Applying Local Discretization Methods in the NASA Finite-Volume General Circulation Model

The general circulation model, developed at the NASA Goddard Space Flight Center for climate simulations and other meteorological applications, emphasizes conservative and monotonic transport and achieves sufficient accuracy for the global consistency of climate processes.

You can simulate the atmosphere's activities, *climate modeling*, by programming approximate solutions to the physical laws that govern it. An atmospheric model usually has two parts: a dynamical core that solves a set of partial differential equations for an idealized atmosphere and a set of physical parameterizations that provides realistic forcing (such as precipitation, surface friction, and solar radiation) to this atmosphere. These two parts are usually treated separately. Recently, designing computing algorithms for climate modeling, which requires massive computation for long-term simulations, has come to rely on efficiently implementing parallel computation with distributed memory. Although numerical methods based on local memory have parallel efficiency with distributed memory, fundamental issues arise when applying these local methods to global climate modeling. (See the related sidebar.)

To address these issues, we developed a general circulation model (GCM) at the NASA Goddard Space Flight Center using monotonic finite-volume transport schemes. The physical quantity choices are conservative following the motion in the idealized smooth atmosphere. To establish transport in one dimension, we adopted a set of finite-volume schemes, including Sergei Godunov's piecewise constant scheme,[1] Bram van Leer's piecewise linear scheme,[2] and Phil Colella and Paul Woodward's piecewise-parabolic method (PPM).[3] We based our model's dynamical core on Shian-Jiann Lin and Richard Rood's work in the 1990s[4–7] and based the physical parameterizations on those of the community climate model developed by the National Center for Atmospheric Research. In this article, we present the NASA finite-volume dynamical core's basic ideas, concentrating on how to use Lagrangian conservation to improve the approximate solutions' accuracy for the idealized atmosphere.

1521-9615/02/$17.00 © 2002 IEEE

Kao-San Yeh
University of Maryland
Shian-Jiann Lin and Richard B. Rood
NASA Goddard Space Flight Center

Transport algorithms

We can uniquely specify an idealized atmosphere's status with a set of state variables such as air mass density, air temperature, and wind velocity. Starting with data for the *grid boxes*—computational units of the atmosphere—a numerical method aims to predict the state vari-

Fundamental Issues

When adopting local methods for climate modeling, maintaining global consistency among the climate phenomena is a key concern. To achieve this without using global information to constrain the numerical solutions, a local method must closely follow physics' conservation laws. The finite-volume method approximates a conservation law's integral over the volume of each grid box, a computational unit of the atmosphere. We can use this method for successful climate modeling because it maintains physical consistency in numerical solutions through *local conservation*. Furthermore, to improve the solutions' accuracy, we can use Lagrangian conservation, a special case of local conservation that conserves physical quantities contained in a fluid element following the motion. A fluid element's physical quantity is conservative following the motion only when no sources or sinks occur during the transport process.

Simulating atmospheric motions with computers often generates spurious noise in the solutions. This noise contaminates the simulation with unrealistic features, so climate modelers have developed various techniques to mitigate the problem. However, we can avoid the noise by maintaining the physical quantity distributions' monotonicity during the transport process. In other words, the numerical approximation creates no new local maxima or minima. Unfortunately, monotonic transport schemes are often quite diffusive and can be less accurate than nonmonotonic ones. However, for scalar transport where sources and sinks aren't present, the continuous governing equations dictate that solutions be monotonic, so it can be desirable for the discrete model to maintain this property.

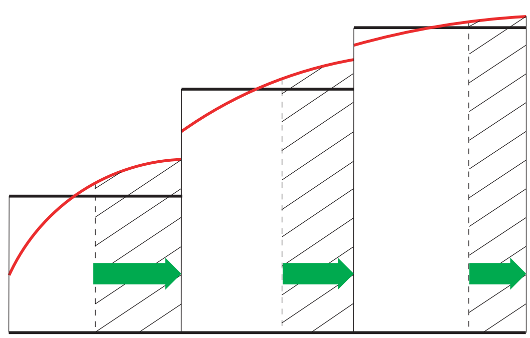


Figure 1. The piecewise-parabolic method transport mechanism in one dimension. We first construct detailed subgrid distributions (red curves) from the given overgrid distribution of mean values (black line segments) for the grid intervals A, B, and C. We then calculate the fluxes crossing the grid interfaces during transport, with the subgrid distributions' volume integrals (shaded areas) over the upstream ranges implied by the given velocity field (green arrows).

able values for the grid boxes in a short period of time, say, five to 60 minutes. Then, we make a simulation with a sequence of such small time steps.

