AN ADAPTIVE GRID MODEL FOR URBAN TO REGIONAL SCALE AIR QUALITY PROBLEMS

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ABSTRACT

An adaptive grid, urban-to-regional scale air quality model has been developed. The adaptive grid algorithm increases the grid resolution dynamically and automatically in regions where the errors are large. This assures accurate estimates of pollutant concentrations with optimal use of computational resources throughout the simulation. The movement of the grid is controlled by a weight function formed as a linear combination of errors in various pollutant species. In preliminary applications involving dispersion and chemistry of plumes and puffs, the algorithm proved to be more accurate and efficient than fixed grid models. This paper reports preliminary results from a simulation performed as part of the model's verification.

Key Words: Regional Study, Multiscale Modeling, Point Source Emissions

1. INTRODUCTION

Inadequate grid resolution can be an important source of uncertainty in the predictions of air quality models (AQMs). A large grid size could lead to significant errors in the concentrations of pollutant species, especially those that are formed via non-linear chemical reactions. To address this issue, multi-scale modeling and grid nesting techniques have been developed (Odman and Russell, 1991; Odman et al., 1997). These techniques use finer grids in areas that are presumed to be of interest (e.g., cities) and coarser grids elsewhere (e.g., rural locations). Limitations include loss in accuracy due to grid interface problems and inability to adjust to dynamic changes in resolution requirements. Adaptive grids are not subject to such limitations and do not require a priori knowledge of where to place finer resolution. Using grid clustering or grid enrichment techniques, they automatically allocate finer resolution to areas of interest. Adaptive grid AQMs can capture the details of atmospheric dynamics and chemistry more efficiently than their fixed grid counterparts. The vicinities of emission sources are of particular interest with their large pollutant concentration gradients and rapid chemical kinetics.

The adaptive grid methodology used here is based on the Dynamic Solution Adaptive Grid Algorithm (DSAGA) of Benson and McRae (1991). It employs a structured grid with a constant number of grid nodes. In two-dimensional space, a rectangular domain is partitioned into $N \times M$ quadrilateral grid cells. The nodes move throughout the simulation. This changes the length of the links and the area of the grid cells, but the connectivity between the nodes remains the same. The movement of the nodes is controlled by a weight function whose value is proportional to the error in the solution. The nodes are clustered around regions where the weight function bears large values, thereby increasing the resolution where the error would be large. Since the number of nodes is fixed, refinement of grid scales in some regions is accompanied by coarsening in other regions where the weight

function has smaller values. This results in optimal use of computational resources and yields a continuous multiscale grid where the scales change gradually. Unlike nested grids, there are no grid interfaces, which may introduce numerical problems due to the discontinuity of grid scales.

The adaptive grid algorithm was applied to problems with increasing complexity and relevance to air quality modeling. First, it was applied to pure advection tests (Srivastava et al., 2000). In a rotating cone test, the adaptive grid solution was more accurate than a fixed, uniform grid solution using the same number of grid nodes. The error in maintaining the peak was only 13% compared to 39% with the fixed grid. The same level of accuracy could only be achieved by using 22 times more grid nodes in the fixed uniform grid. In a second test, concentric conical puffs of NO_x and VOC introduced in a rotational wield field were allowed to react and form ozone (Srivastava et al., 2001a). The parameters of this problem are such that, after a certain time, ozone levels drop below the background near the base of the conical puffs but they peak near the vertex of the cones. This feature was resolved by the adaptive grid solution while it was completely missed by the uniform fixed grid solution. Srivastava et al (2001b) conducted a third test where a power-plant plume was simulated. A two-dimensional plume with a VOC/NO_x emission ratio of 14% was advected with uniform winds and diffused over a background with a VOC/NO_x ratio of 35. Other parameters were chosen to make the dispersion as realistic as possible. After about 12 hours of simulation, the composition of the plume was analyzed taking cross sections at various downwind distances. At 10 km downwind, the adaptive grid solution showed a NO_x rich, but ozone deficient core. This feature was completely missed in the uniform grid solution, which artificially diffused the NO_x and displayed highest ozone levels at the core of the plume. The adaptive grid, on the other hand, had ozone bulges developing near the plume edges. At a downwind distance of 30 km, these bulges continued to grow as NO_x diffused slowly from the core to the edges (at a rate more in line with physical diffusion) and radicals were entrained into the plume. This plume structure started disappearing after about 80 km. At a downwind distance of 135 km, the peak ozone concentration was larger than the one predicted by the fixed uniform grid. A similar plume evolution was observed in the fixed uniform grid solution when the number of grid nodes was increased by a factor of nine. However, this solution was about five times more expensive than the adaptive grid solution and yet not as accurate.

