

SIAM Activity Group Uncertainty Quantification Charter Renewal Application

This CHARTER RENEWAL APPLICATION applies to the SIAM Activity Group on Uncertainty Quantification. The SIAM Activity Group (or SIAG UQ) to which this renewal applies was originally formed under the aegis of SIAM in December 2010 by the SIAM Council and by the SIAM Board of Trustees with its initial operating period beginning December 11, 2010 and ending December 31, 2012. Its charter has been renewed by the Council and Board five times thereafter.

This SIAG has 741 members, including 287 student members, as of December 31, 2021.

According to its Rules of Procedure, the objective(s) of the SIAG are:

- It is the purpose of the SIAM Activity Group on Uncertainty Quantification to foster activity and collaboration on all aspects of the effects of uncertainty and error on mathematical descriptions of real phenomena. It seeks to promote the development of theory and methods to describe quantitatively the origin, propagation, and interplay of different sources of error and uncertainty in analysis and predictions of the behavior of complex systems including biological, chemical, engineering, financial, geophysical, physical, and social/political systems. The SIAG serves to support interactions between mathematicians, statisticians, engineers, and scientists working in the interface of computation, analysis, statistics, and probability.
- Together with its partner UQ Interest Group in ASA, the SIAG organizes a biennial conference, sponsors minisymposia at conferences, publishes a newsletter biannually, and maintains an electronic discussion group.

Within the framework of SIAM, the SIAG will conduct activities that implement its purposes. The SIAG on Uncertainty Quantification will organize activities in uncertainty quantification.

The SIAG is expected to:

1. Organize minisymposia at the SIAM Annual Meeting in years where there is no SIAG conference.
2. At least once every seven years either organize a track of at least six Minisymposia at the SIAM Annual Meeting or have an activity group meeting held jointly with the annual meeting. The VP for Programs and the VP at Large will coordinate the scheduling with the SIAG chair.
3. Organize a biennial SIAM Conference on Uncertainty Quantification. 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 chairperson 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. 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 (including advisory board, if relevant).

Chair: Ralph Smith

Vice-Chair: Elisabeth Ullmann

Program Director: Daniela Calvetti

Secretary: Rebecca Morrison

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 quantification of uncertainties associated with large-scale computer models now permeates most facets of predictive science, thus leading to continued growth in the broad field of uncertainty quantification (UQ). Whereas aspects of uncertainty quantification have been investigated for decades, the field experienced significant growth with the development of theory and numerical algorithms for engineering and science applications, whose large-scale simulation models precluded direct reliance on sampling-based methods. The role of sensitivity analysis (SA) and uncertainty quantification has continued to grow rapidly as verified and validated simulation models are increasingly employed for: (i) next generation energy systems including nuclear power plant designs, advanced wind harvesting, and solar designs, and advanced carbon sequestration systems; (ii) quantification of rare events including tsunami predictions; (iii) social and economic predictions including the use of scenarios analogous to those employed by the IPCC; (iv) biomedical applications including precision medicine with individual treatment regimes and simulation-based drug discovery; and (v) model-based risk analysis and policy. The growing field has relied on several synergistic advances, including the development and improvement of novel numerical and statistical algorithms, improved computer architectures, and the realization within various disciplines that uncertainty quantification is critical for simulation-based inference, prediction, validation, and design for emerging applications. Aspects of this growth in engineering science, biomedical, and social sciences have resulted from interdisciplinary collaborations with SIAG/UQ.

Specific areas of growth within the last two years are reflected in topics and plenary presentations at the 2022 SIAM UQ conference. Applications include advances in uncertainty quantification and parameter estimation for climate and greenhouse gas models, advanced energy systems, characterization of rare events in complex systems, earth remote sensing, sensitivity analysis for Quantitative Systems Pharmacology (QSP), and lockdown strategies during the COVID-19 pandemic. Novel theoretical advances include advanced transport methods for stochastic modeling and inference, simulation and theory for rare events, surrogate models for complex coupled systems, high-dimensional Bayesian inference and nonlinear filtering, physics-informed data-driven models with quantified uncertainties, advances in sensitivity analysis, and the synthesis of uncertainty quantification and deep learning.