To illustrate, consider the PPM transport mechanism of the air in one dimension (see Figure 1). Suppose we have the mean density of air mass over the grid intervals at an initial time, and we wish to determine the mean density of air mass over the grid intervals after a short transport time. We first notice that a grid interval's air mass is simply its mean density times its length. We can readily determine the mean density after transport if we know the grid interval's inflow and outflow during transport. We also notice that a grid interval's outflow across a grid interface equals the adjacent grid interval's inflow across the same interface. This is the *air mass flux*. The issue is then determining the air mass fluxes across the grid interfaces during transport; the approximate solution's accuracy to the mean density after transport depends on how the algorithm calculates the air mass fluxes.

The PPM transport algorithm first constructs a detailed structure of air mass density in each grid interval using the given mean values. In this article, we'll call these structures *subgrid distributions* and the collection of mean values *overgrid distribution*. The subgrid distribution in a grid interval is constructed so the area under the curve equals the rectangular area under the line segment; the integral of a subgrid distribution over the corresponding grid interval equals the air mass contained in this grid interval. Additionally, each subgrid distribution is monotonic in the corresponding grid interval and adjacent subgrid distributions are monotonic across the grid interfaces. The subgrid distributions' monotonicity results from the monotonicity of the given overgrid distribution.

If we know the airflow velocity everywhere, we know exactly which air particle crosses a grid interface during transport. Suppose the airflow moves from grid interval A to grid interval B in Figure 1—we then know how far upstream in grid interval A an air particle would reach the interface I_1 between A and B. The air contained in this upstream range is exactly the flux across interface I_1 during transport. So, the flux F_1 across interface I_1 equals the subgrid distribution's *volume integral* over the upstream range in grid interval A. This integral corresponds to the shaded area under the curve.

Similarly, we can determine the flux F_2 across the interface I_2 between grid intervals B and C in Figure 1. If the airflow moves from B to C, the flux F_2 is an outflow leaving B during the transport. Given the air mass M contained in grid interval B before transport, we see that ($M - F_2$) is the amount of air remaining in B after transport—that is, the volume integral of the subgrid distribution over B's remaining section. It corresponds to the blank area under the curve in grid interval B. With F_1 being the inflow and F_2 the outflow during transport, the air mass in grid interval B after transport is simply $M' = M + F_1 - F_2$, and we divide the resulted air mass M' by the grid interval's length to obtain the mean density over B after transport.

If the overgrid distribution of the mean values before transport is monotonic, overgrid distribution of the mean values after transport is monotonic; the monotonic construction of subgrid distributions maintains monotonicity. Furthermore, to obtain each mean value after transport, we combine the neighboring volume integrals of the subgrid distributions that conserve the material within the corresponding grid intervals, conserving the transported material locally. Because these constructed subgrid distributions are not the actual ones for the smooth fluid to be simulated, errors occurred during the numerical transport. These errors would be greater if the transported material were not conservative following the motion in the smooth fluid system. The actual distribution would have changed during transport, but the approximate subgrid distributions were constructed with the overgrid distribution given at the initial time.

In multidimensional transport, using the 1D schemes to estimate the fluxes in each dimension separately could amplify the 1D transport errors. Lin and Rood designed a multidimensional transport algorithm to exploit dimensional splitting's efficiency while reducing the associated errors by considering the contributions from other dimensions during the transport.[4] This multidimensional algorithm also maintains the relationship between air mass and other transported physical quantities, and thereby promotes the computational fluid system's physical consistency. To further improve both accuracy and efficiency in multidimensional transport, Lin and Rood adopted the Lagrangian coordinates in the vertical direction—namely, the altitudes of horizontal material surfaces which evolve during the transport.[7]

Dynamics system

Not all physical quantities in the atmosphere's continuous dynamics system are conservative following the motion. For instance, the momentum (mass times velocity) in an air parcel is not conservative following the motion because of external forcing, such as the pressure gradient force due to pressure differences surrounding the parcel. If we conserved momentum in the discrete numerical system through explicit transport with the wind velocity, interaction with the pressure gradient force would amplify the errors in inertial transport. We wouldn't localize the conservation of momentum in the discrete system as well as in the inertial case.

