Implicit solver formulations for shallow-water equation

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2022-02-08

Contents

These notes are taken from a final report for a KONWIHR funding from 2020 and should serve the purpose to explain the current REXI and implicit time integrators which includes the Coriolis effect and requires solving a system of equations. This can be done in spherical harmonics space. An original attempt for the REXI method was done [1, 2], but this version shows an optimized one which is based on the formulation in [**?**] (developed for implicit methods).

1 Application: SWE on rotating sphere

For the development of atmospheric simulations, methods are first developed with a **single-layer atmospheric model**. Although this model first sounds inappropriate for weather simulations, it is used in standard test cases of dynamical cores to assess numerical and performance properties in the horizontal dimension (see [**?**]). These equations can be directly related to the shallow-water equations on the rotating sphere

$$\begin{bmatrix} \frac{\partial \Phi}{\partial t} \\ \frac{\partial \mathbf{V}}{\partial t} \end{bmatrix} = \underbrace{\begin{bmatrix} -\overline{\Phi}\nabla\cdot\mathbf{V} \\ -\nabla\Phi \end{bmatrix}}_{L_g(U)} + \underbrace{\begin{bmatrix} 0 \\ -f\boldsymbol{k}\times\mathbf{V} \end{bmatrix}}_{L_c(U)} + \underbrace{\begin{bmatrix} -\mathbf{V}\cdot\nabla\Phi' \\ -\mathbf{V}\cdot\nabla\mathbf{V} \end{bmatrix}}_{N_a(U)} + \underbrace{\begin{bmatrix} -\nabla\Phi'\cdot\mathbf{V} \\ \end{bmatrix}}_{N_d(U)}$$

with $\boldsymbol{V}$ the velocity, Φ the geopotential, $\boldsymbol{k}$ the vector perpendicular to the earth's surface and f related to the Coriolis effect (a force induced on moving objects perpendicular to the horizontal moving direction due to the rotation of the earth). We will use these equations in their vorticity-divergence formulation and refer to [**?**, **?**] for further information.

2 Discretization: Spherical harmonics

We use spherical harmonics for the discretization in space. This is also used by the European Centre for Medium-Range Weather Forecasts (ECMWF) which belongs to one of the world's best quality weather forecasting systems.

To keep things short, we just want to introduce the most important terms relevant for this work. Spherical harmonics yield an efficient representation of a solution on the sphere with orthogonal basis functions. The continuous series of spherical harmonic functions are given by

$$\xi(\lambda,\mu) = \sum_{m=-M}^{M} \sum_{n=|m|}^{N(m)} \xi_n^m P_n^m(\mu) e^{im\lambda}$$

with N the highest degree of the Legendre function and M different variants of the associated Legendre polynomial. Using spherical coordinates, the coefficient λ denotes the longitude and μ is the Gaussian latitude ($\mu(\phi) = \sin\phi$). The spectral representation ξ_n^m can be determined via

$$\xi_n^m = \int_{-1}^{+1} \frac{1}{2\pi} \int_0^{2\pi} \xi(\lambda,\mu) e^{-im\lambda} d\lambda P_n^m(\mu) d\mu$$

where the inner integral

$$\xi^m(\mu) = \frac{1}{2\pi} \int_0^{2\pi} \xi(\lambda,\mu) e^{-im\lambda} d\lambda$$

is a Fourier transformation. The outer integral of the Legendre polynomials can be evaluated using Gaussian quadrature, hence accurate for sufficient number of quadrature points. The associated Legendre polynomials (ALP) are given in their non-normalized form by

$$P_n^m(x) \quad = \quad (-1)^m \frac{1}{2^n n!} \left(\sqrt{1-x^2}\right)^m \frac{d^{n+m}}{dx^{n+m}} \left(x^2-1\right)^{n+m}.$$

Here, n specifies the degree of the polynomial and m the variant of the function.

