91

Domain Decomposition of an Atmospheric Transport–Chemistry Model

Andreas Müller

1 Introduction

The simulation of temporal and spatial distribution of reactive constituents of the atmosphere relies on a set of coupled nonlinear partial differential equations in space, time and the considered species. The numerical approach to the solution of these equations of balance is the discretization of space and time. A numerical solution of this system has especially to consider that the temporal scales relevant to the meteorological processes differ largely from those relevant to chemical processes. Therefore the system of balance equations is split into two systems - a transport- and a chemistry system. In every time–step the model first solves for each species the transport component. The transport–system uses extensively the concept of operator–splitting - the transport–equation is split into an advection- and a diffusion–equation ([Str68]). Each of these three–dimensional equations is decomposed into a series of it's one–dimensional components. The one–dimensional advection–equations are solved by the FCT–method, the diffusion–equations are solved by a modified second–order Lax-Wendroff–method ([BB76],[vL74]). After this at each grid point the rate of change of each species concentration resulting from the chemical kinetics - expressed by a set of coupled, nonlinear ordinary differential equations - is solved by the chemistry solver. Because of the stiffness of the system a semi–implicit method is used ([GJM82]).

At the Institut für Meteorologie und Klimaforschung of the Research Center Karlsruhe and of the University Karlsruhe for regional scales a sophisticated numerical model system consisting of the meteorological model KAMM [AF73], the transport model DRAIS [TD88] and the chemical reaction model RADM [CBI$^+$87] has been developed since years. KAMM models the velocity field necessary for DRAIS whereas RADM evaluates the chemical interaction equations. The presentation at hand concentrates on the model parts DRAIS and RADM because these parts need nearly the whole computation time of the model.

Typical grids consist of 50000–100000 grid points on which the physical processes are

Ninth International Conference on Domain Decomposition Methods
Editor Petter E. Bjørstad, Magne S. Espedal and David E. Keyes

simulated with time-steps up to 20 seconds. In contrast the chemistry simulation works with time-steps between 0.1 and 5 seconds. A one-day simulation with 26 species takes about 12 hours computing time by using the vector computer VP400. An overview of explicit meteorological applications and visualization of numerical results is given in [Fie93].

The method of domain decomposition is used to parallelize the solution process of the model system. It will be shown that the use of domain decomposition is a good possibility to shorten the response time on parallel computers strongly. Another advantage of this method is that on parallel computing systems it can be engaged to simulate larger problems because of the data can be maintained on the local memories of the computing system.

2 Governing Equations

Neglecting molecular diffusion the spatial and temporal distribution of the concentration field $c_s(\boldsymbol{r}, t)$, $s = 1, \dots, n$ of a set of n species is given by the system of balance equations:

$$\frac{\partial c_s}{\partial t} + \boldsymbol{\nabla} \cdot (c_s \boldsymbol{v}) = S_{c_s}, \qquad s = 1, \dots, n, \tag{2.1}$$

where $\boldsymbol{v}$ is the wind velocity and S_{c_s} are source and sink terms due to for example emissions, chemical reactions or deposition at the ground.

Due to the typical different time scales relevant to the various processes under consideration each equation is split into an homogeneous and an inhomogeneous part in view of the numerical solution of the system. The homogeneous part of the balance equations refers to the meteorological transport and the inhomogeneous part to the chemical reactions. The latter is accepted to be independent of spatial derivations. Thus the solution of (2.1) will be the replaced by solving (2.2) and (2.3) successively

$$\frac{\partial c_s}{\partial t} + \boldsymbol{\nabla} \cdot (c_s \boldsymbol{v}) = 0 \qquad s = 1, \dots, n \tag{2.2}$$

$$\frac{\partial c_s}{\partial t} = S_{c_s} = f_s(c_1, \dots, c_n, t) \qquad s = 1, \dots, n. \tag{2.3}$$

Applying these equations to the turbulent system of the atmosphere all variables ϕ are decomposed into a mean $\overline{\phi}$ and a fluctuating part ϕ' (Reynolds–decomposition). In chemistry the fluctuating parts are neglected. The turbulence is closed with a first order parameterization ([MY74]). So under the assumption of shallow convection ([DF69]) we can write the equations of conservation (2.2) as

$$\frac{\partial \overline{c_s}}{\partial t} + \boldsymbol{\nabla} \cdot (\overline{c}_s \overline{\boldsymbol{v}}) - \overline{c}_s (\boldsymbol{\nabla} \cdot \overline{\boldsymbol{v}}) = \boldsymbol{\nabla} \cdot (\mathcal{K} \cdot \boldsymbol{\nabla} \overline{c_s}), \tag{2.4}$$

with $\mathcal{K}$ the tensor of diffusion. Because of the generally not flat bottom of the model terrain following systems of coordinates are used. By a transformation of the irregular z-coordinate the model volume is transformed into a cube ([GCS75]). Because of that numerical methods for structured grids can be employed.

