Semi-Lagrangian exponential integration for geophysical flows

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Abstract:

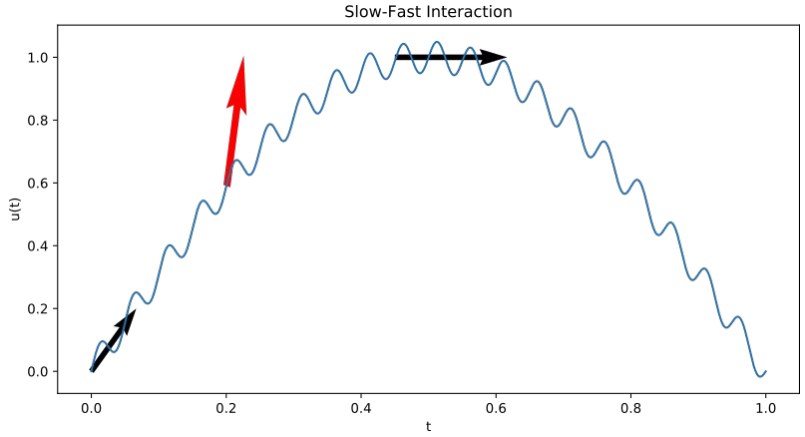
Weather and climate models must handle both highly oscillatory linear dynamics and important nonlinear advection effects while maintaining computational efficiency. To achieve large time-step sizes, models often use semi-Lagrangian advection methods combined with semi-implicit treatments of oscillatory linear dynamics. However, this can lead to dispersion effects, such as the attenuation of wave speed in fast atmospheric waves. Exponential integrators are numerical methods that can accurately solve highly oscillatory linear dynamics, allowing for large time steps and potential added parallelism. However, when these integrators are used with nonlinear dynamics, they typically require smaller time steps. In this talk, we present a class of Semi-Lagrangian Exponential schemes. These schemes handle the exponential of the linear operator within a Lagrangian framework at each time step, aiming to bypass the time-step limitations of traditional exponential schemes and improve the solution of linear oscillatory dynamics compared to classic semi-implicit methods. The framework was first proposed in Peixoto & Schreiber (2019) and applied to the shallow water equations on an f-plane, demonstrating the feasibility of large time steps with exponential schemes. Recent work by Steinstraesser, Peixoto, and Schreiber (2024) has enhanced the accuracy and stability of these schemes, applying them to the rotating shallow water equations on the sphere. This new approach leverages the strengths of exponential integrators for linear dynamics and semi-Lagrangian methods for nonlinear advection, promising more efficient numerical simulations of geophysical fluid dynamics.

Motivations: NWP

Numerical Weather Prediction (NWP)

Ultimate goal: Solve 3D compressible Euler equations on the sphere

Dynamics are highly influenced by **oscillatory dynamics (linear waves)** and **nonlinear advection.**



$$\frac{D\mathbf{u}}{Dt} = -2\,\boldsymbol{\Omega} \times \mathbf{u} - \frac{1}{\rho}\nabla p + \mathbf{g} + \mathbf{F}_r \text{ (Momentum)}$$

$$\frac{D\rho}{Dt} = -\rho \nabla \cdot \mathbf{u} \text{ (Continuity)}$$

$$c_v \frac{DT}{Dt} = -\frac{p}{\rho}\nabla \cdot \mathbf{u} \text{ (Thermodynamics)}$$

- $\mathbf{u} = (u, v, w)$: wind velocity
- p: pressure
- ρ: density
- T: temperature
- $D/Dt = \partial/\partial t + \mathbf{u} \cdot \nabla$: Material derivative

Motivation: NWP

Desirable numerical properties:

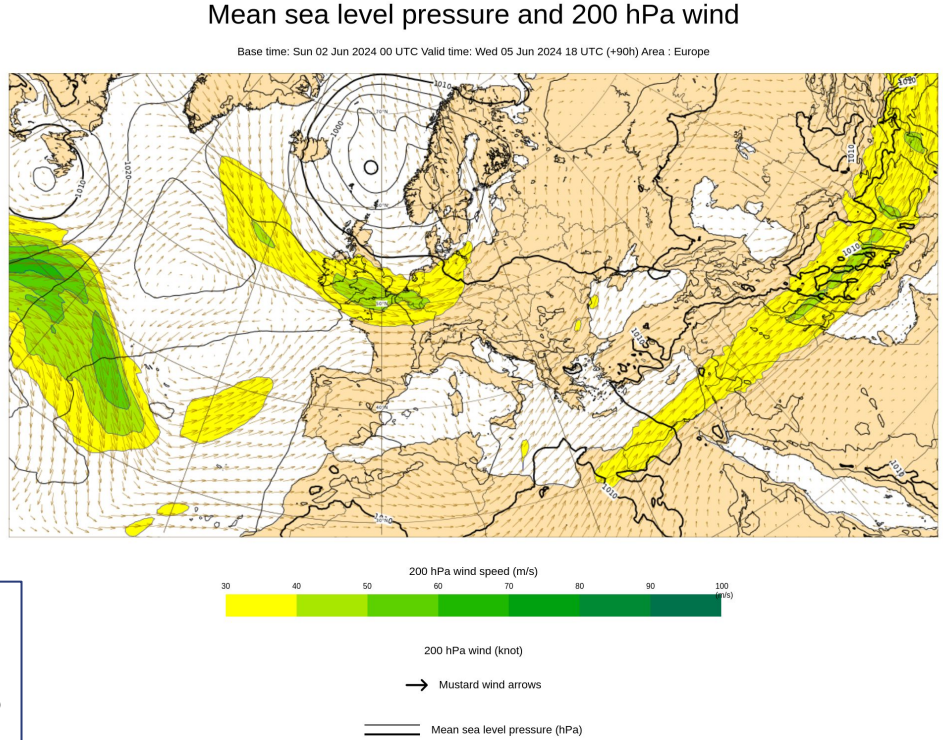
- Large timestep sizes
- Accurate dispersion relations

Spectral Models:

IFS-ECMWF / Brazilian Atmosphere Model (BAM)

- semi-Lagrangian
- semi-implicit linear operator (Crank-Nicolson)
- spectral (spherical harmonics)

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



Motivation: General Numerical Methods

Exponential integrators solve accurately **linear problems**

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

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

- Different possibilities for approximating exp(L)
- Large time steps
- Potential for added degree of parallelism

Nonlinear equations:

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

Approximation of nonlinear terms:

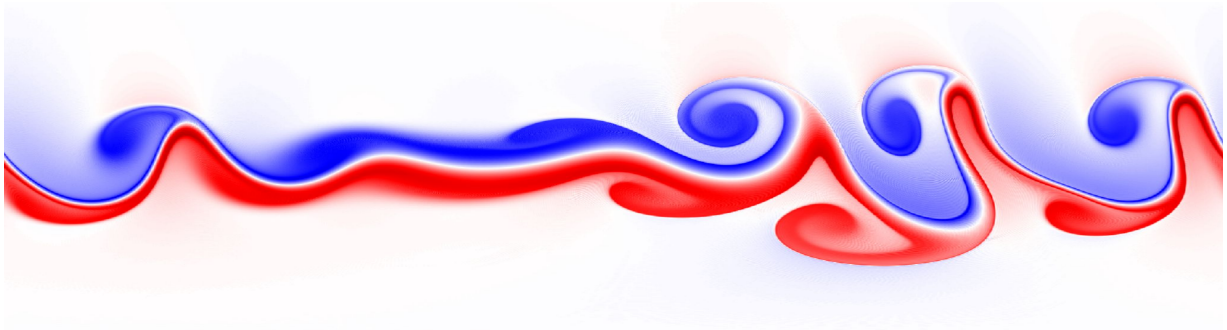
- Limitations of time step size

General Goal

Build a general class of **semi-Lagrangian exponential** schemes:

- Precise solution of linear **oscillations/waves** (hyperbolic)
- Accurate representation of **nonlinear advection** considering very large time step sizes

Target application: NWP & Climate, Atmospheric dynamics



Classic Exponential Integrators

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

If L does not depend on time, then

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

“variation-of-constants” formula.

