Comparison of Two Local Refinement Methods for Large Scale Air Pollution Simulations

Anton Antonov¹, Krassimir Georgiev², Emilia Komsalova², and Zahari Zlatev³

Wolfram Research Inc.
100 Trade Center Drive, Champaign, IL 61820-7237, USA antonov@wolfram.com
² Central Laboratory for Parallel Processing Bulgarian Academy of Sciences
Acad. G. Bonchev, Bl. 25-A, 1113 Sofia, Bulgaria georgiev,emilia@parallel.bas.bg
³ National Environmental Research Institute Frederiksborgvej 399, DK-4000 Roskilde, Denmark zz@dmu.dk

Abstract. Two methods for Large Scale Air Pollution (LSAP) simulations over static grids with local refinements are compared using the object-oriented version of the Danish Eulerian Model. Both methods are based on the Galerkin finite element method. The first one is over a static locally refined grid – we call it Static Local Refinement Algorithm (SLRA). We compare SLRA with the Recursive Static-Regridding Algorithm (RSRA), in which regular grids with finer resolution are nested within a coarser mother grid. RSRA and SLRA are compared with the translational and rotational cone tests. The drawbacks and advantages of the methods are discussed.

Keywords: Air pollution modeling, rotational test, translational test, local refinement.

Subject Classifications: 65N30, 76R05.

1 Introduction

The base grids of all known large-scale air pollution models are uniform and too coarse to represent the local phenomenon well enough. For example, the mesh size of the grid in the operational two-dimensional version of the Danish Eulerian Model (DEM) is 50~km. It is difficult to resolve on this grid the enhancement (the supply of more details) of concentrations and depositions in urban areas, resulting from the local emissions. In fact, the point source emissions are smeared out over the corresponding grid cell (which is too big) and as a result an unnatural diffusion is introduced into the model. The local phenomenon can be represented if much finer grid is used. However, an uniform finer grid about 10~km mesh step size, leads to 25 times more grid squares and will increase correspondingly the computational time of the algorithm. The concept of local grid refinement is a compromise between better resolution and computational expense in terms of

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the computational time. In fact, higher resolution is mostly needed only inside certain subdomains of the model domain, such as the areas around the point sources and areas where strong gradients in the concentration field are observed. It is much more difficult to organize local refinement in some specific (user defined or with strong gradients) areas than to refine the whole model domain uniformly. The former though leads to much "cheaper" solution than the later, while both solutions are comparable.

In this paper two algorithms for Large Scale Air Pollution (LSAP) simulations over static grids with local refinements are compared and discussed. They are both implemented in the object-oriented version of the Danish Eulerian Model [1,11].

Both algorithms are based on the Galerkin Finite Element Method (GFEM). The first algorithm use a static locally refined grid. This algorithm is called Static Local Refinement Algorithm (SLRA). We compare SLRA and the Recursive Static-Regridding Algorithm (RSRA; see [6]).

RSRA is designed for time evolution problems involving partial differential equations that have solutions with sharp moving transitions, such as steep wave fronts and emerging or disappearing layers [6]. A version of it is used in the LSAP model called EURopean Operational Smog model (EUROS) [3,4].

Both SLRA and RSRA use grids concentrated just over the areas of interest. The construction of the grids is based on the principle of local uniform grid refinement, i. e. locally uniform refinement on some subdomains of an uniform grid. The refinements also could be nested.

The remainder of the paper is organized as follows. Section 2 gives descriptions of the algorithms. Section 3 focuses on the rotational test – numerical results are presented and discussed. Section 4 describes two translational tests and their results. Conclusions and future plans can be found in the last section, Section 5.

