### SIAM Activity Group 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 eight times thereafter.

This SIAG has 2292 members, including 1156 student members, as of December 31, 2015.

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 CS&E 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 CS&E. The SIAG will work with other professional societies to promote CS&E. 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 CS&E 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.

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: Lois Curfman McInnes, Argonne National Laboratory, USA (1/1/2015 12/31/2016)
  - Vice Chair: Hans De Sterck, Monash University, Australia (1/1/2015 12/31/2016)
  - **Program Director:** Jan Hesthaven, École Polytechnique Fédérale de Lausanne, Switzerland (1/1/2015 – 12/31/2016)
  - Secretary: Suzanne Shontz, University of Kansas, USA (1/1/2015 12/31/2016)

## 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?

Over the past two decades the field of computational science and engineering (CSE) has penetrated the worlds of academia, industry, and laboratory—of research basic and applied—to advance discovery, optimize systems, support decision-makers, and educate the scientific and engineering workforce. Informed by centuries of theory and experiment, it performs theoretical experiments to answer questions that neither theory nor experiment alone is equipped to answer. Attracting scientists and engineers of all persuasions, it cross-fertilizes them with algorithmic inventions and software systems that transcend disciplines and scales. Carried on a wave of digital technology, it brings the power of parallelism to bear on troves of data. Mathematics-based advanced computing has become a prevalent means of discovery and innovation in essentially all areas of science, engineering, technology, and society; and the CSE community is at the core of this transformation. However, a combination of disruptive developments—including the architectural complexity of extreme-scale computing, the data revolution that engulfs the planet, and the specialization required to follow the applications to new frontiers—is redefining the scope and reach of the CSE endeavor. See discussion in a draft report (released in March 2015 and currently under revision) from a workshop on *Future Directions in CSE Education and Research*, organized by the 2013-14 SIAG-CSE officers (see details below).

During the last two decades, several universities in the US and abroad have started graduate and undergraduate programs in CSE. These interdisciplinary programs are currently quite diverse. The SIAG has played an important role in defining the setup and the curricula of these programs by providing a template in the form of the SIAM report on "Graduate Education for Computational Science and Engineering," Petzold et al., 2001 (see DOI:10.1137/S0036144500379745). Minisymposia on education in CSE have been held regularly at the SIAM CSE conferences to provide a forum for discussion and exchange of experiences. The draft report mentioned above discusses issues in next-generation CSE education.

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?

As of December 31, 2015, the SIAG-CSE has 2292 members, including 1156 students. SIAG-CSE membership has increased by 279 members (nearly 14%) since December 31, 2013, when the SIAG had 2013 members. Non-student membership in the SIAG increased slightly from 1129 members in 2013 to 1136 members in 2015; student membership increased from 884 (44% of SIAG members) in 2013 to 1156 (50% of SIAG members) in 2015. About 73% of non-student members are from academia, while over 14% of non-student members are from government, and 9% are from industry. Overall female membership (students and non-students) is about 15%.

One of the main activities of the SIAG is the biennial CSE conference. Through this highly active conference we keep the SIAG current to trends in the field and help foster newly emerging areas. For example, at the SIAM CSE15 conference, the invited speakers brought a range of expertise in a vast number of applications areas, from multiscale and multiphysics simulations in science, engineering, and industry to big data and extreme-scale architectures. The conference remains attractive to the membership because it invites a broad range of participation, while focusing on the advancements and impact of CSE. The attendees can showcase their work in a variety of related areas that would otherwise not interact, and they are able to see new ideas in new areas at the forefront of CSE. A variety of events at the CSE15 conference targeted students

and early-career researchers, including a job fair, a career panel, minitutorials, and an expanded poster session.

SIAM strengthens the interactions among mathematics, science, and technology. The CSE SIAG is an excellent forum for these interactions, particularly through its conference series. In the past several years, we have strived to maintain a balance on the organizing committees with applied mathematicians, computer scientists, and application scientists. This has been valuable in reaching out to different communities and ensuring the multidisciplinary nature of the SIAG.

