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M. Brachet, J.-P Croisille

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A CENTER COMPACT SCHEME FOR THE SHALLOW WATER EQUATIONS ON THE SPHERE

M. BRACHET† AND J.-P. CROISILLE‡

Abstract. We consider the Shallow Water Equations (SWE) on a rotating sphere and their approximation by a finite difference scheme. The discrete unknowns are located at the vertices of the equiangular Cubed Sphere grid, [11, 12]. The standard fourth order Hermitian difference derivative [24] is used along a set of suitable great circles. No one sided difference formula is used at any point. All differential operators on the sphere (gradient, divergence and curl) are approximated in a centered fashion. The approximation procedure is close in spirit to the one of compact schemes used in Computational Aeroacoustics. Numerical results on a series of numerical test cases for SWE on the sphere are presented. A particular attention is devoted to the temporal scheme. In particular two Rosenbrock exponential time schemes are used and compared to the RK4 scheme.

The results demonstrate the interest of the present approach in a variety of situations of interest in numerical climatology.

Keywords: Cubed Sphere grid - Compact finite difference scheme - Hermitian derivative - Rosenbrock time scheme - Spherical Shallow Water equations

1. Introduction

In this paper a new finite difference scheme for the Shallow Water Equations (SWE) on the rotating sphere is considered. The SWE equations represent the basic propagation system of interest in numerical climatology at global scale, [17, 26]. This system is routinely solved by spectral methods [23] with models of various complexity (single or multilayer, hydrostatic or nonhydrostatic, etc.). Over the past twenty years, many efforts have been devoted to renew numerical schemes for Global Circulation Models (GCM) by adapting ideas from Computational Fluid Dynamics (CFD) to Geophysical Fluid Dynamics (GFD). Solving (SWE) in the two dimensional spherical setup was a first step in this direction. To assess the accuracy of the numerical methods, several series of test cases have been suggested, [7, 14, 45].

Conservative approximation frameworks have been considered as a suitable platform to develop new methods for GCM. A natural option is the finite volume method. It can be considered on various kinds of grids in [4, 8, 35]. The Discontinuous Galerkin method is also considered in [2]. Another possibility is the spectral element method. It is explored and analyzed in [18, 19]. Another point of view recently developed in [13, 39] is the one of discrete differential topology and the associated Mimetic Finite Element (orFinite Volume) framework. In all these methods, referred to as the conservative approach, there is a primal grid supporting discrete averages. Numerical degrees of freedom are attached to this primal grid or alternatively to a second grid in dual position with the primal grid. In the conservative approach, discrete conservation holds ab initio, at least for the mass.

In the present work, we do not start from a discrete flux form of (SWE). Instead we consider a direct finite difference approximation. The equiangular Cubed Sphere is used as the sole grid. All the discrete unknowns are located at the vertices of the Cubed Sphere in a finite difference fashion. There is no staggered nor mean value variables in the cells of the Cubed Sphere. A center compact formula is then applied at each vertex of the Cubed Sphere to calculate approximate derivatives. The geometric structure of the Cubed Sphere plays a central role in our approximation. This approach is directly inspired by high order finite differencing in Computational Aeroacoustics (CAA) [5, 24]. In CAA, the main goal is to ensure an accurate numerical
propagation of linear waves or of weakly nonlinear waves. This is also a central objective in Geophysical Fluid Dynamics: linear waves related to SWE must be numerically advected over long physical intervals of time. Therefore a numerical scheme based on the same premises than compact schemes in CAA seems highly desirable, also in the GFD context.

Our finite difference approximation follows the principles introduced in [11, 12]. The basic idea is to use high order differencing along a set of great circles suitably associated to the structure of the equiangular Cubed Sphere. This great circles approach permits to handle the full sphere with the same periodic treatment. Doing so, there is no need of any one sided difference formulas to handle interpanel boundaries. This has been proved to be of great importance to preserve the accuracy over a large number of time iterations.

Compact formulas for the derivatives are commonly centered formulas. Enhancing stability is obtained by adding some numerical dissipation. A typical practice in CAA is to add a high frequency filtering at each time step. In our approach, performing such a filtering step has been found efficient as well.

The objective and the summary of this paper are as follows. In Section 2, we recall the background of our centered differencing along great circles on the Cubed Sphere [11, 12]. The three operators that are approximated are grad, div and curl also denoted as ∇, ∇T r and ∇T x, respectively. In the three cases, the approximation principle is similar.

In Section 3, the two time stepping used in our simulations are described. First, the explicit RK4 scheme is our reference time scheme. A CFL condition must be used with this scheme. Our second time stepping consists of two exponential schemes belonging to the Rosenbrock family. They have been compared with the RK4 scheme.

In Section 4, numerical results for (SWE) are shown for the isolated mountain, the Rossby-Haurwitz and the barotropic instability test cases. In each case, we show that our scheme compares favourably with high order conservative upwind methods, such as [2, 25, 41]. The accuracy is well preserved over a large number of time steps. In addition, all conserved quantities at the continuous level are as well remarkably well preserved at the discrete level. This includes the mass, the total energy, and the potential enstrophy. The meaning of this conservation is related to the quadrature formula on the Cubed Sphere in [29].

All the computations were performed in Matlab on a desktop computer.

2. A CENTER COMPACT SCHEME FOR THE SHALLOW WATER EQUATIONS ON THE CUBED SPHERE

Let \( S_a \) be the sphere of radius \( a \), \( (a = 6371 \text{ km for the earth}) \). The Shallow Water Equations let evolve the height and (tangent) wind velocity \((t, x) \in [0, +\infty] \times S_a \rightarrow (h(t, x), u(t, x)) \) by \((g \text{ is the gravity constant})\),

\[
\frac{\partial h^*}{\partial t}(t, x) + \nabla_T \cdot (h^*(t, x)u(t, x)) = 0
\]

\[
\frac{\partial u}{\partial t}(t, x) + \nabla_T \left( \frac{1}{2} |u(t, x)|^2 + gh(t, x) \right) + \left(f(x) + \zeta(x, u(t, x))\right)n(x) \times u(t, x) = 0
\]

This is the vector form of the Shallow Water Equation, [45]. The three given functions in (SWE) are

\[
\begin{align*}
  x \in S_a &\mapsto n(x) \in TS_a^\perp, \text{ exterior normal} \\
  x \in S_a &\mapsto f(x) \in \mathbb{R}, \text{ Coriolis force} \\
  x \in S_a &\mapsto h_s(x) \in \mathbb{R}_+, \text{ bottom topography.}
\end{align*}
\]

The relative vorticity \(\zeta(x, v(x))\) associated with the velocity field \(v(x)\) is the function defined by

\[
\zeta(x, v(x)) = (\nabla_T \times v(x)) \cdot n(x).
\]

The total height of the atmosphere is

\[
h^*(t, x) = h(t, x) - h_s(x).
\]

Denoting \((t, x) \in [0, +\infty] \times S_a^2 \rightarrow q(t, x) = [h(t, x), u(t, x)]^T \in \mathbb{R}^4\), (1) is expressed as

\[
\frac{\partial}{\partial t} q(t, x) = J(x, q(t, x)),
\]
with
\[ J(x, q(x)) = - \left( \begin{array}{c}
\nabla_T \cdot \left( (h(x) - h_s(x))u(x) \right) \\
\nabla_T \left( \frac{1}{2} |u(x)|^2 + gh(t, x) \right) + (f(x) + \zeta(x, u(x)) n(x) \times u(x)) \end{array} \right). \]

The notation \( C\mathbb{S}_a,N \) stands for the equiangular Cubed Sphere grid with radius \( a \) and parameter \( N \). \(^1\) We consider on \( \mathbb{S}_a \) the six panels \( k = (I),..., (VI) \) matching the faces of a cube. A typical panel is represented in Fig. 1. The local chart of each panel is the system of angles \((\xi, \eta)\) (local coordinates) are such that \(-\pi/4 \leq \xi, \eta \leq \pi/4\), with origin at the center of the panel. The vertices in panel \( k \) are denoted \( s_{k,j}^i \). The integer \( i \) (resp. \( j \)) denotes the index in the \( \xi \) direction (resp. \( \eta \) direction). A gridfunction defined on \( C\mathbb{S}_a,N \) consists of \( 6N^2 + 2 \) data located at \( s_{k,j}^i \), \(-N/2 \leq i, j \leq N/2 \) and \((I) \leq k \leq (VI) \). The step size is \( \Delta_N = \Delta\xi = \Delta\eta = \frac{\pi}{2N} \).

