Semi-Lagrangian Exponential Integration

with application to the rotating shallow water equations

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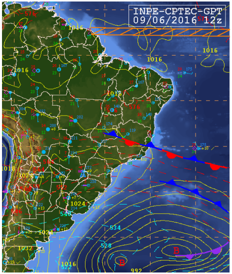
Motivation 1 - the application perspective

- Weather forecasts :
  3D compressible Euler equations on the sphere
- Important horizontal terms:
  - Linear hyperbolic operator
  - Nonlinear advection
- Desirable numerical properties:
  - Large timestep sizes
  - Accurate dispersion relations
- Today's state-of-the-art scheme (IFS-ECMWF):
  - semi-Lagrangian
  - semi-implicit linear operator (Crank-Nicolson)
  - spectral (spherical harmonics)



Goal1

How to improve wave dispersion damped by the Crank-Nicolson scheme preserving large time steps of the semi-Lagrangian semi-implicit?

Motivation 2 - Exponential integration with nonlinear advection

- Exponential integrators solve accurately **linear** problems
  - Usually allows very large timesteps

$$\frac{dU}{dt} = LU, \quad U(0) = U_0,$$

$$U(t_{n+1}) = e^{\Delta t L} U(t_n),$$

- For nonlinear equations
  - Usually nonlinearity limits timestep sizes

$$\frac{dU}{dt} = LU + N(U), \quad U(0) = U_0,$$

$$U(t_{n+1}) = e^{\Delta t L} U(t_n) + e^{\Delta t L} \int_{t_n}^{t_{n+1}} e^{-(s-t_n)L} N(U(s)) ds,$$

Goal2

How to treat N if dominated by nonlinear advection, in way to allow large time step sizes?

Semi-Lagrangian Exponential Integrator

Main Goal

Build a general semi-Lagranginan exponential class of schemes that allow:

- Precise solution of linear oscillations (hyperbolic)
- Accurate representation of nonlinear advection

considering very large time step sizes

Summary

Non-linear exponential integration

Basic concept

$$\frac{dU}{dt} = \underbrace{LU}_{\text{Linear Discrete}} + \underbrace{N(U)}_{\text{Nonlinear Discrete}} \quad , \quad U(0) = U_0$$

If L does not depend on time, then

$$U(t_{n+1}) = e^{\Delta tL}U(t_n) + e^{\Delta tL}\int_{t_n}^{t_{n+1}} e^{-(s-t_n)L}N(U(s))ds,$$

"variation-of-constants" formula.

Keep in mind that $N(U)$ may include nonlinear advection $\vec{v} \cdot \nabla U$

Exponential-Time-Differencing (ETDRK)

Assume precise calculation of the matrix exponential

Moler and Van Loan, (2003) - Nineteen Dubious Ways to Compute the Exponential of a Matrix, Twenty-Five Years Later

EDT1RK

$$
\begin{aligned}
U(t_{n+1}) &= e^{\Delta t L} U(t_n) - \left(\int_{t_n}^{t_{n+1}} L^{-1} \frac{d\left(e^{-(s-t_{n+1})L}\right)}{ds} ds \right) N(U(t_n)) + \mathcal{O}(\Delta t) \\
&= e^{\Delta t L} U(t_n) + L^{-1} \left(e^{\Delta t L} - I \right) N(U(t_n)) + \mathcal{O}(\Delta t),
\end{aligned}
$$

Second Order Exponential-Time-Differencing

EDT2RK

$$
\begin{aligned}
U_1^{n+1} &= \varphi_0(\Delta t L)U^n + \Delta t\, \varphi_1(\Delta t L)N(U^n), \\
U^{n+1} &= U_1^{n+1} + \Delta t \varphi_2(\Delta t L)\left(N(U_1^{n+1}) - N(U^n)\right),
\end{aligned}
$$

$$
\varphi_k(z) = z^{-k}(e^z - t_{k-1}(z)), \quad t_k = \sum_{l=0}^{k} \frac{z^l}{l!}
$$

Limited time step size due to CFL of nonlinear advection.

