Abstracts of scientific publications,

with which Assoc. Prof. Krasimir Todorov Georgiev participates in the competition for the occupation of the academic position of "Professor" in the field of higher education 4. "Natural sciences, mathematics and informatics", professional field 4.5. Mathematics, scientific specialty "Mathematical modeling and application of mathematics (in ecology)", announced in the State Gazette no. 49 / 21.06.2019 for the needs of section "Scientific Computations"of IICT-BAS

B4. Scientific publications in journals that have been referenced and indexed in world-renowned scientific databases (Web of Science, Scopus, Zentralblatt, MathSciNet, ACM Digital Library, IEEE Xplore, and AIS eLibrary) equivalent to habilitation work

1. Konstantinos Liolios, Vassilios Tsihrintzis, Konstantinos Moutsopoulos, Ivan Georgiev, and Krassimir Georgiev, A Computational Approach for Remediation, Procedures in Horizontal Subsurface Flow Constructed Wetlands, LNCS 7116, pp. 299–306, 2012, Springer-Verlag Berlin Heidelberg (SJR)

A large-scale computational approach for groundwater flow and contaminant transport and removal in porous media is presented. Emphasis is given to remediation procedures in horizontal subsurface flow constructed wetlands. For the numerical procedure, the MODFLOW computer code family is used. Application is made for the simulation of horizontal subsurface flow wetlands pilot-scale units, constructed and operated in Democritus University of Thrace, Xanthi, Greece. The effects of the inlet and outlet recharge positions to the optimum contaminant removal are also numerically investigated.

2. Liolios, K; Tsihrintzis, V; Georgiev, K; Georgiev, I, A Computational Investigation of the Optimal Reaction Type Concerning BOD Removal in Horizontal Subsurface Flow Constructed Wetlands, Studies in Computational Intelligence, Vol: 648, Pages: 29-45, DOI: 10.1007/978-3-319-32207-0_3, 2016 ***(SJR)***

A numerical simulation of Biochemical Oxygen Demand (BOD) removal in Horizontal Subsurface Flow Constructed Wetlands (HSF CW) is presented. Emphasis is given to select the optimal type of the reaction concerning the BOD removal. For this purpose, a computational investigation is realized by comparing the most usual reaction type, the first-order one, and the

recently proposed Monod type, with simulated experimental data obtained from five pilot-scale HSF CW units. These units were operated for 2 years in the facilities of the Laboratory of Ecological Engineering and Technology (LEET), Democritus University of Thrace (DUTh), Xanthi, Greece. For the numerical simulation the Visual MODFLOW family computer code is used, and especially the RT3D code.

3. Liolios, K; Tsihrintzis, V; Angelidis, P; Georgiev, K; Georgiev, I, Numerical Simulation for Horizontal Subsurface Flow Constructed Wetlands: A Short Review Including Geothermal Effects and Solution Bounding in Biodegradation Procedures, AIP Conference Proceedings, Vol: 1773, Article Number: 110009, DOI: 10.1063/14965013, 2016 ***(SJR)***

Current developments on modeling of groundwater flow and contaminant transport and removal in the porous media of Horizontal Subsurface Flow Constructed Wetlands (HSF CWs) are first reviewed in a short way. The two usual environmental engineering approaches, the black-box and the process-based one, are briefly presented. Next, recent research results obtained by using these two approaches are briefly discussed as application examples, where emphasis is given to the evaluation of the optimal design and operation parameters concerning HSF CWs. For the black-box approach, the use of Artificial Neural Networks is discussed for the formulation of models, which predict the removal performance of HSF CWs. A novel mathematical prove is presented, which concerns the dependence of the first-order removal coefficient on the Temperature and the Hydraulic Residence Time. For the process-based approach, an application example is first discussed which concerns procedures to evaluate the optimal range of values for the removal coefficient, dependent on either the Temperature or the Hydraulic Residence Time. This evaluation is based on simulating available experimental results of pilot-scale units operated in Democritus University of Thrace, Xanthi, Greece. Further, in a second example, a novel enlargement of the system of Partial Differential Equations is presented, in order to include geothermal effects. Finally, in a third example, the case of parameters uncertainty concerning biodegradation procedures is considered and the use of upper and a novel approach is presented, which concerns the upper and the lower solution bound for the practical draft design of HSF CWs.

4. Liolios, K; Tsihrintzis, V; Georgiev, K; Georgiev, I, Geothermal Effects for BOD Removal in Horizontal Subsurface Flow Constructed Wetlands: A Numerical

Approach, Studies in Computational Intelligence, Vol: 681 Pages: 115-125, DOI: 10.1007/978-3-319-49544-6_10, 2017 ***(SJR)***

A simplified numerical approach is presented for the simultaneous groundwater flow, geothermal energy (heat) transport and contaminant transport and removal in shallow unconfined aquifers. Emphasis is given to Biochemical Oxygen Demand (BOD) removal in Horizontal Subsurface Flow Constructed Wetlands (HSF CW), under non-isothermal conditions. The system of the governing non-linear partial differential equations is treated numerically by using the family computer code Visual MODFLOW. In a numerical example, where BOD is injected in entering geothermal water, the so-resulted computational results are compared with available experimental data.

5. Liolios, K; Tsihrintzis, V; Angelidis, P; Georgiev, K; Georgiev, I, Total Phosphorus Removal in Horizontal Subsurface Flow Constructed Wetlands: A Computational Investigation for the Optimal Adsorption Model, Studies in Computational Intelligence, Vol: 728 Pages: 109-121, DOI: 10.1007/978-3-319-65530-7_11, 2018 (SJR)

A numerical simulation concerning Total Phosphorus (TP) removal in Horizontal Subsurface Flow Constructed Wetlands (HSF CWs) is presented. For the phenomenon of absorption, a comparison between the results of a linear and a non-linear model is realized. The purpose is to investigate which one of these two adsorption models is the optimal one for the computational simulation of TP removal. The simulations concern five pilot-scale HSF CWs units, which were constructed and operated in the facilities of the Laboratory of Ecological Engineering and Technology (LEET), Department of Environmental Engineering, Democritus University of Thrace (DUTh), Xanthi, Greece. Concerning the numerical simulation, the Visual MODFLOW computer code is used, which is based on the finite difference method. Finally, a comparison between computational and available experimental results is given.

Γ7. Scientific publications in publications that have been referenced and indexed in world-renowned scientific databases (Web of Science, Scopus, Zentralblatt, MathSciNet, ACM Digital Library, IEEE Xplore, and AIS eLibrary), other than publications under item B4

1. Antonov, A; Georgiev, K; Komsalova, E; Zlatev, Z, *Comparison of two local refinement methods for Large Scale Air Pollution simulations*, Lecture Notes in Computer Science, Vol: 2907 Pages: 287-294, 2003 (IF, Q4)

Two methods for Large Scale Air Pollution (LSAP) simulations over static grids with local refinements are compared using the object-oriented version of the Danish Eulerian Model. Both methods are based on the Galerkin finite element method. The first one is over a static locally refined grid – we call it Static Local Refinement Algorithm (SLRA). We compare SLRA with the Recursive Static-Regridding Algorithm (RSRA), in which regular grids with finer resolution are nested within a coarser mother grid. RSRA and SLRA are compared with the translational and rotational cone tests. The drawbacks and advantages of the methods are discussed.

