

Computer-Aided-Nano-Design Education in the Engineering Curriculum: Scope and Challenges

Raghu V. Pucha¹ and Tristan T. Utschig²

Abstract – With many nanotechnology initiatives by government, industry and academia, there is an increasing trend of nanotechnology products using both *top-down* and *bottom-up* manufacturing methodologies. The US National Academies Report “*Triennial Review of the National Nanotechnology Initiative* (NNI)” has concluded that nano-materials and devices of moderate complexity can be designed and manufactured today using *bottom-up molecular manufacturing* approaches and self-assembly. Realization of these new technological systems requires integration of design knowledge with CAD/CAE tools that can explore targets for development well in advance of their physical feasibility. Therefore, it is essential that our nation prepare its engineers for tomorrow’s bottom-up nano-technology product development through Computer-Aided-Nano-Design Education. To address this issue, the authors (i) Describe how emerging needs for engineering expertise relate to the process of systematic curriculum design (ii) Review various efforts in academia that will contribute to Computer-Aided-Nano-Design and related courses (iii) Review available engineering tools that can be integrated into the Computer-Aided- Nano-Design curriculum and (iv) Analyze the challenges associated with the scoping and integration of Computer-Aided-Nano-Design Education in the engineering curriculum.

Keywords: Nano-Design Education, Curriculum Development

INTRODUCTION

Developing bottom-up fabrication technologies that enable the construction of a wide range of atomically precise engineering components and systems is a fundamental goal of nanotechnology. However, the present technologies cannot build complex structures containing billions of atoms, each occupying a predictable location. Most of the current research activities are directed towards nanoscience. In the absence of molecular manufacturing technologies and devices, both the design and theoretical/computational methods can play a leading role in the development of molecular nanosystems, guiding and speeding component fabrication technologies and system integration techniques. Realization of these new technological systems requires that design knowledge and CAD/CAE tools that can be used to explore and examine potential targets for development well in advance of their physical feasibility.

Theoretical/computational modeling in the context of nanomaterials and systems can be categorized by (i) Models that fit a given physical system with pre-existing properties that relate cause to effect (Science Models in Top-Down Manufacturing) and (ii) Models based on systems concepts, which relates desired effects to required causes [1], to develop a physical system with desired properties (Design Models in Bottom-UP Manufacturing) (see Figure 1). While the science and manufacturing of molecular nanocomponents and systems is still in its infancy, design and CAD/CAE modeling can provide concrete descriptions and specifications required, realizing the fabrication of nano-mechanical components and systems (see Figure 2).

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While the research developments in the design –for – implementation towards nano-physical systems are happening at a reasonable pace, the incorporation of nano-design education in the engineering curriculum is not getting attention in academia. It is estimated that about 2 million nanotechnology workers will be needed worldwide by 2015 and nanotechnology has the potential to create 5 million additional related jobs in the global market [2]. Are we ready to train our engineering graduates for tomorrow’s nano-manufacturing needs? Is it not the right time to revisit the traditional engineering design curriculum with a nano-systems focus? What are the challenges and pedagogical needs of curriculum development in this highly emergent field? What is the path for the process of systematic curriculum design and instructional resource development that is commensurate with the emerging needs of Nano-manufacturing? What are the developments in academia around the world in this direction? What are the available engineering tools today that can be integrated into the nano-design curriculum? What are the scope and associated integration challenges of such a curriculum?

In this paper the authors address some of these issues. The framework presented here illustrates how design engineers are always confronted with new demands due to the application of new technologies [3]. This discussion is then placed in the context of the current status of nano-engineering education. Finally, implications stemming from the nexus of these two pieces are discussed. Thus, this work provides value to the engineering education community beyond the specifics of Computer-

Aided-Nano-Design. The generic aspects of the process may be viewed as a template for integrating new demands on engineers into the engineering curriculum.

