CHARTER RENEWAL APPLICATION

SIAM Activity Group on Computational Science and Engineering (CS&E)

This CHARTER RENEWAL APPLICATION applies to the SIAM Activity Group on Computational Science and Engineering (CS&E). The SIAM Activity Group (or SIAG) to which this renewal applies was originally formed under the aegis of SIAM on July 12, 2002 by the SIAM Council and July 13, 2002 by the SIAM Board of Trustees with its initial operating period beginning January 1, 2003 and ending December 31, 2004. Its charter has been renewed by the Council and Board once thereafter and is chartered to operate until December 31, 2006. This SIAG had 1,127 members as of December 31, 2005.

According to its Rules of Procedure, the objective(s) of the SIAG 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; and
> 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 purposed functions were to:
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.
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.
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.
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.
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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. 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 three years?

Computational science as a field continues to grow as simulation is increasingly recognized as the third pillar of science, complementing theory and experiment. As medium and large-scale computational resources become more widespread and increase in capacity, we are seeing increased activity in two areas. First, the range of activities to which computational techniques are being applied is growing. Not only are the traditional areas of physical science remaining strong, for example, physics, chemistry, material sciences, etc., new areas are being explored as well. For example, computational techniques are increasingly being applied in the biological, social sciences, and artistic domains as well. These new areas are both taking advantage of well-established techniques to make new advances in their fields and are also

pushing the boundaries of existing computational methods to increase the applicability to their domain. Second, as the capability of computational resources continues to grow so, too, must the algorithms and mathematics change to keep pace. For example, increasing the realism of simulations often now requires the representation of many different physical phenomenon and many different scales. This in turn drives the need for new mathematics to link these multi-physics, multi-scale phenomenon. Furthermore, the sheer volume of data produced by simulations requires new mathematical techniques for mining the data to gain insight into the produced solution. Finally, the largest machines of today and tomorrow have 100,000 processors or more, which requires new algorithms and methods to take us to the promise of ultra-scalable computing. Finally, there is an increasing recognition of the power of multi-disciplinary computational science teams such as those evidenced by the DOE SciDAC program. This program is widely viewed as successful and new programs and initiatives in this area will likely continue to utilize this partnership/teaming model.

There are many examples of success in computational science in the past several years. In particular, consider the DOE SciDAC program in which successes range from large scale engineering projects such as the design of a new generation of high energy accelerators and magnetically confined plasma reactors to new explorations of basic science, with the promise of explaining and understanding at a level of detailed science such phenomena as supernova explosions. None of these examples would have been made possible without input from the mathematics and computer science communities. More details of these and other successes can be found on the online proceedings of the 2005 SciDAC Conference (http://www.iop.org/EJ/toc/1742-6596/16/1).

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?

The SIAG has been and continues to do well. It was founded in 2001 and the membership grew quickly to be the largest SIAM SIAG. There are currently 1127 members and this number has remained approximately constant for the past two years. Of these 1127 members, 648 (57%) are regular members and 479 (43%) are student members. For the 542 out of the 648 regular SIAG/CSE members for whom we have information, 30% are affiliated with government or industry, as compared to 21% of all SIAM members.

The primary activity of the SIAG is the biannual CS&E conference. It is primarily through this forum that we keep the SIAG current with changes in the field. For example, at the SIAM CSE05 conference, our organizing committee and invited speakers reflected a broad range of activities in many different application areas. This allows attendees to see the full spectrum of activities being pursued in the community and also potentially identify unifying themes. In particular, one of the interesting themes that emerged from the CSE05 was the need for and current research in multiscale mathematics.

SIAM exists to ensure the strongest interactions between mathematics and other scientific and technological communities through its activities. Because of the inherent multi-disciplinary nature of computational science, the CS&E SIAG offers an excellent forum for these interactions, particularly through its conference series. In the past several years, we have made a particular effort to include computational scientists as well as applied mathematicians on the organizing committees to ensure diverse conference attendance. This has allowed us to reach out into to different communities to increase overall membership in SIAM; for example the CSE05 conference resulted in 44 new SIAM memberships.

3. 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.

SIAM Conference on CS&E, February 10-13, 2003, San Diego had 505 paid attendees.
SIAM Conference on CS&E, February 12-15, 2005, Orlando had 536 paid attendees.

The SIAM CSE conference series has been highly successful. We have attracted over 500 attendees at each of the last two meetings. At CSE05 there were over 500 presentations in 82 minisymposia sessions and 52 contributed sessions along with 20 posters.

There are a few issues that should be considered for future conferences. First, there are a large number of parallel sessions at these meetings which is one of the biggest complaints from attendees. In addition, the conference tends to be held over the course of a week and it is difficult for university attendees to attend the full conference.

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 tract of minisymposia at an annual meeting?

For the SIAM06 Annual conference held in Boston, the CSE and Optimization SIAGs jointly organized a tract of 7 minisymposia with 10 sessions total. Organizers included a number of researchers with joint membership in both SIAGs. The CSE SIAG did not formally organize any sessions at the 2005 annual conference as that was our SIAG conference year.

