Semi-Lagrangian Exponential Integrator

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1 Introduction

Purpose: show a possible method to solve the nonlinear SWE with a semi-Lagrangian exponential integrator.

2 Shallow Water Equations

Consider the shallow water equations for a planar domain written as

$$\begin{aligned} u_t + uu_x + vu_y &= fv - g\eta_x, & (1)\\ v_t + uv_x + vv_y &= -fu - g\eta_y, & (2)\\ \eta_t + u\eta_x + v\eta_y &= -\bar{\eta}(u_x + v_y) - \eta(u_x + v_y), & (3) \end{aligned}$$

where the total fluid depth h was decomposed into $h = \eta + \bar{\eta}$, where $\bar{\eta}$ is a constant mean fluid depth and η is the perturbation. The velocities are given by $\vec{v} = (u, v)$ and the gravity g is assumed constant. The Coriolis parameter f is a function of y.

Let the variables to be in a Lagrangian reference frame, $\vec{v} = \vec{v}(t, \vec{r}(t))$ and $\eta = \eta(t, \vec{r}(t))$, where $\vec{r}(t) = (x(t), y(t))$. Then we have for η (and analogously for u and v) that the total derivative is given as

$$\frac{d\eta}{dt} = \frac{\partial \eta}{\partial t} + \nabla\eta \cdot \vec{v} = \frac{\partial \eta}{\partial t} + u\frac{\partial \eta}{\partial x} + v\frac{\partial \eta}{\partial y}, \tag{4}$$

where we have used that $\vec{r}\,'(t) = (x'(t), y'(t)) = \vec{v}$. Considering the total derivatives given along flow trajectories, we will call γ the parametrized trajectory curves in (t, x, y) space,

$$\gamma(s) = (s, x(s), y(s)). \tag{5}$$

So the total derivative can be written as

$$\frac{d}{dt} = \gamma'(t) \cdot \left(\frac{\partial}{\partial t}, \frac{\partial}{\partial x}, \frac{\partial}{\partial y}\right), \tag{6}$$

with

$$\gamma'(s) = (1, x'(s), y'(s)) = (1, u(s), v(s)). \tag{7}$$

Also, we may express the linear wave operator as a matrix operator given by

$$L = \begin{pmatrix} 0 & f & -g\partial_x \\ -f & 0 & -g\partial_y \\ -\bar{\eta}\partial_x & -\bar{\eta}\partial_x & 0 \end{pmatrix}. \tag{8}$$

This allows the shallow water equations to be written as

$$\frac{dU}{dt} = LU + N(U), \tag{9}$$

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where

$$U = \begin{pmatrix} u \\ v \\ \eta \end{pmatrix}, \tag{10}$$

$$N(U) = \begin{pmatrix} 0 \\ 0 \\ -\eta \nabla \cdot \vec{v} \end{pmatrix}. \tag{11}$$

3 General semi-Lagrangian formulation

For a review and details about semi-Lagrangian methods, please see [?] and [?].

3.1 Trajectory calculations

To calculate the trajectories one needs to solve the following ODE problem for $\vec{r}(t) = (x(t), y(t))$,

$$\frac{d\vec{r}(t)}{dt} = \vec{v}(t, \vec{r}(t)), \tag{12}$$

with

$$\vec{r}(t_0) = (x(t_0), y(t_0)). \tag{13}$$

This can be done through many of existing techniques (see [?] and [?]). We will discuss two possibilities in this section.