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

**CSE15 Conference:** The SIAM Conference on CSE has seen dramatic growth since its inception in 2000. CSE15 (see <u>https://www.siam.org/meetings/cse15/</u>), held at the Salt Palace Convention Center in Salt Lake City, Utah, was in fact the largest SIAM conference to date. The 1687 registered attendees reflect a 23% increase over CSE13—and a four-fold increase since 2000. CSE15 incorporated some elements of the SIAM Annual meeting, as no annual meeting was held during 2015 due to ICIAM being held that year.

The CSE15 program offered an enormous diversity of topics across computational science and engineering. Popular themes among the 301 minisymposia included CSE software, big data analytics, physics-compatible numerical methods, high-accuracy numerical methods, and compressed sensing. Recordings of synchronized slides with audio for invited plenary speakers, featured minisymposia, and a few other sessions are available from the conference website, <u>https://www.siam.org/meetings/cse15/</u>). The *SIAM Journal on Scientific Computing (SISC)*, in conjunction with CSE15, will devote a section of an upcoming issue to the conference's two special themes: *CSE software* and *big data analytics*. There were 47 submissions to the SISC special section for CSE15. The CSE15 organizers gratefully acknowledge conference sponsorship by Intel, HP, Mathworks, Kitware, KAUST, and the University of Utah's Scientific Computing and Imaging Institute. An article in the July 2015 issue of SIAM News summarizes the meeting, including the following conference elements:

- Celebrating 15 Years of SIAM CSE, including a *featured presentation by Linda Petzold*.
- **Pilot program on Broader Engagement for CSE**, summarized in the October 2015 issue of SIAM News, organized by Sustainable Horizons Institute, a nonprofit organization founded by Mary Ann Leung, a longtime SIAM member and member of the CSE15 Organizing Committee. The inaugural cohort, which consisted of nearly 50% female and 3% American Indians/Alaska Natives, 16% Asian, 28% Black/African American, 11% multiple race, 39% white, and 31% percent Hispanic, benefitted from networking and mentoring activities at CSE15. Many participants in the Broader Engagement program were first-generation college scholars.

- Featured Minisymposia, solicited by the CSE15 organizing committee to provide overview presentations on fundamental advances in fields related to the conference themes. Featured minisymposium topics and organizers were *Big Data Analytics* (Han-Wei Shen, The Ohio State University); *CSE Software* (Hans Petter Langtangen, Simula Research Laboratory and University of Oslo); *Distributed Methods for Optimization* (Wotao Yin, UCLA); *Fast Multipole Methods Maturing at 30 Years* (Lorena Barba, George Washington University); *Modeling and Computing Complex Flows* (Gretar Tryggvason, University of Notre Dame); and *Physics-compatible Numerical Methods* (Mikhail Shashkov, Los Alamos National Laboratory).
- Hands-on Minitutorials: To promote cross-disciplinary education for both students and experienced CSE practitioners, CSE15 featured two hands-on minitutorials on the conference's special themes. *Python Visual Analytics for Big Data*, led by Jonathan Woodring (Los Alamos National Laboratory); *Lab Skills for Scientific Computing*, led by Greg Wilson (Software Carpentry Foundation, www.software-carpentry.org).
- Panel: Data Science: What Is It and How Is It Taught? summarized in the July 2015 issue of SIAM News.
- Expanded poster sessions: CSE15 introduced several features designed to make poster sessions more useful for networking and sharing ideas, and as a means to handle conference growth. Poster presenters were invited to include demos with their posters, using their laptops to demonstrate CSE simulations and software. The CSE15 poster call also included a new submission category: a "minisymposterium" (that is, a minisymposium of posters), a collection of three or more posters by different presenters with a central theme. CSE15 poster sessions included 14 minisymposteria on a broad range of themes, with 4 to 16 posters per group. An <u>online "poster sizzle" video</u> shows that CSE15 poster sessions fostered a vibrant exchange of ideas.