2. Georgiev, K, On an Implementation of the TM5 Global Model on a Cluster of Workstations, Lecture Notes in Computer Science, Vol: 4310, pp. 451–457, 2007. (IF, Q4)

TM5 is a global chemistry Transport Model. It allows two-way nested zooming which leads to possibility to run the model on relatively very fine space grid ($1^{\circ} \times 1^{\circ}$) over selected regions (Europe is most often used in up to now experiments but North America, Africa and Asia can be treated separately or in combinations). The boundary conditions for the zoomed subdomains are provided consistently from the global model. The TM5 model is a good tool for studying some effects due to the grid refinement on global atmospheric chemistry issues (intercontinental transport of air pollutants, etc.). The huge increase in the number of the multi-processor platforms and their differences leads to a need of different approaches in order to meet the requirements for the optimality of the computer runs. The paper is devoted to an implementation of a parallel version of the TM5 model on a cluster of SUN Workstations and to the developing of a new parallel algorithm. It is based on the decomposition, in some sense, of the computational domain supposing that the zoomed regions are more than one. If it is assumed that the number of zoomed regions is N and the number of the processors available is p. The processors are divided in N/p groups and each group is responsible for the whole computational domain and one of the zoomed regions. Some communications are needed in order to impose the inner boundary conditions. The new algorithm has better parallel feathers than the old one

which is used in the inner level. Some results concerning the CPU time, speed up and efficiency can be found.

3. I. Dimov, K. Georgiev, Tz. Ostromsky, Z. Zlatev, Computational challeneges in the numerical treatment of large air pollution models, Ecological Modelling, 179 (2004)187 – 203, Elsevier, DOI: 10.1016/j.ecolmodel.2004.06.019, (IF, Q2)

The air pollution, and especially the reduction of the air pollution to some acceptable levels, is an important environmental problem, which will become even more important in the next 10-20 years. This problem can successfully be studied only when high-resolution comprehensive models are developed and used on a routinely basis. However, such models are very time-consuming, also when modern high-speed computers are available. Indeed, if an air pollution model is to be applied on a large space domain by using ne grids, then its discretization will always lead to huge computational problems. Assume, for example, that the space domain is discretized by using a (480x480) grid and that the number of chemical species studied by the model is 35. Then several systems of ordinary differential equations containing 8064000 equations have to be treated at every time-step (the number of time-steps being typically several thousand). If a three-dimensional version of the same air pollution model is to be used, then the above figure must be multiplied by t h e n umber of layers. It is extremely difficult to treat such large computational problems even when the fastest computers that are available at present are used. There is an additional great difficulty, which is very often underestimated (or even neglected) when large application packages are moved from sequential computers to modern parallel machines. The high-speed computers have normally a very complicated memory architecture and, therefore, the task of producing an efficient code for the particular high-speed computer that is available is both extremely hard and very laborious. The use of standard parallelization tools in the solution of the problems sketched above is discussed in this paper. Results obtained on different types of parallel computers are given. It is demonstrated that the new efficient parallel algorithms allow us to solve more problems and bigger problems.

4. Zlatev, Z; Georgiev, K, Treatment of large scientific problems: An introduction, Lecture Notes in Computer Science, Volume: 3732, Pages: 828-830, 2006 (IF, Q4)

The computers are becoming faster and faster. Their capabilities to deal with very large data sets are steadily increasing. Problems that require a lot of computing time and rely on the use of huge files of input data can now be treated on powerful workstations and PCs (such problems had to be treated on powerful mainframes only 5-6 years ago). Therefore, it is necessary to answer the following two important questions: Are the computers that are available at present large enough? Do we need bigger (here and in the remaining part of this introduction, "a bigger computer" means a computer with larger memory discs, not a physically bigger computer) and faster computers for the treatment of the large-scale scientific problems, which appear in different fields of science and engineering and have to be resolved either now or in the near future?

5. Georgiev, K; Kosturski, N; Margenov S, On the numerical solution of the heat transfer equation in the process of freeze drying, Lecture Notes in Computer Science, Vol: 4818 Pages: 410-416, DOI: 10.1007/978-3-540-78827-0_46 , 2008 (SJR)

The coupled process of vacuum freeze drying is modelled by a system of nonlinear partial differential equations. This article is focused on the submodel of heat and mass transfer in the absorption camera. The numerical treatment of the related parabolic partial differential equation is considered. The selected numerical results well illustrate the specific issues of the problem as well as some recently obtained results. Brief concluding remarks and prospectives for future investigations are given at the end.

6. Zlatev, Z; Ebel, A; Georgiev, K, Editorial: large-scale computations in environmental modelling, INTERNATIONAL JOURNAL OF ENVIRONMENT AND POLLUTION, Vol: 32 Issue: 2 Pages: 135-138, 2008 (IF, Q1)

The protection of our environment is one of the most important problems faced by the modern society. The importance of this problem has been increasing steadily for the past three to four decades, and protecting the environment is becoming even more important in the 21st century. Reliable and robust control strategies for keeping the pollution caused by harmful chemical compounds below certain safe levels have to be developed and used in a routine way. Large mathematical models, in which all the important physical and chemical processes are adequately described, can successfully be used to support this task. However, the use of large-scale mathematical models in which all the important physical and chemical processes are

adequately described leads, after the application of appropriate discretisation and splitting procedures, to the treatment of huge computational tasks. In a typical simulation, one has to perform several hundred runs. In each of these runs, one has to carry out several thousand time-steps and at each time-step, one has to solve numerically systems of coupled ordinary differential equations containing up to several million equations. Therefore, it is difficult to treat demanding mathematical models numerically even when fast modern computers are available.

7. Farago, I; Georgiev, K; Thomsen, P.G; Zlatev, Z, Numerical and computational issues related to applied mathematical modelling – Preface, APPLIED MATHEMATICAL MODELLING, Vol: 32 Issue: 8 Pages: 1475-1476, 2008, DOI: 10.1016/j.apm.2007.06.035 (IF, Q1)

Mathematical models are powerful tools when different relationships in the nature and in the society have to be studied. This is why such models are commonly used in many fields of science and engineering. Analytical solutions of the mathematical models are normally not available. Therefore, the mathematical models are to be treated numerically on computers. The computers are becoming more and more powerful. This allows the scientists and the engineers to build up more and more comprehensive models. This means that the development of more powerful computers stimulates the scientists and the engineers to develop more advanced, more complex and more comprehensive mathematical models.

8. Zlatev, Z; Ebel, A; Georgiev, K; Jose, RS, Large scale computations in environmental modelling: Editorial introduction, ECOLOGICAL MODELLING, Vol: 217 Issue: 3-4 Pages: 207-208, DOI: 10.1016/j.ecolmodel.2008.06.001, 2008 (IF, Q2)

Environmental problems are becoming more and more important for the modern society, and their importance will certainly be increased in the near future. High pollution levels (high concentrations and/or high depositions of certain harmful chemical species) may cause damages to plants, animals and humans. Moreover, some eco-systems can also be damaged (or even destroyed) when the pollution levels become very high. This is why the pollution levels must be carefully studied in the efforts

- to predict the appearance of high pollution levels, which may cause different damages in our environment and/or

- to decide what must be done in order to keep the harmful concentrations and/or depositions under prescribed acceptable limits.

9. Georgiev, K; Kosturski, N; Margenov, S; Stary, J, On adaptive time stepping for large-scale parabolic problems: Computer simulation of heat and mass transfer in vacuum freeze-drying, JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS, Vol: 226 Issue: 2, Pages: 268-274, DOI: 10.1016/j.cam.2008.08.020, 2009 (IF, Q1)

The work is motivated by the problem of freeze-drying, which is a process of dehydrating frozen materials by sublimation under high vacuum. In particular, it concerns the mathematical modelling and computer simulation of the heat and mass transfer with the core in solving the time-dependent nonlinear partial differential equation of parabolic type.

