WP4: Monte Carlo methods for sensitivity analysis of large mathematical models

1. Major results

Task 4.1. Generation of mesh function for different climate scenarios (pollutants, chemical reactions) using two and three dimensional version of UNI-DEM (Unified Danish Eulerian Model). According to Task 4.1 a special version of UNI-DEM model for obtaining sensitivity analysis mesh functions SA-DEM is developed. Figure 1 shows the distribution of ozone concentrations over Europe for July 1998. The results presented on similar plots for various important pollutants allow us to identify the computational mesh-points where each pollutant reaches its maximum. A large number of parallel numerical experiments are performed. The results are used to compute Sobol's total sensitivity indices. The aim of the experimental results is to study the influence of the dimensionality of data-table (values of pollution concentrations) on the approximation error and the values of sensitivity indices. Presented results are obtained by varying perturbation parameters of three different chemical rate constants in the interval в [0.6; 1.4] ^{3}. CBM IV chemical scheme is chosen to present chemical reactions (Tz. Ostromsky, I. Dimov, R. Georgieva). Results obtained are published in [DG_09a, ODGZ_09a, DG_09]. An MPI version of the Unified Danish Eulerian Model for long-range transport of air pollutants is developed for the IBM BlueGene/P computer (K. Georgiev and Tz. Ostromsky). The results are documented in [ODGZ_09a, GZ_09a, GZ_09a2]. The above results are compared with results obtained on other parallel computers [GZ_09s]. A large number of computer experiments are obtained with real meteorological and emission data for Europe. Some typical scenarios for the period 1989 – 1998 are considered. For the same period some climatic scenarios are run on the area of South-East Europe. A special technique dealing with sparse matrices is studied. Some results are documented in [GZ1_09p, GZ2_09p].

Task 4.2. Techniques for approximation of mesh function and error estimation. Different techniques for approximation are studied. We have chosen minimization of discrete integral norm as a satisfactory technique (functions are relatively smooth, but they may have areas with "computational irregularities"). Polynomials of 3rd and 4th degree and spline-functions are used as approximation tool. The error of approximation is studied numerically for different multi-dimensional cubes (I. Dimov, R. Georgieva). Some results are published in [DG_09a].

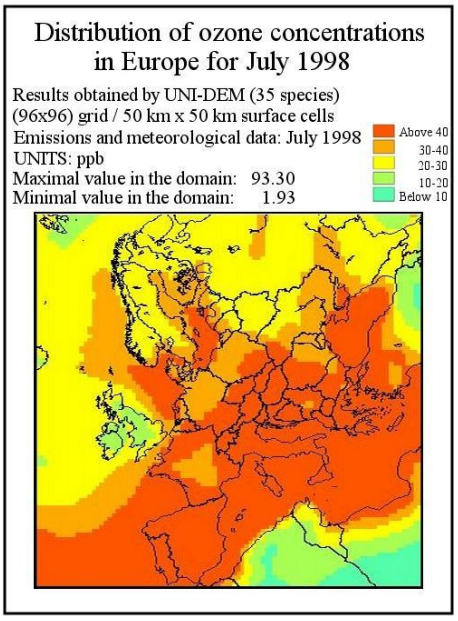

Fig 1. Distribution of ozone concentrations in Europe for July 1998.

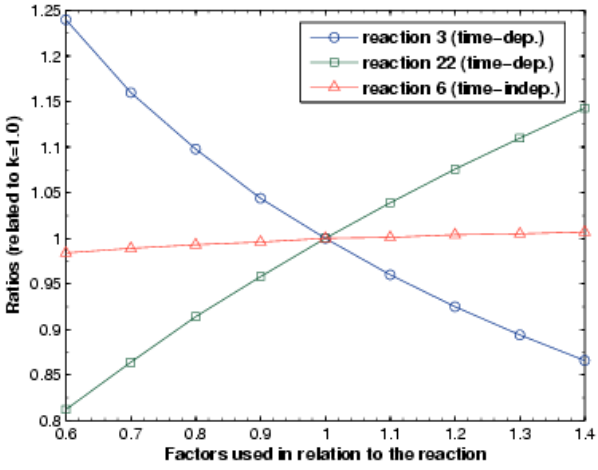

Fig. 2: Sensitivity of ozone concentrations to changes of chemical rates.

Task 4.3. ***Analysis of the UNI-DEM output parameters according to the emission levels and supporting the decision makers in developing ecological directives.*** Adaptive Monte Carlo algorithm for evaluating sensitivity indices (first order and total indices) using Sobol' method and its modifications is developed. It is studied numerically how various chemical rate reactions influence the values of air pollution concentrations. An example is shown on Figure 2. Numerical experiments applying two approaches for small sensitivity indices (in order to overcome loss of accuracy in the case of small sensitivity indices) are carried out. Plain and adaptive Monte Carlo technique are applied for numerical integration of model function that describes distribution of air pollutants concentration according to values of chemical rates. SIMD-oriented Fast Mersenne Twister generator (SFMT) is used for random number generation (I. Dimov, R. Georgieva). The obtained results are published in [DG_09a]. A systematic procedure for sensitivity analysis is performed and it is applied for UNI-DEM. A comparison of results obtained using the proposed scheme for sensitivity analysis and results obtained using the available software tool for sensitivity analysis SA - R language and environment for statistical computing is done. Our scheme has significant priorities over the existing approach in some cases (for relatively small sensitivity indices). The main reason that one would prefer our approach is that we are able to control the accuracy at each stage of the computations (R. Georgieva, I. Dimov, S. Ivanovska). The obtained results are documented in [DG_09, DG_09a, DGIOZ_09s, ODGZ_p].
Some of the results are given in Section „Sensitivity analysis of an air pollution model" of R. Georgieva's PhD Thesis entitled „Computational complexity of Monte Carlo algorithms for multidimensional integrals and integral equations" (supervisor: Prof. I. Dimov).

