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Introduction

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Multiscale modelling, simulation and computing: from the desktop to the exascale

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This short contribution introduces a theme issue dedicated to 'Multiscale modelling, simulation and computing: from the desktop to the exascale'. It holds a collection of articles presenting cutting-edge research in generic multiscale modelling and multiscale computing, and applications thereof on high-performance computing systems. The special issue starts with a position paper to discuss the paradigm of multiscale computing in the face of the emerging exascale, followed by a review and critical assessment of existing multiscale computing environments. This theme issue provides a state-of-the-art account of generic multiscale computing, as well as exciting examples of applications of such concepts in domains ranging from astrophysics, via material science and fusion, to biomedical sciences.

This article is part of the theme issue 'Multiscale modelling, simulation and computing: from the desktop to the exascale'.

1. Introduction to Theme Issue

Multiscale modelling, simulation and computing has been a major activity in the computational sciences over the last two decades, and will remain so in years to

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come [1]. Usually, these efforts are driven forward by the needs of specific applications or application domains, resulting in tailored solutions for these domains.

At the same time, there have been research efforts to define generic environments for multiscale modelling and simulation (e.g. [2–5]), which have been quite successful in achieving their goals, which merit a much stronger uptake by scientific communities. With this in mind, the guest editors of this theme issue organized a dedicated workshop to Multiscale computing, from the desktop to the exascale that was held from 16 to 20 April 2018 in the Lorentz Center in Leiden, the Netherlands,[1] which laid the foundations for this theme issue.

In 2014, this journal published a first theme issue on generic multiscale computing [6], in which Hoekstra *et al*. wrote a position paper [7] where they maintained that 'notwithstanding some notable successes, in our opinion, the field of multiscale modelling does have a number of unresolved questions that, although they are deemed important for the field, have so far hardly been explored'. These questions included a generic theory or calculus of multiscale modelling, verification, validation, and uncertainty quantification of multiscale models, and more efficient and well-defined multiscale computing environments. Two years later, a further issue dedicated to multiscale was published in this journal, entitled Bridging the gaps at the physics–chemistry–biology interface [8]. Although driven forward by challenging applications at the interface between physics, chemistry, biology, it also acknowledged and discussed the need for multiscale paradigms that would support applications at this PCB interface.

Over the last 4 years, and triggered in part by the 2014 special issue, we have witnessed exciting new developments pushing the envelope of multiscale modelling, for instance towards exascale performance levels [5], towards uncertainty quantification [9] (see also the recently started VECMA project[2]), and towards exciting new concepts for high-performance multiscale computing [10]. These are just a few examples of the now wide-ranging research into multiscale computing.

All this led to the organization of the 2018 Lorentz Center workshop and to bringing together a series of papers dedicated to Multiscale modelling, simulation and computing: from the desktop to the exascale into this theme issue. Hoekstra, *et al*. [11] have written a position paper in which they first investigate if generic multiscale modelling and simulation frameworks are possible (they conclude *yes*) and on where in the simulation-based science cycle the best opportunities can found. Next, they discuss scalability of applications towards the exascale, in relation to multiscale computing.

Groen *et al.* [12] not only provide a review of 22 available sets of multiscale computing software, they also review common steps in multiscale application development, and critically assess how these software environments may or may not be beneficial for these common steps.

Neumann *et al.* [13] and van Elteren *et al.* [14] introduce two challenging application domains, weather/climate and astrophysics, respectively, discuss the complex multiscale nature of problems addressed in those domains, and demonstrate if and how multiscale computing towards exascale performance would be able to provoke next big steps in these fields. Another equally complex and relevant field with potential impact, which could benefit tremendously from advanced multiscale computing, is that of soft flowing crystals. Montesorri *et al.* [15] highlight the challenges in modelling such systems, as well as when simulating realistic systems, and if and how exascale performance helps to meet those challenges.

Allowayed *et al.* proposed the vision of multiscale computing patterns to facilitate efficient high-performance multiscale computing [5] and provided a first proof of concept for two of those multiscale computing patterns, so-called extreme scaling and replica computing [10]. This special issue holds a few contributions that further elaborate the vision of multiscale computing, providing further evidence that this approach holds promises for high-performance multiscale computing towards exascale performance. First, Vasseux *et al.* [16] develop a heterogeneous

[1]See https://www.lorentzcenter.nl/lc/web/2018/993/info.php3?wsid=993&venue=Snellius.

[2]See https://www.vecma.eu.

multiscale modelling approach for inelastic polymer materials, and apply it to fracturing of such materials. This model is an example of a third multiscale computing pattern, called heterogeneous multiscale computing [5]. Luk *et al.* [17] discuss in detail a multiscale fusion plasma model and how the extreme scaling pattern enabled efficient high-performance multiscale computing for this application. The multiscale computing patterns provide generic means to schedule and deploy a multiscale simulation in a most efficient way on available computing resources. All users of supercomputers know that execution time is not the only metric that determines the overall throughput time of a simulation but also the time needed when a job is sitting in a queue, waiting to be executed. Alowayyed *et al*. already suggested that taking such waiting time into account in the multiscale computing patterns would help reach much more optimized scheduling decisions [10]. Jancauskas *et al.* [18] propose a method for predicting waiting times in queues of a production supercomputer (SuperMUC), and test it in scenarios relevant to high-performance multiscale computing.

We expect that an important use case scenario on exascale computers will be sensitivity analysis and uncertainty quantification of current multiscale models running at the peta scale. For simulation-based science to become a predictive science on which decisions can be based, its output needs to be enriched with clear measures of uncertainties, due to uncertain initial conditions and uncertain model parameters. But even at the exascale a brute-force, quasi Monte Carlo approach may fail due to huge computational demands, certainly when the number of uncertain parameters becomes large. Nikishova *et al.* [19] propose a method, called semi-intrusive uncertainty quantification, to reduce the computational demands of multiscale uncertainty quantification, by exploiting the multiscale structure and reducing calls to the most expensive micro-scale models.

Finally, in the periphery of the workshop, and following up on a paper by Coveney *et al.* [20], an ongoing discussion was on the impact of big data on simulation-based science. This led to a discussion paper where Coveney & Succi argue that 'the boldest claims of Big Data are in need of revision and toning-down' [21]. This paper has been included in this issue, as it touches on some quite fundamental issues that are relevant for all exascale computing initiatives.

We hope that this theme issue will contribute to further advancing the field of multiscale computing and that it will inspire readers in their own inquiries into the multiscale nature of the systems they study.

Data accessibility. This article has no additional data.

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