Numerical Simulation of Global-Scale Atmospheric Chemical Transport with High-Order Wavelet-Based Adaptive Mesh Refinement Algorithm

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Abstract

High computational cost associated with numerical modeling of multiscale global atmospheric chemical transport (ACT) imposes severe limitations on the spatial resolution of fixed nonadaptive grids. Recently it has been shown that the interaction of numerical diffusion caused by the crude resolution with complex velocity field of atmospheric flows leads to large numerical errors. To address the described difficulties, the authors have developed a wavelet-based adaptive mesh refinement (WAMR) method for numerical simulation of two-dimensional multiscale ACT problems. The WAMR is an adaptive method that minimizes the number of grid points by introducing a fine grid only in the locations where fine spatial scales occur and uses high-order spatial discretization throughout the computational domain. The algorithm has been tested for several challenging ACT problems. Particularly, it is shown that the method correctly simulates dynamics of a pollution plume traveling on a global scale, producing less than 1% error with a relatively low number \((7 \times 10^5)\) of grid points. To achieve such accuracy, conventional nonadaptive techniques would require more than three orders of magnitude more computational resources. The method possesses good mass conservation properties; it is shown that an error in the total pollutant mass does not exceed 0.02% for this number of points. The obtained results demonstrate the WAMR’s ability to achieve high numerical accuracy for challenging ACT problems at a relatively low computational cost.

1. Introduction

An accurate numerical simulation of global atmospheric chemical transports (ACTs) is crucial for addressing problems and issues related to atmospheric air quality (Li et al. 2002), climate forcing (Hansen et al. 2000), and greenhouse gases budget (Thompson 1992). A number of different chemical transport models (CTMs) and computational codes have been used for numerical simulations of local and global atmospheric chemical transport: the Goddard Earth Observing System (GEOS) three-dimensional model of tropospheric chemistry (GEOS-Chem; Bey et al. 2001), the Model of Ozone and Related Chemical Tracers (MOZART; Horowitz et al. 2003), the Weather Research and Forecasting (WRF) Model coupled with Chemistry (WRF-Chem; Grell et al. 2005), the Met Office’s Numerical Atmospheric-dispersion Modelling Environment (NAME; Jones et al. 2007), Tracer Model 5 (TM5; Huijnen et al. 2010), etc. The majority of these models, except WRF-Chem, which offers some nesting capability, use uniform or quasi-uniform fixed grids.

It is well known that accurate simulation of these CTMs requires enormous computational resources since the governing equations are extremely stiff, nonlinear, and involve a large number of unknowns. The high computational cost associated with such simulations imposes severe limitations on the spatial resolution of the CTMs implemented on uniform or quasi-uniform grids. This relatively crude spatial resolution results in significant numerical diffusion introduced into the system, which is shown to noticeably distort the pollutant mixing and transport dynamics for typically used grid resolutions (refer to Rastigejev et al. 2010). In this paper, the authors have shown that in order to achieve a high convergence rate and accuracy, the mesh spacing in numerical simulation of global pollution plume transport must be decreased to a few
kilometers. It is very hard to achieve such fine resolution on uniform or quasi-uniform grids at a global scale since it would require us to increase the computational speed by at least several orders of magnitude. For instance, recent numerical simulations of the global atmospheric transport (Mueller et al. 2015) required 700,000 cores on the supercomputer Mira at the Argonne National Laboratory to attain the spatial resolution of several kilometers. To tackle the resolution problem, novel methods such as adaptive grids have to be developed and implemented.

Recently, efforts have been made in application of adaptive resolution (AR) algorithms for multiscale numerical modeling in atmospheric sciences. These algorithms include stretched grid (Fox-Rabinovitz et al. 1997), nested grid (Rowley and Ginis 1999), and adaptive mesh refinement (AMR) methods (Nikiforakis 2005; Jablonowski et al. 2006). All these methods use nonuniform adaptive grids with higher resolution over the areas of interest without requiring a fine grid throughout the entire domain. Therefore, the AR techniques are computationally more efficient than the methods that use uniform or quasi-uniform grids since the AR methods require a significantly lower number of points to achieve a given numerical accuracy. Even though the classical adaptive methods offer great advantages in computational speed and storage over methods that use uniform or quasi-uniform grid, they have a number of shortcomings, which are especially conspicuous for the problems with rapidly developing spatial scales. Specifically, the total number of grid points stays constant in the stretched and nested grid methods during the numerical code execution. As a result, these techniques have difficulty maintaining satisfactory resolution throughout the computational domain, especially in the problems where small spatial scales dynamically occur and rapidly develop. This deficiency may lead to high numerical errors and numerical instability. Moreover, often these techniques require a priori information about the solution, which is often not available for the CTM problems.

The conventional AMR methods have been widely used for multiscale problems in computational fluid dynamics (Berger and Colella 1989; Quirk 1996; Baeza et al. 2012; Pau et al. 2012), but only recently have been applied to atmospheric flow simulations (Rosenberg et al. 2006; Koper and Giraldo 2014) and especially CTM problems (Constantinescu et al. 2008). The AMR methods have been largely free from the described difficulties associated with the stretched or nested grids since these methods use local refinement (i.e., the grid points are added or removed dynamically during the algorithm execution). However, the traditional AMR techniques also have deficiencies. Particularly, it is difficult to estimate computational errors in the AMR algorithms so as to directly control the grid refinement and computational accuracy since a mathematically rigorous criterion for mesh adaptation is not available. Instead, heuristic criteria based on ad hoc estimates of magnitudes of gradients of physical variables are used. As a consequence, the actual error of AMR often is not estimated accurately, and the adaptation criteria necessitate a posteriori error estimates.

Even though it is challenging to construct high-order schemes using finite-volume formulations, a noticeable progress has been made recently in developing these techniques (St-Cyr et al. 2008; McCorquodale and Colella 2011; Koper and Giraldo 2014). High-order schemes are particularly desirable for the ACT models since they enable one to reduce numerical diffusion and, therefore, numerical error significantly without resorting to over-refined grids. We show in this paper that the implementation of the higher-order wavelet-based adaptive mesh refinement (WAMR) scheme, unlike that of higher-order AMR algorithms based on finite-volume formulation, is straightforward.

Wavelet-based multiscale numerical methods form a novel class of the adaptive multiresolution techniques (Holmstrom 1999; Singh et al. 2001; Rastigejev and Paolucci 2006b,a) procedures. Galerkin methods, while very accurate, are somewhat computationally expensive and have difficulty with the treatment of general boundary conditions, nonlinear terms, and complex geometries. On the other hand, collocation methods have been shown to be free from these difficulties—they use a wavelet representation of a solution only for the grid adaptation and solve PDEs in the physical space.

