6.5 A Model for Local to Global to Local Scale Atmospheric Dispersion

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1. ABSTRACT

Dispersion is inherently a multiscale phenomenon. Most sources are constrained in their spatial and temporal extent, but the pollutant may travel long distances before it re-interacts with the local terrain to deposit on the surface. This range of scales makes the simulation of the processes involved difficult. The usual method of surmounting this difficulty is to use grid nesting, though this requires prior knowledge as to where to put the nests. This paper discusses an approach that has been used for a number of years now – the application of adaptive unstructured grids – that has been extended to support local to global to local scale dispersion. The Operational Multiscale Environment model with Grid Adaptivity (OMEGA) consists of an atmospheric forecast and simulation system designed around an adaptive unstructured grid with an embedded Lagrangian Atmospheric Dispersion Model (ADM). Originally designed for regional forecasts and simulations, OMEGA / ADM now supports full global problems with both static and dynamic adaptive resolution providing appropriate resolution to model the local processes.

2. INTRODUCTION

Dispersion is a problem that depends critically upon the details of the atmospheric state. Where traditional weather forecasting typically consists of predictions of the surface pressure, temperature, and wind speed and direction, dispersion requires much more information on the state of the boundary layer including the thermal lapse rate, the profiles of wind speed and direction, the surface fluxes, and the boundary layer turbulence profile. Thus, any improvement in our ability to forecast dispersion is intimately linked to improvement in our ability to forecast the atmospheric condition with increased horizontal, vertical, and temporal resolution and greater physical fidelity.

In the early days of computing, numerical weather prediction (NWP), was a dominant factor in the design of computer architecture and algorithms. This early work focussed initially on solving a finite difference equation on a uniform rectilinear computational grid and later on spectral methods. After the initial work of Charney (1948), von Neumann (Charney *et al.,* 1950), and Arakawa (1966), however, the focus shifted from the basic algorithms for the numerical solution of the fundamental differential equations to improvements in the model physics. Further work on fundamental numerical algorithms shifted to other disciplines – predominately the then emerging aerospace community. As a result, for 40 years the NWP community has been using numerical techniques that are virtually unchanged; spectral models have traditionally been used for global modeling and structured rectilinear grids have been used for regional modeling.

The fact that the numerical techniques have not changed does not imply, however, that progress has not been made. Indeed, over the past forty years numerical weather prediction has undergone a decade-by-decade advance. The 1960's saw the initial success of the barotropic model. Limited area, multi-layer primitive equation models were put into operational use in the 1970s and 1980s by the US National Weather Service (NWS) and other forecasting centers around the world. These models, first the Limited-area Fine Mesh (LFM) (Gerrity and McPherson, 1971) and later the Nested Grid Model (NGM) (MacPherson and Kelly, 1976) were the first operational nested models in which high resolution was applied to local regions. In parallel with this operational trend, a number of flexible modeling systems with physics intended for high resolution applications were developed. These included the Regional Atmospheric Modeling System (RAMS) (Pielke *et al.,* 1992), and the Penn State/NCAR Mesoscale Model now in its fifth version (MM5) (Grell *et al.,* 1994). In the 1980's increased computational power allowed the introduction of more elaborate model physics. In the 1990's mesoscale models drove toward finer and finer resolutions, mostly through the use of nested grids (e.g., the ARPS model (Xue *et al.,* 1995)) or variable horizontal resolution (e.g., the GEM model (Côté *et al.,* 1998ab). Nested grid models, however, are not sufficient to forecast multiscale phenomena because the nests are fixed and hence unless high resolution is used everywhere, which eliminates the benefits of grid nesting, only specific scales of motion can be resolved in each nest. Thus, while they represented the best possible solution at the time, the application of the output of these models to atmospheric dispersion has been less than ideal.

