Editorial: large-scale computations in environmental modelling

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1 Introduction

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. Combined research by specialists from the fields of:

- environmental and ecological modelling
- numerical analysis and
- scientific computing

must be carried out in an attempt to resolve successfully the challenging computational problems that appear when comprehensive environmental studies are to be performed.

In some areas of Europe, as well as in some other parts of the world, the pollution levels are so high that preventive actions are urgently needed. Therefore, robust and reliable control strategies must be developed to find out *where* and by *how much* the emissions of harmful pollutants should be reduced. The solutions found must be optimal (or, at least, close to optimal), because the reduction of the emissions is as a rule to expensive process. This means that great economical problems may appear when the task of optimal reduction of the emissions is not correctly solved. Optimal (or nearly optimal) solutions can successfully be found only by performing a long series of simulation experiments consisting of many hundreds of runs of several comprehensive mathematical models. Then, the results obtained by different models must be carefully compared to answer the following questions:

- Are there any discrepancies and
- What are the reasons for discrepancies?

In a few cases, where the answer to the first question is positive, the needed corrections of some of the models have to be made and the simulation experiments must be repeated for the corrected models. This shows that the process of finding an optimal solution will in general be very long and, thus, efficiency of the codes is highly desirable. Achieving efficiency of the codes by selecting faster (but still sufficiently accurate) numerical algorithms and by improving the performance on different high-speed computers is one of the topics of this special issue of the International Journal of Environment and Pollution.

Computer architectures are steadily becoming more efficient. Supercomputers that have top performance of several T-flops will become broadly accessible in the near future. New and efficient numerical methods, by which the great potential power of the parallel computers can be better exploited, are also gradually becoming available. However, many unresolved problems still exist. One of the most important problems is the great gap between the top performance of a modern supercomputer and the speeds actually achieved when large application codes are run. The task of achieving high computational speeds close to the top performance of the computers available, is very difficult and at the same time, challenging for the comprehensive mathematical models (not only for the large-scale environmental models). This is also true for the heterogeneous computations, where it is possible to achieve very high computational speed when the computational process is properly organised.

A few non-realistic simplifying assumptions are always needed and made, in all the existing large-scale ecological and environmental models, to be able to treat them numerically on the computers that are available. Many such assumptions are no longer absolutely necessary, because both the computers and the numerical algorithms are much faster than before, and will become even faster in the near future. Therefore, it becomes more and more essential to describe all the important physical and chemical processes in an adequate way (according to the present knowledge) and to try to solve the problems by exploiting extensively the modern computational and numerical tools.

Moreover, many new modules have permanently to be added to the large-scale environmental models:

- modules for treatment of particles (including secondary organic aerosols)
- modules for performing data assimilation

- modules for achieving refinement in certain sub-domains of particular interest, etc.

The addition of such modules not only leads to more advanced but also to more complicated models. The treatment of the new advanced models is a challenging task even when modern supercomputers are available.

Finally, in many comprehensive studies, it is necessary to run a large number of scenarios. This also implies large-scale computations. The computations are to be carefully organised in the efforts to resolve the huge computational tasks arising when comprehensive environmental studies are to be carried out.

Both the improvements of numerical methods for environmental models and comprehensive studies performed with several advanced large-scale air pollution methods are discussed in the papers included in this special issue. Most of the papers were presented at the Fifth International Conference on Large-Scale Scientific Computations, LSSC'05, held in Sozopol (Bulgaria) on 5–10 June 2005.