In this work we have developed a dynamic multilevel WAMR method (Rastigejev and Paolucci 2006b) for numerical modeling of atmospheric chemical transport. The WAMR method introduces a fine grid in the regions where sharp transitions occur and a cruder grid in the regions of smooth solution behavior. Therefore, the algorithm enables the minimization of the number of degrees of freedom for a prescribed accuracy and results in much more accurate solutions than those obtained using conventional numerical methods implemented on uniform or quasi-uniform grids. The algorithm is based on...
the mathematically well-established wavelet theory. This enables one to provide error estimates of the solution that are used in conjunction with an appropriate threshold criterion to adapt the nonuniform grid. Other essential features of the numerical algorithm include the following: an efficient high-order wavelet spatial discretization that allows the minimization of the number of points for a prescribed accuracy, a fast algorithm for computing wavelet coefficients, a fast algorithm for grid construction, and efficient and accurate high-order upwind discretization schemes on a nonuniform grid. Specifically, the advection operator is approximated with up to the seventh-order upwind scheme at each point of the adaptive grid. These high-order schemes result in significantly lower errors for advection and, therefore, in significantly reduced numerical dissipation and dispersion, which eliminates the need for an excessive refinement of the spatial grid. In this paper, we demonstrate that the adaptive method produces much more accurate solutions than conventional numerical techniques implemented on uniform or quasi-uniform grids with the same or lower number of points.

The WAMR method uses more rational refinement algorithm than conventional AMR methods since the WAMR, unlike conventional AMR methods, refines individual grid cells, not large blocks of uniform or quasi-uniform grids. The conventional AMR methods, on the other hand, employ a sequence of locally nested refined subgrids or patches that are organized in a hierarchy of progressively finer levels of resolution. Because of a simple, often rectangular, geometrical shape of these subgrids, it is difficult to efficiently cover complex geometric features of multiscale flows. As a result of that, often excessively large subgrid blocks are refined, and, thus, a vast amount of computational resources is wasted.

The developed algorithm has been tested for several benchmark problems including numerical simulation of inert pollution plumes propagating in convergent–divergent flows, nonstationary deformational flow with a nonzero divergence, and realistic atmospheric flows over the Pacific Ocean. The East Asian region is a significant source of various atmospheric emissions. Recent studies have indicated that some of these pollution plumes are lifted into the free troposphere and transported to North America over the Pacific Ocean (Jaffe et al. 1999; Hsu et al. 2012) where they may significantly affect the surface air quality over the United States (Jacob et al. 1999; Lin et al. 2012). The generated plumes are diluted due to turbulent mixing as they advect. Despite this dilution, observations from aircraft, sondes, and satellites show that the pollution plumes in the remote free troposphere can preserve their structure as well-defined layers for a week or more as they are transported on intercontinental scales (Colette and Ancialet 2005). It has been shown that the presently used conventional global CTMs implemented on uniform or quasi-uniform nonadaptive grids are incapable of reproducing such layered structures because of the large numerical diffusion smearing the physical non-uniformity of atmospheric flows (Rastigejev et al. 2010). The present study demonstrates that the WAMR algorithm applied to traveling plumes, on the contrary, accurately reproduces their dynamics over their entire lifetime. The results of numerical simulations obtained with the WAMR algorithm have been compared with conventional global CTM computations that use fixed grids, specifically, the GEOS-Chem simulations (Rastigejev et al. 2010) and the third-order discontinuous Galerkin transport scheme (Nair and Lauritzen 2010). It is shown that the WAMR solutions with the accuracy comparable to that of conventional numerical techniques are obtained with several orders of magnitude reduction in the number of grid points.

The paper is organized as follows. The governing equations for atmospheric transport are formulated in section 2. The WAMR method is described in section 3. The time integration scheme for the advection equation is explained in section 4. The data structure and parallel algorithms discussion is given in section 5. The plume decay due to numerical diffusion is discussed in section 6. The numerical results for the convergent–divergent and the deformational flows with nonzero divergence, and for the realistic atmospheric flow are presented in sections 7, 8, and 9, respectively.

2. Governing equation

The following set of two-dimensional advection–diffusion–reaction equations describes the evolution of the mass mixing ratio $c_i$ of the $i$th chemical species (also referred as concentration below) by the horizontal wind in the atmosphere in the absence of convection:

$$\frac{\partial c_i}{\partial t} + \mathbf{u} \cdot \nabla c_i = \nabla \cdot D \nabla c_i + \omega_i + s_i, \quad i = 1, \ldots, N,$$

where $\mathbf{u}$ is the wind velocity, $D$ is the turbulent diffusivity, $\omega_i$ is the net chemical production rate, and $s_i$ is the local emissions and nonchemical sinks. The wind velocity $\mathbf{u}$ is typically provided by assimilated meteorological databases [e.g., NASA GEOS for GEOS-Chem (Bey et al. 2001) or ECMWF operational forecast data for TM5 (Huijnen et al. 2010)].

To demonstrate the versatility of the WAMR approach first we consider propagation of an inert plume...
of a single chemical species with mass mixing ratio $c$ in the free troposphere in the absence of turbulent mixing. Such plumes are described by a simple advection equation

$$\frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = 0. \tag{2}$$

In this work we use the longitude–latitude grid that is based on the standard spherical coordinate system (SCS). This spherical domain is mapped into the corresponding rectangular domain $\{(x, y) \mid 0 \leq x \leq 2\pi$, $0 < y < \pi\}$, hence, the wavelet basis, two-dimensional SWR, and corresponding sparse grid are constructed in this rectangular domain. In this system of coordinates, Eq. (2) takes the following form:

$$\frac{\partial c}{\partial t} + \frac{u}{r \sin y} \frac{\partial c}{\partial x} + \frac{v}{r} \frac{\partial c}{\partial y} = 0. \tag{3}$$

Here $\mathbf{u} = (u, v)$ is the horizontal velocity and $r$ is the radius of the earth.

Although, the SCS is widely used for nonadaptive global chemical transport calculations: GEOS-Chem (Bey et al. 2001), WRF-Chem (Skamarock et al. 2008), TM5 (Huijnen et al. 2010), etc.), the SCS has a difficulty related to singularities in the polar regions. As these singularities are approached, the longitudinal grid spacing tends to zero, which may lead to numerical instabilities. Recently, there has been an increased interest in constructing more isotropic spherical grid systems that are free from singularities or at least contain much weaker singularities (Ronchi et al. 1996; Rančić et al. 1996). This approach is based on nonconformal or conformal transformations that map the spherical surface onto the surface of the circumscribed cube, thus, it is often referred to as a cubed sphere method (CSM). The method performs calculations in six separate computational subdomains that correspond to the sides of the cube.

Even though, the approach enables stable calculations of the atmospheric flow in the polar regions of the earth, it results in significantly more complicated and computationally expensive numerical algorithms due to the need for an intensive data exchange between the computational subdomains. Application of the WAMR algorithm in conjunction with the CSM does not present any additional difficulties associated with the data exchange between subdomains compared with the CSM implemented on a uniform grid. This is due to the fact that all calculations associated with the adaptive grid rearrangement and approximation of derivatives are performed via one-dimensional Lagrange interpolations on uniform stencils of different sizes and, therefore, are identical to the analogous operations on the fixed uniform grid. Even though, the hybrid WAMR–CSM method can be used for simulation of the chemical transport in the polar regions, the implementation of this method is beyond the scope of this paper.

