

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 five times thereafter.

This SIAG has 279 members, including 108 student members, as of December 31, 2021.

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 even year (the 2022 SIAM MS was not held because 2020 was held in 2021 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.
4. With the approval of the SIAM Program Committee, the SIAG may organize special sessions at SIAM meetings. Other SIAG meetings may be organized only with the approval of the SIAM president and vice president for programs.

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: Felix Otto

Vice Chair: Maria Emelianenko

Program Director: Dmitry Golovaty

Secretary: Lin Lin

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 text from the previous charter renewal still perfectly reflects the state of the field, so much that we essentially repeat it here:

The field covered by the activity group remains healthy and vital. The discovery, development, and refinement of new materials and 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 is critical in exploring the design space. Second, machine learning is being adopted across materials sciences. While the early focus has been on refining regression or using neural nets to replace empirical models, less black-box approaches that embrace these new tools and combine them with our knowledge, e.g., on symmetries and conservation laws, 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 held every other year, and our membership oscillates around a relatively stable (slightly growing) average over a two-year period. Enthusiasm for our meetings remains high – the registration at these meetings has grown steadily. The virtual 2021 SIAM MS meeting had 815 participants vs. 511 at the 2018 SIAM MS conference that was held concurrently with the SIAM annual meeting. The 2021 conference had a number of mini-symposia and plenary talks on the emerging areas in the field. Our membership draws from mathematicians, physicists and engineers. The previous SIAG officers identified Europe as a large untapped source of increasing the SIAG membership, and the conference proved successful in generating interest on this continent. The virtual format of the meeting, however, was not conducive to converting the conference participants into SIAG members. Extensive European participation in 2021 SIAM MS indicates that a successful membership drive can be held at a physical gathering in Europe four years from now. Further recruitment opportunities include students and employees of national labs.

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

The opportunities to hold or sponsor meetings were sparse in the last two years due to the ongoing COVID-19 pandemic. Two major events were sponsored/organized by the SIAG.

- In 2021, the SIAM Conference on Mathematical Aspects of Materials Science (MS21) was held virtually at the Basque Center for Applied Mathematics (Bilbao, Spain). The meeting attracted 815 attendees, out of which 672 were paid, with almost half of all

participants coming from Europe.

- In 2022, the SIAG organized the Materials Science track at the AN22 in Pittsburgh. The event involved 7 minisymposia with over 90 speakers.
- A minisymposium on quantum algorithms for materials was organized for the Joint Math Meetings 2022 conference in January 2022, later canceled to COVID-related change of time and modality.
- SIAG members are involved in organizing the Multiscale Materials Modeling (MMM10) conference to be held in Baltimore in October 2022 (postponed from 2020). This international event is expected to draw more than 750 participants this year working in areas of interest to our SIAG.

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.

Given that SIAM MS 22 was cancelled because of the COVID-19 pandemic, the activity group organized a Materials Science track at the 2022 SIAM AN with 7 minisymposia that covered a range of topics, including recent advances in peridynamics modeling and analysis of materials, mathematics of transforming structures and metamaterials, participation of women in the mathematics of materials, geometric variational problems and their applications, as well as problems arising in liquid crystals and soft matter.

The last time the SIAM MS meeting was held concurrently with SIAM AN was in 2018.

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 has been actively promoting scientific opportunities through SIAM Engage and Facebook platforms. SIAG Facebook currently has 715 members, and SIAG Engage lists 248 members.

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

After consulting with two dozens of experienced and particularly committed members of the SIAG, the officers devised a concept for an early career award. The side constraints specific to the MS-SIAG is that 1) there should be a symbiosis between the award and the conference, which in absence of a journal is the defining activity of the SIAG, 2) the set-up of the award should be adapted to the scientific diversity of our SIAG (experiments-theory-simulation, mathematics-engineering). We hope that the proposal finds the full support of SIAM.

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

SIAM's help with establishing and promoting the first SIAG early career prize will go a long way in terms of ensuring the longevity of the efforts undertaken by the SIAG members and attracting junior scientists to this highly interdisciplinary research area.

We applaud that SIAM is returning to in-person conferences. This is essential for the exposure and casual networking of our young members. As a positive side effect for SIAM, it will increase student membership.

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

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

A handwritten signature in blue ink that reads "Felix Otto". The signature is written in a cursive style with a large initial 'F'.

Felix Otto, SIAG/MS Chair
[05/20/2022]