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Isogeometric shape design optimization of nanoscale structures using continuum-based shell theory considering surface effects

Seung-Ho Ahn, Myung-Jin Choi, Seonho Cho*

Department of Naval Architecture and Ocean Engineering, Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul 151-744, Republic of Korea

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ABSTRACT

Considering surface effects on nanoscale structures, an isogeometric shape optimization method is developed for curved structures using Naghdi's shell formulation. Since the curved structures are very sensitive to geometrical changes, the geometric exactness of isogeometric approach successfully prevents the loss of higher-order geometric information in design sensitivity analysis (DSA). A direct differentiation method is employed for the DSA, where the control points are selected as the design variables and describe the flexible modeling of free-form shell surfaces. Through numerical examples, we verified the accuracy of isogeometric analysis whose framework shows better convergence rate than finite element analysis due to the exact geometry and the higher order geometric information in the DSA formulation. The surface Lamé constants turns out to alter the ratio between the portion of membrane and bending energies. Also, the optimal shape is dependent on the residual surface stress that affects its stress state.

1. Introduction

Nowadays, nanoscale structures such as resonators, mass and biochemical sensors, and NEMS (Nano Electro Mechanical Systems) are widely used in various fields, which requires the accurate prediction of nanoscale behaviors for structural analysis. Also, to obtain the better performance of nanoscale designs, necessity for structural design optimization has continuously increasing. Molecular dynamic (MD) simulation method is generally employed to obtain the physical properties and behaviors of nanoscale structures that the continuum based approach cannot handle. However, the MD simulations are computationally expensive for large scale practical structures.

To overcome the difficulty of computational costs in MD simulation, the continuum based formulations of nanoscale structures have been developed. Although the conventional continuum models provide simple formulas and have advantage on computational time, the application of these continuum models directly to practical model is questionable due to surface effects. The difference of coordination of atoms between bulk and surface results in the surface effects that are negligible in macro-sized structures since surface-to-volume ratio is small. However, as the ratio increases in nanoscale structures, the influences of surface have to be taken into account. Miller and Shenoy [1] showed that continuum formulations of plate in the nanoscale are reliable by comparing with the MD simulation results. However, it is observed that accuracy is somewhat decreased in considering bending energy. Dingreville et al. [2] showed that material properties have size dependence due to the increasing importance of surfaces as the scale of structures become comparable with the atomic scale. To analyze the nanoscale structures using the continuum model with the size effects, the conventional elasticity theory has been extended to various theories such as Gurtin and Murdoch theory [3], Nonlocal theory [4], Strain gradient elasticity [5] and couple-stress theory [6]. Wang et al. [7] showed that the decreased accuracy can be improved by considering residual surface stress in the formulation. He and Lilley [8] and Jing et al. [9] experimentally showed that the continuum theory of Gurtin and Murdoch is reliable. Material properties obtained from the continuum formulation were compared with those measured by AFM (Atomic Force Microscopy) facility, which showed fairly good agreement. In this paper, the continuum theory by Gurtin and Murdoch is employed to develop a shape optimization method for nanoscale structures.

Curved structures are a generalized form in nanoscale and a curved graphene with curvature is one example to show the importance of curvature in nanoscale structures. Graphene is a one-atom-thick planar sheet of carbon atoms, densely packed together into a honeycomb shaped crystal lattice. Some researchers showed that the curvature of the curved graphene affects the properties of graphene. Kolesnikov and Osipov [10] showed that the curvature of the graphene changes the electron density, so the electrical properties can be improved. Gosálbez-Martínez et al. [11] discussed that a curved graphene with constant curvature is generated by unzipping carbon nanotubes, and the curvature affects the spin-orbit coupling and bandwidth. Since the curvature of nanoscale structures fairly affect the properties of structures, the

* Corresponding author.
E-mail address: secho@snu.ac.kr (S. Cho).

