j}^1, \qquad \triangle Q_{i,j}R_{i,j}S_{i,j} = \triangle_{i,j}^2,$$
$$\triangle P_{i,j}Q_{i,j}R_{i,j} = \triangle_{i,j}^3, \qquad \triangle R_{i,j}S_{i,j}P_{i,j} = \triangle_{i,j}^4$$

the general functional over the grid can be written as

$$F=\sum_{i=1}^{m-1}\sum_{j=1}^{n-1}\sum_{k=1}^{4} f\left(\triangle_{i,j}^{k}\right).$$

Finally, we have that the length functional adopts the form

$$F_L=\sum_{i=1}^{m-1}\sum_{j=1}^{n-1}\sum_{k=1}^{4} \lambda\left(\triangle_{i,j}^{k}\right)$$

the area and reciprocal functionals

$$F_A=\sum_{i=1}^{m-1}\sum_{j=1}^{n-1}\sum_{k=1}^{4} \left(\alpha\left(\triangle_{i,j}^{k}\right)\right)^2, \qquad F_{A^{-1}}=\sum_{i=1}^{m-1}\sum_{j=1}^{n-1}\sum_{k=1}^{4} \frac{1}{\alpha(\triangle_{i,j}^{k})},$$

the orthogonality functional

$$F_O=\sum_{i=1}^{m-1}\sum_{j=1}^{n-1}\sum_{k=1}^{4} \left(o\left(\triangle_{i,j}^{k}\right)\right)^2$$

and the smoothness functional

$$F_S=\sum_{i=1}^{m-1}\sum_{j=1}^{n-1}\sum_{k=1}^{4} \frac{\lambda(\triangle_{i,j}^{k})}{\alpha(\triangle_{i,j}^{k})}.$$

In the study of the behavior of these functionals the following quantities are important:

$$\alpha_+(G)=\max_{\triangle\in G}\bigl(\alpha(\triangle)\bigr), \qquad \alpha_-(G)=\min_{\triangle\in G}\bigl(\alpha(\triangle)\bigr).$$

Relevant properties of these functionals and a deeper presentation can be found in [6,10,11]. We just want to point out that convexity cannot be guaranteed when they are applied on arbitrary regions. In the next section, we present the proposal by Tinoco-Ruiz and Barrera-Sánchez (see [11]) of some other form of the area and smoothness functional, which guarantee convexity on very irregular regions.

1.2.2. New functionals

The main problem at this point is how to guarantee convexity on the grid we are working with. In order to solve this problem, Tinoco-Ruiz and Barrera-Sánchez proposed a variation of the previous functionals which they called adaptive, introducing a parameter k to control the non convexity, as we briefly present next.

Bearing in mind the definitions given in the previous section, we introduce

$$D_k=\bigl\{G \mid G\in M, \alpha_-(G)>-k\bigr\},$$

where M is the set of all the grids defined over the region Ω. If $k<k'$, we have $D_k\subset D_{k'}$, besides if

$$k\leqslant -\bar{\alpha}=-\frac{\text{Area}(\Omega)}{(m-1)(n-1)}$$

then $D_k=\phi$. Therefore the set of real numbers k such that $D_k\neq\phi$ is nonempty and bounded below; if we set $k_-=\text{glb}\{k \mid D_k\neq\phi\}$. It can be said that the set of convex grids over Ω is nonempty if $k_-<0$.

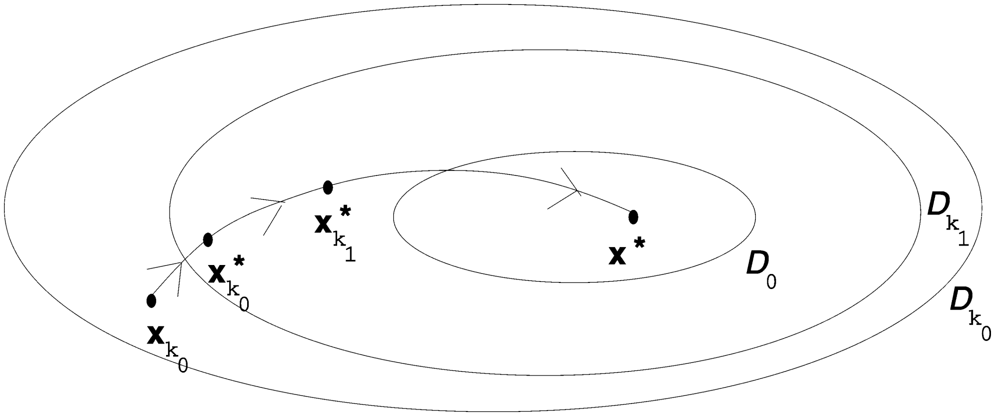

Fig. 2. An expected trajectory.

