DEVELOPMENT AND APPLICATION OF PARALLEL PLUME-IN-GRID MODELS

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1. INTRODUCTION

The inability of traditional grid models, such as CMAQ, to simulate sub-grid scale processes is well recognized. Plume-in-Grid (PiG) modeling has been demonstrated to be an effective approach to resolve sub-grid scale effects associated with discrete sources (e.g., Seigneur et al., 1983; Sillman et al., 1990; Kumar and Russell, 1996; Gillani and Godowitch, 1999; Karamchandani et al., 2002; 2006; Godowitch, 2004). These effects are important for a variety of air quality issues including ozone, fine particulate matter ($PM_{2.5}$), mercury, and near-roadway air toxics concentrations. However, the computational overhead associated with PiG modeling has limited its use to a few selected studies. PiG modeling can require significantly more computational resources than traditional grid modeling, particularly for long-term simulations or when a large number of sources are explicitly treated with the plume component of the model. To use PiG models for such applications, it is necessary to minimize their computational overhead.

This paper presents one approach to minimize the computational costs associated with PiG modeling. The approach, based on parallelization of the PiG code, relies on the widespread availability of multi-processor workstations and workstation clusters that are commonly used today for air quality model simulations. A fully parallel PiG code allows efficient utilization of all the available compute cycles in these modern computer systems.

In the following sections, we describe the parallelization of a PiG model based on CMAQ that has been developed over the last few years and has been applied for ozone, $PM_{2.5}$ and mercury modeling. The parallel version of the PiG model is currently being applied for multiple annual simulations in the eastern United States for approximately 100 large point sources.

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2. PLUME-IN-GRID MODEL

The plume-in-grid model consists of the latest version (Version 4.6, released October 2006) of the Community Multiscale Air Quality (CMAQ) (Byun and Schere, 2006) as the host 3-D grid model and the Second-Order Closure Integrated puff model with CHEMistry (SCICHEM) (Karamchandani et al., 2000) as the embedded reactive plume model. The model is referred to as CMAQ with Advanced Plume Treatment (CMAQ-APT). There are two versions of CMAQ-APT, both of which were parallelized in this study. The first version uses the AERO3 module of CMAQ for the treatment of aerosols and is referred to as CMAQ-AERO3-APT. The second version uses the Model of Aerosol Dynamics, Reaction, Ionization and Dissolution (MADRID) (Zhang et al., 2004) for aerosol treatment and is referred to as CMAQ-MADRID-APT. The suite of models, consisting of CMAQ-AERO3-APT, CMAQ-MADRID, and CMAQ-MADRID-APT, is referred to as the Advanced Modeling System for Transport, Emissions, Reactions & Deposition of Atmospheric Matter (AMSTERDAM).

SCICHEM, the embedded reactive plume model in CMAQ-APT, simulates plume transport and dispersion using a second-order closure approach to solve the turbulent diffusion equations. The plume is represented by a myriad of three-dimensional puffs that are advected and dispersed according to the local micrometeorological characteristics. Each puff has a Gaussian representation of the concentrations of emitted inert species. The overall plume, however, can have any spatial distribution of these concentrations, since it consists of a multitude of puffs that are independently affected by the transport and dispersion characteristics of the atmosphere. The model can simulate the effect of wind shear since individual puffs will evolve according to their respective locations in an inhomogeneous velocity field. As puffs grow larger, they may encompass a volume that cannot be considered homogenous in terms of the meteorological variables. A puff splitting algorithm accounts for such conditions by dividing puffs that have become too large into a number of smaller puffs. Conversely, puffs may overlap significantly,

thereby leading to an excessive computational burden. A puff-merging algorithm allows individual puffs that are affected by the same (or very similar) micro-scale meteorology to combine into a single puff. Also, the effects of buoyancy on plume rise and initial dispersion are simulated by solving the conservation equations for mass, heat, and momentum. The formulation of nonlinear chemical kinetics within the puff framework is described by Karamchandani et al. (2000). Chemical species concentrations in the puffs are treated as perturbations from the background concentrations. The chemical reactions within the puffs are simulated using a general framework that allows any chemical kinetic mechanism to be treated. The puff chemical mechanism is the same as the host grid model mechanism for consistency.

Additional details on the plume-in-grid model can be found in Karamchandani et al. (2002; 2006a; 2006b) and Vijayaraghavan et al. (2006) who describe the development of the various configurations of AMSTERDAM and its applications for ozone, $PM_{2.5}$, and mercury. CMAQ-APT has also been recently adapted to simulate the sub-grid scale transport and fate of toxic air pollutants near roadways (Karamchandani et al. 2007; 2008). In the following section, we discuss the approach adopted to parallelize the plume-in-grid component of the model.