Cox, S. M., & Matthews, P. C. (2002)

Summary

Oscillatory equations with nonlinear advection

$$\underbrace{\frac{\partial U}{\partial t} + \vec{v} \cdot \nabla U}_{\text{Advective nonlinear}} = \underbrace{LU}_{\text{Linear oscilatory}} + \underbrace{\tilde{N}(U)}_{\text{Nonlinear}}$$

$$\underbrace{\frac{DU(t, \vec{r}(t))}{Dt}}_{\text{Material derivative}} = L(U(t, \vec{r}(t))) + \tilde{N}(U(t, \vec{r}(t)))$$

$$\frac{d\vec{r}(t)}{dt} = \vec{v}(t, \vec{r}(t), U(t, \vec{r}(t))), \quad \vec{r}(0) = \vec{r}_0.$$

$\vec{r}(t)$ describes a particle trajectory along the flow.

Semi-Lagrangian semi-implicit

Used in IFS-ECMWF model (European Centre for Medium-Range Weather Forecasts)

Stable Extrapolation Two-Time-Level Scheme (SETTLS) of Hortal (2002)

$$\frac{U^{n+1} - U^n_*}{\Delta t} = \frac{1}{2}\left((LU)^{n+1} + (LU)^n_*\right) + \tilde{N}^{n+1/2},$$

where

- X^{n+1} is assumed to live in grid points.
- X_* denotes interpolation at departure points.
- Extrapolation:

$$\tilde{N}^{n+1/2} = \frac{1}{2}\left(\left[2\tilde{N}^n - \tilde{N}^{n-1}\right]_* + \tilde{N}^n\right),$$

- SETTLS also proposes an iterative scheme to solve the trajectory equation to calculate departure points from arrival grid points (2nd order accurate)

Summary

General formulation

$$\underbrace{\frac{DU(t,\vec{r}(t))}{Dt}}_{\text{Material derivative}} = \underbrace{L(U(t,\vec{r}(t)))}_{\text{Linear oscilatory}} + \underbrace{\tilde{N}(U(t,\vec{r}(t)))}_{\text{Nonlinear}}$$

If L commutes in time*

$$U(t_{n+1},\vec{r}(t_{n+1})) = e^{\Delta tL}U(t_n,\vec{r}(t_n)) + e^{\Delta tL}\int_{t_n}^{t_{n+1}} e^{-(s-t_n)L}\tilde{N}(U(s,\vec{r}(s)))ds + E_L.$$

where $\vec{r}(t)$ defines a particle trajectory.

This is the basis for Semi-Lagrangian exponential integrator methods.

*If this is not the case, approximate versions can be built (e.g. constant in within each time-step), so we have the error term E_L.

SL-EXP-SETTLS

The semi-Lagrangian exponential integrator:

$$U^{n+1} = e^{L\Delta t}(U)^n_* + e^{L\Delta t}\int_{t_n}^{t_{n+1}} e^{-(s-t_n)L}\,\tilde{N}(U(t,\vec{r}(t)))\,dt.$$

Stable Extrapolation Two-Time-Level Semi-Lag (Hortal et al 2002):

$$U^{n+1} = e^{L\Delta t}U^n_* + \frac{\Delta t}{2}\,e^{L\Delta t}\left[2\tilde{N}^n - e^{L\Delta t}\tilde{N}^{n-1}\right]_* + \frac{\Delta t}{2}\tilde{N}^n$$

$*$ indicates calculation at departure points.

Can be simplified to use require only 2 exponentials per timestep.

SL-ETDRK

SL-ETD1RK

$$U_1^{n+1} = \varphi_0(\Delta t L)\left[U^n + \Delta t\, \varphi_1(-\Delta t L) N(U^n)\right]_*^n,$$

SL-ETD2RK

$$U_2^{n+1} = U_1^{n+1} + \Delta t\, \varphi_0(\Delta t L)\left[\psi_2(\Delta t L) N(U_1^{n+1}) - \left(\psi_2(\Delta t L) N(U^n)\right)_*^n\right],$$

where

$$\psi_2(\Delta t L) = -\varphi_2(-\Delta t L) + \varphi_1(-\Delta t L).$$

Can be coded to use only 2 exponentials/φ evaluations per timestep.

