ON A TWO-WAY NESTING METHOD FOR AIR POLLUTION MODELLING. APPLICATION TO THE ESCOMPTE AREA

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INTRODUCTION

Air quality numerical models involve a considerable number of equations and variables. Because of computer limitations and time-consuming calculations, a high grid resolution over a large area is not always affordable. To improve numerical accuracy, various methods of local grid refinement can be found in the literature. But most of them do not allow any feedback from fine to coarse resolution. Methods that allow information exchange only from coarse to fine resolution are commonly called one-way nesting or passive embedding methods.

In order to see the influence of local finer resolutions over coarse areas, more advanced decomposition methods, known as two-way nesting methods, can be applied. Using a finite volume formulation, such a decomposition method has been developed and included in the model MAPOM (Multiscale Air POllution Model). MAPOM is a three dimensional Eulerian model including topography variations. It can solve transport, diffusion and gas-phase chemistry.

A rough description of the model is made in order to present its main features. Next, the two-way nesting method is described and the one-dimension algorithm is given. The two-way nesting method and MAPOM have been applied to the ESCOMPTE area (Marseille-Lake of Berre), using two grids. Results are presented for passive tracers and a comparison with coarse simulations and one-way nesting simulations is made. Finally, the conclusions will be drawn and further developments will be introduced.

MODEL DESCRIPTION

MAPOM is a multiscale air pollution model including two-way nesting procedures. Therefore, it is possible to run simulations over large domains with local refinements in order to increase accuracy in areas where it is required. Then, two-way nesting procedures allow a feedback from the locally refined areas up to the coarse levels.

MAPOM uses offline meteorological models (currently MM5 from the NCAR [Dudhia, 1993; Grell, Dudhia and Stauffer, 1995]) as meteorological drivers for transport and diffusion. It recalculates vertical fluxes to ensure the air mass conservation. Then, it resolves transport, vertical diffusion and gas phase chemistry.

In order to speed up the calculation and to restrain the use of complex numerical methods needed to solve strong non-linearities, MAPOM uses operator splitting. The classical Strang's operator splitting (Strang, 1968) has been implemented following the sequence Transport-Diffusion-Gas chemistry / Gas chemistry-Diffusion-Transport.

The resolution of the transport problem is based on a finite volume scheme. Using the conservation of air mass, it is possible to write a conservative form of the transport equation to ensure the conservation of the pollutant mass. Thus, the problem is to solve the following equation:

$$\frac{\partial C_i}{\partial t} + div(\vec{u} \cdot C_i) = Sources + Sinks \quad (1)$$

Where C_i is a generic name for the product of the air density r_a with the mixing ratio of the ith species, and $\vec{u}$ is the wind velocity. To calculate diffusion, MAPOM assumes that horizontal diffusion is much smaller than numerical diffusion due to transport effects. Thereby, it calculates only the diffusion on a column of air along the vertical. This calculation is also based on a finite volume formulation. At last, the gas chemistry module uses the Regional Atmospheric Chemistry Mechanism (RACM [Stockwell, Kirchner, Khun and Seefeld, 1997). RACM is a box model that includes 77 chemical compounds (organic and inorganic compounds) reacting through 237 reactions. Photolysis rates are calculated by the Tropospheric Ultraviolet-Visible model (TUV [Mandronich and Flocke, 1998). Further developments will lead to the implementation of dry deposition and aerosol chemistry.

THE TWO-WAY NESTING PROCEDURE

Local refinement is made on the horizontal plane. Refinement along the vertical has not been considered first because the vertical resolution of the model is thought to be high enough, and secondly because a grid refinement in 3D has a huge cost in term of data structuring, storage and computational time.

As mentioned before, the diffusion is calculated only on columns of air and RACM solves the gas chemistry on each cell (box model). Therefore these processes are not affected by any exchange of information due to a local refinement. Only the transport calculation includes an exchange of information between the various levels of resolution.