CSE15 organizing committee members Luke Olson, Pavel Bochev, and Tom Bartol coordinated the teams of judges who selected the recipients of poster prizes from nearly 300 candidates—a new CSE conference record. Monetary awards for poster prizes were generously sponsored by HP. Eight prizes were awarded in three categories:

- Best Poster Awards: Computational Methods to Study the Coordination of Mechanical Forces Involved in Amoeboid Cell Migration (Calina Copos, University of California, Davis); Computational Homogenization for the Modeling of Soft Matter Materials (Christian Linder, Stanford University); The Sparse Grid Combination Technique for Solving Eigenvalue Problems (Christoph Kowitz, Technische Universität München); Dolfin-Adjoint (Simon Funke, Simula Research Laboratory).
- Best Minisymposterium Awards: Scalable Finite Element Assembly, chaired by Irina Demeshko and Eric Cyr (Sandia National Laboratories), 7 posters by various presenters; CSE Software, chaired by Anders Logg (Chalmers University of Technology), 16 posters by various presenters.
- Best Poster Design and Presentation Awards: Finite Element Methods for the Evolution Problem in General Relativity (Vincent Quenneville-Belair, University of Minnesota); Inducing Approximately Optimal Flow Via Truthful Mediators (Ryan Rogers, University of Pennsylvania).

Workshop on Future Directions in CSE Education and Research. As a major initiative to explore future CSE directions, the 2013-14 SIAG-CSE officers (U. Rüde, K. Willcox, L.C. McInnes, and H. De Sterck) organized a workshop on Future Directions in CSE Education and Research, held August 4-6, 2014, in Breckenridge, Colorado, USA. This invitation-only workshop, sponsored by SIAM and the European Exascale Software Initiative (EESI), focused on future directions in CSE education and research in light of recent advances in highperformance computing and CSE application areas. The workshop brought together leaders in the CSE field to update the SIAM report on "Graduate Education for Computational Science and Engineering," Petzold et al., 2001 (see DOI:10.1137/S0036144500379745). Workshop discussions included possible new strategies and new directions for the CSE discipline—both in education and in research—in light of new disruptive developments that include extreme-scale challenges, big data/big computing, and a significant broadening of the application fields of CSE and that are redefining the scope and reach of the CSE endeavor. As a first step in collecting material, participants were requested to submit a two-page position paper prior to the meeting. An outcome of the workshop was a consolidated draft document that was posted on the CSE wiki and presented in a minisymposium at CSE15, which included discussion and feedback from the community. The workshop organizers are currently revising the draft report to address community input and will provide an updated version later in 2016. We anticipate that the outcomes of this workshop will help to guide the further development of the CSE field and the SIAG's focus and activities over the coming decade.

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.\*

SIAG-CSE organized a MS track with five sessions during the 2014 SIAM Annual Meeting; we did not organize a MS track during 2015 or 2016.

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?

**Proposed SIAG-CSE Early-Career Prize in Computational Science and Engineering,** Current SIAG-CSE officers submitted a proposal to SIAM in February 2016 for a *SIAG-CSE Early-Career Prize in Computational Science and Engineering*, in recognition of an individual who has made outstanding contributions to the development and use of mathematical and computational tools and methods for the solution of science and engineering problems, within 7 years of receiving the PhD or equivalent degree as of January 1 of the year of the award. We proposed that the prize be awarded every second year (starting in 2017) at the biennial SIAM Conference on Computational Science and Engineering. The award would consist of a certificate containing the citation; there would be no cash award. As of the time of submitting this charter renewal document, the proposed prize is still under consideration by the SIAM Major Awards Committee, who are also considering several other early-career prize proposals. In order to meet the timeline of selecting the prize recipient at least 6 months prior to the proposed award date at CSE17 (March 2, 2017), we need to move ahead rapidly with revisions to the award proposal (to address feedback from SIAM), so that we have sufficient time to announce the call for nominations and establish the prize committee.

