

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 six times thereafter.

This SIAG has 218 members, including 75 student members, as of December 31, 2023.

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 or three years. 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: Irene Fonseca

Vice Chair: Carlos Garcia-Cervera

Program Director: Kaushik Dayal

Secretary: Miranda Holmes-Cerfon

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?

We recall from the 2023 charter renewal: “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.”

This SIAG continues to offer a forum for the design, discovery, and development of novel materials through mathematical modeling, computation and experiment. Significant advances have been made in the understanding of liquid crystals, thin films, multiscale materials structures and homogenization, and contemporary areas also include the study of metamaterials, hard and soft materials, defects in complex materials and at grain boundaries, electronic structure theory, quantum computing, quantum chemistry and quantum embedding theories, electronic and mechanical properties of graphene and other Dirac materials, and machine-learning-enhanced design of materials.

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 main activity of this SIAG is its periodically held conference, and here, as the program of the upcoming MS 24 Conference in Pittsburgh shows, main areas of the mathematics of materials, as discussed in 1., are well represented.

However, the rapidly decline of this SIAG’s membership since 2020 is worrisome. Being a small activity group (the 4th smallest SIAG), losing so many members so fast needs a careful analysis and, possibly, the adoption of measures to correct this trend. Until 2020, the SIAG’s membership increased steadily to reach a total of 360 members, with 203 nonstudents and 157 students. In 2023 the total number of members was 218, of whom 143 were nonstudent and only 75 students. The members are mostly in academia (86.1%) and mostly in mathematics departments (75.9%). Perhaps the engineering participation, now 16.9%, could be enhanced, and the “free” students’ memberships could be better advertised. Further, the percentage of women nonstudent is rather low (16%), although the number of students is a little better (28%), but the latter may not be very significant since the overall number is so small.

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.

MS21 (virtual): <https://www.siam.org/conferences/cm/conference/ms21>

Rescheduled virtual conference originally scheduled to be held at the Basque Center for Applied Mathematics in Bilbao in 2020. Final attendance: 672 (a record for SIAG/MS). Quoting the organizer Arghir Zarnescu:

“Despite the challenges presented by the online format of the conference, the conference can be considered a success as the overall impression of most of the attendees was either

very positive (40.63%) or positive (43.75%), as based on the final evaluation survey of the MS21 conference.” (The survey is attached).

MS24: Scheduled to take place in Pittsburgh, Pennsylvania, May 19-23, 2024.

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?

SIAG/MS last ran a track at the Annual Meeting in 2022 (hybrid in Pittsburgh, Pennsylvania). The track contained 23 sessions, many of which were parts of multi-session minisymposia.

We don't have a record of SIAG/MS-sponsored sessions held during AN21 (virtual).

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, which currently lists 224 members. In February 2023 we discussed how to keep the SIAG-MS community engaged and connected during the period between conferences. It was discussed that (a) the SIAM Engage platform is difficult to use, and does not lend itself to easy discussions; (b) many members do not have the time/desire to use social media such as Facebook or Twitter/X. For lack of better options, it was determined that a more up-to-date website would be appropriate, which lists conferences, workshops, summer schools, internships, postdoc positions, etc. Plans for the website are underway.

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

Three main efforts and activities lead by members of this SIAG members are:

- (i) The establishment of the Ericksen prize.

By initiative of John Ball, Kaushik Bhattacharya (initial officer of this SIAG, 2010), Irene Fonseca (initial officer of this SIAG, 2010), and Richard James, in 2021 SIAM established the Jerald L. Ericksen prize

<https://sinews.siam.org/Details-Page/siam-establishes-the-jerald-l-ericksen-prize>

which will first be awarded at the 2025 SIAM Annual Meeting. Principal guidelines read: *The Jerald L. Ericksen Prize is awarded every 5 years for the original formulation of a mathematical theory of a significant scientific or engineering problem. The prize may recognize either a formulation that enables the application of deep mathematical ideas, or a formulation that raises new questions in mathematics. The prize is awarded for research in the preceding fifteen years. The prize is awarded every fifth year normally at the annual meeting of the society. The initial funds for this award were contributed by the students, friends, colleagues, and family of Jerald Ericksen in recognition of his fundamental contributions to the development of mathematical and continuum theories of nonlinear elasticity, liquid crystals, non-Newtonian fluids and crystalline solids, in admiration for his ability to bring to bear deep and abstract mathematical ideas to physical phenomena, and in deep appreciation for his encouragement, mentorship and generosity.*

(ii) MS24 Conference in Pittsburgh, May 19-23, 2024 (as of Apr 19, 2024)

We discussed that SIAG-MS conferences should highlight students' and postdocs' work, e.g., by holding a poster blitz, poster competition, submission of abstracts, etc. However, this upcoming Co-Chairs decided not to organize a blitz or competition, given that there are only 9 posters and, therefore, not enough to have a blitz and competition. We suggest that this be better advertised by the next organizers so as to ensure a critical mass.