The observation that pollution plumes in the remote troposphere, where turbulent mixing is suppressed, can propagate as well-defined layered structures for a week or more as they circle the globe is explained by the fact that in the absence of diffusion, the mass mixing ratio at each material point remains constant in time along the trajectory $(x, t)$ of this material point originated at $x_0$:

$$c(x, t) = c(x_0, 0). \tag{4}$$

Certainly, numerical integration cannot reproduce these dynamics exactly due to the discretization error that introduces either dispersion or diffusion into the solution resulting in plume dissipation. More importantly, as it was shown in Rastigejev et al. (2010), this dissipation is much faster for low resolutions typically used for fixed grids, than one would expect from the discretization order of the advection scheme because of the interaction between numerical diffusion and the atmospheric flow stretching. This numerical diffusion is shown to noticeably distort the pollutant mixing and transport dynamics for spatial resolutions typically used for fixed non-adaptive grids. In the current paper, we demonstrate that this difficulty can be efficiently resolved through application of the WAMR algorithm, which uses a multilevel adaptive grid, to a numerical simulation of the global atmospheric chemical transport.

### 3. The WAMR method

Below we briefly describe the WAMR method used in this study, more details of which can be found in Rastigejev and Paolucci (2006b,a). The method is a numerical technique for efficient numerical integration of multiscale problems described by partial differential equations. It consists of several essential parts: the construction and adaptation of a multilevel nonuniform grid, the spatial discretization of the governing equations on the nonuniform grid, and a time-integration scheme. In this section, we describe the first part of the WAMR method—the construction and adaptation of the multilevel sparse grid. We begin with the discussion of a one-dimensional case and later proceed with a two-dimensional case.

The construction of the adaptive grid is based on a wavelet decomposition of a solution function $[c(x)$ in our case] that dissects the solution function into components of different spatial scales corresponding to different levels of resolution $0 \leq l < \infty$. The zeroth level ($l = 0$)
spanned by the set of so-called scaling functions \( \phi_{0,k}(x) \) describes the largest spatial features of the solution, while the other levels \( (l \geq 1) \) spanned by the set of the so-called wavelets \( \psi_{l,k}(x) \) describe its finer features. The Deslauriers–Dubuc (DD) wavelet bases (Donoho 1992; Beylkin and Saito 1992; Daubechies 1992) of different orders \( p \) have been used in this paper. Figure 1 presents a cartoon picture of the fourth-order DD basis; the four lowest levels \( (l = 0, 1, 2, \text{and} 3) \) are shown with five scaling functions on the zeroth level of resolution corresponding to locations \( k = 0, 1, 2, \text{and} 3 \). The locations of every individual scaling function \( (x_s) \) and those of a wavelet function \( (x_w) \) at \( l \text{th} \) level of resolution are defined by the value of parameter \( k \). Specifically,

\[
\begin{align*}
x_s &= k/2^l, \quad (5) \\
x_w &= (2k + 1)/2^l. \quad (6)
\end{align*}
\]

The maxima of the DD scaling and wavelet functions are usually scaled to unity [i.e., \( \max[\phi(x)] = \max[\phi(x)] = 1 \)]; however, for illustration purposes, the wavelets shown in Fig. 1 are dilated proportionally in both horizontal and vertical directions.

The scaling function \( \phi(x) \) of order \( p \) is computed numerically using the interpolating subdivision scheme (Daubechies 1992). The corresponding wavelet is defined as

\[
\psi(x) = \phi(2x - 1). \quad (7)
\]

The translated and dilated scaling functions and wavelets are defined by the following expressions:

\[
\begin{align*}
\phi_{l,k}(x) &= \phi(2^l x - k), \quad (8) \\
\psi_{l,k}(x) &= \phi(2^{l-1} x - k). \quad (9)
\end{align*}
\]

The spaces spanned by \( \phi_{l,k} \) and \( \psi_{l,k} \) over the whole range of parameter \( k \in \mathbb{Z} \) values at a fixed level of resolution \( l \) are commonly denoted as

\[
\begin{align*}
V_l &= \text{span}_{k \in \mathbb{Z}}(\phi_{l,k}), \quad (10) \\
W_l &= \text{span}_{k \in \mathbb{Z}}(\psi_{l,k}), \quad (11)
\end{align*}
\]

so that \( V_l \) can form a ladder of embedded subspaces of increasing resolution:

\[
V_0 \subset V_1 \subset V_2 \subset \cdots. \quad (12)
\]

Note, the space \( W_{l+1} \) is a nonorthogonal complement to \( V_l \) in \( V_{l+1} \), that is,

\[
V_{l+1} = V_l \oplus W_{l+1}, \quad (13)
\]

where \( \oplus \) is a direct sum. From Eq. (13), it follows that

\[
V_{l+1} = V_0 \oplus W_1 \oplus W_2 \oplus \cdots \oplus W_{l+1}. \quad (14)
\]

This choice of the basis ensures that the computation of the expansion coefficients in the wavelet series reduces to the efficient use of the local Lagrange interpolation formula of order \( p \) (Dubuc 1986).

The wavelet basis can be used for approximating the solution function \( c(x) \) (Daubechies 1992) as follows:

\[
c'(x) = \sum_k b_{0,k} \phi_{0,k}(x) + \sum_{l=1}^J \sum_k d_{l,k} \psi_{l,k}(x), \quad (15)
\]

such as

\[
\lim_{J \to \infty} c'(x) = c(x). \quad (16)
\]

Here \( b_{0,k} \) and \( d_{l,k} \) are the scaling function and wavelet coefficients accordingly, \( c'(x) \) is a wavelet approximation of the function \( c(x) \), and \( J \) is the highest level of resolution.

Most of the coefficients corresponding to the wavelets located in the regions where the solution is smooth are small—and, therefore, can be disregarded without upsetting numerical accuracy (Donoho 1992). Hence, the approximation can be decomposed into two parts that represent wavelets whose coefficients are above (essential wavelets) and below (nonessential wavelets) the specified threshold \( \epsilon \):

\[
c'(x) = c'_e(x) + R'_e(x), \quad (17)
\]

where

\[
\begin{align*}
c'_e(x) &= \sum_k b_{0,k} \phi_{0,k}(x) + \sum_{(l,k) \in \mathcal{E}} d_{l,k} \psi_{l,k}(x), \quad (18) \\
R'_e(x) &= \sum_{(l,k) \in \mathcal{I}(\epsilon)} d_{l,k} \psi_{l,k}(x), \quad (19) \\
\mathcal{I}(\epsilon) &= \{ (l,k) : |d_{l,k}| \geq \epsilon \}. \quad (20)
\end{align*}
\]

Here \( c'_e(x) \) is the sparse wavelet representation (SWR) of function \( c(x) \). It can be shown (Donoho 1992)
that the error associated with the SWR is of the order of $\varepsilon$.

