A Characteristic Adaptive Wavelet Method for Aerosol Dynamic Equations

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***Abstract*—In this paper, a characteristic adaptive wavelet method is developed for solving aerosol dynamic equations. The proposed method combines the adaptive multi-resolution technique and the characteristic method to obtain the fully adaptive multi-resolution scheme, in which the solution is represented and computed in dynamically evolved wavelet bases along the characteristic curves. It overcomes numerical dispersions and can use large time steps. The efficiency and accuracy of the new algorithm is verified by numerical experiments. The developed characteristic adaptive wavelet algorithm in the paper has great applications in the modelling of aerosol dynamics.**

Keywords–Aerosol dynamic equation; the characteristic technique; adaptive multi-resolution method; wavelet.

I. INTRODUCTION

Aerosols are now clearly identified as an important factor in many environmental aspects of climate and radiative forcing processes, as well as in the health effects of air quality [7][8][11][15][17]. The aerosol dynamics with respect to size distribution is a nonlinear partial differential and integral equation.

Numerical methods have been proposed to solve the aerosol dynamic equations such as sectional method [9], moment method [1][14], modal method [18], finite element method [16], and stochastic approach [5], etc. The modal and moment approaches have the high numerical efficiency but only applied to some particular cases. When the distribution function is required, sectional methods are popular technique in aerosol dynamic modelling. But the treatment of condensation by sectional approaches usually leads to extra numerical diffusion, while smears the steep fronts. Sandu and Borden [16] developed a framework of finite element methods for numerical solutions of the aerosol dynamic equations, Liang et al. [13] developed the characteristic finite element methods for aerosol dynamic equations, and Liang et al. [12] developed a splitting wavelet method for solving the general aerosol dynamic equations on time, particle size and vertical spatial coordinate.

The size of atmospherical aerosols spans order of magnitude and the mechanisms for different size regions are totally different, so the aerosol size distribution is highly uneven distributed, such as multiple lognormal distributions in some regions. Thus, the most important problem encountered in the solutions of aerosol dynamic equations is how to efficiently solve the equations in size and time since the aerosol distributions vary very sharply in the size direction. Another problem is to approximate the advection process caused by the condensation growth term.

Multiresolution methods have been recognized to be important adaptive techniques in the applications to solutions of Partial Differential Equations (PDEs). For many real problems, solutions often exhibit localized singular features, such as sharp peaks. Uniform basis function space is not a practical option since high resolution is only needed in small regions. For improving the accuracy, the localization property of the wavelets both in space and in frequency makes the adaptivity efficiently [2][3][6][10].

In the paper, a characteristic adaptive wavelet method is developed to solve the aerosol dynamic equations, in which the time derivative and the condensation advection are transferred to the directional derivative along the characteristics and then discretized by the difference along the characteristics. For approximating size distribution, the differential systems of equations in time variable are obtained based on the wavelet bases. Owe to the advantage of characteristics method, we can refine the adaptive wavelets at the next time step along the characteristic curves. Adaptive space refinement strategy can follow the flow of solution over time. It reduces temporal errors and eliminates the excessive numerical dispersion. Compared with the uniform mesh method, the characteristic adaptive wavelet method has higher computational efficiency. Numerical experiments show the excellent performance of the developed algorithm in simulating aerosol dynamics.

The paper is arranged as follows. The mathematical model of aerosol dynamic system is presented in Section 2. In Section 3, the characteristic adaptive wavelet scheme is proposed for the aerosol dynamic equations. Numerical experiments are given in Section 4. Finally, we address some conclusions in Section 5.

