

REVIEW

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Role of cyberinfrastructure in educating the next generation of computational materials scientists

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Abstract

An overview of cyberinfrastructures developed to advance the field of materials modeling is presented. The role of cyberinfrastructures in educating the next generation of the workforce is also discussed, with an emphasis on the Cyberinfrastructure for Atomistic Simulation (CAMS). The paper concludes with a summary regarding the future outlook of cyberinfrastructures, especially with regard to education.

Keywords: Cyberinfrastructure; Material modeling; Education

Background

The last decade has witnessed tremendous growth in the development and utilization of cyberinfrastructures in a variety of science and engineering disciplines. This includes the materials modeling community, where cyberinfrastructures have been used to enable the sharing of information to advance a specific objective within a team of researchers, or within a specific community to distribute information or establish best practices. For example, the Atomic-scale Friction Research and Education Synergy Hub (AFRESH) [1] was developed to share links to computational tools, data provided by users and mined from the literature, and best practices for modeling friction with atomic-scale simulations.

Cyberinfrastructures have additionally been used to host databases generated from a particular experimental apparatus, from a computational program, and/or from published literature. Having extensive, specialized data gathered in a single location and available to other researchers is extraordinarily beneficial for subsequent material design and discovery. This has therefore been a common way in which cyberinfrastructure has been used, at least in part. For instance, the Materials Project at MIT [2] provides access to databases of material properties generated using first-principles calculations. The focus is primarily on materials for energy storage applications, although the information may be useful for a variety of applications. Another example is the AFLOWLIB [3] cyberinfrastructure, hosted at Duke University, that provides access to an extensive database of metal alloy properties and phase diagrams. AFLOWLIB also hosts databases of material properties that include structural, electronic, and thermoelectric characteristics, to name just a few.

An important use of cyberinfrastructures for computational materials science has been to give broad access to computational tools of various types. For example, in the

case of AFRESH access to tools for displaying the output of atomic-scale simulations and examples for their optimal use were provided. Additionally, both the Materials Project and AFLOWLIB allow users to carry electronic structure calculations through the cyberinfrastructure itself at computers located at the hosting institution. Cyberinfrastructures may further serve to organize and disseminate information that is critical for the optimal use of a computational method. This is exemplified by the openKIM project [4] and the NIST Interatomic Potentials Repository Project [5] that catalog interatomic potentials for classical simulations in a unique way so that they may be clearly identified when they are used. These cyberinfrastructures further host their organizational systems in a user friendly way and propagate information to the community as a whole.

An additional important application of cyberinfrastructure in computational materials science and engineering is to enhance the education of the next generation of computational materials scientists. For example, the openKIM project has held several workshops, primarily students and postdocs, about the openKIM cataloging system, including information on how to migrate potentials to the cyberinfrastructure, and to how to fully use the of the openKIM system for potential development.

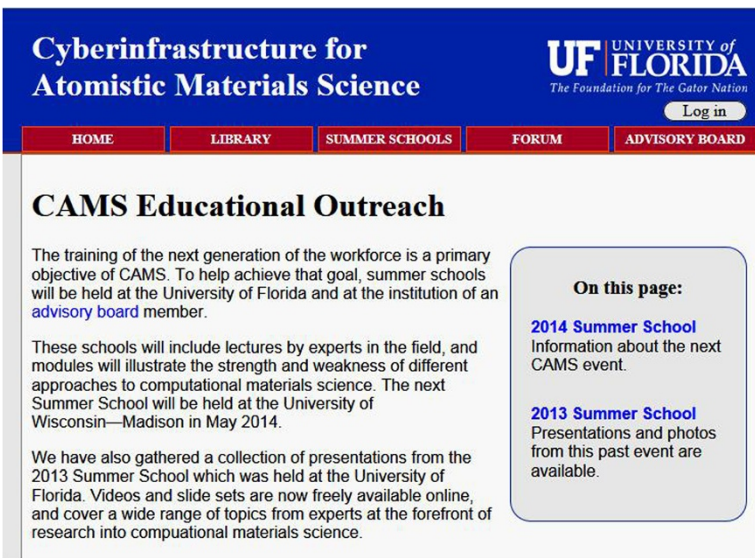
This educational role is critical and will deepen the understanding of newcomers to the field, assist them with learning to use important technical software for computing and data analysis, and provide a forum for them to share information. Educating the next generation in this manner is also a critical step to ensure the long-term viability of the cyberinfrastructure itself. Indeed, it will ultimately be this next generation who will use, maintain, and expand these platforms.