The points on the sparse grid are positioned exactly in the locations of the essential wavelets ensuring a one-to-one correspondence between the nonuniform grid of points and the set of essential wavelets. It can be shown that the functional values at the missing points at each level of resolution could be calculated using the local Lagrange interpolation of order $p$ (Dubuc 1986). To resolve small moving spatial structures the nonuniform grid has to adapt dynamically following the temporal evolution of the numerical solution. To achieve the grid adaptation, we discard nonessential points and preserve only essential points and the so-called neighboring region at every time step [refer to Rastigejev and Paolucci (2006b) for more detail]. The neighboring region is constructed by adding several wavelets that are located next to the essential wavelets at the same and higher levels of resolution. The inclusion of these neighboring wavelets enables the method to capture dynamically the formation and development of small spatial scales. The essential and neighboring wavelets constitute a set of active wavelets. The SWR that includes all active wavelets is referred to as an extended SWR below. Then the nonuniform adaptive grid $G^{(n)}$ consists of the collocation points corresponding to all active wavelets used by the extended SWR at any given time $t_n$.

The algorithm can be easily extended to higher-dimensional spaces by introducing a multidimensional multilevel wavelet basis that is constructed as a tensor product of the basis elements [for more detail refer to Rastigejev (2002); Santos et al. (2004); Domingues et al. (2010)]. For a three-dimensional case we may adopt SCS for the spherical surface discretization and the generalized vertical coordinate (e.g., $\sigma$ or $\sigma - \rho$) (Kasahara 1974) for discretization in the vertical direction. This curvilinear orthogonal system of coordinates can be easily mapped to Cartesian coordinates where the wavelet basis and the corresponding adaptive grid are constructed.

Specifically, the two-dimensional scaling function $\phi_{ij}(x)$ at level $l$ and a vector of three corresponding wavelets $\Psi(x) = \{\psi^r(x); r = 1, 2, 3\}$ at level $l + 1$ are defined as follows:

$$\phi_{ij}(x) = \phi_{ij}(x)\phi_{ij}(y),$$

$$\phi_{l+1,i,j}(x) = \phi_{l+2,i,j}(x)\phi_{l+1,2,i,j}(y),$$

$$\phi_{l+1,2,i,j}(x) = \phi_{l+2,2,i,j}(x)\phi_{l+1,2,2,i,j}(y),$$

$$\phi_{l+1,2,2,i,j}(x) = \phi_{l+2,2,2,i,j}(x)\phi_{l+1,2,2,2,i,j}(y).$$

The two-dimensional grid shown in Fig. 2 consists of collocation points corresponding to scaling functions and wavelets at some level of resolution $V_l = V_{l-1} \oplus W_l$ and is constructed similarly to the one-dimensional case. Collocation points at the $V_{l-1}$ level of resolution are shown by black circles, while collocation points at the $V_l$ level of resolution are drawn as triangles.

The two-dimensional wavelet basis can be used for multiscale approximation of any sufficiently smooth function $c(x)$ in a rectangular domain:

$$c_i(x) = \sum_{ij} b_{ij} \phi_{ij}(x) + \sum_{l=1} \sum_{ij} d_{ij} \Psi_{ij}(x),$$

where $d_{ij} = (d_{1,ij}, d_{2,ij}, d_{3,ij})$ is the set of wavelet coefficients corresponding to $\Psi_{ij}(x)$. The algorithm for constructing two-dimensional SWR and a nonuniform sparse grid is similar to the one-dimensional one described above.

4. Time-integration scheme

In this section we describe a finite-difference scheme for numerical integration of advection in Eq. (3) on the nonuniform adaptive grid. For time $t^n$ at each grid point $(i, j)$ this equation is approximated by the second-order trapezoidal rule:

$$\frac{c_i^{n+1} - c_i^n}{\Delta t} + \frac{\Lambda}{2} (c_i^{n+1} + c_i^n) = 0,$$

where $\Lambda$ is the advection operator discretized with the $m$th-order diffusive upwind finite-difference formula (Durran 2010). For instance, the expression for the advection operator takes the following form for $m = 3$:

$$\Lambda c_{ij} = \frac{u_{ij}}{r \sin y_{ij}} \frac{c_{i-2,j} - 6c_{i-1,j} + 3c_{i,j} + 2c_{i+1,j}}{6h_1} + \frac{v_{ij}}{r} \frac{c_{i,j-2} - 6c_{i,j-1} + 3c_{i,j} + 2c_{i,j+1}}{6h_2}. $$

FIG. 2. Two-dimensional collocation grid corresponding to the $V_l$ level of resolution. Positions of wavelets at the $W_l$ level of resolution and at lower levels of resolution are shown by triangles and circles, respectively.
for $u_{ij} \geq 0$ and $v_{ij} \geq 0$. Spatial steps $h_1$ and $h_2$ in the longitudinal $x$ and latitudinal $y$ directions are defined as the distances from point $(i, j)$ to the nearest neighboring point on the nonuniform grid in the corresponding direction. Then the local uniform spatial stencils of a certain number of equally spaced points are reconstructed in each spatial direction. If a necessary point is absent on the nonuniform grid, it is recreated, and the functional value at this point is interpolated from the coarser levels of resolution by using Eq. (18). These local uniform stencils at this point is recreated, and the functional value number of equally spaced points are reconstructed in direction. Then the local uniform spatial stencils of a certain

Let us assume without loss of generality that

more detail. Note that the uniform stencils may have number of equally spaced points are reconstructed in direction. Then the local uniform spatial stencils of a certain

where $c$ is a vector of mass mixing ratio values at the collocation points of the nonuniform adaptive grid at time moment $t^{n+1}$. While a number of different numerical techniques can be used, here we solve this system, using Jacobi method:

$$c^{(k+1)} = D^{-1}[b - (L + U)c^{(k)}],$$  

where $k$ is the iteration number; and $U$, $L$, and $D$ are the upper triangular, the lower triangular, and the diagonal matrices correspondingly of $A$, respectively:

$$A = L + D + U.$$  

The adaptive numerical algorithm for solving the PDE may now be summarized as follows:

1) Solve the system of difference Eq. (26) iteratively to obtain the approximate solution $c^{n+1}$ on the adaptive grid $G^{(n)}$. The solution from the previous time step $c^n$ is used as an initial condition.

2) Construct the new sparse grid $G^{(n+1)}$ that is based on the extended SWR of $c^{n+1}$.

3) Compute the values of $c^{n+1}$ at new collocation points of $G^{(n+1)}$ by the SWR. Increment time and go back to step 1.