Proceeding along the method of lines, (1) is first approximated in space by the semi-discrete system
\[ \frac{d}{dt} q(t) = J_{\Delta_N}(s, q(t)). \]

The semidiscrete function \( q(t) \) \(^2\) is \( q(t) = [h(t), u(t)]^T \) where
\[ h(t) = [h_{k,j}^i(t)]^T, \quad u(t) = [u_{k,j}^i(t)]^T, \quad -N/2 \leq i, j \leq N/2, k \in \{(I),..., (VI)\}. \]

For \( f, g \), two given (scalar or vector) gridfunctions, the gridfunction \( \{ f \bullet g \} \) is defined by
\[ \{ f \bullet g \}_{k,j}^i = f_{k,j}^i g_{k,j}^i, \quad -N/2 \leq i, j \leq N/2, k \in \{(I),..., (VI)\}. \]

In the case of vector gridfunctions, one has \( \{ f \bullet g \}_{k,j}^i = f_{k,j}^i \cdot g_{k,j}^i \). Similarly \( \{ f \times g \}_{k,j}^i = f_{k,j}^i \times g_{k,j}^i \). The approximation of \( J \) on \( C\mathbb{S}_a,N \) is \( J_{\Delta_N} \) defined by
\[ J_{\Delta_N}(s, q) = - \left( \begin{array}{c}
\nabla_T,\Delta_N \left( h - \{ h_s(s) \bullet u \} \right) \\
\nabla_T,\Delta_N \left( \frac{1}{2} \{ u \bullet u \} + gh \right) + \{ (f(s) + \zeta_{\Delta_N}) \bullet (n(s) \times u) \} \end{array} \right). \]

\(^{1}\)Refer to [30] for different Cubed Sphere grids.

\(^{2}\)We adopt the fraktur font for gridfunctions, i.e. functions defined at the vertices of \( C\mathbb{S}_a,N \).
The gridfunction $\zeta_{\Delta N}$ is
\begin{equation}
\zeta_{\Delta N} = (\nabla_T, \Delta_N \times u) \cdot n(s).
\end{equation}
In (10), the operators $\nabla_{T,\Delta N}$, $\nabla_{T,\Delta N}$, and $\nabla_{T,\Delta N} \times$ are centered approximations of the operators $\nabla_T$, $\text{div}_T$ and $\text{curl}_T$, respectively. These approximations are defined as follows. Consider for example the discrete gradient $\nabla_{T,\Delta N}$. Let $\mathbf{x} \in \mathbb{S}_a \mapsto f(\mathbf{x})$ be a given function. The value of $f$ at the vertex $s_{i,j}^k$ is $f_{i,j}^k = f(s_{i,j}^k)$. Consider the panel (I) in Fig. 1. Fix an "horizontal" coordinate line (iso-$\eta$ line $\eta = j_0 \Delta_N$). This coordinate line is a great circle section. Consider next the extension of this coordinate line to the full great circle around the sphere $\mathbb{S}_a$. On panel (III), opposite to panel (I), this great circle again matches an iso $\eta$ coordinates line, this time with index $N - j_0$. On the contrary, on panels (II) and (IV), both adjacent to panel (I), this great circle does not coincide with any coordinate line. Next, define along this great circle a one dimensional grid associated with a set of data. On the panel (I) the grid coincides with the Cubed Sphere vertices $s_{i,j}^{(I)}$. The data at these vertices are the values $f_{i,j}^{(I)}$. We proceed similarly on panel (III). On panel (II), the great circle intersects each "vertical" coordinates line $\xi = \xi_i$. This intersection defines a point to which some interpolated value, deduced from data in panel (II) is assigned. A similar procedure is performed on panel (IV). Summing up, this results in a grid of size $4N$ of the considered great circle with constant step size $\Delta \xi = \Delta N$ and in a set of $4N$ periodic data along this circle. Then the finite difference $\delta_H^f f_p^k$, is applied to these data, using the relations
\begin{equation}
\frac{1}{6} \delta_H^f f_{p-1} + \frac{2}{3} \delta_H^f f_p + \frac{1}{6} \delta_H^f f_{p+1} = \frac{f_{p+1} - f_{p-1}}{2 \Delta \xi}.
\end{equation}
where the index $p = 1...4N$ stands for the index of the $4N$ periodic data along the great circle. The formal truncation error for $\delta_H^f f_p$ satisfies (assuming exact data at the gridpoints), [3]
\begin{equation}
\delta_H^f f_p - \partial_\xi f(s_p^k) = O(\Delta_N^4).
\end{equation}
Remark 2.1. The data on panels (II) and (IV) only serve as "ghost values". They permit to apply the periodic differencing (12) without taking care of any cut-off in panels (II) and (IV). After solving (12), only the finite difference values $\delta_H^f f$ located in panels (I) and (III) are retained and the values located in panels (II) and (IV) are discarded. We refer to [11, 12] for more details.

The computational procedure above is repeated for all the coordinate lines in the $\xi$ direction for panels (I), (II) and (V); and similarly in the $\eta$ direction for the same panels (I), (II) and (V). Due to the spherical symmetry, the couple of partial derivatives $(\partial_\xi f, \partial_\eta f)$ is approximated at each vertex of $\text{CS}_{a,N}$. Note that this way to proceed ensures a perfect symmetry in the calculation.

Considering effective accuracy, according to (13), one may expect fourth order accurate for the approximate derivative. However, due to the interpolation of the data in panels (II) and (IV), the accuracy possibly could drop to 3. In fact, the value $f_p$ assigned to point $m_p$ on the great circle satisfies
\begin{equation}
\begin{cases}
  f_p = f(m_p) & \text{if } m \text{ belongs to panels (I) or (III)}.
  f_p = f(m_p) + O(\Delta_N^3) & \text{if } m \text{ belongs to panels (II) or (IV)}.
\end{cases}
\end{equation}
Therefore it turns out that ($\Delta \xi = \Delta N$)
\begin{equation}
\frac{f_{p+1} - f_{p-1}}{2 \Delta \xi} = \frac{f(m_{p+1}) - f(m_{p-1})}{2 \Delta \xi} + O(\Delta \xi^3),
\end{equation}
which gives at the least
\begin{equation}
\delta_H^f f_p = \partial_\xi f(m_p) + O(\Delta \xi^3).
\end{equation}
In practice however, fourth order accuracy has been numerically observed so far. See also Section 4.6. The approximate gradient, divergence and curl are then calculated as follows. On the panel $k$, the local basis at the vertex $s_{i,j}^k$ is $(g_\xi, g_\eta)$ given by
\begin{equation}
g_\xi(s_{i,j}^k) = \frac{\partial \mathbf{x}}{\partial \xi}(s_{i,j}^k), \quad g_\eta(s_{i,j}^k) = \frac{\partial \mathbf{x}}{\partial \eta}(s_{i,j}^k).
\end{equation}
Refer to [11, 6] for the analytic expression of \((g_\xi, g_\eta)\). Let \(x \in S_\alpha \mapsto f(x)\) be a given function. We denote by \(f^*\) the restriction of \(f\) to the Cubed Sphere vertices:

\[(f^*)_k^{i,j} = f(s_k^{i,j}).\]

The divergence of \(f(x)\) is expressed at \(s_k^{i,j}\) in terms of the dual basis \((g_\xi, g_\eta)\) by

\[
\nabla_T f(s_k^{i,j}) = \frac{\partial f}{\partial \xi}(s_k^{i,j}) g_\xi^{i,j} + \frac{\partial f}{\partial \eta}(s_k^{i,j}) g_\eta^{i,j}.
\]

The partial derivatives \(\frac{\partial f}{\partial \xi}(s_k^{i,j})\) and \(\frac{\partial f}{\partial \eta}(s_k^{i,j})\) are approximated by the divided differences calculated by the above "great circle" procedure.

\[
\frac{\partial f}{\partial \xi}(s_k^{i,j}) \simeq \delta_\xi (f^*)_k^{i,j}, \quad \frac{\partial f}{\partial \eta}(s_k^{i,j}) \simeq \delta_\eta (f^*)_k^{i,j},
\]

Similarly, consider a vector function \(v(x)\). The associated gridfunction is \(v^*\) with components \((v^*)_k^{i,j} = v_k^{i,j}\).