In this paper, we describe how the adaptive grid algorithm was implemented in an urban-to-regional scale AQM. After a brief discussion of important model components, we report preliminary results from the first application of the adaptive grid AQM.

2. METHODOLOGY

There are two important steps in a simulation with the adaptive grid AQM: the adaptation step and the solution step. During the adaptation step, the grid nodes move while the solution (i.e., concentration fields) remains unchanged. A weight function that can detect the error in the solution determines how much to move each node and clusters them in regions where the error is large. The current weight function considers the error in the concentrations of NO only, but we could use any linear combination of errors in different chemical species. In preparation for the solution step, the fields of meteorological inputs and emissions must be mapped onto the new grid locations. This mapping is also considered part of the adaptation step. During the solution step, the grid nodes remain fixed while the solution is advanced in time. Ideally, the adaptation step should be repeated after each solution step because the errors in the concentration fields thus grid resolution requirements change. However, since the mapping of meteorological and emissions data that has to be performed with each

adaptation step is costly, one may choose to apply the adaptation step less frequently. Currently, we apply the adaptation step once every hour of the simulation but we advance the solution by one hour in several time steps. We require that the Courant number is less than unity in determining the time step of the solution. The rest of this section consists of a detailed description of the adaptation and solution steps.

2.1. Adaptation Step

The key to adaptation is a weight function that can detect where grid nodes need to be clustered in order to achieve a more accurate solution. Such a weight function, w, can be built from a linear combination of the errors in the concentrations of various chemical species:

$$w \propto \sum_n \alpha_n \nabla^2 c_n \tag{1}$$

where ∇^2, the Laplacian, represents the error in c_n, the computed value of the concentration of species *n*. The chemical mechanisms used in AQMs usually have a large number of species. Due to non-homogeneous distribution of emissions and disparate residence times, each species may have very different resolution requirements. Determining α_n such that pollutant concentrations (e.g., ozone) can be estimated most accurately is a current research topic. Here, all α_n are set to zero, except the one for NO. Further, the grid adaptation is restricted to the horizontal plane and the same grid structure, which is determined by the surface layer NO concentrations, is used for all vertical layers. This combined with the requirement that the Courant number should be less than unity may result in very small solution time steps because of high wind speeds in the upper layers. Adaptation in the vertical direction is possible but significantly more complicated.

Repositioning of the grid nodes is accomplished by using the weight function. The new position of the grid node *i*, $\vec{P}_i^{new}$, is calculated as

$$\vec{P}_i^{new} = \sum_{k=1}^{4} w_k \vec{P}_k \Big/ \sum_{k=1}^{4} w_k \tag{2}$$

where $\vec{P}_k$, $k = 1,\ldots,4$, are the original positions (i.e., before the movement) of the centroids of the four cells that share the grid node *i* and w_k are the values of the weight function at those locations. After repositioning of the grid nodes, the concentration values must be recalculated for the cells of the adapted grid. This can be achieved by using the concentration values at the old grid locations and interpolating to the new locations. Note that holding the concentration fields fixed and moving the grid is equivalent to advection on a fixed grid. Therefore, we use a high-order accurate and monotonic advection scheme known as the piecewise parabolic method (Collela and Woodward, 1984) for interpolation.