Three physical quantities in the atmosphere's continuous dynamics system are conservative following the motion: air mass, *potential temperature*, and *absolute vorticity*. Potential temperature is a measure of molecular motions respecting a reference thermodynamic state of the atmosphere. Absolute vorticity is a measure of a fluid element's rotation relative to an inertial frame such as the space containing Earth. We chose to conserve these three quantities in the NASA finite-volume dynamical core to promote transport accuracy and conservation localization.

Because they are directly related to primary variables, we can achieve local conservation and monotonicity of air mass and of potential temperature through finite-volume transport. Absolute vorticity is, however, a quantity derived from velocity. To achieve the local conservation and monotonicity of absolute vorticity with velocity being a primary variable, we must apply the *circulation theorem*. This theorem says that

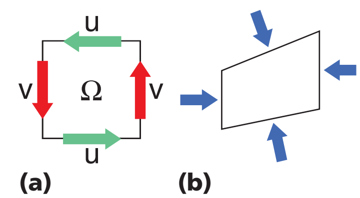


Figure 2. Theorem applications: (a) D-grid configuration for applying the circulation theorem in two dimensions. The absolute vorticity (Ω) is a mean value over the grid box, and the wind components (*u*, *v*) are predicted along the boundary. (b) Schematic for applying Green's theorem with vertical Lagrangian coordinates. We obtain the external force acting on a fluid element by integrating the surrounding pressure (blue arrows).