At the same time meteorology was benefiting from this research and technology boom, computational fluid dynamics (CFD) researchers were creating new innovative numerical techniques designed to model fluid flows around complex geometries. In the 1970s and early 1980s the models developed for aerospace engineering and plasma physics were surprisingly similar to their counterparts in the atmospheric sciences. The grids were composed of regular, rectangular cells extending from no-slip or free-slip surfaces. As more computational power became available and atmospheric modelers were implementing more physics into their models, CFD practitioners were busy refining complex gridding techniques around irregular surfaces. One of the methodologies developed was the use of

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unstructured triangular grids (Baum *et al.,* 1993; Luo *et al.,* 1994).

In the last few years, this new paradigm of unstructured adaptive grids has been applied to atmospheric simulation. This paradigm has the advantage of tremendous flexibility in providing high resolution where required by either static physical properties (terrain elevation, coastlines, land use) or the changing dynamical situation. The first application of this paradigm was the Operational Multiscale Environment model with Grid Adaptivity (OMEGA), an atmospheric simulation and forecasting tool (Bacon *et al.,* 2000) with an embedded Atmospheric Dispersion Model (ADM). Conceived out of a need to advance the state-of-the-art in numerical weather prediction in order to improve our capability to predict the transport and diffusion of hazardous releases (Boybeyi *et al.,* 2001), the OMEGA dynamically adapting grid has since been applied to hurricane track forecasting (Gopalakrishnan *et al.,* 2002). Originally designed for regional simulations, this paper describes the extension of the modeling system to one capable of the ultimate multiscale modeling challenge – global to local scale atmospheric simulation using a dynamically adapting grid.

3. DISPERSION

Dispersion is primarily the coupling of the processes of advection and diffusion. Advection is a well-understood physical process and given a perfect high-resolution, four-dimensional wind field the computation of the advection of a contaminant is straightforward. Similarly, the process of diffusion of an initial delta-function distribution of a contaminant, given a fixed and known diffusivity, is solvable analytically and is represented as a Gaussian distribution with a width determined by κ, the diffusivity. The problem in real situations is that the four-dimensional flow field (the mean wind and turbulence fields) is not known accurately at high spatial and temporal resolution, and the diffusion is not dominated by molecular diffusion but by turbulent diffusion, which is inherently known only in an average sense.

Much is known about homogeneous, isotropic turbulence. The theory for fully developed turbulence has provided useful guidance for many decades. Transient phenomena and developing turbulence are different issues. The atmosphere is constantly changing and the turbulent spectrum is highly variable in space and time. This is one of the reasons for the major difference between chronic and episodic dispersion. When the emission is chronic (continuous over time), one can make assumptions about long time averages and exploit statistical approximations based on observations. When the emission is episodic, the average values are useful as general guidance, but not sufficient to properly understand the evolution of the threat.

4. DISPERSION AND METEOROLOGY

As mentioned in the previous section, the solution of the advection and diffusion equations is relatively straightforward if the four-dimensional flow field is known. Unfortunately, the atmospheric circulation is usually either poorly known at the level of detail important to dispersion, or, for long-range dispersion, poorly forecast. For this reason, the only way to improve our ability to simulate and/or forecast dispersion is to improve our ability to simulate and/or forecast the weather.

The weather is a product of many processes operating over a wide range of scales. If we are concerned with a chronic situation, we can average all of these processes over long times; if we are concerned with a single specific episodic event, then of necessity we must understand these processes down to the scale of the initial dispersal – typically a kilometer or less.

The forces that drive the atmosphere are actually quite small perturbations on a much larger background state. This provides some important scale analyses for consideration in emergency response situations (*cf.* Table 1). The mean sea level pressure for the atmosphere is 1013.25 mb. However, most synoptic (meso-α) forcing is of the order of only 0.01 mb/km. The mesoscale (meso-β and non-hydrostatic cloud scale (meso-γ) forcings are of the order of 0.10 and 0.50 mb/km, respectively.