2 The Two Algorithms

2.1 Recursive Static-Regridding Algorithm (RSRA)

When the solution advances from the time level t_0 to $t_0 + \Delta t$, the version of RSRA we use for the tests in the article has the following steps (see [6] for the original version of RSRA):

- 1. Integrate by GFEM on the coarse grid with time step Δt .
- 2. Integration is followed by regridding. For the applications of RSRA described in this article, the regridding is always over the same subdomain. (This differs from the description in [6], where the domain of the refinement is chosen according to the sharp gradients of the coarse solution.)
- 3. Regridding is followed by interpolation. Since the fine grid is static, we interpolate the concentrations at time level t_0 and specify boundary values for the fine grid cells that abut on the coarse cells. We impose on these grid interfaces Dirichlet boundary conditions via interpolation of the values of

the concentrations at the time level t_0 . Since we use rectangular grids, the interfacing cells form stripes along the edges of the finer grids. In the experiments reported in this article the width of these stripes is two cells (three points).

4. Finally, GFEM is applied on the finest grid over the time interval $t_0 \leq t \leq t_0 + \Delta t$. The so found refined values of the concentrations are injected in the coarse grid points.

Multiple levels in RSRA are handled in a recursive fashion. It is clear from step 4 that when this algorithm is employed, the simulations over the refined domain influence the solution through the injection of the fine grid results. We can say that RSRA assumes that after the injection of the refined grid solution into the coarser grid solution, the result will be nearly the same as the one with global refinement.

The advantage of RSRA is that the same algorithm can be used for the coarse and the fine grids. This means that if we have an algorithm for simulations on the coarser regular grid, it can be reused in an algorithm for refined simulations. This is an algorithm which is easier to develop than one that seeks global solutions on the locally refined grid. The algorithms for regular two dimensional grids can use some splitting procedure to become simpler and faster.

2.2 Static Local Refinement Algorithm (SLRA)

The SLRA algorithm can be defined as follows.

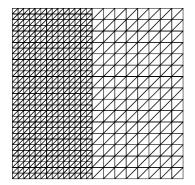
First, the coarse grid over the whole computational domain is generated. Then, a rectangular subdomain of the main domain that contains the region of interest is extracted. Finally, the grid cells belong to the selected subdomain are refined to the desired resolution. The refined subdomain is plugged in the coarse grid and then we generate the grid description suitable for our simulation code. Clearly, this algorithm can be applied for several regions of refinement as far as the refined regions do not overlap. (Let us mention that the RSRA algorithm has the same requirement.) Then GFEM is applied with basis functions generated on the obtained locally refined grid.

3 Rotational Test

The rotational test ([2,5]) is the most popular tool among the researchers in the fields of meteorology and environmental modeling for testing the numerical algorithms used in the large air pollution models. From the mathematical point of view, it is a pure advection problem which creates difficulties in the numerical treatment. We have changed the test to use the domain used in DEM: a square with size $4800 \ km$. The test governing partial differential equation is:

$$\frac{\partial c}{\partial t} = -(2400 - y)\frac{\partial c}{\partial x} - (x - 2400)\frac{\partial c}{\partial y},\tag{1}$$

where $0 \le x \le 4800 \ km$, $0 \le y \le 4800 \ km$. The initial cone has a center in the point $(0.25, 0.5) * 4800 \ km$ and radius $1/8 * 4800 \ km$. Its height is $100 \ m$. All the test experiments presented bellow are inside the **Object-oriented version of DEM** (OODEM) [1]. Crank-Nicholson method and Restart GM-RES(30) are used to solve the discretized problem. In fact, the codes are taken from the Portable, Extensible Toolkit for Scientific computation (PETSc), which is a suite of uni- and parallel-processor codes for solving large-scale problems modeled by partial differential equations (see [9, 10]). The pre- and post processing procedures, including visualization tools, are made using Mathematica ([8]).



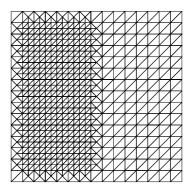


Fig. 1. 16×16 coarse grid models of the refined grids used for the rotational tests. The grids used in the tests have 96×96 coarse, mother grids. On the left – RSRA-2:1; on the right – SLRA-2:1.

Six numerical experiments are done in the framework of the rotational test. For each of the grids RSRA-2:1 and SLRA-2:1 (see Fig. 1) one complete rotation of the cone for 400, 800, and 1600 number of steps was performed.

