XXI Congreso de Ecuaciones Diferenciales y Aplicaciones
XI Congreso de Matemática Aplicada
Ciudad Real, 21-25 septiembre 2009
(pp. 1–8)

A comparison of high-order time integrators for the Boussinesq Navier-Stokes equations in rotating spherical shells.

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Palabras clave: Time integration methods, backward differentiation-extrapolation formulae, Krylov methods, spectral methods, spherical shells, thermal convection.

Resumen

The efficiency of implicit and semi-implicit time integration codes based on backward differentiation and extrapolation formulae for the solution of the three-dimensional Boussinesq thermal convection equations in rotating spherical shells is studied. The use of Krylov techniques allows the implicit treatment of the Coriolis term with low storage requirements. The results show that high order methods, either with or without time step and order control, increase the efficiency of the time integrators, and allow to obtain more accurate solutions.

1. Introduction

The study of the thermal convection in rotating spherical geometries is fundamental to explain many geophysical and astrophysical phenomena, such as the generation of the magnetic fields, or the differential rotation observed in the atmosphere of the major planets. The difficulties related with the experimental studies enhance the importance of the three-dimensional numerical simulations in these fields. For this reason the development and improvement of the numerical techniques is basic for this research.

The exclusive use of time integrations is not sufficient to establish the origin of the laminar flows and their dependence on the parameters, specially in the case of subcritical

or multicritical transitions. In these situations pseudo-arclength continuation methods [9], and the linear stability analysis of the time dependent solutions [10, 3] provide powerful instruments to clarify the dynamics. However, these techniques require to find accurate solutions, and, even if one is only interested in low precision time evolutions, high order methods can be more efficient than low order approximations.

In this note we perform a study of the efficiency of different multistep methods of either constant time step size or variable step size and variable order (VSVO) based on backward differentiation formulae (BDF), which are widely used for obtaining high order solutions for very stiff problems. In our own time integration codes, we apply backward differentiation-extrapolation (BD-E) formulae, with the nonlinear terms of the equations taken explicitly, in order to avoid to solve nonlinear equations at each time step. The Coriolis term is treated either semi-implicit or fully implicit, giving rise to the different algorithms presented. The use of *matrix-free* methods facilitates the implementation of a suitable order and time step size control.

2. Mathematical model and spatial discretization

The thermal convection of a spherical fluid shell differentially heated, rotating about an axis of symmetry with constant angular velocity $\mathbf{\Omega} = \Omega\mathbf{k}$, and subject to radial gravity $\mathbf{g} = -\gamma\mathbf{r}$, where γ is a constant, and $\mathbf{r}$ the position vector, is considered. The mass, momentum and energy equations are written by using the same formulation and non-dimensional units as in [7, 11]. The units are the gap width, $d = r_o - r_i$, for the distance, $\nu^2/\gamma\alpha d^4$ for the temperature, and d^2/ν for the time, ν being the kinematic viscosity, α the thermal expansion coefficient, and r_i and r_o the inner and outer radii, respectively. The velocity field $\mathbf{v}$ is expressed in terms of toroidal, Ψ, and poloidal, Φ, scalar potentials $\mathbf{v} = \nabla\times(\Psi\mathbf{r}) + \nabla\times\nabla\times(\Phi\mathbf{r})$, and $\Theta = T - T_c$ is the temperature perturbation from the conduction state $\mathbf{v} = \mathbf{0}$, $\quad T_c(r) = T_0 + R\eta/\sigma(1-\eta)^2 r$, with $r = ||\mathbf{r}||_2$.

With the functions $X = (\Psi, \Phi, \Theta)$ expanded in spherical harmonic series up to degree L, the equations written for their complex coefficients are

$$\partial_t \Psi_l^m = \mathcal{D}_l\Psi_l^m + \frac{1}{l(l+1)}\left[2E^{-1}\left(im\Psi_l^m - [Q\Phi]_l^m\right) - [\mathbf{r}\cdot\nabla\times(\boldsymbol{\omega}\times\mathbf{v})]_l^m\right], \tag{1}$$

$$\partial_t \mathcal{D}_l\Phi_l^m = \mathcal{D}_l^2\Phi_l^m - \Theta_l^m + \frac{1}{l(l+1)}\left[2E^{-1}\left(im\mathcal{D}_l\Phi_l^m + [Q\Psi]_l^m\right) + [\mathbf{r}\cdot\nabla\times\nabla\times(\boldsymbol{\omega}\times\mathbf{v})]_l^m\right], \tag{2}$$

