Available online at www.sciencedirect.com

SciVerse ScienceDirect

Procedia Engineering 00 (2015) 000–000

Procedia Engineering

www.elsevier.com/locate/procedia

24th International Meshing Roundtable (IMR24)

On curving high-order hexahedral meshes

Abel Gargallo-Peiró[a,b], Eloi Ruiz-Gironés[a], Xevi Roca[b,c], Jose Sarrate[a,*]

[a] Laboratori de Càlcul Numèric (LaCàN), Departament de Matemàtica Aplicada III (MA III), Universitat Politècnica de Catalunya (UPC), Campus Nord UPC, 08034 Barcelona, Spain.

[b] Computer Applications in Science and Engineering, Barcelona Supercomputing Center, 08034 Barcelona, Spain.

[c] Aerospace Computational Design Laboratory, Department of Aeronautics and Astronautics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA.

Abstract

We present a new definition of distortion and quality measures for high-order hexahedral (quadrilateral) elements. This definition leads to two direct applications. First, it can be used to check the validity and quality of a high-order hexahedral (quadrilateral) mesh. Second, it allows the generation of high-order curved meshes composed of valid and high-quality hexahedral (quadrilateral) elements. We describe a method to simultaneously smooth and untangle high-order hexahedral (quadrilateral) meshes by minimizing the proposed mesh distortion. Finally, we analyze the behavior of the proposed distortion measure and we present several results to illustrate the benefits of the mesh generation framework.

Peer-review under responsibility of organizing committee of the 24th International Meshing Roundtable (IMR24).

Keywords: unstructured high-order methods, hexahedral mesh generation, CAD, mesh optimization, mesh quality, curved meshing

1. Introduction

Although several valid approaches have been developed to generate curved high-order tetrahedral meshes [1–5], these techniques have not been extended to high-order hexahedral meshes. This drawback is partially due to the fact that a fully unstructured hexahedral mesh generator is still an unreachable goal. See [6–11] for a review and a classification of the main hexahedral mesh generation methods. In this work, we focus on developing a methodology that allows the generation of curved high-order hexahedral meshes. Specifically, we will adopt the *a posteriori* approach to generate high-order hexahedral meshes. Note that in industrial applications, the process for obtaining an initial tri-linear hexahedral mesh is often the most time-consuming task of the whole analysis. Nevertheless, hexahedral elements are preferred in a wide range of applications. For instance, in computational fluid dynamics, hexahedra perform better than stretched tetrahedra capturing the anisotropy of the flow field over such viscous regions. In computational solid mechanics, hexahedral elements reproduce better than tetrahedra the anisotropic properties of composite materials. Moreover, the spectral element method explodes the characteristics of hexahedral elements to improve the efficiency of the code.

* Corresponding author.
E-mail address: jose.sarrate@upc.edu

1877-7058
Peer-review under responsibility of organizing committee of the 24th International Meshing Roundtable (IMR24).

In contrast with the generation of high-order triangle/tetrahedral meshes, fewer approaches to generate high-order quadrilateral/hexahedral meshes have been developed [5,12–14]. Reference [13] formulates a local optimization approach that uses the surface geodesics to compute the location of the nodes of high-order quadrilaterals of any polynomial degree. Stepping to both quadrilaterals and hexahedra, reference [5] solves an optimization problem for the node locations according to an objective function. Alternatively and strictly oriented for shell-like structures, in [14] it is proposed a method to generate high-order hexahedral meshes taking advantage of the fact that having a valid surface mesh, the hexahedral shell mesh generated through a sweeping does present a minimal distortion.