The calculation of the weight function, the movement of the grid nodes and the interpolation of concentration values to the new grid locations are three distinct tasks of an iterative process. Unless the maximum movement of all grid-nodes is below a preset tolerance, the process is reiterated. The grid is considered to have resolved the solution sufficiently when the movement tolerance is met. Note that the adapted grid is non-uniform; this makes the solution step more complicated compared to uniform grid AQMs. Further, since the weight function used in adapting the grid is a function of evolving concentration fields, there is no a

priori knowledge of where the nodes would be located at any given time. Therefore, meteorological and emissions inputs must be re-gridded after each adaptation in contrast to fixed grid AQMs where those inputs are gridded once before the simulation. We identify three more tasks that must be performed in preparation for the solution step.

First, the meteorological inputs (e.g., temperature, wind and humidity fields) must be prepared for the new grid locations. The ideal solution would be to run a mesoscale meteorological model (MMM), which can operate on the same adaptive grid, in parallel with the AQM. This would assure dynamic consistency of meteorological inputs. However, since such a MMM is currently nonexistent, our choices are limited. We are using hourly data from a very high resolution fixed grid MMM simulation and interpolating the necessary inputs to the adaptive grid locations. For mass conservation, as a minimum requirement, the vertical wind components are readjusted later during the solution step as described in Odman and Russell (2000).

Second, the emission inputs must be mapped onto the adapted grid. Here, we treat all emissions in two categories: point and area source emissions. For simplicity, we lump the mobile sources into the area-source category, but treating them in a third category of line sources would yield better resolution. For the point sources, the grid cell containing the location of each stack must be identified. The search may be quite expensive if there are thousands of stacks in the modeling domain. However, assuming that the cell containing the stack before adaptation would still be in close proximity of the stack after adaptation, the search can be localized. Therefore, we start the present search from the cell where the stack was found in the last search and continue with that cell's neighbors and the neighbors' neighbors and so on. This local search provides significant savings over more general, global searches. The area source emissions are first mapped onto a high-resolution grid using geographic information systems. This "emissions grid" remains fixed throughout the simulation. Around each adaptive grid cell there is a box of emissions grid cells E_i, $i = 1, \ldots, n$, as illustrated in Figure 1. The major task in processing area source emissions is to find the polygon S_i, which is.the intersection of the adaptive grid cell with E_i. Once this is done, the total mass emitted into the adaptive grid cell can be calculated by summing the products of the area of S_i by the emission flux of E_i.

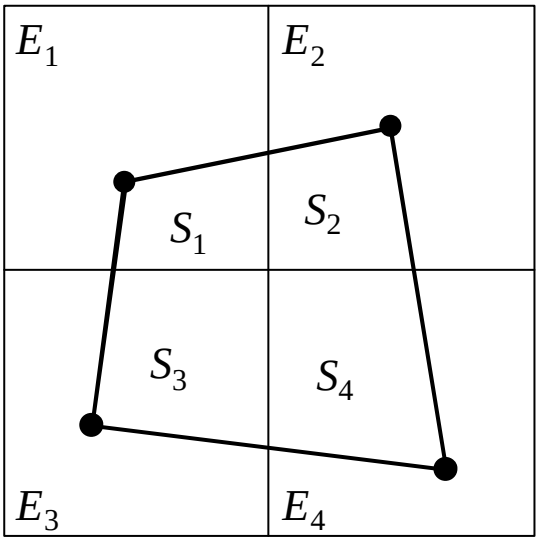

Figure 1. Intersection of an adapting grid cell with the area-source emissions grid.

The third task in preparation for the solution step is reestablishing a uniform grid for easy computation of the solution. This requires computation of a transformation from the (x, y) space where the grid is non-uniform to the (ξ, η) space where the grid would be uniform. The calculation of the Jacobian of the transformation and other necessary metrics (i.e., $\partial\xi/\partial x, \partial\xi/\partial y, \partial\eta/\partial x, \partial\eta/\partial y$) concludes the adaptation step.

