INSTITUTE OF PHYSICS PUBLISHING MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING

Modelling Simul. Mater. Sci. Eng. **13** (2005) R53–R69 doi:10.1088/0965-0393/13/2/R01

TOPICAL REVIEW

Current status and outlook of computational materials science education in the US

K Thornton[1] **and Mark Asta**[2]

[1] Department of Materials Science and Engineering, University of Michigan, Ann Arbor, MI 48109, USA
[2] Department of Materials Science and Engineering, Northwestern University, Evanston, IL 60208, USA

Received 4 April 2003, in final form 18 October 2004
Published 7 February 2005

Abstract
We examine the current state of computational materials science education based upon information compiled from top universities in materials science and engineering (MSE). We find that there is a large variation in the emphasis on computational modelling between universities. It is reported that a relatively large course offering is the result of changes in the curriculum made in the last five years, showing a rapid pace in the implementation of computational courses at these departments. We also collected information from industry and national labs regarding their current and future needs in MSE graduates, and the results are summarized. This paper also provides a list of resources that are currently used in computational materials science education.

1. Introduction

Materials science and engineering (MSE) is a discipline which has grown substantially from its original roots in metallurgy and ceramic and polymer engineering. Traditionally, significant research breakthroughs in this discipline have been driven mainly by advances in experimental techniques, rather than theory or modelling. However, recent advances in theoretical and numerical methods, coupled with an explosion in available computational resources, has led to enormous progress in the development and integration of modelling techniques applicable to the study of a wide range of materials systems and properties. Modelling and simulation tools are thus finding increasing applications not only in fundamental materials-science research, but also in real-world design and optimization of new materials. The relatively new field of computational materials science is continuing to find a growing number of practitioners not only in academia and national labs but also, increasingly, in industry.

The growing impact of computation in materials research is clear. In surveying the publications in *Acta Materialia* during 2003, one out of five articles included at least one of the two words ‘simulat*’ and ‘comput*’ in the key words (including the title and the abstract) [1].

The same survey applied to 1991 publications in *Acta Metallurgica et Materialia* produced only about one out of ten. In the US, a recognition of the growing role of modelling and simulation in materials research has led to a substantial expansion in the number of computational materials science faculties in universities across the country. In fact, many leading programmes now include multiple faculties in this area. As specific examples, both MIT and the University of Michigan have recently completed hires leading to the presence of four full-time modelling faculties in their MSE programmes. With this growth in the number of faculties has come a sizeable increase in the rate at which PhD students are being trained in the field. What has been slower to evolve, however, is the development of curriculum which could lead to more general training of materials-science graduates in the application of modelling tools. At present, efforts are under way in many MSE departments to develop and/or refine such curricula; it is a premise of this article that such efforts would benefit from increased knowledge of the ongoing progress at peer institutions.

We thus provide a survey of the current state of computational materials science education at undergraduate and graduate levels, based on surveys from a number of top-rated programmes in the USA. To our knowledge, this paper is the first to compile results of this kind. An analysis of these survey results shows many similar trends in the overall approach to computational materials education and allows identification of methods that have proven particularly successful. These surveys have also allowed us to develop a list of text books and software resources currently used by the programmes surveyed, as given in the appendix. In the continuing development of computational-materials-science curricula, it is clearly of vital importance to consider the needs of industry and national labs who represent the future employers of materials-science graduates. Therefore, we also include in this article a survey of researchers in industry and national labs, concerning the desired level of training of materials graduates in computational methods. Due to the broad nature of the field, we acknowledge that the results and analyses presented here are in no way exhaustive. We nevertheless hope that this paper proves useful in identifying successful approaches and further needs in the development of computational-materials curricula. At the very least it is hoped that the results may serve as a stimulus for further discussion on the topic.

2. Current state of computational materials science education

The survey (reproduced in appendix A) was sent to at least one faculty member at each of the top 20 MSE departments as determined by *US News and World Report* [2]. Responses were received from Carnegie Mellon University, Cornell University, Georgia Tech, Lehigh University, Massachusetts Institute of Technology, North Carolina State, Northwestern University, Ohio State (partial response), Penn State, Purdue University, the University of California Berkeley, the University of Florida, the University of Illinois at Urbana Champaign, the University of Michigan, the University of Pennsylvania and the University of Wisconsin (partial response). Those with partial responses provided information only about one of the courses offered; for statistical purposes these were excluded from the tables and figures. We have summarized the results in tables 1 and 2. For both undergraduate and graduate programmes, there was a general consensus for changes in the curriculum to address the increase of computation in MSE. Some universities have recently implemented changes in the curriculum or course offerings, while others were still defining the needs and had not yet implemented extensive changes to the curricula. In the following two sections, we will discuss the responses for undergraduate and graduate curricula. The survey explicitly requested information about the courses offered on a regular basis within the MSE departments, which may include those that have multiple listings in different departments. This is to remove as

Table 1. Survey results for undergraduate courses (14 responses).

Programmes offering computational undergraduate MSE courses (Only those offering at least one course on a regular basis are included)			
# Programmes	With lab components	# Requiring	
6	6	2	
Undergraduate MSE courses with computational components (Only courses offered within MSE departments on a regular basis are included)			
	Average	Maximum	Minimum
# offered	0.8	4	0
# with labs	0.4	2	0

Table 2. Survey results for graduate courses (14 responses).

