SIAM Activity Group on Computational Science and Engineering Charter Renewal Application

This CHARTER RENEWAL applies to the SIAM Activity Group on Computational Science and Engineering. The SIAM Activity Group (or SIAG) to which this renewal applies was originally formed under the aegis of SIAM on December 15, 2000 by the SIAM Council and December 2, 2000 by the SIAM Board of Trustees with its initial operating period beginning January 1, 2001 and ending December 31, 2003. Its charter has been renewed by the Council and Board twelve times thereafter.

This SIAG has 2051 members, including 1164 non-student members, as of December 31, 2023.

According to its Rules of Procedure, the objective(s) of the SIAM Activity Group on Computational Science and Engineering are to:

- Foster collaborations among applied mathematicians, computer scientists, domain scientists and engineers in those areas of research related to the theory, development, and use of computational technologies for the solution of problems in science and engineering.
- Promote and facilitate Computational Science and Engineering as an academic discipline.
- Promote computational simulation as a peer to theory and experiment in the process of scientific discovery.

Within the framework of SIAM, the SIAG will conduct activities that implement its purposes. The SIAG on CSE will undertake a number of activities, including:

- 1) Organize minisymposia at the SIAM Annual Meeting on years where there is no SIAG conference. The SIAG will organize a track of at least six minisymposia at the SIAM Annual Meeting at least once every seven years. The VP for Programs and the VP at Large will coordinate the scheduling with the SIAG Chair.
- 2) Organize a biennial SIAM Conference on Computational Science and Engineering. The SIAG will consider dovetailing specialized workshops and conferences with the SIAM Annual Meeting or other SIAG conferences. The Chair of the Conference Organizing Committee shall be either the Program Director or the Chair of the SIAG or their designee. The organizing committee must be approved by the VP for Programs at least 16 months before the conference.
- 3) With the approval of the SIAM Program Committee, the SIAG may organize special sessions at SIAM meetings, and conduct special one--- or two---day meetings immediately before or after a regular SIAM meeting. Other SIAG meetings may be organized only with the approval of the SIAM President and Vice President for Programs.
- 4) Broker partnerships between academia, industry, and government laboratories. The SIAG will seek to facilitate the establishment of academic programs in CSE to foster its development as an academic discipline. The SIAG also will facilitate the placement of undergraduate and graduate students in internships in industry and government laboratories.
- 5) Work with other societies to promote CSE. The SIAG will work with other professional societies to promote CSE. For example, SIAM and another society might organize a workshop on a topic of mutual interest. The SIAG also would attempt to increase government support for CSE through various outreach activities.

6) Disseminate information. The SIAG may publish a newsletter, offer a members' list serve or maintain a Website to facilitate the exchange of information among its members and other interested parties. SIAG meetings, workshops, and conferences may be organized only with the approval of the SIAM President and the SIAM Vice President for Programs.

The SIAG has complemented SIAM's activities and supported its proposed functions. The answers to the questions below indicate how this was accomplished and what the officers propose as the future directions for the SIAG.

List all current officers of the activity group.

Chair: Judith Hill

Vice Chair: Philipp Birken

Program Director: Edmond Chow

Secretary: Sara Pollock

1) How is the field covered by the activity group doing? Is it growing, is the focus shifting? What have been the significant advances over the last two years?

The field of computational science and engineering, involving the development and use of mathematical methods and computational techniques to solve complex problems, continues to grow and play a vital role in industry, academia, and government research facilities around the world. This growth can be attributed to many factors, including:

- Advancement in Computing Power: Advances in computing hardware, software tools that take
 advantage of that hardware, and the underlying algorithms have enabled researchers and
 practitioners to answer increasingly complex questions through modeling and simulation. More
 recently, the increase in cloud computing resources is democratizing access to compute capabilities.
- Emergence of Machine Learning and AI Methods: The proliferation of data in almost every field has
 created a demand for sophisticated machine learning methods to analyze, interpret, and derive
 insights from large datasets. The further integration of machine learning and artificial intelligence
 techniques with computational methods has opened up new possibilities for predictive modeling,
 optimization, and automation in various domains.