These topics convey the depth and breadth of significant advances in the field of uncertainty quantification over the last two years. Two broad areas of growth include the synthesis of uncertainty quantification and machine learning for complex systems and the use of digital twins and virtual populations to provide highly effective and unique prototyping and design capabilities.

Whereas there are numerous regimes where deep learning complements and extends uncertainty quantification, one area of research has focused on employing machine learning to augment empirical or phenomenological model components to reduce model discrepancy and improve the predictive capabilities of large-scale simulation models. Similarly, the integration of equation learning, and physics-informed model inadequacy terms has produced significant advances for applications ranging from epidemiology to coupled multi-physics designs for next generation nuclear power plant designs. The current emphasis in this area is quantified by the fact that there were 10 sessions focused on the integration of uncertainty quantification and deep learning at SIAM UQ22.

Validated digital twin technologies have significantly impacted aeronautic designs by providing platforms for efficiently evaluating aircraft performance using highly comprehensive models with quantified uncertainties.

Within the last two years, similar digital twin technologies have been developed and implemented for the simulation-based design of nuclear reactors. This constitutes a critical advance in the field, which leverages validated high-fidelity models to provide simulation data for regimes in which it is difficult or impossible to collect physical data, e.g., boron deposits on rods during power plant operation. There is a synergistic but unrelated focus in Quantitative Systems Pharmacology (QSP) to generate and rigorously validate virtual population platforms to facilitate safe and efficient drug development regimens. The role of sensitivity analysis and uncertainty quantification for virtual population development is substantial and will most certainly expand over the next two years.

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 /UQ is vibrant and thriving. At the end of 2021, it had 741 members, making it the 7th largest of the 22 SIAM SIAGS. Moreover, it had 287 student members, which is the 6th largest number among the SIAGS and indicates significant potential for the future. Whereas the membership varies by year, the SIAG membership is stable and at a natural number for the size of the field. When reporting these numbers, we note that the SIAG started in 2010, so it is one of the more recent SIAM activity groups.

The top three represented disciplines in the SIAG are mathematics (61.8%), engineering (20.7%), and statistics (6.5%). We note that statistics serve a central role in the SIAG, and one of the three program chairs for each SIAM UQ conference is an American Statistical Association (ASA) member. The SIAG/UQ continues to focus on increasing ASA and statistics participation in the activity group. One past example is the Statistical and Mathematical Sciences Institute (SAMSI) Program on *Model Uncertainty: Mathematical and Statistics (MUMS)* in 2018-19, which had leadership from the SIAG/UQ. Other efforts have focused on soliciting statistics plenary presentations and minisymposia at the SIAM UQ conferences and participation by SIAG members in the ASA Annual Meeting. As noted in Item 6, we will continue to build on these efforts in the future.

The SIAG membership is 72.6% academic, 11.4% laboratory, and 7.5% industry, with the remaining members coming from government and other positions. We will continue to solicit nonacademic members, and we expect these numbers to continue growing as the central role of

uncertainty quantification is increasingly established in government laboratories, industry, and the government sectors.

For the 2021 membership, 17.2% of the members and 22.6% of the students reported being female. These percentages represent an increase from 15% and 20% in the 2019 membership but are still low. We discussed these issues and trends during the Business Meeting at SIAM UQ22 and summarize suggested future initiatives in Item 6.

The SIAG/UQ is keeping up with changes in the field and initiating some of these changes through a variety of mechanisms. The first is that SIAG/UQ members are providing research leadership for a number of emerging applications in engineering, science, biology, and biomedical sciences. One example is the article on digital twins in the September 2021 *SIAM News*, written by SIAG members. Secondly, due to the highly interdisciplinary nature of the discipline, SIAG/UQ members participate in leading conferences associated with essentially all the application areas. One example pertains to the growing emphasis on sensitivity analysis and uncertainty quantification in the field of Quantitative Systems Pharmacology (QSP), as noted in Item 1. The SIAG chair gave two overview presentations on sensitivity analysis and parameter estimation for biological models at the American Conference on Pharmacometrics and presented a QSP seminar to the Food and Drug Administration in 2021. Similar examples exist for a wide range of SIAG members presenting their research in a broad range of applications; hence, the SIAG is strongly poised to continue keeping up with and leading changes in the field.