The divergence and curl operators are expressed in local coordinates as [36]

\[
\begin{align*}
\nabla_T \cdot v &= \partial_\xi v \cdot g_\xi + \partial_\eta v \cdot g_\eta, \quad (a) \\
\nabla_T \times v &= g_\xi \times \partial_\xi v + g_\eta \times \partial_\eta v \quad (b).
\end{align*}
\]

The partial derivatives \(\partial_\xi v\) and \(\partial_\eta v\) are approximated at \(s_k^{i,j}\) by

\[
\partial_\xi v(s_k^{i,j}) \simeq \delta_\xi v_k^{i,j}, \quad \partial_\eta v(s_k^{i,j}) \simeq \delta_\eta v_k^{i,j}.
\]

The approximations considered in the sequel to the gradient, the divergence and the curl, are the gridfunctions \(\nabla_{T,A_N}\), \(\nabla_{T,A_N}^*\), and \(\nabla_{T,A_N} \times\), with components

\[
\begin{align*}
\left(\nabla_{T,A_N} f^*\right)_k^{i,j} &= (\delta_\xi f^*)_k^{i,j} g_\xi^{i,j} + (\delta_\eta f^*)_k^{i,j} g_\eta^{i,j} \quad (a), \\
\left(\nabla_{T,A_N} \cdot v^*\right)_k^{i,j} &= (\delta_\xi v^*)_k^{i,j} \cdot g_\xi^{i,j} + (\delta_\eta v^*)_k^{i,j} \cdot g_\eta^{i,j}, \quad (b), \\
\left(\nabla_{T,A_N} \times v^*\right)_k^{i,j} &= g_\xi^{i,j} \times (\delta_\xi v^*)_k^{i,j} + g_\eta^{i,j} \times (\delta_\eta v^*)_k^{i,j} \quad (c).
\end{align*}
\]

**Remark 2.2.** As mentioned in Remark 2.1, one may wonder if the redundancy in the "great circle" procedure could be avoided. For example, considering a small number of ghost points beyond the limit of a panel could give a smaller computational effort. In this spirit, the following alternative formula for the spherical divergence was suggested in [12], to which we refer for more details.

\[
\left(\nabla_T v^*\right)_k^{i,j} = \frac{1}{\sqrt{\det G}} \left( \partial_\xi \left( \sqrt{\det G} \cdot g_\xi^{i,j} \right)_k^{i,j} + \partial_\eta \left( \sqrt{\det G} \cdot g_\eta^{i,j} \right)_k^{i,j} \right).
\]

We have adopted here (23)\(_b\) in order to have an homogeneous treatment of all differential terms in (SWE).

### 3. Time discretisation

#### 3.1. Basic setup.

In Section 2, the spatial approximation of (1) was considered. Two kinds of time discretizations are used in Section 4. The reference time scheme is the standard RK4 scheme. The basic time marching algorithm is given in Algorithm 1.
Algorithm 1: Explicit Runge-Kutta Scheme of order 4 with filter

1: $q^0 = q^{(0)}$ given
2: for $n = 0, 1, \ldots \text{itemax}$ do
3:   $K^{(1)} = J_{\Delta N}(q^n)$,
4:   $K^{(2)} = J_{\Delta N}\left(q^n + \frac{\Delta t}{2}K^{(1)}\right)$,
5:   $K^{(3)} = J_{\Delta N}\left(q^n + \frac{\Delta t}{2}K^{(2)}\right)$,
6:   $K^{(4)} = J_{\Delta N}\left(q^n + \Delta tK^{(3)}\right)$,
7:   $q^{n+1} = F\left(q^n + \frac{\Delta t}{6}\left(K^{(1)} + 2K^{(2)} + 2K^{(3)} + K^{(4)}\right)\right)$.
8: end for

In line 7, at the end of each time step a filtering step is applied. The function $F$ is the filtering function. As already mentioned, this filtering step is commonly used in CAA\textsuperscript{3} simulations. For details, refer to [5] and the references therein. The filter step enhances the stability of the scheme, but with accuracy preserving. The design of the filter function $F$ in one dimension is recalled in Section 6.3. In two dimensions, the filter function is obtained by tensor product. In the case of the Cubed Sphere $CS_{a,N}$ we have used the following symmetric filter

$$F = \frac{1}{2}\left(F_\xi \circ F_\eta + F_\eta \circ F_\xi\right),$$

where the functions $F_\xi$ and $F_\eta$ correspond to a 10-th order filter in the last line in Table 4 in Section 6.3. This choice has been proved to be a good compromise between accuracy and stability.

Remark 3.1. The filter function $F_\xi$ operates along the great circles as a periodic difference operator in a fashion similar to the difference operator $\delta^H_\xi$; and similarly for $F_\eta$.

3.2. Two Rosenbrock time schemes. Beyond the RK4 time scheme mentioned above, we also have used two schemes of the Rosenbrock family [44, Ch. 7]. These schemes are particular examples of exponential time schemes. Recenlty, they have received interest for stiff problems as an alternative to implicit schemes. For flows over a sphere, refer to [9, 15]. With exponential time schemes, the stability constraint on the time step, related to the CFL condition in our case, is relaxed as when using an implicit time schemes. The damping of high frequency modes, which is a main goal of implicit time-stepping, is replaced with exponential schemes by the exact integration of the linear part of the source term. The design and convergence analysis of such schemes has been extensively documented. We refer to [22] for a recent review.

Consider the nonlinear differential system

$$\frac{dq}{dt} = F(q), \quad q(0) = q_0.$$  

where $t \geq 0 \mapsto q(t) \in \mathbb{R}^n$ is the semidiscrete vector in (7). The function $F : \mathbb{R}^n \mapsto \mathbb{R}^n$ represents the spatial discretisation in the RHS of (7). Consider the calculation of $q^{n+1}$ with $q^n$ assumed to be known. The source term $F(q)$ is decomposed as

$$F(q) = \mathcal{L}_n(q) + \mathcal{N}(q),$$

where $\mathcal{L}_n$ is the Jacobian of $F$ at $q^n$

$$\mathcal{L}_n = \text{Jac}_q F(q^n).$$

The system (26) is rewritten for $t \in [t^n, t^{n+1}]$ as

$$\begin{cases}
\frac{dq(t)}{dt} = \mathcal{L}_n(q(t)) + \mathcal{N}(q(t)) \\
q(t^n) = q^n
\end{cases}$$

}\textsuperscript{3}\text{Computational AeroAcoustics}
The exact solution of (27) is \( q(t^{n+1}) \). It is expressed at time \( t^{n+1} \) by

\[
q(t^{n+1}) = \exp(L_n \Delta t) q(t^n) + \int_0^\Delta t \exp(L_n(\Delta t - \tau) ) \mathcal{N}(q(t^n + \tau)) d\tau.
\]

The integral in the right-hand side of (30) is then approximated but with integrating the exponential "exactly". The function \( \mathcal{N} \) is approximated in a Runge-Kutta fashion.

The two following Rosenbrock schemes are used in the sequel:

- The exponentially fitted Euler method is given by
  \[
  q^{n+1} = q^n + \Delta t \varphi_1(\Delta t L_n) F(q^n),
  \]
  where the function \( z \mapsto \varphi_1(z) \) is
  \[
  \varphi_1(z) = (\exp(z) - 1)/z.
  \]
  
  The scheme (31) is second order in time. It requires one matrix vector product per time iteration.