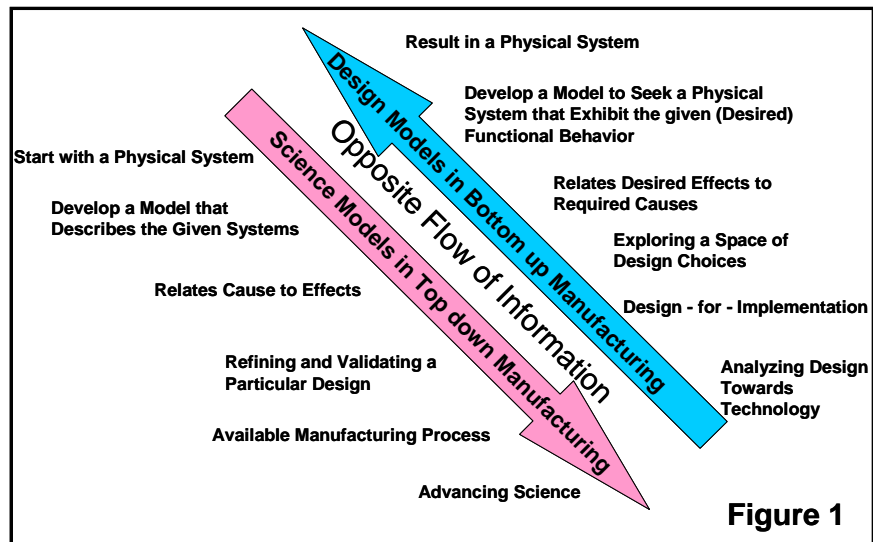


Figure 1

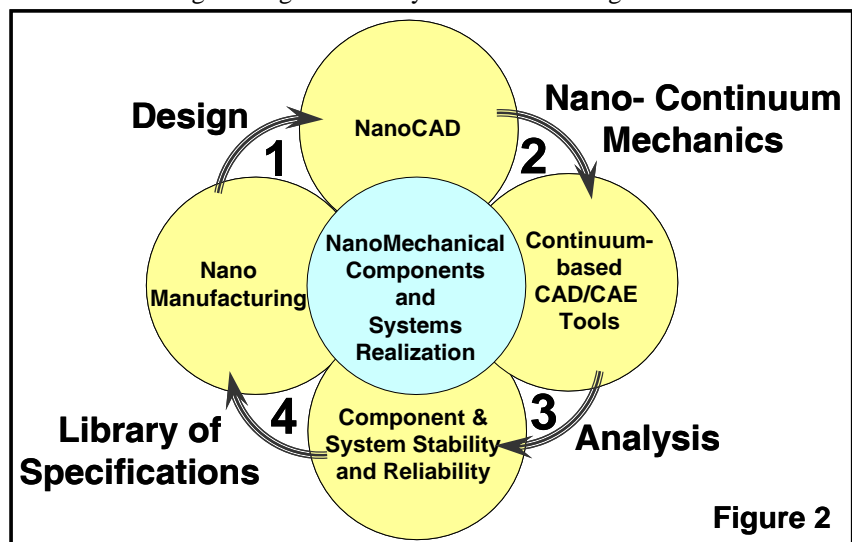


Figure 2

EMERGING NEEDS AND CURRICULUM DEVELOPMENT CHALLENGES

Because computer-aided-nano-design is an emerging field (Figures 1 and 2) it will naturally have a relatively low level of consensus about key content and processes that need to be learned by the students when compared to more traditional areas within engineering. The implications on teaching and learning due to this lower consensus are described in [4] and state that instruction within low-consensus fields may benefit from the inclusion of more general intellectual development (in this case as it applies to skills needed for nano-engineering design) along with embedding current research within the scope of a course. This status of emergence then also indicates that students

who pass through the curriculum will have significant needs for continued learning and adaptation as the field develops. In short, students entering the nano-fabrication and design workforce need to be eminently trainable “self growers”. This concept is not new, of course. It is simply more prominently visible in an emergent field. Figure 3 is a concept map representing how the content and processes in computer-aided-nano-design relate to curriculum design for the field. The concept map is described in more detail below.

