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Computational Multiscale Methods

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Abstract. Almost all processes in engineering and the sciences are characterised by the complicated relation of features on a large range of non-separable spatial and time scales. The workshop concerned the computer-aided simulation of such processes, the underlying numerical algorithms and the mathematics behind them to foresee their performance in practical applications.

Mathematics Subject Classification (2010): 65, 35B, 74Q, 70F, 76A, 76M.

Introduction by the Organisers

Many processes in geophysics, material sciences, biology and quantum mechanics are multiscale in nature and it is the complex interplay of effects at a large range of non-separable scales in space and time that characterises their relevant and surprising properties. Since this complex interplay is intractable analytically, their understanding and control is intrinsically tied to numerical simulation. However, in many interesting applications, computers are not able to resolve all details on all relevant scales. In the foreseeable future, the observation and prediction of physical phenomena from multiscale models will require sophisticated numerical techniques for the effective representation of unresolved scales, i.e., computational multiscale methods.

Computational multiscale methods are a systematic approach to the modelling and simulation of multiscale problems that includes the derivation of detailed models (fine scale discretisation) adapted to all relevant scales, the derivation of reduced models of feasible computational complexity, e.g. the compression/filtering to coarse scales of interest while still maintaining its essential features (upscaling/homogenisation/coarse graining), the reconstruction of fines scale information from coarse scale computations (downscaling), and the fast simulation of the detailed/reduced model by iterative up- and downscaling (multilevel method) or concurrent coupling.

This workshop concerned the design of such efficient numerical algorithms and the mathematics behind them to foresee and assess their performance in engineering and scientific applications. For this purpose, the workshop broad together researchers with very different scientific backgrounds including numerical analysis, mathematical modelling, scientific computing, and computational mechanics. Amongst the particular trends of the workshop were numerical homogenization, discrete multiscale mathematical modelling, the coupling or blending of mathematical models on different scales, and the impact of randomness on models and numerical methods.

Computational homogenization refers to a class of numerical methods for partial differential equations with multiscale data aiming at the determination of macroscopic (effective) approximations that account for the complexity of the microstructure. While many approaches are empirically successful and robust for certain multiscale problems, there is an extremely high current interest for rigorous numerical analysis of those methods. This interest was reflected, e.g., by the lectures of Abdulle, Arbogast, Efendiev, Frederick, Hackbusch, Målqvist and Owhadi in the context of linear and non-linear problems. We have seen the high efficiency of numerical methods when structural knowledge of the problem is available but also the added value of computational homogenization when compared with classical analytical techniques, i.e., its applicability, reliability, and accuracy in the absence of strong assumptions such as periodicity and scale separation.

Multilevel approaches for the acceleration of the numerical solution of detailed models were addressed by Spillane for a linear model problem and also by Cancès and Henning in the context of the Kohn-Sham and the non-linear Schrödinger equation. The presentations of Gorb and Tsai presented network-type approaches to the effective numerical modelling of multiphase media. The lectures of Berlyand, van Brummelen, Heitzinger, Schmuck and Wheeler discussed the multiscale mathematical and numerical modelling of various multiscale and multiphysics problems. The estimation of modelling errors was addressed by Szepessy in the context of molecular dynamics simulations.

A major difficulty in multiscale problems is when fine scales and coarse scale are described by different equations. The lecture of Bochev and Luskin discussed the coupling of molecular and continuum models, Gunzburger and Lipton presented the intermediate model of peridynamics. Stochastic aspects and uncertainty quantification were also included in many lectures; Legoll addressed random homogenization, Bal studied the propagation of stochasticity in numerical homogenization, and Samaey discussed variance reduction methods for kinetic equations.

Most of the research presented during the week was motivated by applications such as the mechanical analysis of composite and multifunctional materials, transport processes in porous media, e.g. reservoir modelling or the transport of charged species in microfluidic devices, motility in biosystems, as well as the simulation of quantum mechanical systems. The range of related mathematical models included the minimisation of convex and non-convex energy functionals, inverse problems, non-linearly coupled systems as well as linear and non-linear eigenvalue problems. The large variety of applications and mathematical problems clearly demonstrated that the field of Computational Multiscale Methods is very active. Many promising results were presented and it is clear that in the future challenging multiscale problems and more general multiphysics applications will be investigated.

This workshop was well attended with 46 participants from 14 different countries (15 participants from the United States, 14 from Germany, 3 from France, 3 from Sweden, 2 from Switzerland, and respectively 1 from Austria, Belgium, Chile, China, England, Korea, Netherlands, Norway and Scotland). 26% of the participants were students or young postdocs (less than 3 years after their PhD).

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