The broader interests of SIAM are reflected in various SIAG/UQ activities. The first is that due to its breadth, the field of uncertainty quantification spans numerous SIAM research areas. Hence there are UQ-related minisymposia at a number of conferences, with substantial participation at the SIAM CSE Conference. At the 2021 CSE Conference, there were 13 minisymposia with UQ in the title with many others, which reflected research related to the field.

Secondly, we detail in Item 6 proposed activities to increase the SIAG's impact both with respect to SIAM and the broader mathematics and scientific communities. This includes initiatives pertaining to equity, diversity, and inclusion (EDI).

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

- SIAM UQ20: This conference was scheduled for March 24—27 at the Garching campus of the Technical University of Munich but had to be cancelled due to COVID-19. The size of the scheduled program is established by the fact that it would have featured 823 presentations, organized as 157 minisymposium sessions, 136 contributed talks, and 59 posters.
- SIAM UQ22: This conference took place on April 12—15 at the Westin Peachtree Plaza in Atlanta, GA. There were 865 registered attendees, of which 329 attended onsite and 536 attended virtually. This is the largest total attendance of the five SIAG/UQ meetings since the first in 2012. This was the first hybrid meeting hosted by SIAM, which posed some technological challenges for remote attendees. It is anticipated that these challenges will be addressed for future hybrid meetings.

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?

The last SIAG/UQ-sponsored track at the SIAM Annual Meeting was at AN17, which included 10 minisymposium sessions. The SIAG is next scheduled to sponsor a track at AN24.

There was only 1 SIAG/UQ-organized minisymposium specifically focused on uncertainty quantification at the 2020 SIAM Annual Meeting, co-sponsored by the Canadian Applied and Industrial Mathematics Society (CAIMS). However, several minisymposia focused more broadly on applications in which UQ plays a role. We hypothesize that COVID-19 significantly reduced SIAG/UQ organization of minisymposia at this meeting.

At the 2021 SIAM Annual Meeting, there were 10 minisymposia, which directly pertained to uncertainty quantification in the sense that they had “Uncertainty Quantification” or “Inverse Problems” in the title. Of these, 6 were organized by SIAG/UQ members, while the others included activity group members as speakers. The topics included UQ Strategies for Data-Driven, Large-Scale Problems, Advances in UQ with Model Order Reduction Methods, and Inverse Problems and Uncertainty Quantification in Biological and Medical Applications.

To complement the 2021 SIAM Annual meeting, we noted in Item 2 that there were 13 UQ minisymposia at the 2021 SIAM CSE Conference with several others that reflected the research in the field. In combination, this represented a significant organization of minisymposia by the SIAG in the off year from the SIAM UQ 2022 Conference.

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 2020 SIAG/UQ Early Career Prize was awarded to Björn Sprungk from the Technical University Bergakademie Freiberg. Dr. Sprungk was scheduled to give the Prize Lecture “Noise-Level Robust Sampling Methods for Bayesian Inverse Problems” at the 2020 SIAM UQ Conference, which was cancelled due to COVID-19.
- The 2022 SIAG/UQ Early Career Prize recipient was Mengyang Gu from the University of California Santa Barbara. Dr. Gu gave the Prize Lecture “Scalable Gaussian Process for Computer Model Emulation and Uncertainty Quantification” at the 2022 SIAM UQ conference in Atlanta, GA.
- SIAG members organized a SIAM minisymposium, comprised of 6 presentations, at the 2022 Joint Mathematical Meeting (JMM) sponsored by the American Mathematical Society (AMS). This supported SIAM’s serving as a partner for this meeting.

The SIAG/UQ electronic mailing list and SIAM Engage remain the primary form of communication between members. This medium has been very active and successful. Recent postings have included descriptions of research positions and postdocs, “Careers in Industry: Meet and Greet with the SIAM Industry Committee,” and congratulations to SIAG/UQ 2022 SIAM Fellows. Activity group activities are also maintained on the SIAG/UQ website.

