

SIAM Activity Group on Computational Science and Engineering Charter Renewal Application

This CHARTER RENEWAL applies to the SIAM Activity Group (SIAG) on Computational Science and Engineering (CSE). The 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.

SIAG Statistics:

- This SIAG has 2751 members, including 1442 student members as of December 31, 2019.
- Of the non-students, there are 186 female, 1056 male, and 1 non-binary member of this SIAG.
- Of the non-students, there are 902 domestic members and 407 international members.

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

- Fostering 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.
- Promoting and facilitating Computational Science and Engineering as an academic discipline.
- Promoting 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. Its proposed functions are

- Organizing a biennial SIAM Conference on computational science and engineering. A Chair of the Conference Organizing Committee shall be the Program Director, the immediate past Program Director, the Chair of the SIAG, or their designee. The organizing committee must be approved by the VP for Programs at least 26 months before the conference.
- SIAG CSE Early Career Prize: The SIAG CSE Early Career Prize is awarded to an outstanding early career researcher in the field of CSE for distinguished contributions to the field, within seven years of receiving a PhD or equivalent. The candidate's work must be a significant research contribution to the development and use of mathematical and computational tools and methods for the solution of science and engineering problems. The prize is awarded every second year at the biennial SIAM Conference on Computational Science and Engineering. The first award was made in 2017.
- SIAG CSE Best Paper Prize: The SIAM Activity Group on Computational Science and Engineering Best Paper Prize is awarded every two years to the author(s) of the best paper, as determined by the prize committee, on the development and use of mathematical and computational tools and methods for solving problems that may arise in broad areas of science, engineering, technology, and society. The prize recognizes a paper that makes an outstanding and potentially long-lasting contribution to the field. The selection criteria emphasize multidisciplinary work opening new areas of research, and potential broad impact, in addition to novelty, creativity, and overall scientific advancement and quality. The first award was made in 2019.
- Organizing minisymposia at the SIAM Annual Meeting on years when there is no SIAG conference.
- Organizing 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.

Other activities can include

- Organizing special sessions at other SIAG conferences and conducting special one- or two-day meetings immediately before or after the SIAM Annual meeting. Such SIAG meetings may be organized only with the approval of the SIAM President and Vice President for Programs.
- Brokering partnerships between academia, industry, and government laboratories. The SIAG can facilitate the establishment of academic programs in CSE to foster its development as an academic discipline. The SIAG also can facilitate the placement of undergraduate and graduate students in internships in industry and government laboratories.
- Working with other professional societies to promote CSE. For example, SIAM and another society might organize a workshop on a topic of mutual interest.
- Disseminating information. The SIAG may publish a newsletter, offer a members' mailing list 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 SIAM's proposed functions. The answers to the questions below indicate how these activities were accomplished and what the officers propose as the future directions for the SIAG.

1. List all current officers of the activity group.

Chair: Karen Devine

Vice Chair: Suzanne Shontz

Program Director: Stefan Wild

Secretary: Judith Hill

2. 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 continues to grow and play a vital role in industry, academia and government research facilities across the globe. The US DOE Exascale Computing Project, for example, includes researchers at all US National laboratories and many universities in an effort to make exascale computing a reality for real applications (energy, science, health, cyber security) by 2021.

The European Extreme Data and Computing Initiative, part of the EU's Horizon 2020 program, brings together researchers in extreme-scale hardware, programming languages, numerical solvers, and multiphysics applications to enable better policy decisions and industrial innovation; the follow-on Horizon Europe program was endorsed by the European Parliament in April 2019. More than eighteen countries are represented in the top 100 entries of the November 2019 Top500 Supercomputer list. Clearly, computational science and engineering is an international phenomenon.

The ongoing COVID-19 pandemic demonstrates the multi-faceted international impact that computational science can have on medicine, logistics, and policy making. Computational science is being used across the world to estimate pandemic spread, predict hospital usage, simulate proteins to understand corona virus' infection of cells, sequence the SARS-CoV-2 genome, identify potential drugs to treat patients, and understand and learn from clinical data in the hope of finding a vaccine.