	Average	Maximum	Minimum
Computational graduate MSE courses (Only courses offered in materials science departments on a regular basis are included)			
# offered	1.3	3	0
# with labs/projects	1.3	3	0
Graduate level courses including courses in other departments[a]			
# offered	1.9	4	0
Graduate MSE courses with computational components (Only courses offered in materials science departments on a regular basis are included)			
# offered	0.5	2	0
# with labs	0.2	1	0

[a] We did not solicit this information explicitly, but it was offered by some of the respondents. Therefore, while this count is likely to be inaccurate, it is nonetheless offered for completeness.

much ambiguity from the comparisons as possible. In addition, graduate-level courses offered by other departments but reported to be widely taken by MSE students are also listed separately (see footnote ‘a’ of table 2).

2.1. General findings

Generally, MSE curricula have been updated very recently. All respondents (a total of 10 responses for this question) reported that updates occurred after 2000, and most of those were 2003 or later. Four responded that the curricula are updated continuously, often with small changes. This shows that many departments are indeed responding to the substantial changes occurring in the field of MSE, and illustrates that changes are possible despite the inherent barriers in updating curricula in higher education.

2.2. Undergraduate curriculum

The survey shows that most universities are planning to introduce CMS in their undergraduate programmes, even though few of them currently offer such an opportunity. Table 1 shows that very few schools offer courses that have significant computational components (i.e. accompanied with computational labs or assignments or integrated with a module on computational approaches), and even fewer courses focus on computational topics. There are six programmes each offering one CMS focused course, all of which are accompanied by some lab components. The survey showed active changes occurring in MSE undergraduate curricula. Six out of ten have plans for further introduction of computational components into the

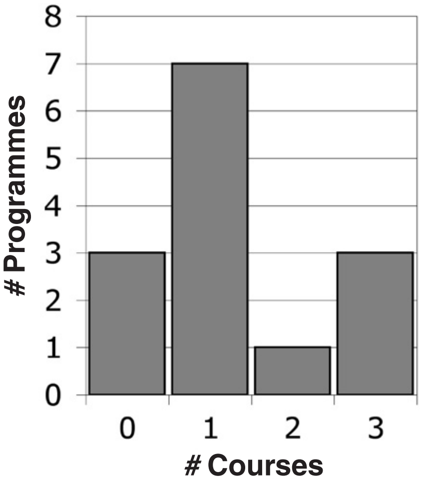

Figure 1. Histogram showing the number of programmes versus the number of graduate-level computational materials science courses offered within the department.

undergraduate curriculum. There are two main approaches reported and the choices are equally split. One approach is to integrate computational components into current MSE courses. Such changes were reported by three out of six programmes with plans. Three others reported that they were planning to introduce a new undergraduate-level course. The different choices stem in part from the long list of required courses typical of an undergraduate curriculum. In addition, the survey shows that there is less flexibility for undergraduate students to pursue courses outside their department without delaying their graduation. Two respondents reported specifically that, because of this reason, they are pursuing integration of CMS-related aspects into their existing courses. This will be discussed in more detail in section 4.

2.3. Graduate curriculum

Table 2 shows the variations in the number of course offerings at the graduate level. Significantly, most departments are now offering at least one course focused on computational MSE, showing the gradual but steady spread of education in this field. The same is reflected by the number of courses that are often taken by MSE students but offered by other departments. On the other hand, the traditional MSE courses have not been implementing computational components, possibly reflecting the technical difficulties associated in such integration as discussed in section 2.4.

More details of the data are shown by the distribution of the number of CMS courses offered in figures 1 and 2. Eleven out of 14 institutions offer at least one regularly taught course in computational MSE. The specific coverage of the courses depends largely on the faculty available to teach them. Seven courses are introductory courses covering at least two topics. As a focal topic, atomistic modelling had by far the largest number of courses, at six. Other course topics included *ab initio* electronic-structure methods, computational thermodynamics, continuum modelling and computational materials design. The number increases significantly when courses that are often taken by MSE students but offered by other departments are included, as shown in figure 2. Since the information regarding courses outside MSE departments was not explicitly solicited, the result bears large uncertainty and likely reflects the minimum rather than the actual figure.

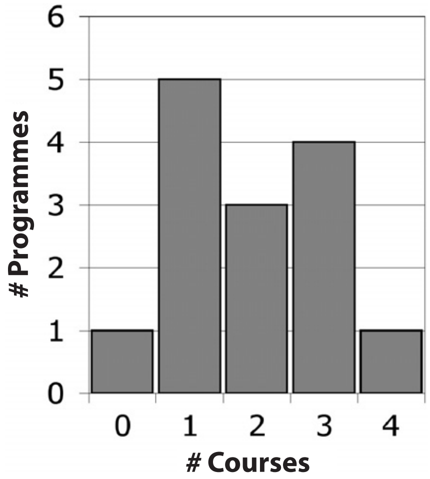

Figure 2. Similar to figure 1, but including the equivalent courses offered by other departments (see footnote 'a' in table 2).

