



Phenomenological multiscale finite element for single layer graphene



T.C. Theodosiou^{a,*}, C. Galiotis^{b,c}, D.A. Saravanos^a

^a Dept. of Mechanical Engineering & Aeronautics, University of Patras, GR-26500 Rion-Patras, Greece

^b Institute of Chemical Engineering Sciences, Foundation of Research and Technology-Hellas (FORTH/ICE-HT), Stadiou Street, GR-26504 Platani-Patras, Greece

^c Dept. of Chemical Engineering, University of Patras, GR-26500 Rion-Patras, Greece

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ABSTRACT

A novel multiscale finite element is developed for the prediction of single layer graphene mechanical response. The introduced model implements a coarse-grained multiscale approach and targets computational efficiency via dimensionality reduction. Recovery of the full atomistic configuration is also possible. The element employs a set of molecular mechanics based finite elements previously developed for the prediction of the elastic response and fracture of graphene at atomistic level simulations. The development of a simple multilevel finite element is described and predictions are validated against theoretical and experimental data. Results appear to be in a very good agreement.

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1. Introduction

The discovery of stable single layer graphene [1,2] has boosted effort towards the development of computational tools for the simulation of its response. Fortunately, graphene has been theoretically studied for decades before its discovery, as a starting point for graphite and fullerenes. Despite the strong theoretical background, various issues arise when practical applications are considered. Traditional modeling approaches like molecular dynamics and tight-binding have been successfully employed and various aspects of the graphene behavior have been highlighted; although very successful, the required amount of computational power and resources grows exponentially with the number of atoms involved. Furthermore, if graphene-based Nanodoped Polymer Composites are considered, fully atomistic simulations are rather impossible for dimensions of practical interest. Multiscale modeling has proved to be a major asset for the investigation of large scale atomic systems.

As the name implies, multiple material scales are combined and coupled. Generally, based on the scale-bridging methodology, multiscale methods can be divided into two major categories: (i) Hierarchical and (ii) Concurrent methods. Hierarchical methods are based on the two-scale convergence concept [3] and its generalization to multiple scales [4]. This is actually a “bottom-up” approach, according to which, material properties are initially derived from a fully atomistic representation and then fed sequentially as input

across multiple higher scales until the macroscopic behavior is obtained. These methods are particularly useful for macroscopically homogeneous materials. Typical examples are the Asymptotic Homogenization [5], the Quasi-Continuum (QC) Method [6], Coarse-Grained Molecular Dynamics (CGMD) [7], etc. On the other hand, Concurrent methods employ multiple scale models simultaneously in the same analysis. The problem domain is divided into atomistic and continuum sub-domains connected to each other with special transitional areas; among others, the Ghost Force Correction Method [8], the Force-Based coupling [9], Blending Schemes [10], etc. have been proposed for the coupling of the individual sub-domains. Concurrent methods are particularly useful for the investigation of localized phenomena and typical examples include the Heterogeneous Multiscale Method (HMM) [11], the Macroscopic Atomistic Ab-Initio Dynamics (MAAD) [12,13], the Bridging Scale Methods (BSM) [14,15], the FE^2 method [16,17], etc.

Considering multiscale analysis of graphene, numerous works can be found in the literature. To begin with, existing Carbon Nanotube (CNT) models are generally applicable to graphene with minor modifications. More focused investigations require consideration of graphene's special characteristics like its 2D nature and its lattice structure. Arroyo and Belytschko have developed a methodology for single layer crystalline films [18] which later became the basis for other works. Belytschko et al. have also demonstrated coupling methods for bridging atomistic and continuum scales [10,19] using a “handshake” area for the coupling. Based on the Cauchy–Born rule, Larsson and Samadikhah [20] have employed an atomistic unit lattice and treated graphene as homogenized 2D membrane. Sfyris and Galiotis [21] have also

* Corresponding author. Tel.: +30 2610 969445; fax: +30 2610 969417.

E-mail address: dozius@mech.upatras.gr (T.C. Theodosiou).

incorporated lattice curvature by considering a two-lattice structure.

Although, the methodologies for continuum and homogenized modeling are well-established, the atomistic part of multiscale analysis still remains a challenge. Various computationally efficient techniques have been successfully demonstrated. Finite Element based methods become very popular, as they take advantage of similarities in the formulations between strain energy and molecular potential. A common, yet rather simplistic, method models graphene using classical rod and beam finite elements whose nodes represent carbon atoms by replacing stretching, bending and torsion stiffness terms with effective quantities calculated from molecular potential equations [22]. In a more comprehensive approach, specialty molecular finite area elements have been reported encompassing the molecular potential, either through homogenization [23], or based on the repetitive hexagonal pattern of the graphitic lattice [24]. More recently, the authors have published a new formulation, amenable to the investigation and simulation of graphene failure, where each atomistic interaction type is represented by a special finite element; this modeling approach encapsulates all atomistic details and proved to yield a reasonably good approximation of graphene response, including graphene fracture [25,26].

