

# Integrated Computational Materials Engineering (ICME): A “Model” for the Future?

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“The committee believes that the MSE discipline is at a critical crossroad and that computationally driven development . . . can be a core activity of materials professionals in the upcoming decades.”<sup>1</sup>

—Committee on *Integrated Computational Materials Engineering*



Integrated Computational Materials Engineering, or ICME, is an emerging discipline that was recently the subject of a National Materials Advisory

Board (NMAB) study, an excerpt from which is quoted above. TMS has been a leader in facilitating the development of this area and is in fact recognized in the recently released report for these efforts. TMS, too, is at a crossroad in determining our role in aiding further growth of ICME. In this month’s edition of “Presidential Perspective,” I am soliciting your inputs as we consider how to move ahead.

First, let me provide some context and background. ICME is an overarching approach to bridge length and time scales in computational materials science and engineering, with multiscale modeling and materials informatics being two other important approaches being actively pursued. There are many similarities between ICME and multiscale modeling, with much of the progress to date in multiscale modeling providing a good basis for ICME techniques. Typically, ICME has had an engineering focus while multiscale modeling efforts have largely been science focused. Materials informatics is much more data focused. Figure 1 illustrates the various communities and the landscape of computational MSE.

## TMS AND ICME

Recent TMS efforts have recognized the importance of all approaches to spanning length and time scales, with ICME coverage at the TMS Annual Meeting and in *JOM* including aspects of Materials Informatics and Multiscale Modeling.

How did these events within TMS begin? In late 2005, the TMS Board of Directors commissioned the Integrated

Computational Materials Engineering Technical Advisory Group, or ICME TAG, under the leadership of TMS Past President John Allison. The charge of the ad hoc ICME TAG was to provide recommendations to the TMS Board of Directors along with Technical Divisions and Committees for incorporation in the TMS Strategic Plan and execution of key initiatives.

The TAG recognized that TMS is well positioned to take a leading role in advancing ICME for the benefit of its members and the materials profession. This is because:

- TMS members are actively involved in computational modeling, both in individual components and in the integrated whole, through their professional work and in TMS technical committees with a computational focus.
- TMS has historically been at the interface between applied science, engineering, and industrial application, consistent with the stage of development of ICME.
- Bringing interdisciplinary aspects of technology to TMS members is an increasing emphasis and focus. By definition, ICME is interdisciplinary in nature.
- TMS has a history of leveraging information technology capabilities for the benefit of members.
- TMS has the heritage of strong interpersonal and professional relationships and can lead in areas where the development of communities of practice is important.

In February 2006, the ICME TAG made several recommendations to the TMS Board of Directors. Specifically, the group recommended that TMS establish a Technology Coordination Group for ICME (ICME TCG); de-

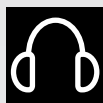


### President’s Blog

[www.tms.org/president](http://www.tms.org/president)

This month at the TMS President’s Blog Zone, readers are invited to post comments on the following questions:

- What do you see as the primary role of professional societies in engaging emerging areas such as ICME?
- Do you see computational components as critical additions to MSE education? We would especially like to hear from our university community.
- TMS is historically a collaborative society. Who do you see as candidates for cooperation in ICME?



### President’s Podcast

[www.tms.org/president](http://www.tms.org/president)

Readers can download the President’s Podcast, in which Apelian discusses the topics presented here in more detail.

velop an integrated three-year plan for information dissemination on ICME; become the professional home for the ICME community; facilitate educational development in ICME; and facilitate technical development of ICME.

In the past two years, significant activity in the ICME area has been underway at TMS. Here is a summary in a few categories.

### Technical Programming

TMS 2007 Annual Meeting symposia included:

- Integrated Computational Materials Engineering: Lessons from Many Fields: ICME in Materials Science
- NMAB ICME Town Hall Forum

TMS 2008 Annual Meeting symposia included:

- Creating the ICME Cyberinfrastructure: An Interdisciplinary Technology Forum
- Frontiers of Computational Materials Science (Sponsored by the American Physical Society—APS)
- 9th Global Innovations Symposium: Trends in Integrated Computational Materials Engineering for Materials Processing and Manufacturing
- Materials Informatics: Enabling Integration of Modeling and Experiments in Materials Science (sponsored by TMS and APS)
- Computational Thermodynamics and Kinetics

### Publication in *JOM*

In November 2006, *JOM* presented a series of papers on ICME. In 2008, the journal is planning a two-part series on materials informatics. In March, *JOM* presented part one, a series of articles that provided a broad look at materials informatics. In December, a second series of articles targeting specific materials science platforms is planned.