Remarks

Be careful when deriving such schemes!

- Lack of commutation: $e^{\Delta t L} U_*^n \neq \left(e^{\Delta t L} U^n\right)_*$
- Avoid application of operators on irregular grids (departure/midpoints) $(\varphi(\Delta t L) N(U^n))_*$
- Operators on advected quantities are ok: $e^{\Delta t L} U_*^n$
- Simple midpoint rule:

$$\int_{t_n}^{t_{n+1}} T(s) w(s)\, ds \approx \begin{cases} A_1 = & \Delta t\, T(t_{n+1/2}) \left[w(t_{n+1/2})\right]_\dagger ✗ \\ A_2 = & \Delta t \left[T(t_{n+1/2}) w(t_{n+1/2})\right]_\dagger ✓ \end{cases},$$

† interpolation to traj. midpoints

Summary

Shallow Water Equations

Rotation non-linear SWE (f is rotation/Coriolis parameter):

$$\begin{aligned} u_t + uu_x + vu_y &= fv - g\eta_x, \\ v_t + uv_x + vv_y &= -fu - g\eta_y, \\ \underbrace{\eta_t + u\eta_x + v\eta_y}_{\text{Nonlinear } D/Dt} &= \underbrace{-\bar{\eta}(u_x + v_y)}_{\text{Linear } \mathcal{L}} - \underbrace{\eta(u_x + v_y)}_{\text{Nonlinear } \tilde{\mathcal{N}}}, \end{aligned}$$

- Well established 2D test case for atmospheric dynamical models.
- Linear waves can be solved very precisely with exponential of linear terms.
- Nonlinear advection can have long time steps with semi-Lagrangian
- Stability constraints related to nonlinear divergence ($\tilde{N}$).

Exponential of $\mathcal{L}$

Fourier basis operator symbol:

$$\mathcal{L} U_{\vec{k}} = \begin{pmatrix} 0 & f & -gik_1 \\ -f & 0 & -gik_2 \\ -\bar{\eta} ik_1 & -\bar{\eta} ik_2 & 0 \end{pmatrix} \hat{U}_{\vec{k}},$$

Eigen-decomposition:

$$e^{\mathcal{L}(i\vec{k})} = Q e^{\Lambda} Q^{-1},$$

Eigenvalues (Λ):

$$\omega_f(\vec{k}) = 0, \quad \omega_g(\vec{k}) = \pm i \sqrt{f^2 + g\,\bar{\eta}\,\vec{k}\cdot\vec{k}},$$

φ functions:

$$\varphi_n(\Delta t\, \mathcal{L}(i\vec{k})) = Q \varphi_n(\Delta t\, \Lambda) Q^{-1},$$

* It is possible to do a *similar* exponential calculation on the sphere with Spherical Harmonics!

Methods

- RK-FDC: Energy conversing finite differences C-grid with Runge-Kutta
- SL-SI-SETTLS: Semi-Lagrangian, semi-implicit (Crank-Nicolson) spectral discretization.
- SL-EXP-SETTLS: Exponential version of SL-SI-SETTLS
- ETD2RK: Original ETD2RK scheme, with spectral in space.
- SL-ETD2RK: Semi-Lagrangian version of ETD2RK
- REF: Reference solution. 4th order Runge-Kutta forth order in time, high resolution Eulerian spectral space.

