

Multiscale Computing: From the desktop to the Exascale

16 - 20 April 2018 @Snellius

The goal of this workshop was to bring together a group of computational scientists and scientists from several different scientific disciplines to further explore generic methods, algorithms, specification and modelling languages, and software environments for multiscale computing. By building upon the current understanding of multiscale modelling the focus of the workshop is mainly on multiscale computing on state-of-the-art computing resources, with focus on high end HPC/Cloud ecosystems.

A main scientific output of the workshop will be a special issue in the Philosophical Transactions of the Royal Society A, on "Multiscale Modelling, Simulation & Computing: from the Desktop to the Exascale", expected to be published in the beginning of 2019. This special issue will feature a position paper summarizing the main the conclusions of the workshop, as well as a collection of ten research papers dedicated to the theme of the workshop and written by participants of the workshop.

A main theme within the workshop was to identify generic algorithms and techniques for multiscale computing, and we agreed that the vision of multiscale computing patterns is very useful for a large range of multiscale models, independent of specific application domains. We also realised that such execution patterns would be broader applicable than only in a multiscale computing setting, but that such patterns should be applicable in any scenario where coupled components need to be executed on HPC environments, certainly when either the number of components or their coupling is dynamic, or both. This triggered deeper discussion on how generic software environments for multiscale computing could be developed, and how to make such environment useful in the context of HPC. This was based on existing systems such as the MMSF/Muscle or AMUSE, but also by mirroring such environments with the needs from different communities (e.g. from weather and climate, biomedicine, materials, fusion).

The workshop featured plenary lectures on specific topics, working sessions in smaller groups with rapporteurs making notes in a google doc shared among all participants. The working sessions were planned in detail (topics for discussion, intended outcomes), nominating participants to take part in specific working sessions to foster contacts and cross-disciplinary discussions. Two months before the workshop the organizers distributed relevant papers to participants and asked them to study this material, and to form their opinion on specific issues identified by the organisers. We also asked all participants to bring one (or more) posters of their current (and if relevant, past work) and put these on display. We organized a few speed sessions where participants get 5 minutes to present their poster to draw attention to their work and to trigger discussions. These speed sessions are always just before a scheduled break, so that discussions can immediately start. Overall we were satisfied with this format, although the speed sessions and poster presentations were not very crowded, meaning that most participants unfortunately did not bring a poster. This would probably work better in a larger setting, e.g. in Oort, and less so in Snellius.

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