3 Numerical Solution

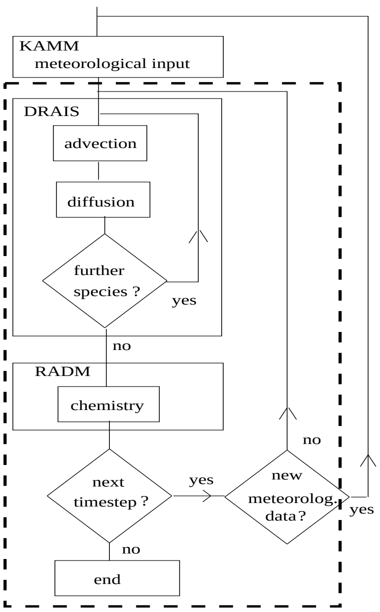

Figure 1 Flowchart of the simulation

Figure 1 shows the sequence of calculation. In order to solve the meteorological transport equation (2.4) this equation is decomposed into a three–dimensional advection and into a three–dimensional diffusion equation ([Str68]). Both are solved in a transport–step. After this the rate of change of the species concentrations is calculated by the chemistry–simulator. The numerical scheme at the n–th step we can express by operators:

$$\boldsymbol{c}_{n+1} = \mathcal{C} \circ (\mathcal{A} + \mathcal{D})\boldsymbol{c}_n$$
$$\mathcal{D} = \sum \mathcal{D}^i$$

with the operators $\mathcal{A}, \mathcal{C}$ and $\mathcal{D}$ referring to advection, diffusion and chemical composition. The index i characterizes the spatial direction.

The transport–simulator splits the three–dimensional advection- and diffusion equations in the one–dimensional compounds ([Str68]). The time–integration of these equations uses forward-Euler discretization. The one–dimensional equations of advection are solved by the FCT–method (flux–corrected–transport). The diffusion equations are solved by a modified second order Lax–Wendroff difference–method ([BB76],[vL74]). The transport equations have to be solved for each species. Their solution is independent of each other.

To model the chemistry a stiff system of nonlinear ordinary equations

$$\frac{\partial c_s}{\partial t} = f_s(c_1, \ldots, c_n, t) \quad , s = 1, \ldots, n. \tag{3.5}$$

has to be solved. On the assumption of a production rate a_s of a species s (independent of its own concentration) and a loss rate $b_s \cdot c_s$ we can write equation 3.5 in the following form:

$$\frac{dc_s}{dt} = f_s(c_1, \ldots, c_n, t) = a_s - b_s \cdot c_s \quad , s = 1, \ldots, n. \tag{3.6}$$

Because of the coupling of different species by chemical reactions the functions a and b are in general not constant but dependent on the concentrations of other species. The algorithm is a predictor-corrector integration scheme with internal self-adaptive time–steps. [GJM82].

4 Domain Decomposition

The topological regular grid is decomposed into sub–grids by hyper-planes parallel to planes formed by two coordinate axes.

Now we want to discuss the use of a different number of coordinates for domain decomposition (dimension) with regard to the parallelization of the problem. So the aim of this work is to investigate the benefit the domain decomposition for acceleration without changing anything in the physical and the numerical processes of modeling and solution.

For the first we consider a transport–step of the constituents. In a transport–step three one–dimensional advection and three one–dimensional diffusion equations are solved by explicit schemes. Meanwhile a transport–step the solution of advection and diffusion equations in a sub-domain doesn't need any data of an other sub-domain [Mül96].

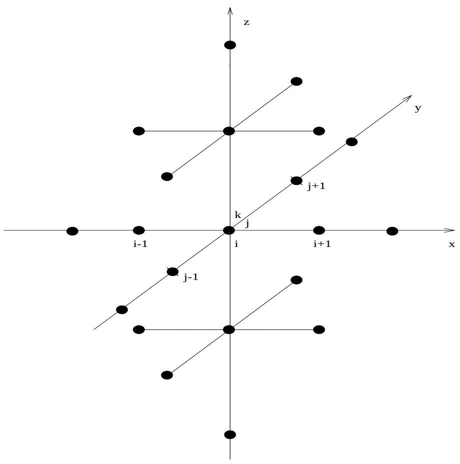

Figure 2 Structure of data dependence in a grid point G_{ijk} for a transport–step

The union of all six difference stars at a grid point G_{ijk} (figure 2) gives the grid points from which the calculation scheme for the transport at a fixed interior grid point needs data from the foregoing chemistry step. Between different solution steps of a transport–step their is no communication necessary. Because of the equal number of arithmetical operations for the calculation of the transport in each grid point a homogeneous distribution of the grid points on different processors leads also to a good balance of the numerical load between the processors. By domain decomposition we distribute the domain (one–dimensional) in the following way.