II. AEROSOL DYNAMIC EQUATIONS

The aerosol dynamic equations can be described as [7]

$$\begin{aligned}\frac{\partial n(v,t)}{\partial t} &= -\frac{\partial[G(v)n(v,t)]}{\partial v} - n(v,t)\int_{V_{min}}^{V_{max}} \beta n(w,t)dw \\ &+\frac{1}{2}\int_{V_{min}}^{v-V_{min}} \beta n(v-w,t)n(w,t)dw, \qquad (1)\end{aligned}$$

with boundary and initial conditions

$$\begin{aligned} n(V_{min},t) &= 0, \quad t\in(0,T], \qquad (2)\\ n(v,0) &= n_0(v), \quad v\in\Omega. \qquad (3)\end{aligned}$$

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where $t > 0$ is the time, v is the aerosol particle volume, and $T > 0$ is the time period. $n(v, t)$ is the number concentration distribution associated with particles volume v at time t. In practice, one assumes that the particle population has a nonzero minimal volume and a finite maximal volume, i.e., in a finite volume interval $[V_{min}, V_{max}]$, where V_{min} and V_{max} are chosen as lower and upper limits of the aerosol volume respectively. The condensation growth rate $G(v)$ is defined as the rate of change of the volume of a particle of volume v and $G(v) = \sigma_0 v$ will be considered in this paper due to the important application of linear growth rate. Coagulation of aerosol particles occurs through a variety of mechanisms such as Brownian motion, turbulent diffusion, etc. The coefficient β is the coagulation kernel.

III. THE CHARACTERISTIC ADAPTIVE WAVELET SCHEME

A. The Characteristic Method

For treating the condensation advection efficiently, we first propose the characteristic semi-discretization scheme in time. Denote the number of time steps by the positive integer Q and the time level by $t^q = q\Delta t$, $q = 0, 1, \cdots, Q$, where Δt is the time step size. For any particle size x at time $t = t^{q+1}$, the characteristics curve $X(x, t; \tau)$ passing through (x, t) satisfies:

$$\begin{cases} \frac{dX}{d\tau}(x, t^{q+1}; \tau) = a\sigma_0 X(x, t^{q+1}; \tau), \\ X(x, t^{q+1}; t^{q+1}) = x. \end{cases} \tag{4}$$

where τ is the characteristics direction. Let $\hat{x}$ be the intersection point of tracking back along the characteristic curve from the point (x, t^{q+1}) to time level $t = t^q$.

For the aerosol dynamic equations in logarithmic coordinates, the characteristic semi-discretization scheme is defined as

$$\begin{aligned} &\frac{n(x, t^{q+1}) - n(\hat{x}, t^q)}{\Delta t} = -\sigma_0 n(x, t^{q+1}) \\ &+ \frac{\beta}{2} \int_0^{aln(e^{x/a}-1)} \frac{e^{(y-b)/a}}{a} n(x^*, t^q) n(y, t^q) dy \\ &- \beta n(x, t^q) \int_0^1 \frac{e^{(y-b)/a}}{a} n(y, t^q) dy \end{aligned} \tag{5}$$

with initial value $n(x, 0) = n^0(x)$ and the boundary condition $n(x, t) = 0$.

Let $\tilde{V}^{q+1}(\Omega)$ be wavelet space at $t = t^{q+1}$ defined in the next section. Then, the characteristic wavelet scheme is to find $n(x, t^{q+1}) \in \tilde{V}^{q+1}(\Omega)$ such that

$$\begin{aligned} &\big((1 + \sigma_0 \Delta t) n(x, t^{q+1}), \xi(x)\big) = (n(\hat{x}, t^q), \xi(x)) \\ &+ \tfrac{\Delta t \beta}{2} \left(\int_0^{aln(e^{x/a}-1)} \tfrac{e^{(y-b)/a}}{a_2} n(x^*, t^q) n(y, t^q) dy, \xi(x) \right) \\ &- \Delta t \beta \left(n(x, t^q) \int_0^1 \tfrac{e^{(y-b)/a}}{a} n(y, t^q) dy, \xi(x) \right) \end{aligned} \tag{6}$$

with $n(x, 0) = n_0(x)$.

B. The Characteristics Adaptive Wavelet Algorithm

In this section, we shall construct an adaptive multiresolution scheme of Haar wavelets for (6).