Instead of a uniform discretization of the considered time interval, an adaptive time-stepping procedure is applied in an effort to optimize the whole simulation. The procedure is based on the local comparison of the Crank–Nicolson and backward Euler approximations. The results of numerical experiments performed on a selected real-life problem are included.

10. Georgiev, K; Zlatev, Z, Runs of UNI-DEM Model on IBM Blue Gene/P Computer and Analysis of the Model Performance, Lecture Notes in Computer Science, Vol: 5910, Pages: 188–196, DOI: 10.1007/978-3-642-12535-5_21, 2010 (SJR)

UNI–DEM is an Eulerian model for studying long range transport of air pollutants. The computational domain of the model covers Europe and some neighbour parts of Atlantic ocean, Asia and Africa. The model mainly is developed in the National Environmental Research Institute of Denmark, located at Roskilde. If UNI–DEM model is to be applied on a large space domain by using fine grids, then its discretization leads to a huge computational problem. If the space domain is discretized by using a (480 x 480) grid and the number of chemical species studied by the model is 35, then several systems of ordinary differential equations containing 8 064 000 equations have to be treated at every time-step (the number of time-steps being typically several thousand). If a three-dimensional version of the same air pollution model is to be used, then the figure above must be multiplied by the number of layers. This implies that such a model as UNI–DEM must be run only on high-performance computer architectures, like IBM Blue Gene/P. The implementation of such complex large–scale model on each new

computer is a non trivial task. Analysis of the runs of UNI–DEM performed until now on IBM Blue Gene/P computer is presented and some preliminary results on performance, speed ups and efficiency are discussed.

11. Georgiev, K; Zlatev, Z, Studying an Eulerian Computer Model on Different High-performance Computer Platforms and Some Applications, AIP Conference Proceedings, Vol: 1301 Pages: 476-+, 2010 (SJR)

The Danish Eulerian Model (DEM) is an Eulerian model for studying the transport of air pollutants on large scale. Originally, the model was developed at the National Environmental Research Institute of Denmark. The model computational domain covers Europe and some neighbour parts belong to the Atlantic Ocean, Asia and Africa. If DEM model is to be applied by using fine grids, then its discretization leads to a huge computational problem. This implies that such a model as DEM must be run only on high-performance computer architectures. The implementation and tuning of such a complex large-scale model on each different computer is a non-trivial task. Here, some comparison results of running of this model on different kind of vector (CRAY C92A, Fujitsu, etc.), parallel computers with distributed memory (IBM SP, CRAY T3E, Beowulf clusters, Macintosh G4 clusters, etc.), parallel computers with shared memory (SGI Origin, SUN, etc.) and parallel computers with two levels of parallelism (IBM SMP, IBM BlueGene/P, clusters of multiprocessor nodes, etc.) will be presented. The main idea in the parallel version of DEM is domain partitioning approach. Discussions according to the effective use of the cache and hierarchical memories of the modern computers as well as the performance, speed-ups and efficiency achieved will be done. The parallel code of DEM, created by using MPI standard library, appears to be highly portable and shows good efficiency and scalability on different kind of vector and parallel computers. Some important applications of the computer model output are presented in short.

12. Ganzha, M; Georgiev, K; Lirkov, I; Margenov, S; Paprzycki, M, Highly Parallel Alternating Directions Algorithm for Time Dependent Problems, AIP Conference Proceedings, Vol: 1404, DOI: 10.1063/1.3659922, 2011 (SJR)

In our work, we consider the time dependent Stokes equation on a finite time interval and on a uniform rectangular mesh, written in terms of velocity and pressure. For this problem, a parallel algorithm based on a novel direction splitting approach is developed. Here, the pressure

equation is derived from a perturbed form of the continuity equation, in which the incompressibility constraint is penalized in a negative norm induced by the direction splitting. The scheme used in the algorithm is composed of two parts: (i) velocity prediction, and (ii) pressure correction. This is a Crank-Nicolson-type two-stage time integration scheme for two and three dimensional parabolic problems in which the second-order derivative, with respect to each space variable, is treated implicitly while the other variable is made explicit at each time sub-step. In order to achieve a good parallel performance the solution of the Poison problem for the pressure correction is replaced by solving a sequence of one-dimensional second order elliptic boundary value problems in each spatial direction. The parallel code is implemented using the standard MPI functions and tested on two modern parallel computer systems. The performed numerical tests demonstrate good level of parallel efficiency and scalability of the studied direction-splitting-based algorithm.

13. Zlatev, Z; Dimov, I; Farago, I; Georgiev, K; Havasi, A; Ostromsky, T, Richardson Extrapolated Numerical Methods for Treatment of One-Dimensional Advection Equations, Lecture Notes in Computer Science, Vol: 6046 Pages: 198-+, 2011 (SJR)

Advection equations are an essential part of many mathematical models arising in different fields of science and engineering. It is important to treat such equations with efficient numerical schemes. The well-known Crank-Nicolson scheme will be applied. It will be shown that the accuracy of the calculated results can be improved when the Crank-Nicolson scheme is combined with the Richardson Extrapolation.

14. Georgiev, K; Zlatev, Specialized Sparse Matrices Solver in the Chemical Part of an Environmental Model, Lecture Notes in Computer Science, Vol: 6046 Pages: 158-166, 2011 (SJR

A two-dimensional advection-diffusion-chemistry module of a large-scale environmental model (Danish Eulerian Model for studying the transport of air pollutants on large scale - UNI-DEM) is taken. The module is described mathematically by system of partial differential equations. Sequential splitting is used in the numerical treatment. The non-linear chemistry is most the time-consuming part during the computer runs and it is handled by six implicit algorithms for solving ordinary differential equations. This leads to the solution of very long sequences of systems of linear algebraic equations. It is crucial to solve these systems

efficiently. This is achieved by applying four different algorithms, which are developed, tested and discussed.

15. Georgiev, K; Zlatev, Z, Studying air pollution levels in the Balkan Peninsula area by using an IBM Blue Gene/P computer, INTERNATIONAL JOURNAL OF ENVIRONMENT AND POLLUTION, Vol: 46 Issue: 1-2 Pages: 97-114, DOI: 10.1504/IJEP.2011.042611, 2011 (IF, Q4)

The Unified Danish Eulerian Model (UNI–DEM) is an appropriate model for investigating both the transport on long distances and the transformations in the atmosphere of pollutants, which are potentially harmful. This mathematical model was developed at the National Environmental Research Institute (NERI, Roskilde, Denmark). The spatial domain of the model covers Europe and some its neighbouring parts. The parallel code of UNI–DEM is created by using the MPI standard library. It is highly portable and performs very efficiently on different kind of parallel computers. An IBM Blue Gene/P computer is used in this study.

