Face Page (ORNL)

1. TITLE OF PROPOSED RESEARCH:

   New Methods for Global Atmospheric Dynamics on Parallel Computers

2. ER PROGRAM ANNOUNCEMENT TITLE:

   DOE LAB 98-05 Climate Change Prediction Program

3. NAME AND ADDRESS OF LABORATORY:

   Oak Ridge National Laboratory
   P.O. Box 2008, MS 6367
   Oak Ridge, Tennessee 37831-6367

4. PRINCIPAL INVESTIGATOR TITLE, ADDRESS AND PHONE NUMBER

   John B. Drake

Title	:	Research Staff, Computer Science and Mathematics Division
Address	:	Oak Ridge National Laboratory
		P.O. Box 2008, Bldg. 6012
		Oak Ridge, Tennessee 37831-6367
Phone	:	423-574-8670
Fax	:	423-574-0680
E-mail	:	drakejb@ornl.gov

5. CERTIFYING REPRESENTATIVE'S NAME, TITLE, AND PHONE NUMBER

   Michael A. Kuliasha

Title	:	Acting Division Director, Computer Science and Mathematics Division
		Division Director, Computational Physics and Engineering Division
Phone	:	423-574-5304
Fax	:	423-574-9646
E-mail	:	kuliashama@ornl.gov

6. REQUESTED FUNDING FOR EACH YEAR AND TOTAL REQUEST

FY1998	FY1999	FY2000	FY2001	Total
\$133,524	\$266,542	\$285,038	\$298,263	\$983,367

7. USE OF HUMAN SUBJECTS IN PROPOSED PROJECT: **No**

8. USE OF VERTEBRATE ANIMALS IN PROPOSED PROJECT: **No**

9. The following signatures certify that personnel and facilities are available as stated in the proposal, if the proposal is funded.

Signature of Principal Investigator

Signature of Certifying Representative

Date

Date

Contents

1 Narrative **1**
- 1.1 Background and Significance . . . 1
- 1.2 Preliminary Studies . . . 2
  - 1.2.1 Semi-Lagrangian Models . . . 2
  - 1.2.2 Grid-Point Models . . . 3
  - 1.2.3 Spectral Models . . . 3
  - 1.2.4 Comparisons of Accuracy . . . 4
  - 1.2.5 Cartesian Method . . . 5
- 1.3 Research Design and Methods . . . 6
  - 1.3.1 3-D Baroclinic Equations . . . 8
  - 1.3.2 Isentropic-Sigma Vertical Coordinates . . . 9
  - 1.3.3 Parallel algorithms . . . 11
  - 1.3.4 Impact and long term research . . . 11
- 1.4 Subcontractor Consortium Arrangements . . . 12

2 Literature Cited **13**

3 Budget Explanation **16**
- 3.1 Senior Personnel . . . 16
- 3.2 Secretarial/Clerical . . . 16
- 3.3 Fringe Benefits . . . 16
- 3.4 Travel . . . 16
- 3.5 Publication Costs . . . 16
- 3.6 Other - Organization Burden Administration . . . 16
- 3.7 Indirect Costs . . . 17

4 Other Support of Investigators **17**

5 Biographical Sketches **17**
- 5.1 John B. Drake . . . 17
- 5.2 Patrick H. Worley . . . 19
- 5.3 Eduardo F. D'Azevedo . . . 21

6 Description of Facilities and Resources **22**

Abstract

The simulation of climate on decadal to century time scales remains one of the most computationally demanding tasks in science. To satisfy the demands for improvements in these simulations new mathematical and computational methods are proposed. This proposal addresses area (3) of the proposal solicitation DOE LAB 98-05:

> The development of improved mathematical techniques, model formulations and computer algorithms for atmosphere, ocean and coupled atmosphere-ocean general circulation models (GCM) that more accurately and efficiently describe and predict global climate system behavior on the time and space scales mentioned above using advanced, parallel-processing scientific supercomputers.

The proposed research has three goals:

1. To develop new formulations and numerical methods that improve existing climate modeling techniques. In particular, to develop a 3-D baroclinic formulation for the spectral/semi-Lagrangian, grid-point/semi-Lagrangian and icosahedral Cartesian methods in the horizontal together with a hybrid isentropic sigma vertical coordinate system.

2. To develop parallel algorithms with scalable performance on advanced computer architectures and to build dynamical cores of atmospheric climate models using the new methods.

3. To install and test hybrid isentropic-sigma vertical coordinates in a semi-Lagrangian equivalent of the NCAR Community Climate Model.

1 Narrative

1.1 Background and Significance

The demands for reliable prediction of global and regional climate change have forced the research community to improve climate modeling techniques and to take advantage of advances in computer hardware. The search for new methods that improve the dynamics of climate models while at the same time performing well in a parallel computing environment is an important part of the advance in climate simulation. The advent of supercomputers and the incredible advances in microelectronics have been responsible for many of the improvements. But work on algorithms fitted to the new computing environments is also required.

In the context of new computing environments it has been found that some methods are able to more effectively exploit massive parallelism or vector constructs and that, by carefully choosing the method, an increase in model throughput can be achieved. This, in turn, increases the productivity of climate scientists studying scenarios that may have significant climatic and social impacts.

This proposal seeks to continue our earlier work by extension of three methods to dynamical cores of atmospheric models and to complete atmospheric climate models.

In previous work sponsored by the DOE/CHAMMP program, numerical algorithms and model formulations were developed in the context of the shallow water equations in a spherical geometry. The shallow water equations are a simple setting appropriate to test methods with potential for atmospheric and ocean climate models without the complexity and ambiguities of a full model. This approach proved very successful for the development of parallel algorithms [19] and in fact parallel algorithms developed for a spectral shallow water model were implemented in the parallel atmospheric climate code PCCM2 [6, 4, 3].

Our previous work explored a systematic approach to the development of future climate models. The approach is essentially collaborative in that the strengths and weaknesses of methods are displayed in the simplest possible setting for other researchers. The mathematical setting encourages numerical analysts, mathematicians, computer scientists, meteorologists and climate dynamicists to collaborate on joint definition of problems and solutions. Indeed, our previous contributions would not have been possible without significant interactions with atmospheric model developers at the National Center for Atmospheric Research (NCAR) and with computer scientists at Argonne National Laboratory. This proposal further elaborates the approach to the development of new methods for climate modeling.

Looking beyond the NCAR Community Climate Models CCM2 and CCM3 towards future atmospheric general circulation models, the spectral/semi-Lagrangian method was investigated for parallel performance and numerical properties by ORNL researchers [5]. The application in a full climate simulation was considered by collaborators at NCAR [35, 34, 32]. A formulation of the semi-Lagrangian method that replaced the spectral method in favor of a grid point approximation was developed. These methods were applied to the standard test cases developed for the shallow water equations. Both the spectral/semi-Lagrangian methods with a linear grid and the grid-point/semi-Lagrangian method are strong contenders for the dynamics algorithms of next generation climate models. In addition, a novel method based on a 3-D embedding of the horizontal dynamics equations was discovered and tested. Dubbed the "Cartesian method" for its use of 3-dimensional Cartesian velocities, the new method performed surprisingly well in accuracy, conservation and efficiency tests. Instead of the traditional lon-lat grid, this method uses an icosahedral grid.

The research issues concerning these three methods in the context of shallow water models are largely settled. Each has its strengths and weaknesses. For example, the semi-Lagrangian methods allow longer time steps but this must be balanced against the error and computational cost introduced by interpolation. Semi-implicit spectral formulations have higher accuracy but, unfortunately, higher operation counts than grid point methods. For the evolution of these methods to be complete, the trade-offs between numerical properties and computational efficiency need to be considered in the more realistic setting of a 3-D model based on the baroclinic primitive equations.

Our proposal is to formulate, construct and test dynamical cores based on three methods for horizontal dynamics and a new hybrid isentropic-sigma vertical coordinate. In particular, advantages of the semi-Lagrangian method for accurate horizontal advection will be investigated when the coordinate surface is a Lagrangian surface. The new research will be facilitated by the development of baroclinic (dry) atmospheric test cases for dynamical cores as being proposed by Held and Suarez [13], and others [1]. Our research will be complementary to the development of community climate models at NCAR. As part of our proposal we will modify a semi-Lagrangian version of the CCM by the introduction of hybrid isentropic-sigma coordinate.

1.2 Preliminary Studies

As part of a CHAMMP research project on numerical methods for climate modeling a set of test cases for shallow water equation models was defined [33] and several models implemented [20, 36, 8, 37]. Three methods proved particularly promising. We will briefly describe each of these methods that form the basis for our research proposal.