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

Exponential integration

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

\+ Lots of more recent developments, including potential added parallelism within exponential calculation

Rational Approximations

$$e^{\tau \mathcal{L}} U(t) \approx \underbrace{\sum_{n=0}^{N} \gamma_n (\alpha_n + \tau \mathcal{L})^{-1} U(t)}_{\text{Parallelizable sum}}$$

Eigen-decomposition

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

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

Schreiber, Peixoto, Haut and Wingate, 2017: Beyond spatial scalability limitations with a massively parallel method for linear oscillatory problems (International Journal of High Performance Computing)

Exponential-Time-Differencing (ETDRK)

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

Accurate (Exp)

Approximated (Taylor)

EDT1RK

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

Cox, S. M., & Matthews, P. C. (2002). Exponential time differencing for stiff systems. Journal of Computational Physics, 176(2), 430-455.

Second Order Exponential-Time-Differencing

EDT2RK

Second order expansion of nonlinear term

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

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

Limited time step size due to CFL of nonlinear advection.

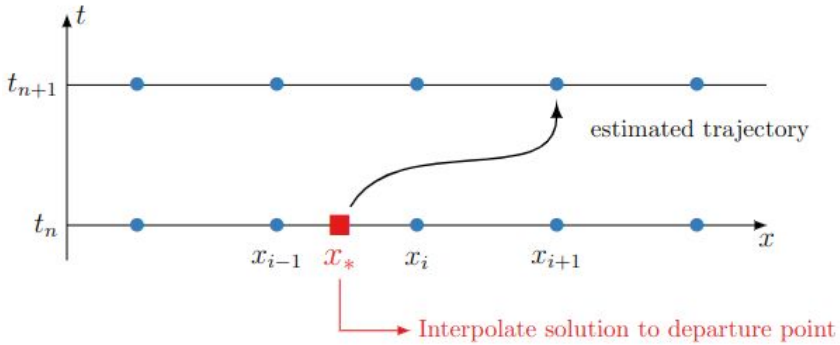
Cox, S. M., & Matthews, P. C. (2002). Exponential time differencing for stiff systems. Journal of Computational Physics, 176(2), 430-455.

Classic Semi-Lagrangian Integrators

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

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

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



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

Semi-Lagrangian Semi-Implicit

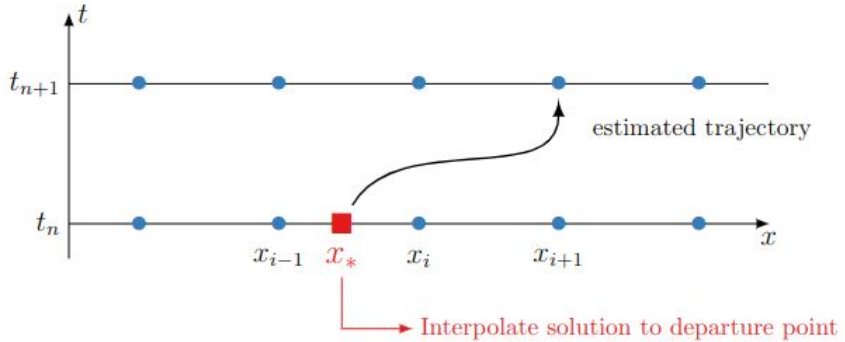
Used in IFS-ECMWF model (European Centre for Medium-Range Weather Forecasts)

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

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

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

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



Hortal, M. (2002). The development and testing of a new two-time-level semi-Lagrangian scheme (SETTLS) in the ECMWF forecast model. *Quarterly Journal of the Royal Meteorological Society: A journal of the atmospheric sciences, applied meteorology and physical oceanography*, *128*(583), 1671-1687.