Similar to fast Helmholtz solvers in Fourier space (see e.g. [?] related to this work), we can use the Spherical Harmonics for directly solving equations of a particular form in spectral space due to, e.g.,

$$\Delta P_n^m = \frac{-n(n+1)}{r^2} P_n^m$$

leading to a modal-wise treatment in spectral space. This is, e.g., used in ECMWF's weather forecasting system. We will exploit such a strategy also in this work, however resulting in matrices which are not directly diagonal. Nevertheless, due to a very low matrix bandwidth, this allows using direct solvers.

3 Efficient REXI solver using spherical harmonics

For REXI time integration we need to solve for terms of the form

$$\left(\alpha_i I + \Delta t L\right)^{-1} U(t).$$

An efficient[1] REXI solver using spherical harmonics has been developed (see [?]) which is, however, based on transformations from/to physical space. In this work, we considered the interpretation of the REXI terms from the implicit time integration point of view

$$\frac{U(t+\Delta t) - U(t)}{\Delta t} = LU(t+\Delta t)$$
$$U(t) = (I - \Delta t L)\, U(t+\Delta t)$$

[1]Efficient here refers to more efficient than iterative solvers by exploiting properties of spectral space

where REXI-like terms can be easily related to this structure.

Hence, we adopted a formulation of [?] which describes an implicit time integration including the Coriolis effect for spherical harmonics which does not require transformations from/to physical space, but stays entirely in spectral space, hence overcomes the computationally expensive spherical harmonics transformations.

We can use this framework to embed REXI into the implicit time integration by choosing e.g. a complex-valued time step size. Dividing both sides by $-\Delta t$ we get

$$\frac{U(t)}{-\Delta t} = \left(\frac{1}{-\Delta t} + L\right) U(t + \Delta t)$$

where we can find a REXI matching formulation by setting $\alpha = -\frac{1}{\Delta t}$ or $\Delta t = -\alpha^{-1}$. Hence, we can rescale Δt with a possibly complex value to get a more efficient REXI solver based on an implicit complex-valued time stepper. This is briefly described next.

4 Implicit time integration with Spherical Harmonics

In what follows, we will further investigate the steps from [?] and [?] in detail. For the implicit time integration, we then get

$$\begin{bmatrix} I & \Delta t\overline{\Phi}\nabla^i\cdot & \Delta t\overline{\Phi}\nabla^j\cdot \\ \Delta t\nabla^i & I & -\Delta t f \\ \Delta t\nabla^j & \Delta t f & I \end{bmatrix} U(t + \Delta t) = U(t).$$

Given the divergence $\delta(u, v) = \nabla^i \cdot u + \nabla^j \cdot v$ and relative vorticity $\zeta(u, v) = \nabla^i \cdot v - \nabla^j \cdot u$ we get (see [?] and [?])

$$\begin{aligned} \Phi + \Delta t\overline{\Phi}\delta &= \Phi^0 \\ u + \Delta t\nabla^i\Phi - \Delta t f v &= u^0 \\ v + \Delta t\nabla^j\Phi + \Delta t f u &= v^0. \end{aligned}$$

4.1 Velocity from vorticity/divergence

We first derive an explicit formulation of the velocities based on the vorticity and divergence via

$$\mathbf{V} = \mathbf{k} \times (\nabla\psi) + \nabla\chi$$

with

$$\begin{aligned} \psi &= \nabla^{-2}\zeta \\ \chi &= \nabla^{-2}\delta. \end{aligned}$$

We can write

$$\mathbf{V} = \mathbf{k} \times \left(\nabla\nabla^{-2}\zeta\right) + \nabla\nabla^{-2}\delta$$

to get

$$\begin{aligned} u &= -\nabla^j\nabla^{-2}\zeta + \nabla^i\nabla^{-2}\delta \\ v &= \nabla^i\nabla^{-2}\zeta + \nabla^j\nabla^{-2}\delta. \end{aligned}$$

4.2 Computing F

Later on we also need a spectral formulation for

$$F = \Delta t 2\Omega \left(\mu - \frac{1}{r^2} \left(1 - \mu^2\right) \frac{d}{d\mu} \nabla^{-2} \right)$$

where we can use spherical harmonics representation to get

$$\begin{aligned} \mu - \frac{1}{r^2} \left(1 - \mu^2\right) \frac{d}{d\mu} \nabla^{-2} &= \mu - \frac{1}{r^2} \left(1 - \mu^2\right) \frac{d}{d\mu} \frac{r^2}{-n(n+1)} \\ &= \mu + \left(\left(1 - \mu^2\right) \frac{d}{d\mu} \right) \frac{1}{n(n+1)}. \end{aligned}$$

Computing the P_n output mode will be based on P_{n-1} and P_{n+1} input modes.