1.2.1 Semi-Lagrangian Models

The semi-Lagrangian transport (SLT) method is now an important part of many climate and weather models [24]. A three time level semi-Lagrangian method for the shallow water equations was described in Ritchie [21]. An extension of this using spatial averages in semi-implicit, semi-Lagrangian schemes was discussed in [26]. For meteorological models the form of their method was based on a division of terms in the equations between those involved in the fast moving waves, e.g. gravity waves, and the slower moving Rossby waves.

Let G denote the fast moving wave terms and R the slower wave terms. Then an advected scalar field F is represented by the equation

$$\frac{dF}{dt} + G = R. \tag{1}$$

Let subscripts $()_A$, $()_M$ and $()_D$ represent quantities evaluated at the arrival point, midpoint and departure point, respectively. Let superscripts $\tau - 1$, τ and $\tau + 1$ represent the time levels at which quantities are evaluated. Integrating the equation (1) along the trajectory between the departure point and the arrival point

$$\int_{t^{\tau-1}}^{t^{\tau+1}} \frac{dF}{dt} + \int_{t^{\tau-1}}^{t^{\tau+1}} G = \int_{t^{\tau-1}}^{t^{\tau+1}} R. \tag{2}$$

The first term reduces exactly by the fundamental theorem of calculus,

$$\int_{t^{\tau-1}}^{t^{\tau+1}} \frac{dF}{dt} = F_A^{\tau+1} - F_D^{\tau-1}, \tag{3}$$

while the G and R terms must be approximated using a quadrature rule. Interesting quadrature rules are the midpoint, trapezoidal and Simpson's rule. For example, the trapezoidal rule for G and a midpoint rule for R gives the following semi-implicit formulation.

$$\frac{F_A^{\tau+1} - F_D^{\tau-1}}{2\Delta t} + \frac{G_A^{\tau+1} + G_D^{\tau-1}}{2} = R_M^{\tau}. \tag{4}$$

These three time level "centered" approximations result in an $O(\Delta t)$ approximation to (1); the approximation to F is $O(\Delta t^2)$. This approximation is the basis for most three level semi-implicit SLT methods. Ritchie's [21] three level spectral shallow water model was based on this approximation.

Another approximation can be obtained by replacing the R_M^{τ} term with a spatial average at time level τ. This approximation has been shown to be advantageous in numerical weather prediction models [26] to reduce distortion produced by topographically forced waves. The spatial average introduces a further approximation error $O(\Delta P^2)$ where ΔP is the length of the trajectory and not the spatial resolution. But since the trajectory length is proportional to the time step Δt this is thought to be an acceptable error.

The assignment of terms of the shallow water equations to G and R results in different numerical algorithms. If we take $G \equiv 0$, then the algorithm is *explicit* in time. The explicit method requires small timesteps to stably follow the gravity wave components of the solution. A *semi-implicit* method results by assigning selected terms to G, terms that give rise to the gravity waves. In the momentum equation (24) the gravity wave component is identified with the $\nabla\phi$ term and the Coriolis term is identified with the R. We take

$$R = \begin{pmatrix} fv - \frac{1}{a\cos\theta}\frac{\partial \phi_s}{\partial \lambda} + S_u \\ -fu - \frac{1}{a}\frac{\partial \phi_s}{\partial \theta} + S_v \\ -(\phi' + \phi_s)\nabla\cdot\mathbf{v} + S_\phi \end{pmatrix}, \tag{5}$$

$$G = \begin{pmatrix} \frac{1}{a\cos\theta}\frac{\partial\phi'}{\partial\lambda} \\ \frac{1}{a}\frac{\partial\phi'}{\partial\theta} \\ \bar{\phi}\nabla\cdot\mathbf{v} \end{pmatrix} \tag{6}$$

where $\phi = \bar{\phi} + \phi_s + \phi'$ and $\bar{\phi}$ is a constant reference value.

Another algorithm is obtained by moving the Coriolis term into the implicit G.

$$R = \begin{pmatrix} -\frac{1}{a\cos\theta}\frac{\partial\phi_s}{\partial\lambda} + S_u \\ -\frac{1}{a}\frac{\partial\phi_s}{\partial\theta} + S_v \\ -(\phi' + \phi_s)\nabla\cdot\mathbf{v} + S_\phi \end{pmatrix}, \tag{7}$$

$$G = \begin{pmatrix} \frac{1}{a\cos\theta}\frac{\partial\phi'}{\partial\lambda} - fv \\ \frac{1}{a}\frac{\partial\phi'}{\partial\theta} + fu \\ \bar{\phi}\nabla\cdot\mathbf{v} \end{pmatrix}. \tag{8}$$

This can be called the *implicit* algorithm, reserving the terminology *fully implicit* for the case when $R \equiv 0$.

1.2.2 Grid-Point Models

The algorithmic options available for approximation of the time derivatives may be combined with options for approximating spatial derivatives in the R and G terms. We are interested in higher order approximations for at least some of the terms. The geopotential gradient term, which balances the Coriolis term, should be higher order to give an accurate geostrophic wind. But other terms may not require such accuracy. A grid point model based on variable order spline approximation, similar to [17], has been developed to study this and other issues.

Key to the differences between implicit and semi-implicit algorithms are the methods used to solve the implicit part of the equations. In the context of the semi-implicit system, a Helmholtz equation results. A more complicated elliptic system results from the implicit algorithm and solution strategies for this based on a quasi-mimimum resdiual (QMR) iterative technique have been considered as well [7].

1.2.3 Spectral Models

The combination of the semi-Lagrangian method with the spectral transform method is a powerful technique, providing easy solution of the semi-implicit equations, high spatial accuracy, and effectively double the resolution of a pure spectral transform method with the same cost. Williamson [32] has observed that the semi-Lagrangian treatment of the advection of momentum eliminates the nonlinear aliasing of terms in the spectral representation. This allows use of more terms of the spectral expansion but using the same physical grid, effectively doubling the horizontal resolution at little extra cost. The CFL condition that results from a non-Lagrangian treatment of momentum advection is also removed, allowing longer timesteps with a semi-Lagrangian treatment.

In the derivation of the semi-implicit, semi-Lagrangian method where a spectral approximation is used for spatial derivatives, the notation will be simplified by omitting the source term as well as the surface geopotential. In vector form the semi-implicit formulation is,

$$\mathbf{v}_A^{\tau+1} + \Delta t \nabla \phi'^{\tau+1}_A = \mathbf{v}_D^{\tau-1} - \Delta t[(f\vec{k} \times \mathbf{v})_A^\tau + (f\vec{k} \times \mathbf{v})_D^\tau + \nabla \phi'^{\tau-1}_D] \equiv N_{\mathbf{v}}, \tag{9}$$

and

$$\phi'^{\tau+1}_A + \Delta t \bar{\phi} \nabla\cdot\mathbf{v}_A^{\tau+1} = \phi'^{\tau-1}_D - \Delta t[(\phi'\nabla\cdot\mathbf{v})_A^\tau + (\phi'\nabla\cdot\mathbf{v})_D^\tau + \bar{\phi}\nabla\cdot\mathbf{v}_D^{\tau-1}] \equiv N_\phi, \tag{10}$$

To avoid pole problems with the vector representation of the velocity and to maintain compatibility with the scalar spectral transform method, we introduce the vorticity $\zeta \equiv k \cdot \nabla\times\mathbf{v}$ and the divergence $\delta \equiv \nabla\cdot\mathbf{v}$. The coordinate system used is the $\lambda - \mu$ spherical coordinates where $\mu = \sin\theta$ and θ is the co-latitude. We define $U = u\cos\theta$ and $V = v\cos\theta$. Let $N_U = \vec{i} \cdot N_{\mathbf{v}} \cos\theta$ and $N_V = \vec{j} \cdot N_{\mathbf{v}} \cos\theta$.

Taking the curl $(k \cdot \nabla \times \mathbf{v})$ and divergence $(\nabla \cdot)$ of the discrete momentum equation (9) gives the following equations ,

$$\zeta_A^{\tau+1} = \frac{1}{a(1-\mu^2)} \frac{\partial(N_V)}{\partial\lambda} - \frac{1}{a}\frac{\partial(N_U)}{\partial\mu}, \tag{11}$$

and

$$\delta_A^{\tau+1} + \Delta t \nabla^2 \phi'^{\tau+1}_A = \frac{1}{a(1-\mu^2)} \frac{\partial(N_U)}{\partial\lambda} + \frac{1}{a}\frac{\partial(N_V)}{\partial\mu} \tag{12}$$

These two equations can be solved together for the advanced time level values in spectral space of δ_n^m and ϕ_n^m. For each mode a 2×2 system of equations

$$\begin{bmatrix} 1 & -\Delta t \frac{n(n+1)}{a^2} \\ \Delta t \bar{\phi} & 1 \end{bmatrix} \begin{bmatrix} (\delta_n^m)_A^{\tau+1} \\ (\phi_n^m)_A^{\tau+1} \end{bmatrix} = \begin{bmatrix} H \\ Q \end{bmatrix}. \tag{13}$$

This is the same system found in the semi-implicit spectral method of Hack [10].