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representation of exact geometry and the accurate prediction of mechanical behaviors are highly significant. In this paper, to analyze the curved structures in nanoscale, we introduce a continuum shell formulation considering surface effects, where the interfacial surface is modeled as a shell [12] whereas a membrane is modeled in Gurtin and Murdoch [3]. Altenbach and Eremeyev [13] discussed the derivation of the governing nonlinear shell equations considering surface effects. Zhang et al. [14] presented the general equations of piezoelectric shells considering the surface effects in an orthogonal curvilinear coordinate system.

Finite element analysis (FEA), one of the widely used numerical analysis methods, has difficulties in dealing with curved structures due to the linear approximation of the geometry. The framework of IGA that has capability to overcome this difficulty is developed by Hughes et al. [15]. The IGA adopts the same NURBS (Non-Uniform Rational B-Spline) basis function as used in CAD and does not require any further communication with the CAD systems during refinement process. Furthermore, Cho and Ha [16] developed an IGA-based shape optimization method that can prevent the loss of higher-order geometric information such as normal vector and curvature. Also, the developed method is applied to heat conduction problems [17] and built-up structures [18].

The continuum models for nanoscale structures are also advantageous in structural optimization. Since most of optimization schemes require some iterations of analysis process, the application of MD simulations to the optimization process results in computationally expensive costs. Furthermore, due to the discrete nature of shape variations at the atomic level, it is difficult to directly extend the continuum-based DSA method to the MD simulations. To overcome the difficulty of discrete nature in atomic structures, Jang and Cho [19] developed a method to transform the discrete spatial variations into the non-shape variations of MD systems. Some continuum based optimization methods considering nanoscale effects have been presented in recent years. Evgrafov et al. [20] considered the kinetic theory in topology optimization of heat conducting devices at nanoscale. An average distance travelled by a particle between collisions with other particles is considered in continuum formulation to consider nanoscale effects. Nanthakumar et al. [21] introduced a coupled XFEM/level set method to perform topology optimization of nanostructures considering nanoscale surface effects. They showed different optimal topology by considering the surface effects but physical interpretations for the obtained optimal topology at nanoscale are not presented.

The paper is organized as follows: in Section 2, we introduce the equilibrium equations for shell theory considering surface effects in the IGA framework. In Section 3, the isogeometric shape design sensitivity is derived for the shells with surface effects. In Section 4, we give some numerical examples, where the influence of surface effects is demonstrated and verified with exact solutions. The shape optimization problem of minimum strain energy is formulated and its optimal solution is verified with exact optimal solution.

2. Isogeometric analysis of shells

2.1. NURBS basis function

Consider a set of knots ξ in one-dimensional case.

$$\xi = \{\xi_1, \xi_2, \ldots, \xi_{n+p+1}\}, \tag{1}$$

where p and n are the order of the basis functions and the number of control points, respectively. B-spline basis function can be defined, recursively, as

$$N_i^0(\xi) = \begin{cases} 1 & \text{if } \xi_i \le \xi < \xi_{i+1} \\ 0 & \text{otherwise} \end{cases} \tag{2}$$

and

$$N_i^p(\xi) = \frac{\xi - \xi_i}{\xi_{i+p} - \xi_i} N_i^{p-1}(\xi) + \frac{\xi_{i+p+1} - \xi}{\xi_{i+p+1} - \xi_{i+1}} N_{i+1}^{p-1}(\xi), \ (p = 1, 2, 3, \ldots). \tag{3}$$

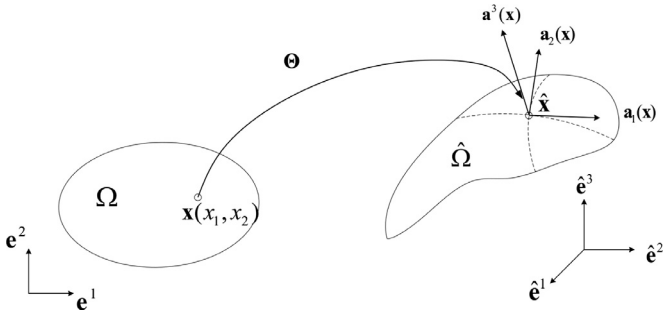

Fig. 1. Definition of the middle surface of the shell.