As a result of the above factors and others, many industries, including aerospace, automotive, pharmaceutical, finance, and energy, rely on computational methods to optimize processes, design products, and make informed decisions. This reliance drives the continually increasing demand for computational scientists and engineers which has resulted in:

- Increasing Academic Programs with CSE components: Many universities around the world are
 expanding their offerings in computational science and engineering, either through standalone
 certificates or degree programs or by integrating computational components into existing
 disciplines. This expansion reflects the rising demand for professionals with expertise in
 computational methods.
- <u>Strong Funding Support for CSE programs</u>: Government funding agencies, private foundations, and industry sponsors continue to invest significant resources in relevant applied math and computer research. Recent examples of national-scale efforts include the US Exascale Computing Project (ECP), the European High-Performance Computing Joint Undertaking (EuroHPC JU), and Australia's National Computational Infrastructure (NCI).
 - 2) How is the activity group doing? Is it remaining vibrant? Is the size of the SIAG stable or increasing? How is the SIAG keeping up with the changes in the field? How are the broader interests of SIAM reflected in the activities of the SIAG?

With 2,051 members, SIAG CSE remains the largest and one of the most vibrant SIAGs in SIAM. However, despite this vibrancy, the SIAG has experienced a 14% decrease in membership compared to two years ago. This overall decrease is due to a 17% drop in student members and a 12% drop in non-student members over the same period. While the SIAG continues to have the largest number of non-

student members amongst all of the SIAGs, we hypothesize that the emergence of new SIAGs may be impacting the student membership.

Of the 887 students, there are 237 (26%) female, 559 (65.8%) male, 4 (<1%) non-binary, 56 (6.2%) not-indicated, and 14 (1.5%) prefer-not-to-disclose members. Of the 1,164 non-students, there are 199 (17%) female, 886 (76%) male, 5 (<1%) non-binary, 48 (4%) not-indicated, and 22 (2%) prefer-not-to-disclose members. The larger percentage of females in the student member population compared to the non-student population is heartening as the SIAG strives for better gender representation in our profession.

The SIAG's biennial conference is SIAM's largest SIAG meeting. The broad interests of the SIAG are best reflected by the minisymposia submitted to its biennial conference. At SIAM CSE 2023, there was a strong representation of a broad array of science and engineering fields, including biology, biomechanics, chemistry, climate, energy, fluid dynamics, geophysics, materials, and medicine. Scientific computing, including numerical methods and their analysis, continued to be the core of the conference, but there was also a significant increase in the number of minisymposia discussing topics in data-driven techniques and machine learning. Several minisymposia addressed high-performance computing and emerging architectures, and many addressed various aspects of software, from building communities to software sustainability.

3) Please list conferences/workshops the activity group has sponsored or co-sponsored over the past two years, and give a brief (one sentence or phrase) indication of the success or problems with each.

The 2023 SIAM Conference on Computational Science and Engineering was held February 26 – March 3, 2023 in Amsterdam, The Netherlands. The SIAM CSE conference seeks to enable in-depth technical discussions on a wide variety of major computational efforts on large-scale problems in science and engineering, foster the interdisciplinary culture required to meet these large-scale challenges, and promote the training of the next generation of computational scientists. SIAM CSE23 was the first SIAM CSE conference held outside of the United States, and the first in-person conference since the beginning of the COVID-19 pandemic. Participation was extremely strong, including:

- 2,0543 registered participants (an 8.5% increase over CSE19, the last in-person CSE conference)
- 1,944 speakers in 422 minisymposia
- 6 two-part minitutorials (solicited through an open call for participation)
- 121 poster presentations
- An evening public outreach event, The Role of Mathematics in Solving the World's Main Challenges, open to the broader Amsterdam community.
- A hackathon, held in the two days prior to CSE23, focused on creating cutting-edge
 mathematical solutions to real-world problems in industry. Over 100 students, post-docs and
 early career professionals collaborated with six sponsor companies on problems of interest to
 the company.

4) Please indicate the number of minisymposia directly organized by the activity group at the last two SIAM annual meetings. When did the SIAG last organize a track at an annual meeting or meet jointly with the SIAM Annual Meeting?