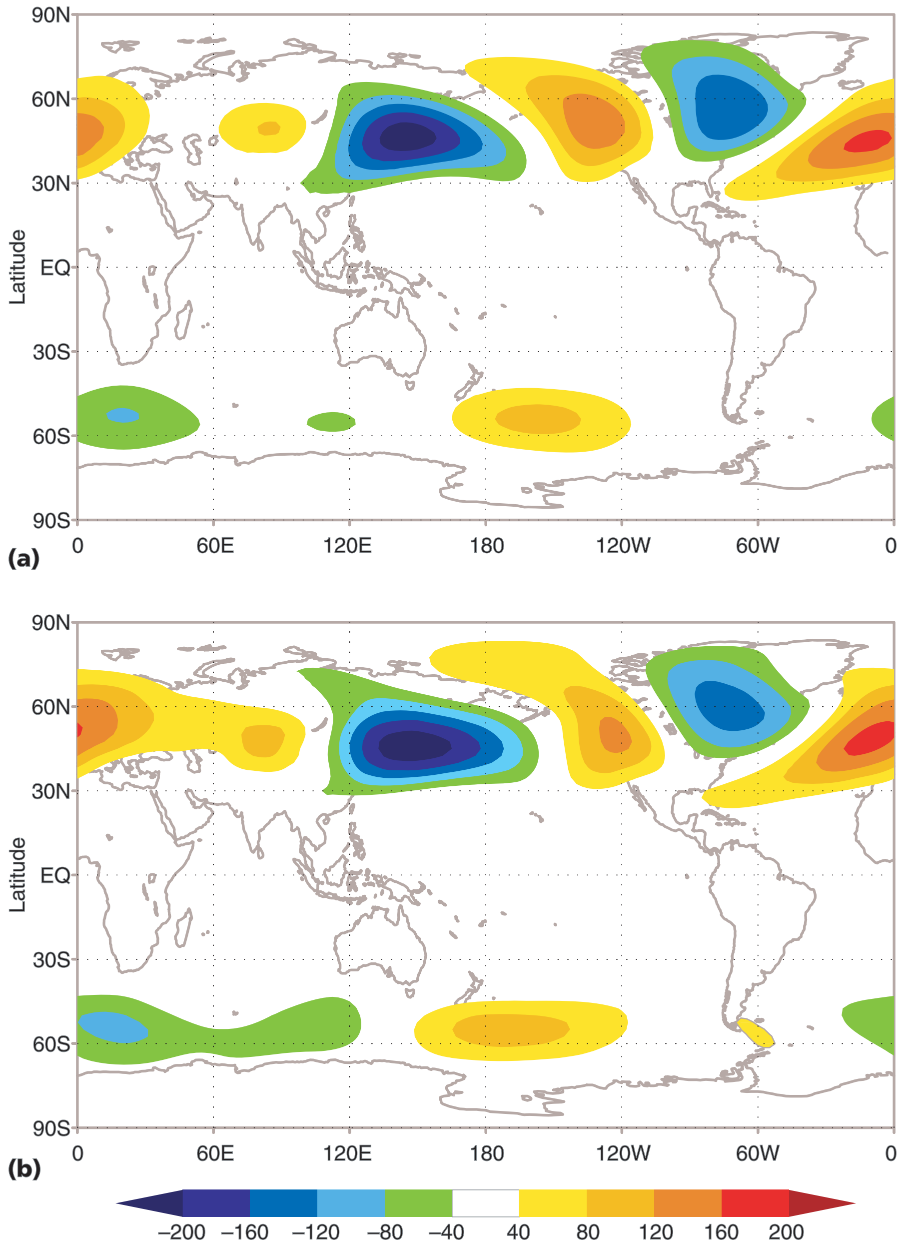


Figure 3. Climatology of the Atmospheric Model Intercomparison Project II (a) simulated with the NASA finite-volume general circulation model and (b) the corresponding analysis from the European Center for Medium-Range Weather Forecast, demonstrated with an average of 500-hPa eddy height (*m*) over December, January, and February. The simulation is produced with a 15-year run at the resolution of 2.5 x 2.0 degrees with 55 layers in vertical direction.

the integral of vorticity over an area equals the integral of velocity along the boundary enclosing the area. By using the so-called D-grid configuration Figure 2a shows, we can predict velocity directly along the area's boundary while conserving absolute vorticity. Lin and Rood[5] demonstrated such an approach's advantages in two dimensions with an excellent simulation of the Rossby-Haurwitz waves, which the modeling community has recognized as a standard test for modeling atmospheric dynamics.[8]

To extend the 2D dynamics to three dimensions, we adopted the Lagrangian coordinates[7] in the vertical direction. The vertical coordinates are the altitudes of horizontal material surfaces, and we can assume from hydrostatic equilibrium that the difference of the pressure at the material surfaces balances the weight of the air confined between two material surfaces. The 3D atmosphere is thus decoupled into inertial horizontal layers. We can treat the dynamics in each layer as we would the 2D dynamics, except when calculating pressure gradient force. We calculate the pressure gradient force in a Lagrangian layer[6] with Green's theorem, which says that the integral of pressure difference over the volume contained in a grid box equals the integral of pressure over the surface surrounding the grid box (see Figure 2b). So, we obtain the net external force acting on a fluid element by integrating the surrounding pressure.

The NASA finite-volume dynamical core is ultimately a collection of finite volumes, where dynamical processes are calculated as integrals of simple, locally continuous functions. The dynamical core reduces many of the finite-difference and spectral methods' inherent errors, and a high degree of consistency of primary variables and dynamical quantities exists. Figure 3 demonstrates the climatology of the NASA finite-volume GCM with the 500-hPa eddy height—that is, the height at 500-hPa pressure level relative to its own zonal mean—for December, January, and February. We produced the simulation with a 15-year run at the resolution of 2.5 degrees in longitude and 2.0 degrees in latitude. The atmosphere's vertical dimension is covered with 55 Lagrangian layers up to the pressure level of one Pascal. The time step is 7.5 minutes for the dynamical core and 30 minutes for the physical parameterizations. We adopted the PPM to found transport in one dimension. The 500-hPa eddy height represents the wave patterns and magnitudes in middle troposphere, and the simulated climatology is quite realistic according to the analysis from the European Center for Medium-Range Weather Forecast. You can find additional results from this model at http://dao.gsfc.nasa.gov/NASanCAR.

Our experience with the NASA finite-volume GCM indicates that the adopted monotonic transport schemes' diffusion effects are often too strong for simulating small-scale atmospheric phenomena. We developed new monotonic finite-volume transport schemes to address this issue and have incorporated some of them in the model as options; some are not yet published or implemented.