The B-spline has some useful properties as a basis function such as the partition of unity, compactness and non-negativity. Using the B-spline basis function $N_i^p(\xi)$ and the corresponding weight w_i, a NURBS basis function $R_i^p(\xi)$ is defined as

$$R_i^p(\xi) = \frac{N_i^p(\xi) w_i}{\sum_{j=1}^{n} N_j^p(\xi) w_j}. \tag{4}$$

For the given l pairs of the pth order NURBS basis function R_i^p and the corresponding control point $\mathbf{B}_i$, a NURBS curve is obtained as

$$\mathbf{C}(\xi) = \sum_{i=1}^{l} R_i^p(\xi) \mathbf{B}_i. \tag{5}$$

Similarly, a NURBS surface $\mathbf{S}$ is defined as a tensor product of coordinates,

$$\mathbf{S}(\Xi) = \sum_{i=1}^{l} \sum_{j=1}^{m} R_i^p(\xi) R_j^q(\eta) \mathbf{B}_{i,j} = \sum_{I}^{CP} W_I(\Xi) \mathbf{B}_I, \tag{6}$$

where $\mathbf{B}_I$ is the location of control point and W_I is introduced for the brevity of expression. CP and Ξ denote the number of control points and the set of parametric coordinates for surfaces, respectively.

2.2. Kinematics of Naghdi's shell

A generic point $\hat{\mathbf{x}}^*$ in a shell is represented by

$$\hat{\mathbf{x}}^*(x_1, x_2, x_3) = \hat{\mathbf{x}}(x_1, x_2) + x_3 \mathbf{a}^3(x_1, x_2), \tag{7}$$

where $\hat{\mathbf{x}}(x_1, x_2)$ is a material point in the middle surface and $\mathbf{a}^3(x_1, x_2)$ is a unit normal vector at the point and $\boldsymbol{\Theta}$ is an one-to-one mapping such that $\boldsymbol{\Theta}(\Omega) = \hat{\Omega}$ as shown in Fig. 1.

The corresponding covariant base vectors are obtained by

$$\mathbf{g}_\alpha = \hat{\mathbf{x}}^*_{,\alpha} = (\hat{\mathbf{x}} + x_3 \mathbf{a}^3)_{,\alpha} = \mathbf{a}_\alpha + x_3 \mathbf{a}^3_{,\alpha}, \quad (\alpha = 1, 2), \tag{8}$$

where $(\bullet)_{,\alpha}$ denotes the partial derivative with respect to the curvilinear coordinates x_α. $\mathbf{a}_\alpha$ and $\mathbf{a}^\alpha$ are the covariant and the contravariant base vectors on the middle surface, respectively, and utilized to construct surface metric tensors as

$$a_{\alpha\beta} = \mathbf{a}_\alpha \cdot \mathbf{a}_\beta, \ a^{\alpha\beta} = \mathbf{a}^\alpha \cdot \mathbf{a}^\beta. \tag{9}$$

In the Naghdi's shell model [22], a displacement vector is represented by

$$\hat{\mathbf{z}}^* = u_\alpha \mathbf{a}^\alpha + x_3 \psi_\alpha \mathbf{a}^\alpha + w \mathbf{a}^3 = (u_\alpha + x_3 \psi_\alpha) \mathbf{a}^\alpha + w \mathbf{a}^3, \tag{10}$$

where u_α, w, and ψ_α are the in-plane, out-of-plane, and rotational displacement measures, respectively. The membrane, bending, and shear strain measures are given by

$$\varepsilon_{\alpha\beta} = \frac{1}{2}\left(u_\alpha \|_\beta + u_\beta \|_\alpha - 2 b_{\alpha\beta} w \right), \tag{11}$$

$$\omega_{\alpha\beta} = \frac{1}{2}\left(\psi_\alpha \|_\beta + \psi_\beta \|_\alpha \right) - \frac{1}{2} b^\gamma_\alpha \left(u_\mu \|_\beta - b_{\beta\gamma} w \right) - \frac{1}{2} b^\gamma_\beta \left(u_\gamma \|_\alpha - b_{\alpha\gamma} w \right),$$