Basic 2-time-level

A simple approach uses fixed point iterations using the method of [?], but following a two-time level method as in [?]. Integrating from time t_n to time t_{n+1} we have that

$$\vec{r}(t_{n+1}) - \vec{r}(t_n) = \int_{t_n}^{t_{n+1}} \vec{v}(t, \vec{r}(t)) dt. \tag{14}$$

Numerically we can calculate departure points $\vec{r}_d = \vec{r}(t_n)$ using the arrival grid points $\vec{r}_a = \vec{r}(t_{n+1})$ and the trajectory midpoint $\vec{r}_m = \vec{r}(t_{n+1/2})$ as

$$\vec{r}_a - \vec{r}_d = \vec{v}(t_{n+1/2}, \vec{r}_m)\Delta t, \tag{15}$$

and

$$\vec{r}_a - \vec{r}_m = \vec{v}(t_{n+1/2}, \vec{r}_m)\frac{\Delta t}{2}, \tag{16}$$

and solving iteratively the equation for the midpoints with

$$\vec{r}_m^{k+1} = \vec{r}_a - \vec{v}(t_{n+1/2}, \vec{r}_m^k)\frac{\Delta t}{2}, \tag{17}$$

with $\vec{r}_m^0 = \vec{r}_a$. Two or three iterations are usually enough to obtain a good estimate for the midpoint. The departure point can then be estimated by

$$\vec{r}_d = \vec{r}_m - \vec{v}(t_{n+1/2}, \vec{r}_m)\frac{\Delta t}{2} = 2\vec{r}_m - \vec{r}_a. \tag{18}$$

Extrapolation methods are required to obtain the velocity at the trajectory midpoints, this may be obtained as

$$\vec{v}(t_{n+1/2}, \vec{r}_m^k) = \left(\frac{3}{2}\vec{v}(t_n) - \frac{1}{2}\vec{v}(t_{n-1})\right)_m, \tag{19}$$

where the sub-index $_m$ indicates that once the extrapolation is done, it is then interpolated to the trajectory midpoints $\vec{r}_m^k$.

Stable Extrapolation Two-Time-Level Scheme

The extrapolation scheme shown above tends to be unstable for large time steps for the nonlinear shallow water equations [**?**]. An alternative is the Stable Extrapolation Two-Time-Level Scheme (SETTLS) of [**?**], used in the ECMWF global model IFS.

This approach uses as extrapolation method along the trajectories, for any given function ϕ,

$$\phi(t_{n+1/2}, \vec{r}_m) = \frac{1}{2}\left(2\phi(t_n, \vec{r}_d) - \phi(t_{n-1}, \vec{r}_d) + \phi(t_n, \vec{r}_a)\right). \tag{20}$$

So the velocity at the midpoints may be approximated as

$$\vec{v}(t_{n+1/2}, \vec{r}_m) = \frac{1}{2}\left(2\vec{v}(t_n, \vec{r}_d) - \vec{v}(t_{n-1}, \vec{r}_d) + \vec{v}(t_n, \vec{r}_a)\right). \tag{21}$$

The departure point can be obtained through an iterative procedure as before with,

$$\vec{r}_d^{\,k+1} = \vec{r}_a - \frac{\Delta t}{2}\left(2\vec{v}(t_n, \vec{r}_d^{\,k}) - \vec{v}(t_{n-1}, \vec{r}_d^{\,k}) + \vec{v}(t_n, \vec{r}_a)\right), \tag{22}$$

with first guess given using $\vec{r}_d^{\,0} = \vec{r}_a$.

The fields to be calculated at the departure points, such as $\vec{v}(t_n, \vec{r}_d^{\,k})$, will be done first calculating $\vec{v}(t_n)$ at the usual grid points, and then this will be interpolated to the departure points $\vec{r}_d^{\,k}$. We will denote this interpolation to departure points with a $*$, to give the following formulas

$$\vec{r}_d^{\,k+1} = \vec{r}_a - \frac{\Delta t}{2}\vec{v}(t_n) - \frac{\Delta t}{2}\left(2\vec{v}(t_n) - \vec{v}(t_{n-1})\right)_*. \tag{23}$$

A second order interpolation for the velocity is usually enough to ensure an overall second order accurate semi-Lagrangian method [**?**].

3.2 Integrating factor

Let I be defined as the solution to the problem

$$\frac{dI}{dt} = -IL, \tag{24}$$

subject to

$$I(t_n) = \mathrm{Id}, \tag{25}$$

where Id is the identity matrix.