Haar wavelets, which are Daubechies wavelets of order 1 (see [4]), consist of piecewise constant functions and are therefore the simplest orthonormal wavelets with a compact support. Because of the advantages of Haar wavelets, we will apply Haar wavelets as the basis functions in the scheme (6). Let $\psi(x)$ be the Haar wavelet, and the corresponding scaling function $\phi(x)$ The adaptive space $\tilde{V}^{q+1}(\Omega)$ composed by the Haar scaling functions is the cell-average multiresolution representation, where $J_0 \le j \le J$ and J_0 is the coarsest resolution level and J is the highest resolution level. The scaling coefficients $c_{j,k}^{q+1}$ are cell-average values. Find $\tilde{n}^{q+1}(x) \in \tilde{V}^{q+1}(\Omega)$ with

$$\tilde{n}^{q+1}(x) = \sum_{(j,k)\in\tilde{\Lambda}^{q+1}} c_{j,k}^{q+1} \phi_{j,k}(x) \tag{7}$$

in the scheme (6), where $\tilde{\Lambda}^{q+1}$ is the index set of scaling functions at $t = t^{q+1}$. Once $\hat{\Lambda}^q$ is determined, which is the final index set at $t = t^q$, we initialize $\tilde{\Lambda}^{q+1}$ from $\hat{\Lambda}^q$ by tracking along the characteristics.

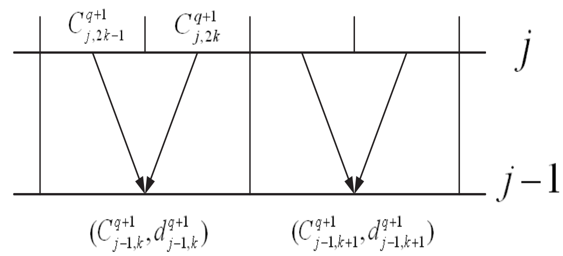


Figure 1. The operator P_j^{j-1}.

To estimate the cell-averages and detail information at level $j-1$ from the ones of the level j, we use the multiresolution transform P_j^{j-1}, see Figure 1, as

$$c_{j-1,k}^{q+1} = \frac{1}{\sqrt{2}} \left(c_{j,2k-1}^{q+1} + c_{j,2k}^{q+1} \right), \tag{8}$$

$$d_{j-1,k}^{q+1} = \frac{1}{\sqrt{2}} \left(c_{j,2k-1}^{q+1} - c_{j,2k}^{q+1} \right). \tag{9}$$

Then, we have $\tilde{n}^{q+1}(x)$

$$\begin{aligned} \tilde{n}^{q+1}(x) = \sum_{(j,2k),(j,2k-1)\in\tilde{\Lambda}^{q+1}} &[c_{j-1,k}^{q+1} \phi_{j-1,k}(x) \\ &+ d_{j-1,k}^{q+1} \psi_{j-1,k}(x)]. \end{aligned} \tag{10}$$

A threshold parameter ϵ is prescribed for the adaptive procedure

$$\epsilon_j = \epsilon / 2^{j-J_0}, \quad J_0 \le j \le J-1.$$

If $|d_{j-1,k}^{q+1}| < \epsilon_j$, we reduce $\phi_{j,2k-1}$ and $\phi_{j,2k}$ from the space $\tilde{V}^{q+1}(\Omega)$; while if $d_{j-1,k}^{q+1}$ is big, then we add $\phi_{j+1,4k-3}$, $\phi_{j+1,4k-2}$ $\phi_{j+1,4k-1}$ and $\phi_{j+1,4k}$, based on operator P_j^{j+1}, see Figure 2. The space after adjustment is called as $\hat{V}^{q+1}(\Omega)$ and the corresponding index set is $\hat{\Lambda}^{q+1}$.

The important feature of the characteristic adaptive wavelet algorithm is that it adjusts the approximation wavelet space

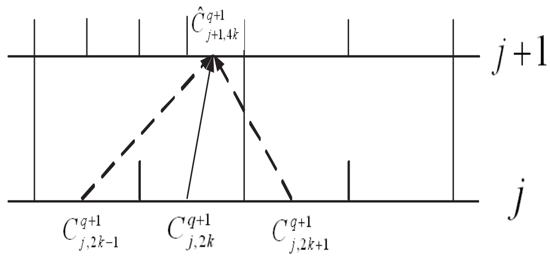


Figure 2. The operator P_j^{j+1}.

at next time level by tracking back along the characteristics, which is further refined or coarsened by the adaptive wavelet technique. The highly accurate approximation can be obtained by the new algorithm even large time step sizes are used, while other classic algorithms need to use very small time steps.