For P_{n-1} we get

- μ is represented by ϵ_n^m in spectral space
- $\left(1 - \mu^2\right) \frac{d}{d\mu}$ is represented by $(n+1)\,\epsilon_n^m$ in spectral space

We then get

$$\begin{aligned} \mu + \left(\left(1 - \mu^2\right) \frac{d}{d\mu} \right) \frac{1}{n(n+1)} &\Rightarrow \epsilon_n^m + \frac{n+1}{n(n+1)} \epsilon_n^m \\ &= \frac{n+1}{n} \epsilon_n^m. \end{aligned}$$

For P_{n+1} we get

- μ is represented by ϵ_{n+1}^m in spectral space
- $\left(1 - \mu^2\right) \frac{d}{d\mu}$ is represented by $-n\epsilon_{n+1}^m$ in spectral space.

We get

$$\begin{aligned} \mu + \left(\left(1 - \mu^2\right) \frac{d}{d\mu} \right) \frac{1}{n(n+1)} &\Rightarrow \epsilon_{n+1}^m - \frac{n}{n(n+1)} \epsilon_{n+1}^m \\ &= \frac{n}{n+1} \epsilon_{n+1}^m \end{aligned}$$

For matrix elements related to P_{n+1} we then get

$$\frac{n}{n+1} \epsilon_{n+1}^m.$$

To summarize, the upper and lower diagonal elements of the matrix F are then given by

$$\boxed{F = \Delta t 2\Omega \left(\mu - \frac{1}{r^2} \left(1 - \mu^2\right) \frac{d}{d\mu} \nabla^{-2} \right) = \begin{cases} f_n^- = \frac{n+1}{n} \epsilon_n^m & \text{for } P_{n-1} \\ f_n^+ = \frac{n}{n+1} \epsilon_{n+1}^m & \text{for } P_{n+1}. \end{cases}}$$

4.3 Geopotential

For sake of completeness, we repeat the continuity equation

$$\boxed{\Phi + \Delta t \overline{\Phi} \delta = \Phi^0}$$

which can be directly written in matrix form.

4.4 Divergence

Computing the divergence on the velocity equations yields

$$\nabla^i \cdot \left(u + \Delta t \nabla^i \Phi - \Delta t f v\right) + \nabla^j \cdot \left(v + \Delta t \nabla^j \Phi + \Delta t f u\right) = \nabla^i \cdot u^0 + \nabla^j \cdot v^0$$
$$\Delta t \nabla^2 \Phi + \delta - \Delta t \nabla f \cdot (v, -u)^T - \Delta t f \zeta = \delta^0$$

where we used $\zeta = curl(V) = \nabla \cdot (v, -u)^T$.

Next, we search for a vort/div representation of

$$\Delta t \nabla f \cdot (v, -u)^T = -\Delta t \nabla^j f u.$$

Using $\nabla^j f = 2\Omega \nabla^j \mu$ and $\mu = \sin\phi$ we first get

$$\nabla^j \mu = \nabla^j \mu = \frac{\sqrt{1-\mu^2}}{r} \frac{\partial \mu}{\partial \mu} = \frac{\sqrt{1-\mu^2}}{r} = \frac{\cos\phi}{r}$$

and therefore

$$\Delta t \nabla f \cdot (v, -u)^T = -2\Omega \Delta t \frac{\cos\phi}{r} u.$$

Using also

$$u = -\nabla^j \nabla^{-2} \zeta + \nabla^i \nabla^{-2} \delta$$

with the vort/div formulation, we get

$$\Delta t \nabla f \cdot (v, -u)^T = -2\Omega \Delta t \frac{\cos\phi}{r} u = 2\Omega \Delta t \frac{1}{r^2} \left(1 - \mu^2\right) \frac{d}{d\mu} \left(\nabla^{-2} \zeta\right) - 2\Omega \Delta t \frac{1}{r^2} \frac{d}{d\lambda} \left(\nabla^{-2} \delta\right).$$