- The second Rosenbrock time scheme used in Section 4 is
  \[
  \begin{align*}
  a^n &= q^n + \Delta t \varphi_1(\Delta t L_n) F(q^n), \\
  q^{n+1} &= a^n + 2\Delta t \varphi_3(\Delta t L_n) (\mathcal{N}(a^n) - \mathcal{N}(q^n)).
  \end{align*}
  \]
  
  The function \( \varphi_3(z) \) is
  \[
  \varphi_3(z) = (\exp(z) - 1 - z - z^2/2)/z^3.
  \]
  
  The scheme (33) is third order in time. Two matrix vector products are required per time step.

For (31) and (33), the filtering step takes place after each time step. In each case, the time stepping has the following form:

\begin{algorithm}
\caption{Algorithm 2 : Rosenbrock time scheme of order 2 or 3 with filtering step}
1: \( q^0 = q^{(0)} \) given, \\
2: \textbf{for} \( n = 0, 1, \ldots, \text{itemax} \) \textbf{do} \\
3: \hspace{1em} Compute \( \tilde{q}^{n+1} \) using (31) or (33) \\
4: \hspace{1em} Compute \( q^{n+1} = F(\tilde{q}^{n+1}) \). \\
5: \textbf{end for}
\end{algorithm}

In the particular case of (1), the linear operator \( L_n \) is given by discretizing the continuous Jacobian of \( F(q) \) at the gridfunction \( q^n = [b^n, u^n]^T \) with perturbation \( q' = [b', u']^T \). It is given by, (see (9) for the notation),

\[
L_n(q') = - \begin{bmatrix}
\nabla_{T,A} \Delta_N \left( \{u^n \cdot b'\} + \{u' \cdot (b^n - h_s(s))\} \right) \\
\n\nabla_{T,A} \Delta_N \left( gh' + \{u^n \cdot u'\} \right) + \left\{ f(s) + \zeta_{\Delta_N}(s,u^n) \right\} \cdot (n(s) \times u') + \left\{ \zeta_{\Delta_N}(s,u') \cdot n(s) \right\} \times u^n
\end{bmatrix}.
\]

The function \( (s,u) \mapsto \zeta_{\Delta_N}(s,u) \) is given in (11).

Remark 3.2. The operator \( L_n \) in (35) acting on a gridfunction \( q' \) can be equivalently defined as the linearisation at \( q^n \) of the discretisation \( F(q) \).

3.3. Krylov method in Rosenbrock schemes. As explained in [28], implementing a Rosenbrock scheme such as (31) or (33) relies on efficiently evaluating matrix vector products of the form \( \varphi_1(A)b \) with \( A \) the matrix \( \Delta t L_n \Delta t \), and \( b \) a vector. The function \( z \mapsto \varphi_1(z) \) is a complex function related to the exponential \( z \mapsto \exp(z) \). Approximating \( \varphi_1(A)b \) is based on the Krylov method.

For \( A \in \mathcal{M}_N(\mathbb{R}) \) a given matrix and \( b \in \mathbb{R}^N \), fix \( m \leq N \). The Krylov space \( \mathcal{K}_m = \mathcal{K}_m(A,b) \) is the subspace of \( \mathbb{R}^N \) defined by

\[
\mathcal{K}_m(A,b) = \text{Span} \left\{ b, Ab, A^2b, \cdots, A^{m-1}b \right\}.
\]

The integer \( m \) is selected as follows, [21, 40]. First \( m \) must be picked small enough to efficiently evaluate \( \varphi_1(H_m) \). On the other hand it must be large enough to have an accurate approximation of \( Ab \). Typical
values of \( m \) are reported in Section 4. Krylov spaces are commonly used to approximate a matrix vector product \( f(A)b \) by the Arnoldi method. This idea is the basis for the resolution of large sparse linear systems [32, 33, 42] in the GMRES method. Here the Arnoldi algorithm [32] is used as follows

- Calculate the matrix \( H_m \in \mathbb{M}_m(\mathbb{R}) \), the projection of \( A \) on \( \mathcal{K}_m \). The matrix \( H_m \) is expressed as
  \[
  H_m = V_m^T A V_m.
  \]
  where the matrix \( V_m \in \mathbb{M}_{N,m}(\mathbb{R}) \) has orthonormal columns.
- Approximate \( A \) by
  \[
  A \approx V_m H_m V_m^T.
  \]
- Approximate the vector \( \varphi_l(A)b \) by
  \[
  \varphi_l(A)b \approx V_m \varphi_l(H_m)V_m^T b = \|b\|_2 V_m \varphi_l(H_m)e_1
  \]
  where \( e_1 \in \mathbb{R}^m \) is the first vector in the canonical basis of \( \mathbb{R}^N \).

The evaluation of \( \varphi_l(H_m) \) is obtained by the method in [37]. A rational Padé approximation of \( \varphi_l(z) \) is used. In addition, scaling and squaring are used to avoid errors in the case where \( \|H_m\| \gg 1 \).

4. Numerical results for the Shallow Water equation

4.1. Introduction. In this section, we report numerical results obtained for (1) using the scheme (7) and either the time scheme RK4 or one of the two Rosenbrock scheme (31) or (33).

Four standard test cases are considered. The three first test cases are the tests 2, 5 and 6 in [45]. They are referred to as the time-independent geostrophic flow, the isolated mountain and the Rossby-Haurwitz case. The fourth test case is the barotropic instability in [14]. In all cases, our numerical results are compared to the ones in the literature. The conservation properties of our scheme are numerically evaluated.

The physical constants are \( a = 6.37122 \times 10^6 \text{m} \) (earth radius), \( \Omega = 7.292 \times 10^{-5} \text{s}^{-1} \) (earth angular velocity), and \( g = 9.80616 \text{m} \cdot \text{s}^{-2} \) (gravity constant). The Coriolis force in (2) is given by \( f(x) = 2\Omega \sin \theta \), where \( \theta \) is the latitude angle. We call \( I_1, I_2 \) and \( I_3 \) the following mean values, which are invariants of (1).

\[
\begin{align*}
\text{mass} : I_1 & = \int_{s_2} (h - h_s) ds, \\
\text{energy} : I_2 & = \int_{s_2} \left( \frac{1}{2} (h - h_s)|u|^2 + \frac{1}{2} g(h^2 - h_s^2) \right) ds, \\
\text{potential enstrophy} : I_3 & = \int_{s_2} \frac{(\zeta + f)^2}{2(h - h_s)} ds.
\end{align*}
\]

The numerical error for \( I_1, I_2 \) and \( I_3 \) is reported using the relative value

\[
\frac{I_{p}(t) - I_{p}(0)}{I_{p}(t)} \quad \text{for } p = 1, 2, 3.
\]

Since the discrete unknown is the gridfunction \( q^n \), and not discrete averages in cells, the meaning of the discrete version of the averages must be given. All the approximate averages in (40) are calculated using the Cubed Sphere quadrature rule \( Q_\alpha \) in [29].

4.2. Time-independent geostrophic flow. Our first test consists in calculating a particular time independent geostrophic flow of (1) (test 2 in [45]). There is no bottom topography i.e. \( h_s(x) = 0 \). The Coriolis force is

\[
f(x) = 2\Omega (-\cos \lambda \cos \theta \sin \alpha + \sin \theta \cos \alpha).
\]

The angles \((\lambda, \theta)\) are the lon/lat system of coordinates. The parameter angle \( \alpha \) is the angle between the zonal axis with the \( Oz \) axis. Picking up different values of \( \alpha \) permits to evaluate the influence of the position of the
Cubed Sphere with the solution. In our case, it permits to see if there is some interpanel parasitic reflection with our scheme. The exact solution is \( q(x) = [h(x), u(x)]^T \), with \( u(x) = u(x)e_\lambda(x) + v(x)e_\theta(x) \) and

\[
\begin{align*}
    h &= h_0 - \frac{1}{g} \left( a\Omega u_0 + \frac{u_0^2}{2} \right) (-\cos \lambda \cos \theta \sin \alpha + \sin \theta \cos \alpha)^2, \\
    u &= u_0(\cos \theta \cos \alpha + \cos \lambda \sin \theta \sin \alpha), \\
    v &= -u_0 \sin \lambda \sin \alpha.
\end{align*}
\]

The constants \( h_0 \) and \( u_0 \) are given by \( gh_0 = 2.94 \times 10^4 \text{m}^2\text{s}^{-2} \) and \( u_0 = 2\pi a/(12\text{days}) \) (in m \cdot s\(^{-1}\)). Starting from (43) as initial data, the scheme (26) is used, integrated in time by the RK4 scheme. A calculated asymptotic in time state is compared to the initial data. Fig. 2 shows the convergence slope for the relative error \( |h - h^*|/|h^*| \) between the steady state \( h \) computed with the RK4 scheme and the exact value \( h^*(s) \) at the grid vertices. Our finest grid is \( 64 \times 6 \times 6 \) with a time step \( \Delta t = 300 \) seconds, corresponding to CFL \( \simeq 1 \) at the equator. The asymptotic state is observed at day 5. This approximately corresponds to 1500 iterations in time. As seen in Fig. 2 both values \( \alpha = 0 \) and \( \alpha = \pi/4 \) give a sharp 4-th order accuracy. A very good error level is obtained in both cases. Furthermore, there is no visible influence of the angle \( \alpha \).