Terrain forcing can be considerably larger than the synoptic and non-hydrostatic components. Near sea level, the surface pressure decreases by roughly 100 mb per kilometer of elevation leading to a near-surface forcing in complex terrain of 5.00 mb/km for a 5% grade. An analysis of the effects of thermal forcing of land/sea breezes is equally illuminating. The thermal wind, or difference in the geostrophic wind arising from a horizontal difference in temperature, can be related to an effective pressure gradient using the geostrophic wind speed relation. In a coastal situation with a 2.5 K temperature gradient over a kilometer, the effective forcing at 1 km altitude would be roughly 1.00 mb/km.

Urban areas add considerable forcing to the atmospheric circulation. The most obvious is the mechanical forcing due to the urban geometry. A more subtle, but in general more important, forcing is due to the differential heating and cooling that is associated with surface features. The mechanical forcing can be estimated using the dynamic pressure:

Table 1. A hierarchy of atmospheric forcing processes.

Scenario	**ΔP (mb)**	**ΔX (km)**	**ΔP / ΔX (mb / km)**
Synoptic (meso-)	10	1000	0.01
Mesoscale (meso-)	10	100	0.10
Urban Scale – Mechanical Light Wind (2 kt)	0.006	0.05	0.12
Cloud Scale (meso-g)	2	4	0.50
Land / Sea Boundary	1	1	1.00
Urban Scale – Thermal 2 K Urban Heat Island	24	20	1.20
Urban Scale – Mechanical Strong Wind (10 kt)	0.16	0.05	3.20
Terrain Elevation 5 % Grade	5	1	5.00

$$P_{dyn} = \frac{1}{2} \rho \, \mathrm{v}^2 \qquad (1)$$

The urban mechanical forcing is thus of the order of 0.12 mb/km for a 1 m/s wind (2 kt), rising to 3.20 mb/km for a 5 m/s (10 kt) wind.

The thermal forcing in urban situations is more subtle and takes longer to influence the urban circulation, but it is far more common. The nature of the urban environment is such that cities are generally warmer than their surroundings. This is due to the lower albedo of the city surface (daytime), the higher heat capacity of the city (nighttime), and anthropogenic heat (always). An estimate of the thermal forcing can be made using the adiabatic relationship between temperature and pressure:

$$T^{\gamma} \, P^{-(\gamma-1)} = T_0^{\gamma} \, P_0^{-(\gamma-1)} \Rightarrow \frac{dT}{T} = \frac{(\gamma-1)}{\gamma} \frac{dP}{P} \qquad (2)$$

where $\gamma = \frac{c_P}{c_V}$ (= 1.4 for an ideal gas).

This implies that the change in pressure due to a change in temperature is roughly 12 mb/K leading to an estimated forcing of 1.2 mb/km. A critical factor in the thermal forcing is that it is always present given sunlight; urban canyon effects occur only when there is ambient wind.

It is at the smaller scales that micrometeorological factors become important, and sometimes dominant, considerations. Over a typical landscape, terrain relief gives rise to organized flows that may well be different from the predictions of models driven by synoptic features alone. At night, when the surface cools and air in contact with it becomes stratified, downslope winds are typical. Pollutants will tend to drift towards lower elevations, unless they themselves are lighter than air and are released in sufficient amounts to significantly modify the density of the mixture they form with the air. During a sunny day, the air is well mixed in the vertical, and the tendency for upslope winds is therefore often masked by the consequences of synoptics, especially winds driven by pressure gradients.

It is the behavior of the air layer near the ground that generates most modern concern, since it is within this layer that people live and breathe. This planetary boundary layer (PBL) is the region of the atmosphere most influenced by local terrain and obstacles that interrupt the wind flow. It also has the greatest impact on the two major physical variables that control local dispersion – the transport vector and the diffusion rate. The PBL is driven by a mixture of mechanical and thermal forcing. The mechanical forcing is defined by the shape and texture of the terrain: the elevation, surface roughness, and canopy. The thermal forcing is defined by the albedo and heat capacity of the surface, the land/water fraction and vegetation coverage, plus any low solar elevation angle and shadowing effects.