Semi-Lagrangian Exponential

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

If L commutes in time*

$$L_{\vec{r}(t)} L_{\vec{r}(s)} = L_{\vec{r}(s)} L_{\vec{r}(t)}$$

Integrating Factor Problem

$$\frac{D(P_n(t)\,U(t,\vec{r}(t)))}{Dt} = P_n(t)\tilde{N}(U(t,\vec{r}(t))), \quad P_n(t_n) = I.$$

$$P_n(t) = e^{-\int_{t_n}^{t} L_{\vec{r}(s)}\, ds}$$

Assume L constant along trajectories

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

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

*Error due to lack of commutation of L in time

Semi-Lagrangian Exponential

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

Caution:

- Exponential and interpolation on departure point does not commute $e^{\Delta tL}U^n_* \neq \left(e^{\Delta tL}U^n\right)_*$
- Applications of differential operator on irregular grids (midpoints/departure points) are problematic: build method avoiding it!
- Midpoint rule along trajectories $(\varphi(\Delta tL)N(U^n))_*$

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

† interpolation to traj. midpoints

Semi-Lagrangian Exponential

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

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

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.

Peixoto, Schreiber, 2019: Semi-Lagrangian Exponential Integration with application to the rotating shallow water equations (SIAM Journal on Scientific Computing)

SL-EXP - Accuracy

Nonlinear advection + Linear operator

$$\frac{Du}{Dt} = Lu, \qquad \frac{D}{Dt} := \frac{\partial}{\partial t} + v\frac{\partial}{\partial x}$$

Local truncation error:
1st order accurate only

Semi-Lagrangrangian Exponential scheme

$$U^{n+1} = \varphi_0(\Delta t L)[U^n]^n_*$$

with 3rd order space interpolation on departure point.

Proof bases on writing:

$$U_j^{n+1} = \varphi_0(\Delta t L) \sum_{k=-r}^{q} \beta_k U^n_{j-p+k}$$

Steinstraesser, Peixoto, Schreiber, 2024: A second-order semi-Lagrangian exponential scheme with application to the shallow-water equations on the rotating sphere (In review at SIAM Sci. Comp.)

SL-EXP - Accuracy

Nonlinear advection + Linear operator

$$\frac{Du}{Dt} = Lu, \qquad \frac{D}{Dt} := \frac{\partial}{\partial t} + v\frac{\partial}{\partial x}$$

How to get 2nd order?

$$\varphi_0(\Delta t L/2)\varphi_0(\Delta t L/2) = \varphi_0(\Delta t L)$$

Semi-Lagrangrangian Exponential scheme

$$\varphi_0(\Delta t L)[\boldsymbol{U}^n]_*^n \neq \varphi_0\left(\frac{\Delta t L}{2}\right)\left[\varphi_0\left(\frac{\Delta t L}{2}\right)\boldsymbol{U}^n\right]_*^n$$

$$U^{n+1} = \varphi_0\left(\frac{\Delta t L}{2}\right)\left[\varphi_0\left(\frac{\Delta t L}{2}\right)U^n\right]_*^n$$

with 3rd order space interpolation on departure point.

Local truncation error:
2nd order

Steinstraesser, Peixoto, Schreiber, 2024: A second-order semi-Lagrangian exponential scheme with application to the shallow-water equations on the rotating sphere (In review at SIAM Sci. Comp.)

