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Elastic buckling behavior of skew shaped single-layer graphene sheets

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ABSTRACT

A continuum based approach is presented for buckling analysis of single layer graphene sheets with skew shape. The straight-sided quadrilateral graphene field is mapped into a square domain in the computational space using a four-node graphene element. Then, the governing equations and boundary conditions of the graphene are transformed from the physical domain into a square computational domain by using the geometric transformation. Some numerical examples related to buckling loads of skew shaped graphene are presented for different geometric parameters. Results related to buckling loads of the single layer graphene with skew shape have been presented which can serve as benchmark solutions for future investigations.

1. Introduction

The extra-ordinary mechanical, chemical, thermal and electrical properties of carbon based nanostructures have led to a wide interest in their potential applications in microelectro-mechanical system (MEMS), biomechanics, microcomputers and nanocomposites. In the past five years great deals of studies have been devoted on mechanical properties of graphene sheets [1–7]. The nanoscaled controlled experimental studies are very difficult. Also, the molecular dynamic and atomic simulation approaches are highly computationally expensive. So, many researchers have used the continuum based techniques for modeling of nanoscaled structures [8–12]. Arbitrary shaped graphenes such as skew and rhombic have been widely used in modern industries such as biomedical devices, nanoelectro mechanical applications, actuators and sensors. Thus, understanding mechanical behaviors such as bending and buckling of these elements are an important task for design stage. While the majority of work on graphene sheets has related on buckling and vibration of rectangular and circular graphene [11–19], the buckling analysis of skew shaped graphene has not yet been studied. In the past ten years continuum models have been widely used for modeling of nanoscaled structures such as micro beams and micro plates, carbon nanotubes and microtubules [20–27]. In this paper, a geometric mapping methodology is used for transformation of the skew geometry [28–33]. A major advantage of the method proposed here for the analysis of arbitrary-shaped plates is that it does not require any mesh discretion. Thus, it needs only a few of input data to carry out the computations. The resulting governing equation for buckling of skew graphene is solved by numerical method. Some results for elastic buckling values of skew shaped graphene have been presented which can serve as benchmark solutions for future investigations in the field of nanomechanics.

2. Discrete singular convolution (DSC)

Singular convolutions (SC) are a special class of mathematical transformations, which appear in many science and engineering problems, such as the Hilbert, Abel and Radon transforms [34–37]. In fact, these transforms are essential to many practical applications, such as computational electromagnetics, signal and image processing, pattern recognition, tomography, molecular potential surface generation and dynamic simulation [38–40]. It is the most convenient way to discuss the singular convolution in the context of the theory of distributions. Wei and his co-workers first applied the DSC algorithm to solve solid and fluid mechanics problem [40–49]. These studies indicate that the DSC algorithm works very well for numerical solution of the partial differential equation [50–62]. Furthermore, it is also concluded that the DSC algorithm has global methods' accuracy and local methods' flexibility for solving differential equations in applied mechanics. In a general definition, numerical solutions of differential equations are formulated by some singular kernels. The mathematical foundation of the DSC algorithm is the theory of distributions and wavelet analysis. Consider a distribution, T and $\eta(t)$ as an element of the space of the test function. A singular convolution can be defined by [37]

$$F(t) = (T*\eta)(t) = \int_{-\infty}^{\infty} T(t-x)\eta(x)dx, \tag{1}$$

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where $T(t-x)$ is a singular kernel. For example, singular kernels of delta type [38]

$$T(x) = \delta^{(n)}(x); \quad (n = 0, 1, 2, \ldots,). \tag{2}$$

Kernel $T(x) = \delta(x)$ is important for interpolation of surfaces and curves, and $T(x) = \delta^{(n)}(x)$ for $n > 1$ is essential for numerically solving differential equations. With a sufficiently smooth approximation, it is more effective to consider a discrete singular convolution [39]

$$F_\alpha(t) = \sum_k T_\alpha(t-x_k) f(x_k), \tag{3}$$

where $F_\alpha(t)$ is an approximation to $F(t)$ and $\{x_k\}$ is an appropriate set of discrete points on which the DSC (3) is well defined. Note that, the original test function $\eta(x)$ has been replaced by $f(x)$. This new discrete expression is suitable for computer realization. The mathematical property or requirement of $f(x)$ is determined by the approximate kernel T_α.

2.1. Regularized Shannon's delta (RSD) kernel

Recently, the use of some new kernels and regularizer such as delta regularizer [40] was proposed to solve applied mechanics problem. The Shannon's kernel is regularized as

$$\delta_{\Delta,\sigma}(x-x_k) = \frac{\sin[(\pi/\Delta)(x-x_k)]}{(\pi/\Delta)(x-x_k)} \exp\left[-\frac{(x-x_k)^2}{}2\sigma^2\right]; \quad \sigma > 0. \tag{4}$$

where Δ is the grid spacing. It is also known that the truncation error is very small due to the use of the Gaussian regularizer, the above formulation given by Eq. (4) is practically and has an essentially compact support for numerical interpolation. Eq. (4) can also be used to provide discrete approximations to the singular convolution kernels of the delta type [41]

$$f^{(n)}(x) \approx \sum_{k=-M}^{M} \delta_\Delta(x-x_k) f(x_k), \tag{5}$$

where $\delta_\Delta(x - x_k) = \Delta\delta_\alpha(x - x_k)$ and superscript (n) denotes the n*th*-order derivative, and $2M + 1$ is the computational bandwidth which is centered around x and is usually smaller than the whole computational domain.