16. Georgiev, K; Zlatev, Z, Ebel, A, Editoral, INTERNATIONAL JOURNAL OF ENVIRONMENT AND POLLUTION, Vol: 46 Issue: 1-2 Pages: 1-5, DOI: 10.1504/IJEP.2011.042611, 2011 (IF, Q4)

The control of the pollution levels in highly developed regions of Europe, Eastern Asia (first and foremost, China and Japan) and North America is a very challenging task for the modern society. This task is also very important or, at least, will soon become very important for many other highly industrialised regions of the world. Its relevance has been steadily increasing during the last two to three decades. The need of establishing reliable control strategies for the pollution levels in order to prevent damaging effects on plants, animals and human beings will become even more significant in the future. Large-scale environmental models for studying the harmful effects that are caused or may be caused by high pollution levels can successfully be used, when several conditions are satisfied, to design robust and reliable control strategies. In many cases, the application of advanced models is the only means by which many important physical and chemical processes can be investigated. The influence of future climatic changes on the high pollution levels is one example for a situation in which only models can be used. Both the development of modern modelling systems and, even to a greater degree advanced

applications of such systems in different environmental studies are employed in many countries by researchers from different scientific areas. Studies and simulations related to:

- implementation and use of data assimilation
- use of advanced computer architectures to handle modelling systems numerically
- impact of climatic changes on pollution levels
- damaging effects caused by aerosols
- dust simulation
- sensitivity analysis
- forest fires, etc.

are major topics of investigations in the area of environmental modelling.

17. Georgiev, K; Zlatev, Z, Implementation of sparse matrix algorithms in an advection-diffusion-chemistry module, JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS, Vol: 236 Issue: 3, Pages: 342-353, DOI: 10.1016/j.cam.2011.07.026, 2011 (IF, Q2)

A two-dimensional advection–diffusion–chemistry module of a large-scale environmental model is taken. The module is described mathematically by a system of partial differential equations. Sequential splitting is used in the numerical treatment. The non-linear chemistry is most time-consuming part and it is handled by six implicit algorithms for solving ordinary differential equations. This leads to the solution of very long sequences of systems of linear algebraic equations. It is crucial to solve these systems efficiently. This is achieved by applying four different algorithms. The numerical results indicate that the algorithms based on a preconditioned sparse matrix technique and on a specially designed algorithm for the particular problem under consideration perform best.

18. Zahari Zlatev, Ivan Dimov, Istvan Farago, Krassimir Georgiev, Agnes Havasi, and Tzvetan Ostromsky, Solving Advection Equations by Applying the Crank-Nicolson Scheme Combined with the Richardson Extrapolation, Hindawi Publishing

Corporation, International Journal of Differential Equations, Volume 2011, Article ID 520840, 16 pages, doi:10.1155/2011/520840

Advection equations appear often in large-scale mathematical models arising in many fields of science and engineering. The Crank-Nicolson scheme can successfully be used in the numerical treatment of such equations. The accuracy of the numerical solution can sometimes be increased substantially by applying the Richardson Extrapolation. Two theorems related to the accuracy of the calculations will be formulated and proved in this paper. The usefulness of the combination consisting of the Crank-Nicolson scheme and the Richardson Extrapolation will be illustrated by numerical examples.

19. Ostromsky, Tz; Georgiev, K; Zlatev, Z, An Efficient Highly Parallel Implementation of a Large Air Pollution Model on an IBM Blue Gene Supercomputer, AIP Conference Proceedings, Volume: 1487 Pages: 135-142 DOI: 10.1063/1.4758951, 2012 (SJR)

In this paper we discuss the efficient distributed-memory parallelization strategy of the Unified Danish Eulerian Model (UNI-DEM). We apply an improved decomposition strategy to the spatial domain in order to get more parallel tasks (based on the larger number of subdomains) with less communications between them (due to optimization of the overlapping area when the advection-diffusion problem is solved numerically). This kind of rectangular block partitioning (with a square shape trend) allows us not only to increase significantly the number of potential parallel tasks, but also to reduce the local memory requirements per task, which is critical for the distributed-memory implementation of the higher-resolution/finer-grid versions of UNI-DEM on some parallel systems, and particularly on the IBM BlueGene/P platform - our target hardware. We will show by experiments that our new parallel implementation can use rather efficiently the resources of the powerful IBM BlueGene/P supercomputer, the largest in Bulgaria, up to its full capacity. It turned out to be extremely useful in the large and computationally expensive numerical experiments, carried out to calculate some initial data for sensitivity analysis of the Danish Eulerian model.

20. Georgiev, K; Zlatev, Z, Numerical Experiments with Applying Approximate LU-factorizations as Preconditioners for Solving SLAEs with Coefficient Matrices from

the "Sparse Matrix Market", AIP Conference Proceedings, Vol: 1487, pp 104-111, 2012 (SJR)

The solution of systems of linear algebraic equations (SLAEs) is very often the most time-consuming part of the computational process during the treatment of the original problems, because these systems can be very large (containing up to many millions of equations). It is, therefore, important to select fast, robust and reliable methods for the solution of SLAEs when large applications are to be run, also in the case where fast modern computers are available. Since the coefficient matrices of the systems are normally sparse (i.e., most of their elements are zeros), the first requirement is to exploit efficiently the sparsity. However, this is normally not sufficient when the systems are very large. The computation of preconditioners based on approximate LU-factorizations and their use in the efforts to increase further the efficiency of the calculations will be discussed in this paper. Computational experiments based on comprehensive comparisons of many numerical results that are obtained by using ten well-known methods for solving SLAEs (the direct Gaussian elimination and nine iterative methods) when the coefficient matrices are chosen from the "Sparse Matrix Market" are reported in this paper. Most of the methods are preconditioned Krylov sub-space algorithms.

21. Krassimir Georgiev, Tzvetan Ostromsky, and Zahari Zlatev, New Parallel Implementation of an Air Pollution Computer Model – Performance Study on an IBM Blue Gene/P Computer, LNCS 7116, pp. 283–290, 2012, Springer-Verlag Berlin Heidelberg (SJR)

A new parallel version of the Danish Eulerian model for long transport of air pollutants over the territory of Europe (UNI–DEM) is presented. It is based on the domain partitioning of the space domain both in the *Ox* and *in Oy* directions. This new approach gives possibilities to use large number of processors (or cores) on the IBM BlueGene/P computer. The new version of the parallel code of the UNI–DEM is created by using MPI standard library, appears to be highly portable, and shows good efficiency and scalability. Discussions according to the performance, speed-ups and efficiency achieved in the first testing runs of the new parallel code on an IBM Blue Gene/P computer are presented.

22. Zlatev, Z; Georgiev, K; Dimov, I, Influence of climatic changes on pollution levels in the Balkan Peninsula, COMPUTERS & MATHEMATICS WITH APPLICATIONS,

Volume: 65 Issue: 3 Pages: 544-562, DOI: 10.1016/j.camwa.2012.07.006, 2013 (IF, Q1)

The aim of the paper is to study the influence of future climatic changes on some high pollution levels that can cause damages on plants, animals and human beings. The particular area of interest is the Balkan Peninsula. Four important quantities have been selected: (a) annual concentrations, (b) AOT40C (high AOT40C values can cause damages on plants and, first and foremost, crops), (c) AOT40F (high AOT40F values can cause damages on forest trees), (d) number of ‘‘bad days’’ (large numbers of ‘‘bad days’’ can cause damage to people suffering from asthmatic diseases).

Critical levels for the quantities from (b), (c) and (d) are legislated by several directives of the European Parliament (see, for example, [European Parliament Directive 2002/3/EC of the European Parliament and the Council of 12 February 2002 relating to ozone in ambient air, Official Journal of the European Communities L67 (2002) 14–30]). We are mainly interested in cases where the prescribed in the directives critical values are exceeded.

An advanced mathematical model was used to run fourteen scenarios over a period of sixteen years. Results, which are obtained in the selected domain, the Balkan Peninsula, with some of these scenarios, are carefully studied. The major conclusion is that the increase of the temperature, alone or in combination with some other factors, leads to rather considerable increases of some pollution levels, which might become dangerous for the environment.