It is important that the numerical methods which are applied to the cone test keep the height of the cone close to its initial one. The cone heights after the final steps of the six experiments are shown in Table 1.

steps	400	800	1600
RSRA-2:1	92.2317	92.3666	92.2938
SLRA-2:1	92.5299	92.0869	92.2268

We were not able to observe differences between the RSRA-2:1 results and those of SLRA-2:1 using 3D plots. Nevertheless, on very detailed contour plots

of the results obtained with the 1600 experiments, the RSRA-2:1 results look slightly better – see Figure 2.

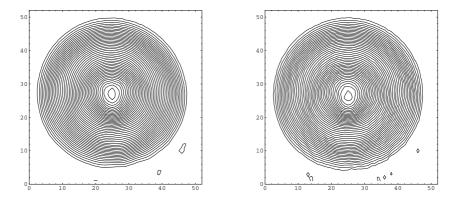


Fig. 2. Contour plots when the cone enters the refined region. On the left – RSRA-2:1; on the right – SLRA-2:1. The contours are at the concentration values 5, 7, 9, 11, ..., 95.

Another interesting phenomenon is the increase of the number of iterations in the RSRA-2:1 rotational experiment over the refined region when the cone is not on it – see Figure 3. The number of iterations become more uniform when the rotational steps are increased – for 1600 steps rotation they vary between 3 and 5. Obviously this happens because of the convergence tester. With real data simulations this will not happen.

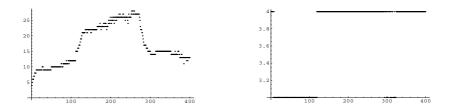


Fig. 3. Number of iterations for RSRA-2:1 rotational test with 400 steps. Fine grid – left, coarse grid – right.

4 Translational Test

Another way to compare the methods is using a translational test, i.e. a test in which the cone is translated **in** and **out** of the finer grid. As in the rotational test, we study how the described above two algorithms keep the height and shape of the cone close the initial ones. We did two experiments corresponding to the

two grids – RSRA-2:1 and SLRA-2:1 – each with constant wind magnitude 10 m/s that is close to the typical maximum wind magnitudes in DEM. The wind has zero y-component, and it changes its x-direction every 240 steps. As in the rotational cone test, the cone initial position is on the finer grid at the point $(0.25, 0.5) * 4800 \ km$. The time step is $1000 \ s$, which is close to the time step 900 s used in DEM. The number of the steps is 240 in order the change in the wind direction to be at the points $(0.25, 0.5) * 4800 \ km$ and $(0.75, 0.5) * 4800 \ km$. The results are shown on Table 2. We can see that RSRA-2:1 cone height decreases much faster than the SLRA-2:1 cone height, which stays close to the initial one.

We can explain these results in the following way. Let us assume we have RSRA grids with several levels of refinement. If a puff is located inside the most refined region, some of the concentrations it consists of will lie only on the refined grid but not on the coarser one. After the injection on step 4 of RSRA is done, the puff generally will be aliased with a smoother concentration distribution on the coarser grid. If the puff is blown away from the region of the refinement the detailed information will be lost – it will be only sampled on the coarser grids. If SLRA is used the blown away puff will be "incorporated" in the SLRA solution.

To confirm the reasoning above we did further translation experiments. RSRA was used with three squares, telescopically nested grids. Each of the finer grids is twice finer than the one it is nested within. The region of the refinement was placed in the middle of the base grid. The width of the transition stripes for the finer grids is 3. The side size of the second grid is 1/4-th of the base one; the third, finest grid covers the inner non-transitional area of the second. We denote RSRA with these grids with RSRA-1:2:4. The corresponding SLRA grid is denoted with SLRA-1:2:4.

step	RSRA-2:1		SLRA-2:1	
	finer grid	coarser grid	finer grid	coarser grid
0	100		100	
240		93.4417		95.6048
480	96.8807		99.6673	
720		93.5301		95.6
960	96.0226		99.5504	
1200		93.592		95.5989
1440	94.555		99.487	

Table 2. Maximum cone values for the translation tests.