Considering the integral as being element-wise in L, it is easily verified that the problem has solutions of the form

$$I = e^{-\int_{t_n}^{t} L(\gamma(s))\,ds}, \tag{26}$$

where $\gamma(s)$ is the trajectory curve parametrization related to d/dt. This I will be denoted as the integrating factor.

We will also need the inverse of the integrating factor, which we will call J, defined as

$$J = e^{\int_{t_n}^{t} L(\gamma(s))\,ds}, \tag{27}$$

for which one readily sees that IJ is the identity matrix.

3.3 Semi-Lagrangian method

Using the above defined integrating factor I, we may write the shallow water equations as

$$I\frac{dU}{dt} = ILU + IN(U), \tag{28}$$

which, using the definition of the integrating factor and the properties of the derivative, can be transformed to

$$I\frac{dU}{dt} = -\frac{dI}{dt}U + IN(U), \tag{29}$$

$$\frac{d(IU)}{dt} = IN(U). \tag{30}$$

To derive the semi-Lagrangian formulation we assume that the solution is known at grid points at a time step t_n and wish to calculate the solution at time t_{n+1}. Integrating the above equation along trajectories gives us

$$(IU)^{n+1} - (IU)^n_* = \int_{t_n}^{t_{n+1}} I(t, \vec{r}(t))\, N(U(t, \vec{r}(t)))\, dt, \tag{31}$$

where $*$ indicates that this value should be at trajectories departure points and the integral is along trajectories. The integrating factor I is the identity at the departure points, so the resulting method for calculation of the new values at grid points can be calculated as

$$U^{n+1} = J^{n+1}(U)^n_* + J^{n+1} \int_{t_n}^{t_{n+1}} I(t, \vec{r}(t))\, N(U(t, \vec{r}(t)))\, dt. \tag{32}$$

We see that this is very similar to the usual exponential integrator equation in Eulerian forms.

To solve this equation, the trajectories and departure points may be calculated with any of the several existing flavours. We will discuss possible approximation for the right hand side of the equation in what follows.

4 Non-divergent flow case

Here we will analyse the case when the flow is non-divergent, therefore, $N(U) = 0$, and we need to solve only

$$\frac{dU}{dt} = LU, \tag{33}$$

where all the non-linearities are in the material derivative.

4.1 On a f-plane

Consider the shallow water equations given for a bi-periodic plane with f constant. In this case L is constant along the trajectories, so

$$U^{n+1} = J^{n+1} U^n_*, \tag{34}$$

with

$$J^{n+1} = e^{L\Delta t} \tag{35}$$

and the method may be written as

$$U^{n+1} = e^{L\Delta t}(U)^n_*. \tag{36}$$

Since $e^{L\Delta t}$ is constant, we can allow ourselves to apply it as

$$U^{n+1} = (e^{L\Delta t}U)^n_*, \tag{37}$$

which means that in practice we can first calculate $e^{L\Delta t}U$, with any given matrix exponentiation method, and then interpolate this to quantity to the departure points.

4.2 On a variable f scenario

We will now allow the Coriolis parameter f to vary in the y direction, for example as in the β-plane approximation $f = f_0 + \beta y$ or, on the spherical case, $f = 2\Omega \sin\theta$, where θ is the latitude, and Ω is the rotation rate of the Earth. In this case, L is no longer constant along trajectories and the integrating factor needs to be approximated.

4.2.1 f constant along trajectories

Considering that the trajectories spam a small region in space for which the variation of f is small, we may approximate the integrating factor considering the Coriolis parameter given for the trajectory midpoint. That is

$$J^{n+1} = e^{\int_{t_n}^{t_{n+1}} L(\gamma(t))dt} \approx e^{L(\gamma(t_{n+1/2}))\int_{t_n}^{t_{n+1}} dt} = e^{L^{1/2}\Delta t}, \tag{38}$$

where $L^{1/2}$ is the linear operator calculated at the trajectory midpoint $\vec{r}_m$. The resulting method is similar to the f-plane case,

$$U^{n+1} = (e^{L^{1/2}\Delta t}U)^n_*. \tag{39}$$

The problem with this approach is that the exponential integrator will depend on the trajectory points, which can make it impractical with REXI, since these the midpoints are not necessarily grid points.