Accumulating everything leads to

$$\Delta t \nabla^2 \Phi + \delta - \Delta t \nabla f \cdot (v, -u)^T - \Delta t f \zeta = \delta^0$$
$$\left(1 + \Delta t 2\Omega \frac{d}{d\lambda} \nabla^{-2}\right) \delta - \Delta t 2\Omega \left(\mu - \frac{1}{r^2} \left(1 - \mu^2\right) \frac{d}{d\mu} \nabla^{-2}\right) \zeta + \left(\Delta t \nabla^2\right) \Phi = \delta^0.$$

Using spherical harmonics representation we can write this in matrix form

$$\boxed{J\delta - F\zeta - L\Phi = \delta^0}$$

with

$$J = 1 + \Delta t 2\Omega \frac{d}{d\lambda} \nabla^{-2}$$
$$= 1 - \Delta t \frac{im 2\Omega}{n(n+1)}.$$

Note, that $J_0^{-1} = 1$ for $n = 0$ and hence $m = 0$ (due to spherical harmonics properties). Furthermore, we get

$$L = -\left(\Delta t \nabla^2\right)$$
$$= \Delta t n(n+1)/r^2$$

with F given by the formulation above.

4.5 Curl

Applying the curl operator $curl(V) = \nabla \cdot (v, -u)^T$ on the velocity equations, we get

$$\nabla^i \cdot \left(v + \Delta t \nabla^j \Phi + \Delta t f u\right) - \nabla^j \cdot \left(u + \Delta t \nabla^i \Phi - \Delta t f v\right) = \nabla^i \cdot v^0 - \nabla^j \cdot u^0$$
$$\zeta + \Delta t f \delta + \Delta t \nabla f \cdot \boldsymbol{V} = \zeta^0.$$

We need to find a direct formulation for $\nabla f \cdot \boldsymbol{V}$ only depending on the vorticity or divergence. We get

$$\nabla f \cdot \boldsymbol{V} = \nabla^j f v$$

where we next use $\nabla^j f = 2\Omega \frac{\cos\phi}{r}$. Using also

$$v = \nabla^i \nabla^{-2} \zeta + \nabla^j \nabla^{-2} \delta$$

with the vort/div formulation, and bringing things together we get

$$\left(1 + \Delta t 2\Omega \frac{1}{r^2} \frac{d}{d\lambda} \nabla^{-2}\right) \zeta + \Delta t 2\Omega \left(\mu - \frac{1}{r^2}\left(1 - \mu^2\right) \frac{d}{d\mu} \nabla^{-2}\right) \delta = \zeta^0$$

and in matrix form

$$\boxed{J\zeta + F\delta = \zeta^0.}$$

Regarding the vorticity, we get a trivial formulation for a spectral solver.

4.6 Solver for divergence

We can use the previously derived equations (see also [?])

$$\Phi + \Delta t \overline{\Phi} \delta = \Phi^0 \quad (1)$$
$$J\delta - F\zeta - L\Phi = \delta^0 \quad (2)$$
$$J\zeta + F\delta = \zeta^0 \quad (3).$$

Rewriting (1) to

$$\Phi = \Phi^0 - \Delta t \overline{\Phi} \delta$$

and using this in (2) we get

$$J\delta - F\zeta - L\left(\Phi^0 - \Delta t \overline{\Phi} \delta\right) = \delta^0 \quad (4).$$

Rewriting (3) to

$$\zeta = J^{-1}\zeta^0 - J^{-1} F \delta \quad (5)$$

and using this in (4) we get

$$J\delta - FJ^{-1}\zeta^0 + FJ^{-1}F\delta - L\left(\Phi^0 - \Delta t \overline{\Phi} \delta\right) = \delta^0$$

$$\boxed{\left(J + FJ^{-1}F + \Delta t \overline{\Phi} L G\right) \delta = \delta^0 + FJ^{-1}\zeta^0 + L\Phi^0.}$$

Given the solution for the divergence δ, we can simply compute the vorticity and geopotential based on it.