A majority of the respondents (seven out of nine) noted deficiencies in the background of typical MSE graduate students for CMS courses. The specific deficiencies noted were a lack of mathematical and physics backgrounds (five out of seven responses above), with computational skills being secondary (two responses). Two of the responses commented on the difficulties in balancing the important topics in the curricula. The topics suggested for providing a solid background for CMS courses included quantum mechanics statistical mechanics and solid mechanics, as well as relevant math and applied math courses. Obviously, it would be a heavy burden if a student must take all these courses. Often, for this reason, students are discouraged from gaining any background at all in CMS. Another point often brought up is the comfort level that students have with computational methods, as compared with experimental ones. After all, MSE students take several laboratory classes, and therefore they are familiar with the techniques, tools, methodologies and potential strengths and weaknesses of different methods. On the other hand, few graduate students are familiar with computational approaches and thus do not feel comfortable pursuing research projects in this area. This is a Catch-22 situation; since students do not feel comfortable with computational methods, they do not pursue courses or projects in this area, and thus they remain unfamiliar with the methodology. As mentioned in section 2.5, for some students it takes only one course to break this barrier.

2.4. Course materials

Most courses are taught based on instructor notes, journal articles and text-books. Books that are reported in the survey are listed in appendix B. Many courses at the undergraduate level utilize Excel, Matlab and Mathematica for simple analysis. Others and graduate-level courses adopt ThermoCalc, DICTRA and a host of other simulation codes for molecular dynamics, *ab initio* calculations and continuum simulations. In-house codes are also widely utilized.

As in any newly developed courses, the material covered in CMS classes varies significantly. At the undergraduate level, it is still undecided how best to prepare the students. As will be discussed in detail in section 4, some courses emphasize an overview, some details in a topic, others hands-on use of software tools. In particular, two respondents emphasized the importance of *active learning* or 'learning by doing'. At the graduate level, there seems to be a list of books on focused topics that are commonly used (see appendix B). However, class notes are also used extensively. The significant diversity in student preparation may require instructors to cover both basic and advanced topics, making instructor-developed notes necessary for filling the gaps in students' backgrounds.

One of the respondents pointed out that the fact that many MSE faculties do not feel comfortable with CMS techniques poses a significant barrier in planning systematic introduction of computational components throughout the curriculum; it was suggested that the development of collections of *well documented and tested* teaching tools and course materials could provide a remedy.

2.5. Effects and effectiveness

In discussing the effects and effectiveness of CMS education, let us attempt to build a framework of a CMS education that consists of three components: (1) modelling, (2) methods and (3) general approaches that are different from those in experimental work. In area (1) we imply development of physical understanding relevant to modelling materials science phenomena. The methods, (2), include basic math, applied math, programming or simply learning what packages are available for different types of material modelling. The general approaches, (3), are rather difficult to define precisely, but they would involve, for example, how to test the models or to validate simulation results for the system under examination. Since these three areas are distinctive, students must gain very different knowledge and skill sets in order to be proficient in computational work. There was a general consensus in our survey that effective education in the area of CMS should emphasize the basics, i.e. the underlying physics (quantum mechanics, statistical mechanics and solid mechanics) in (1), and basic and applied numerical methods in (2).

The effectiveness of undergraduate-level CMS courses or components within courses were reported from only a few programmes since many schools do not have a significant offering in this area, as shown in table 1. The main consensus is that CMS courses stimulate interest in computational materials science and thus are an effective recruitment tool in the CMS community. Also reported is the benefit of adding a positive element in students' resumes especially for those interested in the materials processing industries.

The effectiveness of graduate-level CMS courses varied from 'unclear' (one response) to 'useful for students pursuing CMS projects' (five responses) to 'significant broader impact' (four responses). The reason for the variation of the effectiveness of CMS courses was not clear from the responses, and further investigation is needed to determine it with certainty. One likely reason is the level of the courses taught. Those focusing on advanced topics may be accessible only to those pursuing computational theses and therefore do not have a broader impact. It is beyond the scope of this article to examine how to optimize the effectiveness of these courses. However, interestingly, the most notable impact is reported when experimentalists take a CMS course that requires an extensive project within their interest. Allowing the students to apply the methods learned in the course to their thesis topics provides a practical purpose for the project, an additional component to their theses and an extended hands-on experience that teaches the general approaches, (3) mentioned above. Furthermore, by combining experiments and simulations, students may generate novel insights not seen by experiments alone. One of the authors (KT) observed these effects while teaching a graduate-level CMS course at MIT, where, as a result, some students changed their theses' emphasis from experimental to theoretical work or added computational components to their experimental theses, and others published the results of work that began as a class project in journals [3–5]. Similar experience is reported at UIUC, where several graduate students pursuing experimental theses completed publishable work as a class project and added significant computational components to their theses.

In conclusion, systematically teaching computational approaches and their physical bases, as well as offering an opportunity for applying the main concepts to a topic of interest (requiring support for technical issues that inevitably arise) all within a course framework, provides the experience and confidence a student needs to pursue and succeed in a CMS-based project. Also, such courses can become a forum for exploring the effectiveness of computational approaches in various fields and may accelerate advances in computational materials science in general.

3. Perspectives of employers of materials science and engineering degree holders

In this section, we discuss the benefit of computational materials science education in nonacademic settings. The national laboratories and industry are two major employers of MSE degree holders, and thus they are discussed below in turn. The information presented is obtained from only a few individuals; as such, it is meant to be informative, but not exhaustive. However, we hope that the information will provide insights into the goals of computational materials science education that can be considered when designing a curriculum.