IV. Numerical simulation

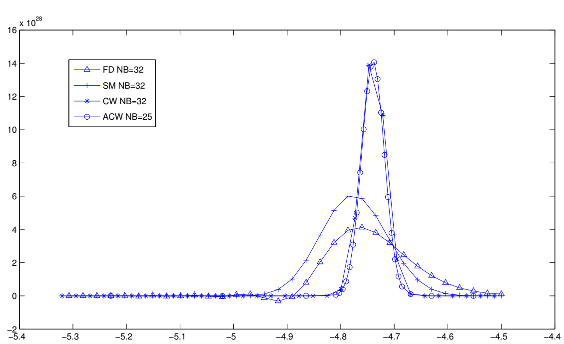
In this section, numerical examples are taken to illustrate the performance of the characteristic adaptive wavelet algorithm.

Example 1.

In this example, we consider the condensation process with initial single mode distribution. The initial distribution is a log-normal distribution on the volume domain $[1 \times 10^{-16} m^3, 1 \times 10^{-13.5} m^3]$ described by

$$n_0(v,t) = \frac{N_0}{3\sqrt{2\pi}\ln\sigma} \exp\left(-\frac{\ln^2(v/v_g)}{18\ln^2\sigma}\right)\frac{1}{v} \tag{11}$$

with the volume concentration $N_0 = 5 \times 10^{10}$particles$/m^3$, the geometric average volume $v_g = 1 \times 10^{-15} m^3$ and the standard deviation $\sigma = 1.05$. We choose coarsest level $J_0 = 2$ and highest level $J = 6$ for our method.

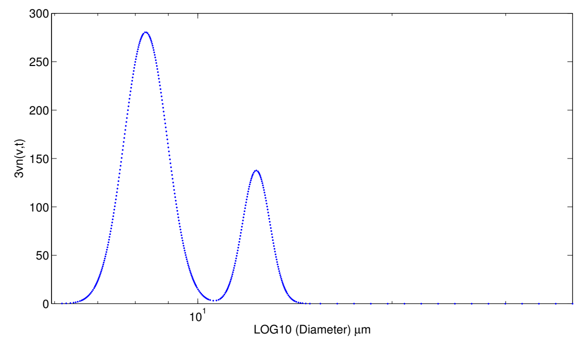


(a) $\sigma_0 = 1.8/h$ and $\Delta t = 0.05h$

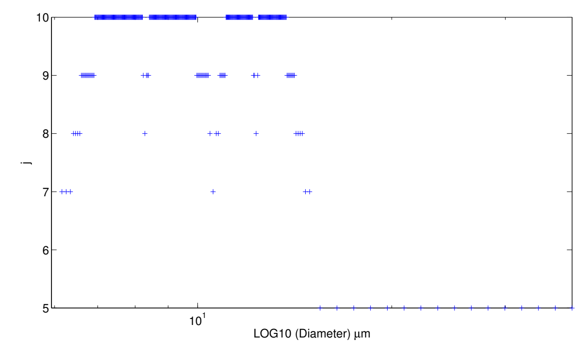
Figure 3. Comparison of number distribution $3vn(v,t)$ by different methods.

We take the numerical experiment of our Characteristic Adaptive Wavelet (CAW) method with threshold parameter $\epsilon = 10^{-2}$ and compare with other methods including upstream Finite Difference (FD) method, Sectional Method (SM) in [9] and the Characteristics Wavelet (CW) method, where the number of the bins NB is 32 for the last three methods. Figure 3 shows the numerical computations after 1h for different growth rates and time step sizes, where the vertical coordinate represents numerical distribution $3vn(v,t)$ and the horizontal coordinate is the logarithmic diameter of the aerosol particles.

From Figure 3, where the growth rate σ is $1.8/h$, numerical distributions obtained by the characteristic wavelet method and our characteristic adaptive wavelet algorithm are excellent. but both of the finite difference method and sectional method suffer from numerical diffusion greatly. Moreover, our characteristic adaptive wavelet method is only with the number of the bins $NB = 25$, however the characteristic wavelet method requires the number of the bins $NB = 32$. The numerical solutions by our algorithm with less number of bins show much better numerical efficiency even with a large time step and growth rate.