Smoothness and reciprocal area functionals generate convex grids if the initial mesh is convex, which is an important limitation for their use.

If, for each triangle, α is greater than k, then $1/(\alpha + k)$ is positive, and so this way

$$f_{A_k^{-1}}(\triangle) = \frac{1}{k + \alpha(\triangle)}, \qquad f_{S_k}(\triangle) = \frac{\lambda(\triangle)}{k + \alpha(\triangle)},$$
$$F_{A_k^{-1}} = \sum_{i=1}^{m-1}\sum_{j=1}^{n-1}\sum_{l=1}^{4} f_{A_k^{-1}}\left(\triangle_{i,j}^{l}\right), \qquad F_{S_k} = \sum_{i=1}^{m-1}\sum_{j=1}^{n-1}\sum_{l=1}^{4} f_{S_k}\left(\triangle_{i,j}^{l}\right)$$

are non-negative. For both functionals, it can be shown [9] that for k positive, if $D_k \neq \phi$, $F_{A_k^{-1}}$ and F_{S_k} have a minimum on D_k. Hereinafter, $F_{A_k^{-1}}$ and F_{S_k} will be referred to as the k-area (kA) and the k-smoothness (kS) functionals, respectively.

The use of these new functionals produced good grids, meaning convex and smooth, by calculating an appropriate k, then optimizing and afterwards updating k, until a convex grid is built. Details and more properties of $F_{A_k^{-1}}$ and F_{S_k} can be found in [11]; an implementation is available as part of UNAMALLA system [12]; the process can be summarized in a short algorithm:

1. Get $\alpha_-(G_0)$ as initial grid.
2. Calculate $k = -1.005\alpha_-(G_0) + \varepsilon$, with a convenient ε.
3. Get G_k as $F_k(G_k) = \min_{G\in D_k}(F_k(G))$.
4. Go to step 2 until convexity of G_k is achieved.

Thinking each one of the grids G_k obtained in every step as trajectory points in the set of all grids over Ω, the convex grid generation can be considered as the problem of finding a suitable trajectory from the initial grid to the subset of convex grids on Ω, as sketched in Fig. 2.

So, at this point, a trusty algorithm to generate convex grids is at hand. However, watching these grids one can think that there should be a way to modify them slightly to get real rectangles within the original region, which is the motivation for some of the ideas of the following sections.

1.2.3. Combination of functionals

When optimizing one of the functionals introduced, we try to find a grid having a geometric property given by the features associated to optimal values of each of them [6,9,11]. It would be desirable to have more than just one property on our grids. In order to accomplish this convex combinations of functionals have been proposed and employed with good results in many cases; the general form to combine (two) F_1 and F_2 is given by

$$F = \sigma F_1 + (1 - \sigma) F_2,$$

where $0 \leqslant \sigma \leqslant 1$.

It is of great importance to point out that in those combinations, the magnitude of the values of the functionals could lead to an inappropriate sum, since they have different magnitude orders, this is a very important point if we really want to combine the geometrical properties. To avoid any trouble, functionals must be previously normalized according to their optimal values; the better normalization the better grids. Details of how it can be done for the classical and new functionals are available in [6,11].

2. Orthogonal grid generation

2.1. Orthogonality

In order to solve PDEs numerically over a grid, this one must be convex. If in addition, the grid is orthogonal or almost orthogonal, the implementations of solution algorithms are easier and numerical errors on the solution are diminished; some early works in the generation of orthogonal grids were made by Eiseman, Brackbill and Saltzman in 1982 (see [3]).

However, the use of the orthogonality functional presented in Section 1.2.1 as a first approach has some difficulties. In the general case, when orthogonality criteria are used in order to get meshes, the meshes generated are quite nonconvex, since those criteria produce folding in the grids when they try to fit the inner angles of each cell to be $\pi/2$. As an example of how bad the situation can turn out when orthogonality is the only geometrical criterion in the optimization, we can see Fig. 3: an “almost” standard rectangle twists into a nonstandard origami figure.

The ideas presented in Section 1.2.2 show, so far, that construction of convex meshes can be guaranteed over irregular plane regions, but orthogonality obviously can not. Now a basic analytic concept will be used in order to get as much orthogonality as possible.