4.3. Isolated mountain test case. This is the test 5 in [45]. It is a time dependant case without analytical solution. The initial data is (43) with the parameters \( h_0 = \text{5960m}, u_0 = 20\text{m} \cdot \text{s}^{-1} \) and \( \alpha = 0 \). This initial data is perturbed by a conic mountain located at the point \((\lambda_c, \theta_c)\) on \( S_a \). The bottom topography function \( h_s(x) \) is

\[
\begin{align*}
    h_s(x) &= h_{s_0} \left( 1 - \frac{r(x)}{r_0} \right), \quad h_{s_0} = 2000\text{m}, \\
    r &= \min \left( r_0, \sqrt{\lambda - \lambda_c)^2 + (\theta - \theta_c)^2} \right), \quad r_0 = \pi/9, (\lambda_c, \theta_c) = (3\pi/2, \pi/6).
\end{align*}
\]

Fig. 3 reports the total height \( h(x) \) at day 15. A coarse Cubed Sphere \( 32 \times 32 \times 6 \) is used. The time schemes RK4 and the two Rosenbrock schemes (31) and (33) are used. The isolines are close to those obtained by the conservative schemes in [8, 41]. Fig.4 shows the conservation history for the approximate values \( I_p, p = 1 \ldots 3 \). At day 15, the relative mass conservation is below \( 10^{-5} \) in all cases. The mass curve is increasing for the RK4 scheme. It is slightly decreasing with the two Rosenbrock schemes whose curves are superposed. This indicates a good mass conservation property of the spatial approximation. The energy error curves...
Figure 3. Isolated mountain test case at time of 15 days. The total height $h$ is represented. The coarse Cubed Sphere $32 \times 32 \times 6$ is used. The contour line are plotted from 5050m to 5950m with interval of 50m. Top Left : solution using the Rosenbrock time scheme (31). Top Right : Rosenbrock time scheme (33). In both case the time step is $\Delta t = 4h$ (CFL $\simeq 20$). Bottom : solution using RK4 with $\Delta t = 1\text{min}$ (CFL $\simeq 0.9$). The results are almost identical.

present a behaviour similar to the mass error curves with the same relative error magnitude. At day 15, the magnitude of the relative error in potential enstrophy is $10^{-5}$ ($N = 32$) using the Rosenbrock time scheme (31) or (33). The RK4 curve shows a larger dissipation in the enstrophy, reaching a relative error of $10^{-4}$. This is the same error level than with a FV scheme [8, 41], the magnitude of this error is $10^{-4}$. The curves clearly show that the magnitude of the errors depend on the time scheme. The two Rosenbrock schemes give better conservation results in all cases.

Finally, we report in Table 1 the numerical data used in the Arnoldi method when using the Rosenbrock schemes (31) and (33).

Figure 4. Isolated mountain test case with a grid Cubed Sphere $32 \times 32 \times 6$. Conservation error $(I_q(t) - I_q(0))/I_q(0)$. Left panel : mass ($q = 0$). Center panel : energy ($q = 1$). Right panel : potential enstrophy ($q = 2$). Exp. Int. 3 and Exp. Int. 2 correspond to Rosenbrock methods (33) and (31) respectively, both with $\Delta t = 4h$ (CFL $\simeq 20$). The scheme RK4 is considered with $\Delta t = 1\text{min}$. (CFL = 0.9).
4.4. Rossby-Haurwitz test case. The Rossby-Haurwitz is the test 6 in [45]. It is an analytical solution of the nonlinear barotropic vorticity equation [27]. Although this equation is different from the equation (1), it is used to assess the qualitative behaviour of numerical schemes for (1). The initial velocity is $u(x) = u(x)e_\lambda(x) + v(x)e_\varphi(x)$ with

$$
\begin{align*}
    u(x) &= a_\omega \cos \theta + aK \cos \theta \cos \theta \sin \theta \cos R\lambda, \\
    v(x) &= -aKR \cos \theta \sin \theta \sin R\lambda.
\end{align*}
$$

The initial height $h(t = 0, x)$ is:

$$
h(t = 0, x) = gh_0 + a^2 A(\theta) + a^2 B(\theta) \cos R\lambda + a^2 C(\theta) \cos 2R\lambda.
$$

The functions $A$, $B$ and $C$ are:

$$
\begin{align*}
    A(\theta) &= \frac{\omega}{2}(\Omega + \omega) \cos^2 \theta + \frac{1}{4} K^2 \cos^2 \theta \left[ (R + 1) \cos^2 \theta + (2R^2 - R - 2) - 2R^2 \cos^2 \theta \right], \\
    B(\theta) &= \frac{2(\Omega + \omega)K}{(R + 1)(R + 2)} \cos \theta \left[ (R^2 + 2R + 2) - (R + 1)^2 \cos^2 \theta \right], \\
    C(\theta) &= \frac{1}{4} K^2 \cos 2R\theta \left[ (R + 1) \cos^2 \theta - (R + 2) \right].
\end{align*}
$$

The constants are $\omega = K = 7.848 \times 10^{-6}$ s$^{-1}$, $h_0 = 8 \times 10^3$m and $R = 4$. The function $h$ at day 14 is reported in Fig. 5 with a Cubed Sphere $80 \times 80 \times 6$. The time schemes RK4, and the two Rosenbrock schemes (31) and (33) have been used. For this test, the minimal resolution for accurate results has been found as $80 \times 80 \times 6$. With this grid, the conservation history is reported in Fig. 6 for the first 14 days. The mass conservation is excellent in all cases. As for the isolated mountain, the mass conservation error level is even smaller when using any of the two Rosenbrock schemes ($10^{-8}$) than with the RK4 scheme ($6 \times 10^{-8}$). The energy error curves display an oscillating behaviour for each of the two the Rosenbrock schemes. In all cases, the magnitude of the relative energy error is below $2.5 \times 10^{-6}$, which is very good. This is one order of magnitude better than $5 \times 10^{-4}$, obtained in [15]. The magnitude of the relative error on the potential <potential > is $8 \times 10^{-4}$ compared to $5 \times 10^{-4}$ obtained in [15]. For the enstrophy, the RK4 scheme and the two Rosenbrock schemes perform similarly. Table 2 reports the numerical data used when using the Rosenbrock schemes (31) and (33).

<table>
<thead>
<tr>
<th>Method</th>
<th>Time step</th>
<th>CFL</th>
<th>Number of Krylov vectors</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rosenbrock scheme (31)</td>
<td>$\Delta t = 2h$</td>
<td>CFL $\simeq 27$</td>
<td>56 for $\varphi_1$</td>
</tr>
<tr>
<td>Rosenbrock scheme (33)</td>
<td>$\Delta t = 2h$</td>
<td>CFL $\simeq 27$</td>
<td>56 for $\varphi_1$ and 50 for $\varphi_3$</td>
</tr>
</tbody>
</table>

Table 2. Rosenby-Haurwitz case on a Cubed Sphere $80 \times 80 \times 6$ (38402 points). The final time is 14 days. Maximum number of Krylov vectors used to calculate $\varphi_l(L_n)b$. The matrix $L_n$ is full.