3.1. Perspectives from National Laboratories

We summarize here the discussions with Dr Elizabeth Holm at Sandia National Laboratory, Albuquerque, Dr James Warren at the National Institute of Standards and Technology and Dr Michael Baskes at Los Alamos National Laboratory.

National laboratories hire a significant number of MSE graduates, especially at the PhD level. Computational investigations are quite common at many of the national laboratories. In particular, computational methods are uniquely important when experiments are difficult or impossible, as in nuclear weapon stewardship. One of the respondents reported a hiring goal aimed at building an organization in which up to 25% of the staff have backgrounds in modelling and simulation. In fact, computation was reported as one of the four fastest growing fields along with nanotechnology, microtechnology and biology. Currently, only about 50% of the staff computational materials scientists come from MSE departments, as reported by a respondent, due to a shortage of appropriate candidates. Therefore, a stronger computational background will expand the job opportunities for MSE PhDs regardless of their research field, computational or experimental.

Similar issues raised by university researchers are again of concern in national lab settings, including the lack of mathematical abilities, and background in physics and chemistry. The common concerns about the backgrounds of researchers are understandable, given that the research done at national labs is very similar in scope to that done at universities. Additional points made, some of which are also relevant in university settings, include the following:

- *Interdisciplinary education.* Many approaches and methods used in CMS are developed in other fields of science, engineering and mathematics. Therefore, a researcher must be capable of understanding subjects outside MSE in order to understand the bases on which a computational method is developed, in addition to its applicability to the specific problem at hand. Basic mathematics and physics backgrounds are also valued, as in academic research. This aspect belongs to (1) in the framework introduced in section 2.5.
- *Knowledge of available methods.* In order to choose the best method for the problem, researchers should be knowledgeable about the relative advantages, disadvantages and

capabilities of different computational approaches. As mentioned, most of the current offerings in computational materials courses focus on one or two methods, typically those in which the instructor is actively involved in his/her own research. Therefore, students often lack a broad perspective in computational materials science. An instructor may make an effort to introduce students to other methods, either as an overview module of a course or by inviting guest speakers on various topics. This aspect belongs to (2) in the framework described above.

- *Critical examination of the applicability of the results to real materials.* The complexity of materials should be emphasized. The relevance of simulation results derived for often somewhat idealized situations must therefore be examined critically using experimental data. This aspect belongs to item (3) in the above framework.
- *Interpretation skills.* The results obtained must be interpreted and applied. Doing so often requires connecting the raw simulation results to real materials by nontrivial analyses. Furthermore, since we often work with computational constraints, we must consider corrections necessary to apply the results to the system of interest. This aspect also belongs to element (3) in the above framework.
- *Familiarity with CMS in experimentalists.* With the proliferation of computational tools, basic knowledge and understanding of CMS methodologies are also desired in experimentalists. This will facilitate collaborations with computational counterparts, as well as allowing them to apply packaged codes to augment and guide experimental research. In addition, the same skills are desirable for MS materials scientists who are hired as analysts or technicians, but it is reported that they often lack experience in this area.

As is evident above, there is significant emphasis at national laboratories on the relation of simulations to ‘real’ materials that were not specifically raised in the survey of the universities. This can likely be attributed to the often very close ties of national-lab research to engineering problems.

3.2. Perspectives from industry

Dr John Allison of Ford, Dr Clifford Bampton of Boeing and Dr Charles Kuehmann of QuesTek Innovations, Inc. contributed to this section via survey and interview. Understandably, industry’s needs are somewhat different from those of academic research or national laboratories. These employers often focus on development and research with short-term goals. Furthermore, there is increasing economic pressure on companies to downsize their research divisions and outsource research and development either to academia or to companies specialized in research. In addition, there is a significant variation in how extensively computational methods are used in their research. All these factors induce a wide range of responses. Nevertheless, we have attempted to extract the essential points below.

From the respondents’ points of view, these skills were valuable for those who pursue computational MSE in a research and development setting.

- *Model building ability.* If one is involved with developing a simulation, the first step is examining the model and the physical assumptions. He/she needs to be able to choose the modelling approach. This can be classified under (1) of the framework introduced in section 2.5.
- *Optimization ability.* They need to select optimal methods to design a code that is numerically efficient and robust. This aspect belongs to (2) in the framework of the previous section.

- *Validation ability.* They need to be able to examine the models and programmes for accuracy. There are two components to this: one is the applicability of the assumptions made in the model, and the other is ensuring the accuracy of implementations into computer codes. They should be familiar with the general approaches in these tasks. Sensitivities to input parameters should also be characterized. This point is a part of (3) in the framework above.

Although these points above have some features in common with the perspectives of the national laboratory respondents, there was a more definite emphasis on robustness and validation. Such aspects are very important when a software product must be sold to and used by end-users.

4. Recent changes to advance computational materials science

Integrating changes in curriculum is a challenging task. In many cases, implementation must be carried out gradually over a period of time. However, the most difficult step is often the initial step of installing the first course that focuses on computational methods. In this section, we outline approaches reported by universities.

