AC 2007-1702: ENGINEERING EDUCATION AND ELEMENTARY MULTI-SCALE MECHANICS

Ghodrat Karami, North Dakota State University
Dr. Karami is an Associate Professor in the Department of Mechanical Engineering and Applied Mechanics at North Dakota State University.

Robert Pieri, North Dakota State University

Engineering Education and Elementary Multiscale Mechanics

Abstract

Classical Mechanics addresses the foundation of engineering education at conventional scales. To include mechanics at smaller scales and especially nanoscience as part of engineering education, curriculum development or enhancement has been launched at many institutions by introducing new nanoscience/technology courses. Although such efforts are necessary and valuable in their place, however, efforts should also be directed at bridging the gap between nanoscience and engineering to provide future engineers with the necessary educational background in multiscale technologies.

Classical elementary engineering mechanics courses (statics, dynamics and mechanics of materials) are taught in most engineering disciplines as essentials for the professional development of engineering students. This paper will focus on the implementation of some ideas and modules for material mechanics to include problems at the nanoscience mechanics. The paper will explain how all this was done by introducing the concepts of multiscale engineering and adding new modules containing example problems at micro and nano-scales within the topical framework of existing courses and using existing resources. The efforts will be substantiated and facilitated using the simulation capabilities of Computer Aided Engineering and Drawing techniques and simulation. Studies on students' understanding of nanoscience and technology and the correlation with continuum technologies have been made before and after the implementation of these modules to such courses.

Introduction

Newtonian mechanics has been and is the most fundamental branch of science governed by the laws of nature. Its principles provide the foundation for most hardware technological developments. These principles provide the foundation for engineering mechanics, which describe the interactions of entities in terms of energies, forces, positions, deformations, material characteristics, and other defined/derived parameters.

Recent technological discoveries demonstrate a shifting concern from macroscopic phenomena to an ever decreasing physical scale, i.e. from the overall strength of a structure to the maximum theoretical material strength derived from atomic packing within an advanced material. This shift will not abandon the basic laws observed in engineering mechanics, but new terms, concepts and definitions should be introduced to bridge the commonly understood laws and the principles that could be implemented at all scales. Therefore a need for multiscale analysis and design, especially multiscale mechanics, seems to be necessary. In this respect, calls for engineering curriculum renewal have been made from both industry, as well as university communities in the past decade,[1,2] and obviously among the items of reform to be considered is the inclusion of current and future technological advances in engineering disciplines is of prime importance.

Although, multiscale education seems to be demanding and useful,[3,4,5] there are many questions regarding implementation procedures, the level of students' understanding and their preparedness. For example, engineering mechanics at the level of continuum is difficult and demanding by itself. Another problem is how much the students are prepared and what will be the benefits of overloading the students with advanced materials. These concerns become the focus of results that will be published in the future.

There is a general feeling that the elementary courses of engineering mechanics including statics, dynamics and mechanics of materials (Fig.1) can be revised to be more computer-based and to include some multiscale modules in concepts, problems and exercises[6-11]. Perhaps the main objectives will be to prepare engineers and researchers for the future of multiscale technology by:

1) Development, at an early stage, of students' internalized ease with the scale,
2) Development of students' visualization of the problems under consideration.

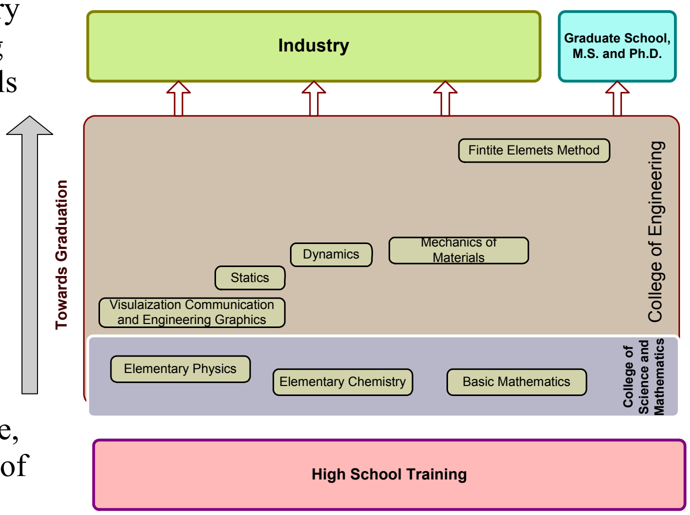

Fig. 1. Courses of Mechanics in Engineering Curriculum

Further objectives should focus on how the faculty of engineering mechanics courses can develop the associated pedagogy for multiscaling mechanics education. Therfore a careful and a systematic plan to revitalize the multiscale mechanics curriculum should be undertaken with the following thrusts:

- Introducing new modules to mechanics courses to conclude multiscale mechanics,
- Applying computer aided engineering (CAD) and finite elements method (FEM) technology to the construction of virtual space simulations illustrating solution possibilities,
- Enhancing student and academic community awareness and attitude toward multiscale mechanics and its employment in emerging nanotechnology opportunities.

In this paper, we will focus mainly on the concepts that can be implemented at the intermediate course of mechanics of materials. The mechanics of materials is an essential course that is offered to second-year engineering students in most engineering disciplines. Relying upon the framework of existing courses and by using existing physical and intellectual resources, an array of educational activities will be suggested to provide such an opportunity for undergraduate engineering students.

In the modules to be developed, a simplified, but not "dumbed-down", mechanics of nanostructures and elements can be demonstrated in parallel with the conventional examples at the macromechanics level, illustrating the universality of these concepts. Examples will include the mechanics of nanocarbon materials and structures and typically available nanomachines. Two common threads of these experiences will be visualization and scale application. These can be enacted through new pedagogies that connect the courses above to graphical communications via 3-D modeling of nanoscale visualization examples. Also, FEM[13-14] and Molecular Dynamics (MD)[15-17] analysis power will be brought to bear to demonstrate the mechanical behavior of some structures and nanostructures.

Student's Preparedness

Prior to implementation of the idea of multiscale mechanics education, questionnaires were given to students. The questions were targeted at three broad areas of: familiarity and knowledge, preparation and expectation. Following are the questions sent to a group of material mechanics students.

1. Do you know what nanotechnology and nanoscience is?
2. Do you know why nanotechnology is becoming so important in engineering?
3. Do you know some applications of nanotechnology?
4. Do you know why material properties such as Young's modulus and heat conductivity coefficients of nano-sized materials are superior to common materials?
5. Are you familiar with any nano-sized material?
6. Do you know how large nano-size is?
7. Do you know the size of an atom?
8. Do you think that the forces that hold you to the earth any different from the forces that hold a grain of sand to the earth?
9. What do you think the ratio is between goal posts of a football field and the distance between the earth and our sun?
10. Did you have any classes in HS which was related to nanoscience and were you instructed?
11. Have you taken any courses related to nanoscience in College?
12. Have you read any scientific facts about nanoscience? Elaborate on the program, such as News, self reading, TV programs
13. Do you a clear idea how nanoscience is related to courses of mechanics you will take at college?
14. Do you think mechanics of materials has any relation with nanotechnology? And if yes in what aspects?
15. Do you think will it more beneficial if we extends the mechanics of materials to nano-sized and multiscale analysis?

The results are plotted in Figs. 2 and 3. As expected, and from the analysis of the results, one can see that most students are exposed to the importance of nanotechnology and have heard or watched news articles about improvements generated by nanotechnology, but they are "not clear on the matter". As far as their preparation and understanding of nanotechnology is concerned, it is not encouraging at any level. Obviously, one does not expect students be prepared for mechanics and nanomechanics before entering engineering courses. However, there are some introductory courses in physics and chemistry focusing on the atomic and molecular structures of matters. It seems that students treat these courses as science- and knowledge-based "non-engineering major courses" that obviously will not focus on nanomechanics or its applications in a meaningful way. Also, it seems the historic approach of the upper level courses on "Nano-Whatever" create separate islands of thought that will not serve multiscale fluency and the innate grasping of opportunities afforded through the application of nanotechnology. For that reason it can be argued that the suitable place to generalize Newton's laws of motion and mechanics to all scales is in the introductory courses of mechanics[21-23]. It is comparable to learning English as a second language vs. having it as one of several languages spoken since birth. The statistics show that the students are willing to learn multiscale mechanics if the classroom approach is appropriate.