We highlight that the main challenge of *a posteriori* mesh deformation methods is to repair the invalid elements that may arise from displacing the boundary nodes of the initial straight-sided mesh. In some cases, these elements may be excessively distorted, having an adverse effect on the accuracy of the finite element solutions, or may even be invalid in which case the mapping between the master element and the curved deformed element is not invertible. A first requirement to repair invalid elements is an algorithm to detect them and to quantify the level of distortion. Specifically for quadratic quadrilaterals, reference [15] provides sufficient conditions for the invertibility of 8-node quadrilaterals, whereas [16] analyses their distortion in terms of the parameters of that define the mapping from the reference quadrilateral to the physical one. Alternatively, [17] presents a method to verify the non-singularity of the element representation, and [18] provides non-degeneracy conditions for bi-quadratic (9-nodes) quadrilaterals with one curved edge are determined.

Herein, we focus both on quantifying the validity of quadrilateral/hexahedral meshes, and on the *a posteriori* curving of the high-order mesh. In particular, we extend the definition of quality measure for high-order triangle/tetrahedral elements presented in [19] to high-order quadrilateral/hexahedral elements of any polynomial degree. We present a regularized [20–22] point-wise distortion measure of the high-order mesh, which is used to determine the validity of the mesh elements. Moreover, similarly to the work presented in [23] for tetrahedra, we also use the point-wise regularized distortion measure to formulate a global optimization procedure (smoothing and untangling) that allows curving the high-order mesh in order to obtain a valid final configuration that matches the boundary geometry.

2. Validation of high-order hexahedral meshes: distortion measure

2.1. Distortion measures for linear simplices

In this work, we define the quality of a high-order quadrilateral or hexahedral element by means of a generalization of the Jacobian-based quality measures for linear simplexes presented in [24]. To define a Jacobian-based measure for linear tetrahedra, three elements are required: the master, the ideal, and the physical. The master element (E^M) is the element from which the iso-parametric mapping is defined, the ideal tetrahedron (E^I) represents the target configuration, and the physical (E^P) is the element to be measured. First, the mappings between the ideal and the physical elements through the master element are obtained. Specifically, the mapping between the ideal and physical element is determined by the composition

$$\boldsymbol{\phi}_E : E^I \xrightarrow{\boldsymbol{\phi}_I^{-1}} E^M \xrightarrow{\boldsymbol{\phi}_P} E^P.$$

In this work, we use a regularized version [20] of the shape distortion measure [24]:

$$\eta_\delta(\mathbf{D}\boldsymbol{\phi}_E) = \frac{\|\mathbf{D}\boldsymbol{\phi}_E\|_F^2}{n|\sigma_\delta|^{2/n}}, \qquad \sigma_\delta(\sigma) = \frac{1}{2}\left(\sigma + \sqrt{\sigma^2 + 4\delta^2}\right). \tag{1}$$

where n is the space dimension, $\|\cdot\|_F$ is the Frobenius norm, and $\sigma = \det(\mathbf{D}\boldsymbol{\phi}_E)$. The value of δ parameter depends on the problem and can be selected using [20,21,23].

2.2. Distortion and quality measures for high-order hexahedra

To define a distortion measure for high-order elements, we interpret the regularized distortion measure of a linear tetrahedra, see Equation (1), as a point-wise measure of the distortion of a deformation map between the ideal element and the physical one. We define the distortion at a point $\mathbf{y} \in E^I$ for a high-order element with nodes $\mathbf{x}_1, \ldots, \mathbf{x}_{n_p} \in \mathbb{R}^3$, as:

$$\mathrm{M}\boldsymbol{\phi}_E(\mathbf{y}) := \eta_\delta \left(\mathbf{D}\boldsymbol{\phi}_E(\mathbf{y})\right). \tag{2}$$

We point out that $\mathrm{M}\boldsymbol{\phi}_E$ is a function of $\mathbf{y}$, and that it also depends on $\mathbf{x}_1, \ldots, \mathbf{x}_{n_p}$, since $\boldsymbol{\phi}_E$ does. Note that the point-wise distortion, Equation (2), can be defined using any distortion measure for linear tetrahedra that is expressed explicitly in terms of of the Jacobian (Jacobian-based) or that can be casted to an expression in terms of the Jacobian.

