United States
Environmental Protection
Agency

Atmospheric Sciences Research
Laboratory
Research Triangle Park NC 27711

Research and Development

EPA-600/S3-84-112 Jan. 1985

EPA

Project Summary

Evaluation of Two Numerical Integrator Schemes

A. A. N. Patrinos and M. J. Leach

This report compares the performance of two numerical integrator schemes that have been used in air pollution simulations. The schemes are the integrator used in the Northeast Regional Oxidant Study and a version of the pseudospectral integrator; both schemes have been considered candidates for the Regional Acid Deposition Model. The two schemes are discussed in some detail, along with their principal advantages and drawbacks. An objective methodology is then developed to provide quantitative measures of the schemes' performances on accuracy, conservation, and efficiency. Representative results are given from two test simulations: the advection-diffusion of a single puff in a uniform wind field and the continuous plume in a uniform wind field. Although less efficient, the Northeast Regional Oxidant Study integrator demonstrated superior consistency in accuracy and conservation over the pseudospectral scheme.

The Project Summary was developed by EPA's Atmospheric Sciences Research Laboratory, Research Triangle Park, NC, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

An important focus of the National Acid Precipitation Assessment Program is the development of the Regional Acid Deposition Model (RADM). This model is expected to integrate state-of-the-art knowledge of the important chemical reactions leading to acid deposition precursors with state-of-the-art routines describing atmospheric processes The end product will be a Eulerian grid model capable of performing assessment calculations and alternative scenario simulations. The choice of a suitable numerical scheme for the transport simulations of RADM is a critical one, and a decision was made to compare two candidates for that role on the basis of an objective evaluation methodology. The schemes were the NEROS (Northeast Regional Oxidant Study) integrator and a version of the pseudospectral integrator. The NEROS scheme may be described as a Lagrangian, upwind differencing scheme employing bi-directional quintic polynomials. The pseudospectral integrator employs the traditional, finite Fourier series expansion coupled with a coordinate transformation to eliminate the need for periodic boundary conditions.

Evaluation Procedure

The evaluation methodology concentrated on three criteria; accuracy, conservation, and efficiency. Accuracy was judged by three numerical measures borrowed from the nomenclature of applied mathematics, L_1, L_2, and L_∞. The first two are measures of the global performance of a scheme, the third is important where the forecasting of peak values is crucial In selecting the test cases for comparison, an important requirement was the availability of the exact solution in order to effectively assess accuracy Two test cases were formulated. one involved the advection-diffusion of a "spline" puff and the other the constant point source in a uniform wind, particularly the early transient part prior to the development of the steady state plume

Within the framework of the two cases mentioned above, the schemes were tested in a variety of parametric changes, including wind speed, diffusivity, time step, and position of point source. Every effort was made in creating fair comparison circumstances. Various filtering algorithms for the pseudospectral integrator were also attempted.

Conclusions

The importance of an objective evaluation methodology is emphasized. This should include a variety of test cases such as "solid body" rotation, transport across boundaries, and point and areal sources. Puffs should be of general shape, and symmetric flow characteristics should be avoided It is important, however, that the exact solution be available in analytical closed-form terms or in simple and verifiable numerical form.

The NEROS integrator demonstrated a more consistent performance than the various versions of the pseudospectral integrator. This consistency was maintained throughout most parametric changes and particularly for simulations involving transport across boundaries. Although more than twice as expensive, the NEROS integrator demonstrated superior accuracy and conservation properties. The performance of the filtering algorithms for the pseudospectral integrator was erratic; only high diffusion appears to favor this integrator, but at the price of efficiency, since computational stability restrictions decrease the allowed time step.

RADM is expected to be dominated by the chemical reaction simulations in terms of computer time demands. It is essential to keep this in perspective in attempting to optimize the advection-diffusion integrator. The "best" integrator may in fact be the one which allows better optimization of the chemical reaction simulations while maintaining reasonable standards of accuracy and conservation for the transport terms

A. A. N. Patrinos and M. J. Leach are with Brookhaven National Laboratory, Upton, NY 11973.
***F. Binkowski** is the EPA Project Officer (see below).*
The complete report, entitled "Evaluation of Two Numerical Integrator Schemes," (Order No. PB 85-138 196; Cost: $8.50, subject to change) will be available only from:
National Technical Information Service
5285 Port Royal Road
Springfield, VA 22161
Telephone: 703-487-4650
The EPA Project Officer can be contacted at:
Atmospheric Sciences Research Laboratory
U.S. Environmental Protection Agency
Research Triangle Park, NC 27711

United States
Environmental Protection
Agency

Center for Environmental Research
Information
Cincinnati OH 45268

BULK RATE
POSTAGE & FEES PAID
EPA
PERMIT No G-35

Official Business
Penalty for Private Use $300