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 nine times thereafter.

SIAG Statistics:

- This SIAG has 2762 members, including 1488 student members, and 1274 non-student members as of December 31, 2017.
- Of the non-students, there are 172 female and 1046 male members of this SIAG.
- Of the non-students, there are 904 domestic members and 370 international members.

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. Its proposed functions are:

- 1) Organize minisymposia at the SIAM Annual Meeting on years where there is no SIAG conference.
- 2) Organize a track of at least six minisymposia at the SIAM Annual Meeting at least once every five years. The VP for Programs and the VP at Large will coordinate the scheduling with the SIAG Chair.

Other activities can include:

- 3) 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.
- 4) 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.
- 5) 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.

- 6) 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.
- 7) 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.
- 8) SIAM/ACM Prize in Computational Science and Engineering (with ACM): The SIAM/ACM Prize in Computational Science and Engineering, established in 2002, is awarded by the Society for Industrial and Applied Mathematics (SIAM) and the Association for Computing Machinery (ACM) in the area of computational science in recognition of outstanding contributions to the development and use of mathematical and computational tools and methods for the solution of science and engineering problems. This prize is awarded at the biennial SIAM Conference on Computational Science and Engineering.
- 9) SIAG CSE Early Career Prize: The SIAG CSE Early Career 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 years of receiving the 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 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.

1. List all current officers of the activity group (including advisory board, if relevant).

Chair: Hans De Sterck, Monash University, Melbourne, Australia Vice Chair: Lorena Barba, George Washington University, USA Program Director: Suzanne Shontz, University of Kansas, USA Secretary: Karen Devine, Sandia National Laboratories, USA

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. China and Japan have five of the ten most powerful computers in the Nov 2017 Top 500 list. And Australia recently announced significant investments in next-generation supercomputers for research in medical science, engineering, geoscience, marine science, chemistry, and agriculture. Clearly, computational science and engineering is an international phenomenon. The explosion of interest in the application of data sciences to engineering and scientific computing only increases the need for the exchange of ideas enabled by the SIAM CSE SIAG.

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?

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 29%.

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 2017, 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 and vector processors, were also strongly represented. New emphasis on data analysis for scientific computing was reflected in numerous sessions on tensor decomposition and graph analytics. And an important emphasis on reproducibility and sustainability in our software products was communicated through plenary and minisymposium talks, as well as mini-tutorials on software productivity topics such as git, Jupyter, and Julia. Most important, recent CSE conferences have expanded diversity, education, and outreach efforts through Broader Engagement mentoring programs, career fairs, and even minisymposia including junior researchers such as "Model Order Reduction: Perspectives from Junior Researchers."

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. This list of conferences may be found at: http://www.siam.org/activity/cse/archive.php

The 2017 SIAM Conference on Computational Science and Engineering was held February 27-March 3, 2017, in Atlanta, GA. With 1724 registered attendees, attendance increased a moderate 2% over the 2015 meeting (which, because of ICIAM in 2015, incorporated some aspects of the SIAM Annual meeting). Some highlights include:

- 327 minisymposia and 23 contributed paper sessions on conference themes of Applications in Science, Engineering, and Industry, CSE Education, Data Analytics and Visualization, Data-Driven Modeling and Prediction, Multiphysics and Multiscale Computations, Novel Discretizations and Fast Solvers, Numerical Linear/Multilinear Algebra, Scientific Software and High-Performance Computing, Simulations on Emerging Architectures, Surrogate and Reduced-order Modeling, Verification, Validation, and Uncertainty Quantification
- Nine invited presentations with speakers from the US, Europe and Asia

- Minitutorials on software productivity practices, processes, and tools
- One-day career fair and student careers panel session with participation from 20+ laboratories, universities and companies
- Broader Engagement mentoring program to increase diversity and engagement in the community; program included funded travel, workshops, affinity groups and community events
- Poster session with regular and electronic posters, and six "minisymposteriums" (collections of related posters)
- Inaugural awarding of the SIAM CSE Early Career award
- Awards for Best Posters and Best Minisymposterium.

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.

For the SIAM Annual Meeting 2018, the following track containing four minisymposia and one minisymposterium was organized at the invitation of the activity group:

MS-1 Current topics in cardiovascular modeling and simulation

MS-32 Machine learning for Scientific Computing, Part I

MS-50 Machine learning for Scientific Computing, Part 2

MS-19 PinT – Parallel in Time Methods for Large-Scale Problems

PP-3 Minisymposterium: Current trends in mathematical modeling and simulation of problems in cardiovascular medicine

For the SIAM Annual Meeting 2017, SIAG CSE did not organize a track.