The latter is further extended in this paper towards a MultiScale Finite Element (MSFE) model targeting both accuracy and computational efficiency. The most important features of the introduced formulation are summarized in the following:

1. *Lack of assumptions regarding the homogeneity and periodicity.* The majority of existing models for graphene rely on assumptions like the Cauchy–Born rule and assume homogeneous deformations. Although this approach generally gives reasonably accurate results, it can also be the source of numerical errors and artifacts associated with the deformation gradient [9], especially when nonlinearities and instabilities occur. On the contrary, the MSFE approach makes no assumptions for the homogeneity or periodicity of deformations, but performs a full nanoscale analysis on finite systems and obtains accurate atomistic configurations.
2. *Bidirectional approach.* Most homogenization methods usually employ a bottom-up approach; i.e. the atomistic configuration feeds an effective continuum model. The presented approach employs a nonlinear regression model and provides a reverse mapping from the MSFE representation to an accurate atomic configuration. This is particularly useful for the investigation of localized phenomena in full atomistic detail.
3. *Computational efficiency.* Owing to dimensionality reduction and formulation simplification, the MSFE representation requires significantly less computational effort than a typical molecular mechanics simulation. The efficiency of the multiscale model is quantified in terms of timing and resource allocation. Furthermore, the presented formulation can be easily incorporated into commercial FE codes that support user-defined constitutive models; such codes are highly optimized and can boost speed even more.

The developed MSFE in its current state can be used for the prediction of graphene response. Ultimately, it may be incorporated in other successful methodologies dealing with multiscale simulations of graphene and even nanotube composites [27,28] in order to facilitate the computationally demanding nanoscale calculations. To avoid any misleading conclusions, the MSFE approach does not intend to replace the Molecular Mechanics methodology; instead, it provides a fast numerical tool to speed up calculations regarding structural deformation of graphene. Calculations that strongly rely on the exact atomic configuration, should still be

conducted using the atomic configuration, as recovered from the MSFE assembly.

This ultimate goal of this work is not only to introduce the MSFE, but also to describe the methodology concept in a stepwise fashion, so that other independent researchers may reproduce the envisioned approach and further develop it. To this end, all technical details – including employed parameter sets and derived coefficients – are provided. The rest of the paper is organized as follows: Section 2 provides the effective molecular mechanics representation of graphene, which will be the basis for the multiscale model. This has been previously published by the authors [25,26], but some basic features have to be included herein, in order to make the paper self-consistent. Section 3 describes the Atomic-to-MSFE Mapping and the numerical solution procedure. Section 4 describes the reverse mapping from the MSFE model to atomic configuration. Section 5 demonstrates validation cases and quantification of computational efficiency.

2. Molecular mechanics formulation

The mechanical response of graphene depends on a number of atomic interactions, including bond stretching, angle bending, dihedral angles, improper angles, non-bonded interactions, electrostatic interactions, etc. Existing numerical formulations represent such interactions as contributions of respective energy terms in coupled or uncoupled form; typical choices for the modeling of atomic interactions in graphene are the very popular and successful Tersoff–Brenner [29] and AIREBO [30] potentials, and various Morse-type formulations. The number of interactions considered within an analysis determines the accuracy of a model, as well as its computational efficiency. Intuitively, incorporation of too many energy terms can lead to very accurate, but computationally prohibitive formulations.

For the needs of the present work, the energy terms are limited to bond stretching, angle bending and dihedral angles in uncoupled form. Previous works [25,26] proved that this set of energy terms is adequate for a reasonably accurate description of graphene, including out-of-plane deformations and fracture. The energy terms for bond stretching (V_{str}) and angle bending (V_{ang}) are dominant, while the weaker term for dihedral angles (V_{dih}) is only activated for out-of-plane deformations. Following this, the total potential (V) of a graphene flake can be expressed as

$$V = \sum V_{str}(r_{ij}) + \sum V_{ang}(\theta_{ijk}) + \sum V_{dih}(\phi_{ijkl}). \quad (1)$$

where r_{ij} is the Euclidean distance between atoms i, j , which is equal to the bond length of the respective atoms; θ_{ijk} is the angle formed by atoms i, j, k ; and ϕ_{ijkl} is the dihedral angle formed by the planes defined by θ -angles.

The individual energy terms are further expanded to

$$V_{str}(r_{ij}) = D \cdot \left[e^{-a(r_{ij}-r_0)} - 1 \right]^2 \quad (2)$$

$$V_{ang}(\theta_{ijk}) = \frac{k}{2} \cdot (\theta_{ijk} - \theta_0)^2 - \frac{k'}{3} \cdot (\theta_{ijk} - \theta_0)^3 \quad (3)$$

$$V_{dih}(\phi_{ijkl}) = \frac{1}{2} k_d \cdot (\phi_{ijkl} - \phi_0)^2. \quad (4)$$

The employed parameter set for Eqs. (2)–(4) is obtained from previous successful works [31,32]; to ensure high accuracy, the coefficients for the dominant terms (V_{str}, V_{ang}) have been derived from DFT-based calculations. All constants are listed in Table 1. Minimization of the total energy provides the equilibrium state under any loading condition.

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