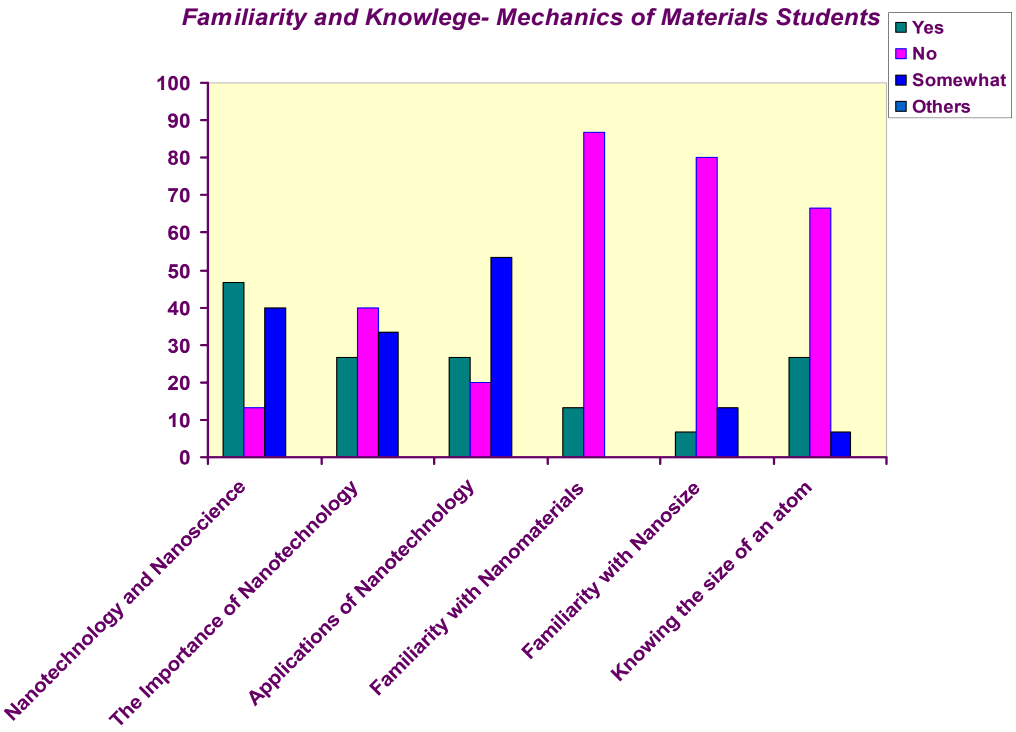

Fig.2. Familiarity and Knowledge- student's survey

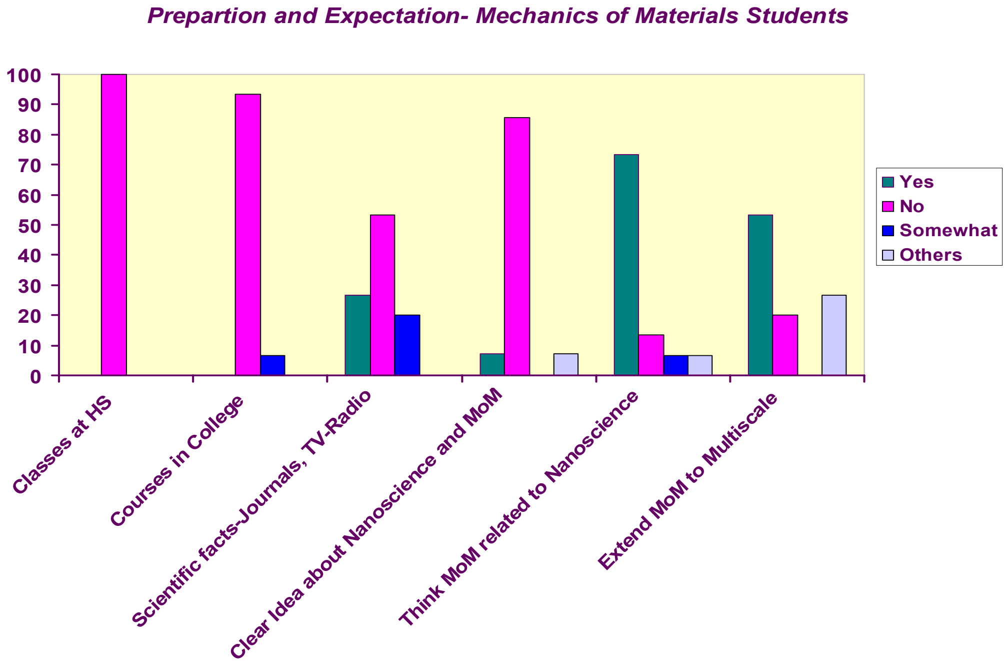

Fig.3. Preparation and Expectation- student's survey

Modules Topics Correlated To Mechanics of Materials

As mentioned above in regards to the process of integrating Nano/micromechanics into a classical engineering education, the development and evaluation of modules are essentials, as the educational materials for classical education is well established.

The Scales: Nano, Micro and Macro Scales: Scales and size range are the prime materials to be introduced. In Greek, *nano* means dwarf, but in science, nano means 1billionth ($\times 10^{-9}$). A nanometer is a unit of spatial measurement that is 10^{-9} meter, or one billionth of a meter. An average human hair is about 80,000 nanometers wide.

By referring to demonstrated figures and tables, one can introduce that nanoscale is concerned with the objects within the range of 10^{-7}-10^{-9}. Below this range is *pico,* which is concerned with matters of size from 10^{-9}-10^{-12}. Above nano range is *microscale,* which concerns the scales from 10^{-5}-10^{-7}. Also the size of some objects and distances can be presented (some typical size ratios are shown in Table 1) for clarification.

Sample	**Measurement (meters)**
Uranium nucleus (diameter)	10^{-13}
Water Molecules	10^{-10}
DNA molecule (width)	10^{-9}
Protozoa	10^{-5}
Earthworm	10^{-2}
Human	2
Earth (diameter)	12.76×10^{6}
Dist. from Fargo to New York	2.3×10^{5}
Dist. from earth to Sun	1.5×10^{8}
Dist. from the Sun to Pluto	10^{13}

Table.1 Comparison of objects and distances

Transition from Nanoscale to Macroscale: The physical transition across the scales should be demonstrated. Transition from macro to nanoscale is acknowledged as the transition from a continuous world to a world of discretized atoms and molecules. The assumption of continuity of the domain of the structures is acknowledged in macroscale, but at smaller scales each