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

Many of the planned and proposed activities will fall under the leadership of the next set of SIAG/UQ officers, however, several are broad enough that they can be addressed by the general activity group.

- I. Initial planning for the SIAM UQ 2024 Conference is underway, with discussions regarding site selection. Potential locations in Europe are under consideration, and SIAG will continue to obtain information for site selection.
- II. The SIAG will closely coordinate with SIAM leadership, including the Vice President for Equity, Diversity, and Inclusion (EDI), regarding EDI initiatives. The following suggestions were proposed during the 2022 SIAG/UQ Business Meeting both to expand activity group impact and as part of the broad SIAM mission.

The need to actively organize events to expand and retain diverse demographics and those not normally attending existing events was discussed and will be pursued by the SIAG. One model is the “Women in Inverse Problems” Workshop held at the Banff International Research Station on December 5-10, 2021. There was also discussion regarding potential efforts to establish direct contact with diverse demographics and promote SIAG opportunities. These efforts will build on recent SIAG/UQ leadership demographics, which included three female Program Co-Chairs for the UQ 2020 Conference and three of the present SIAG officers being female and will closely coincide with the SIAM initiative to form a new SIAM Activity Group on Equity, Diversity, and Inclusion (SIAG/EDI).

- III. During the 2022 SIAG Business Meeting, a suggestion was made to establish one or more SIAG/UQ student awards. We will coordinate with SIAM leadership and industrial affiliates to pursue this goal.
- IV. We noted in Item 2 that the American Statistical Society (ASA) contributes strongly to the SIAG/UQ and broad SIAM communities, as evidenced by the fact that one of the three SIAG Conference Co-Chairs is always an ASA member and the ASA co-sponsors and co-manages the *SIAM-ASA Journal on Uncertainty Quantification*. Despite these close ties, statistics presently accounts for approximately 6.5% of the SIAG membership. We will pursue various initiatives to increase statistics participation in the SIAG. First, SIAG/UQ members are increasingly joining the ASA and participating in the ASA Annual Conference. Secondly, we will continue to co-sponsor or coordinate activities such as the 2018-19 SAMSI Program on *Model Uncertainty: Mathematical and Statistics (MUMS)*. Through such efforts, we anticipate continued integration of the mathematics and statistics communities in the SIAG.
- V. We will continue to focus on expanding the functionality of the SIAG/UQ website. Potential ways to achieve this include advertising conferences, workshops, and summer schools, posting model or challenge problems and UQ case studies, advertising employment opportunities, and providing a moderated forum for communications and questions among SIAG/UQ members.

- VI. We noted in Item 3 a SIAM News Article focused on UQ activities pertaining to Digital Twins. We will continue to solicit articles highlighting activities and future directions for UQ research.

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

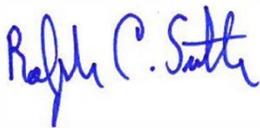
The SIAM leadership and staff have provided exemplary assistance and support for all SIAG activities, including: the SIAM UQ Conferences, the SIAG/UQ Early Career Prizes, the *SIAM-ASA Journal on Uncertainty Quantification* – which, while not sponsored by the SIAG/UQ, greatly benefits the SIAG – and the SIAM mailing list and SIAM Engage. For the future activities, we will need to coordinate closely with SIAM leadership regarding the proposed EDI initiatives and extensions to the website. We will also need to coordinate closely to increase ties with other organizations, such as the ASA, CAIMS, and GAMM.

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

As we detailed in Items 1 and 2, the field of uncertainty quantification permeates simulation-based predictive science across a broad range of disciplines. By providing a cohesive organization to synthesize emerging theory, algorithms, and best practices for a wide range of applications, this activity group is providing SIAM with substantial leadership capabilities to promote uncertainty quantification to the broad mathematics and scientific communities.

This SIAG requests that the SIAM Council and Board of Trustees renew its charter for a two-year operating period beginning January 1, 2023.

Signed,



Ralph Smith, SIAG/UQ Chair

May 16, 2022