1.2.4 Comparisons of Accuracy

As an example of a study [7] to investigate the accuracy of the explicit, semi-implicit and implicit methods consider (Test case 2 from [33]) a steady, non-linear zonal flow rotated through an angle $\alpha = \frac{\pi}{4}$. The velocity and geopotential for this test case are exactly representable with the spherical harmonics of second order. So the local spherical harmonic approximations for the derivative operators are able to capture the steady state solution extremely well. This eliminates the spatial accuracy of the derivative approximation from consideration and allows a comparison of the time truncations of the algorithms.

The Asselin filter must be used to stabilize the computation for several of the methods. Figure 1 shows the relative error in the geopotential as a function of time for all the schemes *without* the time filter. The explicit-midpoint method(EX-MID) and the implicit methods (IM-SA and IM-MID) have better initial error than the semi-implicit methods (SI-SA and SI-MID). These methods keep the geostrophic balance consistently at interpolation points while the semi-implicit method splits the balance term, approximates and then combines. The leap frog instability evident in the explicit and semi-implicit methods point to the need for time filtering.

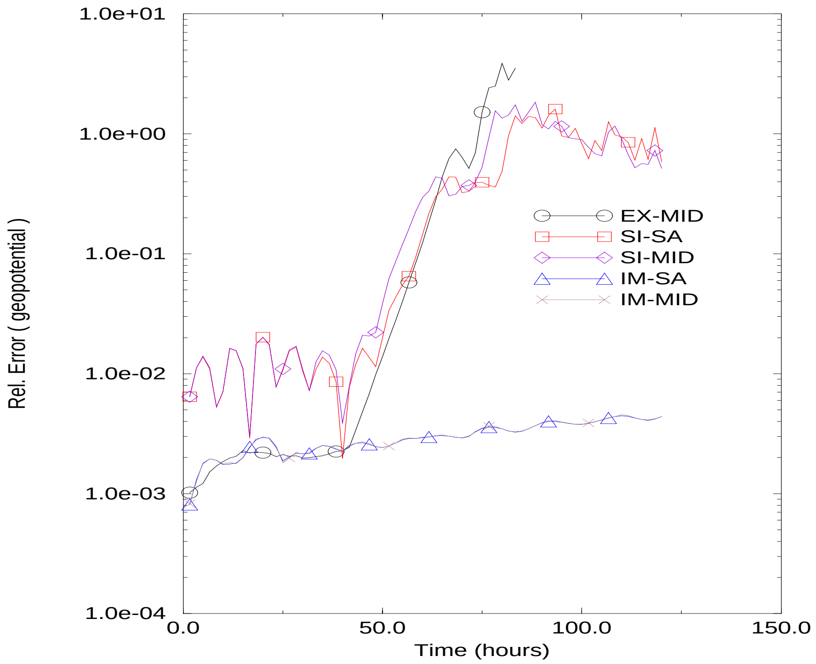

Figure 1: Non Filtered: Relative Max Error in ϕ, Test Case 2, T21

These studies serve to indicate the breadth of algorithmic options available for modeling the shallow water equations using the semi-Lagrangian transport method. Though some methods can be shown to be inappropriate or unsuitable even for these simple equations, there is no clear winner. Other considerations, such as the parallel algorithm performance or numerical properties in a more realistic setting, are needed to choose a best algorithm.

The preliminary studies also suggested many questions and areas of fruitful research that could have a direct impact on the development of future climate models. The use of local higher order methods for approximating selected derivatives in the grid-point semi-Lagrangian method and spatial filters for the control of stability could be significant. The iterative solution of the implicit and semi-implicit systems is also important for the computational performance of the algorithms.

1.2.5 Cartesian Method

Another promising method we have worked on is based on a triangular tessellation of the sphere. The use of triangular meshes for the solution of PDE's on a spherical domain is attractive for several reasons. Triangles allow nearly uniform meshes while rectangular meshes suffer the problem of varying resolution near the poles. Secondly, triangular meshes easily resolve irregular features. Adapting a mesh to fit a coastline is an obvious example.

Several early papers investigated the use of icosahedral-triangular meshes [22, 23, 27, 28, 29, 30]. The barotropic vorticity equation and the shallow water equations on the sphere served as the primary equation sets for testing the numerical methods because of their relevance in atmospheric flow models. A review article [31] gives further references to that early work.

More recently an icosahedral method based on the stream function and velocity potential formulation of the shallow water equations with a control volume discretization has been proposed by Masuda [18]. The method was refined and tested on the standard set of cases [33] by Heikes and Randall in [11, 12]. Other icosahedral methods have also been proposed in [2].

The Cartesian form of the shallow water equations was proposed by Swarztrauber in [33] and further developed in [25]. This alternative formulation avoids the singularity in the velocity at the pole by expressing velocities in a 3-D Cartesian form instead of in spherical coordinates. The introduction of 3-D velocities necessitates a change of the form of the shallow water equations. At first sight this form appears more complicated and probably more expensive computationally. But a closer examination shows the Cartesian formulation to be compact and computationally simple.

The pole problem can also be partially addressed by introducing new scalar variables derived from the velocity. The stream function/velocity potential or the vorticity/divergence function are the usual choices. The resulting system of equations then involves elliptic equations relating the new scalar variables. Since there is no introduction of new scalar variables in the Cartesian formulation, the introduction of elliptic equations is avoided. Thus, the Cartesian method has a significantly lower operation count than those methods requiring the solution of an elliptic equation.

Let $\mathbf{V} = (X, Y, Z)^T$ be the velocity in Cartesian coordinates (x, y, z). Then the spherical coordinate velocity is related by

$$\mathbf{v}_s = \mathbf{Q}\mathbf{V} \tag{14}$$

where

$$\mathbf{Q} = \begin{pmatrix} \cos\theta\cos\lambda & \cos\theta\sin\lambda & \sin\theta \\ -\sin\theta\cos\lambda & -\sin\theta\sin\lambda & \cos\theta \\ -\sin\lambda & \cos\lambda & 0 \end{pmatrix}. \tag{15}$$

The shallow water momentum equation can be developed around the vorticity and the kinetic energy. The vorticity ζ is defined in the spherical coordinate system as $\zeta \equiv \mathbf{k}\cdot\nabla\times\mathbf{v}$. Using the vector identity

$$\mathbf{v}\cdot\nabla\mathbf{v} = \nabla(\frac{\mathbf{v}\cdot\mathbf{v}}{2}) + \zeta\mathbf{k}\times\mathbf{v}, \tag{16}$$

the momentum equation can be written

$$\frac{\partial\mathbf{v}}{\partial t} = -(\zeta + f)\mathbf{k}\times\mathbf{v} - \nabla(\phi + \frac{\mathbf{v}\cdot\mathbf{v}}{2}) + \mathbf{F}_{\mathbf{v}}. \tag{17}$$

Changing variables to Cartesian velocities, the resulting Cartesian equation is

$$\frac{\partial \mathbf{V}}{\partial t} + \mathbf{Q}^T(\mathbf{\Lambda} + \boldsymbol{\gamma} + \mathbf{\Delta}) = 0. \tag{18}$$

In this equation

$$\mathbf{Q}^T\mathbf{\Delta} = \frac{(\zeta + 2\Omega z)}{a^2} \begin{pmatrix} 0 & -z & y \\ z & 0 & -x \\ -y & x & 0 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix}, \tag{19}$$

and

$$\mathbf{Q}^T\mathbf{\Lambda} = \mathbf{P}\nabla_c(\phi + \frac{\mathbf{V}\cdot\mathbf{V}}{2}). \tag{20}$$

Since the *curl* is invariant under coordinate transformation we have that $\zeta \equiv \mathbf{k}\cdot\nabla_c \times \mathbf{V}$. The Cartesian *curl* is the standard,

$$\nabla_c \times \mathbf{V} = \begin{pmatrix} \frac{\partial Z}{\partial y} - \frac{\partial Y}{\partial z} \\ \frac{\partial X}{\partial z} - \frac{\partial Z}{\partial x} \\ \frac{\partial Y}{\partial x} - \frac{\partial X}{\partial y} \end{pmatrix}. \tag{21}$$

Similarly the continuity equation in Cartesian form is

$$\frac{\partial \phi^*}{\partial t} + \mathbf{V}^T\mathbf{P}\nabla_c\phi^* + \phi^*\nabla_c \cdot \mathbf{V} = F_\phi, \tag{22}$$

where $\phi = \phi^* + \phi_s$ is the total geopotential, and ϕ_s is the surface geopotential. The matrix $\mathbf{P}$ projects an arbitrary Cartesian vector onto a plane that is tangent to the sphere at the point (x, y, z).

