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Multiscale Modelling and Simulation, 13th International Workshop

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Abstract

Multiscale Modelling and Simulation (MMS) is a cornerstone in the today's research in computational science. Simulations containing multiple models, with each model operating at a different temporal or spatial scale, are a challenging setting that frequently require innovative approaches in areas such as scale bridging, code deployment, error quantification, and scientific analysis. The aim of the MMS workshop is to encourage and consolidate the progress in this multidisciplinary research field, both in the areas of the scientific applications and the underlying infrastructures that enable these applications. Here we briefly introduce the scope of the workshop and highlight some of the key aspects of this year's submissions.

Keywords: modelling,simulation,multiscale,multiphysics,coupling

1 Introduction to the workshop

Modelling and simulation of multiscale systems constitutes a grand challenge in computational science, and is widely applied in fields ranging from the physical sciences and engineering to the life science and the socio-economic domain. Most of the real-life systems encompass interactions within and between a wide range of space and time scales, and/or on many separate levels of organization. They require the development of sophisticated models and computational techniques to accurately simulate the diversity and complexity of multiscale problems, and to effectively capture the wide range of relevant phenomena within these simulations.

Additionally, these multiscale models frequently need large scale computing capabilities as well as dedicated software and services that enable the exploitation of existing and evolving

computational ecosystems. Through this workshop we aim to provide a forum for multiscale application modellers, framework developers and experts from the distributed infrastructure communities to identify and discuss challenges in, and possible solutions for, modelling and simulating multiscale systems, as well as their execution on advanced computational resources and their validation against experimental data.

The workshop is a successor of the series of workshops on Simulation of Multiphysics Multiscale Systems organized during 2002-2015 [1]. This year's edition attracted 10 accepted presentations, covering a range of application domains, but also an unusually large fraction of cross-disciplinary research on multiscale simulation.

These cross-disciplinary talks include a review of multiscale coupling tools to improve scientific productivity, a general-purpose computational framework for scale bridging in multiscale simulations, and an software approach which helps automate the creation and execution of complex multiscale applications. Given the nature of the workshop, we look forward to lively discussions as the communities from different disciplines will have the opportunity to exchange ideas on general-purpose approaches from different angles.

In addition, we are pleased to host a range of contributions on cutting-edge applications of multiscale modelling, including multiscale models of organic electronics, stochastic slow-fast dynamics, rolling-contact fatigue, small-scale plasticity, ground water-land surface-river processes, laser propagation in optically active semiconductors, and electrokinetic transport in porous media. With representation from leading institutions across three different continents present this year, the 13th workshop on multiscale modelling and simulation is indeed at the forefront of computational science.

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