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Quality parameters to control algebraic surface grids

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Dedicated to Prof. Laura Gori on the occasion of her $70th$ birthday

Abstract: *In this paper we discuss a strategy to provide geometrical control of algebraic grid surfaces by means of a re-parametrization procedure combined with the use of quality parameters for grid surfaces. The re-parametrization phase is based on a tensor product transformation following given directions. The free parameters in the tensor product are set by solving an optimization problem that uses objective functions based on grid quality measure parameters.*

1 – Introduction

In dealing with the numerical grid generation for the approximation of partial differential equations, we have developed methods and tools mainly for 2D structured grid generation. We have defined either algebraic or elliptic approaches and recently their combination in an algebraic-elliptic algorithm [2]. In this paper we present and discuss a mixed algebraic method for the representation of surfaces in $\mathbb{R}^3$ in order to move the first step towards the surface grid generation for which several methods have been proposed, for example, in [8] and [9]. Indeed the numerical generation of complex grids quite always needs surface discretizations to be carried out. Thinking of volume grid generation it

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results of evidence the role of surface grids as basic components of the whole discretization process. However a satisfactory surface grid can be achieved only by an appropriate parametric representation of domain geometries which guarantees times by times geometrical surface characteristics to be saved.

Given a physical surface $S: [0,1]^2 \rightarrow \Omega \subset \mathbb{R}^3$, we assume information on the surface geometry is available in some way, for instance an appropriate set of interior and boundary data. We look for a simple algebraic transformation $X: [0,1]^2 \rightarrow \Omega$ able to represent the physical surface. Unfortunately, the available algebraic schemes mainly produce parametric surfaces with a very poor parametrization so that the generated grid usually has no particular properties (as orthogonal feature or constant aspect ratio). Therefore, a re-parametrization phase is necessary. Following the idea discussed in [3] in this paper a re-parametrization technique based on tensor product of B-spline bases is proposed and applied to an algebraic method for numerical grid generation. Thus, a new parameter distribution (of arbitrary size) is produced simply through a sampling phase of the tensor product surface. The free parameters (here called control directions) appearing in the tensor product play a key role in the final location of the grid points. More in detail, the control directions used in the tensor product, taken in the parameter domain $[0,1]^2$, are better located in $[0,1]^2$ by solving an optimization problem of small dimension that uses objective functions based on grid quality measure parameters. After the re-parametrization phase the final grid will somehow preserve the features specified by the selected objective functions (see Section 3) and shows a better behavior in the interior of the domain.

The outline of this paper is as follows. In Section 2, an algebraic method used to generate a surface grid from boundary information is given and its properties are investigated. In Section 3, the re-parametrization phase using grid quality measures is discussed. The closing Section 4 is devoted to a few numerical tests showing the effectiveness of the proposed strategy.

2 – Transfinite algebraic surface generation with local control

As well known, transfinite interpolation methods are useful means to construct a three dimensional surface interpolating a net of $\mathbb{R}^3$-curves. With the help of transfinite interpolation methods based on local blending functions, in this section we construct a mixed algebraic surface grid which both conforms to the boundary of a given physical three dimensional domain and possess free parameters for modeling the grid in the interior of the given domain. As already noticed in our previous papers dealing with planar surfaces generated through the so called "mixed schemes" (see for example [1], [5]), free parameters are very helpful to overcome the drawback of classical transfinite interpolation techniques [6] that have no control of the grid quality apart from the boundary. The analytic definition of a so called mixed scheme for generating grids on $\mathbb{R}^3$-surfaces is fully similar to the planar case except for the third component which is now needed. Nevertheless, for completeness, below we shortly discuss the definition of a mixed scheme for $\mathbb{R}^3$ surfaces. It is worthwhile to note that we are going to consider only the Lagrange case even though boundary given directions can be also interpolated assuming they are specified.