5. Data structure and parallel algorithm

A successfully designed data structure and parallel algorithms provide an efficient way to manipulate the data and to perform parallel adaptive calculations. To date, a number of parallel AMR codes [e.g., Parallel Adaptive Mesh Refinement (PARAMESH) (MacNeice et al. 2000), Adaptive Mesh Refinement of Clawpack package (AMRCLAW) (Berger and LeVeque 1998), and Adaptive Mesh Refinement in Object-Oriented C++ (AMROX) (Deiterding et al. 2006)] have been developed. Most of these methods use a hierarchy of uniform progressively refined subgrids that cover the computational domain. These subgrids form the nodes of a tree data structure (Berger and Oliger 1984; Berger and Colella 1989). As the calculation progresses, the tree structure changes (nodes are added or removed) to adapt to the developing numerical solution.

Efficient parallel implementation of the WAMR method introduces the following requirements for the data storage and management:

1) The ability to dynamically allocate and deallocate memory in distributed memory environment.

2) The fast access to any data element.

3) The linear growth of the size of the required computer memory with the number of grid points.

4) The need to balance the computational load dynamically among multiple processes for a shared-memory multiprocessor architecture.

5) The need to minimize communication between different processors.

To satisfy the above requirements, we have designed the composite data structure that is a combination of a $k$-ary (like binary for $k=2$) tree, which is schematically shown for one-dimensional case in Fig. 3, and a linked list that supports grid operations and parallel algorithms, respectively. Here $k = 3^d - 1$ is the maximum number of children for each node, and $d$ is the number of spatial dimensions. Every node in our data structure corresponds to a collocation point on a nonuniform grid and contains the values of physical variables (velocity, mixing ratios of pollutants, etc.), and the information about the point location in both the linked list and the tree. At any instant only nodes corresponding to active points remain in computer memory, therefore, the memory scales linearly with the number of grid points.

We use a $k$-ary tree to perform two searches for each active node of the adaptive grid during the grid rearrangement:

1) locating a set of nodes at coarser levels of resolution $\mathcal{L}_P = \{L_1, L_2, \ldots\}$ that are used for the local Lagrange approximation of functional values at some point (node) $P$, and

2) finding the set of the nearest nodes $\mathcal{D}_P = \{D_1, D_2, \ldots\}$ for a derivative approximation at the same point $P$. 
The locations of nodes $P$, $L_1$, $L_2$, $D_1$, and $D_2$ for the first-degree Lagrangian polynomial and the three-point stencil are schematically shown in Fig. 3.

Our implementation of the parallel algorithm uses the aforementioned linked list data structure. Every node of the linked list contains an address of an individual grid node; therefore, there is one-to-one correspondence between the set of grid nodes and the set of the nodes of the linked list. The linked list is divided into several sublists of equal sizes that are distributed among the available processors and is repartitioned by adding and removing nodes from the sublists during the grid rearrangement. It has been found that the repartitioning procedure requires insignificant CPU time, but enables a dynamic load balancing among all processors.

The parallel code has been tested on the available Dell T-7500 multicore workstation that has a symmetric multiprocessor architecture where all processors connect to a single shared main memory. Multiple numerical experiments have demonstrated that the parallel code has attained the speedup of a factor of 8 on 11 CPUs corresponding to ~72% parallelization efficiency.

6. Numerical decay of inert plume advected by atmospheric flow

To evaluate the rate of numerical diffusion associated with the truncation error of the approximation in Eq. (27), we consider a simple advection problem of an inert pollution plume propagating in the longitudinal direction $(y = \text{const}, v = 0)$ described by the following equation:

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = 0. \quad (31)$$

Replacing the spatial derivative with its approximation in Eq. (27), we obtain the following expression for the differential-difference approximation of Eq. (31):

$$\frac{\partial c_i}{\partial t} + u \frac{c_{i-2} - 6c_{i-1} + 3c_i + 2c_{i+1}}{6h} = 0. \quad (32)$$

After expanding the terms $c_{i=p}$, $p \in \mathbb{Z}$ in Taylor series about $c_i$:

$$c_{i=p} = c_i \pm \frac{\delta c}{\delta x} (ph) + \frac{1}{2} \frac{\delta^2 c}{\delta x^2} (ph)^2 \pm \frac{1}{6} \frac{\delta^3 c}{\delta x^3} (ph)^3 + \frac{1}{24} \frac{\delta^4 c}{\delta x^4} (ph)^4 + O(h^5), \quad (33)$$

and substituting these expansions into the differential-difference equation in Eq. (32), we obtain

$$\frac{\partial c_i}{\partial t} + u \frac{\partial c_i}{\partial x} = -u \frac{\delta c}{\delta x} + O(h). \quad (34)$$

Here $\mathbb{Z}$ is the set of all integers. Equation (34) shows that the differential-difference scheme in Eq. (32) is third-order accurate for the advection equation in Eq. (31) and fourth-order accurate for the modified equation (LeVeque 1992):

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = D \frac{\delta^4 c}{\delta x^4}, \quad (35)$$

where $D = -uh^2/12$ is the numerical diffusivity. Thus, the numerical solution of the differential-difference equation in Eq. (32) approaches the solution of the modified equation in Eq. (35) faster than it approaches the solution of the advection equation in Eq. (31) as $h \to 0$ (Durran 2010). Therefore, the numerical scheme in Eq. (32) models the dynamics of a plume governed by the modified advection-diffusion equation in Eq. (35) more accurately than the original diffusion-free advection problem in Eq. (31).

Let us determine how the plume decay rate depends on the numerical diffusion quantified by the parameter $D$ and the flow stretching. To do that, we expand the solution $c(x, t)$ of the modified equation in Eq. (35) in Fourier series:

$$c(x, t) = \sum_k c_k^0 \exp[-p(k)t] \exp[i k(x - ut)], \quad (36)$$

where $k$ is the wavenumber and $p(k)$ is the damping coefficient. After substituting Eq. (36) into Eq. (35), we obtain the following dispersion relationship:
Fig. 4. Schematic distribution of mixing ratio vs the distance $x$ from the plume center. Here $W$ is the plume width and $r_b$ is the characteristic spatial scale over which the plume concentration decays from the value inside the plume to zero outside of it.

$$p(k) = -D k^4. \quad (37)$$

Note that the considered numerical scheme is non-dispersive since each Fourier mode propagates with the same speed. It is easy to see that the effect of numerical error is analogous to the physical diffusion causing an exponential decay of a plume

$$c \sim e^{-\alpha t}. \quad (38)$$

The plume decay rate $\alpha$ is estimated to be [refer to Rastigejev et al. (2010) for more details]

$$\alpha = \frac{D}{r_b W}, \quad (39)$$

where $W$ is the plume width and $r_b$ is the characteristic length scale over which the concentration decays from the concentration value inside the plume to zero outside (see Fig. 4).

