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Procedia Social and Behavioral Sciences 2 (2010) 7646–7647

Procedia Social and Behavioral Sciences

Sixth International Conference on Sensitivity Analysis of Model Output

Adaptive Monte Carlo Algorithm for Sensitivity Studies of Eulerian Large-scale Air Pollution Models

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Abstract

Sobol' global sensitivity indices have been used here as main numerical indicators for sensitivity of model output to input parameters. Therefore the basic mathematical problem is computing of multidimensional integrals. Numerical results for an Eulerian large-scale air pollution model have been presented. They have been obtained by using an adaptive Monte Carlo algorithm for numerical integration. The results have been compared with SIMLAB implementation of applied approaches for sensitivity analysis.

Keywords: Sobol' global sensitivity indices; Adaptive Monte Carlo algorithm; Eulerian large-scale air pollution models

1. Main text

Mathematical modeling is a powerful field for description of real-world phenomena and sensitivity analysis is an efficient tool for verification and improvement of a model.

A systematic scheme for providing sensitivity analysis has been applied for an Eulerian large-scale mathematical model [4] to analyse the sensitivity of concentrations of some important air pollutants to chemical rate reactions. The model simulates remote transport of air pollutants. The chemical scheme used in the model is the condensed CBM-IV.

Sensitivity analysis computations consist of two steps: approximation and computing of Sobol' global sensitivity indices [2, 3]. Firstly, we obtain tables of values of the model function after numerical tests with the model of atmospheric chemistry under consideration. That is why the initial step of our scheme is to apply an approximation technique to produce a continuous model function as it is required by variance-based sensitivity approaches. Several approximation techniques have been studied. We have used polynomials of third and fourth degree, as well as cubic B-splines. The generated approximate function is smooth but it has a single peak at one of the corners of the domain. It gives us a reason to apply an adaptive Monte Carlo algorithm to compute Sobol´ global sensitivity indices.

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doi:10.1016/j.sbspro.2010.05.159

Plain and adaptive Monte Carlo techniques for numerical integration have been analysed and applied. We have shown that the adaptive algorithm has an advantage over the plain algorithm for a fixed number of samples that confirms reducing variance effect of the applied adaptive technique. Moreover, the approximate values of quantities are sufficiently close to the exact values even for the smallest chosen number of samples. One of the best available random number generators, SIMD-oriented Fast Mersenne Twister (SFMT, [1]) 128-bit pseudorandom number generator of period 2^{19937}-1 has been used to generate the required random points.

Grid implementations have been developed. They have been tested on the available regional South-East European grid infrastructure.

2. References

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