Let $\Omega \subset \mathbb{R}^3$ be such that $\partial\Omega = \cup_{i=1}^{4} \partial\Omega_i$, with $\partial\Omega_1 \cap \partial\Omega_3 = \emptyset$ $\partial\Omega_2 \cap \partial\Omega_4 = \emptyset$ where $\partial\Omega_1, \partial\Omega_2,\ \partial\Omega_3, \partial\Omega_4$ are the supports of four regular curves $\gamma_i : [0,1] \to \partial\Omega_i,\ i = 1, \dots, 4$, taken counterclockwise. Furthermore, we assume that the curve intersections occur only at the end points of the boundary curves $\gamma_i,\ i = 1, \dots, 4$ *i.e.*

$$\gamma_1(0) = \gamma_4(1),\ \gamma_1(1) = \gamma_2(0),\ \gamma_2(1) = \gamma_3(0),\ \gamma_4(0) = \gamma_3(1)\,.$$

We define $\phi_1(\xi) := \gamma_1(\xi),\ \phi_2(\xi) := \gamma_3(1-\xi),\ \xi \in [0,1]$ and $\psi_1(\eta) := \gamma_4(1-\eta),\ \psi_2(\eta) := \gamma_2(\eta),\ \eta \in [0,1]$. Note that each curve has three components, for example $\phi_1(\xi) = (\phi_1^x(\xi), \phi_1^y(\xi), \phi_1^z(\xi))$.

A transfinite blending surface interpolating the four boundary curves is defined by the linear operators P_1 and P_2 blending two "opposite" curves, *i.e.*

$$P_1[\boldsymbol{\phi}](\xi,\eta) := \sum_{i=1}^{2} \alpha_i(\eta)\phi_i(\xi)\,, \quad P_2[\boldsymbol{\psi}](\xi,\eta) := \sum_{j=1}^{2} \alpha_j(\xi)\psi_j(\eta)\,, \tag{2.1}$$

and by the action of P_1 when applied to P_2 blending the four corner points,

$$P_1P_2[\boldsymbol{\phi},\boldsymbol{\psi}](\xi,\eta) := \sum_{i=1}^{2} \alpha_i(\eta) P_2[\boldsymbol{\psi}](\xi, i-1)\,. \tag{2.2}$$

The blending functions $\alpha_j(\xi),\ j = 1,2$ in (2.1) are dilated versions of classical bases with support on $I_0^\xi := [0, \bar{u}_\xi]$ and on $I_1^\xi := [1-\tilde{u}_\xi, 1]$ being $0 < \bar{u}_\xi < 1$ and $0 < \tilde{u}_\xi < 1$, for example the piecewise cubic polynomials

$$\begin{aligned} \alpha_1(\xi) &:= \Big(1 + 2\frac{\xi}{\bar{u}_\xi}\Big)\Big(1 - \frac{\xi}{\bar{u}_\xi}\Big)^2,\ \xi \in I_0^\xi\,, \\ \alpha_2(\xi) &:= \Big(3 - 2\frac{\xi + \tilde{u}_\xi - 1}{\tilde{u}_\xi}\Big)\Big(\frac{\xi + \tilde{u}_\xi - 1}{\tilde{u}_\xi}\Big)^2,\ \xi \in I_1^\xi\,. \end{aligned} \tag{2.3}$$

The blending functions $\alpha_j(\eta),\ j = 1,2$ in (2.1), (2.2) are analogously defined with support on $I_0^\eta := [0, \bar{u}_\eta]$ and on $I_1^\eta := [1 - \tilde{u}_\eta, 1]$. With the above given locally supported bases, the Lagrange blending surface

$$(P_1 \oplus P_2)[\boldsymbol{\phi},\boldsymbol{\psi}](\xi,\eta) = P_1[\boldsymbol{\phi}](\xi,\eta) + P_2[\boldsymbol{\psi}](\xi,\eta) - P_1P_2[\boldsymbol{\phi},\boldsymbol{\psi}](\xi,\eta) \tag{2.4}$$

is interpolating the boundary curves

$$(2.5)\qquad \begin{aligned}(P_1 \oplus P_2)[\boldsymbol{\phi}, \boldsymbol{\psi}](j-1, \eta) = \psi_j(\eta),\ j = 1, 2\,,\\ (P_1 \oplus P_2)[\boldsymbol{\phi}, \boldsymbol{\psi}](\xi, i-1) = \phi_i(\xi),\ i = 1, 2\end{aligned}$$

and shows a localized support *i.e.*

$$(P_1 \oplus P_2)[\boldsymbol{\phi}, \boldsymbol{\psi}](\xi, \eta) = 0 \quad \text{for} \quad (\xi, \eta) \in [\bar{u}_\xi, 1 - \tilde{u}_\xi] \times [\bar{u}_\eta, 1 - \tilde{u}_\eta]\,.$$

