

From Continuum-based to Multiscale-based Engineering Mechanics Education

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The rapid growth in nanoscience and technology and its implementation in modern ‘flat world’ industry and engineering are calling for a new curriculum for engineering education. The change in curriculum involves the introduction of new concepts and examples at scales that are new territories for engineers. These territories were previously acknowledged as the exclusive knowledge-based playground of scientists, in which their explorations broaden the horizon of basic understanding. Engineering mechanics concepts are taught to most engineering disciplines as essentials to basic and practical engineering understanding. At the introductory level engineering mechanics is taught in the courses of statics, dynamics and strength of materials. This paper addresses the need and importance of reforms and revisions of engineering mechanics courses to include experiences in these new territories so that the engineering mechanics education expand beyond continuum and macro-based level to include all the scales. This revision can be done by introducing the concepts of multiscale engineering and development of new lesson modules perhaps including example problems in micro- and nanoscales. Relying upon the framework of existing courses and using the existing physical and intellectual resources, an array of educational activities will be suggested to provide such an opportunity for undergraduate engineering students. The efforts will be facilitated through the visualization capabilities of computer-aided engineering and drawing (CADD) techniques as well as the analysis capabilities of finite element model (FEM) and molecular dynamics (MD) procedures.

Keywords: continuum mechanics; dynamics; engineering mechanics; multiscale mechanics; nanomechanics

INTRODUCTION

CALLS FOR ENGINEERING CURRICULUM RENEWAL have been made from both industry and the university communities in the past decade [1, 2]. Among the reform items to be considered, the inclusion of current and future technological advances in the engineering disciplines is of prime importance. Newtonian mechanics has been, and is, the most fundamental branch of science governed by the laws of nature and its principles provide the foundation for most hardware technological development. These principles provide the foundation to engineering mechanics, which describes the interactions of entities in terms of energies, forces, positions, deformations, material characteristics and other similarly defined parameters.

A brief scan of the recent science discoveries demonstrates a shift of concern from macroscopic phenomena to an ever decreasing physical scale, i.e. from general strength of a structure to the atomic packing within an advanced material. Some of the recent achievements that have revolutionized the practice of applied science and engineering include:

- introduction of new materials;
- advances in information technologies;

- emergence of intelligent systems and sophisticated software;
- revolution in modern engineering design in the field of bioscience;
- advances in manufacturing;
- advent of a formalized approach to nanoscience and nanotechnology;
- the miniaturization of mechanical devices, instruments, sensors and machineries.

Such achievements are dictating revisions and updating in engineering education approaches and particularly the basic engineering mechanics courses. Such revisions would help to prepare the future engineering workforce to be more than just aware of the emerging fields of nanoscience, nanotechnology and nanobiotechnology. In line with such a goal, a major objective in engineering education should be to provide the students with the skills to apply knowledge of multiscale engineering mechanics [4–10] to the design, analysis and manufacture of nanoscaled components and systems in addition to conventional macrostructures. Students should be able to efficiently correlate macro- and nanoscaled structures with engineering fundamentals. 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 nanos-

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structures, while not always applying the proper nanoscience-based relationships, whereas in the latter nanostructures are assembled to build macrostructures that can utilize nanomechanics to fulfil 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 design approaches.

Engineering mechanics courses

Engineering mechanics constitutes a fundamental part of all engineering education. Various concepts of engineering mechanics are presented in several courses in engineering and science, although in current engineering education the essence of this subject will be covered in the introductory courses entitled Statics [11], Dynamics [12] and Mechanics of Materials [13] (see Fig. 1). Departments of Mechanical, Civil and Structural Engineering and Engineering Mechanics are usually the providers of such courses. With the exception of parts of the

dynamics that use the motion of a sparsely defined particle, most activities in these courses utilize practical problems at the macroscale. Therefore, these courses can be described as continuum-based, i.e. dealing with continuous bodies. Under current strategies, students are not expected to learn much about small scale, or multiscale, mechanics. The generalized application of engineering mechanics rules to micro- and nanoscale practical examples should be considered in these courses.

