Journal Pre-proof

Advanced numerical methods for complex scientific and engineering problems: Editorial introduction

Zahari Zlatev, Pasqua D'Ambra, István Faragó, Vladimir Shaydurov, Lubin Vulkov

PII: S0377-0427(19)30601-6
DOI: https://doi.org/10.1016/j.cam.2019.112596
Reference: CAM 112596

To appear in: *Journal of Computational and Applied Mathematics*

Please cite this article as: Z. Zlatev, P. D'Ambra, I. Faragó et al., Advanced numerical methods for complex scientific and engineering problems: Editorial introduction, *Journal of Computational and Applied Mathematics* (2019), doi: https://doi.org/10.1016/j.cam.2019.112596.

Advanced Numerical Methods for Complex Scientific and Engineering Problems: Editorial Introduction

Zahari Zlatev[1)], Pasqua D'Ambra[2)], István Faragó[3)], Vladimir Shaydurov[4)] and Lubin Vulkov[5)]

[1)] Department of Environmental Study, Aarhus University
Frederiksborgvej 399, P. O. Box 358, DK-4000 Roskilde, Denmark
E-mail address: zz@envs.au.dk

[2)] National Research Council of Italy
Institute for Applied Computing "Mauro Picone" (IAC)
IAC-CNR, Via Pietro Castellino 111, I-80131, Napoli, Italy
E-mail address: pasqua.dambra@cnr.it

[3)] Department of Applied Analysis and Computational Mathematics, Eötvös Loránd University
and MTA-ELTE NumNet Research Group
Pázmány P. s. 1/c, 1117 Budapest, Hungary
E-mail address: faragois@cd.elte.hu

[4)] Institute of Computational Modeling of SB RAS, 50/44,
Akademgorodok, Krasnoyarsk, 660036 Russia
E-mail address: shaidurov04@mail.ru

[5)] Department of Applied Mathematics and Statistics, Ruse University,
8 Studentska St., 7017 Ruse, Bulgaria
E-mail address: lvalkov@un-ruse.bg

Complex scientific and engineering models are very useful and very significant tools in the search for answers to many difficult questions which are important for the modern society. These models are often described mathematically by **non-linear systems** of partial differential equations. The discretization of the spatial derivatives in these systems leads to large non-linear systems of ordinary differential equations, which are normally stiff or even very stiff and, therefore, must be solved numerically by implicit methods. This results in non-linear systems of algebraic equations that have to be handled by applying appropriate and quickly convergent iterative methods. Different versions of the well-known Newton Iterative Procedure are often used in the solution of the non-linear algebraic equations (see, for example, [5]). In the inner loop of the iteration process it is always necessary to solve very large systems of linear algebraic equations. This means that **four major tasks** are to be resolved when advanced mathematical models describing complex scientific and engineering problems are handled on computers:

(A) Suitable space-discretization schemes have to be applied. Finite differences and finite elements are commonly used, see for example [6] and [7], but some other methods, for example, the pseudo-spectral discretization algorithms, similar to those described in [3], [9] and [10], can also be selected and successfully used.

(B) The obtained after the discretization of the spatial derivatives non-linear and stiff systems of ordinary differential equations have to be treated by fast and computationally stable implicit numerical methods. The application of variable stepsize variable formula methods, [8], might be suitable and efficient in many situations

(C) Some fast, reliable and convergent iterative methods have to be selected and applied in the treatment of the systems of non-linear algebraic equations (as, for example, the methods discussed in [5]).

(D) The final task can in theory be resolved exactly, but the problem is that the systems of linear algebraic equations are normally very large and can cause great computational difficulties even if modern high-speed computers are used. Therefore, efficient and at the same time sufficiently accurate implementation of fast methods for solving systems of linear algebraic equations is nearly always crucial for the success when complex scientific and engineering problems are handled on computers. Many kernels of the well-known LAPACK Library, [1] and [2], are easily available. Freely available software for linear algebra problems can be obtained from **http://www.netlib.org/utk/people/JackDongarra/la-sw.html.** However, special routines exploiting efficiently the properties of the particular problems that have to be handled can be even more efficient. This possibility is discussed in some of the papers in this special issue.

In spite of the fact that the modern computers are very fast and very powerful, it is still necessary to improve the efficiency of the existing numerical methods and to develop faster and more reliable new algorithms in the efforts to resolve successfully the computational tasks, which are permanently becoming much more difficult and much more time-consuming. The scientists and engineers should not rely **only** on the power of the new computers. They are also challenged to increase their efforts for designing advanced and efficient numerical algorithms, which will allow them to resolve successfully their problems on the computers available at present.

