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Editors' preface for the topical issue "Numerical Methods for Large-Scale Scientific Computing, I"

Editorial Material

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The current issue of the Central European Journal of Mathematics is the first one of a two-part topical collection of papers devoted to recent advances in Numerical Methods for Large-Scale Scientific Computing. This issue contains 14 papers, presenting various theoretical and computational results with contributions from numerical scientists from Austria, Bulgaria, China, Czech Republic, Germany, Hungary, Russia, Spain, Sweden, and the USA.

Many complex problems arising in different fields of science and engineering can be successfully studied by applying large-scale mathematical models. The following are among the crucial issues when solving such problems: (i) robust numerical methods have to be developed in order to approximate the related partial differential equations (PDEs); (ii) scalable solution methods for the related discrete systems of equations are needed; (iii) the reliability of the produced numerical results has to be investigated. The efficient completion of the first task is in particular of primary importance in the case of ill-conditioned parameter-dependent problems. The second task can also raise great problems: let us notice that the size of current real-life applications could reach hundreds of millions or billions of degrees of freedom. For such problems, large-scale scientific computing naturally means parallel computing. The third task is very challenging as well: clarifying the uncertainties of the obtained results is of key importance for their practical applicability.

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This special issue is concerned mainly with the efficient solution of the first and partly of the second and the third tasks. A brief overview of the selected papers is given below.

The first section includes new basic results in advanced numerical methods for PDEs. They are mostly related to finite element methods (FEM) including error estimates, higher order accuracy post-processing, discrete analogues of certain conservation laws, etc. Second-order post-processing approximation of the gradients based on averaging of the linear FEM solution is presented in the paper by Josef Dalík and Václav Valenta. The article by Irina Georgieva, Clemens Hofreither, Christoph Koutschan, Veronika Pillwein and Thotsaporn Thanatipanonda is concerned with a harmonic interpolation along the sides of regular polygons based on Radon projections. The paper of Mingxia Li and Shipeng Mao presents a unified way to derive interpolation error estimates for anisotropic finite elements using orthogonal expansions. A Sobolev gradient method for the steady-state Navier–Stokes equations is elaborated by Robert Renka. The next paper deals with the numerical solution of parabolic problems: a comparison study of the string gradient weighted moving FEM and a moving mesh method is presented by Abigail Wacher. Then Tamás Horváth and Miklós Mincsovics establish the discrete maximum principle for certain interior penalty discontinuous Galerkin methods. In the next paper Marco Buck, Oleg Iliev and Heiko Andrä extend the multiscale FEM to the PDE system of linear elasticity. The paper by Larisa Beilina gives rigorous energy estimates and numerical verification for the stabilized Domain Decomposition FEM/FDM approach for Maxwell's system involving a non-constant electric permittivity function.

The second section is devoted to advanced numerical methods in mathematical modeling, including large scale scientific computing of environmental and life science problems. A mathematical model for the quantitative estimation of the damage to biological resources resulting from a pollutant discharge into an aqueous environment is proposed in the paper by Boris Arkhipov, Viacheslav Solbakov, Mikhail Solov'ev and Dmitry Shapochkin. An implicit-explicit method is developed by István Faragó, Ferenc Izsák, Tamás Szabó and Ákos Kriston for the numerical solution of reaction–diffusion equations with pure Neumann boundary conditions. The results are applied to determine the over-potential in a proton exchange membrane fuel cell. A mathematical model and numerical simulation of surface acoustic wave actuated cell sorting is presented by Thomas Franke and Ronald Hoppe. The inverse problem of determining the velocity characteristic of a medium from a vertical seismic survey is studied in the paper by Vladimir Bogdanov, Wladimir Karsten, Valeriy Miroshnichenko and Yuriy Volkov, including spline approximation of multivariate functions. The next article by Bruno Escribano, Elena Akhmatskaya and Jon Mujika is devoted to the implementation of the generalized shadow hybrid Monte Carlo method into the commonly used molecular dynamics code GROMACS, and to demonstrating the performance and accuracy of the new approach. The last article by Noémi Nagy and Péter Simon is devoted to Monte Carlo simulation and analytic approximation of epidemic processes on large networks based on low dimensional ODE approximations.

The editors would like to thank the authors of all articles in this issue for their valuable contribution. The work of the involved high-quality reviewers is also very highly appreciated.