2.2. Solution Step

The atmospheric diffusion equation in the (ξ, η, σ) space can be written as

$$\frac{\partial(Jc_n)}{\partial t} + \frac{\partial\left(Jv^{\xi}c_n\right)}{\partial\xi} + \frac{\partial\left(Jv^{\eta}c_n\right)}{\partial\eta} + \frac{\partial\left(Jv^{\sigma}c_n\right)}{\partial\sigma} + \frac{\partial}{\partial\xi}\left(JK^{\xi\xi}\frac{\partial c_n}{\partial\xi}\right) + \frac{\partial}{\partial\eta}\left(JK^{\eta\eta}\frac{\partial c_n}{\partial\eta}\right) + \frac{\partial}{\partial\sigma}\left(JK^{\sigma\sigma}\frac{\partial c_n}{\partial\sigma}\right) = JR_n + JS_n \tag{3}$$

where c_n, R_n and S_n are the concentration, chemical reaction and emission terms of species n, respectively, and ó is a terrain-following vertical coordinate. J is the Jacobian of the coordinate transformation:

$$J = \frac{1}{m^2}\frac{\partial z}{\partial\sigma}\left(\frac{\partial x}{\partial\xi}\frac{\partial y}{\partial\eta} - \frac{\partial y}{\partial\xi}\frac{\partial x}{\partial\eta}\right) \tag{4}$$

where m is the scale factor of a conformal map projection in the horizontal. The components of the wind vector in ξ and η directions are v^{ξ} and v^{η}:

$$v^{\xi} = m\frac{\partial\xi}{\partial x}U + m\frac{\partial\xi}{\partial y}V$$
$$v^{\eta} = m\frac{\partial\eta}{\partial x}U + m\frac{\partial\eta}{\partial y}V \tag{5}$$

where U and V are real horizontal wind velocities rotated in the map's coordinate directions. The turbulent diffusivity tensor is assumed to be diagonal and its elements are $K^{\xi\xi}$, $K^{\eta\eta}$ and $K^{\sigma\sigma}$. The last element can be expressed in terms of the vertical diffusivity K^{zz} as

$$K^{\sigma\sigma} = \left(\frac{\partial\sigma}{\partial z}\right)^2 K^{zz} \tag{6}$$

The expressions for v^{σ}, the wind component in the ó direction, as well as $K^{\xi\xi}$ and $K^{\eta\eta}$ are omitted here due to space limitations.

Since the grid is uniform in the (ξ, η) space, solution algorithms can be taken directly from existing AQMs. We use those described by Odman and Ingram (1996).

3. MODEL VERIFICATION

The adaptive grid AQM is being verified by simulating ozone air quality in the Tennessee Valley region for the July 7-17, 1995 period. Meteorological data from a 4x4 km resolution