The efficient solution of the above four tasks, considered either together or separately, is discussed in the papers of this special issue. Therefore, we, the guest-editors of this special issue, believe, that many readers of the "Journal of Computational and Applied Mathematics" will find in the papers published in the Special Issue on "Advanced Numerical Methods for Complex Scientific and Engineering Problems" interesting material which will be useful for them in their efforts to find good solutions of their own problems.

We discussed the computational matters above, but some other issues are also very important. The complications are very often not over when the computations are finished. Extra difficulties arise, because the large-scale models are often producing huge sets of output data, millions and millions of numbers, and the developers should find out what information is hidden in these enormous output files. It is amazing that these difficulties were very precisely foreseen by **Richard Hamming** more than fifty years ago, in 1962, in spite of the fact that the amounts of output data were not very large at that time. He stated consistently and several times in his book, see [4], that

"The purpose of computations is insight not numbers"

Finding what the huge amount of calculated numbers is telling us became a great challenge, one of the greatest challenges, only in the new millennium. Solving this problem requires powerful visualization and animation techniques. Many such techniques were developed during the last decade and many examples for application of visualization of the calculated results can be found in the papers of this volume of the Journal of Computational and Applied Mathematics.

The Special Issue on **"Advanced Numerical Methods for Complex Scientific and Engineering Problems"** that is presented in this volume contains fourteen papers, in which advanced algorithms for handling efficiently the listed above problems are described and discussed.

A very broad range of topics is covered in the papers of this volume and many readers will find interesting algorithms in it, which will hopefully be very helpful for their own research.

We, the guest-editors of this Special Issue, should like to thank very much the authors of all published papers

- for accepting our invitation to submit the papers for publication in this Special Issue,
- for reading carefully the comments of the referees

and

- for taking into account their recommendations during the preparation of the revised papers and for re-submitting the final versions of their manuscripts in time.

We should like also to thank the referees of the papers of the Special Issue (including also the referees of the papers, which were not accepted for publication) for preparing very carefully and in time their reviews and for the constructive criticism, which resulted in considerable improvements of the quality of the accepted papers.

We should like to thank very much the members of the Editorial Board of the **"Journal of Computational and Applied Mathematics"** for the kind permission to prepare the Special Issue on ***"Advanced Numerical Methods for Complex Scientific and Engineering Problems"*** and for helping us permanently during the whole process of preparation of this Special Issue.

Finally, several people from the Publishing Company, Elsevier, helped us many times when we had different difficulties with **EES** (Elsevier Editing System) during our work related to the preparation of this Special Issue. We should like to thank all of them very much.

References:

[1] **E. Anderson, Z. Bai, C Bischof, C. Demmel, J. Dongarra, J. Du Croz, A. Greenbaum, S. Hammarling, A. McKenney, S. Ostrouchov and D. Sorensen:** "LAPACK: Users' Guide", SIAM (Society for Industrial and Applied Mathematics), Philadelphia, **1992**.

[2] **V. A. Barker, L. S. Blackford, J. Dongarra, J. Du Croz, S. Hammarling, M. Marinova, J. Wasniewski and P. Yalamov:** "*LAPACK95: Users' Guide*", SIAM (Society for Industrial and Applied Mathematics) Philadelphia, **2001**.

[3] **B Fornberg:** "*A Practical Guide to Pseudospectral Methods*", Cambridge Monographs on Applied and Computational Mathematics, Cambridge University Press, Cambridge, **1996**.

[4] **R. W. Hamming:** "*Numerical Methods for Scientists and Engineers*", McCraw Hill, New York, San Francisco, Toronto, London, **1962**.

[5] **C. T. Kelley:** "*Solving Nonlinear Equations with Newton's Method*", SIAM (Society for Industrial and Applied Mathematics), Philadelphia **1987**.

[6] **J. Strikwerda:** "*Finite Difference Schemes and Partial Differential Equations*", SIAM (Society for Industrial and Applied Mathematics), Philadelphia **2004**.

[7] **J. W. Thomas:** "*Numerical Partial Differential Equations: Finite Difference Methods*", Texts in Applied Mathematics 22, Springer, Berlin, **1998**.

[8] **Z. Zlatev:** "*Consistency and convergence of general multistep variable stepsize variable formula methods*". Computing, **Vol. 31 (1983)**, pp. 47-67.

[9] **Z. Zlatev, R. Berkowicz and L. P. Prahm:** "*Stability restrictions on time stepsize for numerical integration of first-order partial differential equations*". Journal of Computational Physics, **Vol. 51 (1983),** pp. 1-27.

[10] **Z. Zlatev, R. Berkowicz and L. P. Prahm:** "*Implementation of a variable stepsize variable formula method in the time-integration part of a code for long-range transport of air pollutants"*. Journal of Computational Physics, **Vol. 55 (1984),** pp. 279-301.