As an illustration of the use of the method for modeling the shallow water equations, a test case with orography is used. A 5400m mountain is given through the surface geopotential function, ϕ_s. The simulation used a diffusion coefficient of 5.0×10^5 with a timestep of 600 seconds for the $(q = 4)$ icosahedral mesh.

The following normalized integral quantities are presented as a function of time: mass, total energy, potential enstrophy. The vorticity is presented as an integral without normalization in Figure 2. The conservation properties of the Cartesian method are much better than expected considering that the difference formula used to approximate the conservation of mass are not in flux form and are not guaranteed to preserve the global mass. The excellent conservation of enstrophy and vorticity are also a surprise. It is not evident from Figure 2, but the normalized integral of enstrophy maintains a value near machine zero ($\approx 10^{-13}$) throughout the simulation.

A contour plot of the geopotential ϕ^* at 15 simulated days is given in Figure 3.

This discussion of the gridpoint and spectral Semi-Lagrangian methods and the Cartesian method indicate that these methods are ready to be considered in a more general setting. Our proposal provides this generalization.

1.3 Research Design and Methods

We propose to investigate and compare three numerical models of a (dry) baroclinic atmosphere resulting in the development of dynamical cores for atmospheric climate models. Parallel algorithms for these cores will be implemented and tested on massively parallel scientific supercomputers. Our research will build on previous DOE/CHAMMP sponsored work and be relevant to the ongoing efforts at NCAR to develop Community Climate Models for the atmospheric component of the coupled climate system.

The introduction of the vertical coordinate to our horizontal shallow water models offers an opportunity to address some outstanding issues in climate modeling. Combining the horizontal advection algorithms with the vertical advection affects the accuracy of transport modeling in a fashion depending strongly on the choice of the vertical coordinate system. In addition, the choice of vertical coordinate system effects how well thermodynamic constraints are satisfied. The energy conservation principle has been studied and incorporated in existing climate models. But the entropy principle should also be addressed.

Johnson argues [14] that paying attention to entropy constraints can explain the consistent cold bias at the poles exhibited by nearly all present day climate models. That models should correct this defect before

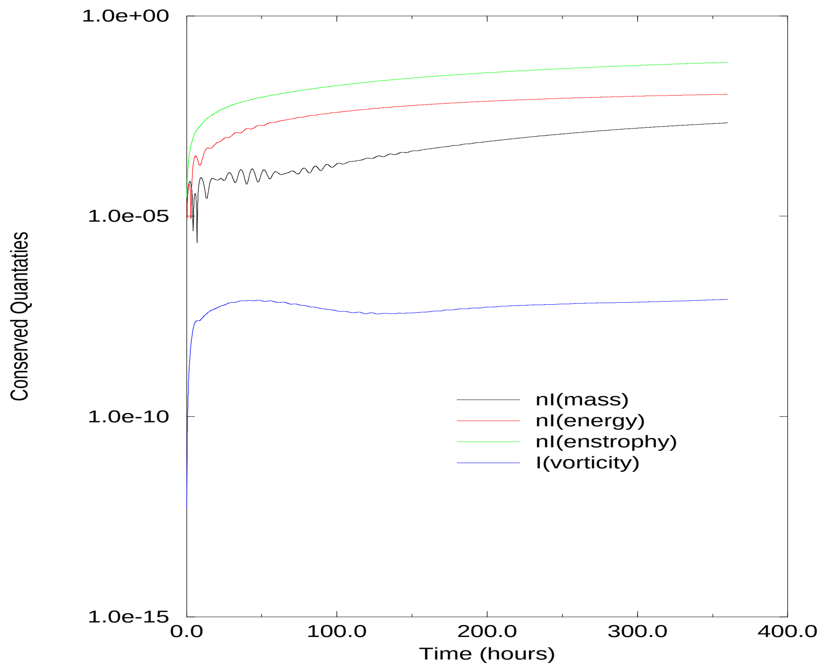

Figure 2: Conserved integral quantities. Test Case 5, $q = 4$. Rotational Form

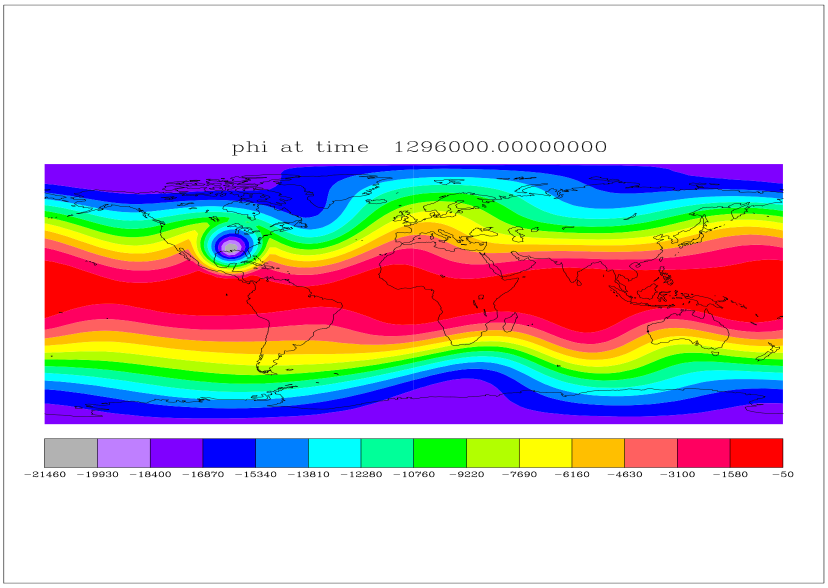

Figure 3: Geopotential at 15 days, Test Case 5, $q = 4$. Rotational Form

attempting regional forecasts seems obvious as the size of the bias is certainly regional in scope. The 3-D baroclinic setting is the simplest mathematical setting to address the issues relating to entropy constraints as well as total advection accuracy and computational efficiency.

The treatment of the vertical advection in an isentropic model is closely tied to the vertical mass flux, which is directly related to heating. The coordinate surface moves in response to heating and, in an adiabatic regime, remains a material surface with no vertical advection. The treatment of vertical advection in other vertical coordinates does not have this nice property. The accuracy of the vertical advection is then a function of method and resolution. It has been suggested [38] that the transport of an inert tracer is inaccurate in many models due to the (non-physical) numerical mixing of the vertical advection method. An isentropic coordinate model may not exhibit the same problems.

The baroclinic models we propose will be based on a generalized meteorological coordinate system varying continuously from a normalized sigma coordinate near the earth's surface to an isentropic coordinate in the free atmosphere. The viability of this type of coordinate system has recently been shown by Konor and Arakawa [16]. The maintenance of terrain following features of the sigma coordinate together with the benefits of the isentropic coordinate for accurate advection and satisfaction of entropy constraints could lead to more efficient and robust climate prediction.

Using a hybrid sigma-isentropic vertical system has practical advantages. By maintaining the sigma coordinate near the earth, no special treatment of massless isentropic layers or subsurface values need be introduced. If a pure isentropic system were used, the earth's surface intersects the vertical layers. From a computational point of view this creates a difficult problem of dealing with the solution of elliptic problems in a topologically complex domain. The terrain following property of the sigma system allows the use of regular meshes. Also, planetary boundary layer models can be easily integrated with the sigma system as is done currently with the hybrid sigma-pressure system in the NCAR CCM2 and CCM3 [15, 9].

To reiterate, *our proposal is to formulate, construct and test dynamical cores based on the three methods for horizontal dynamics and a new isentropic-sigma vertical coordinate. A comparison of the three horizontal methods using the same vertical treatment will provide a clear perspective on the algorithmic alternatives available. In particular, advantages of the semi-Lagrangian method for accurate horizontal advection will be investigated when the coordinate surface is a Lagrangian surface.*

To the extent that a cold bias manifests itself in the 3-D baroclinic setting due to non-physical diffusion and mixing, this too will be studied. For clarity and efficiency it is in this context we will address issues that are important for the development of future atmospheric climate models with improved fidelity as components of coupled climate system models.

The necessity of having good baroclinic test cases for our research is similar to our previous reliance on the shallow water equation test cases. To continue this focus we will begin investigating 3-D test cases that will aid in the understanding of the models ability to forecast regional climate impacts on the 10- 100 year times scale. The test cases and the collection of results will be worked out in collaboration with other modelers through workshops such as the DOE sponsored "PDE's on the Sphere" meeting, and through facilities offered at NCAR and LLNL as part of ongoing climate research activities. We will continue to be involved in the organization of these workshops under the auspicies of this proposal.