Now, to “fill the hole” we take into account a tensor product surface

$$(2.6)\qquad T_P(\xi, \eta) := \sum_{i=1}^{m_p} \sum_{j=1}^{n_p} Q_{ij} B_{i,3}(\xi) B_{j,3}(\eta)$$

with $B_{i,3}(\xi)$ and $B_{j,3}(\eta)$ denoting the usual cubic B-splines with knots $\{\xi_{i-2}, \xi_{i-1}, \xi_i, \xi_{i+1}, \xi_{i+2}\}$, $\{\eta_{j-2}, \eta_{j-1}, \eta_j, \eta_{j+1}, \eta_{j+2}\}$, respectively. The set $\mathcal{Q} = \{Q_{ij}\}_{i,j=1}^{m_p,n_p}$ is a set of control points in $\mathbb{R}^3$. The B-splines knots are taken uniformly distributed except for the end knots that are assumed multiple *i.e.*

$$(2.7)\qquad \begin{aligned}0 = \xi_{-1} = \xi_0 = \xi_1 = \xi_2 < \cdots < \xi_{m_p-1} = \xi_{m_p} = \xi_{m_p+1} = \xi_{m_p+2} = 1\,,\\ \text{with} \quad \xi_{i+1} - \xi_i = \frac{1}{m_p - 3},\ i = 2, \ldots, m_p - 2\,,\end{aligned}$$

and similarly,

$$(2.8)\qquad \begin{aligned}0 = \eta_{-1} = \eta_0 = \eta_1 < \eta_2 < \cdots < \eta_{n_p-1} = \eta_{n_p} = \eta_{n_p+1} = \eta_{n_p+2} = 1\,,\\ \text{with} \quad \eta_{l+1} - \eta_l = \frac{1}{n_p - 3},\ l = 2, \ldots, n_p - 2\,.\end{aligned}$$

The boundary knot repetition is to guarantee the interpolation of the end control points. Next, setting $\bar{u}_\xi = \xi_3 - \xi_2,\ \bar{u}_\eta = \eta_3 - \eta_2,\ \tilde{u}_\xi = \xi_{m_p-1} - \xi_{m_p-2},\ \tilde{u}_\eta = \eta_{n_p-1} - \eta_{n_p-2}$, the tensor product surface is then added to the blending surface to produce the so called mixed surface

$$(2.9)\qquad X(\xi, \eta) := T_P(\xi, \eta) + (P_1 \oplus P_2)\big([\boldsymbol{\phi}, \boldsymbol{\psi}] - T_P\big)(\xi, \eta)$$

where the substraction of the surface

$$(P_1 \oplus P_2)[T_P] := (P_1 \oplus P_2)[T_P(0, \eta), T_P(1, \eta), T_P(\xi, 0), T_P(\xi, 1)]$$

is to keep the boundary interpolation. All considered, the transformation X conforms the boundary as well, *i.e.*

$$(2.10)\qquad X(j-1, \eta) = \psi_j(\eta)\ ,\ j = 1, 2, \quad X(\xi, i-1) = \phi_i(\xi)\ ,\ i = 1, 2\,,$$

and has the property

$$X(\xi,\eta) = T_P(\xi,\eta), \quad \text{for} \quad (\xi,\eta) \in [\xi_3, \xi_{m_p-2}] \times [\eta_3, \eta_{n_p-2}] .$$

The three dimensional grid $\mathcal{X}$ is then obtained by sampling X at a given set of parameter values $\{(\xi_i,\eta_j)\}_{i,j=1}^{m_g,n_g}$ *i.e.*

$$\mathcal{X} := \{ \ X(\xi_i,\eta_j) = (x(\xi_i,\eta_j), y(\xi_i,\eta_j), z(\xi_i,\eta_j)) \ \}_{i,j=1}^{m_g,n_g} .$$

For shortness we will also use the notation $\mathcal{X} = \{ \ X_{i,j} = (x_{i,j}, y_{i,j}, z_{i,j}) \ \}_{i,j=1}^{m_g,n_g}$.

