Available online at www.sciencedirect.com
SCIENCE DIRECT
Atmospheric Environment 40 (2006) 4574–4588
ATMOSPHERIC ENVIRONMENT
www.elsevier.com/locate/atmosenv

An asynchronous time-stepping (ATS) integrator for atmospheric applications: Aerosol dynamics

K. Max Zhang[a,*], Anthony S. Wexler[a,b,c]

[a]Department of Mechanical and Aeronautical Engineering, University of California, Davis, CA 95616, USA
[b]Department of Civil and Environmental Engineering, University of California, Davis, CA 95616, USA
[c]Department of Land, Air, and Water Resources, University of California, Davis, CA 95616, USA

Received 29 September 2005; received in revised form 7 February 2006; accepted 24 March 2006

Abstract

Mixed time integration methods, also known as multiple time-step methods (MTS), have been proposed and implemented successfully to reduce the stiffness of problems in molecular dynamics and solid mechanics, where different time scales are used to integrate different motions or meshes. We apply the similar concept and develop an asynchronous time-stepping (ATS) integrator for atmospheric application. This paper first presents ATS as a generalized ordinary differential equation solver and describes its key components including: (1) global and local time management; (2) dynamic time-scale ordering; and (3) integration and iteration methods. Then we apply ATS to solve stiff problems in aerosol dynamics, where we further introduce several techniques such as grouping particulate species by particle sections to speed up computations. The comparisons between ATS and standard ODE solvers including LSODE, LSODES and VODE in aerosol dynamics simulation are presented, which show that ATS is robust and able to achieve a significant digit average (SDA) value of 2.0 to 3.0 while its speed is around 10 to 100 times faster than LSODE with equivalent accuracy. ATS has been implemented in CMAQ-UCD, a sectional, dynamic aerosol model built on USEPA's CMAQ platform.

Keywords: Stiff problem; Ordinary differential equations (ODE); MTS; Aerosol dynamics; CMAQ-UCD

1. Introduction

Numerical simulations of physical systems often contain high frequency and low frequency degrees of freedom. In molecular dynamics, for example, the bond vibrations usually occur on a time scale which is short compared to that of the translations and rotations (Tuckerman et al., 1990). In path integral simulations of electron salvation, the vibrational force constants arising from the kinetic energy operator increase linearly with the size of the chain (Wu and Smolinski, 2000). Hence, the vibrations of the chain are often fast compared with any other motion in the system. Standard integrators require the choice of time step sufficiently small to guarantee stable solution of the highest frequency motion with the consequence that simulations require a very large number of CPU cycles (Tuckerman et al., 1990). In solid mechanics, the mesh of a finite element model is not uniform in that material properties and element sizes can vary

*Corresponding author. Fax: 530 752 4158.
E-mail address: maxzhang@ucdavis.edu (K.M. Zhang).

1352-2310/$ - see front matter © 2006 Elsevier Ltd. All rights reserved.
doi:10.1016/j.atmosenv.2006.03.048

widely throughout the mesh. For explicit time integration the stable time step is based on the maximum frequency of the mesh and if there is a small region of elements with high frequencies it will set a small critical time step for the entire problem. Also, if a problem has localized loads that vary rapidly, a small time step is necessary to accurately capture the behavior of the load even though far from the load a larger time step may give adequate accuracy (Wu and Smolinski, 2000).

Similar problems also arise in atmospheric applications. The chemical process describing the fate of atmospheric pollutants is mathematically represented through a set of coupled, nonlinear ordinary differential equations (ODEs). A primary source of difficulty in the numerical solution of these equations arises from the fact that the gas chemistry or aerosol dynamics in atmospheric systems involves reactions or gas/particle mass transfer whose characteristic time scales vary orders of magnitude, resulting in highly "stiff" and large systems of equations. For instance, the stiffness ratio for ODEs arising from typical tropospheric photochemistry system is usually of the order of 10^{10}. The system to simulate aerosol dynamics can also be very stiff, partly because atmospheric particle size range spans diameters from a few nanometers to tens of microns. Since the mass transfer rate between gaseous and particulate phases is strongly dependent on particle size, the mass transfer rates for the smallest and the largest particles may differ by several orders of magnitude. The causes of stiffness in simulating aerosol dynamics will be elaborated in Section 3. Further, the spatial dependencies typical of three-dimensional (3D) air quality models require solution of these equations at each computational node of the modeled domain, resulting in an extremely computationally intensive problem. Although computational power has increased tremendously in recent years and significant advances have been made in the numerical solution of stiff ODEs for atmospheric applications (Young and Boris, 1977; Hesstvedt et al., 1978; Hertel et al., 1993; Sun and Wexler, 1998; Capaldo et al., 2000), the emerging long-term studies, such as annual air quality and global climate change simulations, and regulatory studies such as SIPs, which simulate the same episodes numerous times under various control scenarios, pose greater computational demands. So the search for faster and more accurate solution methodologies is of considerable interest to atmospheric modelers, because a major portion of the computational efforts in comprehensive atmospheric chemistry/transport models is devoted to solving these kinetic equations (Mathur et al., 1998).

Mixed time integration methods, also known as multiple time-step methods (MTS), have been proposed and implemented successfully to reduce the stiffness of problems in molecular dynamics (Streett et al., 1978; Tuckerman et al., 1990) and solid mechanics (Belytschko and Mullen, 1976; Neal and Belytschko, 1989; Belytschko and Lu, 1993; Smolinski and Wu, 1998; Wu and Smolinski, 2000), where different time scales are used to integrate different motions or meshes. In this paper, we apply a similar concept and develop an asynchronous time-stepping (ATS) integrator for atmospheric applications, i.e., gas chemistry and aerosol dynamics. The current paper describes the ATS algorithm and compares its predictions to those from established ODE solvers for aerosol dynamics calculations. This paper is organized as follows: we first present ATS as a generalized ODE solver; the causes of stiffness, customized ATS formulations and comparisons to accurate ODE solvers in aerosol dynamics are discussed, respectively. The two following papers will discuss its implementation in simulating aerosol dynamics (Zhang and Wexler, 2006; Nolte et al., 2006) in 3-D air quality models.

2. ATS as a generalized ODE solver

2.1. ATS' computational advantages

Stiffness occurs because there are a wide range of time scales in the solution. A set of ODEs of the form

$$\frac{dc_i}{dt} = f_i(c_j, t), i, j = 1, 2, ..., n \quad (1)$$

is stiff if (1) the eigenvalues of the Jacobian matrix of the system are negative, i.e. $\mathrm{Re}(\lambda_i) < 0$, $i = 1, 2, 3, \ldots, n$; and (2) the ratio of the maximum to the minimum eigenvalues, $\max|\mathrm{Re}(\lambda_i)|/\min|\mathrm{Re}(\lambda_i)|$ 1 (Lambert, 1980). Instead of solving this set of equations simultaneously, multiple time-step (MTS) methods use a small time step δt to advance the fast equations n steps holding the slow variables fixed; the slow degrees of freedom are then updated using a time step $n\delta t$ (Swindoll and Haile, 1984; Teleman and Jönsson, 1986). The main computational advantages of MTS/ATS over other synchronous