Since dispersion depends on the detailed horizontal and vertical structure of the atmosphere, it is especially important that the forcings mentioned above are considered. Some of the most common PBL circulations are those caused by a land-sea boundary, by urban heat islands, by low-level jets, and by boundary layer separation over complex terrain. These localized circulations are especially important for dispersion issues because they occur near the surface and the source. In some cases, where there is a known potential source (*e.g.,* a nuclear power plant), this detailed meteorology is provided by a dedicated mesonet; however, this addresses only the short-range problem. In general, it is necessary to use forecast products to support long-range dispersion analysis.

5. OMEGA MODELING SYSTEM

OMEGA is a high resolution, high fidelity, non-hydrostatic multiscale forecast system (Bacon *et al.,* 2000). The unique capabilities of OMEGA in multiscale atmospheric simulation of atmospheric and aerosol and gas dispersion processes make it an excellent foundation for this effort. The kernel of the system is the OMEGA model – a three-dimensional, time-dependent, non-hydrostatic model of the atmosphere. It is built upon an unstructured triangular grid, which can adapt to a variety of static user-defined fields as well as dynamically during the simulation to the evolving weather. The triangular unstructured grid makes it possible to represent the underlying terrain with great accuracy (Bacon *et al.,* 2000). First, OMEGA does not require the 2-4 ΔX terrain smoothing traditional in mesoscale models such as MM5 (*cf.*, Table 2 from Guo and Chen, 1994). Second, the OMEGA static adaptation provides higher resolution over regions of interest such as complex terrain and complex land/water boundaries. Third, dynamic adaptation increases the spatial resolution only where it is needed, (such as in the region of weather systems or over the region traveled by a plume), automatically during runtime, thus optimizing the use of the computational resources. Figure 1 shows a demonstration of the dynamic adaptation, in this case to the plume resulting from the October, 2002 eruption of Mt. Etna. The dynamic adaptation of the grid to evolving hurricanes was documented in Gopalakrishnan *et al.* (2002).

Table 2. Energy removed by n-passes of the MM5 terrain smoothing algorithms.

Wavelength	**# Passes**		
(ΔX)	**1**	**2**	**3**
Smoother - Desmoother			
2.0	100%	100%	100%
4.0	24%	42%	94%
6.0	5%	11%	43%
8.0	2%	3%	15%
1 – 2 – 1 Smoother			
2.0	100%	100%	100%
4.0	50%	75%	100%
6.0	25%	44%	94%
8.0	15%	17%	79%

The variable resolution and adaptive nature of the OMEGA grid structure give it a unique advantage in simulating the atmospheric circulation. For example, the OMEGA grid can adapt to the terrain and land/water boundary, thus resolving the large-scale dynamics as well as the local scale circulations associated with fine scale representation of the terrain features. This means that OMEGA can simultaneously resolve the meso-α scale (O(100 km)), meso-β scale (O(10 km)), and meso-γ scale (O(1 km)) forcing that drives the local scale wind field. In typical nested-grid models, an a-priori knowledge of the solution is required to strategically place the high-resolution nests over the regions of interest; in OMEGA, the system itself adapts the grid.

OMEGA was developed mainly to address the prediction of atmospheric dispersion over complex terrain regions and in data-void regions. OMEGA includes embedded Lagrangian and Eulerian models for atmospheric dispersion. Unlike other modeling systems, this particle transport model is truly embedded in OMEGA, thus providing increased fidelity (Boybeyi *et al.,* 2001).

OMEGA has been the subject of several model evaluation and verification studies. OMEGA successfully forecasted the weather and dispersion for 12 field tests over the past 5 years. OMEGA was also used to reconstruct past weather events, including data sparse situations. For example, OMEGA was used to simulate the oil fires in Kuwait with the results compared qualitatively against satellite images and quantitatively against all available observational data. The results from this study were presented in Bacon *et al.* (2000). OMEGA has also been evaluated by simulating the European Tracer Experiment (ETEX). Boybeyi *et al.* (2001) compared the OMEGA predicted meteorological and dispersion fields with the atmospheric observations and the ETEX dispersion measurements up to 60 hours after the start of the release (Figure 2). Most recently, the OMEGA system has been extended to support true global to local scale forecasting. For the first time, a single model has the capability of simulating all physical processes using a single, global, and continuously variable adaptive grid. Figure 3 shows a sample global grid with relatively coarse resolution over the globe, but higher resolution over the Southern latitudes surrounding Antarctica.