Review

The Cyberinfrastructure for Atomistic Materials Science (CAMS) [6] is a pilot-project stage platform focused on modeling materials at the atomic scale, with an emphasis on microstructural features. It fills a number of the roles discussed above. For example, it houses an actively curated “virtual library” of microstructure samples, where each sample contains the atomic-scale coordinates of a specified material microstructure. The microstructures that are featured include multiple grain boundaries, surfaces, dislocations, nanocrystalline samples, and related structures. CAMS also links to similar databases to assist the user in finding the structure of interest, reduce duplication across such libraries, and ultimately to encourage the sharing of information across platforms. Users are also encouraged to contribute samples to the CMAS library.

Importantly, CAMS is actively engaged in educational activities (see Figure 1). Part of the motivation for this is to increase use of the virtual library and to grow the number of samples that are contained within it. However, the main motivation is tied to the central mission of CAMS, which is to assist the materials community by serving as a hub for disseminating information on atomic-scale modeling and related methods, especially as they apply to microstructural features within materials. A key target constituency is the next generation of materials modelers, including students, postdocs, junior faculty, and other newcomers to the field.

To reach this audience, in spring 2013 CAMS sponsored and hosted a summer school on “Simulation of Complex Microstructure in Materials” at the University of



The screenshot shows a web page for the Cyberinfrastructure for Atomistic Materials Science (CAMS) at the University of Florida. The header features the CAMS logo and the University of Florida logo with the tagline 'The Foundation for The Gator Nation'. A navigation bar includes links for HOME, LIBRARY, SUMMER SCHOOLS, FORUM, and ADVISORY BOARD. The main content area is titled 'CAMS Educational Outreach' and contains three paragraphs of text. The first paragraph states that the training of the next generation of the workforce is a primary objective of CAMS, and that summer schools will be held at the University of Florida and at the institution of an advisory board member. The second paragraph describes the content of these schools, including lectures by experts and modules illustrating the strength and weakness of different approaches to computational materials science. The third paragraph mentions that presentations from the 2013 Summer School are available online. A sidebar on the right, titled 'On this page:', contains two links: '2014 Summer School' and '2013 Summer School', each with a brief description of the content available on that page.

CAMS Educational Outreach

The training of the next generation of the workforce is a primary objective of CAMS. To help achieve that goal, summer schools will be held at the University of Florida and at the institution of an [advisory board](#) member.

These schools will include lectures by experts in the field, and modules will illustrate the strength and weakness of different approaches to computational materials science. The next Summer School will be held at the University of Wisconsin—Madison in May 2014.

We have also gathered a collection of presentations from the 2013 Summer School which was held at the University of Florida. Videos and slide sets are now freely available online, and cover a wide range of topics from experts at the forefront of research into computational materials science.

On this page:

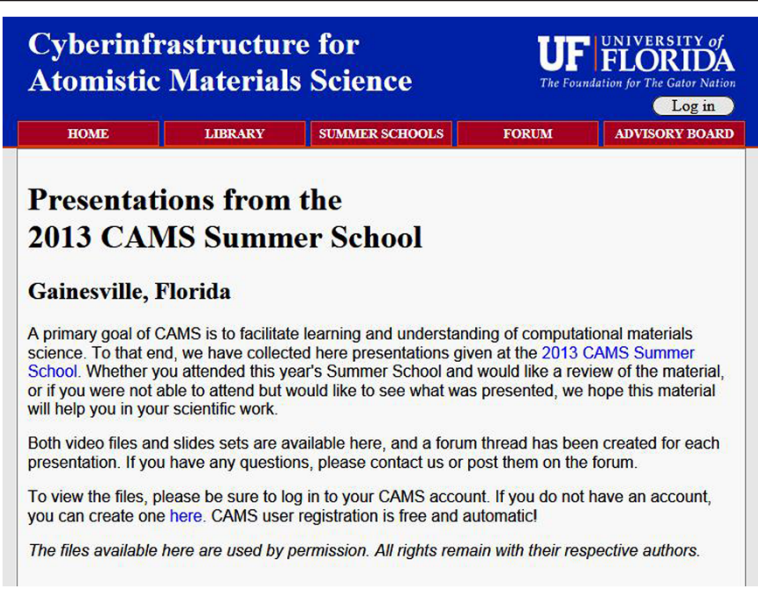
2014 Summer School
Information about the next CAMS event.

2013 Summer School
Presentations and photos from this past event are available.

Figure 1 Information page for CAMS summer school.

Florida. More than 50 participants from 20 different U.S. institutions and one German university participated. The instructors for the week-long school were computational and experimental researchers with considerable expertise from multiple U.S. academic institutions, one German university, and U.S. National Laboratories. After each presentation, participants were charged in working in groups to develop questions for the speakers. In so doing, the group members answered many of each other's questions and reinforced the learning that had taken place in the presentation. The lecturer then returned for an extended question and answer session; the questions that the groups then brought forward were sophisticated and well thought out, and thus initiated extensive and detailed further discussions. Many participants, both students and lecturers, commented on the effectiveness of this approach. In addition, the participants were given a training session on how to use and upload structures to the CAMS virtual library; they were further encouraged to contribute structures to it during and after the school. The participants presented research results from their home institution in a poster session and worked together in teams to develop research proposals based on the topics presented at the school. Awards were given to the best posters and best proposals by a panel of judges populated by a diverse mix of instructors. Lastly, the school set aside time for professional development activities, including a discussion led by a representative of the University of Florida's College of Engineering Entrepreneurship Institute, and discussions of their professional lives by a faculty member at a research-intensive institution and a staff member at a US Department of Energy National Laboratory.