Let the grid be decomposed by $n-1, n \geq 2$ hyper-planes

$$H_j = \{(x,y,z) \in G; y = c_j\},\ j \in J,$$

in n disjunctive sub–grids G_j

$$\begin{aligned} G &= \bigcup_{j \in J} G_j, \\ G_j \cap G_{j'} &= \emptyset \text{ for } j, j' \in J, \\ J &= \{\iota; \iota = 0, \dots, n-1\}. \end{aligned}$$

Each of the n processors gets for simulation the sub–grid G_j defined by

$$G_j := [1, IX] \times [y_r(j), y_s(j)] \times [1, IZ]$$

IX, IY and IZ are the number of grid points in $x-, y-$ and z-direction. With

$$B = \lfloor IY/IYP \rfloor$$

and

$$R = IY \pmod{IYP}$$

we can define the $y-$index of the boundary grid points of the sub-domains by (l:left,r:right):

$$\begin{aligned} y_l(0) &:= 1 \\ y_r(0) &:= \begin{cases} B+1 & \text{for} \quad R > 0 \\ B & \text{for} \quad R = 0 \end{cases} \\ y_l(j) &:= y_r(j-1)+1 \\ y_r(j) &:= \begin{cases} y_l(j)+B+1 & \text{for} \quad j < R \\ y_l(j)+B & \text{for} \quad j \geq R. \end{cases} \end{aligned}$$

The different numerical load at the physical boundary grid points is not relevant for the considered problem size.

After the simulation of the change of the concentrations caused by advection and diffusion the change of the concentration caused by chemistry is calculated. Using the same domain decomposition for the chemistry–module there is no communication from the transport step necessary because the simulation of the chemical interaction runs at each grid point independent of other grid points. Before the beginning of the next meteorological step communication has to take place.

In figure 3 the used computation time for a chemistry–step is shown for different processors summed over all vertical grid point layers of the model. Because of the higher gradients of the concentrations of most species the need of computation time in the layers near the bottom is higher. (The vertical layers are countered from the top.) The reason therefore is a smaller internal time-step for grid points with spatial high gradients and so for a fixed time interval between transport and chemistry locally differing number of iterations of the implicit method.

So we use the common domain decomposition only in one or two horizontal components. The decomposition of the vertical components by horizontal sections on different processors is not suited because of the inhomogeneous distribution of work between the different horizontal layers which is caused by the implicit chemical solver.

The distribution of the calculation of sub-domains to different processors leads to logical boundary grid points. The calculation at these grid points needs data from ghost points which exist in the memory of other processors.

Figure 4 shows the structure of the communication of the two–dimensional decomposition. Data on grid points (ghost points) lying in the dark areas are sent by corresponding processors. Processors dealing with domains without physical boundaries have to communicate with four other processors, others communicate with a corresponding number of processors.

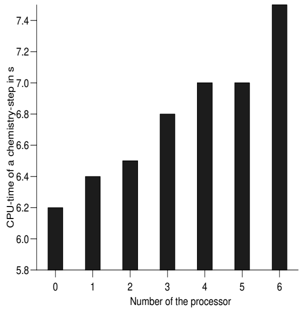

Figure 3 Distribution of CPU-time of a chemistry–step between seven processors

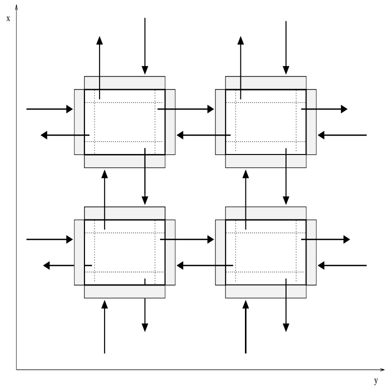

Figure 4 Symbolic representation of the communication of processors dealing with sub-domains without physical boundaries for a two–dimensional decomposition

5 Results

The implementation of the described parallelization has been performed on the MIMD–computer Paragon XP/S using explicit message passing. The grid size is $49 \times 53 \times 25$. In each grid point 26 different species have been considered.