The two-way nesting scheme has to fulfill the following requirements:

- Mass conservation: the procedure should not create or lose mass,
- Positivity: the scheme should not produce any negative value that could lead to instabilities into the chemistry model,
- Monotonicity: the scheme must keep the values of the transported variables between the bounds of the initial conditions (taking into account eventual sources and sinks).

Note that these properties are also required for the transport numerical scheme.

To respect the CFL stability condition, the time step for transport is optimized on each grid according to the local refinement. It implies that grids are not synchronized in time. To allow information exchange between a grid and its nests, resynchronization is automatically done during the transport calculation.

The algorithm for transport in 1D is presented in this paper, as illustrated by Figure1. The passage to higher dimension is straightforward.

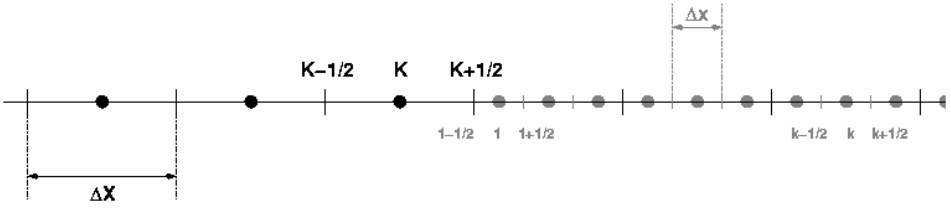

Figure 1: One-dimensional nested grid

The finite volume formulation of the transport problem is:

$$C_K^{n+1} = C_K^n - \frac{\Delta T}{\Delta X} \cdot \left(F_{K+1/2}^n - F_{K-1/2}^n \right) \tag{2}$$

Where:

- C_K^n is the transported variable in the cell K at time n. The cell K is adjacent to the local refinement,
- ΔT and ΔX are the steps in time and in space of the coarse grid,
- $F_{K-1/2}^n$ and $F_{K+1/2}^n$ are the mass fluxes at the edge of the cell K.

The flux $F_{K-1/2}^n$ is calculated by the transport scheme on the coarse level. But $F_{K+1/2}^n$ has to be recalculated using the information available on the fine grid. The integration of this flux has to be done in time, but also in space when in two dimensions. In 1D, the integration gives:

$$F_{K+1/2}^n = \frac{1}{l \cdot \Delta t \cdot u_{K+1/2}^n} \sum_{i=1}^{l} \int_{-i \cdot u_{K+1/2}^n \cdot \Delta t}^{-(i-1) \cdot u_{K+1/2}^n \cdot \Delta t} f(x, T_n) \cdot dx \tag{3}$$

Where:

- l is the ratio between the coarse and the fine time step. It is likely to be equal to the grid ratio (in Figure1, $l=3$),
- Δt is the time step on the fine grid,
- $u_{K+1/2}^n$ is the wind velocity on the interface between the fine and the coarse grid,
- $f(x, T_n)$ is the mass flux to be integrated on the interface during the time step $\Delta T = l \cdot \Delta t$.

Doing so, flux continuity at the interface is ensured. A special calculation is made to take into account topography effects and to avoid inconsistencies at the interface between grids. If the wind is oriented from the coarse grid toward the fine grid, the flow at the interface is a boundary condition. Therefore, the flux is set at the interface using the coarse grid calculation. Various orders of boundary conditions have been tested.

Boundary conditions are calculated using the same interpolation method as the transport algorithm to evaluate the fluxes at the cell faces. It is based on the corrected Piecewise Parabolic Method (Clappier, 1998).

After the synchronization in time of the various grids, results from the refined areas can be used to update the coarser levels. To reinforce numerical stability into the model, the results inside the nests are averaged and reported on the coarser levels.

The two-way nesting algorithm has been checked on the required properties mentioned before (mass conservation, positivity and monotonicity) using the Molenkamp-Crowley test. Various profiles were tried (steps, cones) with several wind fields (diagonal, rotational and parabolic). Several error calculations were looked at in order to test the method efficiency. They were used to appreciate MAPOM capabilities to be mass conservative, and to keep the maximums and the

shape of a given profile. In the following section some preliminary results on the ESCOMPTE area are presented.

