Computers and Mathematics with Applications 67 (2014) 2085–2087

Contents lists available at ScienceDirect

Computers and Mathematics with Applications

journal homepage: www.elsevier.com/locate/camwa

Editorial

Efficient algorithms for large scale scientific computations: Introduction

Complex mathematical models are extensively used in our modern computer age to handle many difficult problems which arise in different fields of science and engineering. These models are typically described by time-dependent systems of partial differential equations (PDEs) and lead after appropriate discretization of the spatial derivatives to the solution of huge systems of ordinary differential equations (ODEs). The number of equations in these systems of ODEs is very often greater than one million. The discretization of the time derivative in the systems of ODEs leads to the treatment of algebraic equations which are as a rule also very large, non-linear and have to be handled by applying iterative methods (very often the well-known quasi-Newton iterative procedure is used). Then huge systems of linear algebraic equations have to be solved during the iterative process. It should also be stressed that the mathematical models have normally to be run

(1) many times,
(2) on long time-intervals and
(3) with different scenarios.

During the last thirty or forty years the size of the mathematical models (and, more precisely, the number of equations which have to be handled after their discretization) was greatly increased in nearly all areas of science and engineering. Here it will be very illustrative to give an example. The work with the mathematical model discussed in [1,2] and [3], which is called **UNI-DEM** and is used for in studying the long-rage transport of air pollutants in a very large spatial domain containing the whole of Europe, was initiated in 1980. The gradually increased computational complexity of this large-scale model in the period 1980–2014 (due both to the refinement of the computational grids and to the larger numbers of involved chemical species) is shown in Table 1. It is seen that the number of the equations that are to be handled at each time-step was increased from 2048 up to 389376000 (i.e. by a factor of 19012.5). It must be mentioned here that the number of time-steps for a run covering meteorological data of one year is 213120. In the runs related to the impact of climatic changes on pollution levels in different parts of Europe [4–8] it was necessary to carry out calculations over a long period of **sixteen** years and to test **fourteen** different scenarios. It should be mentioned here that it is still not possible to run on regular basis the last two versions of the model that are shown in Table 1.

The increase of the computational complexity of an air pollution model in the period 1980–2014 (due to the refinement of the grids and to the involvement of more chemical species in the mathematical description of the underlying processes).

The results presented in Table 1 illustrate clearly that two very important facts had nearly always or at least very often to be taken into account:

(A) the requirements for preparing better and more reliable models are permanently increasing (the speed of this increase being much faster than the increase of the power of the computer architectures)

and

(B) it is very difficult to handle numerically the models (even on the modern computer architectures) when these become very big.

The first of these two facts is not very surprising. It confirms a statement which was made thirty years ago (in 1984) by Arthur Jaffe:

"Although the fastest computers can execute millions of operations in one second they are always too slow. This may seem a paradox, but the heart of the matter is: the bigger and better computers become, the larger are the problems scientists and engineers want to solve."

The scientists are without any stopping continuing to formulate, to develop and to treat computationally bigger and bigger mathematical models that impose very strong requirements for handling larger and larger data sets, because the solutions obtained in this way

http://dx.doi.org/10.1016/j.camwa.2014.05.021
0898-1221/© 2014 Published by Elsevier Ltd.

Table 1

No.	Dimensionality of the model	Number of grid-points	Number of chemical species	Number of equations
1	2-D	32×32	2	2 048
2	2-D	32×32	35	35 840
3	3-D	$32 \times 32 \times 10$	35	3 58 400
4	2-D	96×96	35	3 22 560
5	3-D	$96 \times 96 \times 10$	35	3 225 600
6	2-D	480×480	35	8 064 000
7	3-D	$480 \times 480 \times 10$	35	80 640 000
8	2-D	480×480	56	12 902 400
9	3-D	$480 \times 480 \times 10$	56	1 39 024 000
10	2-D	480×480	169	38 937 600
11	3-D	$480 \times 480 \times 10$	169	3 89 376 000

- will hopefully be ***closer*** to the reality,
- will certainly contain ***more*** details and ***more useful*** details, and
- will surely give ***more reliable*** answers to many questions.

The second fact, fact (B), is also very important. One is often inclined to believe that the development of efficient new computers is going very fast, but the truth is that for many scientific studies it is not fast enough (as was rightly stated many years ago by A. Jaffe). Therefore, it is necessary to resolve the following four tasks:

(a) efficient numerical methods are selected,
(b) parallel techniques are implied,
(c) splitting procedures are applied in order to exploit better the specific properties of the different operators involved in the models and
(d) the cache memories of the modern computer architectures are skilfully taken into account during the preparation of the codes.

It is probably impossible to satisfy the four tasks (a)–(d) in an optimal way and to define a computational procedure suitable for any large mathematical model (here by large we mean a model resulting in more than several millions of equations after applying suitable discretization rules). Therefore, in such a case the choice of a computational procedure for large mathematical models is always a result of some compromise. The need of a suitable compromise can be illustrate by the following two examples:

(A1) Increasing the accuracy of the numerical algorithms, very often leads to more time-consuming algorithms and, furthermore, the stability properties may become poor.
(A2) Applying splitting techniques facilitates the choice of numerical algorithms (for each of the resulting sub-models one can choose the most suitable algorithm) and the parallelization (many parallel tasks appear in a natural way), however the accuracy of these techniques is normally low.