The first step usually occurs with the hiring of faculty members in the area of CMS. Once a CMS researcher joins the faculty, an addition of a computational course seems to follow naturally, especially at the graduate level. The early implementation is typically accomplished by (1) a new advanced course focused on a certain aspect of computational materials science offered upon the arrival of a new faculty member in the field and/or (2) integration of computational aspects or shift of focus within existing courses (e.g. introduction of quantum physics). As mentioned in section 2, the graduate programmes that have a computational faculty member often offer at least one regularly taught course in CMS in the area of his/her research. In the second phase, these expand organically; i.e. there are more computation based courses as the amount of computational research in the department expands, providing more coverage and choices for students.

More detailed planning and coordination for the CMS component of MSE curricula occurs when a critical mass of computationally oriented faculty members is achieved. In the third phase, systematic efforts are put in place to provide solid preparation while balancing other educational requirements. In this phase, one or more of the computation based courses may be included in degree requirements, or a concentration in computational materials science or a new degree programme with an emphasis on computational engineering may be created. Larger departments equipped with more resources are thus at an advantage in moving towards this direction. As seen in the survey, very few universities are approaching this stage, and their success will greatly affect the future direction of CMS education.

The survey was rich with examples of how CMS is being implemented into the existing curriculum. Despite its anecdotal nature, we believe that this information may be valuable to those who are involved in curriculum development. Below, we describe examples from the significant changes that have taken place and are taking place at both undergraduate and graduate levels.

4.1. Undergraduate curriculum

In section 2, we mentioned the trend of incorporating CMS in undergraduate curriculum. Here, we provide the details of progress reported in the survey.

4.1.1. Introduction of new CMS course. MIT updated the undergraduate curriculum in 2003. One outcome of the revision involved the installation of a course titled 'Introduction to Modelling and Simulation', which includes four modules based on approaches in materials science (quantum, atomistic, continuum and statistical). They also plan to introduce computer labs to 'Fundamentals of Materials Science', which includes an introduction to quantum mechanics and statistical mechanics. North Carolina State University has included a junior-level, required course titled 'Computer Applications in Materials Science'. This course introduces students to numerical analysis, numerical methods and materials modelling. Lehigh University also offers a CMS course for undergraduates, and the details of this course are compiled in a JOM-e online article [6]. Courses like these can take away some of the mystery associated with CMS and encourage students to take on opportunities in CMS. Other universities (e.g. UPenn) are also in the process of adding new undergraduate-level courses in CMS.

4.1.2. Implementation of CMS in core courses. At Northwestern, computational thermodynamic methods have been employed for a number of years in the senior-level materials design course taught by Professor Greg Olson. In addition, Northwestern has begun implementing computational tools into a series of core courses. For example, they currently have or plan to introduce 'computational labs' where DICTRA and ThermoCalc [7] are employed in sophomore courses in microstructural dynamics and thermodynamics; finite-element modelling in a junior-level course on mechanical properties; and electronic-structure codes in a junior-level course in solid-state physics. By this approach, they hope to expose students to a range of computational approaches, and the use of the software will also facilitate further learning of the subject. At the University of Michigan, the introduction of finite element simulation as a part of a junior-level Kinetics and Transport course has significantly increased the number of students who wish to use modelling and simulation in Design, which is a senior-level course. Other universities, including Georgia Tech, MIT and University of Florida, are adding CMS components to their existing courses as well.

4.1.3. Cross-departmental listing of courses. Cross-listing is perhaps one of the easiest ways of making computational courses more widely available to students. With this mechanism (1) the course description is typically listed under the departmental listing, which is read by all MSE students, and (2) it removes any unnecessary barriers for a student to take it and to use it fully towards the degree requirement. In the responses to our survey, we found UIUC to have a particularly impressive coordination of cross departmental offerings. For example, Atomic Scale Simulation Methods is listed under MSE, Physics and Computational Science and Engineering (CSE) (which is discussed below). Northwestern also has begun co-listing computational courses between Mechanical Engineering and MSE as part of a new NSF-sponsored 'Integrated Graduate Education and Research Training' (IGERT) programme in 'Virtual Tribology'.

4.1.4. Trend in basic computer programming in Engineering Education. On a negative note, one respondent reported that there is a trend towards de-emphasizing and possibly eliminating the basic programming course requirement in the undergraduate curriculum at his institution, resulting in undergraduates with a weak or no background in programming methodology that involves a rigorous logical thinking process. Since we did not include a question regarding a basic programming course requirement, we are not certain whether this is a widespread trend; our own experience is that most engineering programmes still require programming experience at some level. As pointed out above, basic programming skills are needed, for example, to pursue undergraduate research experience in CMS and may change the willingness of students to pursue computational projects well beyond their undergraduate career.

4.2. Graduate curriculum

As mentioned previously, the addition of CMS courses to the graduate curriculum is typically initiated when a new computational faculty joins a department. The courses typically reflect the instructor's own interests in this case. A few departments (notably those with multiple CMS faculty members) have taken the next step towards offering a comprehensive CMS programme.

4.2.1. Computational Science and Engineering Programmes. As an example, an interesting approach is taken by UIUC, where they offer a separate programme, CSE, which is built around computational modelling and simulation in engineering. Courses are offered within the CSE programme, as well as by other departments such as MSE, Mechanical Engineering, Aerospace Engineering and Physics, and many of them are cross-listed, as mentioned earlier. Although it is a separate programme, the platform provides a consolidated mechanism for coordinating and promoting education in the relevant fields, including CMS.