Our research will be complementary to the development of community climate models at NCAR. As part of our proposal we will modify a semi-Lagrangian version of the CCM by the introduction of an isentropic coordinate. A stepwise approach will be adopted to carefully isolate the affects of each change. First, the vertical isentropic coordiate will be introduced keeping the CCM vertical advection algorithm which is semi-Lagrangian. Then the vertical advection will be replaced with a vertical mass flux algorithm. Simulated climates will be compared using the standard AMIP runs. The effect of these changes on model cold bias and entropy constraints will be investigated.

In order to fix ideas, a sketch of the proposed model formulation and vertical coordinate will be given. Then a discussion of parallel algorithms for the 3-D baroclinic cores will be presented.

1.3.1 3-D Baroclinic Equations

The first steps of our proposed research will include the development of dynamical cores based on a 3-D (dry) baroclinic model. The prognostic variables we choose are p(pressure), p_s(surface pressure), $\mathbf{v}$(horizontal velocity), $(m\dot{\zeta})$(vertical mass flux), and S(entropy). Diagnostic variables are then m(mass),

Φ(geopotential), M(Montgomery potential), Π(Exner function), T(temperature), θ(potential temperature), and $m\mathbf{v}$(horizontal momentum). The two source terms in the equations are Q and $\mathbf{F}$ representing the heating for the energy equation and the momentum forcing, respectively.

The generalized vertical coordinate will be denoted ζ. Using this coordinate the governing equations for a baroclinic model can formulated. The continuity equation can be written in flux form as

$$\frac{\partial m}{\partial t} + \nabla_\zeta \cdot (m\mathbf{v}) + \frac{\partial}{\partial \zeta}(m\dot{\zeta}) = 0. \tag{23}$$

The momentum equation can be written in the form

$$\frac{\partial \mathbf{v}}{\partial t} + (\xi + f)\hat{\mathbf{k}} \times \mathbf{v} + \nabla_\zeta (M + \frac{\mathbf{v}\cdot\mathbf{v}}{2}) - \Pi \nabla_\zeta \theta + \dot{\zeta}\frac{\partial \mathbf{v}}{\partial \zeta} = \mathbf{F}. \tag{24}$$

The thermodynamic energy equation written in terms of the specific entropy S is

$$\frac{dS}{dt} + \dot{\zeta}\frac{\partial S}{\partial \zeta} = \frac{Q}{T}, \tag{25}$$

where Q is the heating per unit mass. This can also be written in terms of potential temperature as

$$\frac{d\theta}{dt} + \dot{\zeta}\frac{\partial \theta}{\partial \zeta} = \frac{Q}{\Pi}, \tag{26}$$

Using the relationship between mass and pressure, an evolution equation for the pressure can be obtained by integrating (23) with respect to the vertical coordinate ζ,

$$\frac{\partial p}{\partial t} = \frac{\partial p_T}{\partial t} + \nabla_\zeta \cdot (\int_{\zeta_T}^{\zeta} m\mathbf{v} d\zeta) + (m\dot{\zeta}) = 0. \tag{27}$$

By setting $\zeta = \zeta_s$, an equation for the surface pressure is obtained,

$$\frac{\partial p_s}{\partial t} = \frac{\partial p_T}{\partial t} + \nabla_\zeta \cdot (\int_{\zeta_T}^{\zeta_s} m\mathbf{v} d\zeta) = 0. \tag{28}$$

Here the mass flux boundary conditions $(m\dot{\zeta}) = 0$ at the top ζ_T of the atmosphere and at the earths surface ζ_s have been used.

1.3.2 Isentropic-Sigma Vertical Coordinates

The vertical coordinate is described by a functional dependence on both entropy and pressure in the equation

$$\zeta = F(S, p, p_s). \tag{29}$$

A continuous isentropic-sigma coordinate system would use a continuous function F. Konor and Arakawa [16] give an explicit construction of a particular form for F. The functional relationship can also be described implicitly. Let σ be defined as a vertically increasing (normalized) pressure coordinate by

$$\sigma \equiv \frac{p_s - p}{p_s - p_T}. \tag{30}$$

Let $A(\zeta)$ and $B(\zeta)$ be continuous functions of a single variable chosen so that

$$S = A(\zeta) + B(\zeta)\sigma. \tag{31}$$

This equation (31) is the implicit definition of ζ in terms of S, p and p_s. The A and B can be chosen in a number of ways to yield an isentropic coordinate system in the free atmosphere and a σ coordinate system near the earth's surface. For convenience we will let $\zeta \in [0, 1]$. At the top of the atmosphere we would like the dependence on σ to vanish, eg. $B(\zeta) \to 0$ as $\zeta \to 1$. Hence $S_T = A(1)$. At the earth's surface $\zeta = 0$ and $\sigma = 0$, so $S_0 = A(0)$.

The functions we choose to satisfy these requirements are

$$B(\zeta) = e^{-\alpha\zeta}, \tag{32}$$

and

$$A(\zeta) = c_p \ln(\frac{\zeta\theta_T + (1-\zeta)\theta_0}{\theta_0}). \tag{33}$$

With $\alpha = 10$, the σ coordinate is largely confined to the boundary layer and an isentropic θ coordinate uniform in potential temperature holds in the free atmosphere. The ζ-coordinate is monotonically increasing with respect to height (and σ) as long as the potential temperature is well behaved. To ensure proper behavior a dry convective adjustment may be required when an unstable stratification occurs.

A relationship to the mass flux can be developed to ensure the consistency of the vertical coordinate with the implicit form. Note that $\dot{\zeta}\frac{\partial S}{\partial \zeta} = -(m\dot{\zeta})\frac{\partial S}{\partial p}$. Hence (when $\frac{\partial S}{\partial \zeta} \neq 0$),

$$\dot{\zeta} = -\frac{\left(\frac{\partial S}{\partial p}\right)}{\left(\frac{\partial S}{\partial \zeta}\right)}(m\dot{\zeta}). \tag{34}$$

In terms of A and B,

$$\dot{\zeta} = \frac{B}{(p_s - p_T)A' + (p_s - p)B'}(m\dot{\zeta}). \tag{35}$$

The implicit part of the vertical dynamics determines the potential temperature, the pressure and the vertical mass flux, in a self consistent manner. This ties the energy equation closely to the mass continuity equation. The basic outline of this implicit algorithm is given by Konor and Arakawa in [16]. A different discretization and iterative algorithm are employed for the determination of the vertical mass flux in what we propose.

The vertical mass flux calculation assumes that the horizontal dynamics update has already taken place. The equations to be solved simultaneously are the update for potential temperature (or entropy), equation (26), pressure, equation (27), the coordinate consistency equation (35) and (31). In the vertical dynamics update step these equations are

$$\hat{S} = \bar{S} + 2\Delta t(m\dot{\zeta}\frac{\partial \hat{S}}{\partial \hat{p}}) \tag{36}$$

$$\hat{p} = \bar{p} + 2\Delta t(m\dot{\zeta}) \tag{37}$$

$$\hat{S} = A(\hat{\zeta}) + B(\hat{\zeta})\frac{p_s - \hat{p}}{p_s - p_T} \tag{38}$$

$$\frac{\hat{\zeta} - \zeta^n}{\Delta t} = \left[\frac{B}{(p_s - p_T)A' + (p_s - p)B'}\right](m\dot{\zeta}) \tag{39}$$

The coordinate consistency equation (35) has been discretized using a two time level Euler scheme for the time derivative $\dot{\zeta}$. These equations (36 - 39) are four non-linear equations in four unknowns $\hat{S}, \hat{p}, \hat{\zeta}$, and $(m\dot{\zeta})$. A Newton method for solving these equations can be formulated.

Once the Newton iteration has converged the mass flux, coordinate system and thermodynamic variables are consistent. With the mass flux determined, the mass (23) or pressure (27 and 28) and the momentum (24) can be updated for the vertical terms. The pressure should then be consistent with mass.

A vertical discretization is now introduced and a numerical procedure for the Newton iteration of a discrete atmospheric column is outlined. At this point we do not need to specify what the particular combination of S, p and p_s are that will define ζ. The continuous coordinate will map $\zeta = \theta$ for an isentropic coordinate in the free atmosphere while near the ground, the map will take $\zeta = \sigma = \frac{p_s - p}{p_s - p_T}$ for a terrain following σ-coordinate. It will be convenient to require that the vertical discretization be uniform in ζ from ζ_T to ζ_s. The levels will be indexed from 1 to K with half levels (half way between) indexed with half value indices. A pictorial representation of the vertical grid is given in Figure (4). All model variables are located on the integer level surfaces while partial derivatives are located on the half levels.

