SIAM Activity Group Mathematical Aspects of Materials Science (MS) Charter Renewal Application

This Charter Renewal Application applies to the SIAM Activity Group on Mathematical Aspects of Materials Science. The SIAM Activity Group (SIAG/MS) was originally formed under the aegis of SIAM on July 10, 2008 by the SIAM Council and July 12, 2008 by the SIAM Board of Trustees. Its charter has been renewed by the council and board four times thereafter.

This SIAG had 286 members as of December 31, 2019; of these, 115 were students and 171 were not students.

According to the Rules of Procedure it is the purpose of the SIAM Activity Group on Mathematical Aspects of Materials Science to bring together mathematicians, engineers and scientists interested in the application of analysis and computation to problems in materials science. Because of the unifying nature of mathematics, the SIAG will serve as a meeting point for mathematicians, engineers and scientists interested in all areas of materials science, thus fostering cross-fertilization between fields, and from diverse venues such as academia, industry and the national laboratories. In this manner, the SIAG provides a unique opportunity for interaction between fields that would be greatly diminished in its absence.

Within the framework of SIAM, the SIAG will conduct activities that implement its purposes.

The SIAG on Mathematical Aspects of Materials Science 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 the SIAM Conference on Mathematical Aspects of Materials Science series, with conferences taking place every two years (normally even years though the 2020 SIAM MS was postponed to 2021 and the 2022 meeting is cancelled due to the ongoing pandemic). The chairs of the conference organizing committee shall be the program director and the chairperson of the SIAG or their designees.

The SIAG/MS 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/MS.

List all current officers of the activity group (including advisory board, if relevant). Chair: Kaushik Bhattacharya Vice Chair: Jianfeng Lu Program Director: Rustum Choksi Secretary: Yekaterina Epshteyn

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?

The field covered by the activity group remains healthy and vital. The discovery, development and refinement of new materials and new phenomena are vital for various technological areas of crucial importance to society. These activities in materials sciences continue to raise interesting questions in mathematics and conversely mathematical and computational approaches provide vital tools in this arena. Four recent examples of mathematics enabling materials science are the development of new multi-modal deforming materials, development of new low-hysteresis shape-memory alloys, understanding of new semi-conducting states in twisted two-dimensional materials and robust algorithms in fracture mechanics.

Materials science is evolving in two major directions, both providing opportunities for mathematical aspects. First, the maturing of 3d printing and other such techniques of net shape synthesis provide properties of making new `meta-materials' with unprecedented properties. Mathematical and computational analysis are critical in exploring the design space. Second, machine learning is being adopted across materials sciences. While the early focus has been in refining regression or using neural nets to replace empirical models, new approaches with embrace these new tools are emerging.

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 activity group remains stable and vibrant. Our meetings are typically held every other year and our membership oscillates around a relatively stable (slightly growing) average with a two-year period. Enthusiasm for our meetings remains high – the registration at these meetings has grown steadily and would have been at an all time high at the postponed 2020 meeting (with the exception when the meeting was held concurrently with the SIAM annual meeting). The postponed 2020 meeting had a number of mini-symposia and plenary speakers speaking on the emerging areas of the field. Finally, our membership draws from mathematicians, physicists and engineers.

There are three recruitment opportunities that we have identified to increase our membership. The first demographic is European members. This was one of the motivations to hold the now postponed SIAM MS 2020 in Bilbao, Spain. The second is student membership, and the third is national laboratory members.

- 3. Please list conferences/workshops the activity group has sponsored or cosponsored over the past three years, and give a brief (one sentence or phrase) indication of the success or problems with each.
- In 2018, the SIAM Conference on Mathematical Aspects of Materials Science (MS18), was held jointly with AN18 in Portland, Oregon, USA. Of the 1336 attendees, 511 indicated they planned to attend MS18.
- In 2019, the SIAG sponsored a symposium on `Mathematical Aspects of Materials Science – Modeling, Analysis and Computations' at the 2019 Spring Meeting of the Materials Research Society. The symposium attracted 72 speakers and was extremely well attended. One issue with this symposium is the high cost of registration for MRS.
- In ICIAM 2019, several minisymposia related to Materials Science were organized by researchers active in SIAG/MS.
- At JMM 2020 in Denver, an invited SIAM special research session "Modeling, Analysis, and Simulation of PDEs with Multiple Scales, Interfaces, and Coupled Phenomena" featured several talks on mathematical aspects of materials science given by researchers active in SIAG/MS.
- Several sessions organized by researchers active in SIAG/MS were planned for WCCM-ECCOMAS 2020 (cancelled due to COVID-19 but may happen at a later date).

SIAG/MS had tried to foster a reciprocal arrangement with Materials Research Society (MRS). This has not worked well because of a lack of interest on the part of MRS leadership. We are now in discussions to create a reciprocal arrangement with the Soft Matter group of American Physical Society (APS), since we see an overlap of researchers.

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?

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.

The 2018 SIAM MS conference was held concurrently with the SIAM Annual Meeting. The 2020 SIAM Annual Meeting had two events related with the SIAG: the DMREF session and the von Karman lecture. 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?

SIAG/MS supports Women in Mathematics of Materials (WIMM) network. During recent SIAM/MS conferences, WIMM organized successful and well-attended networking luncheon (such luncheon was organized during MS18 and MS 16). In addition, WIMM is actively involved in organizing various scientific events for female participants at AWM workshops, SIAM-MS and SIAM annual conferences.

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

As already noted, we have identified three demographic opportunities that we can recruit from to increase our membership. We are also in discussions to have an Early Career prize in our meetings.

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

SIAM can help us seek corporate sponsors for SIAM MS conferences. Travel funds that SIAM contributes for various SIAG/MS conferences and symposia are very helpful, especially for junior researchers and students.

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

The MS activity group will continue its key role in promoting interactions between mathematics and materials science communities to help SIAM promote applied mathematics and computational science. Further, the scientific committee, plenary speakers and mini-symposia of the SIAM MS conferences include physicists and engineers who would not otherwise participate in SIAM.

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

Signed

Kaushik Bhattacharya, SIAG/MS Chair May 29, 2020