Unstable jet on the plane

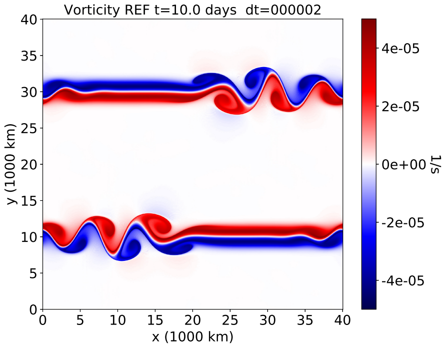
Initial conditions (stationary):

$$u(x,y) = u_0 \left(\sin(2\pi y/L_y)\right)^{81}$$

$$v(x,y) = 0$$

$$\eta(x,y) = -\frac{f}{g}\int_0^y u(x,s)ds.$$

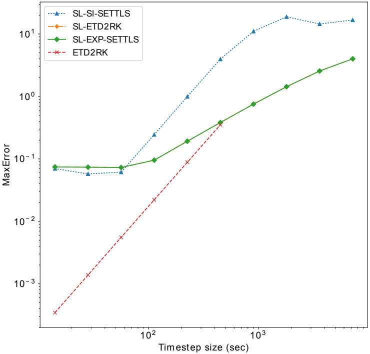
Small Gaussian perturbation to destabilize the flow.

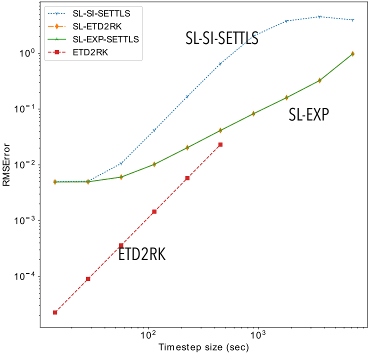


Experiments with $\tilde{N} = 0$

$$\frac{dU}{dt} = LU$$

At 1 day of integration - dominance of linear waves

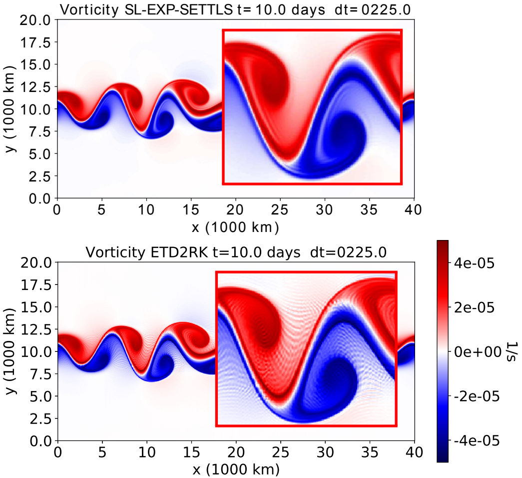




SL-ETD2RK is identical to SL-EXP-SETTLS, since no nonlinear divergence.

Experiments with $\tilde{N} = 0$

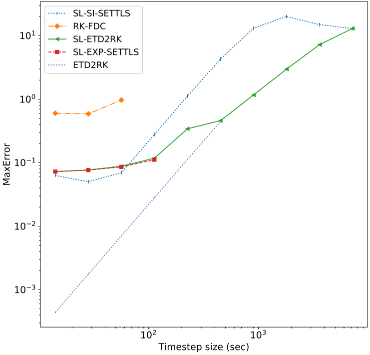
At day 10

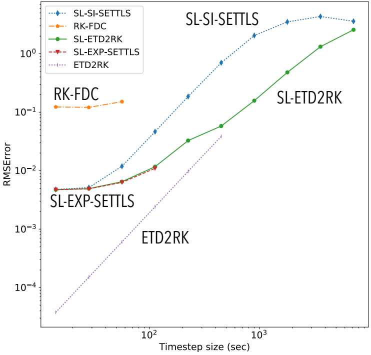


SL-SI-SETTLS/SL-EXP-SETTLS/SL-ETD2RK identically looking

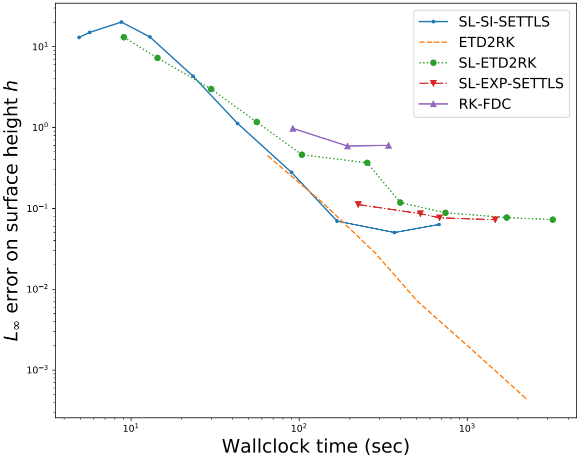
Full SWE

At day 1 of integration (dominance of linear waves)