Because of the number of Activity Groups, the current guidelines are that an Activity Group should organize a track about every seven (7) Annual Meetings or meet jointly with the Annual Meeting within a seven (7) meeting period.

SIAG CSE last organized a track at the 2020 instantiation of the SIAM Annual meeting. The track consisted of the following 8 CSE-sponsored minisymposia:

Advances in High-Performance Mathematical Software for Emerging Architectures - Parts I and II Nonlinear Approximation: Theory and Applications in Computational Mathematics - Parts I and II The Mathematics of Sparse Recovery and Machine Learning - Parts I and II A Deep Look at Neural Networks with Applications in Scientific Machine Learning - Parts I and II

In addition, the SIAG helped organizing committee member Hans de Sterck identify an appropriate plenary speaker representing SIAG CSE (Lars Ruthotto).

SIAG CSE anticipates next organizing a track at the 2026 SIAM Annual Meeting.

5) Please indicate other activities sponsored by the activity group, to include newsletters, prizes and web sites. Have each of these been active and successful?

Prizes. The SIAG awards two prizes biennially; these were most recently awarded in 2023.

The 2023 SIAM Activity Group on Computational Science and Engineering Best Paper Prize was awarded to Matthew J. Colbrook, Andrew Horning, and Alex Townsend. Their award-winning paper "Computing spectral measures of self-adjoint operators" was published in the SIAM Review in 2021. The authors were recognized for the work in developing a robust algorithm for computing smoothed approximations to so-called spectral measures associated with general self-adjoint operators. Among many other things, they used the algorithm to compute a high-resolution picture of a Hofstadter butterfly from a magnetic tight-binding model of graphene.

The 2023 SIAM Activity Group on Computational Science and Engineering Early Career Prize was awarded to Kaibo Hu. Kaibo was recognized for his contributions to the finite element exterior calculus, particularly structure-preserving numerical algorithms for magnetohydrodynamics.

Additionally, two other prize lectures were hosted at CSE23. Carol S. Woodward, Cody J. Balos, Peter N. Brown, David J. Gardner, Alan C. Hindmarsh, Daniel R. Reynolds, and Radu Serban were awarded the 2021 SIAM/ACM Prize in Computational Science and Engineering. Devin A. Matthews and Field G. Van Zee were awarded the James H. Wilkinson Prize for Numerical Software.

<u>Member Communication</u>. The Engage platform continues to be the primary means of communication with and between the broader CSE SIAG. In 2023, there was approximately one email on average each day. The list remains largely unmoderated except when a SIAG CSE member has never interacted with Engage in any community. We encourage the following types of postings to the mailing list: solicitations

for SIAG CSE-sponsored conferences, announcements of CSE-related conferences/events, calls for nominations of prizes, software, open positions, and SIAM announcements such as electronic publication, general conference announcements, and other news.

This year, the SIAG closed its X (formerly Twitter) account due to inactivity at the request of SIAM. Prior to its closing, the SIAG surveyed its members through a survey distributed via Engage to solicit feedback on the SIAG members communication preferences, including its use of social media. Our interpretation of that feedback was that there was not a strong desire amongst the members to receive SIAG information via social media in any form. In particular, there was significant support to divest the SIAG of an affiliation with X (formerly Twitter). A copy of the feedback that we received is attached to this report.

Finally, in 2022, the SIAG migrated its web presence from the difficult-to-maintain wiki webpage to a github-based webpage (https://github.com/SIAGCSE and https://siagcse.github.io). The current officers updated the website at the beginning of their term.

6) What activities are planned and proposed for the next period of the charter? Please describe scheduled and suggested future activities in detail.

White paper on Software and Career Advancement. SIAG CSE, together with SIAG SC, is commissioning a white paper on Software and Career Advancement. We hope that such a white paper would help "move the needle" for software development to be more recognized as a scholarly and impactful activity that should be recognized by tenure and promotion committees and other people who are responsible for evaluating their staff for their technical contributions. Among many things, the white paper could discuss how to evaluate a software contribution, i.e., what constitutes a valuable intellectual product, and best practices for engaging with decision-makers. We have discussed this white paper idea with certain SIAM leaders and have their support. Once the white paper is completed, we hope to be able to use SIAM channels to help disseminate the report to administrators and other decision-makers.