### Materials Technology@TMS

At the TMS 2007 Annual Meeting, TMS launched the ICME community as one of the first six pilot on-line communities of practice as part of the Materials Technology@TMS initiative ([materialstechnology.tms.org/icme/icmeHome.asp](http://materialstechnology.tms.org/icme/icmeHome.asp)).

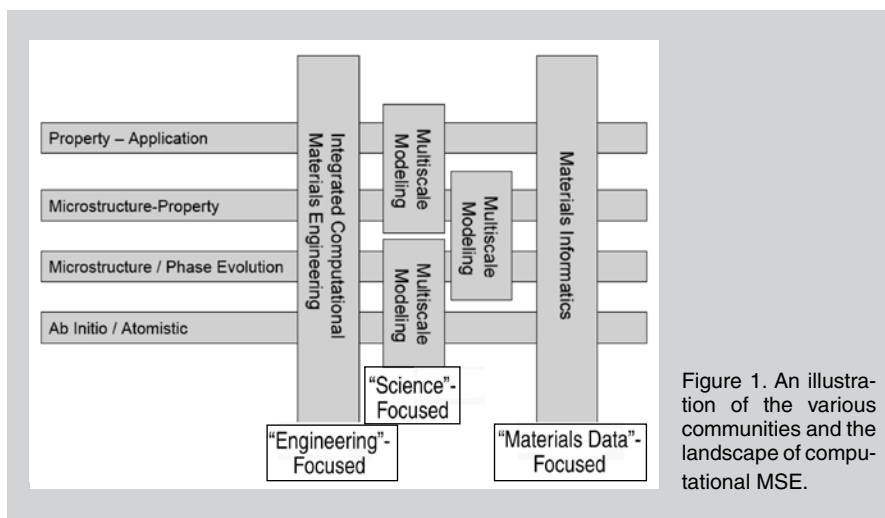


Figure 1. An illustration of the various communities and the landscape of computational MSE.

### THE NMAB REPORT

Of course, another important activity that was underway was the formation of the NMAB committee on ICME. This committee was chaired by TMS Past President Tresa Pollock with Allison acting as vice chair and included many active TMS members. It is the completion of the committee's work and publication of their findings and recommendations that serves as the catalyst for this article. The report is available from the National Academies at [www.nap.edu/catalog/12199.html](http://www.nap.edu/catalog/12199.html) as a free pdf or hard copy for purchase.

The NMAB ICME report does an excellent job of detailing the state of development of ICME, including its application in a range of areas including automotive and aerospace applications. It highlights the roles of industry, government, universities, and professional societies in advancing the area, as many reports of this type do. In my opinion, the report also goes beyond these more typical findings and recommendations in a very significant way. As the title of the report suggests, the committee sees ICME as a "transformational discipline." In fact, and to quote again from the report itself:

"For ICME to succeed, it must be embraced as a discipline by the materials science and engineering community, leading to requisite changes in education, research, and information sharing. . . . [This would] transform the role of the field of Materials Science and Engineering to one of uniting engineering and scientific endeavors into more holistic and integrated activities."<sup>2</sup>

As an educator and one who has been involved in the field for over three decades, I believe that, as a natural evolution of computational MSE, ICME can truly transform the way materials science and engineering is learned and practiced. There are many curricular as well as pedagogical issues that need to be considered and acted upon. Accolades to the NMAB committee for a job well done; the report provides us with a vista for the future that is compelling and exciting.

The NMAB committee recognizes that professional societies like TMS will play an important role in this vision. According to the report, professional materials societies should foster the development of ICME standards and collaborative networks, support ICME-focused programming and publications, and provide continuing ICME education. These issues will be part of this summer's strategic planning discussion, as the TMS Board of Directors looks at the role of TMS in serving the broadening MSE community.

Again, I encourage you to add your voice to the discussion. I have framed some questions to start the dialogue in the "For Further Discussion" sidebar. I look forward to your point of view.

### References

1. National Research Council Committee on Integrated Computational Materials Engineering, *Integrated Computational Materials Engineering: A Transformational Discipline for Improved Competitiveness and National Security*, (Washington, D.C.: National Academies Press, 2008), pp. 1–19.
2. In Ref. 1, p. 1–7.

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