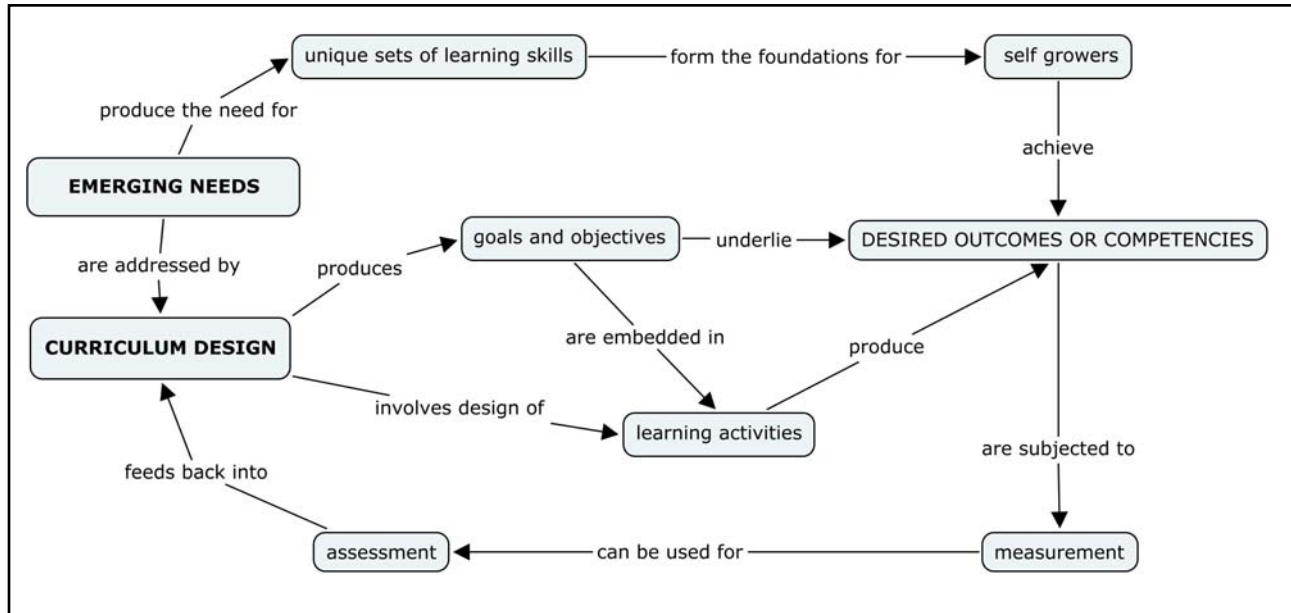


Figure 3 – Relationship of an emergent field to curriculum design.

Creating Self Growers

Within the context of engineering education the ABET accreditation criteria a-k might be considered to represent the self grower’s trainability mentioned above as a need for students to be able to participate in life-long learning [5, 6]. Unfortunately, the literature regarding lifelong learning in this context is limited. Nonetheless, several key offerings from related literature provide some guidance. First, critical thinking skills have been long studied. Numerous sources outline key issues to guide educators and include [7, 8]. These resources point to the need for modeling, coaching, and self-assessment as integral parts of the classroom environment. In the context of nano-engineering design this would mean students need to learn to both develop and use CAD/CAE tools for nano-scale design. For example, projects with various nano-building blocks such as Carbon Nano Tubes (CNT), DNA and Dendrimers in designing nano patterns, components and functional products that include opportunities to improve and iterate based on substantive feedback from instructors will be needed. Criteria for student success on major projects will need to be clearly defined such that students can self-assess their progress in developing expected knowledge and skills.

Secondly, it is only during the college years that brain development reaches its final stages. A recent effort by Jeffries gathered much of what is known about how brain development during the college years may impact instruction [9]. Recommendations include making explicit the disciplinary epistemology, examining how discourse in the field relates to that disciplinary epistemology, and engaging students in challenging and meaningful tasks. In addition, Giedd suggests that the activities students undergo during these late stages of brain development “hard-wire” the brain to be suited for those tasks [10]. Thus, approaches to adult learning need to be incorporated in the curriculum such that students are exposed to these techniques early and can begin to internalize them. Knowles describes the importance of application-oriented instruction and grounding in concrete examples for adult learners [11, 12]. In the case of nano-engineering design, such examples might include things like designing nano drug delivery systems and modeling CNT based fuel cells.