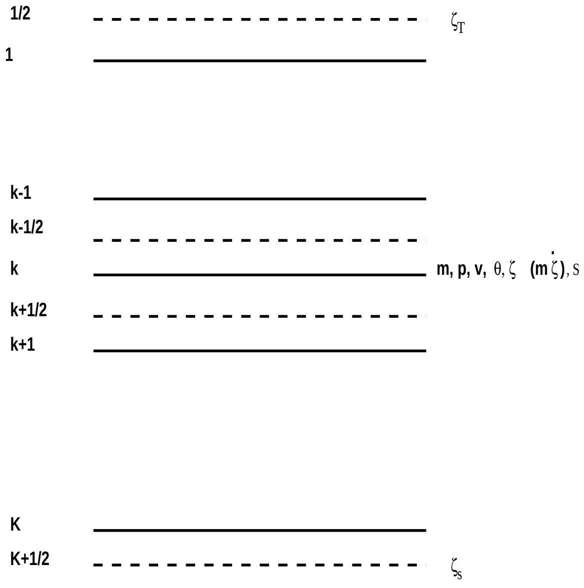

Figure 4: Vertical Grid with Location of Discrete Variables

1.3.3 Parallel algorithms

The computational requirements for decadal to century scale climate modeling demand that atmospheric models be run in parallel computing environments. Thus, we will extend our work on parallel algorithms for climate models to the new formulations and for scalable parallel computer architectures.

Our previous work on parallel spectral algorithms carries over immediately. A 2-dimensional horizontal domain decomposition provides a natural parallelism for the radiation and adjustment physics, treating columns of the atmosphere independently. For grid-point dynamics we will explore a longitude-level-latitude decomposition of the dynamics with a variable chunking of the first two indices. This chunking can be adjusted to gain good performance on vector or cache based machines. It also allows sufficient flexibility to parallelize for machines with very large numbers of processors.

The semi-implicit time integration used with grid point methods requires efficient general iterative solvers. These iterative algorithms must be efficient across shared memory or distributed memory parallel processors. For the grid-point/semi-Lagrangian method, a conjugate gradient like algorithm, the quasi-minimum residual (QMR) will be implemented. For the icosahedral Cartesian method, a multi-grid algorithm seems better suited. Previous work on efficient parallel spectral and semi-Lagrangian methods will also be extended to the new hybrid shared/distributed memory architectures. Dynamical cores will be tested with the available dynamical cores test cases and benchmarked for performance and portability on shared memory and distributed memory scientific supercomputers.

The specification for interchangeable physics modules has greatly aided the development of improved physics in the atmospheric models. We propose to extend this idea to the parallel dynamics, implementing the parallel algorithms developed here in a way that supports swap-able dynamics. This will significantly aid the numerical and parallel research, by minimizing maintenance of multiple codes and supporting fair evaluation of the different algorithmic options. Our experience in this regard will then be used to propose a specification for interchangeable dynamics modules to be used in future climate models.

1.3.4 Impact and long term research

It is not the intent of this proposal to create production models. Rather, we hope to develop and evaluate new ideas and methods that could be used in full models. But, performance issues, both computational and thermodynamic, cannot be fully addressed in a model that does not include columnar radiation and convective adjustment physics. The physics calculations have a dynamic effect on computational load balance, which is not entirely separable from the flow calculations. To further demonstrate the viability of at least one algorithm developed in this proposal we will substitute the hybrid isentropic-sigma vertical coordinate system in a semi-Lagrangian version of the NCAR Community Climate Model.

We will investigate the thermodynamic constraints satisfied in the simulated climate. In particular, we will document the cold bias (or lack thereof) for decadal to century length simulations and study an inert tracer experiment. This will serve to evaluate both the effectiveness of the vertical coordinate system to treat the cold bias problem and the accuracy of semi-Lagrangian transport with this vertical coordinate in a full atmospheric climate model.

In summary, this proposal provides a stepwise development, testing and study of three promising dynamical cores for future atmospheric climate models. It is thought that the numerical properties of the methods will be superior to existing methods particularly in regard to satisfaction of entropy constraints and accuracy of transport. Benchmarking the performance of the dynamical cores on several parallel computing platforms will aid the comparison of methods. At the end of the project, the models developed will be made freely available to the climate research community, and the results will be used to propose new numerical and parallel algorithms for inclusion in ongoing model development efforts like the Community Climate Models at NCAR.

1.4 Subcontractor Consortium Arrangements

There are no arrangements outside plans to collaborate with the CCPP Science and Development Teams.

2 Literature Cited

References

[1] G. J. Boer and B. Denis. Numerical convergence of the dynamics of a GCM. *Climate Dynamics*, 13:359–374, 1997.

[2] I-Liang Chern. A control volume method on a icosahedral grid for numerical integration of the shallow-water equations on the sphere - I. MCS preprint, Argonne National Laboratory, Chicago, IL, 1991.

[3] J.B. Drake, R.E. Flanery, B.D. Semeraro, P.H. Worley, I.T. Foster, J.G. Michalakes, J.J. Hack, and D.L. Williamson. Parallel community climate model: Description and user's guide. ORNL Tech Report ORNL/TM–13271, Oak Ridge National Laboratory, Oak Ridge, TN, 1996.

[4] J.B. Drake, R.E. Flanery, D.W. Walker, P.H. Worley, I.T. Foster, J.G. Michalakes, R.L. Stevens, J.J. Hack, and D.L. Williamson. The message passing version of the parallel community climate model. In *ECMWF Workshop on Parallel Computing*. European Center for Medium Range Weather Forecasting, November 1992.

[5] J.B. Drake, I.T. Foster, J.G. Michalakes, and P.H. Worley. Parallel algorithms for semi-Lagrangian transport in global atmospheric circulation models. In *Parallel Processing for Scientific Computing*, pages 119–124. Society for Industrial and Applied Mathematics, Feb. 1995.

[6] J.B. Drake, I.T. Foster J.J. Hack, J.G. Michalakes, B.D. Semeraro, B. Toonen, D.L. Williamson, and P.H. Worley. PCCM2: A GCM adapted for scalable parallel computers. In *5th Global Change Symposium*. American Meteorological Society, Jan 1994.

[7] J.B. Drake, P.H. Worley, N.M. Nachtigal, and D.L Williamson. Semi-Lagrangian transport algorithms for the shallow water equations in sphereical geometry. ORNL Tech Report ORNL/TM, Oak Ridge National Laboratory, Oak Ridge, TN, to appear.

[8] P.H. Worley D.W. Walker and J.B. Drake. Parallelizing the spectral transform method - Part II. *Concurrency: Practice and Experience*, pages 509–531, 1992.

[9] J. J. Hack, B. A. Boville, B. P. Briegleb, J. T. Kiehl, P. J. Rasch, and D. L. Williamson. Description of the NCAR Community Climate Model (CCM2). NCAR Tech. Note NCAR/TN–382+STR, National Center for Atmospheric Research, Boulder, Colo., 1992.

[10] J.J. Hack and R. Jakob. Description of a global shallow water model based on the spectral transform method. NCAR Technical Note NCAR/TN-343+STR, National Center for Atmospheric Research, Boulder, CO, 1992.

[11] Ross Heikes and David A. Randall. Numerical integration of the shallow-water equations on a twisted icosahedral grid. Part I. *Mon. Wea. Rev.*, 123:1862–1880, 1995.

[12] Ross Heikes and David A. Randall. Numerical integration of the shallow-water equations on a twisted icosahedral grid. Part II. *Mon. Wea. Rev.*, 123:1881–1887, 1995.

[13] Isaac M. Held and Max J. Suarez. A proposal for the intercomparison of the dynamical cores of atmospheric general circulation models. *Bull. Amer. Meteor. Soc.*, 75(10):1825–1830, 1994.

[14] D.R. Johnson. On the general coldness of climate models and the second law: Implications for modeling the earth system. *J. Climate*, to appear.

[15] J.T. Kiehl, J.J. Hack, G.B. Bonan, B.A. Boville, B.P. Briegleb, D.L. Williamson, and P.J. Rash. Description of the NCAR Community Climate Model (CCM3). NCAR Tech. Note NCAR/TN–420+STR, National Center for Atmospheric Research, Boulder, Colo., 1996.

[16] Celal S. Konor and Akio Arakawa. Design of an atmospheric model based on a generalized vertical coordinate. *Mon. Wea. Rev.*, 125:1649–1673, 1997.

[17] P.A. Makar and S.R. Karpik. Basis spline intropolation on the sphere: Application to semi-Lagrangian advection. *Mon. Wea. Rev.*, 124:182–199, 1996.

[18] Y. Masuda and H. Ohnishi. An integration scheme of the primitive equation model with an icosahedral-hexagonal grid system and its application to the shallow water equations. In *Short- and Medium-Range Numerical Weather Prediction*, pages 317–326, 1986.

[19] I.T. Foster P.H. Worley and B. Toonen. Algorithm comparison and benchmarking using a parallel spectral transform shallow water model. In *Sixth Workshop on Parallel Processing in Meteorology*, page to appear. ECMWF, Nov. 1994.

