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Curvilinear mesh generation using a variational framework☆

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ABSTRACT

We aim to tackle the challenge of generating unstructured high-order meshes of complex three-dimensional bodies, which remains a significant bottleneck in the wider adoption of high-order methods. In particular we show that by adopting a variational approach to the generation process, many of the current popular high-order generation methods can be encompassed under a single unifying framework. This allows us to compare the effectiveness of these methods and to assess the quality of the meshes they produce in a systematic fashion. We present a detailed overview of the theory and formulation of the variational framework, and we highlight how such formulation can be effectively exploited to yield a highly-efficient parallel implementation. The effectiveness of this approach is examined by considering a number of two- and three-dimensional examples, where we show how the proposed approach can be used for both mesh quality optimisation and untangling of invalid high-order meshes.

1. Introduction

High-order methods are rapidly increasing in popularity due to their favourable numerical characteristics and ability to more effectively use modern computing hardware than traditional low-order methods. There has been much development of the underlying solvers, which give the ability to simulate fluid flows, acoustic phenomena and many other physical processes. However, these solvers ultimately rely on the partitioning of a domain into elements which, at high polynomial orders, must be: coarse in order to take advantage of the high-order nature of the method; curved to align with the underlying geometry; and valid, so that they do not self-intersect. The lack of development in this area has meant that this is a significant bottleneck in the more widespread use of these methods [1,2]. This is particularly applicable to industrial cases, where complex three-dimensional geometries representing (for example) cars and planes are clearly of significant interest. For these methods to become more popular outside of academia, this bottleneck clearly needs to be addressed.

Research in this area has mostly centred around *a posteriori* approaches, whereby a coarse linear mesh is deformed to accommodate the curvature at the boundary, and is the focus of this study. The challenge in this approach is to determine a method through which this curvature can be incorporated into the interior of the domain. Without this, the mesh is at best of a low quality, and at worst, will self-intersect, rendering it unsuitable for solver-based calculations. Existing work in *a posteriori* generation has broadly centred around two lines of investigation. The first of these focuses around the concept of solid body deformation, whereby the mesh is treated as a solid body which is deformed to incorporate curvature at the boundary. The work in this theme has focused around determining which model is 'best', either in terms of optimal quality or computational efficiency. Some models investigated include linear elasticity by Xie et al. [3] and Hartmann & Leicht [4], non-linear hyperelasticity by Persson & Peraire [5] and more recently by Poya et al. [6], thermo-elasticity by some of the authors of this work [7] and the Winslow equations by Fortunato & Persson [8]. The second theme follows a different route, whereby the mesh is equipped with an associated functional that denotes its energy. A non-linear optimisation problem is then solved in order to minimise this functional and yield a valid mesh. Again, most studies in this area have focused around this choice of functional, which include scaled Jacobian distortion metrics by Dey et al. [9], spring analogies for surface deformation by Sherwin & Peiró [10], unconstrained optimisation of the Jacobian by Toulorge et al. [11] and a number of articles by Roca and collaborators based on a shape distortion metric, e.g. [12–14].

However, what has so far remained unexplored in this area is the connections between these two themes. In the linear mesh generation community, for example in work by Garanzha [15] and Huang & Russell [16], it is known that through the calculus of variations, the elliptic partial differential equations defining these elasticity models can be recast into the minimisation of a energy functional, which takes as its arguments the mesh displacement and its derivatives. However, the use of this approach in high-order

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mesh generation has remained mostly unnoticed, asides from brief remarks in work by Sastry et al. [17].

The purpose of the present study is to examine the connections between these two existing mesh generation themes, by both recasting solid body models in a variational setting and examining other functionals already noted above in the literature. We will show that this approach has several benefits. It first allows us to examine each of the models in a common setting and investigate the relative benefits of each model in turn. Additionally, from a standpoint of robustness, the use of an energy functional that is convex or polyconvex, as investigated by Huang & Russell [16] and Garanzha [18], gives mathematical guarantees of a minimum that may be found using a numerical optimisation procedure. Finally, we note that early work in the 1970s by Felippa [19], who investigated direct energy minimisation methods for mesh generation, concluded that this method is promising but computational power was, at the time, a significant limiting factor in the success of this approach. In the following sections, we will show that modern computing hardware, combined with a suitable choice of numerical optimisation to exploit the denser structure that arises through a high-order discretisation, allows us to overcome this problem. The results we present here highlight that the variational setting allows us to construct a highly efficient and robust parallel framework for high-order mesh generation, permitting the generation of very complex three-dimensional meshes in the order of minutes.

Finally, we note that the groundwork for this study has been outlined in an earlier proceeding [20]. In this article we significantly expand the scope of the work by investigating several additional contributions. These are: the incorporation of optimisation procedures based on analytic gradients and Hessian regularisation; the implementation of an improved regularisation method used to untangle meshes and a detailed discussion of its properties; the extension of the method to permit the mesh nodes connected to the CAD geometry to slide along the curves and across the surfaces on the boundary; and, finally, the inclusion of a wider range of examples, including hybrid prismatic–tetrahedral boundary layer meshes and very high-order quadrilateral meshes.