2018 at Portland co-located with AN 18 had 1336 registered.

2021 at Bilbao virtual had 672 registered (815 attendees, out of which 672 were paid).

Summary of Meeting Registrations by Rate Category for MS24

Reg Category	PRODUCT CODE	Pre-Reg	On-Site	Total	Paid	Free
COMPLIMENTARY	FULL	10	0	10	0	10
CORPMEMBER	FULL	2	0	2	2	0
INVITEDSPEAKER	FULL	11	0	11	0	11
MEMBER	FULL	53	0	53	53	0
MEMBER	FULL_MEMBER	30	0	30	30	0
NONMBR	FULL	96	0	96	96	0
ONEDAYMON	ONEDAYMONDAY	11	0	11	11	0
ONEDAYSUN	ONEDAYSUNDAY	15	0	15	15	0
ONEDAYTHU	ONEDAYTHURSDAY	1	0	1	1	0
ONEDAYTUE	ONEDAYTUESDAY	2	0	2	2	0
SIAG_MBR	FULL	46	0	46	46	0
STUDENT MBR	FULL	26	0	26	26	0
STUDENT NONMBR	FULL	35	0	35	35	0
STUTRAVELAWD	FULL	20	0	20	20	0
TOTALS		358	0	358	337	21

(iii) SIAG-MS “Frontiers of Mathematics of Materials” prize.

This effort was initiated by the previous SIAG’s officers. This SIAG has no journal, therefore this prize would bring visibility and awareness to its very broad (mathematically and scientifically) community. In discussion with SIAM’s leadership in February 2023, the current set of this SIAG’s officers agreed that:

- This prize would be awarded every three years, in tandem with the three year cycle of this SIAG’s conferences.
- Awardees should be within year 6 since their Ph.D. (or equivalent).
- Selection would occur every year. Suppose that the SIAG-MS conference is held in Spring of year x. The SIAG leadership then has been appointed in January year x-2, with term expiring in December year x. The Prize Committee, appointed by this SIAG leadership in year x-2, will select prize winners for years

x-2 -- to be announced in year x-2 in Engage, SIAM News, SIAG website/newsletter, etc.

x-1 -- to be announced in year x-1 in Engage, SIAM News, SIAG website/newsletter, etc.

x -- to be announced in year x in Engage, SIAM News, SIAG website/newsletter, etc.

- At the beginning of the conference in year x, there would be a minisymposium where these three prize winners would present the work that awarded them the prize, although exceptions can be made, for example, the result might have been improved by them or somebody else. They would receive a certificate and no cash award. They would all receive travel reimbursement, including transportation, lodging, meals and/or per diem.
- Prize fund: Felix Otto and Dmitry Golovaty have offered to solicit support from the 25 or so senior SIAG-MS members who they contacted for advice on the award.

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

This SIAG could use SIAM's experience and guidance to:

- (i) improve its membership, both in terms of total numbers as well as in its diversity, as detailed in 2.
- (ii) facilitate the organization of a conference of this SIAG every three years, which has been essentially the pattern since 2008.
- (iii) establish and promote the first SIAG early career prize, as described in 6.
- (iv) facilitate the creating of a website or newsletter.

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

Officers of this SIAG could encourage its members to organize sessions at large conferences (AMS, AAAS, AMS, APS, MRS, SES, SIAM, etc.) to showcase research conducted by this group, and to highlight how applied mathematics, and in particular SIAG MS mathematics, can impact research in other fields. In the same spirit, holding summer schools and poster sessions by graduate students/industry could be considered. These activities would require funding that could be secured by research grants and/or registration fees.

This SIAG requests that the SIAM Council and Board of Trustees renew its charter for a two-year operating period beginning January 1, 2025.



~~Irene Fonseca, SIAG/MS Chair~~

April 26, 2024