Most mechanics laws and conventions are scaleless, although there are conventions and specific relations, such as material parameters, that apply to atomic scales that must be introduced to facilitate multiscale fluency. Practical examples and problems at the new scales within the content of these courses will attract the students' attention and build their confidence in the applicability of the rules and laws at all scales. Although there are some introductory courses in physics and chemistry focusing on atomic and molecular structures of matter, these courses are science and knowledge based and will not focus on nanomechanics applications. The historic approach of the upper level courses on 'Nano-Whatever' creates separate islands of thought that will not serve multiscale fluency and the innate grasping of opportunities afforded through the application of nanotechnology.

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. It is comparable to learning English as a second language versus having it as a language spoken since birth. To develop engineers for all

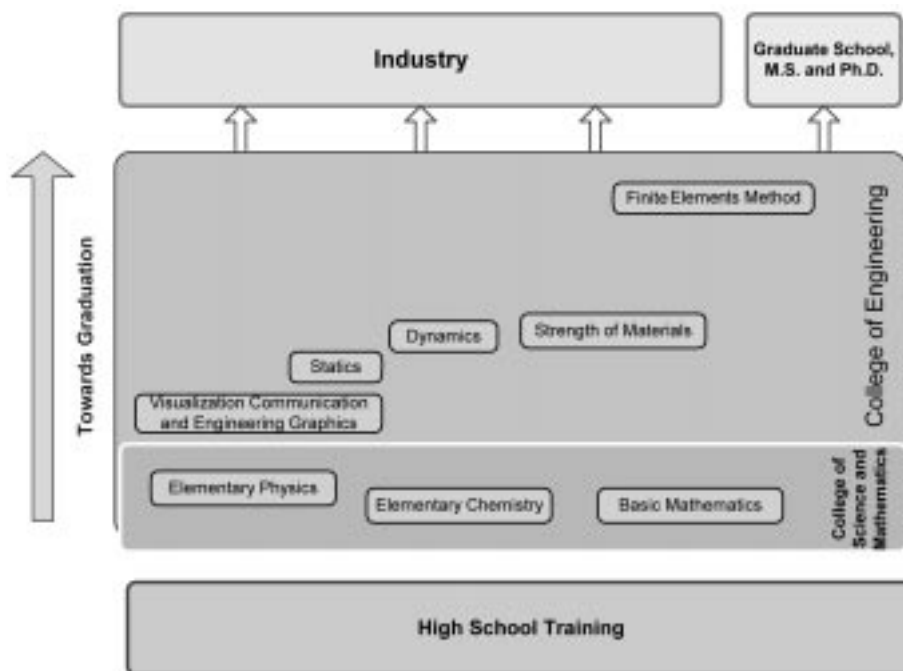


Fig. 1. Courses of mechanics in engineering curriculum.

scales of utilization, multiscale engineering mechanics is essential and the engineering mechanics faculty should be strongly involved in offering such courses. There is a general feeling that the elementary courses of Engineering Mechanics including, Statics, Dynamics and Strength of Materials courses can be revised to be more computer-based and to include some multiscale modules in concepts, problems and exercises [14–20]. Further objectives should be focused on how the faculty of engineering mechanics courses will develop the associated pedagogy for multiscale mechanics education. In a short path, a careful and a systematic plan to revitalize the multiscale mechanics curriculum can be undertaken with the following thrusts:

- introducing new modules to mechanics courses to conclude multiscale mechanics;
- applying computer-aided engineering and drawing (CADD) and finite element model (FEM) technology to construction of virtual space simulations illustrating solution possibilities;
- enhancing student and academic community awareness and attitude toward multiscale mechanics and its employment to the emerging nanotechnology opportunities.

The conventional courses of Statics, Dynamics and Mechanics of Materials are taught in the second year of most engineering curriculums. In the modules to be developed, a simplified, but not dumbed down, mechanics of nanostructures and elements can be demonstrate in parallel with the conventional examples at 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 [21, 22] and molecular dynamics (MD) [23–25] analysis power will be brought to bear to demonstrate mechanical behaviour of some structures and nanostructures.

The challenge continues to be to enhance the content of basic curricula without sacrificing the fundamentals. Because of the rapid pace at which the technology advances, the historic timing of educational developments will take too long to stay abreast of the content advances. Therefore, additional cognizant changes to science pedagogy are necessary to keep pace with the ever expanding technology. The final goals for such an effort will be to prepare engineers and researchers for the future of multiscale technology by:

- development, at an early stage, of students' internalized ease with the scale;
- development of students' visualizations of the problems under consideration.