2. Publications

a) published:

[DG_09] I. Dimov, R. Georgieva, Monte Carlo Algorithms for Evaluating Sobol' Sensitivity Indices, Math. Comput. Simul. (2009), doi:10.1016/j.matcom.2009.09.005.

b) accepted for publication:

[GZ_09a] K. Georgiev, Z. Zlatev, Runs of UNI–DEM Model on IBM BlueGene/P Computer and Analysis of the Model Performance: - In Proceedings of LSSC 2009, LNCS 5910.
[GZ_09a2] K. Georgiev, Z. Zlatev, Comparison results of running of the Danish Eulerian Model for long-range transport of air pollutants on different kind of high-performance computer architectures, Theoretical and Applied Mechanics.

[DG_09a] I. Dimov, R. Georgieva, Monte Carlo Adaptive Technique for Sensitivity Analysis of a Large-Scale Air Pollution Model. - In Proceedings of LSSC 2009, LNCS 5910.
[ODGZ_09a] Tz. Ostromsky, I. Dimov, R. Georgieva, Z. Zlatev, Sensitivity Analysis of a Large-scale Air Pollution Model: Numerical Aspects and a Highly Parallel Implementation. - In Proceedings of LSSC 2009, LNCS 5910.

c) submitted for publication:

[GZ_09s] K. Georgiev, Z. Zlatev, Notes on the Numerical Treatment of Sparse Matrices Arising in a Chemical Model, in: Proc. of BGSIAM meeting, December 21 – 22, 2009.

[DGIOZ_09s] I. Dimov, R. Georgieva, S. Ivanovska, Tz. Ostromsky, Z. Zlatev, Studying the Sensitivity of the Pollutants Concentrations Caused by Variations of Chemical Rates, Journal of Computational and Applied Mathematics.

d) in preparation:

[GZ1_09p] K. Georgiev, Z. Zlatev, Implementation of sparse matrix algorithms in an advection-difusion-chemistry module.
[GZ2_09p] K. Georgiev, Z. Zlatev, Impact of Climate Changes on High Ozone Pollution Levels over the Territory of South-Eastern Europe.
[ODGZ_p] Tz. Ostromsky, I. Dimov, R. Georgieva, Z. Zlatev, Sensitivity Analysis version of an Air Pollution Model:Parallel Implementation and Numerical Results, Journal of Management of Environmental Quality.

3. Presentations and talks

[1] K. Georgiev, *Comparison Results of Running of the Danish Eulerian Model (UniDEM) on Different Kind of Vector and Parallel Computers* (Workshop on Numerical Methods and High Performance Computations – interplay and novel ideas, February 17 – 18, 2009, Sofia).

[2] I. Dimov, R. Georgieva, *Monte Carlo Adaptive Technique for Sensitivity Analysis of a Large-Scale Air Pollution Model* (International conference "Large Scale Scientific Computations", LSSC'09, Sozopol).

[3] K. Georgiev, Z. Zlatev, *Runs of UniDEM Model on IBM BlueGene/P Computer and Analysis of the Model Performance* (international conference "Large Scale Scientific Computations", LSSC'09, Sozopol).

[4] Tz. Ostromsky, I. Dimov, R. Georgieva, Z. Zlatev, *Sensitivity Analysis of a Large-scale Air Pollution Model: Numerical Aspects and a Highly Parallel Implementation* (International conference "Large Scale Scientific Computations", LSSC'09, Sozopol).

[5] K. Georgiev, Z. Zlatev, *Comparison Results of Running of the Danish Eulerian Model for Long Range Transport of Air Pollutants on Different Kind of High-Performance Computer Architectures* (22nd workshop on tropospheric chemical transport modelling, Brescia, Italy, 26-27 November 2009).

4. Other activities

[1] Meetings and discussions with:

a) Colleagues from Centre for Advanced Computing and Emerging Technologies (ACET), University of Reading, Reading, United Kingdom - Prof. Dr. Vassil Alexandrov, Dr. Christian Weihrauch and Dr. Simon Branford;

b) Prof. Istvan Farago, Dr. Agnes Havasi, Dr. Tamas Szabo from Eotvos Lorand University, Hungary, about splitting methods used in UNI-DEM;

c) Colleagues from National Environmental Research Institute (Roskilde, Denmark) – Jurgen Brandt, Lise Marie Frohn, Matthias Ketzel, Lars Moseholm, Michael Evan Goodsite;

d) A. Ebel, A. Strunk, O. Iliev (Germany), G. Dimitriu (Romania), R. San Jose (Spain), F. Deutch (Belgium), P. D'Ambra, G. Candiani (Italy), P. Minev (Canada), I. Farago, I. Piechka, A. Havasi, M. Mincsovics, T. Kurics (Hungary), A. Mishev (FYROM) during the international conference "Large Scale Scientific Computations" (LSSC'09) taken place in Sozopol, June, 2009.

[2] Meetings to discuss the results and forthcoming activities according to package tasks.

[3] Preparation and presentation of personal reports of participants and summarized regular reports on WP4.

[4] Workshops in IPP-BAS devoted to the licensed software to be installed according to the project objectives and tasks.