SIAG CSE and SIAG SC developed a list of potential contributors to the white paper. From this list, we selected and approached a potential Chair to lead the team on the research and writing of the paper. The potential Chair has indicated an interest, and we anticipate that he will accept. SIAG CSE and SIAG SC will help him develop a diverse set of coauthors. We hope the project will be well underway by the end of the year.

<u>Outreach to SIAG CSE members.</u> SIAG CSE has discussed many ways to better connect members of the SIAG CSE community. One way is to help members self-organize into reading groups that could meet online or in person. The reading groups could be an attractive way to learn about recent developments, for example in machine learning, or tools useful for machine learning. Industrial members and students would be good combinations for a study group, where students can meet potential role models and industrial members can recruit from among the students.

We have started this effort in a small way and hope to scale up soon. Sara Pollock (SIAG CSE Secretary) and the SIAM student chapter at her institution advertised through Engage the opportunity for a group

meeting. We are currently experiencing difficulties using Engage to reach all our members. Once this is fixed, we will further seek student chapters to organize study groups open to anyone in the CSE community. We also anticipate asking for curated reading lists from among our members that could be adopted for the study groups.

<u>Updating information about CSE educational programs.</u> Through the Engage platform, we plan to ask members to submit information about CSE educational programs. We will use this information to update/add educational program information on our website.

Consolidating web information. SIAG CSE currently has three resources on the web:

- https://siagcse.github.io/ (managed by the SIAG)
- https://www.siam.org/membership/activity-groups/detail/computational-science-and-engineering (managed by SIAM)
- http://wiki.siam.org/siag-cse/index.php/SIAG-CSE:Community Portal (outdated)

There is some overlap between these three resources and some of the information, especially in the third resource above, is outdated. We wish to discuss with SIAM how to present a more unified web presence for SIAG CSE. In particular, we wish to understand how to control the wiki.siam.org resource and whether it should be merged with our siagcse.github.io resource.

Prizes. Prizes: The SIAG currently has open calls for its two aforementioned prizes. Assuming sufficient nominations, both prizes will have presentations at CSE25. Additionally, SIAM has seemingly formalized the move of other SIAG-relevant prizes to have prize lectures at the SIAG's biennial conference. The 2023 James H. Wilkinson Prize for Numerical Software was awarded at CSE23. The 2023 SIAM/ACM Prize in Computational Science and Engineering was also awarded at CSE23 and will be awarded at CSE25. The 2025 James H. Wilkinson Prize for Numerical Analysis and Scientific Computing will be awarded at CSE25. And the newly formed Ivo & Renata Babuška Prize will be awarded at CSE25. Formalizing these awards at CSE conferences is excellent for planning purposes and to increase the visibility of the awardees. One potential downside is that it may be more difficult for the SIAG to start new prizes (which members often inquire about, given the size of the SIAG) as more of the SIAG's conference footprint is prefilled.

<u>CSE Conference Planning.</u> Because of the size and parallelism of the biennial CSE conference, the SIAG in cooperation with SIAM, moved to a longer planning period for the CSE conference to allow SIAM to site the conference earlier. As a result of this, the planning for CSE25 is well underway and the siting of CSE27 is nearly complete. Given the large participation in CSE23, the SIAG is planning for CSE29 to be located internationally and expect the siting process to begin early in the term of the next slate of SIAG officers.

7) How can SIAM help the activity group achieve its goals?

<u>Facilitating better communication between SIAG members.</u> Notwithstanding the recent problems with members getting unsubscribed from receiving digests from SIAM Engage during the SIAM membership renewal process, we feel that the Engage platform needs improvement. It is not very inviting for

communication and discussion between members. For example, Engage is not integrated with SIAM News, thus commenting on a SIAM News article requires a different login. Also, it does not further self-organization of members into sub-groups within the SIAG. Communication is either to the entirety of the SIAG or individuals must take a conversation "off-line" which is not useful for book club or discussions groups that we envision. Finally, as mentioned above, we wish to streamline the web presence of the SIAG and invite a discussion with SIAM on the deprecation of the SIAG wiki space.