The OMEGA unstructured, dynamically adapting, triangular grid represents the underlying terrain with great accuracy and provides the high resolution, high fidelity surface representations without which it is impossible to accurately simulate the formation of topographically-induced low-level flows. The mixture of static and dynamic adaptation provides multiple ways of ensuring that the model resolution is sufficient to simulate the important physical processes.

OMEGA has demonstrated dynamically adapting resolution to both weather and dispersion variables. The resulting system has been configured to run on a parallel computing platform using the Message Passing Interface.

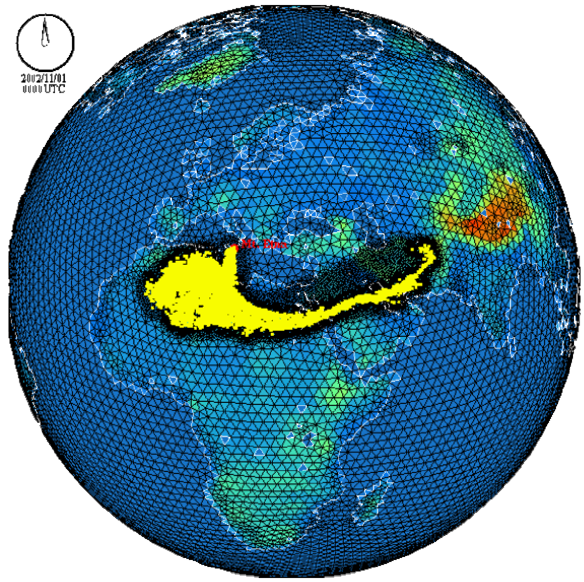

Figure 1. The OMEGA system can also adapt dynamically to the particle field – in this case from the eruption of Mt. Etna in October, 2002.

6. CONCLUSIONS

For the first time, an atmospheric simulation system has been constructed that enables the global to local to global multiscale simulation of the coupled weather and dispersion system. This system has application to both emergency response situations as well as air quality and air pollution studies – especially those involving the transport of trace materials over the ocean from Asia to the Americas.

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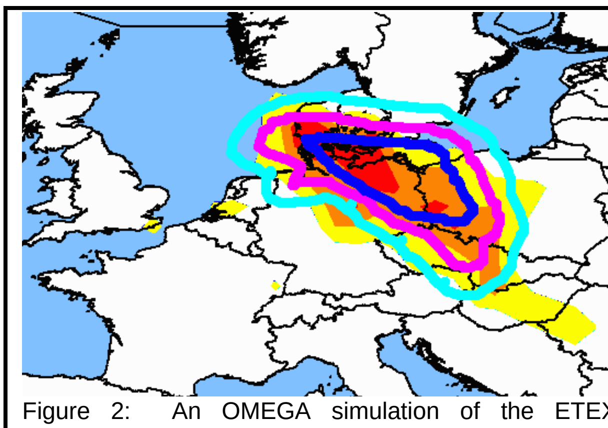

Figure 2: An OMEGA simulation of the ETEX dispersion experiment. Shown are the OMEGA predicted location (cyan / magenta / blue contours) overlaid on a compilation of the equivalent observed ETEX tracer concentration (yellow / orange / red fill) 48 hours after model initialization.