Finally, one can summarize the pedagogical needs for an emergent and evolving field into a simple concept: professionals in computer-aided-nano-design need to be “self-growers”. This concept is integral to the philosophy of process education which is outlined in [13]. Two ideas which have been extensively developed within the process education community are particularly relevant to this discussion. These are the classification of learning skills which manifest themselves in quality learners [14] and the process of assessment [15, 16]. Key cognitive skills directly relating to nano-engineering design would include identifying missing knowledge, integrating and contextualizing information, recognizing patterns, identifying constraints, selecting research methods, selecting tools, defending scholarship. Key social skills would include responding to change, defining purpose, making proposals, team cooperation and compromise, thinking opportunistically, marketing, and projecting the future. Finally, key affective skills would include being curious, responding to failure, seeking assessment, recognizing dissonance, challenging standards, building identity, and self-actualizing.

Emerging Needs Within the Curriculum Design Process

Keeping the concepts about continued learning needs (outlined above) at the forefront of curriculum design is integral to achieving the outcomes one desires in a course or program.

First, we note that essentially all major respected course design methodologies begin with goals and outcomes [17-21]. This is extremely important to note because in an emerging field these outcomes need to include aspects of adaptability and effectively choosing among alternatives. Incorporating these elements into the course goals and outcomes will naturally guide the curriculum towards one that is likely to produce self-growers. Bender and Beitz have carefully outlined how various outcomes (they refer to them as competencies and utilize Beitz and Helbig’s five competency dimensions: subject-specific, methods, systems, personal & social, and practice) in engineering design education for emerging fields can be classified in order of importance from inessential to essential and further identify how student work forms and pedagogical approaches within the design process relate to achieving these competencies [3]. In general the competencies listed above for the engineering design can be extended to nano-design curriculum. Teaching objectives with detailed profiles for each competency need to be developed specific to the emerging field of nano-design and manufacturing,

Bender and Beitz also argue that the subject-specific knowledge must be explicitly connected to both concrete experience and “purposive discussion” or reflection in a social context. This argument is strengthened within the specific context of nanotechnology by Roco who argues that broad connections among concepts to create holistic views for students beginning to learn about nanotechnology will be essential in developing a nanotechnology workforce [22]. Developing a curriculum with emphasis on nano-design concepts and connecting them to create holistic views in nanotechnology can be achieved through enquiry-based and purposive discussions embedded in the curriculum. Specific topics to nano-engineering design which are most relevant include (i) What are the various design parameters that influence the nano-component geometry and stability (ii) How do we relate the nano building blocks (a molecular system with a stable network of bonded atoms) to nano-mechanical components and systems with material-based continuum models (iii) What type of bounding continuum approaches to be used in defining the design-phase estimates of strength, shape, stiffness and surface properties of bulk material properties of nano-structures?

Second, we note that essentially all major respected course design methodologies include work in breaking down the course into specific modules or activities that will encompass the full learning cycle and thus produce maximum growth [23-25]. This is consistent with the need for student knowledge and skills regarding both *bottom-up* and *top-down* approaches in nano manufacturing. As illustrated in the Figure 5, later in the paper, example modules and associated learning activities might include (i) Concepts of bottom-up nano manufacturing and the role of design (ii) CAD of molecular-level nano-components and assemblies and (iii) Introduction to continuum-based CAD and analysis tools for nano-components.

Third and finally, we note that to all major respected course design methodologies include a well-planned and robust measurement system. It is critical that student performance can be accurately measured in order to understand whether a program is achieving its goals. In the developing field of nano-engineering design such measures will be particularly useful if they can be broadly applied across multiple programs. This will foster a coherent needs analysis within the discipline. Extensive resources on education measurement are available via [26].

EFFORTS IN NANO-ENGINEERING EDUCATION AND NANO-DESIGN CURRICULUM

The National Science Foundation (NSF) has supported many nano educational projects covering high school, informal education, undergraduate education and centers of education and learning [22, 28]. Some of these efforts are briefly described here.