Before concluding this section we need to make clearer how to choose the control points. When generating mixed grid on surfaces the location of the control points very much influences the grid shape, even more than in the planar case. Without any additional information we suggest to suitably extract the control points from a bilinear blending surface interpolating the four boundary curves also called Coons patch. For further details and motivation of this choice, though in the planar case, we refer the reader to [1]. Thus, defining the interpolating Coons patch

$$\begin{aligned} L(\xi,\eta) = {} & (1-\eta)\phi_1(\xi) + \eta\phi_2(\xi) + (1-\xi)\psi_1(\eta) + \xi\psi_2(\eta) - \\ & - (1-\eta)\big((1-\xi)\psi_1(0) + \xi\psi_2(0)\big) - \\ & - \eta\big((1-\xi)\psi_1(1) + \xi\psi_2(1)\big) \end{aligned} \tag{2.11}$$

and the parameter value sets $\{\sigma_i\}_{i=1}^{m_p}$ and $\{\tau_j\}_{j=1}^{n_p}$ in $[0,1]$ as

$$\begin{gathered} \sigma_1 := 0, \quad \sigma_2 := \sigma_1 + \frac{1}{3(m_p-3)} \quad \sigma_3 := \sigma_2 + \frac{2}{3(m_p-3)} \\ \sigma_{i+1} := \sigma_i + \frac{1}{(m_p-3)}, \quad i = 3, \dots, m_p - 3 , \\ \sigma_{m_p-1} := \sigma_{m_p-2} + \frac{2}{3(m_p-3)} \quad \sigma_{m_p} := \sigma_{m_p-1} + \frac{1}{3(m_p-3)} = 1 , \\ \tau_1 := 0, \quad \tau_2 := \tau_1 + \frac{1}{3(n_p-3)} \quad \tau_3 := \tau_2 + \frac{2}{3(n_p-3)} \\ \tau_{j+1} := \tau_j + \frac{1}{(n_p-3)}, \quad j = 3, \dots, n_p - 3 , \\ \tau_{n_p-1} := \tau_{n_p-2} + \frac{2}{3(n_p-3)} \quad \tau_{n_p} := \tau_{n_p-1} + \frac{1}{3(n_p-3)} = 1 , \end{gathered} \tag{2.12}$$

the control points are defined as

$$Q_{ij} := L(\sigma_i,\tau_j), \ i = 1, \dots, m_p, \ j = 1, \dots, n_p . \tag{2.13}$$

3 – Re-parametrization by using grid quality measures

The mixed surface grid generation method proposed in Section 2, as well as any other algebraic method, is not always able to produce grids satisfying all the application requirements so that a grid modifications can be looked for. This can be achieved, for example, by a re-parametrization phase based on a B-spline tensor product involving control directions. Thus, a new parameter distribution is produced simply through a sampling phase of the tensor product. The control directions used in the tensor product are better located in $[0,1]^2$ by solving an optimization problem of small dimension that uses objective functions based on grid quality measure parameters. Hence, extending to the surface case the work in [4], in this paper we focus on optimized re-parametrization for algebraic grid surface to control first-order geometrical properties (e.g. cell angles, areas, edge lengths, and aspect ratios). The grid produced this way turns out to show a different behavior in the interior of the physical domain.

To this purpose, we define the Jacobian matrix corresponding to the mapping $X(\xi,\eta) = (x(\xi,\eta), y(\xi,\eta), z(\xi,\eta))$,

$$J := \begin{pmatrix} \dfrac{\partial x}{\partial \xi} & \dfrac{\partial x}{\partial \eta} \\ \dfrac{\partial y}{\partial \xi} & \dfrac{\partial y}{\partial \eta} \\ \dfrac{\partial z}{\partial \xi} & \dfrac{\partial z}{\partial \eta} \end{pmatrix} . \tag{3.1}$$