3. PARALLELIZATION ISSUES AND APPROACH

The traditional approach to parallelizing a grid model such as CMAQ is to perform domain decomposition by subdividing the horizontal domain into a number of roughly equal subdomains, with each subdomain assigned to a separate processor. Each processor then performs the transport/chemistry/removal calculations for the subdomain it owns. However, inter-processor communication is required for I/O purposes and horizontal transport calculations. In CMAQ, this inter-processor communication is accomplished by using the parallel input output (PARIO) management library based on the Message Passing Interface (MPI) library, a communication library for both parallel computers and workstation networks. CMAQ uses the Argonne National Laboratory open-source implementation of MPI, referred to as MPICH, because of its widespread usage and availability.

While the domain decomposition paradigm is appropriate for CMAQ, the plume component (SCICHEM) in CMAQ-APT requires a different approach because it would be unreasonable to expect the puffs to be distributed uniformly among the subdomains. For example, one could expect a larger density of puffs in source regions than in other regions. Thus, using a domain decomposition approach for SCICHEM would result in inefficient utilization of processors. Furthermore, there could be potential issues with puffs crossing subdomain boundaries during a simulation time step.

Thus, we selected “puff decomposition” as the preferred approach for parallelizing the plume component of the model. In other words, the total number of puffs at any given time step is divided roughly equally among the available processors. However, the strongly interactive nature of the puff calculation, including splitting, merging, and overlap calculations posed an additional complication in the parallelization of the plume-in-grid code. Because these puff interactions could occur between puffs distributed among different processors, there would be a significant communication overhead associated with performing the interaction calculations on independent processors.

To overcome this issue, we focused our parallelization effort on the chemistry component of the plume model. This component, which includes gas-phase chemistry, aerosol calculations, and aqueous-phase chemistry, requires more computing resources than any of the other components of the model. Thus, the largest benefit could be expected by conducting these chemistry calculations in parallel.

Based on these considerations, the overall parallelization approach of the embedded plume model consists of the following steps:

1. The grid model subdomain concentrations are collected to construct a full domain 3-D concentration field as background concentrations for SCICHEM.
2. The overall puff stepping control is maintained on the root processor, which performs the puff emissions, transport, dispersion and interaction calculations and assembles the complete meteorology and ambient chemistry fields from the Eulerian subdomains.
3. The root processor distributes the total puffs among itself and the slave processors to perform the chemistry calculations.
4. At the end of the chemistry calculations, the root processor collects the puff information from the individual processors.
5. At the end of the simulation time step, the root processor performs a puff dumping calculation

(if necessary) to adjust the full domain gridded concentration field.

6. The full domain 3-D concentration field is distributed among the various subdomains for the host model parallel computations.

As in the case of the host model, all the inter-processor communication required for distributing and collecting the puff data and subdomain 3-D concentration fields is accomplished using MPI methods.

4. MODEL APPLICATION

The parallelized version of CMAQ-MADRID-APT is applied to a modeling domain that covers the central and eastern United States (see Figure 1). The grid is based on a Lambert Conformal map projection, with the origin located at 97° west longitude and 40° north latitude and reference latitudes at 33° and 45° north latitude. The horizontal grid system consists of 243 x 246 grid cells, with a resolution of 12 km. The vertical grid is pressure-based and extends from the surface to about the tropopause (100 mb or ~15 km) and is discretized using 19 layers of variable thickness. The boundary conditions for the 12-km grid domain are obtained from a coarse grid (36-km resolution) simulation over the continental United States

Figure 1. Modeling domain

Approximately 100 large coal-fired power plants (in terms of SO_2, NO_x and Hg emissions) in the United States are chosen for PiG treatment. Boundary conditions are obtained from simulations with CMAQ-MADRID on a 36 km resolution domain over the entire United States. Base simulations are conducted for calendar year 2002 using “actual” and “typical” emissions inputs. Meteorology is MM5-driven. The 2002 actual simulation is evaluated using ambient concentration and deposition measurements at the AIRS, CASTNET, IMPROVE, NADP and SEARCH monitoring networks. The modeling work is ongoing. Future-year simulations are also planned.

5. SUMMARY

We have developed parallel versions of plume-in-grid models based on CMAQ that offer the capability to conduct long-term plume-in-grid simulations with a large number of point sources practically and efficiently. One configuration of this modeling system, referred to as CMAQ-MADRID-APT, is currently being applied in annual simulations to examine the impact of changes in coal-fired power plant emissions on air quality and deposition in the eastern United States. The simulations are being conducted using four-processor workstations, and are approximately 2.2 times faster than simulations in single processor mode.

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