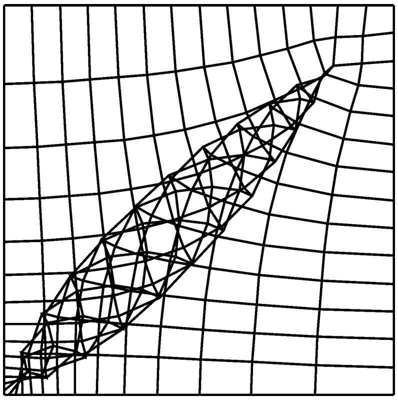

Fig. 3. When orthogonality is used.

Different approaches to get orthogonality by means of conformal mappings can be found in [8], another one was made by Eça in 1996 [6] by rebuilding the distribution of the mesh on the boundaries. But we would like to deal with a fixed boundary distribution, since we think an automatic grid generation algorithm should not modify the original geometrical information, given by the way the region is defined.

2.2. Continuity and functional combinations

It is easy to prove that for a field k, the mapping $\Theta : k \times k^N \times k^N \to k$, given by $\Theta = \sigma F_1 + (1-\sigma) F_2$, with $\sigma \in k$, $F_1, F_2 : k^N \to k$ is continuous; this is the fact we mainly use to "get close" to orthogonality.

As a direct consequence of continuity, $\Theta(\varepsilon, F_1, F_2)$ and $\Theta(0, F_1, F_2)$ are proximal values if ε is small enough. But $\Theta(0, F_1, F_2)$ is nothing but F_2, so if we choose a little value for σ, an approximation to F_2 is obtained. What small means is given by how close we can approach.

Taking F_1 as the k-area or k-smooth functionals, convexity will be guaranteed since O will be bounded in the domain of kS and kA. Besides taking σ in our combination as in the previous paragraph, we expect to get low values for the O functional, recalling that the optimal value for O in an individual cell is obtained when the cell is actually a rectangle, which gives zero for the optimum.

2.3. Some results

The application of such idea to several cases gives promising results; kS-O and kA-O stand for the combinations k-smoothness and k-area with orthogonality, respectively.

Table 1 contains some results of the application of kS-O and kA-O with $\sigma = 0.01$ and $\sigma = 0.50$ to five 40×40 test regions: Russia, Havana Bay, England, South America and a simple polygonal region called "El Gato" [12]; a nice plot of the Havana Bay region, applying kA-O with $\sigma = 0.01$, is shown in Fig. 4. Data in the table are organized in the following way: σ is taken to be the weight of the first functional, kS or kA. NC is the number of nonconvex cells in the grid, convexity is obtained when it is zero; A, L and O stand for the values of area, length, and orthogonality functionals. The last column shows the ratio

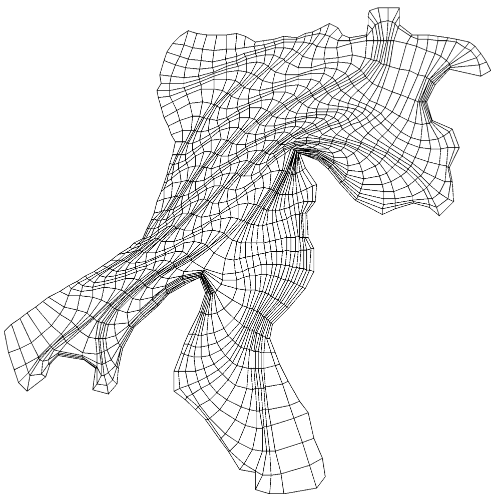

Fig. 4. Havana Bay.

Table 1
Results of kA-O and kS-O

		σ	NC	A	L	O	$\alpha+/\alpha-$
Russia	O		>300	5.00	2.60	0.120	−0.644
	kA-O	0.01	0	1.69	2.05	0.178	1459.3
	kA-O	0.50	0	1.10	2.06	0.526	15.724
	kS-O	0.01	0	1.49	1.89	0.118	112.42
	kS-O	0.50	0	1.47	1.57	0.620	130.80
Havana	O		>300	5.07	2.50	0.053	−0.615
Bay	kA-O	0.01	0	1.87	2.13	0.153	46.479
	kA-O	0.50	0	1.10	2.06	0.526	11.722
	kS-O	0.01	0	1.28	2.33	0.542	70.760
	kS-O	0.50	0	1.80	1.57	0.806	80.537
England	O		>300	17.3	4.54	0.619	−0.390
	kA-O	0.01	0	3.01	3.85	1.480	1158.1
	kA-O	0.50	0	1.55	4.00	2.580	107.24
	kS-O	0.01	0	3.07	3.57	1.540	1230.0
	kS-O	0.50	0	2.17	2.81	3.410	1192.2
South	O		>300	4.46	2.44	0.089	−0.324
America	kA-O	0.01	0	1.57	2.13	0.178	107.39
	kA-O	0.50	0	1.07	2.03	0.428	14.296
	kS-O	0.01	0	1.37	1.87	0.179	118.52
	kS-O	0.50	0	1.25	1.66	0.499	126.88
El Gato	O		>300	5.27	2.62	0.032	−0.556
	kA-O	0.01	0	2.25	2.41	0.114	48.879
	kA-O	0.50	0	1.21	3.10	1.030	37.733
	kS-O	0.01	0	2.24	2.32	0.144	200.00
	kS-O	0.50	0	2.14	1.80	0.997	269.49