The matrix columns are vectors tangent to coordinate lines, therefore their lengths control the edge lengths, their dot products are related to the angles between coordinate lines and the determinant to the area of the cells. We consider the following discretization of the Jacobian matrix at $X_{i,j}$

$$J_{ij} := \begin{pmatrix} x_{i+1,j} - x_{i,j} & x_{i,j+1} - x_{i,j} \\ y_{i+1,j} - y_{i,j} & y_{i,j+1} - y_{i,j} \\ z_{i+1,j} - z_{i,j} & z_{i,j+1} - z_{i,j} \end{pmatrix} \tag{3.2}$$

and construct the corresponding discrete metric tensor $T_{ij} := J_{ij}^T J_{ij}$

$$T_{ij} := \begin{pmatrix} g_{11}^{ij} & g_{12}^{ij} \\ g_{21}^{ij} & g_{22}^{ij} \end{pmatrix} , \tag{3.3}$$

with

$$\begin{aligned} g_{11}^{ij} &= (x_{i+1,j} - x_{i,j})^2 + (y_{i+1,j} - y_{i,j})^2 + (z_{i+1,j} - z_{i,j})^2 , \\ g_{22}^{ij} &= (x_{i,j+1} - x_{i,j})^2 + (y_{i,j+1} - y_{i,j})^2 + (z_{i,j+1} - z_{i,j})^2 , \end{aligned} \tag{3.4}$$

and with $g_{12}^{ij} = g_{21}^{ij}$ given by

$$(x_{i+1,j} - x_{i,j})(x_{i,j+1} - x_{i,j}) + \\ + (y_{i+1,j} - y_{i,j})(y_{i,j+1} - y_{i,j}) + (z_{i+1,j} - z_{i,j})(z_{i,j+1} - z_{i,j}) \,. \tag{3.5}$$

The symmetric matrix T_{ij} determines cell angles, areas, edge lengths, but only *relative* directions (angles which grid lines make with each other). Scalar cell functions associated to the matrix T_{ij} have been defined to measure important local properties of a grid (see, for example, [7]).

Coming to the objective functions, let each grid cell $\mathcal{C}_{ij}$ having vertices $\{X_{i,j},\ X_{i+1,j},\ X_{i,j+1},\ X_{i+1,j+1}\}$ be approximated by the parallelogram $\mathcal{C}_{ij}^p$ as in fig. 1. Defining with $H_{ij}(g_{11}^{ij}, g_{12}^{ij}, g_{22}^{ij})$ the value of an appropriate smooth positive function on the cell $\mathcal{C}_{ij}^p$, an averaged global objective function based on the discrete metric tensor has the general form

$$f_H = \frac{1}{(m_g-1)\times(n_g-1)} \sum_{i=1}^{m_g-1}\sum_{j=1}^{n_g-1} H_{ij}(g_{11}^{ij}, g_{12}^{ij}, g_{22}^{ij}) \tag{3.6}$$

and it specializes according to the quality measure we want to take in to consideration. The global objective functions we worked with are listed below while we refer to [4] for a discussion of grid quality measure parameters,

Length objective function.

$$f_L := \frac{1}{(m_g-1)\times(n_g-1)} \sum_{i=1}^{m_g-1}\sum_{j=1}^{n_g-1} P_{ij}^{le}, \text{ where } P_{ij}^{le} := (g_{11}^{ij} + g_{22}^{ij})\,. \tag{3.7}$$

AO objective function.

$$f_{AO} := \frac{1}{(m_g-1)\times(n_g-1)} \sum_{i=1}^{m_g-1}\sum_{j=1}^{n_g-1} P_{ij}^{ao} \text{ where } P_{ij}^{ao} := g_{11}^{ij} g_{22}^{ij}\,. \tag{3.8}$$

Orthogonality objective function.

$$f_O := \frac{1}{(m_g-1)\times(n_g-1)} \sum_{i=1}^{m_g-1}\sum_{j=1}^{n_g-1} P_{ij}^{sk} \text{ where } P_{ij}^{sk} := \frac{(g_{12}^{ij})^2}{g_{11}^{ij} g_{22}^{ij}}\,. \tag{3.9}$$

Area objective function.

$$f_A := \frac{1}{(m_g-1)\times(n_g-1)} \sum_{i=1}^{m_g-1}\sum_{j=1}^{n_g-1} (P_{ij}^{ar})^2, \text{ where } P_{ij}^{ar} := g_{11}^{ij} g_{22}^{ij} - (g_{12}^{ij})^2\,. \tag{3.10}$$

Condition number objective function.

$$(3.11)\quad f_K := \frac{1}{(m_g-1)\times(n_g-1)}\sum_{i=1}^{m_g-1}\sum_{j=1}^{n_g-1} K_2^2(T_{ij}) \text{ where } K_2(T_{ij}) = \|T_{ij}\|\cdot\|T_{ij}^{-1}\|\,.$$

We conclude with the following objective function having a different form from (3.6) also taking in to consideration the area of the quadrilateral cells.