$$\partial_t \Theta_l^m = \sigma^{-1}\mathcal{D}_l\Theta_l^m + \sigma^{-1}l(l+1)R\eta(1-\eta)^{-2}r^{-3}\Phi_l^m - [(\mathbf{v}\cdot\nabla)\Theta]_l^m, \tag{3}$$

where $\mathcal{D}_l = \partial_{rr}^2 + \frac{2}{r}\partial_r - \frac{l(l+1)}{r^2}$, and the spherical harmonic coefficients of the operator $Q = Q^u + Q^d$ are

$$[Q^u f]_l^m = -l(l+2)c_{l+1}^m D_{l+2}^+ f_{l+1}^m, \quad [Q^d f]_l^m = -(l-1)(l+1)c_l^m D_{1-l}^+ f_{l-1}^m, \tag{4}$$

$$\text{being} \quad D_l^+ = \partial_r + \frac{l}{r}, \quad \text{and} \quad c_l^m = \left(\frac{l^2-m^2}{4l^2-1}\right)^{1/2}.$$

The coefficients of the nonlinear terms of equations (1-3) are obtained following [4]. Non-slip perfect thermally conducting boundaries $\Psi_l^m = \Phi_l^m = \partial_r\Phi_l^m = \Theta_l^m = 0$, are imposed.

The governing parameters are the Rayleigh number R, the Prandtl number σ, the Ekman number E, and the radius ratio η. They are defined by

$$R = \frac{\gamma\alpha\Delta T d^4}{\kappa\nu}, \quad E = \frac{\nu}{\Omega d^2}, \quad \sigma = \frac{\nu}{\kappa}, \quad \eta = \frac{r_i}{r_o},$$

where κ is the thermal diffusivity, and ΔT the difference of temperature between the inner and outer boundaries.

In the radial direction, a collocation method on a Gauss-Lobatto mesh of $N_r + 1$ points is employed ($N_r - 1$ being the inner number of points). A large system of $N = (3L^2 + 6L + 1)(N_r - 1)$ ordinary differential equations must be advanced in time.

3. Time integration methods

In order to simplify the notation, equations (1-3) are written in the form

$$\mathcal{L}_0 \dot{u} = \mathcal{L} u + \mathcal{N}(u), \tag{5}$$

where $u = (\Psi_l^m(r_i), \Phi_l^m(r_i), \Theta_l^m(r_i))$, and $\mathcal{L}_0$ and $\mathcal{L}$ are linear operators including the boundary conditions. The former is invertible, and the latter, for any of the schemes used, includes the diffusive, the buoyancy, and part of the Coriolis terms to be specified below. The operator $\mathcal{N}$, which will be treated explicitly in the BD-E formulae, will always contain the nonlinear terms, and the rest of the Coriolis terms.

The BD-E formulae mentioned before are related to the BDF [2]. They obtain $u^{n+1} \approx u(t_{n+1})$ on a given time level t_{n+1}, $n = 0, 1, 2, \ldots,$ from the previous approximations u^{n-j}, $j = 0, 1, \ldots, k-1$, using the following k-steps formulae

$$\left(\mathcal{I} - \frac{\Delta t_n}{\gamma_0(n)} \mathcal{L}_0^{-1} \mathcal{L}\right) u^{n+1} = \frac{\Delta t_n}{\gamma_0(n)} \mathcal{L}_0^{-1} P_{n,k-1}(t_{n+1}) - \frac{\dot{Q}^0_{n,k}(t_{n+1})}{\dot{L}_{n,k}(t_{n+1})}, \tag{6}$$

where $Q^0_{n,k}(t) = Q_{n,k}(t) - u^{n+1} L_{n,k}(t)$, being $Q_{n,k}$ the interpolating polynomial of degree at most k, such that $Q_{n,k}(t_{n-j}) = u^{n-j}$, for $j = -1, 0, \ldots, k-1$, and $L_{n,k}$ the polynomial of degree at most k taking value 1 at t_{n+1}, and 0 at t_{n-j}, for $j = 0, 1, \ldots, k-1$. Moreover $P_{n,k-1}$ is the interpolating polynomial of degree at most $k-1$, such that $P_{n,k-1}(t_{n-j}) = \mathcal{N}(u^{n-j})$, for $j = 0, 1, \ldots, k-1$, $\mathcal{I}$ is the identity operator, and $\gamma_0(n) = \dot{L}_{n,k}(t_{n+1}) \Delta t_n$, being $\Delta t_n = t_{n+1} - t_n$, $n = 0, 1, 2, \ldots,$ the time step.

