A Parallel Software System for the Numerical Simulation of Air Pollution

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We report on the activity of the *Unità Operativa* leaded by G. Giunta, in Naples, in collaboration with the *Unità Operativa* leaded by A. Murli, in Naples, concerning the development of mathematical software for the simulation of air pollution episodes in mesoscale domains. Computational models are a fundamental tool for understanding the dynamics of pollutants in the atmosphere and for supporting air quality control strategies. A prototypal software package, named *Parallel Naples Airshed Model (PNAM)*, has been developed, for the numerical simulation of the dynamics and the chemical kinetics of air pollutants in urban-scale domains, using parallel distributed-memory machines [1, 2]. PNAM is based on an Eulerian description of the transport and the photochemical transformations of pollutants, leading to time-dependent tree-space dimensional advection-diffusion-reaction equations. A time-splitting approach is applied, which separates the advection from the (coupled) diffusion and chemistry, and the solution is computed using the method of lines and cell-centered finite-difference spatial discretizations. A third-order upwind scheme with flux limiters and a first-order upwind scheme are applied to the horizontal and the vertical advection, respectively, together with an explicit two-stage second-order Runge-Kutta method. The vertical diffusion is semi-discretized using a second-order finite-difference scheme, and the diffusion-chemistry ODEs are treated implicitly using the general-purpose VODE solver [4], modified to take advantage of the structure of the Jacobian matrices involved in the computation. Special attention has been payed to the solution of the diffusion-chemistry operator; results of an extensive comparison among different methods are reported in [3]. The parallel implementation is based on grid partitioning; a dynamic load balancing technique has been also introduced. The software is written in Fortran 90 and uses the *Runtime System Library (RSL)* [5] to manage grid partitioning, data communication and load balancing. Simulations of realistic photosmog episodes in the Campania Region have been performed and the results have been analyzed. A parallel performance evaluation has also been carried out. This research is part of wider, and still ongoing, interdisciplinary research activity carried out at the Center for Research on Parallel Computing and Supercomputers of CNR (CPS-CNR) by a team of atmospheric chemists, meteorologists and computational mathematicians. The next goal of this activity is to develop an operational software system for air quality simulations in the Campania Region, that can be used as an effective tool to help the analysis of the responsibilites of existing pollution levels, the plannning of abatement strategies, and, more generally, the choice of environmental policies.

References

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