If we consider a constant approximation of L along trajectories, with reference values given for the time t_n, then

$$J^{n+1} = e^{\int_{t_n}^{t_{n+1}} L(\gamma(t))dt} \approx e^{L(\gamma(t_n)) \int_{t_n}^{t_{n+1}} dt} = e^{L\Delta t}, \tag{40}$$

then

$$U^{n+1} = (e^{L\Delta t}U)_*^n. \tag{41}$$

where $e^{L\Delta t}U$ is the usual exponential integrator but considering the variations of f given for the time t_n.

The consequences of the latter approximation is that the Rossby waves might not be well represented if the time-step is too large.

5 Full nonlinear case

Considering the above method, where L is constant along trajectories, then we may write the the method for the full non linear case as

$$U^{n+1} = (e^{L\Delta t}U)_*^n + e^{L\Delta t} \int_{t_n}^{t_{n+1}} I(t, \vec{r}(t))\, N(U(t, \vec{r}(t)))\, dt. \tag{42}$$

5.1 Standard Exponential Integrator Scheme

This can be worked out in several ways (like Cox and Mathews). A simple way is to consider a forward Euler method for the nonlinear part, as

$$\begin{aligned}
e^{L\Delta t} \int_{t_n}^{t_{n+1}} I(t, \vec{r}(t))\, N(U(t, \vec{r}(t)))\, dt &\approx e^{L\Delta t} \left(\int_{t_n}^{t_{n+1}} I(t, \vec{r}(t))\, dt \right) N(U(t_n))_* \\
&= e^{L\Delta t} \left(\int_{t_n}^{t_{n+1}} \frac{dI(t, \vec{r}(t))}{dt} L^{-1}\, dt \right) N(U(t_n))_* \\
&\approx e^{L\Delta t} \left(I(t_{n+1}, \vec{r}(t_{n+1})) - I(t_n, \vec{r}(t_n)) \right) L^{-1} N(U(t_n))_* \\
&= e^{L\Delta t} \left(e^{-L\Delta t} - \mathrm{Id} \right) L^{-1} N(U(t_n))_* \\
&= \left(\mathrm{Id} - e^{L\Delta t} \right) L^{-1} N(U(t_n))_* \\
&\approx \left(\left(\mathrm{Id} - e^{L\Delta t} \right) L^{-1} N(U(t_n)) \right)_*,
\end{aligned}$$

where we use that the I is constant along trajectories (but might not be constant in the domain), resulting in

$$U^{n+1} = (e^{L\Delta t}U)_*^n + \left(\left(\mathrm{Id} - e^{L\Delta t} \right) L^{-1} N(U) \right)_*^n. \tag{43}$$

which can be calculated as

$$U^{n+1} = \left(e^{L\Delta t}U + \left(\mathrm{Id} - e^{L\Delta t} \right) L^{-1} N(U) \right)_*^n. \tag{44}$$

The problem with using standard exponential integrator approaches, such as Cox and Mathews, is that they rely on the having L^{-1}, which, in the case of SWE, is not well defined in general, since the kernel is non trivial (it has all the geostrophic modes).

5.2 Alternative scheme

In semi-Lagrangian methods, it is common that the nonlinear terms are discretized as averages of the departure and arrival trajectory points given for the intermediate time $t_{n+1/2}$.

This leads to the following approach,

$$U^{n+1} = (e^{L\Delta t}U)_*^n + \frac{\Delta t}{2} e^{L\Delta t} \left[I(t_{n+1/2}, \vec{r}_a)\, N(U(t_{n+1/2}, \vec{r}_a) + I(t_{n+1/2}, \vec{r}_d)\, N(U(t_{n+1/2}, \vec{r}_d)) \right], \tag{45}$$

which, using the assumption of constant L along trajectories,

$$I(t_{n+1/2}, \vec{r}(t)) = e^{-L\Delta t/2}, \tag{46}$$

may be simplified to

$$U^{n+1} = (e^{L\Delta t}U)_*^n + \frac{\Delta t}{2} e^{L\Delta t/2} \left[N(U(t_{n+1/2}, \vec{r}_a) + N(U(t_{n+1/2}, \vec{r}_d)) \right], \tag{47}$$

or

$$U^{n+1} = \left(e^{L\Delta t}U^n + \frac{\Delta t}{2} e^{L\Delta t/2} N(U)^{n+1/2} \right)_* + \frac{\Delta t}{2} e^{L\Delta t/2} N(U)^{n+1/2}. \tag{48}$$