4.7 Matrix example for FJ^{-1} and FJ^{-1}

For each m partition, we need to compute FJ^{-1} which is given by

$$FJ^{-1} = 2\Omega\Delta t \begin{bmatrix} 0 & f_0^+ & & & \\ f_1^- & 0 & f_1^+ & & \\ & f_2^- & 0 & f_2^+ & \\ & & f_3^- & 0 & f_3^+ \\ & & & f_4^- & 0 \end{bmatrix} \begin{bmatrix} J_0^{-1} & & & & \\ & J_1^{-1} & & & \\ & & J_2^{-1} & & \\ & & & J_3^{-1} & \\ & & & & J_4^{-1} \end{bmatrix} = \begin{bmatrix} 0 & f_0^+ J_1^{-1} & & & \\ f_1^- J_0^{-1} & 0 & f_1^+ J_2^{-1} & & \\ & f_2^- J_1^{-1} & 0 & f_2^+ J_3^{-1} & \\ & & f_3^- J_2^{-1} & 0 & f_3^+ J_4^{-1} \\ & & & f_4^- J_3^{-1} & 0 \end{bmatrix}$$

and for $FJ^{-1}F$ we get

$$FJ^{-1}F = (2\Omega\Delta t)^2 \begin{bmatrix} 0 & f_0^+ J_1^{-1} & & & \\ f_1^- J_0^{-1} & 0 & f_1^+ J_2^{-1} & & \\ & f_2^- J_1^{-1} & 0 & f_2^+ J_3^{-1} & \\ & & f_3^- J_2^{-1} & 0 & f_3^+ J_4^{-1} \\ & & & f_4^- J_3^{-1} & 0 \end{bmatrix} \begin{bmatrix} 0 & f_0^+ & & & \\ f_1^- & 0 & f_1^+ & & \\ & f_2^- & 0 & f_2^+ & \\ & & f_3^- & 0 & f_3^+ \\ & & & f_4^- & 0 \end{bmatrix}$$

$$= (2\Omega\Delta t)^2 \begin{bmatrix} 0 + f_0^+ J_1^{-1} f_1^- & & f_0^+ J_1^{-1} f_1^+ & & \\ & f_1^- J_0^{-1} f_0^+ + f_1^+ J_2^{-1} f_2^- & & f_1^+ J_2^{-1} f_2^+ & \\ f_2^- J_1^{-1} f_1^- & & f_2^- J_1^{-1} f_1^+ + f_2^+ J_3^{-1} f_3^- & & f_2^+ J_3^{-1} f_3^+ \\ & f_3^- J_2^{-1} f_2^- & & f_3^- J_2^{-1} f_2^+ + f_3^+ J_4^{-1} f_4^- & \\ & & f_4^- J_3^{-1} f_3^- & & f_4^- J_3^{-1} f_3^+ + 0 \end{bmatrix}.$$

4.8 Comment on performance comparisons and scalability

The runtime complexity of spherical harmonics transformations, which can be entirely avoided with this formulation, shows that significant speedups can be easily reached for large scale simulations. We should also note, that this puts more pressure on an efficient collective communication to solve for the REXI terms.

References

[1] Martin Schreiber and Richard Loft. A parallel time integrator for solving the linearized shallow water equations on the rotating sphere. *Numerical Linear Algebra with Applications*, 26(2), 2018.

[2] Martin Schreiber, NathanaÃ«l Schaeffer, and Richard Loft. Exponential integrators with parallel-in-time rational approximations for the shallow-water equations on the rotating sphere. *Parallel Computing*, 85:56–65, 2019.