Next, we define the inner product of functions on the ideal element, and its induced norm as,

$$\langle f, g\rangle_{E^I} := \int_{E^I} f(\mathbf{y})\, g(\mathbf{y})\mathrm{d}\mathbf{y}, \qquad \|f\|_{E^I} := \sqrt{\langle f, f\rangle_{E^I}},$$

where E^I is the ideal of element E^P. Using these definitions, the *distortion measure for a high-order element* is

$$\eta_E := \frac{\|\mathrm{M}\boldsymbol{\phi}_E\|_{E^I}}{\|1\|_{E^I}}, \tag{3}$$

where η_E depends on the element nodes $\mathbf{x}_1, \ldots, \mathbf{x}_{n_p}$, since $\mathrm{M}\boldsymbol{\phi}_E$ does. Note that $\|1\|_{E^I}$ is the measure of the ideal element. The *quality measure for a high-order element* is $q_E := 1/\eta_E$.

3. Generation of hexahedral curved high-order meshes: mesh optimization

Given an initial physical mesh $\mathcal{M}_P$ and an ideal mesh $\mathcal{M}_I$, we want to characterize $\mathcal{M}_P$ in terms of $\mathcal{M}_I$. In particular, we seek an optimal element-wise mapping ϕ_h^* from $\mathcal{M}_I$ to $\mathcal{M}_P$, such that for all E^I in $\mathcal{M}_I$, it has an ideal distortion measure. We consider that the curved boundary is prescribed by a surface mesh $\partial\mathcal{M}_P$ determined by the mapping g_h from $\partial\mathcal{M}_I$ to $\partial\mathcal{M}_P$, that we compute using the technique presented in [21,25]. Since we want to obtain a conformal nodal high-order mesh, we seek for the mapping ϕ_h^* in the space of vector functions

$$\boldsymbol{\mathcal{U}} := \{\mathbf{u} \in \left[C^0\left(\mathcal{M}_I\right)\right]^3 \mid (\mathbf{u} \circ \phi_I)_{|_{E^M}} \in [\mathcal{P}^p(I)]^3\,,\ \forall E^M \in \mathcal{M}_M\},$$

where $\mathcal{P}^p(I)$ is the space of polynomials of degree p on the interval I. Note that since we are using hexahedral elements, we assume that the master element, E^M, is the Cartesian product of interval I in such a way that $E^M = I^n$, being n the dimension of the element. $\boldsymbol{\mathcal{U}}$ is the standard space of shape functions for hexahedral elements, defined as polynomials of degree p in the master element, and then mapped to each ideal element using the transformation ϕ_I. Finally, it is worth to notice that $\phi^*_{h|_{E^I_e}} = \boldsymbol{\phi}_{E_e}$, where $\boldsymbol{\phi}_{E_e}$ is the elemental mapping.

In our formulation we seek ϕ_h^* in $\boldsymbol{\mathcal{U}}_D$ such that

$$\phi_h^* = \operatorname*{argmin}_{\phi_h \in \boldsymbol{\mathcal{U}}_D} \|\mathrm{M}\phi_h - 1\|^2_{\mathcal{M}_I}, \text{ where } \boldsymbol{\mathcal{U}}_D := \{\phi_h \in \boldsymbol{\mathcal{U}} \mid (\mathrm{M}\phi_h - 1) \in \mathcal{L}^2(\mathcal{M}_I), \text{and } \phi_h = g_h \text{ on } \partial\mathcal{M}_I\}. \tag{4}$$

In Equation (4) we define the inner product and the corresponding induced norm

$$\langle f, g\rangle_{\mathcal{M}_I} := \sum_{e=1}^{n_E} \langle f_{|_{E^I_e}}, g_{|_{E^I_e}}\rangle_{E^I_e}, \qquad \|f\|_{\mathcal{M}_I} := \sqrt{\langle f, f\rangle_{\mathcal{M}_I}}. \tag{5}$$