Since $N(U)$ is required at an intermediate time-step, this needs to be extrapolated from previous values of $N(U)$ given in time steps n and $n-1$. Using the same extrapolation as in equation (19), the resulting method is

$$U^{n+1} = \left[e^{L\Delta t}U^n + \frac{\Delta t}{2}e^{L\Delta t/2}\left(\frac{3}{2}N(U^n) - \frac{1}{2}N(U^{n-1})\right)\right]_* + \frac{\Delta t}{2}e^{L\Delta t/2}\left(\frac{3}{2}N(U^n) - \frac{1}{2}N(U^{n-1})\right). \tag{49}$$

5.3 Stable scheme

As discussed in section 3.1, using standard extrapolation schemes may lead to an unstable scheme. An option is to use the SETTLS approach, which would give

$$U^{n+1} = (e^{L\Delta t}U)^n_* + \Delta t\, e^{L\Delta t/2}\left[N(U(t_{n+1/2}, \vec{r}_m)\right], \tag{50}$$

where

$$N(U(t_{n+1/2}, \vec{r}_m)) = \frac{1}{2}\left[2N(U(t_n, \vec{r}_d)) - N(U(t_{n-1}, \vec{r}_d)) + N(U(t_n, \vec{r}_a))\right], \tag{51}$$

which may be calculated as

$$N(U(t_{n+1/2}, \vec{r}_m)) = \frac{1}{2}\left[2N(U(t_n)) - N(U(t_{n-1}))\right]_* + \frac{1}{2}\left[N(U(t_n))\right]. \tag{52}$$

The resulting method is

$$U^{n+1} = \left[e^{L\Delta t}U^n + \Delta t\, e^{L\Delta t/2}\left(N(U^n) - \frac{1}{2}N(U^{n-1})\right)\right]_* + \frac{\Delta t}{2}e^{L\Delta t/2}N(U^n). \tag{53}$$

To save on calculations, one may calculate

$$V^n = e^{L\Delta t}U^n \tag{54}$$

$$W^n = e^{L\Delta t/2}N(U^n) \tag{55}$$

and then

$$U^{n+1} = \left[V^n + \Delta t\, W^n - \frac{\Delta t}{2}W^{n-1}\right]_* + \frac{\Delta t}{2}W^n. \tag{56}$$

For the interpolation to departure points, a third order interpolation method is recommended to ensure overall second order accuracy of the semi-Lagrangian scheme [**?**].

6 Lagrangian treatment of Coriolis term

The treatment of variable Coriolis term is complicated with the above approach for 2 reasons: First, it needs to be approximated along the trajectories, which could affect the Rossby waves, second, the exponential integrator has to deal with non constant coefficient solvers, which can be far more complicated and expensive.

For these reasons, here we will briefly describe the possibility of treating the Coriolis term in a Lagrangian fashion.