structure is made of numerous atoms or molecules attracted to each other by force fields usually written in terms of potential fields (see Fig. 4). At such scales, atoms and molecules should be considered individual bodies and entities. With such consideration, implementation of the engineering mechanics formula, kinematics and kinetic terms, such as velocity, acceleration and force, have identical meaning and usage as at the macroscale. However, the material properties in the form of bulk parameters do not apply[18-20]. As an example, the equivalent term to elastic Young's modulus at macroscale is the severity of the attractive potential force field in nanostructures.

Top-down Break down and Bottom up Manufacturing: A module on nano-manufacturing is a necessity. Going across the geometrical scales typically one of two design approaches are used: top-down or bottom-up. The former proceeds by employing ultra-miniaturization to move from macrostructures to nanostructures, while not always applying the proper nanoscience based relationships, whereas in the latter, nanostructures are assembled to build macrostructures that can utilize nanomechanics to fulfill advanced functions. The essence of nanotechnology can be found in "paradigm shift" models, where the top-down and the bottom-up approaches converge. Although, the top-down approach has been more convenient so far, it should be generally recognized that the optimum assemblage and application of nanoscale devices require a drastic shift from simply scaling down to a completely new understanding. In the nanoscale world, new functions are expected to emerge that cannot be seen in the macrostructure world. The bottom-up approach can build up these nanoscale abilities into macroscale structures with expanded abilities. This opportunity is available in various fields of advanced technology, e.g.

biotechnology, information-related devices, and materials. The emerging multiscale engineering mechanics education should address both designs.