Difference area objective function.

$$(3.12)\qquad f_{DA} := \max_{i,j=1,\dots,m_g,n_g} S(C_{ij}) - \min_{i,j=1,\dots,m_g,n_g} S(C_{ij})\,.$$

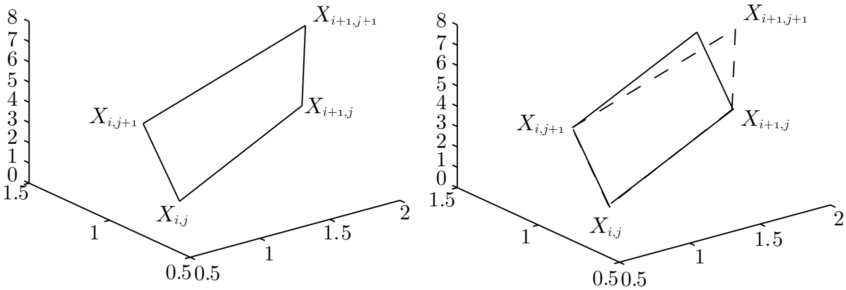

Fig. 1: $\mathcal{C}_{ij}$ (left) and $\mathcal{C}_{ij}^p$ (right).

3.1 – The re-parametrization phase

To improve the quality of an algebraic grid with the help of a tensor product re-parametrization, an univalent map R from the computational domain $[0,1]^2$ in to the parameter domain $[0,1]^2$ is here defined. The idea is to use only uniform grid size on the computational domain and possibly non uniform grid size in to the parameter domain $[0,1]^2$. The tensor product re-parametrization is based on the transformation

$$(3.13)\qquad R:[0,1]^2\to[0,1]^2,\quad R(u,v) := \sum_{i=1}^{m}\sum_{j=1}^{n} D_{ij}B_i(u)B_j(v)$$

where $B_i,\ i=1,\dots,m$ and $B_j,\ j=1,\dots,n$ are, again, B-splines functions with multiple end points. Note that the choice of multiple end points and the linear reproduction of B-splines is enough to guarantee the interpolation of the boundary on $[0,1]^2$. Once the set of functions used in (3.13) is chosen, we need to discuss how to choose the control directions D_{ij}. We assume that $D_{1j},\ D_{mj},\ j = 1,\dots,n$, belong to the boundary curves $s = 0$ and $s = 1$, respectively and $D_{i1},\ D_{in},\ i = 1,\dots,m$ to the remaining boundary curves $t = 0$ and $t = 1$, respectively. The choice of the rest of the control directions will play a key role for making advantage of the re-parametrization phase as it will be clarified in the following algorithm.

Algorithm

1. Input m, n, $mtab$, $ntab$, $\phi_i,\ i = 1,2$, $\psi_j,\ j = 1,2$.

2. Compute X as in (2.9) by using a suitable set of control points $\mathcal{Q}$ (or by means any other algebraic method).

3. Construct the continuous transformation R by using (3.13) with an initial set of $m \cdot n$ control directions D_{ij} in $[0,1]^2$.

4. Compute the grid points $\mathcal{X}_R := \{X(R(l/(mtab-1), k/(ntab-1)))\}_{l,k=0}^{mtab,ntab}$.

5. Compute a new set of $m \cdot n$ control directions D^*_{ij} in $[0,1]^2$ solving an optimization problem with one of the objective functions defined in Section 3 using the grid points $\mathcal{X}_R$.