TRANSITION FROM CLASSICAL TO MULTISCALE MECHANICS EDUCATION

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. 2). At such scales, atoms and molecules should be considered individual bodies and entities. With such consideration implementations of the engineering mechanics formula, kinematic and kinetic terms such as velocity, acceleration and force have identical meaning and usage as at the macroscale. However, the material properties in form of bulk parameters do not apply anymore [26–28]. As an example, the equivalent term to elastic Young's modulus at macroscale is the severity of the attractive potential force field in nanostructures.

As the continuum mechanics literature is dominant and understandable to the public, the analogues of nanomechanics world can be easier found in continuum world than vice versa. For example, a discretized nanostructure can be simulated as atoms of concentrated mass, with their interactions modelled by stiff springs. This is perhaps a crude way of modelling such structures, as the interaction stiffness is a function of distances, distributed in all directions and function of many parameters. But this is how one can start educating students who understand springs and concentrated masses (balls). If we restrict the motion of two atoms to one dimension, along the line connecting them, so that the atoms can only move directly towards or away from one another, the force $f(r)$ between them can be described in terms of the interaction potential $\phi(r)$, defined through:

$$f(r) \equiv \frac{d\phi}{dr} \quad (1)$$

[29]. The typical interaction potential energy for the Lennard–Jones model has the algebraic form:

$$\phi(r) = -\frac{A}{r^6} + \frac{B}{r^{12}} \quad (2)$$

where A and B determine the strength of attractive and repulsive interaction. The simulated engineering mechanics approximation is to think of the atoms being linked by a simple linear spring, with the spring constant k given by:

$$k = \left. \frac{d^2\phi}{dr^2} \right|_{r_0} \quad (3)$$

(see Fig. 3).

The addition of nanomechanics examples to conventional engineering mechanics courses make them more multiscale, interdisciplinary and rela-

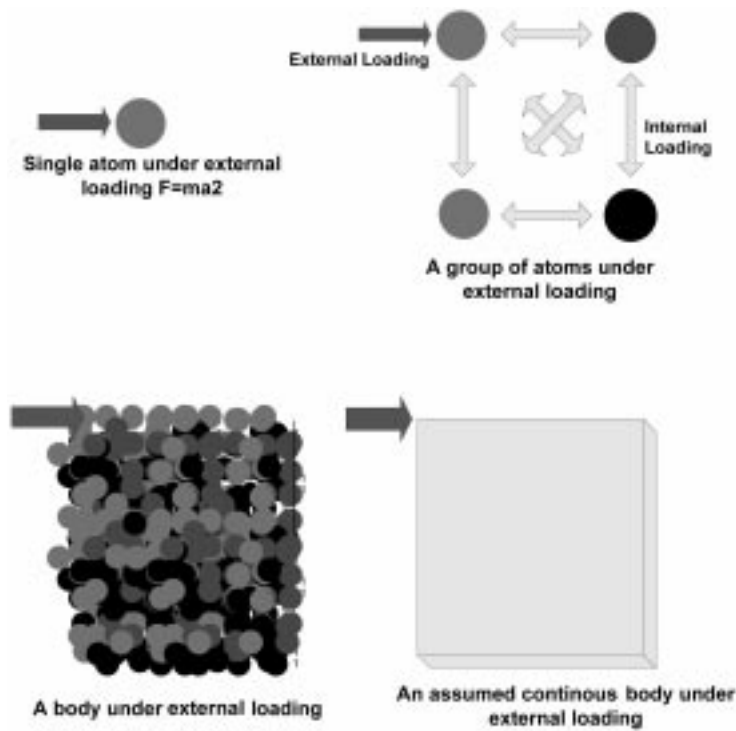


Fig. 2. From a single atom to a continuous body.

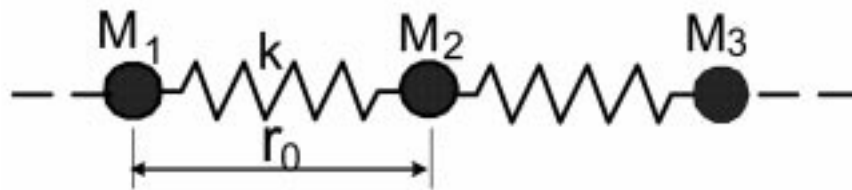


Fig. 3. Representations of a row of atoms by spring and mass.