APPLICATION TO THE ESCOMPTE AREA

The ESCOMPTE project whose main measurement campaign was made in June and July 2001 aims at the setup of a very detailed tridimensional database about emissions of primary pollutants and atmosphere composition and dynamics for typical summer pollution episodes. It covers an area of about 120 by 120 kilometers centered on the zone Marseille-Etang de Berre (France).

MAPOM has been applied on the ESCOMPTE area using passive tracers. The scope of the simulation was to test numerically on a real case, such as the ESCOMPTE area, the effects of a two-way nesting procedure with respect to a coarse simulation and a one-way nesting procedure. To do so, two grids have been set up both centered on Marseille. The coarse grid has on the horizontal 75 by 75 cells with a resolution of 6 by 6 kilometers. It extends from the eastern part of the Pyrenees on the west bound, to the Liguria region in Italy on the east bound. The northern bound is at the latitude of Turin, whereas the southern bound is at about the latitude of Barcelona. There are 18 levels along the vertical direction. The grid is stretched on the vertical, with the finest resolution of 33 meters at ground level. The fine grid has on the horizontal 87 by 87 cells with a resolution of 2 by 2 kilometers. The vertical structure of the fine grid is the same as for the coarse one. Figure2 illustrates the topography of the domain area as well as the position of the nest. The modelled area has the advantage to present a complex topography. The capabilities of MAPOM to deal with topography effects on nested grids are therefore tested.

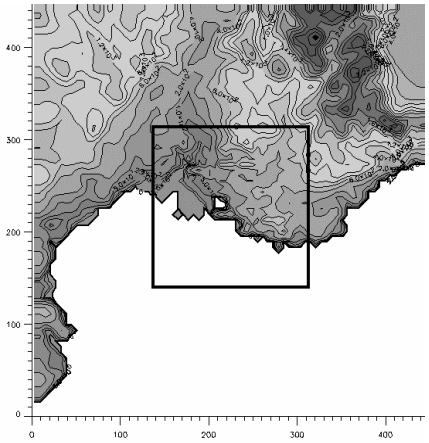

Figure 2: Topography of the domain. The frame indicates the location of the nested grid

The model is using the preliminary emission inventories for the ESCOMPTE project. Gases are used as passive tracers for numerical purposes.

Simulations have been performed using one and two grids in order to compare the results between a two-way nesting approach and a coarse and one-way nested calculation. The gas chemistry module is still under a validation phase. Therefore, comparison with measurements is not yet possible.

Figure 3 illustrates the impact of a nested grid with respect to a coarse simulation. It represents the dispersion of a species emitted at a rate equivalent to the emissions of NO_2 at 8.00 am, on the 23rd of June 2001. At that time, a wind is still blowing seaward. Thus, the transport is mainly done along the north-south axis. Generally, gradients and plumes, after averaging, are still sharper in the nested simulation than in the coarse simulation. Maximums are of the same order but are slightly higher in the nested simulation (3 to 6 ppb). It has also been observed that advected clouds separate from the plume closer to the source point than for the coarse simulation.

Figure 4 presents the impact of the two-way nesting when recirculation processes occur on the boundaries of the nested grid. Considering SO_2 at 8.00 am, on the 24th of June 2001, a recirculation pattern in the southern part of the domain leads to an overestimation of the plume size by the one-way nesting. That is not the case for the simulation done by MAPOM using the two-way nesting.