6.1 Planar case

We may write the momentum equations as

$$\frac{du}{dt} = f(y)v - g\eta_x, \tag{57}$$

$$\frac{dv}{dt} = -f(y)u - g\eta_y, \tag{58}$$

or in vector notation,

$$\frac{d\vec{u}}{dt} + f(y)\vec{k} \times \vec{u} = -\nabla\eta, \tag{59}$$

where $\vec{u} = (u, v)$, and $\vec{k} = (0, 0, 1)$ is a vector normal to the plane. Now notice that

$$\frac{d\vec{r}}{dt} = \vec{v}, \tag{60}$$

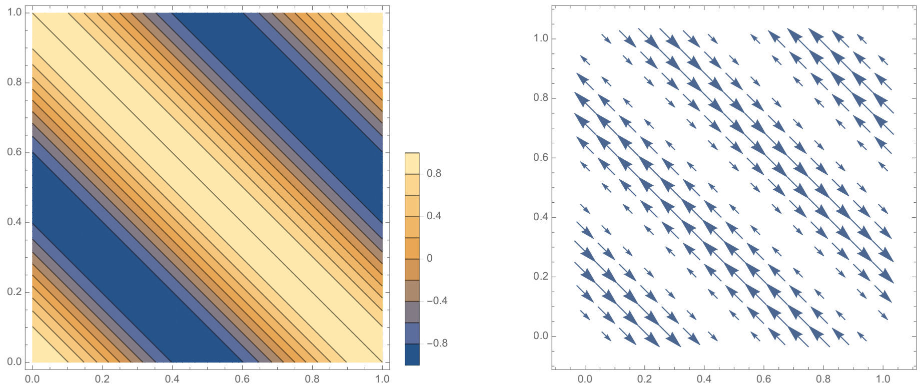

Figure 1: Height and velocity fields for steady state rotated non-divergent flow

so we have that

$$\frac{d\vec{u}}{dt} + f(y)\vec{k} \times \frac{d\vec{r}}{dt} = -\nabla\eta, \tag{61}$$

If $f(y) = f$ constant (f-plane approximation), then

$$\frac{d\left(\vec{u} + f\vec{k} \times \vec{r}\right)}{dt} = -\nabla\eta, \tag{62}$$

which means that the Coriolis term can be solved together with the lagrangian advected quantity.

If f is to be assumed dependent on y, then the above equation (62) only makes sense considering the assumption that $f(y)$ is constant along trajectories.

6.2 Spherical case

Although it is not possible to consider the variable f case lagrangianly on a plane, this is different for the sphere. It is described in [?] how it is possible to treat the Coriolis term in a lagrangian way even in the variable f condition. As a consequence, the exponential computational (REXI) would treat only the gravity waves, but not the Rossby ones.

We will briefly describe this case here (soon).

7 Numerical results

7.1 Non-divergent flows

Geostrophically balanced solution of the nonlinear equations.

$$h = \cos\left(2\pi(x/L_x + y/L_y)\right) + \bar{\eta} \tag{63}$$

$$u = \frac{2g\pi}{f_0 L_y}\sin\left(2\pi(x/L_x + y/L_y)\right) \tag{64}$$

$$v = -\frac{2\pi g}{f_0 L_x}\sin\left(2\pi(x/L_x + y/L_y)\right) \tag{65}$$

This test has trajectories given as straight lines, but these are not coinciding with the grid. Therefore, the departure point calculation is expected to be very accurate, and the errors associated with the semi-lagrangian are mainly related to interpolation errors of the field at the departure points.

Since the flow is non-divergent, the non advective nonlinear term (divergence term of continuity equation) is assumed to be zero.

7.2 Non-divergent Forced flow

$$h = \cos(2\pi x/L_x)\sin(2\pi y/L_y) + \bar{\eta} \quad (66)$$

$$u = -\frac{2g\pi}{f_0 L_y}\cos(2\pi x/L_x)\cos(2\pi y/L_y) \quad (67)$$

$$v = -\frac{2\pi g}{f_0 L_x}\sin(2\pi x/L_x)\sin(2\pi y/L_y) \quad (68)$$

$$(69)$$

with forcings

$$f_h = 0 \quad (70)$$

$$f_u = -\frac{\pi}{L_x}\left(\frac{2\pi g}{f_0 L_y}\right)^2 \sin(4\pi x/L_x) \quad (71)$$

$$f_v = \frac{\pi}{L_y}\left(\frac{2\pi g}{f_0 L_x}\right)^2 \sin(4\pi y/L_y) \quad (72)$$

$$(73)$$

7.3 Divergent flows

8 Concluding remarks