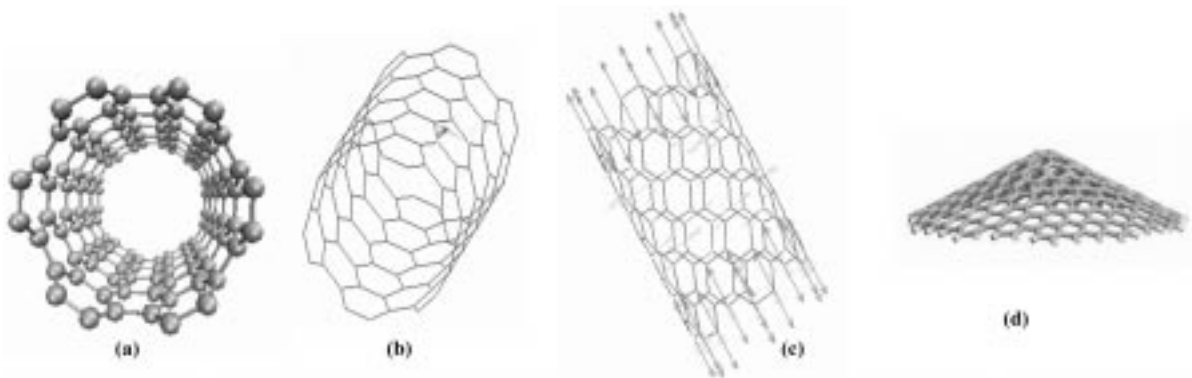


Fig. 4. (a) Molecular representation of carbon nanotube; (b) FEM equivalent structural modelling of CNT; (c) loading distribution from FEM analysis; and (d) a cone nanographene platelet.

tive to the students' existing contextual understanding. Some of the literature and fundamentals have been learned in previous elementary courses such as the basic chemistry or basic physics. However, the method extending engineering mechanics concepts to nanoscales, producing nanomechanics concepts will be new to students.

CADD and FEM capabilities can provide the presentation and demonstration facilities that

capture students' imagination. For example, Fig. 4 shows a molecular representation of a carbon nanotube, its equivalent structural modelling by FEM and the FEM external and internal loading distribution. The visualization power of CADD and the analysis tool of FEM have become basic resources of engineering education in recent years. The scaled-up nanostructures assigned as projects will help the students understanding.

ENGINEERING MECHANICS MODULES

The process to include the nanomechanics into classical engineering education might take some time, as the educators and institutions should be equipped with the necessary facilities and understanding. Relying upon the resources in classical mechanics and the pedagogical and educational facilities (as shown in Fig. 5) this transition period can be shortened. The sequence of some of the recommended tasks for such purpose is shown graphically in Fig.5. The starting point will be to develop the modules to be added to the three courses of Statics, Dynamics and Mechanics of Materials.

Statics

Statics is regarded as the first engineering course. In Statics, the students learn the implemen-

tation of Newton’s first law. They will learn static equilibrium through vector representation of forces, moments and also become familiar with axial and shear forces, torques and bending moments and geometrical parameters such as moment of area [11].

In this course, introductory modules in static equilibrium of nanoelements and structures will be presented. These modules will also include demonstrations, problems, videos and situational simulations, replacing some of more outdated subject approaches.

Dynamics

Dynamics deals with the action of bodies in motion. Dynamic fundamentals obey Newton’s second law of motion. At the undergraduate level, the dynamics of particles, system of particles and continuous bodies are all considered [12]. The