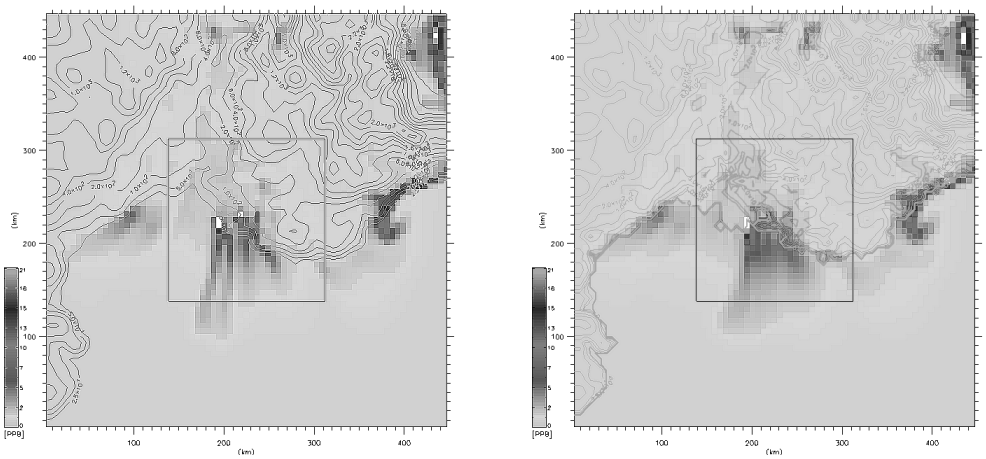

Figure 3: Impact of the two-way nesting procedure with respect to a coarse grid simulation. 23/06/01 - 8.00 am (NO_2 emissions) left: two-way nested simulation; right: coarse simulation

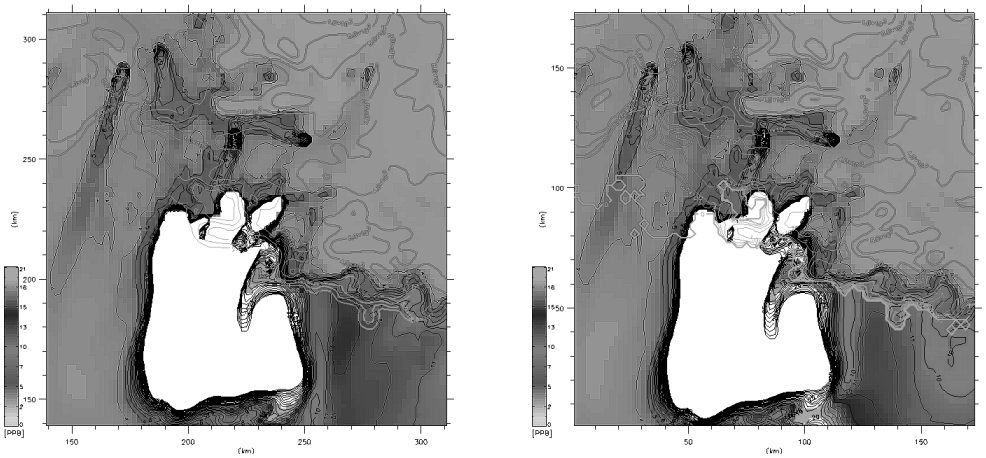

Figure 4: Impact of the two-way nesting on the nest with respect to a one-way nesting method. 24/06/01 - 8.00 am (SO_2 emissions) left: two-way nesting; right: one-way nesting

On the computational side, the major problems remain memory allocation and computational time, as having multiple nest means running the equivalent number of simulations at the same time on the same computer. But these problems are progressively overtaken as computer power increases.

CONCLUSIONS

The two-way nesting method implemented in MAPOM gives consistent concentration fields if compared with a coarse and a one-way nesting simulation. Gradients and plumes are sharper using two-way nesting and maximums are slightly higher. Comparisons with coarse grid simulations show that plumes are more detailed and better tracked with the two-way nesting approach. Moreover, in case of recirculation, the two-way nesting gives better results as the exchange of information is numerically more accurate. However, a comparison with measurements still has to be done in order to appreciate the real improvement represented by two-way nesting procedures. Further work on MAPOM will include the complete validation of the system with the gas chemistry module and with the radiation module. The implementation of other modules dealing with dry deposition and aerosol chemistry is also foreseen. At last, a comparison with data from the ESCOMPTE campaign and other international campaign are planned in order to benchmark MAPOM.

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