4.2.2. Impact of multiple graduate-level courses. At the University of Michigan, three graduate-level courses are now offered in the area of CMS. An increased number of course offerings naturally results in wider accessibility of the material to students. Those who take these courses often continue to use computational approaches in their dissertations, either as a main topic or to supplement experimental theses.

4.2.3. Computational software as a tool for teaching core topics. Multiple respondents mentioned their use of atomistic modelling as a useful tool for the teaching of statistical mechanics. For example, Monte Carlo simulations are ideal for teaching statistical mechanics, partially due to the simplicity of the method and the idea behind it. Using simulation also adds the element of 'learning by doing' (i.e. *active learning*) even for a topic where it is difficult to create a physical laboratory. Some computational tools, such as Cerius2 [8], were mentioned as providing excellent visualization capabilities that can help understanding [9]. There are also other excellent articles describing the experience of integrating computational tools into a course on thermodynamics and kinetics at Pennsylvania State University [10], into teaching processing and diffusion at Penn State [11] and into thermodynamics at University of Wisconsin [12].

5. Discussions and conclusions

Through surveys and discussions with leaders in the field of computational MSE, we assessed the current state of CMS education in the USA. Our findings include the following:

- Research in universities is increasingly adopting computational methods to examine various materials systems.
- Education is following the trend and adopting changes to curricula, although the efforts are understandably lagging behind the growth in research in this area.
- Many educators find that the current core curricula in engineering are in many ways inadequate to properly teach CMS topics. Specific areas that need fortification are mainly in basic and applied math as well as physics.

- National laboratories and industry clearly value CMS education, with an added focus on validation, among other points related to applications to complex engineering problems.
- Opportunities for hands-on projects in computational materials science are found to be effective as a recruiting tool for future PhD candidates.
- A computational materials science course may be a good addition to an undergraduate curriculum for those seeking a position in the materials processing industry.
- Educators may consider adopting computational materials science tools as an active learning platform in the teaching of more traditional MSE topics.
- Some universities are clearly in the process of making ambitious and important changes in their curricula that in many cases include novel integration of computational methods.

One difficulty encountered in implementing extensive changes to curricula required in the advancement of computational materials science is that the accreditation of an engineering programme requires traditional sets of course offerings, leaving limited room for new offerings. However, the *Program Criteria for Materials, Metallurgical, and Similarly Named Engineering Programs* published by the Accreditation Board for Engineering and Technology (ABET) states (italics added) the following:

> The program must demonstrate that graduates have: the ability to apply *advanced science (such as chemistry and physics)* and engineering principles to materials systems implied by the program modifier, e.g., ceramics, metals, polymers, composite materials, etc.; an integrated understanding of the scientific and engineering principles underlying the four major elements of the field: structure, properties, processing, and performance related to material systems appropriate to the field; the ability to apply and integrate knowledge from each of the above four elements of the field to solve materials selection and design problems; the ability to utilize experimental, *statistical and computational methods* consistent with the goals of the program.

In this statement, computational methods are clearly included in the accreditation criteria. Therefore, it can be argued as well that emphasizing physics-based understanding and computational basics will enhance consistency with the accreditation guidelines.

The question of how best to prepare future materials scientists and engineers remains a debatable topic. At the undergraduate level, the consensus in the current survey was an emphasis on basics such as math, physics and chemistry. However, the usefulness of students' exposure to today's computational materials science methods and applications cannot be discarded, especially as a recruiting tool for graduate studies in computational materials science. As the number of computational faculty members increases, this may become an important issue. Even though it is possible to draw candidates from other disciplines (such as physics, or mechanical or chemical engineering), the best policy for sustaining the discipline is to educate the candidates in our own discipline to succeed. In fact, there may be an increasing trend that positions that require independent research, such as university faculty positions and research positions at national labs and some industry labs, are offered to those with educational background in physics and other disciplines instead. If we desire a more well rounded background, enough to evaluate others' work and investigate a new tool if necessary, the best solution may be to create a materials science oriented physics or math course. This is, in effect, what is happening in many of the CMS courses where basic physics and mathematics are covered as a part of the course.

To our knowledge, this is the first publication to provide survey results from multiple institutions regarding the status of computational materials science education. This is only a first step. Advances in computational materials science education must be monitored periodically since the changes are occurring rapidly. Further surveys similar to that performed herein may provide a useful tool for this purpose. A formal forum where educators can gather and discuss the future direction and exchange information is also important. A symposium similar to 'The Symposium on Computational Methods in Materials Education' held during the 2003 TMS Meeting would be another useful tool that should be offered periodically, and education committees of the professional societies can help to encourage such programming. In addition, developing on-line resources that can be publicly accessed may help programmes considering implementing computational or related courses into their curricula. Helpful information includes implementation details (such as a list of courses and who takes them) and course materials such as the syllabus, notes, software, laboratory and other assignments with good documentation and a list of publications and text-books. A central clearing house for such information could have a large impact on the advancement of CMS education.