[20] J.J. Hack R. Jakob and D.L. Williamson. Reference solutions to shallow water test set using the spectral transform method. Ncar tech note, National Center for Atmospheric Research, Boulder, CO, 1993.

[21] H. Ritchie. Application of the semi-Lagrangian method to a spectral model fo the shallow water equations. *Mon. Wea. Rev.*, pages 1587–1598, 1988.

[22] R. Sadourny, A. Arakawa, and Y. Mintz. Integration of the nondivergent barotropic vorticity equation with an icosahedral-hexagonal grid for the sphere. *Mon. Wea. Rev.*, 96:351–356, 1968.

[23] R. Sadourny and P. Morel. A finite-difference approximation of the primitive equations for a hexagonal grid on a plane. *Mon. Wea. Rev.*, 97:439–445, 1969.

[24] A. Staniforth and J. Côté. Semi-Lagrangian integration schemes for atmospheric models – a review. *Mon. Wea. Rev.*, 119:2206–2223, 1991.

[25] P.N. Swarztrauber, D.L. Williamson, and J.B. Drake. The Cartesian method for solving of PDE's in spherical geometry. *Dyn. Atm. Ocn.*, to appear.

[26] M. Tanguay, E. Yakimiw, H. Ritchie, and A. Robert. Advantages of spatial averging in semi-implicit semi-Lagrangian schemes. *Mon. Wea. Rev.*, pages 113–123, 1992.

[27] D. L. Williamson. Integration of the barotropic vorticity equation on a spherical geodesic grid. *Tellus*, 20:642–653, 1968.

[28] D. L. Williamson. Integration of the primitive barotropic model over a spherical geodesic grid. *Mon. Wea. Rev.*, 98:512–520, 1969.

[29] D. L. Williamson. Numerical integration of fluid flow over triangular grids. *Mon. Wea. Rev.*, 97:885–895, 1969.

[30] D. L. Williamson. A comparison of first- and second-order difference approximations over a spherical geodesic grid. *J. Comp. Phys.*, 7:301–309, 1971.

[31] D. L. Williamson. *Numerical Methods Used in Atmospheric Models*, chapter 2, pages 51–120. GARP Pub. Ser. No. 17. JOC, WMO, Geneva, Switzerland, 1979.

[32] D. L. Williamson. Climate simulations with a spectral, semi-Lagrangian model with linear grids. *Atmosphere-Ocean*, page special issue to appear, 1994.

[33] D. L. Williamson, J.B. Drake, J.J. Hack, Rudiger Jakob, and P.N. Swarztrauber. A standard test set for numerical approximations to the shallow water equations on the sphere. *J. Comp. Phys.*, pages 211–224, 1992.

[34] D. L. Williamson and J.G. Olson. Climate simulations with a semi-Lagrangian version of the NCAR Community Climate Model. *Mon. Wea. Rev.*, pages 1594–1610, 1994.

[35] David L. Williamson. A semi-Lagrangian version of the NCAR CCM2 and examples of climate simulations. In *Workshop on Semi-Lagrangian Methods*. Max Plank Institut fur Meteorologie, October 8-9 1992.

[36] P.H. Worley and J.B. Drake. Parallelizing the spectral transform method - Part I. *Concurrency: Practice and Experience*, pages 269–291, 1992.

[37] P.H. Worley and I.T. Foster. Parallel algorithms for the spectral transform method. ORNL Tech Report ORNL/TM–12507, Oak Ridge National Laboratory, Oak Ridge, TN, 1994.

[38] T. H. Zapotocny, A.J. Lenzen, D.R. Johnson, T.K Schaack, and F. M Reames. A comparison of inert trace constituent transport between the university of wisconsin isentropic-sigma model and the NCAR Communtiy Climate Model. *Mon. Wea. Rev.*, 121(7):2088–2114, 1993.

3 Budget Explanation

Cost estimates presented in this proposal have been reclassified in order to be comparable to other research institutions proposals. At Oak Ridge National Laboratory (ORNL), actual costs will be collected and reported in accordance with the Department of Energy (DOE) approved cost accounting system. Total cost presented in this proposal and actual costs totals will be equivalent as will the subtotal of direct and indirect costs.

3.1 Senior Personnel

The ORNL's Cost Accounting System (CAS) incorporates Cost Collect Centers which are built around people performing similar or closely related tasks. The salary figure listed for Senior Personnel represents the average salary for a scientist in the Computer Science and Mathematics Division.

Dr. J. B. Drake is the principal investigator for this project at Oak Ridge National Laboratory. Dr. P. H. Worley and Dr. E. D'Azevedo are senior researchers at ORNL in the Mathematics and Computer Science Division.

3.2 Secretarial/Clerical

The ORNL's CAS incorporates Cost Collect Centers which are built around people performing similar or closely related tasks. The salary figure listed for Secretarial/Clerical represents the average salary for staff secretary/administrative personnel in the Computer Science and Mathematics Division. Level of secretarial/clerical assistance is estimated to be approximately 0.2 full time equivalent (FTE) for every 1.0 FTE of CSMD scientific effort.

3.3 Fringe Benefits

Fringe Benefits for ORNL employees are estimated to be 26.01% (Year 1), 25.93% (Year 2) and 31.92% (Year 3 and 4) of labor costs.

3.4 Travel

Travel costs for the participation in Science Team meetings and workshops are estimated based on one trip of five days to Washington, DC, one trip of five days to San Francisco, CA, and one trip of five days to Denver, CO.

3.5 Publication Costs

Publication and page charges for this project are estimated to be $2,000 per year.

3.6 Other - Organization Burden Administration

Use of cost collection centers in ORNL R&D divisions is the approved method for collection and distribution of direct effort and related costs. These accounts are established to collect costs associated with personnel engaged in a single operation or several closely related operations. The objecctive is to establish uniformity and compatibility in recorded, distributing and reporting direct effort for all ORNL R&D divisions. The types of costs which can be charged to cost collection centers are labor; labor-related costs (fringe benefits); division administration; and general materials/service costs, including, but not limited to, telecommunications, word processing, and copying which are not directly attributable or chargeable to R&D projects. Division administration costs include utilities; managerial, technical ,and administrative oversight; and support personnel such as plant and equipment, instrumentation and controls, environmental, safety, and health, finance and budget, quality, and health physics provided for the general benefit of a division.

The labor and fringe components have been estimated and reported in items above. The organization and administrative burden components have been estimated and reported above. Inclusion of these costs is necessary to provide a full accounting of estimated cost for the project period. All costs will be collected and reported in ORNL's cost accounting system.

3.7 Indirect Costs

ORNL on site overhead is estimated to be 45.15% (Year 1), 42.0% (Year 2), and 40% thereafter. The overhead is applied to all activities performed at the ORNL site.

4 Other Support of Investigators

Two of the investigators involved with this proposal (Dr. Drake and Dr. Worley) are currently supported by the CHAMMP project with minimual involvement in other laboratory projects. Current support for Dr. D'Azevedo is 25% Computational Mathematics project sponsored by DOE/MICS, 25% ETPI project sponsored by DOE, 40% ScaLAPACK project sponsored by DARPA. The CHAMMP extension project and the ScaLAPACK project ends April 1, 1998.

5 Biographical Sketches

5.1 John B. Drake

CONTACT
Mathematical Sciences Section
Oak Ridge National Laboratory
Oak Ridge TN 37831-6367
phone: 423-574-8670
fax: 423-574-0680
e-mail: `drakejb@ornl.gov`
WWW: `http://www.epm.ornl.gov/ bbd/`.

EDUCATION

Ph.D.	(Mathematics)	University of Tennessee,	1991.
M.S.	(Applied Mathematics)	Purdue University,	1979.
B.A.	(Mathematics)	University of Kentucky,	1977.

PROFESSIONAL EXPERIENCE
Research Staff, Mathematical Sciences Oak Ridge National Laboratory, 1984–present.
Research Staff, Engineering Mechanics Oak Ridge National Laboratory, 1979–1984.

PROFESSIONAL ACTIVITIES
Member of SIAM. Host of "PDE's on the Sphere Conference" 1995 and organizing committee for other "PDE's on the Sphere" meetings.
Technical Reviewer for several journals and for proposals from DOE and NSF.

RESEARCH INTERESTS AND EXPERTISE
John Drake's research interests include

- Numerical methods and parallel algorithms for climate modeling.
- Numerical solution of partial differential equations and integral equations.

The development of parallel algorithms for the solution of partial differential equations on distributed memory multiprocessors is the current focus of his work. Fluid flow algorithms for massively parallel, distributed memory computers, used in the simulation of atmospheric flows and in plasma turbulence modeling are the subject of continuing projects. The formulation of atmospheric flow equations to utilize semi-Lagrangian advection algorithms and high order spatial discretizations is also a part of his research. Moving boundary problems associated with change of phase in thermal and fluid flow problems were the focus of his doctoral research. This research employed finite element and control volume methods in a "weak" formulation applied to the Navier-Stokes equations and the equation of energy conservation.