We can always reorder the mesh nodes $\mathbf{x}_i$, $i = 1, \ldots, n_N$ in such a manner that $i = 1, \ldots, n_F$ are the indexes corresponding to the free (interior) nodes, and $i = n_F + 1, \ldots, n_N$ correspond to the fixed nodes (nodes on the CAD surfaces). Note that the coordinates of the fixed nodes are determined by the function g_h, and can be obtained using the technique presented in [21,25]. We can formulate the mesh optimization problem as finding $\{\mathbf{x}_1^*, \ldots, \mathbf{x}_{n_F}^*\} \subset \mathbb{R}^3$ such that:

$$\{\mathbf{x}_1^*, \ldots, \mathbf{x}_{n_F}^*\} = \operatorname*{argmin}_{\mathbf{x}_1, \ldots, \mathbf{x}_{n_F} \in \mathbb{R}^3} f(\mathbf{x}_1, \ldots, \mathbf{x}_{n_F}; \mathbf{x}_{n_F+1}, \ldots, \mathbf{x}_{n_N}) = \operatorname*{argmin}_{\mathbf{x}_1, \ldots, \mathbf{x}_{n_F} \in \mathbb{R}^3} \frac{1}{2}\|\mathrm{M}\phi_h - 1\|^2_{\mathcal{M}_I}, \tag{6}$$

where $\mathbf{x}_i = g_h(\mathbf{y}_i)$ for $i = n_F + 1, \ldots, n_N$. We solve the global minimization problem stated in Equation (6) by mean of a non-linear Gauss-Seidel optimization, as proposed in [23].

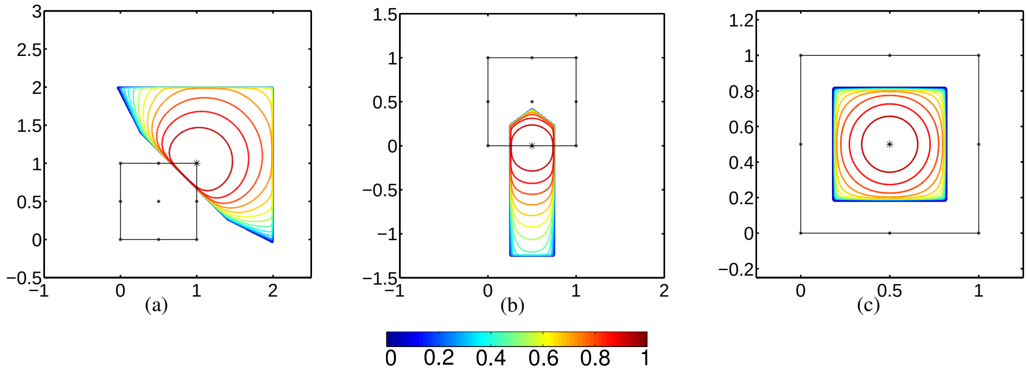

Fig. 1. Level sets for the high-order shape quality measure when the free node is: (a) a vertex node; (b) an edge node; and (c) a face node.

4. Numerical examples

4.1. Behavior of the quality measure for high-order quadrilateral elements

In this example, we analyze the behavior of the shape quality measure for a quadrilateral of polynomial degree two with vertices at $(-1,-1)$, $(1,-1)$, $(1,1)$ and $(-1,1)$. We apply three tests to a quadrilateral of polynomial degree two. In each test we consider a different free node (keeping the rest of nodes fixed in the original location) and compute the quality of the high-order element in terms of the location of this node. In particular, we illustrate the contour plots of the shape quality measure in terms of three different free nodes: a vertex, an edge, and a face node, see Figure 1. Note that the areas outside of the contour plots define the unfeasible region for the given node and, in each case, the quality measure detects the ideal position for the node (where quality equals to 1).

4.2. High-order mesh for a mechanical piece, $p = 5$

We present a hexahedral mesh of polynomial degree five for a mechanical piece. The initial linear mesh is generated using a multi-sweeping method [26]. In this example, the inner nodes of the initial curved high-order mesh are relocated to a random position, see Figure 2(a), and for this reason, all the elements are inverted and the minimum, the maximum and the mean quality are equal to 0. After applying the proposed hexahedral high-order smoother, we recover a mesh without any inverted element, see Figure 2(b), and the minimum quality is 0.72. The maximum quality, the mean quality and the standard deviation of the smoothed mesh are 0.99, 0.98 and 0.03, respectively.