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 inaugural SIAM CSE Early Career Award was presented to Lin (UC Berkeley) at the 2017 SIAM Conference on Computational Science and Engineering. The field of nominated candidates was exceptionally strong: the committee received 14 nominations, and most of them were of very high quality. For example, the nominees who were ranked in the initial top-seven each received more than 600 citations (Google Scholar) within seven years after obtaining their PhD, and more than 200 citations in 2016. Prof. Lin's citation read: "For significant contributions to numerical methods and high-performance computational tools for materials science, enabling scalable electronic structure calculations." A selection committee has been formed for the 2019 award.

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.

The 2019 SIAM CSE Conference will be held February 25 – March 1, 2019, in Spokane, Washington. Like CSE 2015 and 2017, it will include Broader Engagement mentoring activities. Conference themes will include Computational science and machine learning; Statistical modeling, methods, and computation; Multiscale, multiphysics, and multilevel methods; High performance software: packages and design; Algorithms at extreme scales; Tensor Computations; High-order methods, novel discretizations, and scalable solvers; Data science, analytics, and visualization; Applications in science, engineering, and industry; Biological and biomedical computations; Scientific simulation and uncertainty; Numerical optimization: methods and applications; Reduced order modeling; and Emerging trends in CSE education and training.

To complement the SIAM CSE Early Career award, a new CSE Best Paper Award was proposed to SIAM in 2018. Its approval is pending. If approved, the award would first be granted in 2019. The prize recognizes a paper that makes an outstanding and potentially long-lasting contribution to the field. The selection criteria emphasize multi-disciplinary work, opening up new areas of research, and potential broad impact, in addition to novelty, creativity, and overall scientific advancement and quality.

SIAG CSE membership is heavily biased toward researchers working in the United States. To increase participation in SIAG CSE globally, the officers have proposed a six-year rotation for location of the biennial CSE conference. The proposal specifies that the conference location rotate between the eastern US, the western US, and an oversees location over three occurrences of the conference. We are communicating with senior members of the SIAG CSE community, SIAM officers and SIAM staff about details of such a strategy.

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.

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

SIAG CSE continues to be the most significant professional organization for researchers in computational science and engineering. As computation plays an increasingly important role in other fields of mathematics and applications, SIAG CSE will continue to stimulate research and collaboration with professionals in the broader applied mathematics community and beyond. And as computing architectures become more complex, the software, algorithms, and expertise of SIAG CSE researchers

will play an increasingly important role in mathematics and a wide variety of application areas in general.

Over the coming years, SIAG CSE is keen on helping to push SIAM's agenda in the area of Data Science. Data-driven Science and Discovery has quickly become an important part of the CSE research agenda, and the synergy between computational science and data science, which are each centered at the intersection between mathematics and statistics, computer science, and application domain knowledge, holds tremendous promise for cross-pollination between CSE and the emerging Data Science area. Over the past several years, SIAG CSE officers have spearheaded a new report on "Research and Education in Computational Science and Engineering" (https://arxiv.org/abs/1610.02608, to appear in SIAM Review, 2018), which, among several disruptive developments that shape a new agenda for CSE, highlights the synergies between CSE and Data Science, advocating that "the analysis of big data requires efficient and scalable mathematics-based algorithms executed on high-end computing infrastructure, which are core CSE competencies that translate directly to big data applications. CSE education and research must foster the important synergies with data analytics and data science that are apparent in a variety of emerging application areas." Along with other SIAGs with an interest in Data Science, SIAG CSE expects to provide important support to SIAM initiatives in the area of Data Science, and is interested in collaborating on this with SIAG/DMA, which is expected to coordinate most of the SIAM efforts in this area. For example, long-time members of the SIAG CSE community play leading roles in the new SIAM Journal on Mathematics of Data Science (SIMODS) (e.g., the SIMODS editor-in-chief is a recent SIAG CSE chair), and SIAG CSE is keen on supporting the organization of a new SIAM conference on the mathematics of Data Science.

This SIAG requests that the SIAM Council and Board of Trustees renew its charter for a 2 year operating period beginning January 1, 2019.

Signed,

Hans De Sterck

Chair, SIAG/CSE, 2017-2018

May 30, 2018