4.5. Barotropic instability. The last test is the barotropic instability in [14]. The initial condition is $q = \bar{q} + q'$ with the steady state $\bar{q} = (\bar{h} = h^*, \bar{u} = u^*)$ where $(h, u)$ is a time independent zonal solution of
Figure 5. Numerical results of the Rossby-Haurwitz test case with the grid $80 \times 80 \times 6$ at day 14. The contour lines are plotted from 8100m to 10500m with interval of 100m. Top Left: Rosenbrock scheme (33). Top Right: Rosenbrock scheme (31). Both with $\Delta t = 2h$. (CFL $\simeq 27$). Bottom: solution using RK4 with $\Delta t = 300$sec. (CFL $\simeq 1$). The differences between the plots are small.

Figure 6. Rossby-Haurwitz test case with the grid $80 \times 80 \times 6$. Conservation error $(I_q(t) - I_q(0))/I_q(0)$. Left panel: mass ($q = 0$). Center panel: energy ($q = 1$). Right panel: potential enstrophy ($q = 2$). Exp. Int. 3 and Exp. Int. 2 correspond to Rosenbrock methods (33) and (31) respectively, both with $\Delta t = 2h$ (CFL $\simeq 27$). The scheme RK4 is considered with $\Delta t = 300$sec. (CFL $\simeq 1$). In this case, we remark difference in Rosenbrock scheme contrary to previous case.

(1). The perturbation is $q'(t = 0) = (ht, *, 0)$. The steady state $\bar{q} = (\bar{h}^*, \bar{u}^*)$ with $\bar{h}$ and $\bar{u}$ given by in terms of $(\lambda, \theta)$ by

$$
\begin{align*}
\bar{h}(\lambda, \theta) &= h_0 - \frac{1}{g} \int_{\theta}^{\theta} au_\lambda(\tau) \left( f + \frac{\tan \tau}{a} u_\lambda(\tau) \right) d\tau, \\
u(\lambda, \theta) &= u_\lambda(\theta)e_\lambda,
\end{align*}
$$

(48)
with \( u_\lambda(\theta) = u_{\max} \psi(\theta) \) and the function \( \psi(\theta) \) given by

\[
\psi(\theta) = \begin{cases} 
0 & \text{if } \theta \leq \theta_0, \\
\frac{1}{e_n} \exp \left( \frac{1}{(\theta - \theta_0)(\theta - \theta_1)} \right) & \text{if } \theta_0 \leq \theta \leq \theta_1, \\
0 & \text{if } \theta_1 \leq \theta.
\end{cases}
\]

and \((\theta_0, \theta_1) = (\pi/7, \pi/2 - \theta_0), u_{\max} = 80 \text{ m} \cdot \text{s}^{-1}\). The height \( h_0 \) is such that the mean value of \( h \) over the sphere \( \mathbb{S}_n^2 \) be \( 10^4 \text{ m} \). The perturbation \( h'(x) \) is

\[
h'(\lambda, \theta) = \hat{h} \cos \theta \exp \left[ -\left( \frac{\lambda}{\alpha} \right)^2 \left( \frac{\theta_2 - \theta}{\beta} \right)^2 \right],
\]

with \( \hat{h} = 120 \text{ m}, \alpha = 1/3, \beta = 1/15 \) and \( \theta_2 = \pi/4 \). As mentioned in [38], this test is challenging for a Cubed Sphere discretization since the perturbation is located between the two panels (I) and (V), thus possibly giving some interpanel instability. In addition, the largest magnitude of \( \nabla_T h \) is located near panel (V) boundary. In Fig. 7, the contour lines of the vorticity are represented at day 6 for the grid \( 96 \times 96 \times 6 \). The results are similar to those in \([8, 41]\). As mentionned in \([41]\), the grid \( 32 \times 32 \times 6 \) is too coarse to accurately represent the initial data. The history of the conserved quantities is reported in Fig. 8 with the grid \( 96 \times 96 \times 6 \). Again in all cases, the relative errors are better evaluated with the two Rosenbrock schemes than with the RK4 scheme. For the two Rosenbrock schemes, the relative errors for the mass and for the energy are \( 10^{-8} \) and \( 10^{-6} \) respectively. As before, the relative potential enstrophy is challenging to preserve. The relative error at day 6 has an order magnitude of \( 10^{-3} \). The numerical parameters when implementing the Rosenbrock schemes (31) and (33) are given in Table 3.

<table>
<thead>
<tr>
<th>Method</th>
<th>Time step</th>
<th>CFL</th>
<th>Number of Krylov vectors</th>
</tr>
</thead>
<tbody>
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<td>85 for ( \varphi_1 )</td>
</tr>
<tr>
<td>Rosenbrock scheme (33)</td>
<td>( \Delta t = 1h )</td>
<td>CFL ( \approx 16 )</td>
<td>85 for ( \varphi_1 ) and 76 for ( \varphi_3 )</td>
</tr>
</tbody>
</table>

**Table 3.** Barotropic instability case on the Cubed Sphere \( 96 \times 96 \times 6 \), (55298 points). The final time is 6 days. Maximum number of Krylov vectors used to calculate \( \varphi_1(L_n) h \). The matrix \( L_n \) is full.

### 4.6. General comments on the numerical results.
Two conclusions can be drawn from our numerical results. First, the approximation in space shows a very good accuracy. This accuracy is close to 4 as shown in Section 4.2. Furthermore this accuracy is not associated with an interpanel effect of any kind. This is an important property of our spatial approximation. Such an interpanel effect can be present, depending on the type of the Cubed Sphere and on the approximation procedure that are used, [31]. This good behavior is attributed to the Hermitian derivative procedure along the full great circles presented in Section 2. Concerning the stability of the convective term in (1) we never found useful to introduce any upwinding. The mathematical properties of this computational procedure remain to analyze in more detail. Note that an alternative way to interpolate the data of the Cubed Sphere to the set of great circles could be considered. A possibility could be to use some discrete Spherical Harmonics discrete basis associated to the Cubed Sphere. So far however, the cubic spline procedure presented in 2) has been found simple and efficient.

Our second conclusion concerns the Rosenbrock schemes (31) and (33). On the one hand, the numerical results are similar to the ones obtained with the RK4 scheme. However, the relative conservation errors are better with the Rosenbrock schemes than with the RK4 scheme. A much larger CFL number can be used with the Rosenbrock schemes than with the RK4 scheme. This fact is expected, according to the theory of the exponential time schemes [22]. However this is not per se an essential issue, since the choice of the time step also depends on the physical phenomena to be simulated. What is found in the present study is that the test cases considered can be run using large time steps. As mentioned in [15], the real issue is to better analyze the computational cost of the Rosenbrock approach using the Krylov procedure in Section 3.3.
Figure 7. Numerical results of the Barotropic instability with the grid $96 \times 96 \times 6$ at day 6. Contour lines of vorticity are plotted. Top: Rosenbrock scheme (33). Center: Rosenbrock scheme (31). Both with $\Delta t = 1h$ (CFL $\simeq 16$). Bottom: RK4 scheme with $\Delta t = 240s$. (CFL $\simeq 1$). There is no significative differences. Note the absence of interpanel instabilities.

Figure 8. Conservation error for the Barotropic instability with the grid $96 \times 96 \times 6$. The conservation error $(I_q(t) - I_q(0))/I_q(0)$. Left panel: mass ($q = 0$). Center panel: energy ($q = 1$). Right panel: potential enstrophy ($q = 2$). Exp. Int. 3 and Exp. Int. 2 correspond to the Rosenbrock schemes (33) and (31) respectively, both with $\Delta t = 1h$ (CFL $\simeq 16$). The time step for the RK4 scheme is $\Delta t = 240s$. (CFL $\simeq 1$).
5. Conclusion

The finite difference approach in GFD simulations was introduced in early works, [34, 1]. Recently, despite of several contributions as [16], this approach has received significantly less attention than the conservative approach stemming from compressible CFD. The present contribution belongs to this category.