SL-EXP - 2nd order accurate

2019: Partially 1st order SE12

$$\boldsymbol{U}^{n+1}_{\mathrm{SE11}} = \varphi_0(\Delta t \boldsymbol{L}) \left[\boldsymbol{U}^n + \Delta t \psi_1(\Delta t \boldsymbol{L}) \tilde{\boldsymbol{N}}(\boldsymbol{U}^n)\right]^n_*$$

$$\boldsymbol{U}^{n+1}_{\mathrm{SE12}} = \boldsymbol{U}^{n+1}_{\mathrm{SE11}} + \Delta t \varphi_0(\Delta t \boldsymbol{L}) \left[\psi_2(\Delta t \boldsymbol{L}) \tilde{\boldsymbol{N}}(\boldsymbol{U}^{n+1}_{\mathrm{SE11}}) - \left(\psi_2(\Delta t \boldsymbol{L}) \tilde{\boldsymbol{N}}(\boldsymbol{U}^n)\right)^n_*\right]$$

2024: Fully 2nd order SE22

$$\boldsymbol{U}^{n+1}_{\mathrm{SE21}} = \varphi_0\left(\frac{\Delta t L}{2}\right) \left[\varphi_0\left(\frac{\Delta t L}{2}\right) \boldsymbol{U}^n\right]^n_* + \varphi_0(\Delta t L) \left[\Delta t \psi_1(\Delta t L) \tilde{\boldsymbol{N}}(\boldsymbol{U}^n)\right]^n_*,$$

$$\boldsymbol{U}^{n+1}_{\mathrm{SE22}} = \boldsymbol{U}^{n+1}_{\mathrm{SE21}} + \Delta t \varphi_0(\Delta t L) \left[\psi_2(\Delta t L) \tilde{\boldsymbol{N}}(\boldsymbol{U}^{n+1}_{\mathrm{SE21}}) - \left(\psi_2(\Delta t L) \tilde{\boldsymbol{N}}(\boldsymbol{U}^n)\right)^n_*\right].$$

Steinstraesser, Peixoto, Schreiber, 2024: A second-order semi-Lagrangian exponential scheme with application to the shallow-water equations on the rotating sphere (In review at SIAM Sci. Comp.)

SL-EXP - Stability

Stability due to nonlinear effects:

$$\dot{u} = \lambda_{\boldsymbol{L}} u + \boldsymbol{N}(u)$$

$$\dot{u}' = \lambda_{\boldsymbol{L}} u' + \lambda_{\boldsymbol{N}} u'$$

$$u = \overline{u} + u'$$

$$\lambda_{\boldsymbol{L}} \overline{u} + \boldsymbol{N}(\overline{u}) = 0$$

Nonlinear advection effects:

$$\frac{\partial u}{\partial t} + v \frac{\partial u}{\partial x} = \lambda_{\boldsymbol{L}} u + \lambda_{\boldsymbol{N}} u$$