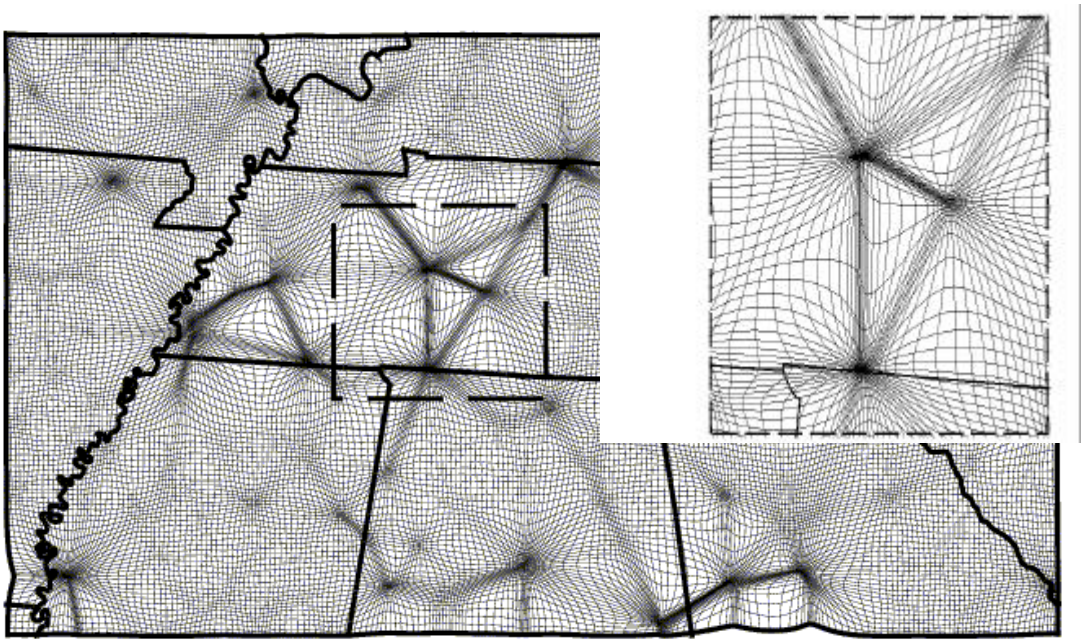

Figure 2. The grid used from 5:00 to 6:00 CST during the simulation of July 7, 1995.

simulation with the Regional Atmospheric Modeling System (RAMS) is being used. The emissions inputs for the region were developed from the Southern Appalachian Mountains Initiative (SAMI) inventory. There are over 9000 point sources in this domain including some of the largest power plants in the U.S.A. The area sources were mapped onto a 4x4 km emissions grid. The AQM grid consists of 225 by 130 cells, initially at 4x4 km resolution. In the vertical, there are 20 unequally spaced layers extending from the surface to 5340 m. Starting with 32 m, the thickness of each layer increases with altitude.

Figure 2 shows the grid at 5:00 CST on July 7. Since the adaptation step is performed once an hour, the grid shown will not change until 6:00 CST. Note that the grid size reduced to 100 m around large point sources. With wind speeds larger than 10 m/s aloft, the solution time step drops below 10 s to keep the Courant number less than unity. Because of this, the simulation is computationally very intense and is progressing very slowly (about 25 hours of CPU time per simulation hour on a SUN Ultra Enterprise 250 with 2x400 MHz CPUs).

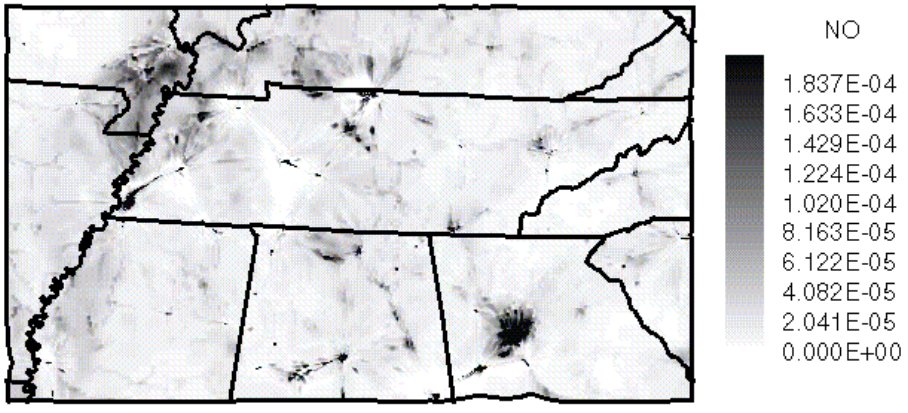

Figure 3. NO concentrations (in ppm) at 5:00 CST that were used to generate the grid above.