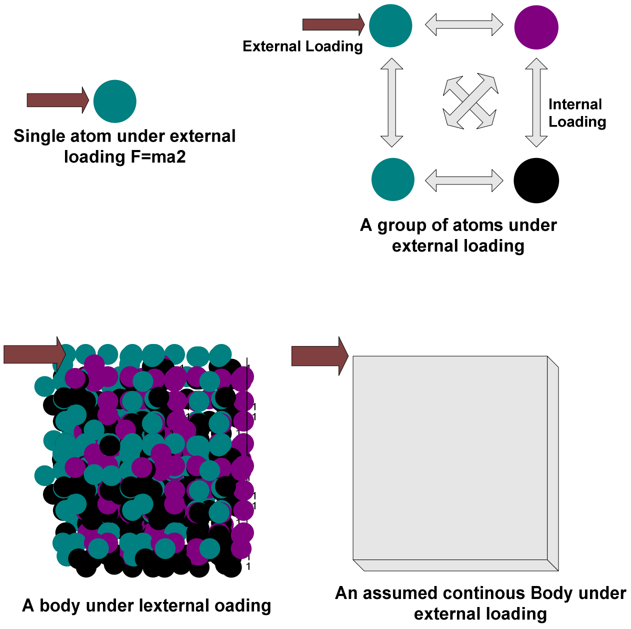

Fig. 4. From a Single atom to a continous body

Material Property Changes and Nanostructured Materials

A module on the change of material properties is necessary. Nano-materials have amazing and useful properties with many structural and nano-structural applications. Nanomaterials have excellent mechanical, electrical, optical, and wear properties. Nanomaterials provide opportunities to develop smaller, faster, lighter and smarter materials and machines to benefit all of humankind. There are two differences in nanoscale behavior:

1. Nanoparticles have a much greater surface area when broken down into tiny particles than they do when whole. Since the chemistry of solids occurs at these surfaces, more surfaces mean increased chemistry reactivity.
2. The smaller the particles get, the greater the changes in particle magnetic, optical and electrical properties.

Some well known nano-materials can be introduced. Nanomaterials can be found in many forms. Distinguished among them are the carbons made materials, which are the most common, and applied nanomaterials in recent years. Fullerenes, Diamond, Graphite, and Carbon Nanotubes are notable nanocarbon materials.

Molecular Dynamics, Energy and Stiffness: Classical mechanics is a sub-field of physics that deals with macroscopic objects moving at slow speeds. Within this domain, classical mechanics can predict the physical behavior of objects with very little error. At the atomic and sub-atomic scale, Newtonian physics begins to break down. This is the domain of quantum mechanics. Originally developed to describe the atom, Quantum mechanics explains the phenomena of errors in classical mechanics within this domain.

Nanomechanics[4-5] utilizes a combination of these two fields of physics called molecular dynamics. Molecular dynamics predicts how atoms will interact with each other. Molecular dynamics predicts the wiggling and jiggling of atoms to determine the movement, structure, and function of molecules. Computer programs based on the laws of molecular dynamics can simulate these interactions. Creating a nanopart out of thousands of atoms might not yet be physically possible, but molecular dynamics can tell us if the structure would be stable or not.