23. Farago, I; Georgiev, K; Havasi, A; Zlatev, Z, Efficient numerical methods for scientific applications: Introduction, COMPUTERS & MATHEMATICS WITH APPLICATIONS, Vol: 65 Issue: 3 Pages: 297-300, DOI: 10.1016/j.camwa.2013.01.001, 2013 (IF, Q1)

Large-scale mathematical models are extensively used in the modern computer age to handle many complex problems which arise in different fields of science and engineering. These models are typically described by time-dependent systems of partial differential equations (PDEs).

The discretization of the spatial derivatives in these systems of PDEs leads to huge systems of ordinary differential equations (ODEs), which are normally solved numerically step by step. The number of steps may be enormous. Furthermore, very often the systems of ODEs are stiff, which implies the use of implicit numerical methods.

If an implicit method for solving linear systems of ODEs is applied, then one or several systems of linear algebraic equations (the number of these systems depends on the particular implicit method for solving stiff systems of ODEs which was selected) have to be solved at every time-step. If the system of ODEs is non-linear, then non-linear systems have to be treated. This is usually done by applying some quasi Newton iterative method and again implies, during each iteration step, the solution of systems of linear algebraic equations. It should also be stressed that the mathematical models have normally to be run (a) many times, (b) on long time-intervals and (c) with different scenarios.

This short analysis is presented, which very clearly shows the four major numerical tasks are to be handled during the treatment of the mathematical models.

24. Zlatev, Z; Georgiev, K, Applying approximate LU-factorizations as preconditioners in eight iterative methods for solving systems of linear algebraic equations, CENTRAL EUROPEAN JOURNAL OF MATHEMATICS, Vol: 11 Issue: 8 Pages: 1510-1530, DOI: 10.2478/s11533-013-0248-2 (IF, Q3)

Many problems arising in different fields of science and engineering can be reduced, by applying some appropriate discretization, either to a system of linear algebraic equations or to a sequence of such systems. The solution of a system of linear algebraic equations is very often the most time-consuming part of the computational process during the treatment of the original problem, because these systems can be very large (containing up to many millions of equations). It is, therefore, important to select fast, robust and reliable methods for their solution, also in the case where fast modern computers are available. Since the coefficient matrices of the systems are normally sparse (i.e. most of their elements are zeros), the first requirement is to efficiently exploit the sparsity. However, this is normally not sufficient when the systems are very large. The computation of preconditioners based on approximate LU-factorizations and their use in the efforts to increase further the efficiency of the calculations will be discussed in this paper. Computational experiments based on comprehensive comparisons of many numerical results that are obtained by using ten well-known methods for solving systems of linear algebraic equations (the direct Gaussian elimination and nine iterative methods) will be reported. Most of the considered methods are preconditioned Krylov subspace algorithms.

25. Zlatev, Z; Georgiev, K; Dimov, I, Stability Properties of Explicit Runge-Kutta Methods Combined with Richardson Extrapolation, Lecture Notes in Computer Science, Vol: 8353 Pages: 428-435, DOI: 10.1007/978-3-662-43880-0_49, 2014 (SJR)

Explicit Runge-Kutta methods of order p with m stages, m=1,2,3,4, are considered. It is assumed that $p=m$ and that Richardson Extrapolation is additionally used. It is proved that not only are the combinations of the Richardson Extrapolation with the selected explicit Runge-Kutta methods more accurate than the underlying numerical methods, but also their absolute stability regions are considerably larger. Sometimes this fact allows us to apply larger time-stepsizes during the numerical solution when Richardson Extrapolation is used. The possibility to achieve such a positive effect is verified by numerical experiments carried out with a carefully chosen example. It is pointed out that the application of Richardson Extrapolation together with explicit Runge-Kutta methods might be useful when some large-scale mathematical models, including models that are arising in air pollution studies, are handled numerically.

26. Georgiev, K; Kosturski, N; Vutov, Y, On the Adaptive Time-Stepping in Radio-Frequency Liver Ablation Simulation: Some Preliminary Results, Lecture Notes in Computer Science, Vol: 8353, Pages: 397-404, DOI: 10.1007/978-3-662-43880-0_45, 2014 (SJR)

Radio-frequency ablation is a low invasive technique for treatment of liver tumors. This work concerns the mathematical modelling and computer simulation of the heat transfer process. The core is solving the time-dependent partial differential equation of parabolic type. Instead of a uniform discretization of the considered time interval, an adaptive time-stepping procedure is applied in an effort to decrease the simulation time. The procedure is based on the local comparison of the Crank Nicholson and backward Euler approximations. Results of some preliminary numerical experiments performed on a selected test problems are presented and discussed.

27. Zlatev, Z; Georgiev, K; Dimov, I, Studying absolute stability properties of the Richardson Extrapolation combined with explicit Runge-Kutta methods, COMPUTERS & MATHEMATICS WITH APPLICATIONS, Vol: 67, Issue: 12 Pages: 2294-2307, DOI: 10.1016/j.camwa.2014.02.025, 2014 (IF, Q1)

Explicit Runge–Kutta methods are considered. It is assumed that the number of stages *m*, *m* = 1, 2, 3, 4, is equal to the order p of the selected method. The impact of the application of the Richardson Extrapolation on the absolute stability properties is studied. The Richardson Extrapolation was used until now only in an attempt to increase the accuracy of the numerical approximations or in order to keep the computational errors under some prescribed in advance level. Another issue, the absolute stability of the Richardson Extrapolation in connection with several numerical methods, is the major topic of this study. It is shown that not only are the combinations of the Richardson Extrapolation with explicit Runge–Kutta methods more accurate than the underlying numerical methods, but also their absolute stability regions are larger. This means that larger time-stepsizes can be used during the integration when Richardson Extrapolation is used. The validity of the theoretical results is confirmed by numerical experiments with three carefully chosen examples. It is pointed out that the application of Richardson Extrapolation together with explicit Runge–Kutta methods might be useful when some large-scale mathematical models, described by systems of partial differential equations, are handled numerically.

28. Zlatev, Z; Dimov, I; Farago, I; Georgiev, K; Havasi, A; Ostromsky, T, Application of Richardson extrapolation for multi-dimensional advection equations, COMPUTERS & MATHEMATICS WITH APPLICATIONS, Vol: 67 Issue: 12 Pages: 2279-2293, DOI: 10.1016/j.camwa.2014.02.028, 2014 (IF, Q1)

A Crank–Nicolson type scheme, which is of order two with respect to all independent variables, is used in the numerical solution of multi-dimensional advection equations. Normally, the order of accuracy of any numerical scheme can be increased by one when the well-known Richardson Extrapolation is used. It is proved that in this particular case the order of accuracy of the combined numerical method, the method consisting of the Crank–Nicolson scheme and the Richardson Extrapolation, is not three but four.

29. Farago, I; Georgiev, K; Havasi, A; Zlatev, Z, Efficient algorithms for large scale scientific computations: Introduction, COMPUTERS & MATHEMATICS WITH APPLICATIONS, Vol: 67 Issue: 12 Pages: 2085-2087, DOI: 10.1016/j.camwa.2014.05.021, 2014 (IF, Q1)

It is state that problem of constructing efficient algorithms for Large-Scale Scientific Computations become more and more important when modern high performance computers are in use It is shown that one of the important topic is the efficient use of the finite element methods applied in the discretization of several types of PDEs or systems of PDEs. Other important topics include 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, and efficient application of splitting procedures.