In the DSC method, the function $f(x)$ and its derivatives with respect to the x coordinate at a grid point x_i are approximated by a linear sum of discrete values $f(x_k)$ in a narrow bandwidth $[x-x_M, x+x_M]$. This can be expressed as [42]

$$\left.\frac{d^n f(x)}{dx^n}\right|_{x=x_i} = f^{(n)}(x) \approx \sum_{k=-M}^{M} \delta^{(n)}_{\Delta,\sigma}(x_i-x_k) f(x_k); (n = 0, 1, 2, \ldots,). \tag{6}$$

where superscript n denotes the nth-order derivative with respect to x. The x_k is a set of discrete sampling points centered around the point x, σ is a regularization parameter, Δ is the grid spacing, and $2M + 1$ is the computational bandwidth, which is usually smaller than the size of the computational domain. For example the second order derivative at $x = x_i$ of the DSC kernels for directly given

$$\delta^{(2)}_{\Delta,\sigma}\left(x-x_j\right) = \frac{d^2}{dx^2}\left[\delta_{\Delta,\sigma}\left(x-x_j\right)\right]\Big|_{x=x_i}, \tag{7a}$$

The discretized forms of Eq. (7a) can then be expressed as

$$f^{(2)}(x) = \left.\frac{d^2 f}{dx^2}\right|_{x=x_i} \approx \sum_{k=-M}^{M} \delta^{(2)}_{\Delta,\sigma}(k\Delta x_N) f_{i+k,j}. \tag{7b}$$

When the regularized Shannon's kernel (RSK) is used, the detailed expressions for $\delta_{\Delta,\sigma}(x)$, $\delta^{(1)}_{\Delta,\sigma}(x)$, $\delta^{(2)}_{\Delta,\sigma}(x)$, $\delta^{(3)}_{\Delta,\sigma}(x)$ and $\delta^{(4)}_{\Delta,\sigma}(x)$ can be easily obtained for x^1x_k. For example, the first- and second-order derivatives are given as [40–46]

$$\begin{aligned}\delta^{(1)}_{\pi/\Delta,\sigma}(x_m-x_k) = {} & \frac{\cos(\pi/\Delta)(x-x_k)}{(x-x_k)} \exp\left[-(x-x_k)^2/2\sigma^2\right] \\ & - \frac{\sin(\pi/\Delta)(x-x_k)}{\pi(x-x_k)^2/\Delta} \exp\left[-(x-x_k)^2/2\sigma^2)\right] \\ & - \frac{\sin(\pi/\Delta)(x-x_k)}{(\pi\sigma^2/\Delta)} \exp\left[-(x-x_k)^2/2\sigma^2)\right]\end{aligned} \tag{8}$$

$$\begin{aligned}\delta^{(2)}_{\pi/\Delta,\sigma}(x_m-x_k) = {} & -\frac{(\pi/\Delta)\sin(\pi/\Delta)(x-x_k)}{(x-x_k)} \exp\left[-(x-x_k)^2/2\sigma^2\right] \\ & -2\frac{\cos(\pi/\Delta)(x-x_k)}{(x-x_k)^2} \exp\left[-(x-x_k)^2/2\sigma^2)\right] \\ & -2\frac{\cos(\pi/\Delta)(x-x_k)}{\sigma^2} \exp\left[-(x-x_k)^2/2\sigma^2\right] \\ & +2\frac{\sin(\pi/\Delta)(x-x_k)}{\pi(x-x_k)^2/\Delta} \exp\left[-(x-x_k)/2\sigma^2)\right] \\ & +\frac{\sin(\pi/\Delta)(x-x_k)}{\pi(x-x_k)\sigma^2/\Delta} \exp\left[-(x-x_k)^2/2\sigma^2\right] \\ & +\frac{\sin(\pi/\Delta)(x-x_k)}{\pi\sigma^4/\Delta}(x-x_k) \exp\left[-(x-x_k)^2/2\sigma^2)\right].\end{aligned} \tag{9}$$

2.2. Lagrange delta sequence (LDS) kernel

This kernel for $i = 0,1,\ldots, N-1$ and $j = -M,\ldots,M$ is given by [38–42]

$$\Re_{i,j}(x) = \begin{cases} \prod\limits_{k=i-M,k\neq i+j}^{i+M} \dfrac{x-x_k}{x_{i+j}-x_k}, & x_{i-M} \leq x \leq x_{i+M}, \\ 0 & \text{otherwise} \end{cases} \tag{10}$$

where $W^{(n)}_{ij}$ is the weighting coefficients and these coefficients for the first derivative can be given as

$$W^{(1)}_{i,j} = \Re^{(1)}_{i,j}; \quad \text{for } i = 0, 1, \ldots, N-1 \text{ and } j = -M, \ldots, M, j \neq 0, \text{ and} \tag{11a}$$

$$W_{i,0}{}^{(1)} = -\sum_{j=-M,j\neq 0}^{M} W^{(1)}_{i,j}; \quad \text{for } i = 0, 1, \ldots, N-1 \text{ and } j = 0. \tag{11b}$$

The weighting coefficients for higher order derivatives are given by [40–43]

$$W^{(n)}_{i,j} = n\left[W^{(1)}_{i,j} W^{(n-1)}_{i,j} - \frac{W^{(n-1)}_{i,j}}{\left(x_i - x_{i+j}\right)}\right] \tag{12}$$

for $i = 0,1,\ldots, N-1$ and $j = -M,\ldots,M, j \neq 0$, and $n = 2,3,\ldots,2M$,

$$W_{i,0}{}^{(n)} = -\sum_{j=-M,j\neq 0}^{M} W^{(n)}_{i,j} \tag{13}$$