Table 1: Nano Education Initiatives and Programs [27-29]

Description	Program / Initiative
Community College	Regional center for nanofabrication manufacturing education (Pennsylvania State University) (Part of NNUN)
Curriculum Development	NSF Nanoscience Undergraduate Education (NUE) (James Madison University)
Curriculum Development	NSF Nanoscience Undergraduate Education (NUE) (Michigan Technological University)
Curriculum Development	One Year Masters Program in Nanoscale Science and Technology (The University of Leeds, UK)
Curriculum Development	Ph.D program in "Analysis of Nanostructured Materials" (Technical University Ostrava, Czech Republic)
Curriculum Development	Bachelor's Degree in Nanotechnology (Flinders University of South Australia)
Curriculum Development	Undergraduate Courses at the Nanobiocenter (Cornell University)
Curriculum Development	Graduate Courses on nanoparticles (Clarkson University)
Develop Instructional Material	NSEE: Nanoscale Science and Engineering Education
Higher Education	Integrative Graduate Education and Research Traineeship (University of Washington, Seattle) – 1 st Ph.D program in NanoTechnology in USA.
Network-based Outreach & Education	NNIN: National Nanotechnology Infrastructure Network
Network-based Outreach & Education	NNUN: National Nanofabrication Users Network
Network-based Outreach & Education	NCN: Network for Computational Nanotechnology (Purdue University)
Outreach Education	Nano Manipulator : University of North Carolina
Outreach Education	NanoKids : CD based interactive video for High School (Rice University)
Outreach Education	Molecularium : Imaging Molecules from the inside (Rensselaer Polytechnic Institute)
Public Education	Making Nanoworld Comprehensible (University of Wisconsin and Discovery World science museum, Milwaukee)
Training	Rensselaer Polytechnic Institute partnerships with industry and several colleges.
Training Modules	Nanomanufacturing processes, using a multimedia classroom integrated laboratory (University of Arkansas)
Training Modules	INSEE: Interactive Nano-visualization in Science and Engineering Education (Arizona State University)
Workshop	K-12 & Informal Nanoscale Science and Engineering Education (NSEE) in the U.S (October 2005)

NSF funds National Science and Engineering Education (NSEE) projects in developing instructional materials for inclusion in grades 7-12 science courses, providing professional development and research opportunities for

secondary teachers, and engaging in multiple forms of outreach to schools and general audiences through exhibits, media presentations, and traveling programs.

The National Nanotechnology Infrastructure Network (NNIN) has established the following goals for its network-based educational outreach and training: Expose young people to advanced and exciting research in nanotechnology and motivate them to educate themselves for careers in the sciences or engineering; train teachers and guidance counselors about the discipline of experimental sciences, provide additional teaching tools, and enhance their enthusiasm for having students pursue careers in science; create and distribute educational materials for children, college students, technical professionals, teachers and the general population, as well as improve the understanding of and involvement with science, technology, engineering and mathematics; and focus these efforts on population segments having disproportionately low employment and education in sciences, including women, disadvantaged minorities, and the economically disadvantaged. NNIN has developed and anticipates continuing development of instructional materials for K-12 schools and teachers.

The Network for Computational Nanotechnology (NCN) is a multi-university initiative that was launched in September 2002 to create a unique, web-based infrastructure to serve researchers, educators, and students. NCN research, education, and outreach programs drive the development of its infrastructure. The NCN hosts collaborative tools and delivers unique educational resources such as online courses, learning modules, lectures, and seminars. Its signature service is online simulation, visualization, and high-performance computing. The NCN is comprised of research themes on nano-electronics, NEMS/nano-fluidics, and nano-bioelectronics – and a cross-cutting computational theme. NCN is collaborating with the National Center for Learning and Teaching (NCLT) in Nanoscale Science and Engineering to support the development of teaching modules for grades 7-16. In particular, NCN is providing expertise, development and resources for interactive and simulation based material that can be integrated in the NCLT modules.

The NCLT has a varied set of objectives in the establishment of a methodology to introduce and evaluate educational material in nanotechnology in grades 7-16, to promote teachers' professional development and to develop educational curricula for future educators in nanotechnology. The goal of NCN is to interact with the NCLT to provide content and interactive software to pursue all of these educational tasks.

The National Nanofabrication Users Network (NNUN), a shared nanotechnology facilities resource, is open to users from across the country. The NNUN university sites, which make up the network, are state-of-the-art user facilities run by a professional engineering staff. The NNUN enables undergraduate and graduate research and education in nanotechnology across the US and thereby strongly impacts nanotechnology workforce development.