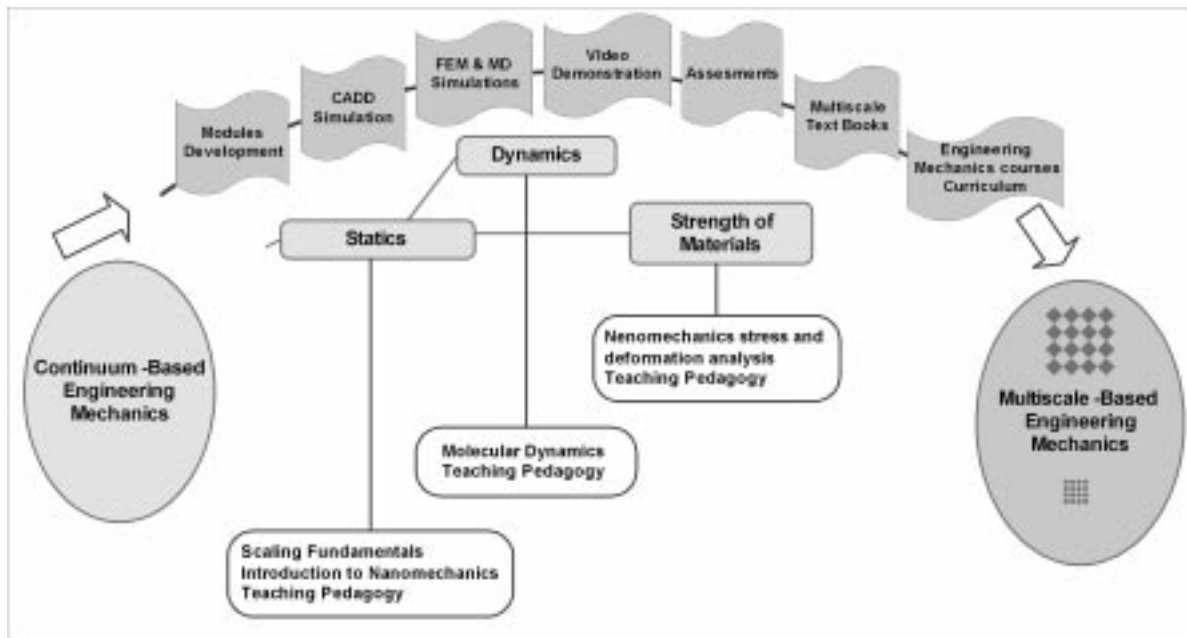


Fig. 5. Facilities for the transition of continuum-based engineering mechanics to multiscale engineering mechanics.

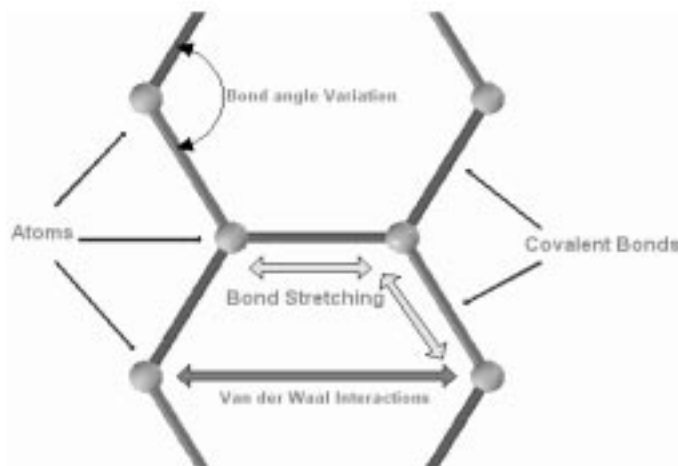


Fig. 6. The bonded forces in molecular structure.

particle or body might be assumed to be an atom or perhaps the earth with its action concentrated at its center of mass. Motion of a single particle or a group of nanoparticles can be analyzed by MD and be shown to students as appropriate for their theoretical backgrounds.

In recent years MD has been routinely used to determine the behaviour of atomic structures. MD can be used to analyse and simulate some conventional nanostructure problems in this programme. In MD, the motion of a molecule is simulated as a function of time. A simple description is that Newton's second law of motion:

$$\mathbf{F}_i = m_i \frac{d^2 \mathbf{x}_i}{dt^2} \quad (4)$$

is solved to find how the position for each atom of the system \mathbf{x}_i varies with time, t . To find the forces, \mathbf{F}_i , on each atom the derivative vector (or gradient) of the potential is calculated. The interaction between atoms thus can be described quantitatively in terms of their force field or potentials (think of a rock rolling down a steep or a shallow hill). The forces are classified as bonded and non-bonded types (as shown in Fig. 6). The forces existing at each bond, as a result of atomic positions, contribute to the total potential energy of the nanostructured material. The molecular potential energy is therefore the sum of the individual energy contributions in the molecular model [26, 27].