If the time steps are constant, the BD-E formulae (6) reduces to

$$\left(\mathcal{I} - \frac{\Delta t}{\gamma_0} \mathcal{L}_0^{-1} \mathcal{L}\right) u^{n+1} = \sum_{i=0}^{k-1} \frac{\alpha_i}{\gamma_0} u^{n-i} + \sum_{i=0}^{k-1} \frac{\beta_i \Delta t}{\gamma_0} \mathcal{L}_0^{-1} \mathcal{N}(u^{n-i}), \tag{7}$$

where the coefficients α_i, β_j and γ_0 do not depend on n, and are listed, for instance, in [9]. In this case the matrix in the system to be solved do not change for all n. On the other hand, changing the step size allows the use of formulae of different orders (step numbers) k, while maintaining accuracy. Then the integration can be started with $k = 1$ (and small Δt_0), when the lack of previously computed values precludes the use of higher order formulae, and then increase the order (and the step length) as the integration advances and previous

approximations u^{n-j} are available. For the fixed-step-size codes, the starting values u^j, $j = 1, \ldots, k-1$ are obtained by time integration from t_{j-1} to t_j with a VSVO code with sufficiently small tolerances.

Once the nonlinear terms are evaluated, equations (1-3) decouple for each azimuthal wave number m, thus, at every time step, $L+1$ linear systems of the form $H^m U^m = V^m, \quad m = 0, ..., L$, have to be solved. The vectors U^m and V^m contain, respectively, the unknowns and the right hand side of the linear system derived from the BD-E formulae (6) or (7), with azimuthal wave number m. For a given order of the unknowns, the size and structure of the matrices H^m depend on which terms of equations (1-3) are treated implicitly.

The inclusion of the diagonal parts of the Coriolis term containing $im\Psi_l^m$ and $im\Phi_l^m$ in $\mathcal{L}$, and of Q in $\mathcal{N}$, gives block-diagonal matrices H^m, whose memory requirements are quadratic in the spherical harmonic truncation parameter L. From now on, the time discretization with this treatment of the operators will be called the Q-explicit method.

By adding Q^u or Q^d (see eq. 4) to $\mathcal{L}$, the matrices H^m become upper or lower block-triangular matrices, respectively. They can be solved, with the same memory requirements and number of operations than the Q-explicit method, by using backward or forward block substitution. In order to implement this possibility in a symmetric way, the two options are used alternately, that is, one step is performed with Q^u implicit and Q^d explicit, and vice-versa in the following step. From now on, this time discretization will be called the Q-splitting method.

By setting Q totally implicit the operator $\mathcal{N}$ only includes the nonlinear terms, and then the matrices H^m become block-tridiagonal. A direct block method for solving these linear systems involves a big amount of memory storage, now cubic in L. However, *matrix-free* methods based on Krylov techniques, GMRES [8] in our case, can be used efficiently, if it is preconditioned with the block diagonal matrix. The increase of the cost in solving the linear systems may be offset by the increase of the time step size. The initial approximation for the solution of the linear system is obtained by extrapolation from the previous steps. From now on this method will be called the Q-implicit method.

The integration with a constant time step can be unnecessarily expensive because the step must be short enough to cope with possible fast transients. To avoid this situation, a refined procedure is to use a VSVO method [5]. In the derivation of the VSVO BD-E formula, the matrices of the linear systems depend on the current time step. They can be solved efficiently, if a Krylov method with a preconditioning matrix depending on a fixed time step Δt^* is used. When the convergence of the iterative linear solver degrades, the preconditioning matrix can be updated with the current time step.

All the semi-implicit methods described before have been implemented with constant time step size, and with variable time step size and order using our own codes (except the Q-splitting VSVO method). From now on, the VSVO implementations of the Q-explicit and Q-implicit methods will be called Q-explicit VSVO and Q-implicit VSVO, respectively.

The last option considered is a fully implicit treatment of the nonlinear terms with a VSVO formulation of the BDF. This leads to the solution of a nonlinear system of equations at each step. See [6] for further details. From now on this method will be called fully implicit method. We will use the DLSODPK code of the ODEPACK package [6]. The linear systems to be solved in this case depend not only on the current time step, but also on the current solution. As before, they can be preconditioned by the block-diagonal

matrices computed with a fixed time step Δt^*. Again, a criterion for recomputing the LU factorizations must be established.

