

## 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 two times thereafter.

This SIAG had 264 members as of December 31, 2015; of these, 120 were students. This reflects about a 20% increase in AG membership from three years ago.

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 five 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 three or four years. 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.

1. List all current officers of the activity group (including advisory board, if relevant).
  - Chair: Qiang Du
  - Vice Chair: John Lowengrub
  - Program Director: We are sad to report the recent passing of the Program Director Peter Smereka.
  - Secretary: Maria Emelianenko
  
2. 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 is continuing to attract interest from the applied mathematics community, helped by the national initiatives such as the Material Genome Initiative (MGI). Federal agencies are funding several programs such as the NSF-DMREF, NSF-OP as well as DOE computational materials science initiatives. There is increasing interest in subjects related to first principles and multiscale modeling and computation, materials design through computation and modeling, and uncertainty quantification. The community thrives at the interdisciplinary boundary between mathematics and the many aspects of materials science. It is represented by a variety of research fields (pure, applied, numerical and computational mathematics; physics, biology, chemistry, and engineering).

How is the activity group doing? Is it remaining vibrant? Is the size of the SIAG/MS stable or increasing? How is the SIAG/MS keeping up with the changes in the field? How are the broader interests of SIAM reflected in the activities of the SIAG/MS? The SIAG-MS remains a vibrant community with a steady increase in membership (going up from the initial 129 members to over 260). The AG is embracing stronger ties with the materials science community through the collaboration between SIAM and MRS. This helps to promote interdisciplinary research and connect modeling, analysis, and computation with applications. To engage the younger generation, the SIAG-MS has improved its online presence with a Wiki page and Facebook page which has over 500 followers. The research represented in the SIAG community shows a very good balance between mathematical modeling, computing, and an increasing trend towards industrial and scientific applications, all within the broader interests of SIAM. The SIAG-MS is continuing its broad appeal to members from diverse disciplines.

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.

- In 2013 – the MS conference was successfully held on May 23-26th in Philadelphia, PA with 437 registered attendees.
- In 2016 - the most recent MS conference was successfully held on May 8-12 in Philadelphia, PA. There were over 519 registered participants for this conference, a new record in attendance.
- Other than the SIAM MS conferences, the AG members organized and actively participated in the 2014 PCMI Summer Program on Mathematics of Materials in Park City, UT. In addition to research talks, the program included training courses for undergraduate, graduate students as well as faculty from undergraduate institutions. It was a big success.
- The inaugural SIAM-MS symposium on Computational Aspects of Materials Science took place successfully in Fall 2014 MRS in Boston. It attracted a variety of participants and was overall a very successful undertaking that will be built upon in the future
- AG officers, in collaboration with NIST, also organized the UQ in Materials Science workshop, January 2016 as part of MGI initiative, which was also quite successful. It brought together experts on various aspects of UQ and was a small size venue aimed at exploring the field frontiers.

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 SIAG-MS members have organized more than 40 minisymposia in SIAM Annual meetings in 2014/2016 and ICIAM 2015.

The SIAG-MS has not been asked to organize a track at the Annual Meeting in the last three years and has been recently informed that it will not get its turn to organize a track in the annual meetings in the next three years, given the increased number of AGs. The group members have continued active participation in SIAM conferences.

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?

To engage the younger generation, the SIAG-MS has improved its online presence with a Wiki-page and a Facebook page. Updated information related to the AG has been regularly posted. There was also a Women in Mathematics of Materials (WIMM) Networking Luncheon organized by female participants of the MS16.

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

SIAM MS19: the next MS conference of the series will take place in 2019. SIAM/MRS workshop/symposium in the spring meeting of 2018. There is a plan to organize a WIMM symposium in 2017.

At the MS16 business meeting, several members suggested that the MS conference series be held every two years. To broaden international participation, it was suggested that the conference can be held in a non-US location every four to six years.

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

SIAM's support of the newly established collaboration with MRS is very helpful to SIAG-MS.

Collaborations with similar organizations such as USACM and USNC-TAM will help promote ties with sister organizations and engage relevant communities. SIAM support of the WIMM activities is also extremely important for increasing female and underrepresented group participation.

There have been suggestions to propose a SIAG-MS prize to further publicize the work represented by the AG. SIAM's help in raising funds for the prize and getting the prize approved would be greatly appreciated. Seeking corporate sponsors for SIAM MS conferences is something SIAM can also help the AG to explore.

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

SIAG-MS will continue its key role in promoting interactions between mathematics and materials science communities to help SIAM promote applied mathematics and computational science.

This SIAG requests that the SIAM Council and Board of Trustees renew its charter for a three year operating period beginning January 1, 2017.

Signed

Qiang Du, Chair,  
On behalf of SIAG officers,  
SIAM Activity Group on Mathematical Aspects of Materials Science  
(May 15, 2016)