Much more examples emphasizing the need of a reasonable compromise when large mathematical models have to be handled numerically can be given. It should be added here that there are as a rule many problems related to the quality of the needed input data as well as with the storage requirements, the visualization and the animation of enormous output data files.

The papers in this **Special Issue** are mainly devoted to the efficient solutions related to the **selection of numerical algorithms**. The tasks related to the improvement of the existing numerical algorithms as well as to the development of new and more efficient numerical algorithms are still extremely important for the numerical analysts. The selected papers deal mainly with the following important topics:

- Finite element methods are applied in the discretization of several types of PDEs or systems of PDEs.
- Iterative methods for the solution of large systems of linear algebraic equations arising after the discretization of elliptic PDEs.
- Application of finite volume schemes for studying particle dispersion in open channel flow.
- Algorithms for applying observation data in an attempt to improve the quality of the calculated by the mathematical models results.
- Treatment of reaction–diffusion models for studying ecosystems composed by one predator and two prey populations.
- Efficient application of splitting procedures.
- Investigation of different types of stability and its impact on the efficiency.
- Treatment of problems arising when multi-scale models are to be handled.
- Techniques related to mesh refinement.
- Difference schemes for convection-reaction–diffusion model.
- Need to solve inverse problems in connection with some classes of epidemic models.
- Solving problems related to nuclear plants.

- Treatment of some problems arising in environmental studies.
- Solving some problems related to three-dimensional elastic structures.
- Handling image reconstruction problems.
- Application of finite element and finite difference schemes in the discretization of the spatial derivatives of PDEs.
- Improving the accuracy of some numerical methods by using Richardson Extrapolation and studying the stability properties of the combination of explicit Runge–Kutta methods and the Richardson Extrapolation is verified.
- The impact of applying Richardson Extrapolation on the accuracy of the Crank–Nicolson scheme.

If the developers of large scale mathematical models are not interested in developing special numerical methods and many scientists and engineers are certainly not willing to do so, then they must have a sufficiently large selection of numerical methods which can be used in their particular case. In such a case, they will be able to select the numerical method which is suitable for their model. The papers in the Special Issue on **"Efficient Algorithms for Large Scale Scientific Computations"** will certainly contribute to the selection of promising numerical methods and computational devices.

Many of the papers in this Special Issue were presented at the International Conference on Large-Scale Scientific Computations held in June 6-10, 2013 (Sozopol, Bulgaria). The conferences on Large Scale Scientific Computations are regularly held in every second year. The last conference was the eighth one. The next conference will be held in June 2015. Sozopol is a very nice and quiet small town on the coast of the Black Sea and normally more than hundred participants from many countries are attending the conferences. We advise the readers of this Special Issue to consider the possibility of attending the next conference in Sozopol.

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

- accepting our invitation to submit their papers,
- reading carefully the comments of the referees and
- taking into account the comments during the preparation of the revised papers and re-submitting the final versions in time.

We should like also to thank the referees of the papers of this Special Issue (including also the referees of the papers which were not accepted for publication) for preparing 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 Editorial Board of the Journal of **"Computers and Mathematics with Applications"** for the kind permission to prepare this Special Issue on "Efficient Algorithms for Large Scale Scientific Computations" and for helping us permanently during the whole process of preparation of this special issue.

References

[1] V. Alexandrov, W. Owczarz, P.G. Thomsen, Z. Zlatev, Parallel runs of large air pollution models on a grid of SUN computers, Mathematics and Computers in Simulations 65 (2004) 557–577.
[2] Z. Zlatev, Computer Treatment of Large Air Pollution Models, Kluwer Academic Publishers, Dordrecht, 1995, (at present this book is distributed by Springer-Verlag, Berlin-Heidelberg).
[3] Z. Zlatev, I. Dimov, Computational and Numerical Challenges in Environmental Modelling, Elsevier, Amsterdam, 2006.
[4] I. Dimov, G. Geernaert, Z. Zlatev, Impact of future climate changes on high pollution levels, International Journal of Environment and Pollution 32 (2) (2008) 200–230.
[5] Z. Zlatev, Impact of future climate changes on high ozone levels in European suburban areas, Climatic Change 101 (2010) 447–483.
[6] Z. Zlatev, K. Georgiev, I. Dimov, Influence of climatic changes on air pollution levels in the Balkan Peninsula, Computers and Mathematics with Applications 65 (3) (2013) 544–562.
[7] Z. Zlatev, Á. Havasi, I. Faragó, Influence of climatic changes on pollution levels in Hungary and its surrounding countries, Atmosphere 2 (2011) 201–221.
[8] Z. Zlatev, L. Moseholm, Impact of climate changes on pollution levels in Denmark, Environmental Modelling 217 (2008) 305–319.
[9] A. Jaffe, Ordering the universe: the role of mathematics, SIAM Rev. 26 (1984) 475–488.

István Faragó
Department of Applied Analysis and Computational Mathematics and MTA-ELTE Numerical Analysis and Large Networks Research Group, Eötvös Loránd University, Budapest, Hungary

Krassimir Georgiev
Institute of Information and Communication Technologies, Bulgarian Academy of Sciences, Sofia, Bulgaria

Ágnes Havasi
Department of Applied Analysis and Computational Mathematics and MTA-ELTE Numerical Analysis and Large Networks Research Group, Eötvös Loránd University, Budapest, Hungary

Zahari Zlatev
Department of Environmental Science, Aarhus University, Roskilde, Denmark