

ICMS Workshop Report

Adaptivity, robustness and complexity of multiscale algorithms

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Organisers.

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1. Significant deviations from the original proposal

The workshop did not deviate from the original proposal.

2. Short Description of the Meeting

Multiscale or multi-physics modeling play a major role in the computational approach of many important problems arising in the geosciences, atmospheric sciences, physical sciences, chemistry, biology and medicine. The computation limitation of multiscale problems arise in many applications in various areas as for example in chemistry (simulation of chemical reactions combining Markov processes with differential equations over disparate time scales) or in material sciences (effect of dislocations in carbone nanotubes on the macroscopic elastic property of novel composite materials) to mention but a few. The past few years has seen increasingly growing research activities aiming at developing novel multiscale computational methods. While new mathematical frameworks for constructing and analyzing multiscale algorithm have emerged and show promise in applications, there is a real need for a better understanding of many challenging issues. The aim of the workshop was to bring together specialists from various area in the broad field of multiscale modeling and computations. This workshop focused on the issues of adaptivity, robustness and complexity of various emerging multiscale algorithms. Each day had a special theme, featuring new advances and challenges of computational techniques in areas as diverse as quasi-continuum methods, multiscale stochastic dynamics, multiscale partial differential equations or molecular dynamics. State of the art and frontiers in multiscale modeling were presented, links between various disciplines were highlighted through many animated discussions both in small and large groups making this workshop highly stimulating for the participants and

a true success.

3. Comprehensive report of the workshop

Structure of the workshop

A broad range of topics in the general field of multiscale modeling and analysis were discussed during this workshop. Each day had a special theme:

- Monday: Quasicontinuum methods;
- Tuesday: Stochastic and statistical multiscale methods;
- Wednesday: Heterogeneous multiscale method;
- Thursday: Adaptive, multilevel and homogenization techniques for PDEs;
- Friday: Controlled molecular dynamics and chemical systems.

It was decided to have rather short talks (around 30 min) allowing for exchanges between each talk. Despite the large number of participants (40 researchers) and presentations, there was still plenty of time for small and large group discussions. Some participants also took advantage of the free afternoon (Wednesday) to work in small groups. The aforementioned structure was quite appreciated by the participants who find it convenient (“easier to follow”) to focus a whole day on a specific topic. We tried to schedule a combination of comprehensive reviews and recent advances to allow each participant to learn from the presentations and to facilitate the possibility for exchanges. We believe also that this structure did help in finding common lines of interest and connection between the various topics. A knowledge transfer networking event was organized (thanks to Helen Bridle) on Wednesday during a buffet lunch, allowing a few selected people from industry to network with delegates from the workshop.

Scientific highlights of the workshop

While several lectures were highlighted by some participants the general feeling (as mentioned in the evaluation) is that the combination of “very high quality” lectures, “very active discussions among participants” and the presence of “world leaders in each topic” made this workshop a unique opportunity to report new advances in multiscale modeling and identify future challenges towards better control of computational methods. This is further documented in the evaluation of the workshop where many participants highlighted the “quality of the speakers, the mix of different fields and the informal discussions with the attending researchers”, the “selected topics at the front of the current research and the people, all very active researchers in their field”, the “interdisciplinary nature of the workshop, bringing together researchers from numerical analysis, stochastic systems, homogenization, and molecular dynamics”, etc.

When possible, we scheduled an overview talk at the beginning of each day related to the specific topic. We mention for example the talk on predictive and efficient quasicontinuum methods which gave an overview of existing approaches as well as recent progress, or the talk on the heterogeneous multiscale method which gave a comprehensive description of the state-of-the-art of this computational framework. The mix between participants, some of them working more on theoretical issues while others were more computationally oriented, was also quite a success. We mention for example a talk about unfolding method for homogenization problems (by an inventor of the method), followed by the presentation of finite element methods based on this new mathematical technique or a presentation on averaging processes for stochastic differential methods followed by a talk on numerical techniques for stochastic problems with multiple scales, etc.

We also mention that several participants presented very recent advances in their field by communicating unpublished work of high interest (as reported in the evaluation). We mention

for examples the talks on multiscale methods for the wave equation, the talk on the existence of modified equations for stochastic differential equations or on Bayesian reduced-order models for multiscale dynamical systems.

Academic value of the workshop

In many results reported by the researchers of the workshop, the role of adaptivity and robustness in multiscale computation proved to be central. Adaptivity is essential for methodology aiming at pushing computation beyond simple physical structural assumptions (as the periodicity in the small scales or the assumption of widely separated scales). It is also of prime importance for the problem of extracting efficiently the coherent information embedded in noisy data, in understanding the effect of uncertainty over long time computation or in deriving efficient computational method capable of handling the transition between atomistic and continuum scales. These presentations emphasized that the topic of the proposed workshop was of paramount importance for the development of reliable algorithms for accurate predictions of physical phenomena.

One of the aim of the workshop was to bring together world leading experts in the mathematical modeling of multiscale problems, stochastic dynamics and adaptivity in order to exchange and confront ideas, identify new directions towards a better understanding of the fundamental issues of robustness and adaptivity in multiscale modeling and computation. We have the impression that these goals were fulfilled. This is also reflected in the evaluation, where participants mentioned the "high academic value with worldwide leading researchers in the scientific disciplines covered by the workshop available for large part of the week for discussions."

Contact between participants, participants involvement

As mentioned in the section related to the structure of the workshop, we tried to favor discussions among participants and interactions in both small or large groups. Often questions and remarks from researchers working in a different area than the speaker shed new light on a topic, allowed to appreciate the difficulties of the presented research but also the potential relation with similar issues in related areas. During almost all lunch breaks, there were animated discussions around the white board of the lecture room. Discussions took also place every afternoon after the last talk until the ICMS closing hour.

As we had participants from four continents (America, Asia, Africa and Europe) the workshop was also a unique opportunity to discuss "live" without the time constraints of the usual conferences and in a friendly and relaxed atmosphere. Many participants mentioned that the meeting allowed them to "sustain a number of existing contacts" and mentioned that there were hoping to "develop new collaborations".

Organisational issues

The organisation of the workshop went very well, thanks to the extremely efficient help of the ICMS staff, and in particular to Johanna Kytöharju, our conference co-ordinator. Her help was crucial prior to the workshop with all issues related to budget, housing and schedule of the presentations and the social events. The help of the ICMS staff was also much appreciated by the participants during the workshop. Many of them reported in their evaluation that they were "deeply impressed by the ICMS staff's professionalism; from the first announcement until the end of the workshop, every event was carefully planned", "ICMS leaves nothing to chance!", "buffet lunch, wine reception, workshop dinner were unforgettable occasions", etc. While many praised the "special atmosphere of the Maxwell House" or mentioned that the "connection to Maxwell was inspiring", some mentioned the size of the lecture room a bit too small for the number of attendees. The organisers were aware of this potential problem but decided that the advantages of the Maxwell's house would compensate this issue. Finally we had also a comment about the wireless slow speed in contrast to the fast fixed connection of the ICMS computers.