$\alpha+/\alpha-$, which is a criterion to measure the regularity and quality of the grids obtained. For the sake of brevity we only present results with $\sigma = 0.01$ or $\sigma = 0.50$; smaller values of σ will result in orthogonality values closer to zero and as we separate from a small weight we expect orthogonality values to increase. A fast look at these data shows that kA-O is a factible choice to do such approximation. Two facts must be noted: first, the grids obtained are convex in all cases as expected, and second, it is important to recall that O is measured in the least squares sense, in such a way that some bad angles can be seen in the grids. However, if that value is small, all the others will be obviously smaller. That is a consequence of the way we are trying to solve the problem, we do not have control over all individual points.

3. Another combination: the classical AO functional

3.1. The AO functional

Among convex combinations of O with other classical functionals, Knupp and Steinberg [10] proposed the so-called AO functional as

$$AO = \frac{1}{2}(A + O).$$

It has been very successful, since despite the fact that A and O do not produce good grids when used alone, AO gives very smooth grids in few steps. However, the main problem of these functionals lays in convexity: it cannot be guaranteed, but encouraged with the results we got adding “some” k-area to orthogonality we can motivate a procedure analogous to the one in Section 2.

Table 2
kA-AO results

		σ	NC	A	L	O	$\alpha+/\alpha-$
Russia	AO		14	1.09	1.96	0.263	−1.155
	kA-AO	0.01	10	1.11	2.02	0.181	−1.722
	kA-AO	0.50	10	1.10	2.02	1.182	−1.600
Havana	AO		14	1.24	2.03	0.378	−2.006
Bay	kA-AO	0.01	0	1.28	2.23	0.259	88.94
	kA-AO	0.50	0	1.25	2.29	0.318	18.039
England	AO		84	1.36	3.65	1.780	−0.451
	kA-AO	0.01	108	1.52	3.78	1.560	−0.361
	kA-AO	0.50	107	1.52	3.77	1.560	−0.360
South	AO		16	1.09	1.96	0.295	−0.690
America	kA-AO	0.01	18	1.08	2.07	0.209	−2.530
	kA-AO	0.50	0	1.08	2.08	0.215	1760.7
El Gato	AO		66	1.30	2.33	0.401	−3.703
	kA-AO	0.01	0	1.27	2.69	0.438	32.07
	kA-AO	0.50	0	1.17	4.51	0.614	82.112

Due to simplicity, AO can be used to get good initial grids in order to apply other functionals or combinations of them.

3.2. Verbatim copy: we wanna be close to AO

Since AO is a good choice to get factible grids, we would like to approach it in order to keep its good properties but getting convexity at the same time. A verbatim copy of the argument given in Section 2.2 suggests again using F_1 as kA and F_2 as AO to accomplish that task; results with this idea are shown in Table 2.

4. Some conclusions

In a way similar to the data in Table 1 for the orthogonal grid generation case, we get convexity when we add small k-area or k-smooth multiples to the orthogonality functional; but we usually lose orthogonality (in the least squares sense, at least). Also it is possible to see a kind of folding in the grid, which causes the "wave" effect within it, it is a consequence of orthogonality since it folds the grids, as has been told. Therefore, we would like to have control on the size of the cells, in order to get more regular grid in terms of the area.

As a future project, we are giving a try to some other continuous but nonlinear combinations, since is a natural question to ask why we only deal with linear combinations. They work well enough, but attempting to combine more effectively if possible the individual functional properties, looking for some other direct approaches to convexity and orthogonality, we must try with some other ways to combine our geometrical properties.

The normalization for the individual functionals is adequate, since the initial values of k-area and k-smooth functionals have the same order of magnitude as orthogonality, so we can effectively consider the combination as a generalization of O. In area-orthogonal grid generation, in the general case, we see that convexity and the properties of the original A-O grid can not be achieved together. Therefore, we cannot think of kA-AO as a straightforward generalization of A-O; but experimental evidence suggests kA-O to be a natural generalization or AO which leads us to one of the goals: convexity and closeness to orthogonality.

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