Table 1 includes the programs listed above and lists additional Nano education initiatives and programs and efforts in US and around the world.

Proposed Computer-Aided-Nano-Design Curriculum

The primary focus of most of the educational efforts (listed in Table 1) has been in developing interdisciplinary teaching/training modules through bridging and synchronizing elementary, middle/high school, undergraduate, graduate and continuing education. These efforts in turn should provide a perfect platform for introducing more specific courses in the engineering curriculum. For nanotechnology to reach its full potential to contribute to our society, it must have a workforce for design and manufacturing. A unified curriculum with a nano-systems focus (Figure 4) that integrates science, provides basic concepts of 'bottom-up' nanofabrication, and encompasses engineering principles of design (Figure 5) is required.

As discussed in the previous section, such a curriculum should include nano-design specific knowledge with a systems focus (Figure 4), providing broad connections among concepts along different planes to create a holistic educational approach. The content and processes the students learn in achieving desired competencies are then also supported by connecting them to current research and purposive discussions.

The design of specific learning activities to achieve the desired competencies in a curriculum will, of course, need to incorporate the appropriate tools. In the context of bottom-up nano design and manufacturing through nano building blocks, the smallest object contains few atoms. Atoms must be periodically adjusted using energy minimization to accurately define the geometry of nano-building blocks. Ensuring the proper arrangement of surface atoms is an

essential design consideration when combining two different molecules for an overall stability of designed nano-components [30]. CAD tools of this nature are currently being developed [31]. Utilization of such nano-CAD tools and linking them to continuum CAD/CAE models (Figure 5) with bounding continuum approaches will facilitate many design and analysis options for nanoscale mechanical components and systems.

CHALLENGES WITH SCOPING AND INTEGRATION

In developing a robust curriculum that will naturally grow and be sustainable within the university environment there are three basic questions which must be answered. These are: Who takes the course? Why do they take it? How can one capitalize on links to K-12 activities? Answering these questions adequately when designing a curriculum within an emerging field will be critical to the success of the program. Some of the other challenges [27-29] associated with curriculum integration in this emerging field include (i) lack of fundamental background knowledge upon which to build an understanding of new knowledge [There is little research available on students' comprehension of this topic] (ii) defining a curriculum and situating this inherently interdisciplinary field within traditionally single discipline courses; (iii) the needed access to fundamental tools and associated costs (iv) difficulty in introducing new required courses without impacting existing content (integration of nanotechnology topics into existing courses might lessen such impact) (v) providing a defined course sequence or track for continued learning.

Collectively, these questions address many issues such as prerequisites and within-major electives, home department or departments, student motivation, recruitment, community integration, etc. Regarding the case of computer-aided-nano-design in engineering curriculum, some of the related background needed for the proposed design courses can be introduced in the freshman seminar classes. With current efforts in K-12 nanotechnology education [28] being systematically implemented, students can build holistic views of their existing knowledge in the freshman seminar classes on specific topics. The traditional undergraduate engineering design courses, which currently focus design concepts at macro- and microscales, need to be augmented with bottom-up nano-design concepts with a systems