The measurements are given in table 1. The two–dimensional parallelization is based on a dividing of the x- and the y-axes. Let IXP and IYP be the numbers of parts IX and IY are decomposed into. Results are given in table 2.

The main loss of efficiency documented in table 1 and 2 is caused by the different calculation efforts at different processors. The main reasons for this are properties of the division of entire numbers (a nonzero remainder leads to a load imbalance between different processors) and the imbalance in the chemistry-model which is a consequence of the implicitness of the solver. So the refinement of the decomposition leads to increasing differences in calculation time meanwhile the chemistry–step between processors dealing with different sub-domains [Mül96].

Up to 70 processors an efficiency greater than 50% has been measured so that this strategy is well suited for parallelizing the model. Grids with a linear increasing number of grid points in the horizontal layers can be expected to be calculated in the same time if an appropriate linear increase of the number of the involved processors is given [Mül96].

Table 1 CPU-time and efficiency for one–dimensional decomposition

processors	computation time	efficiency
1	90.1	1.00
2	46.6	0.97
3	31.9	0.94
5	20.0	0.90
7	14.2	0.91
9	11.7	0.86
13	8.7	0.80
17	7.6	0.70
25	5.8	0.62

Table 2 CPU-time and efficiency for two–dimensional decomposition

$IXP \times IYP$	processors	computation time	efficiency
(2,4)	8	12.8	0.88
(2,12)	24	5.2	0.72
(4,6)	24	5.4	0.70
(2,25)	50	3.4	0.53
(4,17)	68	2.6	0.51
(6,13)	78	2.7	0.43
(4,25)	100	2.2	0.41
(8,17)	136	2.0	0.33

Acknowledgement

This work was been while the author was at the Institute für Meteorologie und Klimaforschung of the Research Center Karlsruhe and of the University of Karlsruhe. The implementation and the measurements of the parallel program were done at the Paragon XP/S of the Research Center Jülich.

REFERENCES

[AF73] Adrian G. and Fiedler F. (1973) Simulation of unstationary wind and temperature fields over complex terrain and comparison with observations. *Beitr. Phys. Atmosph.* 64: 27–48.

[BB76] Book D. L. and Boris J. P. (1976) Flux corrected transport I, SHASTA, A fluid transport algorithm that works. *J. of Comp. Phys.* 22: 517–533.

[CBI+87] Chang J. S., Brost R. A., Isaksen I. S. A., S. Madronich P., Middleton, Stockwell W. R., and Walcek C. J. (1987) A three-dimensional eulerian acid deposition model: Physical concepts and formulation. *J. Geophys. Res.* 92: 14681–14700.

[DF69] Dutton J. A. and Fichtl G. H. (1969) Approximate equations of motions for gases and liquids. *J. Atm. Sci.* 26.

[Fie93] Fiedler F. (1993) Development of meteorological computer models. *Interdisciplinary Science Reviews* 18.

[GCS75] Gal-Chen T. and Sommerville R. C. J. (1975) On the use of a coordinate transformation for the solution of the navier-stokes equations. *J. of Comp. Phys.* 17: 209–228.

[GJM82] G. J. McRae W. R. Goodin J. H. S. (1982) Numerical solution of the atmospheric diffusion equation for chemically reacting flows. *J. of Comp. Phys.* 45: 1–42.

[Mül96] Müller A. (1996) Parallelisierung numerischer Verfahren zur Beschreibung von Ausbreitungs- und chemischen Umwandlungsprozessen in der atmosphärischen Grenzschicht. *Wissenschaftliche Berichte des Instituts für Meteorologie und Klimaforschung der Universität Karlsruhe* 18.

[MY74] Mellor G. L. and Yamada T. (1974) A hierarchy of turbulence closure models for planetary boundary layers. *J. Atm. Sci.* 31: 1791–1806.

[Str68] Strang G. (1968) On the construction and comparison of difference schemes. *SIAM, J. Numer. Anal.* 5: 506–517.

[TD88] Tangermann-Dlugi G. (1988) Numerische Simulationen atmosphärischer Grenzschichtströmungen über langestreckten mesoskaligen Hügelketten bei neutraler thermischer Schichtung. *Wissenschaftliche Berichte des Instituts für Meteorologie und Klimaforschung der Universität Karlsruhe* 2.

[vL74] van Leer B. (1974) Towards the ultimate conservative difference scheme . ii. monotonicity and conservation combined in a second–order scheme. *J. of Comp. Phys.* 14: 361–370.