The other activities sponsored by the activity group include the CSE mailing list, a SIAG Wiki, and articles in SIAM News, SIAM Review, and the SIAM Blog.

**CSE Mailing List.** 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.

**SIAG Wiki.** The CSE SIAG established a Wiki where information relevant to the field can easily be exchanged. Appropriate material for posting includes listings of upcoming meetings of interest to the field, presentation slides from CSE meetings, links to external relevant pages, business meeting notes, etc.

**SIAM News.** The following SIAM News articles (coordinated by G. Corbett, H. De Sterck, and L.C. McInnes) covered topics of the CSE15 Conference:

- <u>Unprecedented Turnout in Salt Lake City as CSE Conference Marks 15th Year</u>, Lois Curfman McInnes, Hans De Sterck, and Chris Johnson, SIAM News, July-August 2015
- *Data Science: What Is It and How Is It Taught?*, Hans De Sterck and Chris Johnson, SIAM News, July-August 2015
- <u>BGCE Prize Finalists in the Spotlight at CSE15</u>, Hans-Joachim Bungartz, Ulrich Rüde, Regina Ammer, and Tobias Neckel, SIAM News, July-August 2015
- <u>Tensor Decompositions in Smart Patient Monitoring</u>, Sabine Van Huffel, SIAM News, September 2015
- <u>Life is a Tensor: Pilot Program Aims at Expanding SIAM Impact</u>, Silvia Crivelli and Mary Ann Leung, SIAM News, October 2015

Additional CSE-related articles in recent issues of SIAM News include:

- <u>*Periodic Table of the Finite Elements*</u>, Douglas Arnold, Anders Logg, SIAM News, November 2014
- <u>A Role for Modeling, Simulation, and Optimization in an Agricultural Water Crisis</u>, Eleanor Jenkins, Kathleen Fowler, SIAM News, December 2014
- <u>Computational Surgery: A Transdisciplinary Approach to Improved Patient Care</u>, Thierry Colin, Marc Garbey, Olivier Saut, SIAM News, May 2015
- New Mathematics for Extreme-scale Computational Science?, Ulrich Ruede, SIAM

News, June 2015

- <u>Computational Sciences in the Upstream Oil and Gas Industry: The ExxonMobil</u> <u>Experience</u>, Thomas Halsey, SIAM News, September 2015
- *Data Assimilation in Numerical Weather Prediction*, Andrew M. Stuart, Sebastian Reich, SIAM News, October 2015
- <u>Applying Mathematics to Data Assimilation Methods</u>, Andrew M. Stuart, Sebastian Reich, SIAM News, November 2015
- <u>SIAM Adopts the Wilkinson Prize for Numerical Software</u>, Jorge Moré, SIAM News, November 2015
- <u>Cardiovascular Blood Flow Simulation: From Computation to Clinic</u>, Alison L. Marsden, SIAM News, December 2015
- <u>See Light Move: Compressed Sensing and the World's Fastest 2-D Camera</u>, Hans Kaper, SIAM News, March 2016
- <u>Computational Modeling of Convection in the Earth's Mantle</u>, Wolfgang Bangerth, Juliane Dannberg, Rene Gassmöller, Timo Heister, SIAM News, March 2016
- <u>Addressing Challenges in Reduced-Order Modeling</u>, Kevin Carlberg, SIAM News, March 2016
- Julia: A Fast Language for Numerical Computing, Alan Edelman, SIAM News, March 2016
- <u>New Initiative Focuses on Computational Science and Advanced Computing</u>, Miriam Quintal, SIAM News, March 2016
- <u>Pushing the Boundaries of Predictions with Data Analytics</u>, Randy Paffenroth, SIAM News, April 2016