It has been shown (Rastigejev et al. 2010) that the numerical dissipation of the pollution plume is strongly enhanced by stretching, which is a common characteristic of complex atmospheric flows. The stretching rate is quantified by the first-order maximal Lyapunov exponent $\lambda$ (Lichtenberg and Lieberman 1992). The Lyapunov exponent is defined as a measure of the rate of convergence or divergence of nearby trajectories of two fluid particles. In this work we use the method described in Leung (2011) to calculate the values of $\lambda$. It can be shown (Benettin et al. 1976) that the distance $\delta$ between the two neighboring fluid particles varies exponentially in time:

$$\delta \sim \delta_0 e^{\lambda t}, \quad (40)$$

where the positive Lyapunov exponent indicates a divergent flow, while the negative one corresponds to a convergent flow. The numerical decay of a pollution plume can be significantly enhanced in a convergent flow ($\lambda < 0$) due to strong flow stretching. As a result of this, the numerical plume decay is much faster than one would predict from the order of the advection scheme for typical resolutions $\sim 1^\circ$ used for global CTMs. More specifically, it was shown that if the plume width $W$ approaches the characteristic length $r_s$, mesh refinement has no effect on the plume decay rate that is set by the value of $\lambda$ until $W$ becomes larger than $r_s$. For such plumes with $W > r_b$ the decay rate decreases like $\sqrt{h}$ or $N^{1/2d}$ regardless of the formal order of a numerical scheme. Here $N$ is the total number of points on a uniform grid and $d$ is the space dimension. The described decay rate dependence on the mesh spacing is explained by the fact that sharp plume boundaries are resolved by only a few mesh points on a quasi-uniform grid, which causes a formally high-order numerical scheme to become effectively just first-order accurate. For better-resolved propagating pollution plumes, the numerical scheme recovers its formal convergence rate. However, since the numerical diffusion is still balanced by the flow stretching, which does not allow $r_b$ to grow, the decay rate decreases with the grid refinement slower than the formal numerical scheme error, specifically, as $\sqrt{h^m}$ or $N^{m/2d}$, where $m$ is the order of the numerical method. Particularly for $d = 2$:

$$\alpha \sim h^{m/2} \sim N^{-m/4}. \quad (41)$$

The WAMR algorithm ensures a very good resolution of all spatial scales; therefore, the numerical diffusion is minimal and its value is much smaller than the flow stretching magnitude. As a result, the plume decay rate is fully determined by the order of the numerical scheme:

$$\alpha \sim h^m \sim N^{-m/2}, \quad (42)$$

where $h$ is the smallest spatial step and $N$ is the total number of points on the adaptive grid.

The maximum numerical error associated with the $i$th fluid element over the whole propagation time $T$ is determined as

$$e_i = \max_{t \in [0,T]} [c_i(t) - c_i(0)], \quad (43)$$

where $c_i(t)$ is the mass mixing ratio of the $i$th fluid element at time $t$. Accordingly, the error $e$ associated with the set of plume elements $E$ is defined as a maximum of the errors associated with the individual fluid elements:

$$e = \max_{i \in E} (e_i) = \max_{i \in E} \left\{ \max_{t \in [0,T]} [c_i(t) - c_i(0)] \right\}, \quad (44)$$

where $E$ is the set of tracked fluid elements. From Eqs. (38), (41), and (42) we obtain the following error estimates.
\( e_f \) and \( e_a \) for fixed and adaptive grids accordingly for not very large travel time \( T \):
\[
e_f \approx \alpha_f T \sim N_f^{-m/4}, \tag{45}
\]
\[
e_a \approx \alpha_a T \sim N_a^{-m/2}, \tag{46}
\]
where subscripts \( f \) and \( a \) refer to fixed and adaptive grids, respectively; \( N_f \) is the total number of points on the fixed grid; and \( N_a \) is the number of active collocation points for the same numerical error. The compression ratio \( \xi \):
\[
\xi = \frac{N_f}{N_a}, \tag{47}
\]
for the same numerical error \( e_f = e_a \), can be estimated from Eqs. (45) and (46) as follows:
\[
\xi = \frac{N_f}{N_a} = N_a. \tag{48}
\]
Equation (48) shows that the compression ratio is proportional to the number of active collocation points \( N_a \). Furthermore, \( N_a \) and the threshold parameter \( \varepsilon \) are related (Rastigejev and Paolucci 2006b) for the \( d \)-dimensional space as
\[
N_a \sim \varepsilon^{-d/m}. \tag{49}
\]
Equations (48) and (49) imply that for the two-dimensional space \((d = 2)\):
\[
\xi \sim \varepsilon^{-2/m}. \tag{50}
\]
In other words, Eq. (50) shows that the compression ratio of the WAMR increases with the accuracy of the adaptive algorithm defined by the threshold parameter \( \varepsilon \).

Below we show that the CPU time \( t_c \) decreases when the stencil size \( m \) increases for a given fixed value of error \( e_a \). This finding has been confirmed by numerical experiments. It is easy to see that the CPU time \( t_c \) required to perform computations with an adaptive grid of \( N_a \) points and a stencil of \( m \) points for moderately large stencil sizes \((m < 10)\) is given by
\[
t_c = amN_a, \tag{51}
\]
where \( a \) is a constant proportionality factor. From Eq. (46) we express \( N_a \) via error \( e_a \) and the stencil size \( m \)
\[
N_a = \left(\frac{e_a}{b}\right)^{-2/m}, \tag{52}
\]
where \( b \) is another constant proportionality factor. After substituting Eq. (52) into Eq. (51) we obtain
\[
t_c = am\left(\frac{e_a}{b}\right)^{-2/m}, \tag{53}
\]
from which it follows that
\[
\ln t_c = \ln a + \ln m - \frac{2}{m} \ln \left(\frac{e_a}{b}\right). \tag{54}
\]
Because the derivative of Eq. (54) with respect to \( m \)
7. Convergent–divergent flow

As a model problem to illustrate the adaptive algorithm performance, we consider an incompressible convergent–divergent flow (Rastigejev et al. 2010) defined by the velocity field:

\[ u = \frac{V}{1 + \epsilon \cos(2x)}, \]

\[ v = -\frac{2V\epsilon(y - y_0)\sin(2x)}{[1 + \epsilon \cos(2x)]^2 \sin(y)}, \]

where \( u \) and \( v \) are the longitudinal and latitudinal velocity components that depend on longitude \( x \in [0, 2\pi] \) and latitude \( y \in [0, \pi] \), respectively. The convergent–divergent flow is smooth and periodic in the \( x \) direction. The flow is characterized by three parameters: the mean wind velocity \( V \), the parameter determining the value of the velocity gradients \( \epsilon \), and the location \( y_0 \) of the stagnation point. We prescribe the following values for these parameters: \( V = 50 \text{ m s}^{-1} \), \( y_0 = \pi/2 \), and \( \epsilon = 5/7 \). The flow velocity field can be divided into the adjacent convergence and divergence regions (see Fig. 5). While passing the convergence region, the plume is squeezed from the initial width \( W_0 \) to

\[ W \approx W_0 \frac{u_{\text{min}}}{u_{\text{max}}} = W_0 \frac{(1 - \epsilon)}{\epsilon (1 + \epsilon)}, \]

where \( u_{\text{min}} \) and \( u_{\text{max}} \) are the minimum and maximum velocities of the flow, respectively. The ratio \( u_{\text{max}}/u_{\text{min}} \) is 6 in our case; consequently, the plume width decreases by a factor of 6 as it passes through the convergence region.