Acknowledgments

This paper was made possible by numerous people who have provided information and insights. We thank Donald Brenner (North Carolina State), Daryl Chrzan (UC Berkeley), Michael Falk (University of Michigan), Duane Johnson (UIUC), Mo Li (Georgia Tech), Jeff Rickman (Lehigh University), Tony Rollett (Carnegie Mellon), Jim Sethna (Cornell University), Susan Sinnott (University of Florida), Vaclav Vitek (University of Pennsylvania), Nicola Marzari (MIT), Matthew Krane (Purdue), Eric Hellstrom (University of Wisconsin), Peter Anderson (Ohio State) and Zi-Kui Liu (Penn State) for gathering information and responding to our survey questions. We also thank those who provided information to the people mentioned above. We thank Charles Kuehmann (QuesTek), John Allison (Ford) and Clifford Bampton (Boeing) for discussing industry's needs. James Warren (NIST), Michael Baskes (Los Alamos) and Elizabeth Holm (Sandia, Albuquerque) provided information regarding national laboratories' needs, and we appreciate their assistance. Both authors acknowledge support from the NSF under programme DMR-0102794. We also thank the editors of *Modelling and Simulation in Materials Science and Engineering* for giving us the opportunity to write this review.

Appendix A. Survey sent to universities

(i) Please list the graduate-level computational materials science courses offered at your institution. Please note whether each course is required or elective.
  (a) Are there any lab components in these courses?
  (b) What books/reading materials do you use in these courses?
  (c) What tools do you utilize in these courses?
  (d) Please list any other resources that are utilized.

(ii) Please list the graduate-level courses that have a significant component of computational materials science. Please note whether each course is required or elective.
  (a) Are there any lab components in the computational part of these courses?
  (b) What books/reading materials do you use in these courses?
  (c) What tools do you utilize in these courses?
  (d) Please list any other resources that are utilized.

(iii) Please list the undergraduate-level computational materials science courses offered. Please note whether each course is required or elective.
  (a) Are there any lab components in these courses?
  (b) What books/reading materials do you use in these courses?

    - (c) What tools do you utilize in these courses?
    - (d) Please list any other resources that are utilized.
- (iv) Please list the undergraduate-level courses that have a significant component of computational materials science. Please note whether each course is required or elective.
    - (a) Are there any lab components in the computational part of these courses?
    - (b) What books/reading materials do you use in these courses?
    - (c) What tools do you utilize in these courses?
    - (d) Please list any other resources that are utilized.
- (v) When, approximately, was the graduate/undergraduate curriculum last updated (if known)?
- (vi) Please indicate plans, if any, to increase computational materials science offerings.
- (vii) Do you allow course substitution or elective credits from math, applied math, computer science, computational/simulation courses from other engineering disciplines, etc. Please elaborate.
- (viii) What are relevant course choices for a typical graduate student who is pursuing a computational thesis?
- (ix) As a thesis adviser for students pursuing computational materials science, do you feel that current undergraduate preparation is adequate? (Please skip if you do not supervise computational projects.)
    - (a) If not, what changes would you like to see?
- (x) Similarly, do you feel that there are any gaps in the course offerings for graduate students pursuing thesis projects in computational materials science?
- (xi) At both undergraduate and graduate levels, have you observed the impact of a computational materials science course or a course with a computational component? (For example, the tools, skills or knowledge learned in the course were applied in research project, or prompted students to pursue a computational project?) Please describe.
- (xii) Any other comments are welcome.

Appendix B. Resources

The majority of resources listed here came to our attention reported by the survey respondents, and in no way should be considered complete. Any additions can be reported to KT, and the updated list can be obtained from her as well.

Textbooks and references

Allen M P and Tildesley D J 1989 *Computer Simulation of Liquids* (Oxford: Oxford University Press)
Arfken G B and Weber H J 1995 *Mathematical Methods for Physicists* (San Diego, CA: Academic)
Atkinson K 1993 *Elementary Numerical Analysis* (New York: Wiley)
Haile J M 1992 *Molecular Dynamics Simulation: Elementary Methods* (New York: Wiley)
Kalos M H and Whitlock P A 1996 *Monte Carlo Methods Volume I: Basics* (New York: Wiley)
Leach A R 1996 *Molecular Modeling: Principles and Applications* (Harlow, England: Pearson Education Limited)
Martin R M *Electronic Structure* 2004 (Cambridge: Cambridge University Press)
Newman M E J and Barkema G T 1999 *Monte-Carlo Methods in Statistical Physics* (Oxford: Oxford University Press)
Fong C Y 1998 *Topics in Computational Materials Science* (Singapore: World Scientific)
Frankel D and Smit B 1996 *Understanding Molecular Simulation* (New York: Academic)
Gaylord R and Nishidate K 1996 *Modeling Nature: Cellular Automata Simulations with Mathematica* (Santa Clara, CA: TELOS)
Gaylord R and Wellin P R 1995 *Computer Simulations with Mathematica: Explorations in Complex Physical and Biological Systems* (Santa Clara, CA: Springer-Verlag TELOS)

Liu W K, Karpov E G, Zhang S and Park H S 2004 An introduction to computational nanomechanics and materials *Comput. Methods Appl. Mech. Eng.* **193** 1529–78

McQuarrie D A 1973 *Statistical Thermodynamics* (New York: Harper and Row)

Parr R G and Yang W 1989 *Density-Functional Theory of Atoms and Molecules* (Oxford: Oxford University Press)

Press W H, Teukolsky S A, Vetterling W T and Flannery B P 1992 *Numerical Recipes in FORTRAN: The Art of Scientific Computing* (Cambridge: Cambridge University Press)

Saunders N and Miodownik A P 1998 *CALPHAD (Calculations of Phase Diagrams): A Comprehensive Guide* (New York: Pergamon)

Starfield A M, Smith K A and Bleloch A L 1994 *How to Model It: Problem Solving for the Computer Age* (Edina, MN: Burgess International Group)

Taylor J R 1997 *An Introduction to Error Analysis: The Study of Uncertainties in Physical Measurements* (Sausalito, CA: University Scientific Books)

Simulation software and tools

Unless noted, the software is publicly available through vendors.