The major contribution to total molecular potential energy of the molecular model comes from the energies associated with bond stretching, angle variation and van der Waals parameters; the result is not unlike the total energy and motion of a bouncing ball. Individual potentials for each type of bonding and non-bonding interactions are expressed in terms of the specific geometrical parameter of the two interacting atoms [26, 27]. For example expressions for the bond-stretching potential terms relating to the separation of nodes for interacting atoms can be simplified to:

$$U^r = \sum_m K_m^r (r_m - R_m)^2 \quad (5)$$

where m stands for the bond number and the terms R_m and r_m refer to the undeformed and deformed interatomic distances, respectively, comparable to atomic springs. The symbol K_m^r represents force

constants associated with the stretching of the bond. Similarly, the van der Waals non-bonding interaction is expressed as:

$$U^{vdW} = \sum_m K_m^{vdW(ij)} \left[\frac{1}{2} \left(\frac{r_m^{ij}}{r_m} \right)^{12} - \left(\frac{r_m^{ij}}{r_m} \right)^6 \right] \quad (6)$$

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 [25, 26], but may not be discussed in these modules for the basic courses.

Strength of Materials

Strength of Materials deals with the deformation of continuous bodies under the influence of external loading or disturbances. In this course the mechanical properties of materials will be introduced, to determine the loading capacity of structures and machine elements. Strength of Materials is a prerequisite course for several advanced courses in structural design of machine elements, their construction and optimization.

The material parameters in nanoscale and continuum scales are related although traditionally defined differently. Bulk properties are characters of continuum scale, although there are means to correlate parameters at different scales, such as different moduli are. A suitable procedure is to pick equivalent representative volumes (RVEs) of the same material at the different scales (see Fig. 7) [26, 28, 30, 31].

Knowing that the change of energy under an equivalent external disturbance should remain the same for RVEs, the material parameters can be related through mechanical laws. The students can be taught the definitions and applicabilities of these parameters and their correlations. FEM can play a distinct role in correlating these parameters. For example in nanocarbon materials, based on the energy equivalence, a linkage between the molecular force field constants and the 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 [27]. The direct relationships between the stiffness properties of the beam

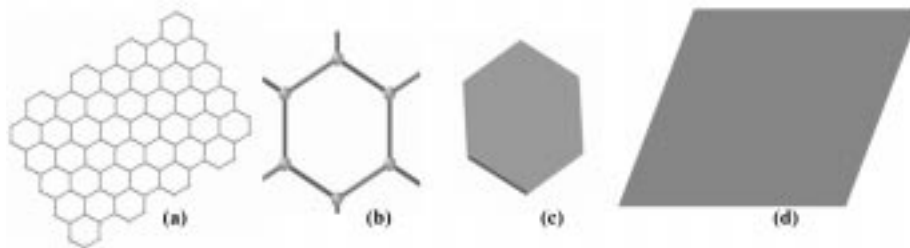


Fig. 7. (a) A single layer of nanographene sheet; (b) and (c) equivalent atomistic and continuum RVEs; and (d) the continuum domain.