Although you can use Lagrangian conservation to enhance the numerical solutions' physical consistency, transport accuracy depends largely on how the dynamics system predicts velocity. Although Lin and Rood provide an accurate way to predict velocity while exploiting the Lagrangian conservation of absolute vorticity,[5,6] their methodology's efficiency is restricted by the time step size of fast-moving gravity waves. Further research might enlarge the time step and improve the overall efficiency.

Furthermore, due to the adoption of the traditional longitude-latitude grid system, global memory is still needed in polar areas where the meridians converge. This affects the efficiency of implementing parallel computation with distributed memory. We are developing a new design of the dynamical core with quasiuniform grids to avoid using global memory and thereby promote parallel efficiency for distributed memory. We must still prove that this approach would gain enough in efficiency while achieving sufficient accuracy for practical applications.

For more information about the NASA finite-volume GCM, see the documentation on the next-generation model at http://dao.gsfc.nasa.gov/pages/atbd.html.

Acknowledgments

We appreciate the comments and suggestions of the editors and several anonymous reviewers. They were very helpful in improving the manuscript.

References

1. S.K. Godunov, "A Difference Scheme for Numerical Computation of Discontinuous Solutions of Equations in Fluid Dynamics," *Maematicheskii Sbornik,* vol. 47, 1959, p. 271.
2. B. van Leer, "Toward the Ultimate Conservative Difference Scheme, Part IV: A New Approach to Numerical Convection," *J. Computational Physics*, vol. 23, no. 3, Mar. 1977, pp. 276–299.
3. P. Colella and P.R. Woodward, "The Piecewise Parabolic Method (PPM) for Gas-Dynamical Simulations," *J. Computational Physics*, vol. 54, no. 1, Apr. 1984, pp. 174–201.
4. S.J. Lin and R.B. Rood, "Multidimensional Flux-Form Semi-Lagrangian Transport Schemes," *Monthly Weather Rev.,* vol. 124, no. 9, Sept. 1996, pp. 2046–2070.
5. S.J Lin and R.B. Rood, "An Explicit Flux-Form Semi-Lagrangian Shallow-Water Model on the Sphere," *Quarterly J. Royal Meteorological Soc.,* vol. 123, no. 544, Oct. 1997, pp. 2477–2498.
6. S.J. Lin, "A Finite-Volume Integration Method for Computing Pressure Gradient Force in General Vertical Coordinates," *Quarterly J. Royal Meteorological Soc.,* vol. 123, no. 542, July 1997, pp. 1749–1762.
7. S.J. Lin and R.B. Rood, "Development of the Joint NASA/NCAR General Circulation Model," *Proc. 13th Conf. Numerical Weather Prediction*, Am. Meteorological Soc., Boston, 1999, pp. 115–119.
8. D.L. Williamson et al., "A Standard Test Set for Numerical Approximations to the Shallow Water Equations in Spherical Geometry," *J. Computational Physics,* vol. 102, no. 1, Sept. 1992, pp. 211–224.

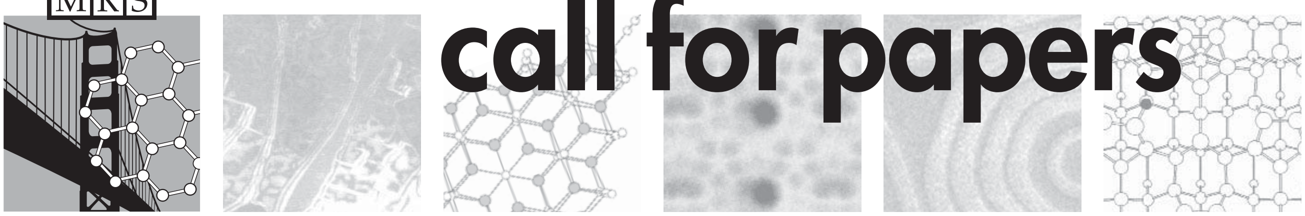
Kao-San Yeh is an assistant research scientist at the Goddard Earth Sciences and Technology Center at the University of Maryland and the Data Assimilation Office at NASA Goddard Space Flight Center. His research interests include numerical methods for geophysical fluid-dynamics modeling, especially the finite-volume method for conservative and monotonic transport in atmospheric models. He has a BS in physics from National Taiwan University, an MS in mathematics, and a PhD in meteorology from Purdue University Contact him at the Data Assimilation Office, Code 910.3, NASA Goddard Space Flight Ctr., Greenbelt, MD 20771; kyeh@dao.gsfc.nasa.gov.