Improving communication between SIAG and SIAM. To reach our mutual goals, we wish for better communication between SIAM and the SIAG. The communication works well when it comes to specific tasks such as the organization the SIAM/CSE conference or the formation of the SIAG prize committees. However, for more forward-looking or strategic activities, there is opportunity for better engagement between the SIAG and SIAM. For example, we only recently learned of the commissioning in 2023 of a Task Force and its subsequent 2024 report on the Future of Computational Science. This is an activity to which the SIAG has a keen interest in and in which the SIAG is a stakeholder. There is opportunity for increased communication with SIAM as an organization. We recommend having a twice-yearly meeting between the SIAG and SIAM leadership or staff to discuss current SIAM and SIAG activities related to computational science and engineering topics, next steps, and opportunities for feedback and participation. We believe this is particularly important in the coming term as we seek to promote the proposed white paper on Software and Career Advancement and would value SIAM's help, potentially engaging with the SIAM Committee on Science Policy.

8) How can the activity group help SIAM in its general role of promoting computational science and engineering?

The scope of this SIAG is intentionally very broad and intersects with many different topics related to other SIAGs. For example, CSE practitioners leverage linear algebra, uncertainty quantification, optimization, discrete mathematics and algorithms, data science and supercomputing to solve physics-based application problems. SIAG CSE enables experts from these many areas to come together to share research and software and build new collaborations that promote scientific discovery. We wish to continue to look for opportunities to further connect these diverse sub-groups of SIAM members and to discuss questions of interest. As described above, SIAG CSE, together with the SIAG on Supercomputing, has started the process of writing a white paper on the importance of valuing scientific software development in academic career promotion. We believe this is an important gap that may impact the future of computational science and engineering education.

We also believe it is time to revisit the state of education in computational science and engineering, particularly as the intersection of CSE and the burgeoning machine learning/AI curricula. These two can be strongly dependent on one another. The emergence of new courses and programs in AI/ML and data science may come at the expense of education in computational mathematics, scientific computing, and modelling and simulation. This SIAG is well placed to spark discussion on this topic and is undertaking an update the current list of Computational Science and Engineering programs on our website (http://wiki.siam.org/siag-cse/index.php/List_of_CSE_Programs). In addition, we believe that promoting the role of software development in the academic promotion process will benefit the broader

community by recognizing the impact of mathematical software and encouraging more computational scientists to pursue academic careers.

This SIAG requests that the SIAM Council and Board of Trustees renew its charter for a two-year operating period beginning January 1, 2025.

Signed,

Gudth CLLU Judith Hill

May 1, 2024

SIAM CE SIAG social media poll results

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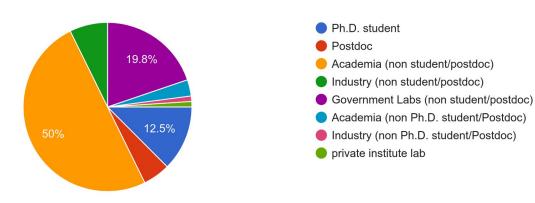
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Employment information

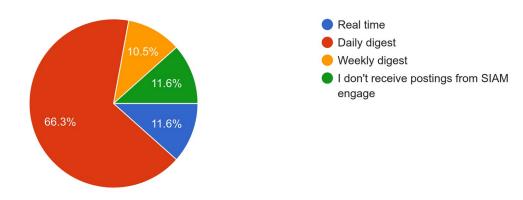
Current employment

96 responses

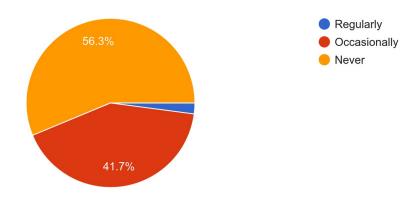


SIAM Engage

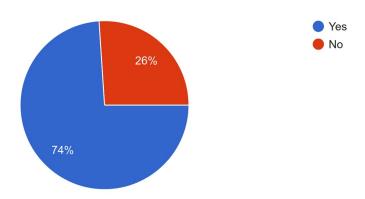
I subscribe to CSE postings on SIAM engage 95 responses