SIAM 2006 Annual Meeting – Joint CSE/Optimization Minisymposia:

(1) George Biros and Alfio Borzi
Title: "Multilevel methods for optimization and inverse problems"
Number of Sessions: 2

(2) Philip E. Gill (with Josh Griffin)
Title: "Iterative trust-region methods for large-scale optimization"
Number of Sessions: 1

(3) Tammy Kolda (with Josh Griffin)
Title: "Derivative-free optimization"
Number of Sessions: 1

(4) Ekaterina Kostina (with Georg Bock)
Title: "Modeling, Simulation and Optimization of Complex Processes"
1. Robustness Aspects
2. Complex optimization applications
3-4. PDE Constrained optimization
Number of Sessions: 4

(5) Ulrich Hetmaniuk and Patrick Knupp
Title: "Impact of mesh on numerical solutions to PDE's"
Number of Sessions: 1

(6) Radu Serban
Title: "Enabling technologies for large-scale dynamically-constrained optimization"
Number of sessions: 1

(7) Todd Munson
Title: "Differential Variational Inequalities"
Number of sessions: 1

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?

The other activities sponsored by the SIAG include our CSE web site, the CSE mailing list, the SIAM/ACM prize in CS&E, and articles in SIAM news.

> CSE Mail List. The CSE mailing list is open to all SIAG members who are automatically subscribed when they joint 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. Information on the list can be found at http://lists.siam.org/mailman/listinfo/siam-cse
> CSE Web page. Our web URL is http://www.siam.org/siags/siagcse.html. Currently this web page contains basic information about our SIAG, but we are working with SIAM to create a web presence with more content. We have been exploring the possibility of including information similar to DSWeb and the Optimization News and Views activities in the Dynamical Systems and Optimization SIAGs.
> SIAM/ACM Prize in CS&E. SIAM and ACM jointly award this prize that recognizes outstanding contributions to the development and use of mathematical and computational tools for science and engineering problems. The prize is awarded at the CSE biannual meeting and in 2005 went to Achi Brandt, Weizman Institute in Revohot.
> SIAM News. We have encouraged our membership to submit articles to SIAM News, particularly in the areas of CS&E education and the undergraduate and graduate levels and on the challenges and tools available in the CS&E domain. One article that appeared recently was an overview of the CSE05 conference in which a number of representative plenary speakers and minisymposium sessions were highlighted with a brief description and pointers for where readers could find additional information.

In addition to these activities, several CSE SIAG officers and members are involved in the SIAM CS&E Book Series on Computational Science and Engineering.

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

The largest activities for the CS&E SIAG over the next two years should include the CSE07 conference and continuing to flesh out the CSE web site to make it a community resource. Plans for the CSE07 conference are already well underway. The conference co-chairs are Bruce Hendrickson, Max Gunzburger, Jill Mesirov and Andy Wathen. The conference will be held in February 2007 in Costa Mesa, CA. The themes have also been decided and again include a wide range of computational science activities (ranging from computational biology and chemistry to computational nanoscience and materials), numerical methods, and applied mathematics topics. Invited speakers are being determined and minisymposium and contributed talks will be solicited shortly. The CS&E SIAG web site should be greatly enhanced to include information such as journals and meetings of interest to SIAG members, other professional societies of interest, links to conference proceedings of interest (for example, the SciDAC conference proceeding mentioned above), links to CS&E educational resources, professional opportunities, book reviews, etc.

The CS&E SIAG is ideally suited to co-sponsoring sessions or conferences with other SIAGs. In addition to sponsoring minisymposia tracts at the annual meeting, the SIAG should also encourage members to submit tracks to conferences such as SIAM Parallel Processing, the SIAM conference on Mathematical and Computational Issues in the Geosciences, the SIAM conference on the Life Sciences, etc.

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

SIAM can best help the CS&E community by continuing to promote CS&E and lobby for increased funding from federal agencies (in particular NSF and NIH) that traditionally have had difficulty supporting the interdisciplinary research essential to CS&E. This could be done as a joint effort among professional societies that emphasize modeling and computation, for example USACM, IEEE, APS, AIChE, ASME...

8. How can the activity group help SIAM in its general role of promoting applied mathematics and computational science?

SIAM is well positioned to be the professional society of choice for CS&E. This community is growing quickly and applied mathematics is an integral part of the field. By providing useful information for professionals in the CS&E field through its conference series, web site, and list serve, the SIAG can be made into a home for a community that, as yet, has no real place to go. This can help broaden SIAM by expanding the base SIAM membership base. By exposing more applied scientists and mathematicians to each other through the CS&E conference, the SIAG can help ensure that new advances in applied mathematics are exposed to potential users of these ideas. In addition, the SIAG could be better utilized in gathering information from the community on a variety of topics and issues. For example, there may be times when input from the community could usefully serve and inform the SIAM Science Policy Board.

The SIAG could also take a more active role in helping SIAM promote CS&E education. Currently, some discussion on this topic occurs at the CS&E conference meetings, but I do not believe the SIAG members have been fully utilized to help ensure this discipline continues to gain footing at leading universities and colleges. Perhaps a call for participation in a CS&E education subgroup to enhance the CS&E education web pages, help formulate official position papers, etc., could be of use to the SIAM Education committee.

This SIAG requests that the SIAM Council and Board of Trustees renew its charter for a two-year operating period beginning January 1, 2007.

Signed
Lori A. Diachin
4.24.2006

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Computational Science and Engineering (CS&E)

The SIAM Activity Group on Computational Science and Engineering (CS&E) fosters collaboration and interaction 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 important problems in science and engineering. The activity group promotes computational science and engineering as an academic discipline and promotes simulation as a mode of scientific discovery on the same level as theory and experiment.

The SIAG on CS&E organizes a biennial conference.

Chair: Lori Freitag Diachin, (1/1/04 - 12/31/06)

Vice Chair: James G. Glimm, (1/1/04 - 12/31/06)

Program Director: Omar Ghattas email (1/1/04 - 12/31/06)

Secretary/Treasurer: Tamara G. Kolda (1/1/04 - 12/31/06)