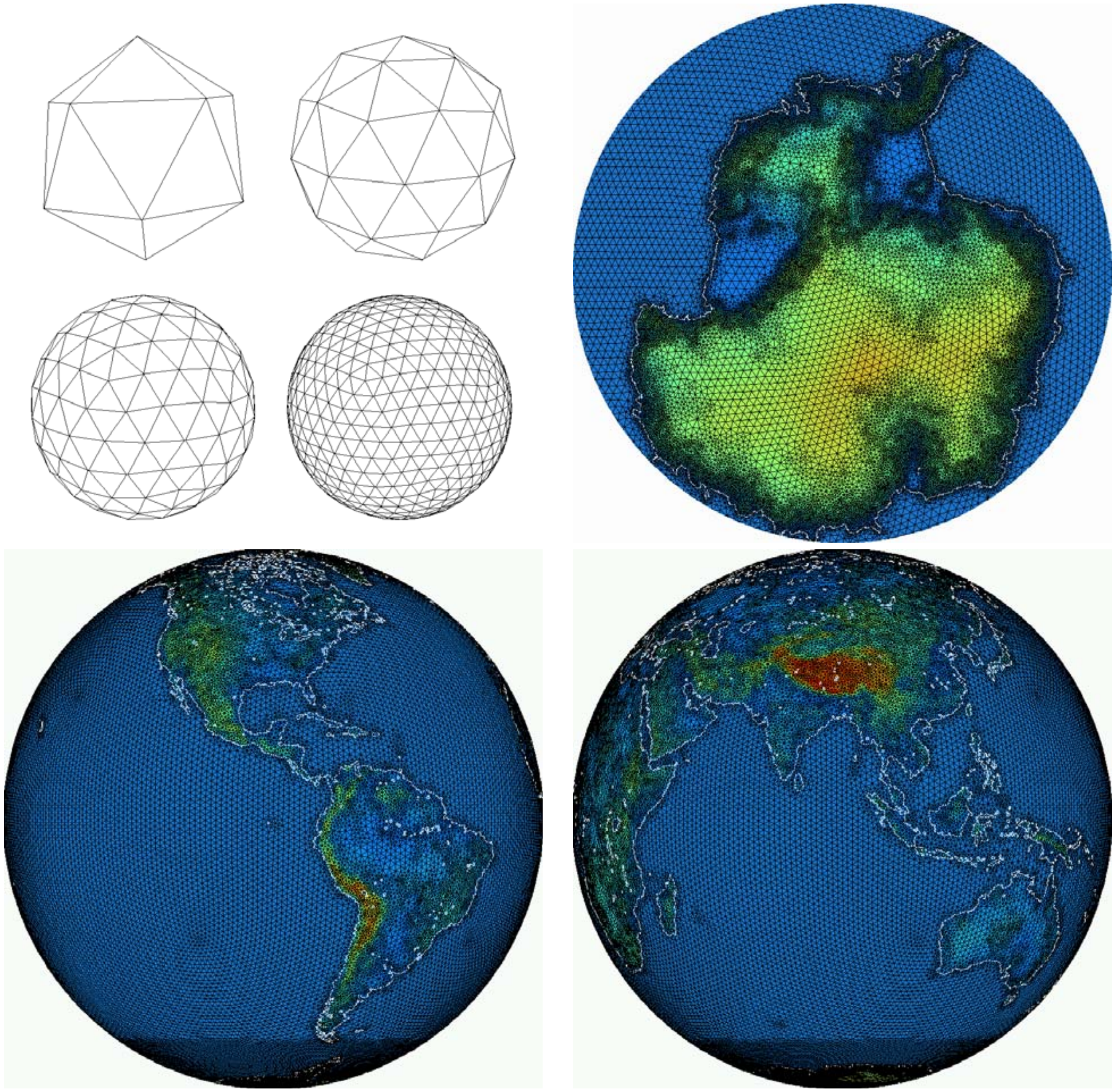

Figure 3. OMEGA can build global grids with higher resolution limited to specific geographic regions such as the Antarctic polar region. Starting from an icosohedron (top left), the mid-points of each triangle are bisected to create four triangles. This process is iterated several times to create a relatively uniform global mesh with a resolution of roughly 100-200 km. The underlying terrain information is then used along with other static criteria to refine the mesh locally. In this case, higher resolution was implemented for regions of complex terrain, coastal areas, and latitudes below 55^{o} S. The top right shows a close up of the grid over Antarctica; the bottom panels show the western and eastern hemispheres, respectively.

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