The paper is structured as follows. Section 2 outlines the formulation of the problem in terms of a solid mechanics analogy. The four energy functionals that we will investigate in this work are introduced in Section 2.1, which overlap with a large number of studies based around high-order mesh generation, and we discuss a regularisation strategy to untangle invalid meshes in Section 2.2. Section 3 describes details of the practical implementation needed in this variational setting. This includes the discretisation and nonlinear optimisation in Sections 3.2 and 3.3, parallelisation strategies in Section 3.4 and allowing surface elements to slide across the CAD geometry in Section 3.5. Section 4 provides a brief analysis of the behaviour of the functional, guiding the choice of some numerical options. Section 5 then examines the application of this method to a number of two- and three-dimensional problems, describing the meshes obtained by each method, the number of iterations and computational time needed for convergence. We finalise the paper in Section 6 with a brief overview and outlook to future work and improvements.

2. Background and formulation

We begin with a brief mathematical overview of the setup of the variational formulation. The ultimate goal is to define an energy functional that will be optimised in order to produce a valid high-order mesh. We therefore first require a coarse mesh $\Omega_I = \bigcup_{e=1}^{N_{\mathrm{el}}} \Omega_I^e$ of N_{el} straight-sided elements. The generation of this coarse grid is beyond the scope of this article but is discussed further in, e.g. Ref. [21]. We equip each element of Ω_I with a high-order polynomial finite element basis, based on standard Lagrange

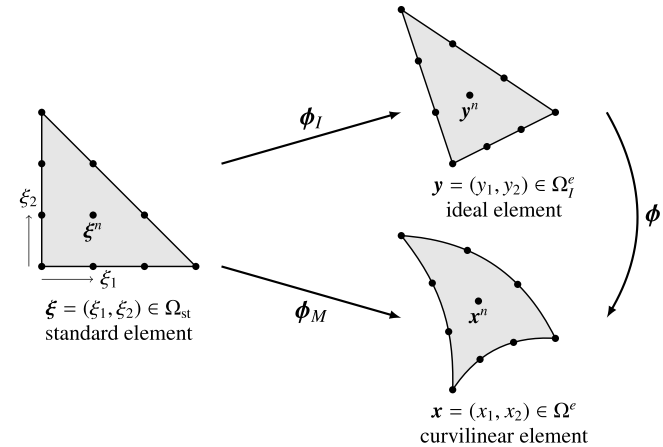

Fig. 1. Notation for mappings used throughout the paper: a triangular element is used for illustration purposes, but the notation is general and applicable to other element types. On the left we map a standard (reference) element Ω_{st} onto the straight-sided element Ω_I^e through the mapping $\boldsymbol{\phi}_I : \Omega_{\mathrm{st}} \to \Omega_I^e$ and onto the curvilinear element $\boldsymbol{\phi}^e : \Omega_{\mathrm{st}} \to \Omega^e$. The deformation mapping $\boldsymbol{\phi} : \Omega_I^e \to \Omega^e$ is then defined through the composition $\boldsymbol{\phi} = \boldsymbol{\phi}_M^e \circ \boldsymbol{\phi}_I^{-1}$.

interpolant basis functions. This gives an initial representation of the domain and serves as the initial configuration for the variational setup. In common with previous approaches [11,14], we define the mapping between a straight-sided mesh Ω_I and a curvilinear mesh Ω, which we subsequently denote by $\boldsymbol{\phi} : \Omega_I \to \Omega$. We refer to each element Ω_I^e as the 'ideal' element as it represents the best quality attainable without the introduction of curvature.

The mapping $\boldsymbol{\phi}$ is constructed by considering each element Ω_I^e separately. We refer to the diagram in Fig. 1, wherein we consider a triangular element and denote the coordinates inside each element as $\boldsymbol{\xi} \in \Omega_{\mathrm{st}}$, $\boldsymbol{x} \in \Omega^e$ and $\boldsymbol{y} \in \Omega_I^e$. These mappings are constructed in an isoparametric fashion, so that the nodes $\boldsymbol{\xi}^n$ that define the Lagrange basis functions on the standard element map to $\boldsymbol{y}^n$ under $\boldsymbol{\phi}_I$ and $\boldsymbol{x}^n$ under $\boldsymbol{\phi}_M$. We note that other element types, such as quadrilaterals in two dimensions and tetrahedra, triangular prisms, pyramids and hexahedra in three dimensions, may use exactly the same definitions as above.

The energy functional is then defined as the integral

$$\mathcal{E}(\nabla\boldsymbol{\phi}) = \int_{\Omega_I} W(\nabla\boldsymbol{\phi})\,\mathrm{d}\boldsymbol{y}, \tag{1}$$

where W depends on the deformation gradient tensor

$$\nabla\boldsymbol{\phi}(\boldsymbol{y}) = \frac{\partial\boldsymbol{\phi}}{\partial\boldsymbol{y}}; \qquad [\nabla\boldsymbol{\phi}(\boldsymbol{y})]_{ij} = \frac{\partial\phi_i}{\partial y_j},$$

and its determinant $J = \det\nabla\boldsymbol{\phi}$, which we hereafter refer to as the Jacobian. In the following section we describe the different forms of the energy that we investigate in this article.

2.1. Forms of the energy functional

This section outlines a key contribution of this work, where we show that many of the existing curvilinear mesh generation methods can be unified in a variational setting through the definition of an energy functional. More importantly, a judicious choice of an energy functional that satisfies the convexity requirements of Ball's existence theory [22] guarantees the existence of a minimiser. We therefore seek to employ energy functionals that are *polyconvex*. A discussion of the properties of such functionals and how to verify them, together with examples of their use in mesh generation can be consulted in section 6.2 of the book by Huang and Russell [16].