30. Liolios, Angelos; Elenas, A; Liolios, A; Radev, S; Georgiev, K; Georgiev, I, Tall RC Buildings Environmentally Degradated and Strengthened by Cables Under Multiple Earthquakes: A Numerical Approach, Lecture Notes in Computer Science, Vol: 8962 Pages: 187-195, DOI: 10.1007/978-3-319-15585-2_21, 2015 (SJR)

A numerical investigation is presented for the seismic analysis of tall reinforced concrete (RC) Civil Engineering structures, which have been degradated due to extreme environmental actions and are strengthened by cable elements. The effects of multiple earthquakes on such RC building frames are computed. Damage indices are estimated in order to compare the seismic response of the structures before and after the retrofit by cable element strengthening, and so to elect the optimum strengthening version.

31. Zlatev, Z; Georgiev, K; Dimov, I, Selecting Explicit Runge-Kutta Methods with Improved Stability Properties, Lecture Notes in Computer Science, Vol: 9374 Pages: 409-416, DOI: 10.1007/978-3-319-26520-9_4, 2015 (SJR)

Explicit Runge-Kutta methods can efficiently be used in the numerical integration of initial value problems for non-stiff systems of ordinary differential equations (ODEs). Let m and p be the number of stages and the order of a given explicit Runge-Kutta method. We have proved in a previous paper [8] that the combination of any explicit Runge-Kutta method with $m=p$ and the Richardson Extrapolation leads always to a considerable improvement of the absolute stability properties. We have shown in: Zlatev, Z., Georgiev, K., Dimov, I.: Improving the absolute stability properties of some explicit Runge-Kutta methods and their combinations with

Richardson extrapolation, (talk presented at the NM&A14 conference in Borovets, Bulgaria, August 2014) that the absolute stability regions can be further increased when $p<m$ is assumed. For two particular cases, $p=3 \wedge m=4$ and $p=4 \wedge m=6$ it is demonstrated that

(a) the absolute stability regions of the new methods are larger than those of the corresponding explicit Runge-Kutta methods with $p=m$, and

(b) these regions are becoming much bigger when the Richardson extrapolation is additionally applied.

The explicit Runge-Kutta methods, which have optimal absolute stability regions, form two large classes of numerical algorithms (each member of any of these classes having the same absolute stability region as all the others). Rather complicated order conditions have to be derived and used in the efforts to obtain some special methods within each of the two classes.

We selected two particular methods within these two classes and tested them by using appropriate numerical examples.

32. Ganzha, Maria; Georgiev, K; Lirkov, I; Paprzycki, M., An application of partition method for solving 3D Stokes equation, COMPUTERS & MATHEMATICS WITH APPLICATIONS, Vol: 70 Issue: 11 Pages: 2762-2772, DOI: 10.1016/j.camwa.2015.04.025, 2015 (IF, Q1)

In our previous work we have studied the performance of a parallel algorithm, based on a direction splitting approach, for solving of time dependent Stokes equation. We used a rectangular uniform mesh, combined with a central difference scheme for the second derivatives. Hence, the proposed algorithm required only solution of tridiagonal linear systems.

In our work, we are targeting massively parallel computers, as well as clusters of multi-core nodes. The somehow slower (experimentally established) performance of the proposed approach was observed when using all cores on a single node of a cluster. To remedy this problem, we tried to use LAPACK subroutines from the multi-threaded layer library, but the parallel performance of the code (while improved) was still not satisfactory on a single (multi-core) node.

Our current work considers hybrid parallelization based on the MPI and OpenMP standards. It is motivated by the need to maximize the parallel efficiency of our implementation of the proposed algorithm. Essential improvements of the parallel algorithm are achieved by

introducing two levels of parallelism: (i) between-node parallelism based on the MPI and (ii) inside-node parallelism based on the OpenMP. The implementation was tested on Linux clusters with Intel processors and on the IBM supercomputer.

33. Liolios, Angelos; Karabinis, A; Liolios, A; Radev,; Georgiev, K; Georgiev, I, A computational approach for the seismic damage response under multiple earthquakes excitations of adjacent RC structures strengthened by ties, COMPUTERS & MATHEMATICS WITH APPLICATIONS, Vol: 70 Issue: 11 Pages: 2742-2751, DOI: 10.1016/j.camwa.2015.08.012, 2015 (IF, Q1)

Civil Engineering systems of adjacent reinforced concrete (RC) structures, which have been environmentally degraded, are considered in order to be seismically strengthened by cable elements (ties). A numerical approach for estimating the effects of pounding (seismic interaction) on the response of such adjacent structures under multiple earthquakes excitation is presented. For the system of the governing partial differential equations (PDE) a double discretization, in space by the Finite Element Method and in time by a direct incremental approach, is used. The unilateral behaviours of both, the cable-elements and the interfaces contact-constraints, are strictly taken into account and result to inequality constitutive conditions. So, in each time-step, a non-convex linear complementarity problem is solved. The decision for the optimal cable-strengthening scheme is obtained on the basis of computed . It is found that pounding and cable strengthening have significant effects on the earthquake response and, hence, on the seismic upgrading of existing adjacent RC structures.

34. Georgiev, K; Iliev, O; Minev, P, Numerical Methods for Scientific Computations and Advanced Applications, COMPUTERS & MATHEMATICS WITH APPLICATIONS, Vol: 70 Issue: 11 Pages: 2619-2620, DOI: 10.1016/j.camwa.2015.11.004, 2015 (IF, Q1)

Some remarks on the connections between the Modern Scientific computing and the Numerical analysis is presented. In the last sixty years Scientific Computing has become a very important and universal approach for scientific studies in every branch of science, engineering, medicine, and even humanities, mainly because:

• It is relatively cheap and efficient as compared to physical experiments;

- It can provide realistic simulations of even more complex systems than those that can be studied experimentally;
- It is an excellent tool for constructing new and improving existing theories and models.

Modern Scientific Computing is one of the most prominent examples of a truly interdisciplinary area involving mathematics, computer science, engineering, physics, chemistry, medicine, etc. In addition, the main instrument allows us to utilize the huge computational resources of the contemporary and future high performance computer systems.

The tools of Scientific Computing are usually based on mathematical models and corresponding computer codes that are used to perform virtual experiments to obtain new data or to better understand existing experimental results. They are particularly important in situations when the cost of the experiments or their complexity is prohibitive. For example, in many cases, it is practically impossible to perform in-vitro experiments in living organisms, or it is extremely expensive to verify experimentally all possible scenarios for the flow, dynamic or electromagnetic response of a modern aircraft. Therefore, numerical simulations revolutionized the development in such areas in recent years.

Numerical Analysis is one of the crucial elements of Scientific Computing. It develops and analyzes numerical methods for discretization of continuous models and their subsequent solution, as well as for approximation of discrete data, such as: data interpolation and extrapolation, methods for solving linear and non-linear systems of algebraic equations (direct and iterative solution methods, preconditioning, multilevel and multigrid methods, etc.), methods for solving systems of ordinary and partial differential equations (finite difference, finite element, and finite volume methods, etc.), methods for solving integral equations, and optimization problems.

Another crucial element of Scientific Computing is the implementation of these numerical methods into computer codes and their customization for the numerous computing systems that are available nowadays. One very recent and important development in this direction is the implementation on various shared or distributed memory parallel computer systems and GPUs that allows for truly large scale scientific computations.