(a) Aerosol number distribution



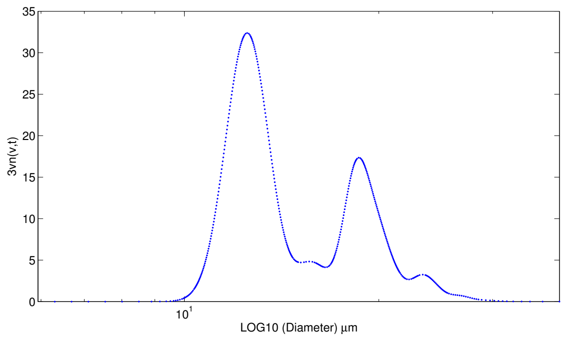
(b) Adaptive mesh

Figure 4. Aerosol distribution for linear condensational growth and constant coagulation kernel.

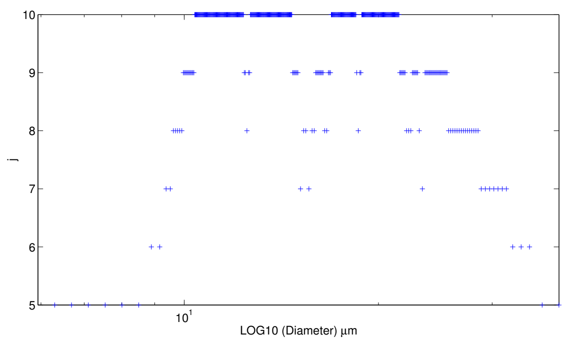
Example 2.

In this example, we consider aerosol dynamic systems evolving both condensation and coagulation processes with the initial two-modal log-normal distribution.

The volume domain is $[10^2 \mu m^3, 10^{4.5} \mu m^3]$. Take time step $\Delta t = 0.1h$, $J_0 = 5$ and $J = 10$. Figures 4 and 5 show the numerical number densities of aerosol distribution and their corresponding adaptive bases at times $T = 0.1h$ and $40h$ with $\sigma = 0.03/h$ and coagulation kernel $\beta_0 = 0.01 \mu m^3/h$. The horizontal coordinate represents logarithm of particle diameter. The vertical coordinate represents the number distribution $3vn(v,t)$ and resolution level separately in the left figures and right figures. In Figure 4, we can see that the multiresolution bases are centered at the places where the two peaks of the two-modal log-normal distributions located. Since the number condensations at the larger particle size region are very small, it's good enough to describe the number condensation with coarsest resolution level.



(a) Aerosol number distribution



(b) Adaptive mesh

Figure 5. Aerosol distribution for linear condensational growth and constant coagulation kernel.

As time goes on, shown in Figure 5, the number condensation moves forward along the size direction, meanwhile number condensation of smaller particles decreases and that of larger particles increases because coagulation is the process whereby two particles collide and form larger particle, as a result, higher resolution level bases are adaptively added to capture the change of the distribution at the larger particle size.

V. Conclusion and Future Work

A new characteristic adaptive wavelet algorithm was developed for solving the aerosol dynamic equations. The considered model is a nonlinear partial differential and integral equation with hyperbolic part from the condensation term.

Using the multiresolution technique, the computational bases are reduced by deleting non-significant wavelet coefficients while keeping the desired accuracy. The adaptive space refinement strategies are simplified and we refine the adaptive bases at the next time step along the characteristic curves, which save computational time and memory.

We demonstrated numerically the efficiency of the characteristic adaptive wavelet algorithm for different tests of the condensation process and the joint effect of condensation and coagulation processes. The method exhibited good shape and high accuracy even when large time steps are used in computations, which has great applications in the modelling of aerosol dynamics.

The proposed characteristic adaptive wavelet method can be further extended to solve aerosol spatial transport problems in atmosphere, where the characteristic adaptive wavelet technique can efficiently treat the transport process. Developing fast and adaptive algorithms for the general aerosol dynamic process will be our another interested work.

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