5. Conclusions

In this work, we have presented a framework to generate and validate high-order hexahedral meshes by adopting an *a posteriori* approach. First, an initial linear hexahedral mesh is generated. This mesh defines the desired shape and size for the elements of the high-order mesh. Then, the polynomial degree of the mesh is increased and the new nodes are projected to the geometry boundary. This operation may induce low-quality and inverted elements and, for this reason, an untangling and smoothing method has to be applied. To this end, we have extended the previous work derived for triangular and tetrahedral high-order meshes into quadrilateral and hexahedral high-order meshes. That is, using a distortion measure for linear simplices, a point-wise distortion measure is defined. The elemental distortion measure is defined as the $\mathcal{L}_2$-norm of the point-wise distortion over the corresponding ideal element. Using this definition, a minimization problem is posed, and a high-quality mesh can be obtained by optimizing it.

References

[1] S. Dey, R. O'Bara, and M. S. Shephard. Curvilinear mesh generation in 3D. *Comput. Aided Design*, 33:199–209, 2001.

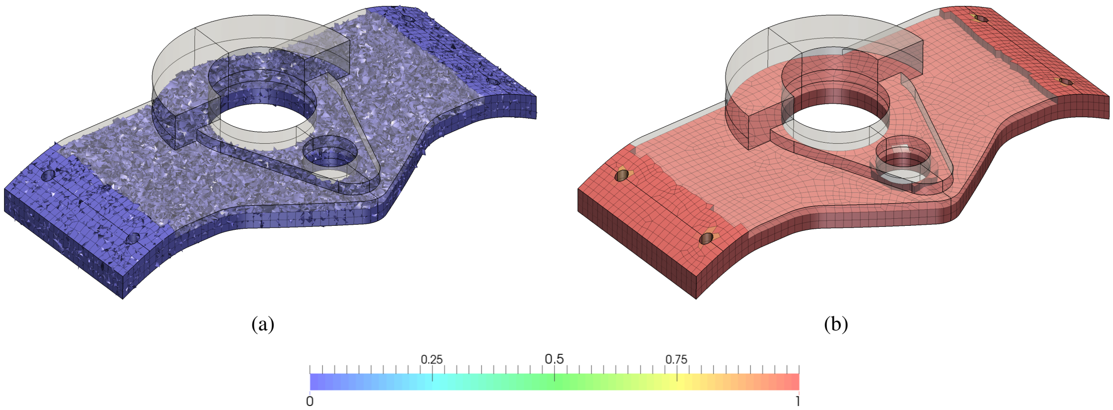

Fig. 2. High-order hexahedral mesh ($p = 5$) for the mechanical piece: (a) initial curved high-order mesh; (b) high-order mesh after applying the smoothing.