6. Construct the new continuous transformation R^* by using (3.13) with the new set of control directions D^*_{ij}.

7. Compute the final grid $\mathcal{X} = \{X(R^*(l/(mtab-1), k/(ntab-1)))\}_{l,k=0}^{mtab,ntab}$.

4 – Examples

In this section some simple surface grids are shown to better stress the capability of using the re-parametrization phase (that is moving the control directions involved in (3.13)) while using the optimization procedure based on some of the objective functions given in the previous section. The left figures we propose refer to surface grids simply obtained by using the analytical expression of the surface. The right figures refer to the surface grid obtained by minimizing the objective functions specified in the caption of the figures. The routine constr of the Matlab Optimization Toolbox is used in all cases. A more detailed investigation of the implementation of the re-parametrization phase and a gallery of resulting grids is in forthcoming paper.

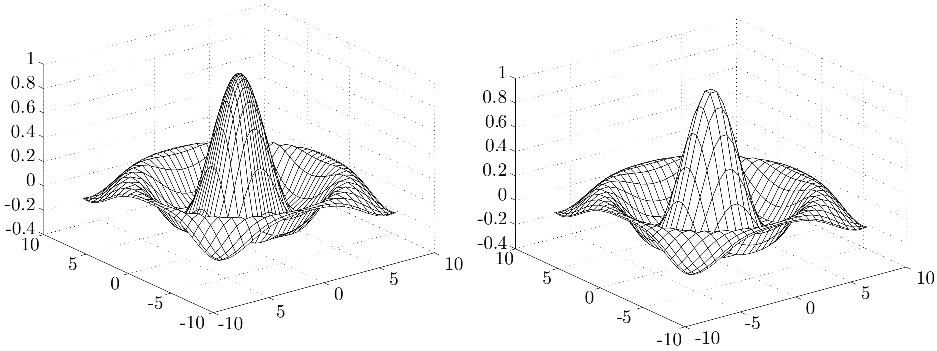

Fig. 2: Initial (left) and optimized grid based on the function f_K (right).

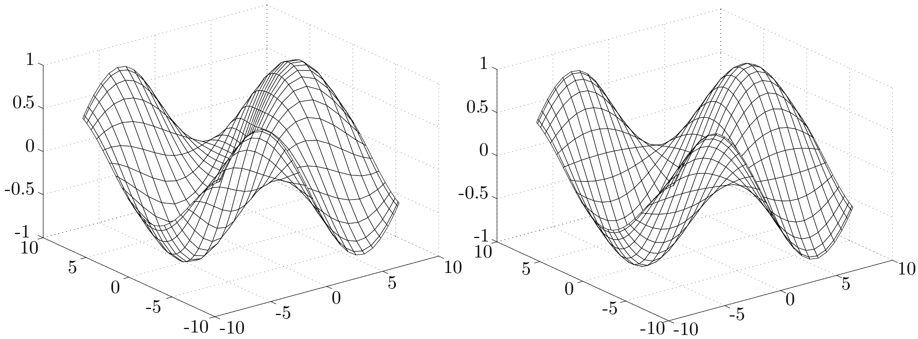

Fig. 3: Initial (left) and optimized grid based on the function f_A (right).

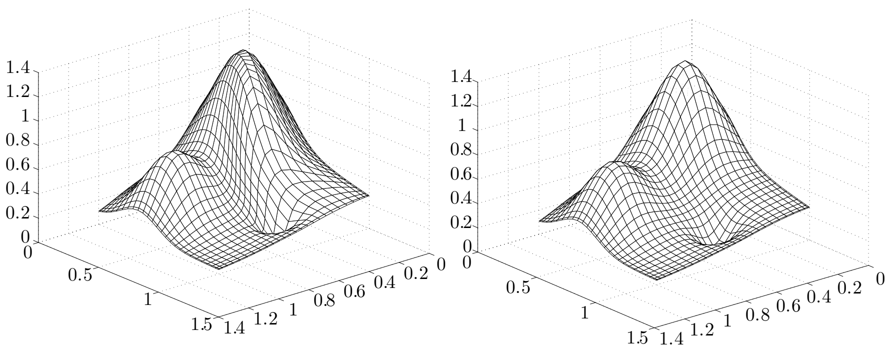

Fig. 4: Initial (left) and optimized grid based on the function f_O (right).

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