4. Results

To compare the time integration schemes presented in the previous section, we integrate the non-magnetic case of [1], where several research groups presented the results of a benchmark study for a convection-driven dynamo problem in a rotating spherical shell. The values of the parameters in our non-dimensional units are $\eta = 0.35$, $\sigma = 1$, $E = 10^{-3}$ and $R = 65000$. By starting from the initial condition recommended, the solution tends, after an abrupt transient, to an azimuthal traveling wave of wave number $m = 4$. We have integrated, discarding the initial transient, with $N_r = 24$, and $L = 32$ ($N = 75095$ equations). From now on, the test case with this resolution, and the parameters of the benchmark will be called C_1. On the second place we integrate with $\eta = 0.35$ and $\sigma = 1$, but with $E = 10^{-4}$, $R = 800000$, $N_r = 48$ and $L = 63$ ($N = 577442$ equations). From now on called C_2 case. The solution tends now to a traveling wave with $m = 7$.

To check the efficiency of the different schemes the relation between the relative error, and the run time is studied. The former is defined as

$$\varepsilon(u) = \frac{||u - u_r||_2}{||u_r||_2}, \tag{8}$$

where u is the solution we want to check, and u_r is an accurate reference solution obtained with the Q-implicit VSVO method.

Fig. 1(a-d) display the efficiency curves for all the methods considered. The relative error $\varepsilon(u)$ is plotted against the run time in seconds. Figs.1(a) and (b) show the results for the constant time step size methods of orders 2 to 5, and Figs.1(c) and (d) those for the VSVO codes together with the constant time step size Q-splitting method for comparison purposes. Plots (a) and (c) are for case C_1, and (b) and (d) for C_2. The decrease of the relative error (8) is achieved by decreasing the constant time step size, or by decreasing the tolerances in the case of the VSVO methods.

Figs.1(a) and (b) show that for approximately $\varepsilon(u) < 10^{-9}$, the $k = 5$ method is the most efficient. The corresponding curves cannot be extended to the left due to stability reasons. If $\varepsilon(u) > 10^{-9}$ the most efficient methods vary from order 2 to 4 depending on the error required.

In the ranges of run time for which all the methods of a given order are available, and for a given run time, all the methods of the same order have similar efficiency, excepting the case $k = 2$ and higher resolution (see Fig.1(b)). Also, for a given constant time step size, the Q-explicit and the Q-splitting methods of all the orders have almost the same computational cost, and therefore the higher order methods should be preferred.

In the Q-implicit method, the predictions of the solution at the end of each step, based on extrapolation using the order of the integrator, are better with increasing order, and then the number of iterations to solve the linear system during the corrections is lower. Moreover, the time step required for a given $\varepsilon(u)$ is larger than for the other methods. All this makes its computational cost comparable to the rest of constant time step size methods.