To test the WAMR performance, we apply the algorithm to a numerical simulation of the inert plume propagating in the described convergent–divergent flow with the initial mixing ratio given by

\[ c(x, y, 0) = \begin{cases} \lfloor \cos(d) + 1 \rfloor/2, & d \leq \pi, \\ 0, & d > \pi, \end{cases} \]

where \( d = k\sqrt{(x-a)^2 + (y-b)^2} \), \( a = 0 \), \( b = 0 \), and \( k = 38 \). Equation (59) implies that the initial plume has the shape of a circle of radius 15° with the density gradually decreasing from 1 at the plume center to 0 at its border.

The mixing ratio \( c(t) \) associated with every fluid element must remain constant in time for the flow without dissipation. The results of calculations performed on a fixed grid (Rastigejev et al. 2010) show, however, that the plume quickly decays, therefore, the value of \( c(t) \) decreases, as the plume passes the convergence zone for typical grid resolutions used for the fixed grids with spatial resolution \( \sim 100 \text{ km} \). Moreover, it was also demonstrated that the plume decay rate drops slowly with the grid refinement for sufficiently strong stretching and low grid resolutions typically used for fixed grids due to poor numerical convergence for such resolutions. The numerical scheme certainly recovers its normal convergence rate if all spatial scales are well resolved.
Below we demonstrate that the WAMR algorithm, unlike conventional nonadaptive methods, can easily achieve such spatial resolutions and produce accurate simulations at a relatively low computational cost.

The evolution of the plume and the corresponding adaptive grid calculated by the WAMR method for the convergent–divergent flow are depicted in Figs. 5 and 6. Initially, the plume propagates in the convergent flow where it is stretched by the flow in the longitudinal direction and compressed in the latitudinal direction for $t < 55$ h. Later the plume enters the divergent flow where it re-expands to its original size. The adaptive grid follows the plume, maintaining a high resolution at the plume location. In our calculations, the numerical method requires us to dynamically add three more levels of resolution (to increase the maximum grid resolution by a factor of 8) for the plume propagating through the convergent flow section compared to the same plume propagating in a uniform flow. This significant local grid refinement is necessary to resolve finer spatial scales that occur as a result of the plume’s fine scales contraction in the convergent flow.

The dependence of numerical error $e$, defined by Eq. (43) for a fluid element corresponding to the maximum plume mixing ratio, versus the total number of grid points $N$ is plotted in Fig. 7. The lines with square and circle markers correspond to the uniform and adaptive grid calculations, respectively. The third-order ($m = 3$) upwind finite differences are used for both grids. It is found that the error decreases with the number of points as $e_f \sim N^{-3.24}$ and $e_a \sim N^{-3.42}$ for the uniform and adaptive grids, respectively. These numerical results agree very well with theoretical estimates for both uniform and nonuniform adaptive grids as in Eqs. (45) and (46), respectively. Results of numerical experiments show that the error associated with the WAMR calculations is at least an order of magnitude lower than that of the calculations performed on a fixed uniform grid for the same number of points. High accuracy of the WAMR method is certainly due to the fact that the nonuniform adaptive grid allows significantly better spatial resolution of the finest scales than the uniform grid. For instance, calculations presented in Fig. 7 produce resolutions in the range $0.1^\circ–1^\circ$ for the adaptive grid.
grid, while similar calculations done on a uniform grid guarantee only the resolution of $3^{m-11}$ for the same number of grid points. Figure 8 shows the dependence of the compression ratio $\xi$ on the threshold parameter $\varepsilon$. This dependence is accurately approximated by the power function $\xi \sim \varepsilon^{-0.7}$ as predicted by Eq. (50). The exponent value of which $-0.7$ agrees well with the theoretically predicted value $-0.66$ given by Eq. (50) for $m = 3$. A high compression ratio allows WAMR to achieve the same accuracy, using significantly lower computational resources compared with the methods that utilize fixed grids.

8. Deformational flow

To test the WAMR algorithm further, we have carried out numerical simulation of the plume propagation in a nonstationary deformational flow with a nonzero divergence suggested by Nair and Lauritzen (2010). This paper proposed a new class of the deformational flows on a sphere for testing different numerical schemes for two-dimensional linear transport problems. We deliberately have chosen the case of a flow with a nonzero divergence since the numerical simulation of the transport in such flow is more complex than that in a divergence-free flow. Therefore, a numerical simulation of the flow with a nonzero divergence provides a more rigorous test for the WAMR algorithm than that of the divergence-free flow. The velocity fields in the tests problem is constructed so that the initial scalar field $c$ undergoes severe deformations making a numerical simulation of the transport very challenging. The flow reverses its course at half-time, and the scalar field returns to its initial position and shape (i.e., the initial and final distributions of $c$ are identical).

In spherical coordinates, the longitudinal $u$ and latitudinal $v$ velocity components are specified as follows:

$$u = -50 \sin^2(x/2) \sin(2y - \pi) \cos^2(y - \pi/2) \cos(\pi t/T),$$

$$v = 25 \sin(x) \cos^3(y - \pi/2) \cos(\pi t/T),$$

where $x \in [0, 2\pi]$, $y \in [0, \pi]$, and $T = 177 \text{ h}$ is the final time. The initial mixing ratio distribution consists of two identical plumes of radius $r = 29^\circ$ defined by Eq. (59) and the background density of 0.1. The plumes are placed at the points $(x_1, y_1) = (3\pi/4, \pi/2)$ and $(x_2, y_2) = (5\pi/4, \pi/2)$, respectively.

Figure 9 shows the pollutant density distribution at initial time (Fig. 9a), half-time (Fig. 9b), and final time (Fig. 9c). This test is challenging for any multiscale method since the initially circular plumes are strongly stretched into thin filaments at half-time, but return to their initial position and shape at the final time of the system evolution. To
simulate the plume structure accurately, the WAMR method requires five levels of resolution which corresponds to the maximum resolution 0.35°. The size of the adaptive grid increases monotonically over the first half of the time interval and reaches its maximum, $3.2 \times 10^4$ points, at half-time (i.e., at the moment when the plumes are most stretched). The average number of grid points is approximately $2 \times 10^4$, which corresponds to the average compression ratio of 26. Our numerical experiments demonstrate that the error defined by $l_2$ norm does not exceed $5 \times 10^{-3}$ for WAMR calculations. This error value is 3 times as small as that reported by Nair and Lauritzen (2010) for their simulations of the same problem performed with the third-order discontinuous Galerkin transport scheme on a fixed grid with resolution of 1.5° at the equator, which corresponds to 38400 points.