35. Liolios, Angelos; Moropoulou, A; Liolios, A; Georgiev, K; Georgiev, I, A Computational Approach for the Seismic Sequences Induced Response of Cultural

Heritage Structures Upgraded by Ties, Studies in Computational Intelligence, Vol: 648 Pages: 47-58, DOI: 10.1007/978-3-319-32207-0_4, 2016 (SJR)

The seismic upgrading of Cultural Heritage structures under multiple earthquakes excitation, using materials and methods in the context of Sustainable Construction, is computationally investigated from the Civil Engineering praxis point of view. A numerical approach is presented for the seismic response of Cultural Heritage industrial buildings of reinforced concrete (RC), which are seismically strengthened by using cable elements (tension-ties). A double discretization, in space by the Finite Element Method and in time by an incremental approach, is used for the system of the governing partial differential equations (PDE). The unilateral behaviour of the cable-elements, as well as the other non-linearities of the RC frame-elements, are strictly taken into account and result to inequality problem conditions. A non-convex linear complementarity problem is solved in each time-step by using optimization methods. The seismic assessment of the RC structure and the decision for the optimal cable-strengthening scheme are obtained on the basis of computed damage indices.

36. Zahari Zlatev, Ivan Dimov, Krassimir Georgiev, Relations between Climatic Changes and High Pollution Levels in Bulgaria, Open Journal of Applied Sciences, 2016, 6, 386-401, Published Online July 2016 in SciRes. http://www.scirp.org/journal/ojapps, http://dx.doi.org/10.4236/ojapps.2016.67040

One of the important consequences of the climatic changes is the potential danger of increasing the concentrations of some pollutants, which may cause damages to humans, animals and plants. Therefore, it is worthwhile to study carefully the impact of future climate changes on the high pollution levels. The major topic of the discussion in this paper is the increase of some ozone levels in Bulgaria, but several related topics are also discussed. The particular mathematical tool applied in this study is a large-scale air pollution model, the Unified Danish Eulerian Model (UNIDEM), which was successfully used in several investigations related to potentially dangerous pollution levels in several European countries. This model is described by a non-linear system of partial differential equations, which is solved numerically by using (a) advanced numerical algorithms and (b) modern computer architectures. Moreover, (c) the code is parallelized and (d) the cache memories of the available computers are efficiently utilized. It is shown that in Bulgaria, as in the other European countries, the climatic changes will result in permanent increases of some quantities related to the ozone pollution. The

important issue is that in our study the changes of the dangerous pollution levels are followed year by year. In this way, an attempt is made both to capture the effect of the inter-annual variations of the meteorological conditions on the levels of the ozone concentrations and to follow directly the influence of the climatic changes on the pollution levels. Moreover, the sensitivity of the pollution levels to variations of the human made (anthropogenic) and natural (biogenic) emissions is also discussed.

37. Blaheta, R; Georgiev, I; Georgiev, K; Jakl, O; Kohut, R; Margenov, S; Stary, J, High Performance Computing in Micromechanics with an Application, CYBERNETICS AND INFORMATION TECHNOLOGIES, Vol: 17 Issue: 5 Pages: 5-16, DOI: 10.1515/cait-2017-0050, 2017 (SJR)

High Performance Computing (HPC) is required for many important applications in chemistry, computational fluid dynamics, etc., see, e.g., an overview in: Mihajlov i c, M., et al. Applications for Ultrascale Computing, International Journal Supercomputing Frontiers and Innovations, Vol. 2, 2015, pp. 19-48. In this paper, we shortly describe an application (a multiscale material design problem) that requires HPC for several reasons. The problem of interest is analysis of the fibre-reinforced concrete and we focus on modelling of stiffness through numerical homogenization and computing local material properties by inverse analysis. Both problems require a repeated solution of large-scale finite element problems up to 200 million degrees of freedom and therefore the importance of HPC computing is evident.

38. Zlatev, Z; Dimov, I; Farago, I; Georgiev, K; Havasi, A, Stability of the Richardson Extrapolation combined with some implicit Runge-Kutta methods, JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS, Vol: 310 Pages: 224-240, DOI: 10.1016/j.cam.2016.03.018, 2017 (IF, Q1)

The implementation of the Richardson Extrapolation in combination with different numerical methods for solving systems of ordinary differential equations (ODEs) is relatively simple, but the important requirement for stability of the computational process may cause serious difficulties. For example, the commonly used by scientists and engineers Trapezoidal Rule has good stability properties, but its combination with the Richardson Extrapolation is unstable. Therefore, it is necessary to study in advance and very carefully the stability of the new numerical methods arising when the scientists and the engineers use this computational device in combination with different algorithms for solving systems of ODEs. We are presenting a

systematic investigation of the implementation of Richardson Extrapolation for two implicit Runge-Kutta methods. Three numerical examples, including an atmospheric chemical scheme used successfully in several extensive environmental studies and described mathematically by a very stiff and badly scaled nonlinear system of ODEs, are presented to illustrate the advantages of the presented approach. The numerical results show that not only are the computations stable, but also the achieved accuracy is higher when the Richardson Extrapolation is additionally applied. It will be possible to derive similar stability and accuracy results for other implicit Runge-Kutta methods.

39. Harizanov, S; Lirkov, I; Georgiev, K; Paprzycki, M; Ganzha, M, Performance analysis of a parallel algorithm for restoring large-scale CT images, JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS, Vol: 310 Pages: 104-114, DOI: 10.1016/j.cam.2016.07.001, 2017 (IF, Q1)

In multiple areas of image processing, such as Computed Tomography, in which data acquisition is based on counting particles that hit a detector surface, Poisson noise occurs. Using variance-stabilizing transformations, the Poisson noise can be approximated by a Gaussian one, for which classical denoising filters can be used. This paper presents an experimental performance study of a parallel implementation of the Poissonian image restoration algorithm, introduced in: Harizanov S., Pesquet JC., Steidl G. (2013) Epigraphical Projection for Solving Least Squares Anscombe Transformed Constrained Optimization Problems. In: Kuijper A., Bredies K., Pock T., Bischof H. (eds) Scale Space and Variational Methods in Computer Vision. SSVM 2013. Lecture Notes in Computer Science, vol 7893. Springer, Berlin, Heidelberg.Hybrid parallelization based on MPI and OpenMP standards is investigated. The convergence rate of the algorithm heavily depends on both the image size and the choice of input parameters (ρ,σ), thus maximizing its parallel efficiency is vital for real-life applications. The implementation is tested for high-resolution radiographic images, on Linux clusters with Intel processors and on an IBM supercomputer.

40. Liolios, A., Liolios, K., Moropoulou, A., Georgiev, K., Georgiev, I., Cultural heritage RC structures environmentally degradated: Optimal seismic upgrading by tention-ties under shear effects, Volume 10665 LNCS, 2018, Pages 516-526 (SJR)

A computational approach is presented for the seismic response of existing Cultural Heritage industrial reinforced concrete (RC) structures, which have been degraded due to extreme actions (environmental, seismic etc.) and are to be seismically upgraded by using cable elements (tension-ties). Emphasis is given to shear effects, which are common for old RC buildings not designed according to new (after 2000) seismic codes concerning Civil Engineering praxis. The unilateral behavior of the cable-elements and the non-linear behavior of the RC structural elements are strictly taken into account and result to inequality constitutive conditions. For the numerical treatment of the system of partial differential relations (PDE), a double discretization, in space by the Finite Element Method and in time by a direct incremental approach, is used. So, in each time-step, a non-convex linear complementarity problem is solved. The decision for the optimal cable-strengthening scheme under seismic sequences is obtained on the basis of computed damage indices, as shown in a numerical example.