FIVE RECENT PUBLICATIONS RELATED TO THIS PROJECT

1. *Parallel Algorithms for Semi-Lagrangian Transport in Global Atmospheric Circulation Models*, with I.T. Foster, J.G. Michalakes and P.H. Worley, in Parallel Processing for Scientific Computing, SIAM, Feb. 1995, pp. 119-124.
2. *Design and Performance of a Scalable Parallel Community Climate Model*, with I.T. Foster, J.G. Michalakes, Brian Toonen and P.H. Worley, Parallel Computing, Vol 21, No.10, pp. 1571-1591, October 1995
3. *Parallel Computing Special Issue: Introduction to Weather and Climate Modeling*, with I.T. Foster, Parallel Computing, Vol 21, No.10, pp. 1537-1544, October 1995
4. *A Parallel Performance Study for the Cartesian Method on a Sphere*, with Matthew P. Coddington, ORNL/TM-13304, February 1997
5. *The Cartesian Method for solving partial differential equations in spherical geometry*, with P.N. Swarztrauber, D.L. Williamson, to appear in Dynamics of Oceans and Atmospheres, 1998.

5.2 Patrick H. Worley

CONTACT

Mathematical Sciences Section
Oak Ridge National Laboratory
Oak Ridge TN 37831-6367
phone: 423-574-3128
fax: 423-574-0680
e-mail: worleyph@ornl.gov
WWW: http://www.epm.ornl.gov/ worley/.

EDUCATION

Ph.D. (Computer Science) Stanford University, 1988.
M.S. (Computer Science) Stanford University, 1983.
B.A. (Computer Science) Indiana University, 1980.
B.A. (Mathematics) Indiana University, 1980.

PROFESSIONAL EXPERIENCE

Research Staff, Oak Ridge National Laboratory, 1987–present.

PROFESSIONAL ACTIVITIES

Member of ACM and SIAM Reviewer for 7 journals, DOE, NSF, and numerous conferences
Moderator of ACM SIGMETRICS Electronic BBoard
Co-chair of 1997 Gordon Conference on High Performance Computing
Member of editorial board for the Electronic Journal of Performance Evaluation and Modelling
Member of PARKBENCH (PARallel Kernels and BENCHmarks) committee
Tutorial speaker on performance evaluation at SC97

RESEARCH INTERESTS AND EXPERTISE

Patrick Worley's research interests are in the design, implementation, and evaluation of parallel algorithms, in the performance evaluation of high performance computer systems, and in the design and evaluation of numerical algorithms for the solution of differential equations.

Worley's parallel algorithm work ranges from theoretical investigations into what is feasible based on information theoretic concepts, including seminal work on the limitations of scalability, to the design and implementation of parallel algorithms in atmospheric and ocean simulation models. He has expertise on the full range of Intel and nCUBE parallel platforms and on the Cray Research T3D and T3E, IBM SP, and Convex Exemplar SPP. He was a coauthor of PCCM2, a massively parallel implementation of the Community Climate Model CCM2.

Worley's work on performance evaluation has three aspects: performance data collection, visualization, and analysis, benchmarking and benchmarking methodology, and performance portability. Worley is the author of the performance data collection facility in the Portable Instrumented Communication Library (PICL), which he continues to maintain and extend this tool for use in evaluation work. Recent research includes constructing and evaluating models for the performance prediction of parallel programs, and comparing the performance characteristics of the Message Passing Interface between parallel systems. Worley was the primary author of the tunable benchmark code PSTSWM, and has an active interest in techniques for "fair" benchmarking and in programming styles and tools that support performance portability.

Worley's numerical work includes research into novel algorithms that are suitable for parallel implementation and the implementation and evaluation of numerical algorithms for use in atmospheric and ocean models. Recent research includes an evaluation of proposed fast Legendre transform algorithms in the context of spectral atmospheric models.

FIVE RECENT PUBLICATIONS RELATED TO THIS PROJECT

1. *Parallel algorithms for the spectral transform method,* with I. Foster Sci. Stat. Comput., 18(3), 1997, pp. 806-837.
2. *Performance of parallel computers for spectral atmospheric models,* with I. Foster and B. Toonen J. Atm. Oceanic Tech., 13(5), 1996, pp. 1031-1045.
3. *A Study of Application Sensitivity to Variation in Message Passing Latency and Bandwidth* with A. Robinson, D. Mackay, and E. Barragy, ORNL Technical Report ORNL/TM-13250, June 1996 (also, Concurrency: Practice and Experience (accepted)).
4. *Performance Modeling for SPMD Message-Passing Programs* with J. Brehm and M. Madhukar, ORNL Technical Report ORNL/TM-13254, June 1996 (also, Concurrency: Practice and Experience (accepted)).
5. *MPI performance evaluation and characterization using a compact application benchmark code* Proceedings of the Second MPI Developers Conference and Users' Meeting, IEEE Computer Society Press, 1996, pp. 170-177.

5.3 Eduardo F. D'Azevedo

CONTACT

Mathematical Sciences Section
Oak Ridge National Laboratory
Oak Ridge TN 37831-6367
phone: 423-576-7925
fax: 423-574-0680
e-mail: e6d@ornl.gov
WWW: http://www.epm.ornl.gov/~efdazedo/.

EDUCATION

Ph.D.	(Computer Science)	University of Waterloo, 1989.
M.Math.	(Computer Science)	University of Waterloo, 1985.
B.Math.	(Computer Science)	University of Waterloo, 1983.
B.Math.	(Combinatorics & Optimization)	University of Waterloo, 1983.

PROFESSIONAL EXPERIENCE

Research Staff,	Oak Ridge National Laboratory,	1991–present.
Postdoctoral Fellow,	Oak Ridge Associated University,	1990-1991.
Postdoctoral Fellow,	University of Waterloo,	1989-1990.

PROFESSIONAL ACTIVITIES

Member of ACM and SIAM.
Member of organizing committee for 7th International Meshing Roundtable.

RESEARCH INTERESTS AND EXPERTISE

Eduardo D'Azevedo's research interests are in the design, and implementation of parallel numerical algorithms, and optimal mesh generation for finite elements computation.

D'Azevedo's parallel algorithm work has included parallel implementation of finite element codes for groundwater modeling, out-of-core library extension to ScaLAPACK, compact storage library extension for ScaLAPACK, efficient implementation of Lagrangian particle tracking and molecular dynamics using emulated shared memory, and development of highly efficient software for parallel I/O.

D'Azevedo's work on optimal mesh generation has included generation of optimal triangular and quadrilateral meshes using anisotropic coordinate transformation. The transformations are derived using the Hessian of data functions or material tensor as the 'metric' tensors. The new technique results in higher than $O(h^2)$ superconvergence bilinear quadrilateral meshes. Anisotropic meshes for problems with strongly anisotropic materials has mesh elements aligned to the characteristic directions and yield better accuracy than isotropic meshes. The resulting assembled matrix is also well conditioned, and thus have fast convergence with iterative solvers.

FIVE RECENT PUBLICATIONS RELATED TO THIS PROJECT

1. *A Study of I/O in a Parallel Finite Element Groundwater Transport Code* with D. Mackay and K Mahinthakumar, ORNL Technical Report ORNL/TM-13440, May 1997 (also, Internal Journal of Supercomputer Applications).

2. *Packed Storage Extension for ScaLAPACK* with J. Dongarra, ORNL Technical Report ORNL/TM-13545, Dec 1997.

3. *Coefficient Adaptive Triangulation for Strongly Anisotropic Problems,* with C. Romine and J. Donato, ORNL Technical Report ORNL/TM-13086, Nov 1995.

4. *Parallelization of a Multiregion Flow and Transport Code Using Software Emulated Global Shared Memory and High Performance Fortran,* with J. Gwo, in Proc. High Performance Computing 1997, A. Tentner (ed.).

5. *Shared memory emulation enables billion atom molecular dynamics,* with C. Romine and D. Walker, in *Applications on Advanced Computers*, edited by Greg Astfalk, SIAM, 1996.

6 Description of Facilities and Resources

The research proposed will be performed at the Oak Ridge National Laboratory. The computing facilities we will use at ORNL for the development of test codes and testing methodology include the Intel Paragons in the Center for Computational Science (CCS), a 4 processor SGI Oynx and local workstation clusters.

Validation of the computational techniques will use the Cray T3E in the National Energy Research Supercomputing Center (NERSC) at LBL and the SGI Origin in the Advanced Computing Laboratory (ACL) at LANL, as well as the Paragon.

We currently have access and sufficient computing time available on all these systems.