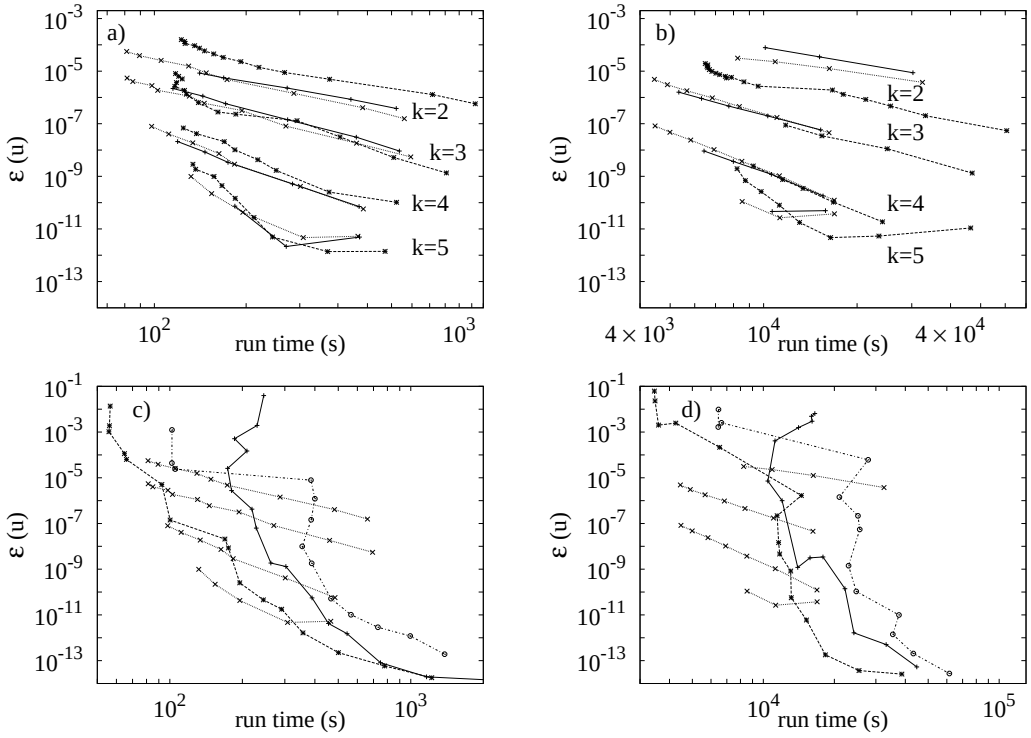

Figura 1: (a) The relative error, $\varepsilon(u)$, plotted versus the run time for constant time step integration, k from 2 to 5, and the lower resolution. (c) Same as (a) for the Q-splitting and VSVO methods. (b), (d) Same as (a) and (c), respectively, for the higher resolution. The symbols mean: Q-explicit ($+$, solid line), Q-splitting ($\times$, dotted line), Q-implicit ($*$, dashed line), Q-explicit VSVO ($+$, solid line), Q-implicit VSVO ($*$, dashed line), and DLSODPK ($\circ$, dash-dotted line).

In the low-cost regions (left of the plots), not all the methods are available due to the constraints of stability. If very small errors are not required, the Q-splitting method, is the most efficient of the constant time step size methods. The cost of the Q-explicit and the Q-splitting methods is essentially the same, but the latter has shown itself to be more stable, allowing for larger time steps, and hence, better efficiency.

In Figs.1(c) and (d) the VSVO methods are compared with the Q-splitting. The fully implicit method using DLSODPK is always more expensive than the Q-implicit VSVO methods because each iteration of the linear solver, and of the Newton's method requires an expensive evaluation of the non-linear terms. The Q-explicit VSVO method is also less expensive than DLSODPK, except for the higher $\varepsilon(u)$, for which the cost of the former increases due to the increase of the number of rejections, and of iterations of the linear solver. Approximately, an evaluation of the nonlinear terms is between 3 and 4 times more expensive than a block-diagonal linear solving. Therefore DLSODPK will never be more efficient than the Q-implicit VSVO method, unless the former could take much larger time steps. Our numerical experiments suggest that this is not the case, especially for very low values of the Ekman number, where very rapid time scales must be resolved to maintain the accuracy.

Fig.1(c) shows that the Q-implicit VSVO method is the best option for the C_1 case. Some constant time step methods can be more efficient, but at the cost of doing some previous experiments to determine the optimal time step. In the C_2 case (Fig.1(d)), there are more eigenvalues of larger imaginary part, and low and negative real part. Therefore, in order to keep the local error below a given tolerance, the Q-implicit VSVO method is forced to use BDF of order 2 in the left part of the curve shown in Fig. 1(d), and 5 in the right part, depending on the tolerance. The abrupt transition between the two parts prevents the Q-implicit VSVO method to be as efficient as the Q-splitting method in the region of intermediate errors. Although the Q-explicit method does not suffer this limitation of availability of orders, it is not more efficient because, as stated before, have a limitation of time step due to the low Ekman number.

5. Conclusions

We have shown that to integrate the thermal convection equations of fast rotating fluid spherical shells, it is possible to handle implicitly the Coriolis term, and even the nonlinear term, thanks to the low memory requirements of the iterative Krylov methods used to solve the linear systems. In this way, the range of Ekman numbers for which it is possible to perform efficient time integrations becomes larger. Otherwise, adapted LU decompositions demand prohibitive amounts of memory in the case of the high resolutions needed to resolve the Ekman boundary layers.

The implementation of high order methods do not reduce the efficiency of the time integrators, and allow to obtain more accurate solutions. In practice the most efficient method depends on the value of E, on the errors accepted for a solution, and even on the type of solution. For instance, if one is just interested in obtaining smooth solutions by direct numerical simulations (DNS), the best choice is to implement a plain Q-explicit or, better, a third or forth order Q-splitting method. However, if the time integration is part of a continuation process, and/or one is interested in calculating the stability of the solutions, low errors must be requested to the time integration. Then the Q-implicit VSVO method will probably be the most efficient option. Moreover, because of the lower run times correspond to the Q-implicit VSVO method with high tolerances, it might also be useful to pass long uninteresting transients, where having a control of the time step size might be important.

Agradecimientos

The research of F. G., M. N. and J. S. has been supported by MEC-DGI project FIS2007-64993 and AGAUR-GENCAT project 2005SGR-01028, and that of B. G.-A. by MEC-DGI project MTM2006-00847.

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