3. 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 2751 members, the SIAM CSE SIAG remains one of the largest, most vibrant SIAGs in SIAM. Since 2015, the SIAG's membership has increased more than 20%. Student membership has increased nearly 25%.

The SIAM CSE 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 2019, traditional scientific computing areas such as simulation of astrophysics, biological systems, climate, fluid dynamics, chemistry and materials were strongly represented. Numerical methods, especially those for emerging computer architectures like GPUs processors, were also strongly represented. New interest in machine learning for scientific computing was reflected in numerous sessions; topics ranged from use of machine learning as a complement to simulations, to computational methods for machine learning, to the mathematical foundations of machine learning. Invited speakers from around the world talked about physical simulations, computational challenges of emerging platforms, and machine learning methods for problems in medicine, climate, renewable energy, and environmental science. Recent CSE conferences have

expanded diversity, education, and outreach efforts through Broader Engagement mentoring programs, and career fairs.

4. Please list conferences/workshops the activity group has sponsored or co-sponsored over the past three years, and give a brief (one sentence or phrase) indication of the success or problems with each. The SIAG [CSE] organizes the biennial conference on CSE.

The 2019 SIAM Conference on Computational Science and Engineering was held February 25-March 1, 2019, in Spokane, WA.

- 1895 attendees (10% increase over SIAM CSE17)
- 401 Minisymposia; 21 contributed paper sessions; six panel sessions; eight invited speakers; four minitutorials; two poster sessions
- One-day career fair; student career sessions; Broader Engagement mentoring program
- Inaugural SIAM CSE Best Paper Award

5. 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.****

SIAM CSE organized a track at the 2019 International Congress on Industrial and Applied Mathematics, at which SIAM held its 2019 annual meeting. The track consisted of 21 CSE-sponsored minisymposia, eight of which were multi-part sessions.

For the 2020 SIAM Annual meeting, the SIAG helped organizing committee member Hans de Sterck identify an appropriate plenary speaker representing SIAG CSE (Lars Ruthotto).

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

The SIAM CSE Early Career award was presented to Steven L Brunton of the University of Washington. The Prize, established in 2016, is awarded to an outstanding early career researcher in the field of CSE for distinguished contributions to the field, within seven (7) years of receiving the PhD or equivalent degree. In a special award session at SIAM CSE19, Steven presented his work: "Data-Driven Discovery and Control of Complex Systems: Uncovering Interpretable and Generalizable Nonlinear Models." There were 14 candidates for this award.

The inaugural SIAM CSE Best Paper prize was awarded to Tobin Isaac, Noémi Petra, Georg Stadler, and Omar Ghattas for their paper, "Scalable and efficient algorithms for the propagation of uncertainty from data through inference to prediction for large-scale problems, with application to flow of the Antarctic ice sheet" (Journal of Computational Physics, 2015). Tobin presented the paper in a special session at SIAM CSE19. The prize recognizes a paper that makes an outstanding and potentially long-lasting contribution to the field. Eight papers were nominated for this new award.

At SIAM CSE19, eight best poster prizes were awarded; five of the awards were given to minisymposia – groups of posters sharing common themes. These awards were chosen from 55 minisymposia and 125 posters submitted to the conference.

The CSE mailing list remains an important communication method for the activity group. The CSE mailing list is open to all SIAG members, who are automatically subscribed when they join the SIAG. 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, new technical reports, papers, software, open positions, and SIAM announcements such as electronic publication, general conference announcements and other news. The list is fully moderated in order to prevent redundant or inappropriate posts. Information on the list can be found at <http://lists.siam.org/mailman/listinfo/siam-cse>.

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

Prize presentations: Because the SIAM Annual Meeting was superseded by ICIAM in 2019, the SIAM/ACM Prize in Computational Science and Engineering and the James H. Wilkinson Prize were both awarded at SIAM CSE19. Conference organizers allowed award winners to give plenary lectures, which were very well received by the audience. As a result, the SIAM CSE21 committee and SIAM agreed that these prizes should remain part of the CSE conference series and will be awarded at future CSE conferences (including CSE21).