41. Zlatev, Z., Dimov, I., Georgiev, K., Blaheta, R., Using advanced mathematical tools in complex studies related to climate changes and high pollution levels, Volume 10665 LNCS, 2018, Pages 552-559 (SJR)

UNI-DEM is a large-scale environmental model described by a non-linear system of partial differential equations (PDEs) and used in many studies of air pollution levels in different European countries. The discretization of UNI-DEM leads to a long series of huge computational tasks, because it is necessary to run the discretized model with many different scenarios during long time-periods of many consecutive years. Therefore, both the storage requirements and the computational work are enormous. We had to resolve four difficult problems in the efforts to perform successfully the required simulations. More precisely, we had to do the following:

(a) to implement fast numerical methods,
(b) to select suitable splitting procedures,
(c) to exploit efficiently the cache memories of the available high-speed computers
(d) to parallelize the computer codes.

We use several runs over sixteen consecutive years and with fourteen scenarios. Our main purpose will be to show the long-range transport of potentially dangerous air pollutants to Bulgaria.

42. Zlatev, Z., Dimov, I., Farago, I., Georgiev, K., Havasi, A., Absolute Stability and Implementation of the Two-Times Repeated Richardson Extrapolation Together with Explicit Runge-Kutta Methods, Lecture Notes in Computer Science, Volume 11386 LNCS, 2019, Pages 678-686, DOI: 10.1007/978-3-030-11539-5_80 (SJR)

Efficient implementation of the Two-times Repeated Richardson Extrapolation is studied in this paper under the assumption that systems of ordinary differential equations (ODEs) are solved numerically by Explicit Runge-Kutta Methods (ERKMs). The combinations of the Two-times Repeated Richardson Extrapolation with the ERKMs are new numerical methods. The computational cost per step of these new numerical methods is higher than the computational cost per step of the underlying ERKMs. However, the order of accuracy of the combined methods becomes very high: if the order of accuracy of the underlying ERKM is p, then the order of accuracy of its combination with the Two-times Repeated Richardson Extrapolation is at least $p+3$ when the right-hand-side function of the system of ODEs is sufficiently many times continuously differentiable. Moreover, the stability properties of the new methods are always better than those of the underlying numerical methods when $p=m$ and $m=1, 2, 3, 4$ (where m is the number of stage vectors in the chosen ERKM). These two useful properties, higher accuracy and better stability, are often giving a very reasonable compensation for the increased computational cost per step, because the same degree of accuracy can be achieved by applying a large stepsize which leads to a considerable reduction of the number of steps when the Two-times Repeated Richardson Extrapolation is used. This fact is verified by several numerical experiments.

43. Zlatev, Z., Dimov, I., Farago, I., Georgiev, K., Havasi, A., Stability Properties of Repeated Richardson Extrapolation Applied Together with Some Implicit Runge-Kutta Methods, Lecture Notes in Computer Science, Volume 11386 LNCS, 2019, Pages 114-125, DOI: 10.1007/978-3-030-11539-5_80 (SJR)

Efficient implementation of the Two-times Repeated Richardson Extrapolation is studied in this paper under the assumption that systems of ordinary differential equations (ODEs) are solved numerically by Explicit Runge-Kutta Methods (ERKMs). The combinations of the Two-times Repeated Richardson Extrapolation with the ERKMs are new numerical methods. The computational cost per step of these new numerical methods is higher than the computational cost per step of the underlying ERKMs. However, the order of accuracy of the combined

methods becomes very high: if the order of accuracy of the underlying ERKM is *p*, then the order of accuracy of its combination with the Two-times Repeated Richardson Extrapolation is at least (*p*+3) when the right-hand-side function of the system of ODEs is sufficiently many times continuously differentiable. Moreover, the stability properties of the new methods are always better than those of the underlying numerical methods when (*p*=*m*\) and (*m*=1, 2, 3, 4) (where m is the number of stage vectors in the chosen ERKM). These two useful properties, higher accuracy and better stability, are often giving a very reasonable compensation for the increased computational cost per step, because the same degree of accuracy can be achieved by applying a large stepsize which leads to a considerable reduction of the number of steps when the Two-times Repeated Richardson Extrapolation is used. This fact is verified by several numerical experiments.

Г8. Публикувани глави от книга

44. Zahari Zlatev, Krassimir Georgiev, Ivan Dimov, Parallel Computations in a Large-Scale Air Pollution Model, in: "Advanced Numerical Methods for Complex Environmental Models: Needs and Availability", István Faragó, Ágnes Havasi and Zahari Zlatev (Eds.), 2013, Bentham Science Publishers, 169-207, DOI: 10.2174/97816080577881130101; eISBN: 978-1-60805-778-8, 2013; ISBN: 978-1-60805-777-1

Large-scale air pollution models, which are normally described mathematically as systems of partial differential equations, must very often be run **efficiently** on high-speed computer architectures. The requirement for efficiency is especially important when some fine discretization of the spatial domain is to be applied. In practice, this means that an efficient implementation of such a model on fast modern computers must nearly always be achieved, because as a rule fine grids are needed in the efforts to avoid the appearance of numerical errors that are comparable with or even larger than the errors which are caused by other reasons (uncertainties of the meteorological data, of the emission data, of the rates of the involved chemical reactions, *etc*.). The organization of the parallel computations will be discussed in this chapter of the book. The major principles, on which the parallelization is based, are rather general and, therefore, some of the discussed techniques can also be applied in connection with some large-scale models arising in other areas of science and engineering.

45. Zahari Zlatev, Krassimir Georgiev, Ivan Dimov, Part C: Sensitivity of European Pollution Levels to Changes of Human-Made Emissions, in: "Advanced Numerical Methods for Complex Environmental Models: Needs and Availability", István Faragó, Ágnes Havasi and Zahari Zlatev (Eds.), 2013, Bentham Science Publishers, 307-333, DOI: 10.2174/97816080577881130101; eISBN: 978-1-60805-778-8, 2013; ISBN: 978-1-60805-777-1

Systematic changes of the human-made emissions in Europe were simulated by applying a carefully chosen series of appropriate scenarios and the impact of these changes on the pollution levels in different parts of the model domain was studied. It was established that, while the changes of the sulphur pollutants correspond in a nearly perfect way to the changes of the emissions, for the most of the other pollutants this was not true. Furthermore, the experiments also indicate that the changes in the different part of Europe can be rather different although the emissions were reduced with the same factor. The conclusions are illustrated by many results presented in tables and plots. Several ideas for future research in this direction are briefly discussed in the end of this chapter.

46. K. Georgiev, PARALLEL ALGORITHM FOR 3D ELASTICITY PROBLEMS BASED ON AN OVERLAPPING DD PRECONDITIONER, in: "Parallel numerical computations with applications", Ed. Tianruo Yang, Springer Science, pp 105 – 117, ISBN 978-1-4613-7371-1 ISBN 978-1-4615-5205-5 (eBook) DOI 10.1007/978-1-4615-5205-5, 1999

In this paper we are mainly concerned with an additive overlapping domain decomposition (DO) algorithm and it implementation on parallel computers with shared and distributed memory including clusters of workstations. The problem under consideration is the numerical solution of 3D elasticity systems but the main ideas, algorithms and codes are applicable to 3D elliptic boundary value problems with discontinuous coefficient~. The system of linear equations which has to be solved after a finite element method discretization is symmetric and positive definite and the Preconditioned Conjugate Gradient method with a preconditioner constructed via Domain Decomposition is used. The algorithm is highly parallelizable. The Message Passing Interface (MPI) standard is used on both shared and distributed memory parallel computer platforms. Results from numerical experiments on two symmetric multiprocessor systems and IBM SP parallel computer with distributed memory are discussed.