There are five different energies that contribute to molecular dynamics. These can be thought of as similar to different energies that are involved in classical mechanics, such as potential energy due to elevation change. The total energy can be a combination of bond stretching, bond bending, bond torsion, van der Waal's forces and electrostatic forces[4-5] (see Fig. 5.), that is, $E=E_{st}+E_b+E_{tor}+E_{vdW}+E_{es}$. When two atoms bond, the bond length is determined by the energy associated with the distance between the two atoms. The atoms seek the lowest energy state. As the bond is stretched past this lowest energy bond length, forces counter this displacement. These forces are what cause the energy known as energy due to bond stretching. This energy is much like a mechanical spring. The force is the product of a spring constant and the displacement. Therefore, the energy in a molecular system is: $E_{st} = \sum_m \frac{1}{2} K_{st}(R_m - R_{0m})^2$ where, K_{st} = stiffness constant, R = bond length and R_o = equilibrium bond length. Also, other types of bonding energies can be formulated in similar forms as a multiplication of associated stiffness times the deformation. For example the energy due to bending is written as $E_b = \sum_m \frac{1}{2} K_b(\theta_m - \theta_{0m})^2$ where, K_b is the bending stiffness and θ as the rotation angle. The nonbonding energies due to van der Waal's forces can be explained by quantum mechanics, which could be written in the form of stiffness as, $E_{vdW} = \sum_m K_m^{vdW(ij)} \left[\frac{1}{2}\left(\frac{R_m^{ij}}{R_m}\right)^{12} - \left(\frac{R_m^{ij}}{R_m}\right)^{6} \right]$, where, the superscripts i and j denote the two atoms involved in an individual van der Waals interaction. The values of the force constants, well depths, natural van der Waals distances, bond lengths, and equilibrium bond angles associated with the carbon and other materials are well established[16-17]. Similarly since the energy due to electrostatic forces for the two particles will have a charge, they will either attract

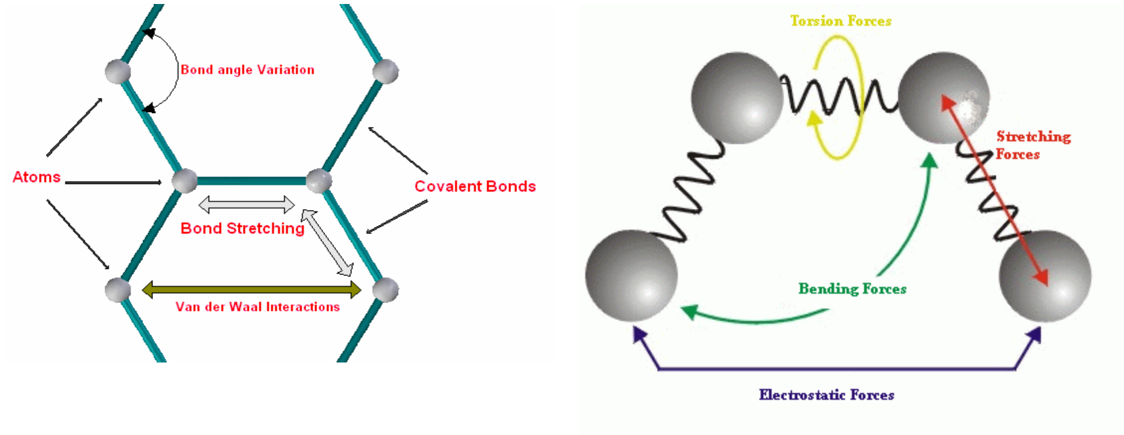

Fig. 5. The bonded forces in molecular structure and their equivalence in conventional mechanics.

or repel each other. There is energy associated with this interaction shown by: $E_{es} = \sum_{m} \frac{q^{1} q^{2}}{R_{12}}$, q = charge, R_{12} = distance between particles.

Examinations: Along with conventional teaching, some specific questions might be put in tests or quizzes; some of them can include:
Why does Young's modulus change at the scales?
How does one compare the Young's modulus of Carbon Nanotube with steels?
How is the strength related to molecular interactions?
How does molecular bonding impact strength?
What is van der Waal's interaction?
Can you compare the deflection of carbon nanotube with a steel bar of the same size?
What is a pico stress and what does TPa stands for?

Educational Facilities- CAD and FEM Simulations

Students will take a course in graphical communication at the freshman/sophomore level. In this course, besides covering the basics of engineering drawing, conventions, codes and standards[24], they will become acquainted with a typical commercial CAD package (in this case ProE, but it also could be AutoCAD, Solid Works or Solid Edge) to do their assigned homework and projects. This course can contribute by teaching some basics of nanomaterials and structures scales and spacing, along with the conventional topics. Examples will include CNTs, nanographene sheet geometries, nanogears, and nanomachines. Through this methodology, the complexity of the nanostructures will be lowered since they become repeated, or "patterned" features in the program. A substantial number of descriptive examples can be inserted into the CAD library for more references. Those who complete this course should be ready to better understand the modules in the engineering mechanics courses.
FEM is a computational analysis tool that will transfer the continuous structures into discretized forms. In fact, the function of FEM might be simulated as transferring the continuous domain back to its original form where it has been naturally discontinuous. In FEM, the material and geometrical properties, such as area, mass, and stiffness, are assigned to nodal points. In a comparison, in a naturally discontinuous material structure, the force field, mass, are also focused towards the atomic points.