[2] S. Sherwin and J. Peiró. Mesh generation in curvilinear domains using high-order elements. *Int. J. Numer. Meth. Eng.*, 53(1):207–223, 2002.
[3] P.-O. Persson and J. Peraire. Curved mesh generation and mesh refinement using lagrangian solid mechanics. In *Proc. 47th AIAA*, 2009.
[4] P. L. George and H. Borouchaki. Construction of tetrahedral meshes of degree two. *Int. J. Numer. Meth. Eng.*, 90(9):1156–1182, 2012.
[5] T. Toulorge, C. Geuzaine, J.-F. Remacle, and J. Lambrechts. Robust untangling of curvilinear meshes. *J. Comput. Phys.*, 254:8 – 26, 2013.
[6] S. J. Owen. A survey of unstructured mesh generation. In *Proc. 7th Int. Meshing Roundtable*, pages 239–267, 1998.
[7] T. D. Blacker. Automated conformal hexahedral meshing constraints, challenges and opportunities. *Eng. Comput.*, 17(3):201–210, 2001.
[8] T. J. Tautges. The generation of hexahedral meshes for assembly geometry: survey and progress. *Int. J. Numer. Meth. Eng.*, 50(12):2617–2642, 2001.
[9] T. J. Baker. Mesh generation: art or science? *Progress in Aerospace Sciences*, 41(1):29–63, 2005.
[10] K. Shimada. Current trends and issues in automatic mesh generation. *Comput. Aided Design and Appl.*, 3(6):741–750, 2006.
[11] J. F. Shepherd. *Topologic and geometric constraint-based hexahedral mesh generation*. PhD thesis, The University of Utah, 2007.
[12] Z. Chen, J. Tristano, and W. Kwok. Construction of an objective function for optimization-based smoothing. *Eng. Comput.*, 20(3):184–192, 2004.
[13] Z. Xie, R. Sevilla, O. Hassan, and K. Morgan. The generation of arbitrary order curved meshes for 3D finite element analysis. *Comput. Mech.*, 51:361–374, 2012.
[14] C. Sorger, F. Frischmann, S. Kollmannsberger, and E. Rank. Tum.geoframe: automated high-order hexahedral mesh generation for shell-like structures. *Eng. Comput.*, 30(1):41–56, 2014.
[15] A. Frey, C. Hall, and T. Porsching. Some results on the global inversion of bilinear and quadratic isoparametric finite element transformations. *Math. Comput.*, 32(143):725–749, 1978.
[16] K.Y. Yuan, Y. Huang, and T. Pian. Inverse mapping and distortion measures for quadrilaterals with curved boundaries. *Int. J. Numer. Meth. Eng.*, 37(5):861–875, 1994.
[17] M. Baart and E. Mulder. A note on invertible two-dimensional quadratic finite element transformations. *Commun. Appl. Numer. M.*, 3(6):535–539, 1987.
[18] L. Branets and G. Carey. Extension of a mesh quality metric for elements with a curved boundary edge or surface. *J. Comput. Inf. Sci. Eng.*, 5(4):302–308, 2005.
[19] A. Gargallo-Peiró, X. Roca, J. Peraire, and J. Sarrate. Distortion and quality measures for validating and generating high-order tetrahedral meshes. *Eng. Comput.*, 31:423–437, 2015.
[20] J. M. Escobar, E. Rodríguez, R. Montenegro, G. Montero, and J. M. González-Yuste. Simultaneous untangling and smoothing of tetrahedral meshes. *Comput. Meth. Appl. Mech. Eng.*, 192(25):2775–2787, 2003.
[21] A. Gargallo-Peiró, X. Roca, and J. Sarrate. A surface mesh smoothing and untangling method independent of the CAD parameterization. *Comput. Mech.*, 53(4):587–609, 2014.
[22] S P . Sastry, S M . Shontz, and S A. Vavasis. A log-barrier method for mesh quality improvement. In *Proc. 20th Int. Meshing Roundtable*, pages 329–346. Springer International Publishing, 2012.
[23] A. Gargallo-Peiró, X. Roca, J. Peraire, and J. Sarrate. Optimization of a regularized distortion measure to generate curved high-order unstructured tetrahedral meshes. *Int. J. Numer. Meth. Eng.*, pages Published online, doi:10.1002/nme.4888, 2015.
[24] P. M. Knupp. Algebraic mesh quality metrics. *SIAM J. Numer. Anal.*, 23(1):193–218, 2001.
[25] A. Gargallo-Peiró, X. Roca, J. Peraire, and J. Sarrate. Defining quality measures for mesh optimization on parameterized CAD surfaces. In *Proc. 21st Int. Meshing Roundtable*, pages 85–102. Springer International Publishing, 2013.
[26] E. Ruiz-Gironés, X. Roca, and J. Sarrate. Using a computational domain and a three-stage node location procedure for multi-sweeping algorithms. *Adv. Eng. Softw.*, 42(9):700–713, 2011.