Initially the cone lies completely in the region with densest refinement. The cone is translated completely out of the refined region and then it is translated back to its initial position. For each method two experiments were made: one with wind being parallel to the x-axis with constant magnitude equal to 10~m/s, and one with the wind being parallel to the diagonal of the grid with constant magnitude equal to $\sqrt{200}~m/s$. The simulation time step is 1000~s. Table 3 shows the maximal values at the initial, intermediate, and final stages of the

		Maximal values		
Method	Wind	Initial	Intermediate	Final
RSRA-1:2:4	x-wind only	100	91.5307	93.6504
RSRA-1:2:4	diagonal	100	90.0830	94.4363
SLRA-1:2:4	x-wind only	100	95.4348	99.9965
SLRA-1:2:4	diagonal	100	94.5626	99.9537

Table 3. Cone translation with horizontal and diagonal winds. The RSRA-1:2:4 values at the initial and final stages are taken from the finest grid; the intermediate value is taken from the base grid.

experiments. On the intermediate stage the wind direction is alternated. We can see that SLRA-1:2:4 preserves the cone height very close to the initial one, and that RSRA-1:2:4 dumps it with 6-7%.

5 Conclusions and Future Plans

Two algorithms for Large Scale Air Pollution (LSAP) simulations over static grids with local refinements using the object-oriented version of the Danish Eulerian Model are compared and discussed – RSRA and SLRA. It is not possible to judge which method is better with the rotational and translational tests we have used. RSRA is easier to implement, but it has the puff smoothing effect described in Section 4. On the other side, in SLRA certain wave components of the puff will be reflected by the inner grid boundaries when the puff passes through them (see [7]). To estimate the significance of these RSRA and SLRA effects, we can extend the described experiments with some that include the chemistry reactions. Another possible extension is to make simulations with real data and to compare the results.

It is easy with RSRA to have dynamic local refinements. To make a corresponding implementation of SLRA would mean dynamic invocation of the grid generator – so far in OODEM the grid generation is a preprocessing step. With RSRA this preprocessing is skipped.

Last, an RSRA implementation with real data can be used to investigate if it is possible to obtain more accurate solutions over the refined region using Richardson extrapolation for the results of the different grids.

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References

- 1. Anton Antonov. Object-Oriented Framework for Large Scale Air Pollution Models. PhD thesis, The Technical University of Denmark, (2001) http://www.imm.dtu.dk/~uniaaa/OODEM/ThesisComplete.ps.gz.
- W. P. Crowley. Numerical advection experiments. Mon. Weth. Rev. 96 (1968) 1–11.
- 3. K. Georgiev. Optimal strategies for parallelization of the EUROS model: design and implementation. Technical Report 2002/TAP/R/041, Flemish Inst. for Technological Research, Mol, Belgium, 2002.
- M. van Loon. Numerical methods in smog predictions. PhD thesis, University of Amsterdam, The Netherlands, 1996.
- 5. C. R. Molenkampf. Accuracy of finite-difference methods applied to the advection equation. Journal of Applied Meteorology, 7 (1968) 160–167.
- R.A. Trompert and J.G. Verwer. A static-regridding method for two dimensional parabolic partial differential equations. Applied Numerical Mathematics 8 (1991) 65–90.
- 7. R. Vichnevetsky. Wave propagation Analysis of Difference Schemes for Hyperbolic Equations: A Review. Numerical Methods in Fluids 7 (1987) 409–452.
- 8. S. Wolfram. Mathematica: a system for doing mathematics by computer. Wolfram Media, Cambridge Univ. Press, Fourth Edition, 1999.
- 9. WWW http://www-unix.Mcs.anl.gov/petsc/ petsc-current/docs/manualpages/ SLES/SLESSolve.html
- 10. WWW http://www-unix.Mcs.anl.gov/petsc/ petsc-current/docs/manualpages/ KSP/KSPGMRESSETRestart.html
- 11. Z. Zlatev. Computer Treatment of Large Air Pollution Models. Kluwer, 1995.