Shian-Jiann Lin is the model development group head and a meteorologist with the Data Assimilation Office at the NASA Goddard Space Flight Center. His research interests include numerical algorithms for geophysical fluid dynamics and cloud microphysics. He has a BS in agricultural mechanical engineering from National Taiwan University, an MS in aerospace and mechanical engineering from the University of Oklahoma, and an MA in geophysical fluid dynamics and a PhD in atmospheric sciences from Princeton University. Contact him at the Data Assimilation Office, code 910.3, NASA Goddard Space Flight Ctr., Greenbelt, MD 20771; lin@dao.gsfc.nasa.gov.

Richard B. Rood is the acting chief of the Earth and Space Data Computing Division at the NASA Goddard Space Flight Center and the acting director of the National Oceanic and Atmospheric Administration-NASA Joint Center for Satellite Data Assimilation. His research interests include the transport of trace constituents in the atmosphere and climate modeling. He has a BS in physics from the University of North Carolina and a PhD in meteorology from Florida State University. He is a member of the American Geophysical Union and the American Meteorology Society. Contact him at the Earth and Space Data Computing Division, Code 930, NASA Goddard Space Flight Ctr., Greenbelt, MD 20771; rrood@dao.gsfc.nasa.gov.

For more information on this or any other computing topic, please visit our digital library at http://computer.org/publications/dlib.

2003 MRS **Materials Research Society Spring Meeting Announcement &**



ABSTRACT DEADLINES

OCTOBER 18
for abstracts sent via fax or mail

NOVEMBER 1
for abstracts sent via the MRS Web site

LATE ABSTRACTS WILL NOT BE ACCEPTED.

CONTACT INFORMATION

MRS
Materials Research Society
506 Keystone Drive
Warrendale, PA 15086-7573 USA
Tel: 724-779-3003
Fax: 724-779-8313 (general)
724-779-3030 (abstract submittal)
E-mail: info@mrs.org

2003 MRS SPRING MEETING • APRIL 21-25, SAN FRANCISCO, CA

The 2003 Materials Research Society Spring Meeting will be held April 21–25, 2003, in San Francisco, California, at the San Francisco Marriott and Argent Hotels. The meeting will include 25 symposia that highlight new advances in the understanding, synthesis, and application of materials in diverse fields.

SCHEDULED SYMPOSIA

ELECTRONIC AND OPTICAL MATERIALS
A: Amorphous and Nanocrystalline Silicon-Based Films—2003
B: Compound Semiconductor Photovoltaics
C: New Applications for Wide-Bandgap Semiconductors
D: CMOS Front-End Materials and Process Technology
E: Materials, Technology, and Reliability for Advanced Interconnects and Low-*k* Dielectrics
F: Chemical-Mechanical Planarization
G: Integration of Heterogeneous Thin-Film Materials and Devices
H: Flexible Electronics—Materials and Device Technology
I: Optoelectronics of Group-IV-Based Materials
J: Microphotonics, Nanophotonics, and Photonic Crystals

MOLECULAR MATERIALS AND BIOMATERIALS
K: Molecular-Scale Electronics and Optoelectronics
L: Organic and Polymeric Materials and Devices
M: Nanotube-Based Devices
N: Biomicroelectromechanical Systems (BioMEMS)
O: Materials Inspired by Biology

NANOSTRUCTURED MATERIALS
P: Self-Assembled Nanostructured Materials
Q: Unconventional Approaches to Nanostructures with Applications in Electronics, Photonics, Information Storage, and Sensing
R: Nanomagnetism
S: Nanoscale Thermal Transport—From Fundamentals to Devices
T: Nanostructuring Materials with Energetic Beams
U: Mechanical Properties Derived from Nanostructuring Materials

GENERAL
V: Semiconductor Spintronics II
W: Multiscale Phenomena in Materials—Experiments and Modeling Related to Mechanical Behavior
X: Frontiers of Materials Research
Y: Advanced Optical Processing of Materials
Z: Mechanisms in Electrochemical Deposition and Corrosion

For symposium descriptions, abstract submission instructions, and updated meeting information, visit the MRS Web site:

www.mrs.org/meetings/spring2003/