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Multiscale Modelling and Simulation, 14th International Workshop

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Abstract

Multiscale Modelling and Simulation (MMS) is a cornerstone in 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 series of workshops devoted to multiscale modelling and simulation is organized annualy from 2002 [1][2]. This year's edition attracted 14 accepted presentations, including one poster presentation. The discussed topics cover a range of application domains as well as cross-disciplinary research on multiscale simulation.

The workshop will contain the presentations about theoretical, general concepts of the multiscale computing and those focused on specific use-cases and describing real-life applications of multiscale modelling and simulation.

The theoretically-oriented presentations will include talks about reusable multiscale computing patterns, dynamic load balancing for heterogeneous hardware infrastructure, a multiscale approach to parabolic equations derivation, and a demonstration on performance monitoring of multiscale applications.

Our second segment will contain talks about specific use-cases in biology and medicine science. It will include presentations about personalized anti-tumor therapy, simulation of intimal hyperplasia with gene dynamics, modelling aortic-valve with stenosis, multiscale modelling systems medicine and the simulations of embryonic branching morphogenesis.

The third segment will focus on engineering, physics and multifactorial optimization problems. In this context the following works will be described: a new strategy to model energetic material deformation with help of surrogate evaluations, the numerical evaluation of local curvature for diffuse interface models of microstructure evolution, the investigation of stability and aggregation phenomena for the silica materials, multiscale modeling of problems in astrophysics with the AMUSE framework, and multiscale modelling of surgical flow in operating rooms.

Given the nature of the workshop, we look forward to lively discussions as communities from different disciplines will have the opportunity meet and to exchange ideas on general-purpose approaches from different angles. We hope that workshop will help participants to get familiar with the latest multiscale modelling, simulation and computing advances from other fields, and provide new inspiration for their own efforts.

With representation from leading institutions across three continents, the 14th edition of Multiscale Modelling and Simulation Workshop is indeed at the forefront of computational science.

Acknowledgments

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