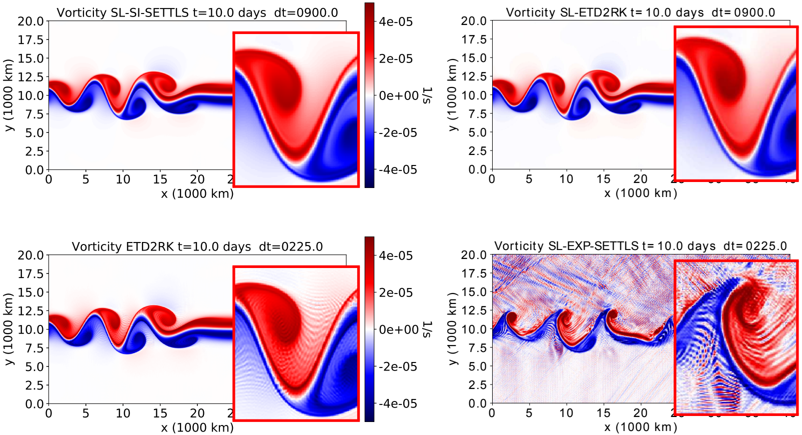


Computational cost



Errors vs. wallclock time at day 1.

Full SWE - Day 10



Vorticity field (implicit diffusion on the nonlinear divergence term with $\mu = 25.6 \times 10^6\,\mathrm{m}^2\mathrm{s}^{-1}$)

Summary

Main conclusion

- Semi-Lagrangian coupling with Exponential Integration possible, but requires a lot of careful design
  - Better linear wave dispersion compared to Semi-Implicit
  - Stability for large time-steps compared to Classic Exponential Integration
  - Energy from non-linear wave interaction may need to be controlled (diffusion).
- Under construction
  - Connections with Lagrangian Laplace Transform Scheme
  - Spherical Shallow Water Model with Spherical Harmonics Exponential
  - Higher order semi-Lagrangian exponential (long term)

Preprint

Semi-Lagrangian Exponential Integration
under 2nd round of review in SIAM Sci. Comp.
`www.ime.usp.br/~pedrosp`

SWEET!

SWEET! Shallow Water Equation Environment for Tests, Awesome!

- Bi-periodic plane and sphere
- Spectral (Fourier/Spherical Harmonics) and finite-difference schemes
- Semi-Lagrangian (SETTLS)
- PINT: PARAREAL, PFASST
- Graphical user interface (GPU)
- Easy-to-code in C++ (HPC hidden)
- Open and collaborative

Main developer: Martin Schreiber

Developers: Pedro Peixoto, Andreas Schmitt, Francois Hamon

`https://schreiberx.github.io/sweetsite/`

Thank you!

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General notation

Continuous initial value problem

$$\frac{du}{dt} = \mathcal{L}(u) + \mathcal{N}(u), \quad u(0) = u_0$$

Semi-Discrete (continuous in time)

$$\frac{dU}{dt} = LU + N(U), \quad U(0) = U_0,$$

Continuous with explicit nonlinear advection ($\vec{v}(u)$)

$$\frac{Du}{Dt} = \frac{\partial u}{\partial t} + \vec{v} \cdot \nabla u = \mathcal{L}(u) + \tilde{\mathcal{N}}(u), \quad u(0) = u_0,$$

Associated Semi-discrete

$$\frac{DU(t,\vec{r}(t))}{Dt} = L(U(t,\vec{r}(t))) + \tilde{N}(U(t,\vec{r}(t))), \quad U(t_0,\vec{r}(t_0)) = U^0,$$

$$\frac{d\vec{r}(t)}{dt} = \vec{v}(t,\vec{r}(t),u(t,\vec{r}(t))), \quad \vec{r}(0) = \vec{r}_0.$$