Cerius^2: a suite of modelling/simulations tools
http://www.accelrys.com/cerius2/

CLAMPS: simulates a classical many particle system
http://web.mse.uiuc.edu/matse485/CLAMPS/index.html

DICTRA: a one-dimensional phase transformation code
http://www.thermocalc.com/

Dynamo and ParaDyn: a molecular dynamics code from Sandia National Lab
http://www.cs.sandia.gov/sjplimp/download.html has this and other software for download

GULP: General Utility Lattice Program
http://gulp.curtin.edu.au/index.cfm

IDL: a computation, data analysis and visualization tool
www.rsinc.com

MathCad: a math, modelling and visualization tool
http://www.mathsoft.com/

Mathematica: a math, modelling and visualization tool
http://www.wolfram.com/

Matlab: a math, modelling and visualization tool
http://www.mathworks.com/

PANDAT: software for multicomponent phase diagram calculation
http://www.computherm.com/

Physica+: continuum modelling code
http://www.multi-physics.com

PWSCF: calculates electronic structure
http://www.pwscf.org

ThermoCalc: calculates phase equilibria from thermodynamic databases
http://www.thermocalc.com/

VASP: calculates electronic structure
http://tph.tuwien.ac.at/vasp/

Online notes and tools

UIUC: http://web.mse.uiuc.edu/matse485

MIT Online OpenCourseWare: http://ocw.mit.edu/OcwWeb/Materials-Science-and-Engineering/

NCSA Education, Outreach and Training Division offers seminars and workshops, as well as online courses: http://www.ncsa.uiuc.edu/Divisions/eot/Training/

Other online resources

The NIST Center for Theoretical and Computational Materials Science: http://www.ctcms.nist.gov/

JOM-e: The Symposium on Computational Methods in Materials Education: http://www.tms.org/pubs/journals/JOM/0312/LiuI/LiuI-0312.html

MatHub: www.mathub.com

Materials Computation Center at UIUC: http://www.mcc.uiuc.edu/

Summer schools, summer programmes and miscellaneous programmes

Materials Research Institute Computational Materials Science and Chemistry Summer Institute at the Lawrence Livermore National Laboratory:

http://education.llnl.gov/MRI/

Summer School on Computational Materials Science

http://www.mcc.uiuc.edu/summerschool/

Industrial Mathematical and Statistical Modelling Workshop for Graduate Students

http://www.ncsu.edu/crsc/imsm/

Los Alamos National Laboratory Mathematical Modelling and Analysis Student Summer Programmes

http://math.lanl.gov/SummerPrograms/

Lawrence Livermore National Laboratory Science and Technology Education Programme

http://internships.llnl.gov/

Argonne National Laboratory Mathematics and Computer Science Division Undergraduate Programme in Computational Science

http://www-fp.mcs.anl.gov/division/information/educational_programs/undergrad-compsci.html

University of Minnesota Supercomputing Institute Undergraduate Internship Programme in Scientific Computing and Graphics

http://www.msi.umn.edu/general/Programs/uip/

UCLA Institute for Pure and Applied Mathematics Research in Industrial Projects for Students

http://www.ipam.ucla.edu/programs/rips2004/

IMA Summer Programme Mathematical Modelling in Industry—A Workshop for Graduate Students

http://www.ima.umn.edu/modeling/

References

[1] ISI Web of Knowledge: www.isiknowledge.com

[2] US News and World Report America's Best Graduate Schools 2004

[3] Allred C L, Yuan X, Bazant M Z and Hobbs L W 2004 Elastic constants of defected and amorphous silicon with the environment dependent interatomic potential *Phys. Rev.* B **70** 134113

[4] Bishop C M and Carter W C 2002 Relating atomistic grain boundary simulation results to the phase-field model *Comput. Mater. Sci.* **25** 378–86

[5] Siem E J and Carter W C 2002 The stability of several periodic surfaces *Interface Sci.* **10** 287–96

[6] Rickman J M and Vinci R P 2003 *A Computational Materials Science Course for Undergraduate Majors* JOM-e

[7] Andersson J O, Helander T, Hoglund L H, Shi P F and Sundman B 2002 THERMO-CALC & DICTRA, computational tools for materials science *CALPHAD* **26** 273–312

[8] http://www.accelrys.com/cerius2/

[9] Knapman K *Educating the Next Generation: The Role of Molecular Modeling in Teaching* http://www.mathub.com/features/education.html

[10] Liu Z-K, Chen L-Q, Spear K E and Pollard C 2003 *An Integrated Education Program on Computational Thermodynamics, Kinetics, and Materials Design* JOM-e

[11] Mohney S E, Miller A J and Gray G L 2003 *Software for Teaching Materials Processing and Diffusion* JOM-e

[12] Chang Y A and Oates W A 2003 *Our Experience in Teaching Thermodynamics at the University of Wisconsin, Madison* JOM-e