FEM is a senior-level course, but the modeling and output of finite element in the analysis of forces, deformations and time-history is also understandable by entry-level students. Examples of nanostructures might also be analyzed by either FEM or MD for representations. Teaching finite elements is not intended at this level.
The addition of nanomechanics examples to conventional engineering mechanics courses make them more multiscale, interdisciplinary and relative to the student's existing contextual understanding. Some of the literature and fundamentals have been learned in previous elementary courses, such the basic chemistry or basic physics. However, the method extending engineering mechanics concepts to nanoscale producing nano-mechanics concepts will be new to students. CAD and FEM capabilities can provide the presentations and demonstrations with facilities that capture students' imagination. For example, Fig. 6 shows a molecular representation of a carbon nanotube, its equivalent structural modeling by FEM and the FEM external and internal loading distribution. The visualization power of CAD and the analysis tool of FEM have become basic resources of engineering education in recent years. The scaled-up

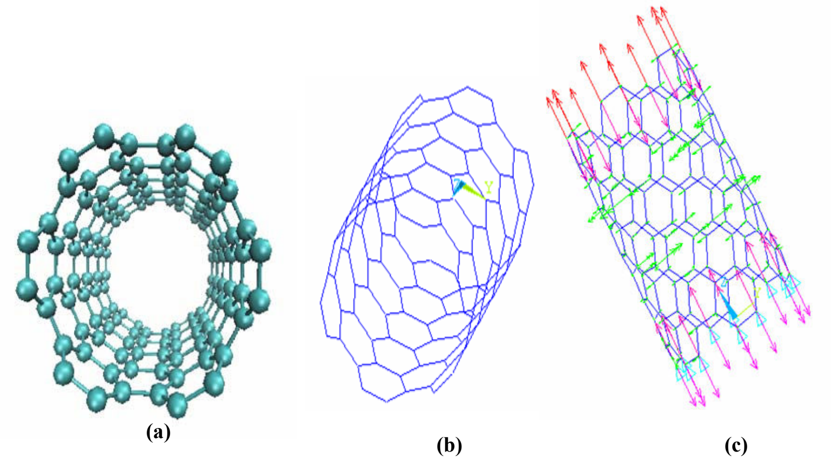

Fig 6. (a) Molecular representation of Carbon nanotube, (b): FEM equivalent structural modeling of CNT, (c) Loading Distribution from FEM analysis.

nanostructures assigned as projects will help student understanding. FEM can play a distinct role in correlating these parameters. For example, in nanocarbon materials, based on the energy equivalence, a linkage between molecular force field constants and structural stiffness properties can be established. The bonded terms are simulated by beam elements, whereas the non-bonded terms will be expressed as two-point force truss members[15]. The direct relationships between the stiffness properties of the beam elements and the force field constants in bonded interactions then becomes, $\left(\frac{EA}{L}\right)_m = (K_{st})_m$, $\left(\frac{EI}{L}\right)_m = (K_b)_m$, $\left(\frac{GJ}{L}\right)_m = (K_{tor})_m$ where L is the bond length, EA and GJ are the cross sectional properties of a beam in axial, bending and torsion, respectively[18-19]. $(K_{st})_m, (K_b)_m$ and $(K_{tor})_m$ are the force field constants for stretching, bending and torsion, respectively. These are typical topics in a continuum approach to the mechanics of materials.

Conclusion

As engineering mechanics is the starting point for engineering education, efforts should be spent to upgrade the classical elementary engineering mechanics courses of statics, dynamics and the mechanics of materials to include multiscale concepts. In this paper, ideas and concepts to be incorporated into the basic course of the mechanics of materials are presented. Students' preparation and expectation were demonstrated. Suggestions were made on the implementation and the necessary modules.

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