LA-SUB--96-69

FINAL REPORT

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MAY 05 1996

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FORWARD IN TIME METHODS FOR GLOBAL CLIMATE RESEARCH Contract #838K0013-35

Purpose

The purpose of this contract has been to demonstrate the feasibility and the utility of nonoscillatory forward-in-time (NFT) methods for modeling the global dynamics of the atmosphere and the oceans. This demonstration includes development of new algorithms, construction of numerical models, and testing these models. A particular aspect of this research is to compare two variants of NFT methods, one based on Eulerian approximations and the other based on semi-Lagrangian approximations.

Background

Three-time-level integration schemes have been widely used in numerical models of the global atmosphere and oceans for more than 30 years. However two-time level (FT) schemes have been preferred in nearly every other field of computational fluid dynamics over the same period. The advantages of two-time level schemes include computational efficiency -- allowing a larger computational timestep, requiring less memory, and not supporting a computational mode -- and greater accuracy due to smaller numerical dispersion. Perhaps the most important advantage of FT schemes is the further development of nonoscillatory options (NFT). All NFT schemes preserve the sign of transported fields and, therefore, guarantee the nonlinear stability of simulations.

A particular class of NFT schemes was originated by Smolarkiewicz more than ten years ago for use in small- and meso-scale simulations of the atmosphere. This approach is named MPDATA for multidimensional positive definite advection transport algorithm. As implied in its name, MPDATA is naturally multi-dimensional and does not require directional splitting. The MPDATA family has been developed over the last decade and now includes a large number of optional features making it a powerful tool for integrating arbitrary flows with, at least, a second-order accuracy.

MPDATA was originally designed for use in Eulerian schemes. More recently Smolarkiewicz and Rasch (1991), and Smolarkiewicz and Grell (1992) have documented that the interpolation aspect of semi-Lagrangian schemes can be accomplished with advection schemes, and that the resulting solutions inherit most of the desired properties of those schemes. The particular use of NFT algorithms as the interpolators with a consistent treatment of the forcing terms for the fluid equations was set forth by Smolarkiewicz and Pudykiewicz (1992). In

general, NFT semi-Lagrangian methods offer better local accuracy while Eulerian NFT methods can be made locally conservative.

Many atmospheric GCMs use spectral transform methods for approximation of spatial derivatives. This is a separate issue from that of temporal differencing. Spectral methods offer high accuracy for smooth flows and are computationally efficient at low resolution on shared memory computers. However they do admit nonphysical oscillations into the solutions; in addition, spectral methods are less efficient when implemented on massively parallel computers with distributed memory. It is an important issue to demonstrate that finite difference methods can be made equivalently efficient.

Technical Progress

Forward-in-time methods in general, and MPDATA in particular, have been successfully applied to mesoscale problems in the atmosphere. Our first task was to demonstrate that the same techniques can be applied to global scale dynamics, where rotation and advection assume a more fundamental role in the overall balance of terms.

We began by constructing explicit models of shallow water on the sphere, one based on Eulerian techniques and the other on semi-Lagrangian. We applied these models to the standardized set of shallow water test problems published by Williamson, et al. (1992) and showed that our NFT models achieved comparable accuracy to more traditional leapfrog methods. Significant aspects of the new algorithms include the extension to a curvilinear coordinate frame, accomplished by a formal mapping of the local coordinates to a logically regular mesh using the metric tensor, and the development of a predictor for the advective velocity based on a low-order integration of the equations of motion. The new advective velocity increases the allowable timestep based on a CFL condition by a factor of two. This work was documented and published in [SM93].

In order to improve the efficiency of our models, we further developed semi-implicit methods in which the fastest waves of the system -- the gravity waves -- are treated implicitly, thus allowing a much larger computational timestep. In order to preserve the linearity of the elliptic equations that result, we used a geometric linearization that preserves the second-order in time accuracy of the algorithm. These implicit systems require solution of a nonsymmetric matrix equation on the mesh, and the ultimate saving of CPU depends strongly on the efficiency of the elliptic solver. We constructed a solver based on conjugate residuals which has proved satisfactory. We believe there is still opportunity for significant speedup of our solver once it is customized for a particular model at hand, particularly by constructing preconditioning operators. This work has been documented and published in [SM94].

In the next phase of this contract, we have extended our techniques to three-dimensional models. We have made continuous improvements to our elliptic solver, and have implemented and tested a reduced grid capability to further improve the computational efficiency. We have ported several of our models to

the massively parallel CM-5. We have begun to implement water vapor processes, including a novel procedure for treating cloud boundaries. Finally, in collaboration with another CHAMMP project and an HPCCI project, we have generalized one of our shallow models to simulate the Green-Naghdi equations -- a dispersive shallow water theory.

Our first three-dimensional model is isentropic, essentially constructed by stacking layers of the explicit Eulerian model. Although this construction is straightforward, the further extension to semi-implicit differencing is more difficult. In particular, it requires a sign-preserving elliptic solver in order to assure nonnegative thickness of each individual layer. The latter is essential for the overall stability and accuracy of semi-implicit fluid models cast in a Lagrangian vertical coordinate.