Our calculations demonstrate that the nonuniform grid adapts very efficiently to the local evolving structures maintaining high resolution at the plume location (where the solution varies the most) and relatively crude grid at other locations (see Fig. 10). Figure 11 shows the distribution of the pollutant mixing ratio field $c$ versus $x$ in the equator cross section $y = 0$ at initial $t = 0$ (solid line) and final $t = 177$ h (squares) times.

9. Atmospheric flow

To demonstrate the efficiency of the adaptive algorithm, we carried out numerical simulations of a pollution plume propagating in a two-dimensional horizontal atmospheric flow. The pollution plume initially located over China is picked up by the westerly wind and
transported across the Pacific Ocean in 7 days (see Fig. 12). The airflow strongly stretches the plume into a thin elongated structure that is preserved during the subsequent trans-Pacific motion. The velocity field on an adaptive nonuniform grid is reconstructed by interpolating the data from cruder uniform grid of $2^\circ \times 2.5^\circ$ to the finer levels of resolution. The velocity field for the uniform grid at the altitude of 4 km on 1 May 2001 is obtained from the GEOS-Chem database. The initial circular plume with the center at 30°N, 110°E and the radius $r = 5^\circ$ is located in the free troposphere with concentration distribution defined by Eq. (59) with $a = 110$, $b = 30$, and $k = 113$. The results of computations with the GEOS-Chem code (Rastigejev et al. 2010) show quick numerical decay of a transpacific plume for resolutions $4^\circ \times 5^\circ$, $2^\circ \times 2.5^\circ$, and $1^\circ \times 1.25^\circ$ typically used for uniform grids. For instance, maximum concentration in the plume decreased to 10% of the original value after 10 days even for the finest uniform grid $1^\circ \times 1.25^\circ$. It was also found that the average numerical plume decay rate $\bar{\alpha} = \int_0^T \alpha \, dt / T$ averaged over time interval $T = 240$ h decreases very slowly with the mesh refinement, $\bar{\alpha} \sim h^{0.25}$ for this range of resolutions.

We employ the seventh-order ($m = 7$) accurate adaptive numerical scheme to run a series of numerical simulations of a pollution plume propagation in the atmospheric flow for different values of the threshold parameter $\varepsilon$ in the range $10^{-1}$–$10^{-4}$ with the finest grid resolution $0.02^\circ$ (~2 km). To evaluate the numerical error in Eq. (44), we tracked three fluid elements of the plume with the initial mass mixing ratios $c = 1, 0.9$, and 0.48. It is found that the error $e_a$ drops very quickly with the total number of points $N$ but somewhat slower than the theoretical estimate in Eq. (42):

$$e_a \sim N^{-5.2/2}. \quad (62)$$

This rapid convergence of the adaptive algorithm enables us to achieve a very high accuracy (numerical error $e_a = 0.8\%$ for the time interval $T = 240$ h) for numerical simulations with relatively small average number of nodes $N = 88\,793$, whereas calculations on a fixed uniform grid with a comparable number of points produce a much larger numerical error $e_f \approx 90\%$ for the same time interval. The pollution plume and the lower levels of an adaptive grid that track large spatial scales for $t = 83$ h and $t = 216$ h are shown in Figs. 13a and 13b, respectively. The upper levels of an adaptive grid that capture smaller spatial scales are shown in Figs. 13c and 13d for the same times. The plots demonstrate that the collocation points adapt very efficiently to the developing local structures; therefore, a fine grid appears only in the regions where the pollutant density varies the most, while the rest of the domain is covered by a relatively sparse grid. The adaptive multilevel grid uses up to nine levels of resolution in these calculations. The total number of grid points as a function of time is plotted in Fig. 14. The total number of grid points varies in time since the points are added or removed dynamically, so that the multilevel sparse grid matches the instantaneous plume shape.

It is explained in section 6 that the numerical dissipation of a plume can be significantly enhanced by the convergent flow stretching that is measured by the value of Lyapunov exponent $\lambda$. Moreover, it was shown in Rastigejev et al. (2010) that for sufficiently strong stretching the numerical decay of the plume is independent of the model grid resolution and is determined by the flow Lyapunov exponent $\lambda$. The value of $\lambda$ and the decay coefficient $\alpha$ along the path of the point corresponding to the maximum plume concentration are plotted in Fig. 15. The plot shows that there is no correlation between $\alpha$ and $\lambda$ unlike in the fixed grid case where a significant correlation between these variables is observed (Rastigejev et al. 2010). The decay rate remains almost zero due to the excellent ability of the WAMR to refine the grid in the locations where the fine spatial scales occur.

To verify how well the method conserves mass, we simulated the propagation of the plume with the initial mass $m(0)$ scaled to unity, during the Pacific Ocean. Figure 16 shows the change in the plume mass $\Delta m = m - 1$ as a function of time $t$. The plot demonstrates that the adaptive method preserves the plume mass well since the error in mass value does not exceed $2 \times 10^{-2} \%$ over the propagation time. We would like to point out that since the present algorithm is based on a collocation approach, the spatial discretization results in a numerical scheme that does not enforce mass conservation to machine precision. However, due to the high accuracy of the numerical method, conservation errors are below the imposed threshold value.
10. Conclusions

We have developed and applied the WAMR method to the numerical simulation of the two-dimensional global atmospheric chemical transport. Difficulties associated with numerical simulations of such problems impose severe limitations on the spatial resolution of fixed numerical grids, which introduces a large numerical diffusion into the system. In combination with strong stretching of the atmospheric flow this causes large numerical errors.

We showed that these difficulties can be efficiently resolved with the WAMR method. The method dynamically introduces a fine grid in the regions where small spatial structures are present and a sparse grid elsewhere. The adaptation algorithm is based on a well-developed wavelet theory, therefore, the algorithm produces an optimal grid that is shown to capture efficiently evolving spatial structures. Unlike traditional finite-volume AMR methods, the WAMR method employs higher-order spatial discretization schemes. Specifically, we use a seventh-order scheme for simulation of a pollution plume propagation in this work. The ability of the algorithm to utilize higher-order schemes is very important for global atmospheric CTM modeling since it enables us to reduce efficiently the numerical diffusion by orders of magnitude, therefore, to decrease the numerical error significantly. As a result, the algorithm enables the minimization of the number of grid points for a prescribed accuracy and leads to very accurate numerical solutions.

The method has been compared with conventional CTM computations. It has been shown that the algorithm allows two orders of magnitude or more for better resolution than conventional fixed grids for the same total number of grid points. Hence, the method produces significantly higher accuracy than conventional numerical techniques using fixed grids. For instance, it has been shown that the error has not exceeded 1% for numerical modeling of trans-Pacific plume propagation. Therefore, the method provides a realistic opportunity to solve numerically the most challenging multiscale problems of the global atmospheric chemical transport on existing computers by producing accurate results at a reasonable computational cost.

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