I have posted announcements on SIAM engage 96 responses

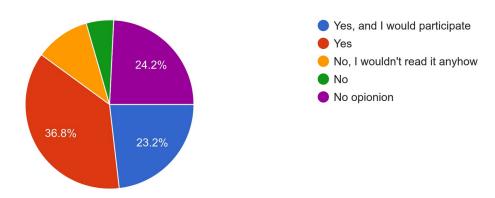


I have connected with useful information on SIAM engage in the past year $_{\rm 96\,responses}$

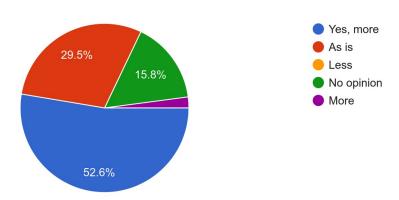


Online discussions and information within the SIAG

I would like to see more online discussions about CSE topics within the SIAG $_{\rm 95\,responses}$

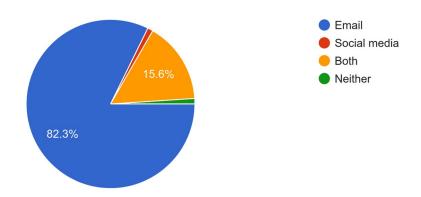


I would like to see more information about CSE topics from the SIAG in SIAM News 95 responses

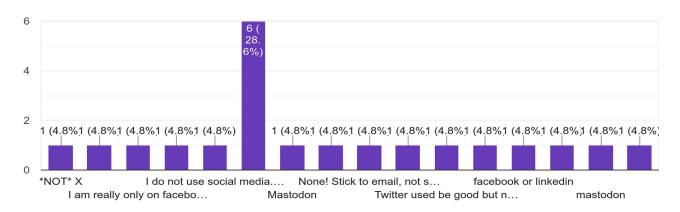


Social Media

I would prefer to receive information from the CSE SIAG via 96 responses

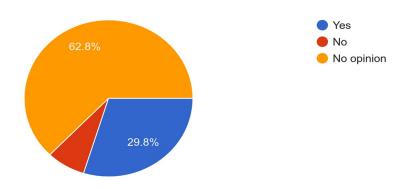


Optional: Do you have a suggested social media platform for the SIAG? 21 responses



I would like the SIAG to do more outreach on CSE topics towards non SIAG members on social media

94 responses



Additional comments and suggestions

Prompt: We welcome any additional comments or suggestions you may have!

I wasn't that aware of the engage platform until recently. Maybe there could be a targeted email or postcard to make members aware of the engage platform and its features

Hold more in-person events. They're more beneficial than online sessions, emails, or social media interactions.

I find the focus of CSE at SIAM (conferences, journals, etc) is often on new numerical methods/tools. And not so much on finding solutions to problems in engineering where one potentially might use a combination of known techniques to tackle a real-world problem. So the focus seems to be less on the E in CSE. This has discouraged me from engaging more with the community such as attending conferences or submitting to SISC.

(I just filled this survey out a minute ago without realizing that SIAM Engage means the SIAM emails that I get. So I am re-submitting since I do receive and benefit from those.)

I view Engage as a mailing list (and liked it better when I could send direct emails to CSE's mailing list). I wish that SIAM would do more to support its SIAGs.

Please seperate about postdoc job posting or position annoucement from every SIAM email-list. Currentry I have receiving several SIAM Email-lists which contain the same those things. Or I hope those job postings should be on the Web.

more engagement with members

Better outreach to students and early career.

I would appreciate having a SIAG speaker series (in person + online). The format would be monthly long-form talks (online) and an annual summary minisymposium at SIAM AN. Invited speakers would be expected to speak at both events.

I'm pretty happy as things stand, but open to change.