The main ideas of the center spatial approximation were introduced in [11, 12] and worked out in [6]. As mentioned in the introduction, this approach is closely related to the standard numerical approach to Computational Aeroacoustics (CAA) by compact schemes. The guiding idea of the present work is that the fluid regime in the test cases presented is closer to the linear regime or to the weakly nonlinear regime than to a strongly nonlinear regime. This makes the GFD flow motion closer from a low Mach number flow than from a shock wave regime. For this reason, centered differencing for the convective term, in a fashion close to the one in CAA, seems a relevant option.

Regarding conservation, the numerical evaluation of integral quantities to be preserved did not reveal any particular misbehaviour with our approach. The numerical results for all the cases tested so far showed sharp fourth order accuracy and very good stability properties. This was found true independently of the particular time stepping scheme used, RK4 or any of the two Rosenbrock schemes considered (31) or (33). These results support the fact that focusing on accuracy in the weakly nonlinear regime is an important challenge for the future of GCM development.

Beyond numerical analysis, many questions remain open. A first question is whether some more nonlinear flow regime in climatology would require more advanced filtering as in [10, 46]. Parallel to this question is which kind of flows in GFD really require upwinding in one form or another.

Another issue is how to efficiently implement the approximation suggested in this paper, as well as how to design some grid refinement procedure. This will be considered in future work. Finally, more complex physical modeling including several layers of shallow water to handle three-dimensional atmospheric flows will be considered as well.

6. Appendix: Numerical analysis

In this section, we gather several numerical analysis facts related to the approximation used in this study. The results are limited to the model problem of the linear convection equation in the periodic setting. Although purely linear and one dimensional, these results were not found in the existing literature.

6.1. Convergence analysis. The approximation in space in Section 2 is based on the standard Hermitian approximate derivative. Consider a regular finite difference grid with stepsize $h > 0$ and periodic data located at point $x_j = jh$, $j = 0, 1, \ldots, N - 1$. To any gridfuncion $w = [w_0, w_1, \ldots, w_{N-1}]$, the Hermitian derivative $\delta^H_w$ is defined by

$$\delta_x w_j - \sigma_x (\delta^H_x w)_j = 0, \quad 0 \leq j \leq N - 1,$$

where the operators $\sigma_x$ and $\delta_x$ are defined by

$$\sigma_x v_j = \frac{1}{6} v_{j-1} + \frac{2}{3} v_j + \frac{1}{6} v_{j+1}, \quad \delta_x v_j = \frac{v_{j+1} - v_{j-1}}{2h}, \quad 0 \leq j \leq N - 1.$$

In it well known that $\delta^H_x w$ is a fourth order approximation to the derivative. It is easily shown that an uniform estimate of the truncation error $\tau$ is given by

$$||\tau||_\infty \leq \hat{C} h^4 ||\partial_x^5 u^*||_{\infty,(0,L)}, \quad \hat{C} = 1/60.$$

Next, consider the linear convection equation for the scalar function $u(t, x)$

$$\partial_t u + c\partial_x u = 0, \quad x \in \Omega = (0, L), \quad t \geq 0, \quad c > 0,$$

with periodic conditions at $x = 0$ and $x = L$. The semidiscrete compact scheme is:

$$\frac{d}{dt} v_j(t) + c\delta^H_x v_j(t) = 0.$$

This scheme is a standard approximation for convection problems. Refer to [24, 20] and the references therein. Note that the total mass $h \sum_{j=0}^{N-1} v_j(t)$ is constant in time, which expresses a conservation property of (55).
An elementary convergence analysis, based on the energy method, for the scheme (55) is now carried out as follows. We denote the norm $|u|_h$

$$|u|_h = \left( h \sum_{j=0}^{N-1} |u_j|^2 \right)^{1/2}, \quad \|w\|_{h,\infty} = \max_{0 \leq j \leq N-1} |w_j|.$$  

The error $e_j(t) = u_j^*(t) - v_j(t)$ evolves along the system

$$\frac{d}{dt} e_j(t) = c \left( \tau_j(t) - \delta_x^h e_j(t) \right), \quad 0 \leq j \leq N - 1.$$  

Taking the $(.,.)_h$ scalar product of (57) with $e(t)$ gives (the antisymmetry of $\delta_x^h$ is used):

$$2 \left( \frac{d}{dt} e(t), e(t) \right)_h = 2c \left( \tau(t), e(t) \right)_h.$$  

Let $\alpha > 0$ be a fixed parameter to be specified latter. The equation (58) implies

$$\frac{d}{dt} |e(t)|^2_h \leq c \left( \alpha |\tau(t)|^2_h + \frac{1}{\alpha} |e(t)|^2_h \right).$$  

Applying the Gronwall Lemma easily gives that for $t$ fixed, $e(t)$ satisfies the estimate

$$|e(t)|^2_h \leq \tilde{C}^2 f_{\min} Lc^2 h^8 \|\partial_x^{(5)} u\|^2_{\infty,[0,T] \times [0,L]}, \quad 0 \leq t \leq T.$$  

where $f_{\min} = \min_{x>0} (x^2(e^{1/x} - 1))$. Is is easily shown that $f_{\min} \leq 1.545$. Defining the constant $\tilde{C} = \sqrt{T_{\min}} \approx 2.08 \times 10^{-2}$, we obtain finally the following

**Proposition 6.1.** Let $u_j^* = u(t,x)$ be the exact solution of (54) at points $x_j$ and $v_j(t)$ be the solution of semidiscrete scheme (55). The error $e_j(t) = u^*(t) - v_j(t)$ satisfies the fourth order error estimate

$$|e_j(t)|_h \leq C(t) h^4 \|\partial_x^{(5)} u\|_{\infty,[0,T] \times [0,L]}, \quad 0 \leq t \leq T,$$

where $C(t) = \tilde{C} \sqrt{T_{\min}}$ and $\tilde{C} \approx 2.08 \times 10^{-2}$ is a universal constant.

The estimate (61) shows a linear evolution of the constant $C(t)$ in time from $t = 0$ to $t = T$.

**Remark 6.2.** The estimate (61) shows fourth order accuracy in the grid dependent norm $|.|_h$. Note that the maximum norm estimate is more difficult to prove. Note also that the practical interest of Prop. 6.1 is limited to the constant velocity and regular grid cases.

### 6.2. Matrix stability analysis of the fully discrete scheme.

In this section, we show how to derive analytically the matrix stability condition for (55) when discretized in time by the RK4 scheme. Let $V(t) = [v_0(t), v_1(t), \ldots, v_{N-1}(t)]^T$. The equation (55) is equivalent to the vector equation

$$\left\{ \frac{d}{dt} V(t) = -\frac{c}{h} J V(t), \right\}$$

$$\quad \quad V(0) = V_0 = [u_0^*, u_1^*, \ldots, u_{N-1}^*]^T,$$

where $J$ is the $N \times N$ matrix defined by $(J v)_j = \delta_x^H v_j$. Let $P$ be the matrix of the left shift operator $u_j \mapsto u_{j-1}$ with $N-$ periodic data.

$$P = \begin{bmatrix} 0 & 1 & (0) & \cdots & \cdots & 1 \\ 0 & 0 & (0) & \cdots & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots & \cdots & \vdots \\ 1 & \cdots & \cdots & 0 & (0) & 1 \end{bmatrix}_{N \times N}.$$  

The matrix $J$ is $J = m(P)$ where

$$m(z) = \frac{1}{2} \frac{z - z^{-1}}{\left( z + z^{-1} \right) + \frac{2}{3}}.$$
The matrices $P$ and $J$ are expressed as

\begin{align}
P &= \sum_{k=\frac{-N}{2}}^{\frac{N}{2}} \omega^k R^k \otimes (R^k)^H, \\
J &= \sum_{k=\frac{-N}{2}}^{\frac{N}{2}} m(\omega^k) R^k \otimes (R^k)^H.
\end{align}

where $R^k = [R^k_0, R^k_1, \ldots, R^k_{N-1}]^T \in \mathbb{C}^N$ is the vector with components

\begin{equation}
R^k_j = \frac{1}{\sqrt{N}} \omega^{kj}, \quad 0 \leq j \leq N - 1, \quad \omega = \exp\left(\frac{2i\pi}{N}\right).
\end{equation}