SIAM Review. Recent CSE-related articles in SIAM Review include:

- A Survey of Projection-Based Model Reduction Methods for Parametric Dynamical Systems, Peter Benner, Serkan Gugercin, and Karen Willcox, SIAM Rev, 57-4 (2015), pp. 483-531, DOI: 10.1137/130932715.
- *Composing Scalable Nonlinear Algebraic Solvers*, Peter R. Brune, Matthew G. Knepley, Barry F. Smith, and Xuemin Tu, SIAM Rev, 57-4 (2015), pp. 535-565, DOI:<u>10.1137/130936725</u>.
- *IFISS: A Computational Laboratory for Investigating Incompressible Flow Problems*, Howard C. Elman, Alison Ramage, and David J. Silvester, SIAM Rev 56-2 (2014), pp. 261-273, DOI:<u>10.1137/120891393</u>.

**SIAM Blog.** SIAG-CSE is also preparing to coordinate contribution of articles on a quarterly basis to the SIAM Blog, with the first article planned to be announcement of the new CSE Early-Career Prize (after the award revision and approval process concludes).

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

**CSE17 Conference:** Plans for the CSE17 Conference are underway. The conference co-chairs are Clint N. Dawson (The University of Texas at Austin, USA); Jan S. Hesthaven (Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland); Xiaoye Sherry Li (Lawrence Berkeley National Laboratory, USA), and Wil H.A. Schilders (Technische Universiteit Eindhoven, Netherlands), and the conference will be held at the Hilton Atlanta in Atlanta, Georgia, USA, during February 27 – March 3, 2017 (http://www.siam.org/meetings/cse17/). The organizing committee and invited speakers represent an interdisciplinary mix of computational science expertise, including applied mathematics, computer science, and domain sciences.

CSE17 will continue with some elements introduced during CSE15: increased emphasis on poster sessions, including demos, thematic groups of posters, and poster prizes; increased profile of the awards ceremony; featured minisymposia; and minitutorials related to the conference themes. The CSE conference series is on a very successful track, with significant growth in participation over the past years. The goals of the conference elements described above are (1) to raise the profile of poster presentations as a mechanism to handle potential conference growth (with poster blitzes and poster sessions as part of the daytime program), and (2) to provide conference attendees with additional rallying points (featured minisymposia, minitutorials) in addition to the traditional minisymposia and invited plenary talks.

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

SIAM can best help the CSE community by continuing to promote CSE and to encourage increased funding from federal agencies that traditionally have had difficulty supporting the interdisciplinary research that is essential to CSE. CSE methods and competence are becoming increasingly relevant for scientists in fields other than mathematics. These include physics, chemistry, computer science and various engineering disciplines, to name just a few. SIAM should consider strategies to attract more members from these disciplines and integrate them under the CSE umbrella.

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

SIAM continues to be the professional society for CSE. Applied mathematics is integral to the community and continues to grow. This SIAG is a medium for professionals to gain information about trends and the cutting edge of research through the CSE conference series and mailing list. As more subfields continue to emerge in CSE, we anticipate that SIAM's membership base and breadth will correspondingly expand. The CSE SIAG will continue to foster research in new areas and to support growth in related subfields. Moreover, this multidisciplinary SIAG will expose a wide range of professionals to applied mathematics.

As encouraged by the prior SIAG CSE charter renewal, the SIAG is now taking an active role in identifying directions for future CSE education and research. The SIAG could also take a more active role in promoting academic activity as far as curriculum and trends. A CSE education

subgroup could be well served to help direct specific issues to the SIAM Education committee, as CSE will continue to be an area of growth in colleges and universities.

This SIAG requests that the SIAM Council and Board of Trustees renew its charter for a 2 year operating period beginning January 1, 2017.

Signed,

Wircufnan Malmos

Lois Curfman McInnes Chair, SIAG/CSE Chair, 2015-16 May 11, 2016