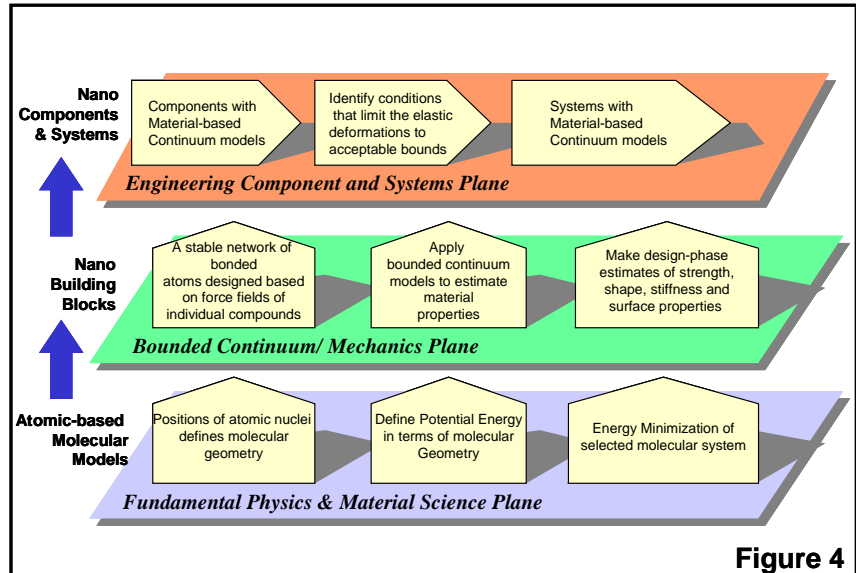


Figure 4

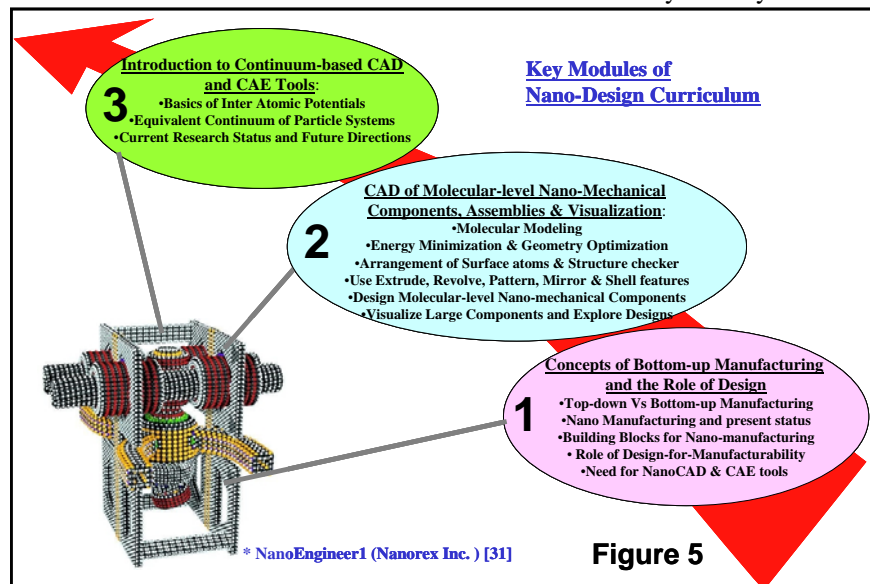


Figure 5

focus. Once such a platform is created the proposed nano-design curriculum discussed in this paper can be introduced as senior level elective courses with appropriate continuity into the graduate level.

Currently, Georgia Tech takes a multidisciplinary approach to the study of nanoscience and nanotechnology by incorporating nanoscale research into a variety of courses through a specialized Nanoscience and Technology (NaST) Certificate program. More efforts within engineering disciplines are needed to incorporate specific nano-design courses and/or content. One model for looking at how to do this is the NSF funded University of Washington's Center for Nanotechnology which has launched the nation's first doctoral degree program in nanotechnology [32]. The program puts in place a Ph.D. nanotechnology track tied closely to other science disciplines. Targeting needs at this level makes it easier to integrate the proposed computer-aided-nano-design curriculum into existing programs. However, ensuring that a workforce coming out of the undergraduate curriculum or a master's level curriculum requires additional planning since many students will not continue to the PhD and, as such, need to be ready to contribute to the field immediately.

SUMMARY

Today's technologies cannot build complex nano-systems containing billions of atoms each occupying a predictable location. In the absence of molecular manufacturing technologies and devices, both design and theoretical/computational methods can play a leading role. Traditional engineering design curricula mainly focus on the analysis and design at macro- and microscales. The incorporation of nano-design education in engineering curricula is not getting attention in academia. In preparing our students to lead the world into the future of nano-fabrication and design, one must also take into account both elements of practice and elements of pedagogy. This will enable rapid skills development that integrates all areas of the technology and can move engineering curricula forward strategically and systematically. This work, at its core, represents the integration of several bodies of knowledge towards a unified purpose of overcoming current challenges regarding the incorporation of computer-aided-nano-design in the engineering curriculum.

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