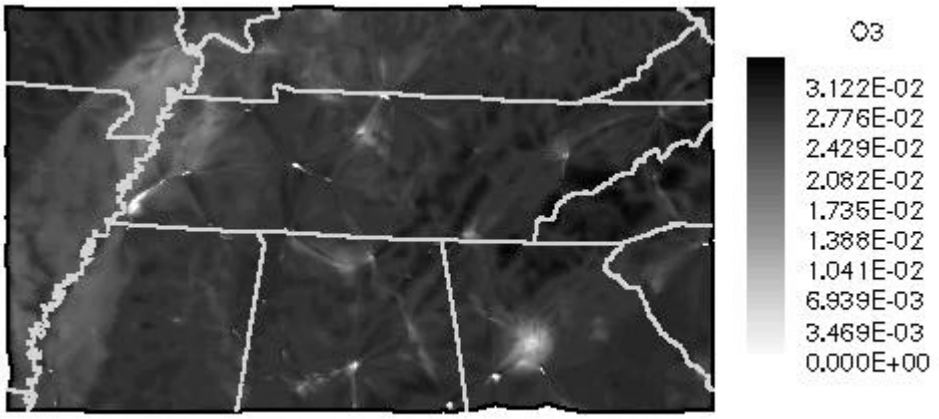

Figure 4. Ozone concentrations (in ppm) at 5:00 CST on July 7, 1995

The surface layer NO concentrations that were used in adapting the grid are shown in Figure 3. NO gradients near source areas are captured with a level of detail that is likely unprecedented for a regional simulation of this scale. It should be noted that some large power plant stacks, such as Cumberland, are emitting above the stable boundary layer at this hour. Since their plumes do not affect the surface layer NO concentrations, no grid clustering is observed in Figure 2 around such stacks. Ozone concentrations that were initialized to 35 ppb everywhere drop below this level since there is no ozone formation at night and O_3 reacts with NO to form NO_2. Figure 4 shows dramatic gradients in ozone near NO sources.

Once this simulation is finished, the results will be compared to those already obtained from a uniform grid AQM simulation with 4x4 km resolution using the same inputs and solution algorithms. To complete the verification, both sets of results will be compared to observations obtained during intensive field studies in the region.

4. SUMMARY AND CONCLUSION

We developed an adaptive grid, urban-to-regional scale AQM. A simulation with this model can be viewed as a repetitive application of two consecutive steps. In the first step, adaptation step, the solution (i.e., concentration fields) is frozen in time. A weight function that can detect the error in the solution is used to move the nodes of a structured grid. The nodes are clustered automatically around regions where the error would be large, increasing the resolution at such regions thereby reducing the error. Iterative movement of the grid nodes continues until further movement does not improve the resolution of the concentration fields. The result is a continuous but non-uniform multiscale grid. In the second step, the solution step, the grid is held fixed and the solution is advanced in time. However, before this can be done, the meteorological and emissions inputs must be mapped onto the adapted grid. For meteorological inputs, we are interpolating data from a very high-resolution mesoscale model simulation. For emissions, we developed efficient search and intersection algorithms to assure proper allocation of point and area sources to the cells of the adapted grid. Using coordinate transformations, the non-uniform grid can be mapped into a space where it becomes uniform. We derived the atmospheric diffusion equation in this new space. Since the form of the equation is very similar to forms in existing AQMs and the grid is uniform, numerical algorithms developed for fixed grid AQMs can be used to advance the solution.

To verify the model, we are simulating the July 7-17, 1995 ozone episode in the Tennessee Valley. So far, the grid is adapting to dynamic changes in the NO fields as expected. Nodes are clustered around major emission sources with grid resolutions around 100 m. The NO and O_3 fields show gradients with a level of detail that is likely unprecedented for a regional simulation at this scale. However, the simulation is progressing very slowly due to very short solution time steps. This will probably necessitate changes in solution algorithms such as using an implicit advection scheme that is not subject to the Courant stability limit. We are also developing adaptation criteria that would consider the errors not only in NO but in other species as well, especially those involved in important ozone formation reactions.

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