The CAMS-run summer school thus contained many opportunities for technical, professional, and interpersonal development on the part of the participants. While travel grants to the participants ensured broad participation, the number of attendees was still limited by the inevitable logistical limitations of any such activity. Therefore, copies of most of the presentations and videos of most of the lectures are provided free of charge on CAMS (see Figure 2) to anyone who goes through a simple registration process. In this way, the impact of the educational effort is disseminated broadly thus further increasing accessibility.



The screenshot shows the website for Cyberinfrastructure for Atomistic Materials Science at the University of Florida. The header includes the site title, the University of Florida logo, and a 'Log in' button. A navigation bar contains links for HOME, LIBRARY, SUMMER SCHOOLS, FORUM, and ADVISORY BOARD. The main content area is titled 'Presentations from the 2013 CAMS Summer School' and is located in Gainesville, Florida. The text explains that the goal of CAMS is to facilitate learning and understanding of computational materials science, and that presentations from the 2013 CAMS Summer School are available. It notes that both video files and slides are available, and a forum thread has been created for each presentation. It also mentions that users can log in to their CAMS accounts or create one if they do not have one, and that CAMS user registration is free and automatic. A disclaimer at the bottom states that the files are used by permission and all rights remain with their respective authors.

Figure 2 Posted presentations for the 2013 CAMS summer school.

In this respect CAMS joins other, more established cyberinfrastructures that are focused on educational activities. For instance, the CAVS CyberDesign effort at Mississippi State University [7] is a comprehensive wiki site devoted to the topic of integrated computational material engineering. Specifically, this cyberinfrastructure is focused on providing access and guidance to computational materials science methods to enable their use in conjunction with design and manufacturing. Several different models are provided related to materials design and educational courses at a variety of educational institutions, highlighting the power of a cyberinfrastructure to enable the sharing of expertise and educational tools among educators. Similarly, the nanoHUB [8] based at Purdue University contains a large number of computational tools, lectures, and other resources in the area of nanoscience and nanotechnology, with a particular strength in the area of electronic devices.

Conclusions

The future of cyberinfrastructures relies on their ability to successfully meet the needs of their constituencies and to provide resources that are deemed to be valuable. Additionally, resources to sustain their maintenance and continued growth have to be available. The ability of cyberinfrastructures to utilize each other's resources is particularly key, as this will allow each one to magnify the effect of the individual effort. It is also important that they work with other, perhaps less formal, efforts in community building. Efforts such as the Materials Innovation @TMS website (<http://materialsinnovation.tms.org/>) greatly assist cyberinfrastructures to connect with one another and achieve this goal.

An example of such cooperation is the spring 2014 summer school titled "Transformational Technologies in Molecular Simulations" that will be held at the University of Wisconsin-Madison (UW). This summer school is co-sponsored by CAMS and the MaterialsHUB [9], a cyberinfrastructure focused on the development

of new theories and computational tools for the rapid calculation of material properties at the atomic scale. The UW Materials Research Science and Engineering Center (MRSEC) Interdisciplinary Computational Group is also co-sponsoring the summer school. This collaborative interaction promises a wider breadth of topics within the common focus area of interest to these cyberinfrastructures and interdisciplinary group. Ultimately, the collaboration should thus enrich the educational experience of the next generation computational materials scientists that participate in the school or access the subsequent electronically disseminated content.

The common initiatives among the cyberinfrastructures described here to catalog, curate, and distribute content from developers, users, and researchers within the field in such a way that each contributor to the cyberinfrastructure receives full credit is an important advance that, if adopted by the next generation of material modelers, will lead to a number of benefits. These include a new avenue to disseminate and to develop computational tools, to clarify the literature for everyone but especially to newcomers, and to ultimately lower the barrier for entry into the field of computational materials science by the non-expert.

The importance of materials modeling cyberinfrastructures is only expected to increase as the use of mobile electronic devices become more widespread, computational methodologies become a common approach in the material structure–property relationship toolbox, and the next generation of the workforce uses these platforms as an expected part of the modern research endeavor.

Competing interests

The authors declare that they have no competing interests.

Authors' contributions

SBS and SRP both contributed to setting up CAMS and writing the present review article. Both authors read and approved the final manuscript. Both authors did indeed read and approve the final manuscript.

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