Using that $V(t) = \exp(-\frac{c}{h} J)V_0$ yields

\begin{equation}
V(t) = \sum_{k=\frac{-N}{2}}^{\frac{N}{2}} \exp\left(-\frac{c}{h} m(\omega^k)t\right)((R^k)^H V_0) R^k.
\end{equation}

Consider now the time stepping of (62) by the RK4 scheme, [44, Chap. IV.2, pp. 16-18]. Since the matrix $-cJ/h$ is constant, the RK4 time stepping coincides with the vector iteration

\begin{equation}
V^{n+1} = r(-\lambda J)V^n,
\end{equation}

where $\lambda = c\Delta t/h > 0$ is the Courant number and $r(z)$ is the truncated exponential series

\begin{equation}
r(z) = 1 + z + \frac{z^2}{2!} + \frac{z^3}{3!} + \frac{z^4}{4!}.
\end{equation}

Using (66) gives that $V^n$ is

\begin{equation}
V^n = \sum_{k=\frac{-N}{2}}^{\frac{N}{2}} [r(-\lambda m(\omega^k))]^n ((R^k)^H V_0) R^k.
\end{equation}

The sequence (71) is bounded if and only if

\begin{equation}
\max_{k=\frac{-N}{2}}^{\frac{N}{2}} |r(-\lambda m(\omega^k))| \leq 1.
\end{equation}

This is equivalent to

\begin{equation}
\lambda \max_{k=\frac{-N}{2}}^{\frac{N}{2}} |m(\omega^k)| \leq K_{RK4},
\end{equation}

where $K_{RK4} = 2\sqrt{2}$ is defined by

\begin{equation}
K_{RK4} = \max \{ b, \text{ where } a + ib \in D_{RK4} \} = 2\sqrt{2},
\end{equation}

where $D_{RK4}$ is the domain of stability of the RK4 scheme, [44, Chap. IV.2, p. 18]. The condition (73) is rewritten as

\begin{equation}
\lambda \max_{k=\frac{-N}{2}}^{\frac{N}{2}} \left( \frac{\sin\left(\frac{2k\pi}{N}\right)}{\frac{2}{3} + \frac{1}{3} \cos\left(\frac{2k\pi}{N}\right)} \right) \leq K_{RK4},
\end{equation}

or equivalently

\begin{equation}
\lambda \leq 2\sqrt{2/3}.
\end{equation}

We have proved the matrix stability analysis result:

\footnote{For $X$ a $n \times m$ matrix, $X^H = X^T$}
Proposition 6.3. The sequence \((V^n)_{n \geq 0}\) is uniformly bounded under the necessary and sufficient condition

\[
\lambda \leq \lambda_\infty, \text{ where } \lambda_\infty = 2\sqrt{2/3}. \tag{77}
\]

6.3. Filtered time-scheme. The preceding stability condition is an indication for a bound of the CFL. However it is only valid for the linear equation (54). In the case of a non constant velocity model, the stability must be reinforced. This is of course not surprising, since the basic scheme is centered. A common treatment consists in adding at each time step a high-frequency filter. Refer to [5] and references therein. This filtering step takes the form (see the last line in Algorithm 1 in Section 3.1):

\[
V^{n+1} = F \left( V^n + \frac{\Delta t}{6} \left( K^{(0)} + 2K^{(1)} + 2K^{(2)} + K^{(3)} \right) \right), \tag{78}
\]

or equivalently

\[
V^{n+1} = F \left( r \left( -\lambda J \right) V^n \right). \tag{79}
\]

The filter function \(F\) is the linear operator acting on periodic sequences defined by

\[
F(u)_i = \sum_{j=0}^{J} a_j \left( u_{i+j} + u_{i-j} \right), \quad 0 \leq j \leq N - 1. \tag{80}
\]

The width of the stencil is the odd integer \(2J + 1\). The first \(J + 1\) coefficients \(a_0, a_1, \ldots, a_J\) must satisfy the \(J + 1\) equations

\[
\begin{cases}
\sum_{j=0}^{J} a_j = 1, & (a)_0 \\
\sum_{j=0}^{J} a_j j^{2k} = 0, & k = 1 \ldots J - 1, & (a)_k \\
\sum_{j=0}^{J} a_j (-1)^j = 0, & (b)
\end{cases} \tag{81}
\]

The \(J + 1\) equations \((a)_k\), with \(k = 0, 1, \ldots, J - 1\) translate the consistency with the identity of the filter function with accuracy \(2J\). These relations are obtained by Taylor expansions near \(x_i\). The additional relation \((81)_b\) translates that the oscillating mode \(v_j = (-1)^j\) is cancelled out by the operator \(F\). The linear system (81) is (we drop the dependence in \(J\) for simplicity)

\[
Aa = b, \tag{82}
\]

<table>
<thead>
<tr>
<th>Order of accuracy</th>
<th>(a_0)</th>
<th>(a_1)</th>
<th>(a_2)</th>
<th>(a_3)</th>
<th>(a_4)</th>
<th>(a_5)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>1/2</td>
<td>1/2</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>10/16</td>
<td>8/16</td>
<td>-2/16</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>44/64</td>
<td>30/64</td>
<td>-12/64</td>
<td>2/64</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>186/256</td>
<td>112/256</td>
<td>-56/256</td>
<td>16/256</td>
<td>-2/256</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>772/1024</td>
<td>420/1024</td>
<td>-240/1024</td>
<td>90/1024</td>
<td>-20/1024</td>
<td>2/1024</td>
</tr>
</tbody>
</table>

Table 4. Examples of filters in the form (80) and their orders of accuracy.


<table>
<thead>
<tr>
<th>$J$</th>
<th>$\lambda_J$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\infty$ (no filter)</td>
<td>1.6329</td>
</tr>
<tr>
<td>10</td>
<td>1.6883</td>
</tr>
<tr>
<td>8</td>
<td>1.7114</td>
</tr>
<tr>
<td>6</td>
<td>1.7485</td>
</tr>
<tr>
<td>4</td>
<td>1.8156</td>
</tr>
<tr>
<td>2</td>
<td>1.9749</td>
</tr>
</tbody>
</table>

Table 5. Maximum CFL number $\lambda_J$ for the vector iteration (79) in term of $J$, the width of the stencil of the filter function $\mathcal{F}$. The function $J \mapsto \lambda_J$ is decreasing. The limit value is $\lambda_\infty = 2\sqrt{2/3} \approx 1.6239$. This limit value corresponds to $J = +\infty$, i.e. the absence of filtering.

Table 4 reports the values of a series of filter coefficients $a_J$ [43]. In addition, a set of approximate values of $\lambda_J$ is reported in Table 5. As expected, the lower $J$, the higher the maximal CFL number $\lambda_J$.

We skip the proof of the following proposition, which states existence and uniqueness of the coefficients $a$:

**Proposition 6.4.** There exists a unique set $[a_0, a_1, \ldots, a_J]^T$ satisfying the relations (81). The filter function $\mathcal{F}$ in (80) operates on each periodic grid function $R^k$ by

\[
\mathcal{F}(R^k)_j = P_J(\cos(\theta))R^k_j,
\]

where $P_J$ is the polynomial

\[
P_J(X) = 1 - \frac{1}{2^J}(1 - X)^J.
\]

Moreover, for all periodic grid function $(w_j)_{0 \leq j \leq N-1}$

\[
\max_{0 \leq j \leq N-1} |\mathcal{F}(w)_j| \leq \max_{0 \leq j \leq N-1} |w_j|,
\]

and the stability condition of the iteration (78) is $\lambda \leq \lambda_J$ where $\lambda_J \geq \lambda_\infty$.

References


‡Université de Lorraine, Département de Mathématiques, F-57045 Metz, France, †Inria, Grenoble, France, ‡C.N.R.S., Institut Elie Cartan de Lorraine, UMR 7502, F-57045 Metz, France

E-mail address: †matthieu.brachet@inria.fr, ‡jean-pierre.croisille@univ-lorraine.fr