We have also constructed a fully nonhydrostatic grid point model. This model is presently in cartesian coordinates. We have now implemented the model on a sphere and are testing its performance. The model consistently incorporates either Eulerian or semi-Lagrangian differencing, at the user's option. The nonhydrostatic formulation will be particularly useful when the grid size is small enough to resolve nonhydrostatic processes---for example: convective instabilities, and internal gravity wave dynamics in deep sheared atmospheres. However we have also found that the nonhydrostatic formulation has numerical advantages on coarser grid, such as the better conditioning of the matrix that must be inverted. In addition, use of the nonhydrostatic equations allows consistency as the mesh is refined, or when using nested grids.

We have used this model as a vehicle to compare the advantages of Eulerian and semi-Lagrangian methods. At present, it appears that each method has advantages for certain classes of problems, and that neither is uniformly superior. The nonhydrostatic model has additional options, including moving boundaries and treatment of moist precipitating processes. This work is documented in [SM 95], recently accepted for publication.

Both the Eulerian shallow water model, and the Eulerian isentropic models have been implemented on the CM-5. Performance, as compared to a shared memory CRAY YMP, depends sensitively on the problem size. In general, performance on 32 nodes of the CM-5 can be equivalent to less than 1.0 YMP processor for small problems, but increases to 1.5 YMP processors for large problems. We have also begun to port the Euclidean version of the non-hydrostatic model to the CRAY T3D.

As part of our efforts to improve the computational efficiency of our models cast on the sphere, we have implemented a reduced grid capability that reduces the number of cells between lines of latitude nearer the pole, thus reducing the Courant number and increasing the allowable timestep. This capability has been implemented in the CM-5 versions of the Eulerian shallow water and isentropic models. There is little if any degradation of accuracy in the use of this technique. This work is documented in [RMS95].

Another CHAMMP project, on "Assessing predictability in global ocean models," has been studying the possible importance of nonhydrostatic effects in long time global integrations. The point is that even though a term in the PDEs is small, its effect may be important if the integration times are long enough. More detailed results supporting this contention will be given in the progress report of this other project. Here we limit ourselves to describing the numerical issues in formulating a model for the Green-Naghdi(GN) equations. The GN equations differ from the usual shallow water equations by the presence of an additional dispersive term in the momentum equations. This term is a third-order mixed derivative of the thickness field. Although this term can be shown to be small based on scale analysis, it is the highest order derivative that appears, making the GN equations a singular perturbation system. We have shown that an explicit treatment of the dispersive term would require a prohibitively small timestep. Instead, we chose to modify one of our semi-implicit shallow water models. Because the dispersive term contains several total time derivatives, we chose the semi-Lagrangian model as our starting point. The dispersive term itself is isolated by an operator splitting, and approximated in a fully implicit manner. This work is documented in [NMS95].

Addendum

The original contract was designed to run for 3 years, and was the mechanism to fund a joint grant awarded by the Department of Energy Office of Energy Research for Margolin and Smolarkiewicz. At the end of the second year, a means to directly fund Smolarkiewicz was implemented, and so this contract was terminated.

References in text

P.K. Smolarkiewicz and P.J. Rasch, 1991: "Monotone advection on the sphere: An Eulerian versus semi-Lagrangian approach," J.Atmos.Sci., 48, 793--810.

P.K. Smolarkiewicz and G. A. Grell, 1992: "A class of monotone interpolation schemes," J. Comput. Phys., 101, 431--440.

P.K. Smolarkiewicz and J. A. Pudykiewicz, 1992: "A class of semi-Lagrangian approximations for fluids," J. Atmos. Sci.49, 2082--2096.

D.L. Williamson J. B. Drake, J. J. Hack, R. Jakob and P. N. Swarztrauber, 1992: "A standard test set for numerical approximations to the shallow water equations on the sphere," J. Comput. Phys. 102, 211--224.

Publications supported by this contract

[SM93] Smolarkiewicz, P.K., and L.G. Margolin, 1994: "On Forward-in-Time Differencing for Fluids: Extension to a Curvilinear Framework," MWR 121, 1847-1859.

[SM94] Smolarkiewicz, P.K., and L.G. Margolin, 1994: "Variational solver for elliptic problems in atmospheric flows," Appl. Math. and Comp. Sci. 4, 527--551.

[SM95] Smolarkiewicz, P.K., and L.G. Margolin, 1995: "On forward-in-time differencing for fluids: An Eulerian/semi-Lagrangian nonhydrostatic model for stratified flows," Atmos.-Ocean, (accepted for publication 10/95)

[RMS95] Reisner, J.M., L.G. Margolin, and P.K. Smolarkiewicz, "A Reduced Grid Model for Shallow Flows on the Sphere," Proceedings of the Parallel CFD95 Conference (reviewed and accepted for publication).

[NMS95b] Nadiga, B.T., L.G. Margolin, and P.K. Smolarkiewicz, 1995: "Dispersive shallow fluid flow over a mountain," Phys. of Fluids., submitted.

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