CSE Conference planning: Because the CSE conference is now SIAM's largest conference, it requires significantly larger facilities and greater levels of organization than most SIAG conferences. Planning further in advance is needed to ensure availability of sufficient resources (venues, speakers, etc.) and enable conference organizers to learn from the experiences of past conference organizers. Thus, we have shifted the conference planning activities of the CSE Program Director to focus on the conference four years ahead. Specifically:

- The Program Director elected to serve from 20XY through 20XY+1 will plan the CSE conference to be held in 20XY+4 (rather than the 20XY+2 conference).
- The Program Director is expected to chair the 20XY+4 CSE Organizing Committee; an appropriate designee may be nominated by SIAG CSE officers and approved by SIAM's VP of Programs.
- The Program Director will work with SIAM to identify an appropriate venue for CSE 20XY+4 by the end of 20XY+1, propose co-chairs, assemble an organizing committee, and begin planning of CSE 20XY+4.
- The Program Director will participate as an observer in 20XY+2 CSE conference planning, to learn from the experiences of the CSE 20XY+2 organizing committee.

Thus, the Program Director elected for 2021-22 will organize the 2025 CSE conference. Following the existing timetable, the 2019-20 Program Director Stefan Wild is co-chairing CSE21. To transition to this new timetable, Stefan led the effort to choose a venue for CSE23; a site has already been approved by SIAM. Current SIAM CSE Chair Karen Devine will serve as co-chair of CSE23.

International representation: Roughly one-third of SIAG CSE membership works outside the United States, yet the SIAM CSE conferences have never been held outside the US. To fairly represent non-US members and increase participation in SIAG CSE globally, the 2017-18 officers proposed a six-year rotation for location of the biennial CSE conference. The proposal specifies that the conference rotate between the eastern US, the western US, and an overseas location over three occurrences of the conference. SIAM CSE19 was held in Spokane, WA, and CSE21 will be held in Dallas, TX. In 2020, SIAM granted SIAG CSE permission to solicit proposals from non-US teams willing to host CSE23. Two proposals were received, and the SIAG officers selected a proposal for CSE23 in Amsterdam, The Netherlands. The contract between SIAM and the Dutch organizers is nearly finalized. Following the rotation, we expect CSE25 will return to the western US.

Risk mitigation: The COVID-19 pandemic is presenting unprecedented challenges to all SIAM conference organizers. SIAM CSE21 is no exception. The hope is that CSE21 can proceed in a normal manner; the call

for minisymposia and presentations was released in Spring 2020. However, the organizing committee is working with SIAM on alternate scenarios for CSE21 in the case that travel restrictions or large public meeting limitations are in effect in February 2021. Such risk assessment and mitigation are a new challenge for all conference organizers going forward.

8. How can SIAM help the activity group achieve its goals?

SIAM can best help the CSE community by continuing to promote CSE through conferences, publications, and student programs. CSE methods and competence are becoming increasingly relevant for scientists in fields other than mathematics; SIAM should consider strategies to attract more members from these disciplines and integrate them under the CSE umbrella. SIAM has a strong record of offering opportunities for leadership, service, and mentoring to under-represented populations; as CSE membership is, perhaps, less diverse than other SIAGs, SIAM can help by continuing to support programs that promote diversity in the CSE community. As the CSE conference grows, the support needed from SIAM grows as well; SIAM can facilitate SIAG CSE's new forward-looking timetable and assist with risk mitigation and disruptions for both near- and far-term activities.

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

SIAG CSE intersects several topics of different SIAGs. 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. Its focus on computation advances deploying mathematical research into software tools that run on the most powerful computers in the world. As computer architectures become more complex, the software, algorithms, and expertise of SIAG CSE researchers will play an increasingly important role in mathematics, science and engineering.

The CSE conferences are large and multi-faceted, providing researchers both a broader view of current capabilities and challenges, and greater opportunities to connect with experts across the spectrum of scientific computation. SIAG CSE is eager to expand these opportunities globally, starting with CSE23 in Europe.

This SIAG requests that the SIAM Council and Board of Trustees renew its charter for a 2-year operating period beginning January 1, 2021.

Karen Devine
Chair, SIAM Activity Group on Computational Science and Engineering
June 1, 2020