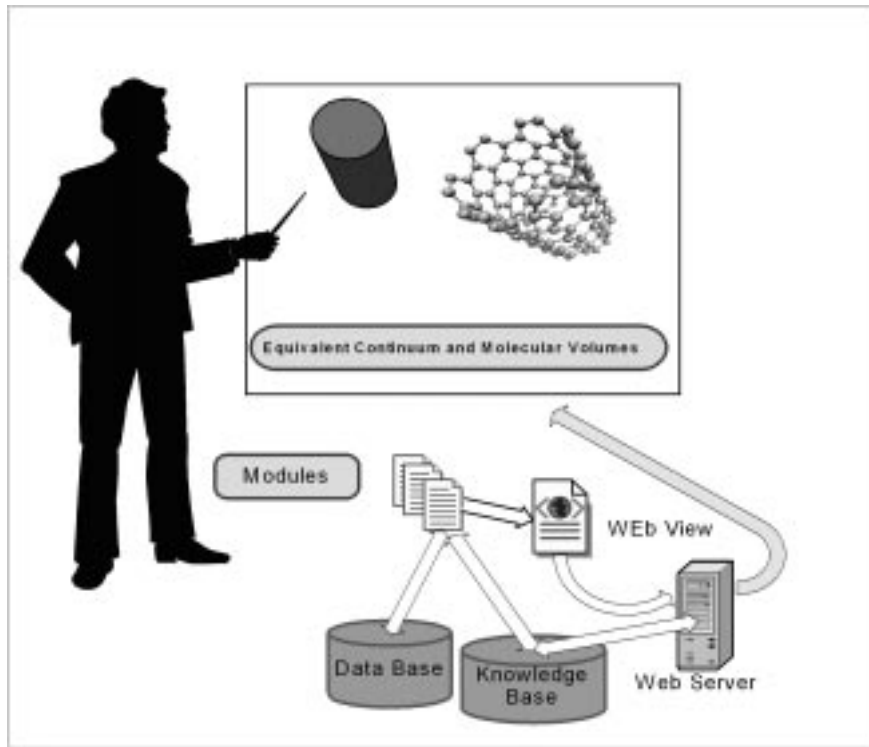


Fig. 8. Teaching pedagogy and resources.

elements and the force field constants in bonded interactions then becomes:

$$\left(\frac{EA}{L}\right)_m = K_m^y, \left(\frac{EI}{L}\right)_m = K_m^\theta, \left(\frac{GJ}{L}\right)_m = K_m^\tau \quad (7)$$

where L is the bond length, EA and GJ are the cross sectional properties of a beam in axial, bending and torsion, respectively. K_m^r , K_m^θ , and K_m^τ are the force field constants for stretching, bending and torsion, respectively. These are typical topics in continuum approach to Mechanics of Materials.

CADD and FEM simulations

The students will take a course of Fundamentals of Visual Communication at the College of Engineering at the freshman level. In this course, besides covering the basics in engineering drawing, conventions, codes and standards [32], they will become acquainted with ProE/AutoCAD/Solid Work/Solid Edge to do their assigned homework and projects. This course can benefit from teaching some basics of nanomaterials and structures, 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 programme. A substantial number of descriptive examples can be inserted in the CADD library for more references. Those who complete this course are 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 [21, 22]. In fact, the function of FEM might be simulated as to transfer 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 modelling and output of finite element in the analysis of forces, deformations and time-history is 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.

DEVISING MULTISCALE TEACHING METHODOLOGY

As nano-based technologies have advanced, a related emergence of new educational pedagogy is driving progressive curriculum upgrades. Science and engineering education is becoming cognitive science based, which will promote technological literacy. A portion of the ongoing research activities of the engineering faculty includes tremendous efforts on nanoscience and nanotechnology. However, efforts on the expansion of education to this new territory have been relatively limited. There is a clear need for exposure of students to

these emerging fields, especially at an early stage, to better prepare them for entry into an evolving modern economy.

According to an NSF/ASME study of the product realization process, industry managers place the highest value on the following elements of engineering: teamwork, communication, design for manufacture (products that assemble as well as they function), Computer-aided design (virtual reality for visualization) and professional ethics [33, 34]. Arguably, these are all traits desirable of the general student population. Studies have also shown [34] that industry practice rarely reduces to the set-piece formulas and algorithms of traditional math and science education. For engineering in particular: most engineering practitioners know that designing is not simply a matter of synthesizing solutions to independent problem sets.

Although few of the complexities of engineering design show up in the undergraduate classroom, the working world of engineers is filled with negotiations across specialties, mixed in with social, political and financial constraints [2, 35]. A significance change in the pedagogy will be how to present the interdisciplinary materials in this programme through presentation schemes to the audience benefiting from the many examples and

problems that are already saved in the library of the course (Fig. 8).

CONCLUSION

As a wide spectrum of stakeholders in engineering are calling for accelerating the pace and substance of curriculum renewal. Since engineering mechanics is the traditional starting point for engineering education, efforts were spent to upgrade the classical courses of Statics, Dynamics and Mechanics of Materials to include multiscale concepts. Nano- and microtechnology will contribute to modern industry and therefore, the new generation of engineering students becomes familiar with it at an early stage of their education. In this paper, methods demonstrating such reforms to these basic courses and the idea of multiscale mechanics were presented. Suggestions were made on implementation of the necessary modules to the basic engineering mechanics courses and the required tasks to follow.

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