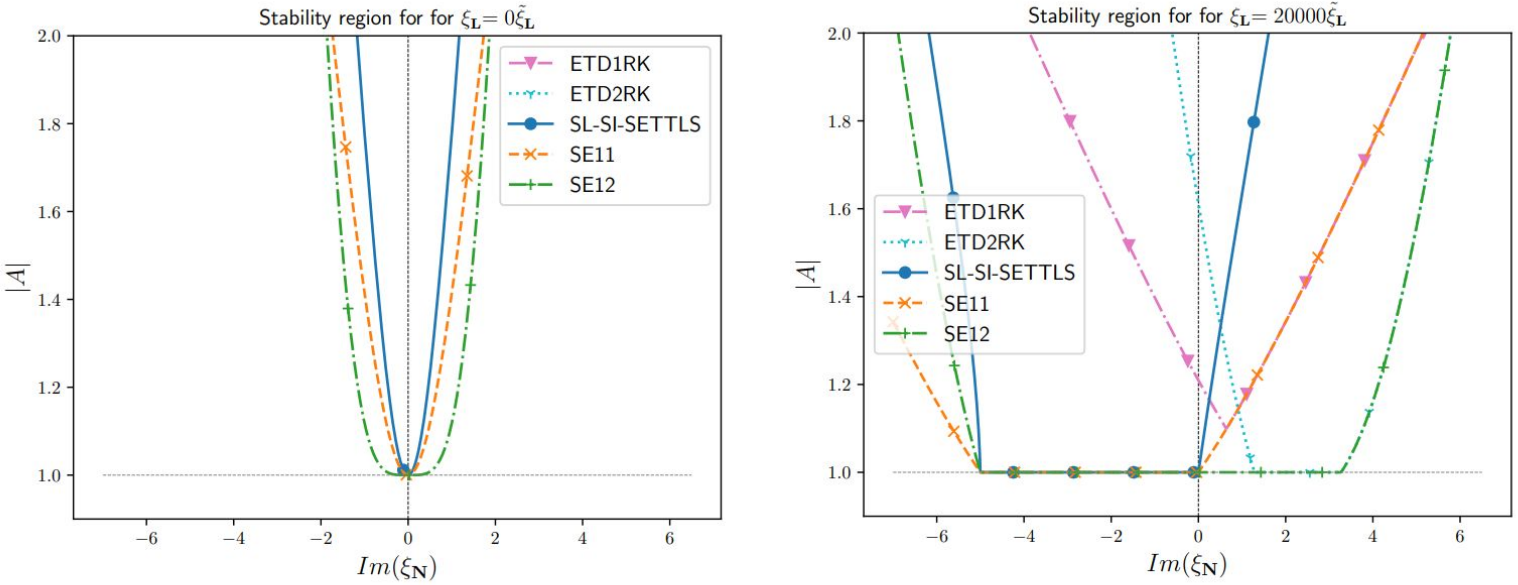
$$u^n = u(t_n, x) = A^n e^{i\kappa x}$$

Amplification factor analysis

$$\left| A(\Delta t \lambda_{\boldsymbol{L}}, \Delta t \lambda_{\boldsymbol{N}}) \right| \leq 1$$

Steinstraesser, Peixoto, Schreiber, 2024: A second-order semi-Lagrangian exponential scheme with application to the shallow-water equations on the rotating sphere (In review at SIAM Sci. Comp.)

SL-EXP - Stability



(a) $\xi_L = 0$ (b) $\xi_L = 20000\tilde{\xi}_L$

SE21 and SE22 have the same region, as for scalars (L=c): $\varphi_0(\Delta t L)[\boldsymbol{U}^n]_*^n = \varphi_0\left(\frac{\Delta t L}{2}\right)\left[\varphi_0\left(\frac{\Delta t L}{2}\right)\boldsymbol{U}^n\right]_*^n$

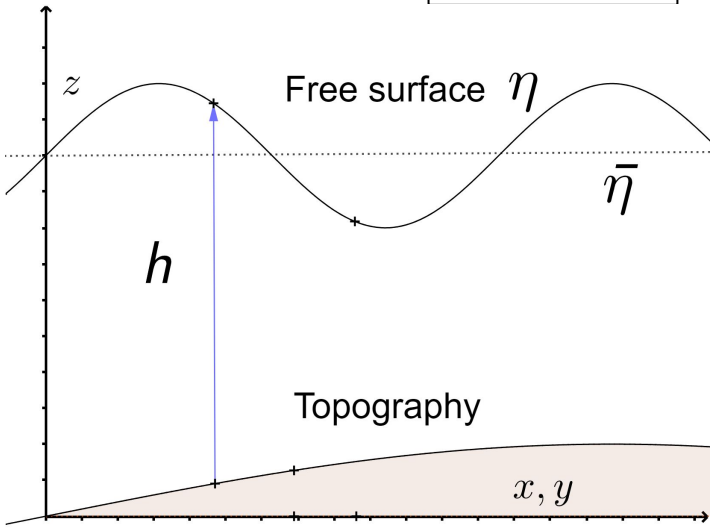
Steinstraesser, Peixoto, Schreiber, 2024: A second-order semi-Lagrangian exponential scheme with application to the shallow-water equations on the rotating sphere (In review at SIAM Sci. Comp.)

Model Problem - Plane

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

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

Vertical Integration (Mean Flow)



Model Problem - Plane

Spectral (Fourier) expansion in space

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

Coriolis is treated within the exponential

Eigenvalues (Λ): $e^{\mathcal{L}(i\vec{k})} = Qe^{\Lambda}Q^{-1}$

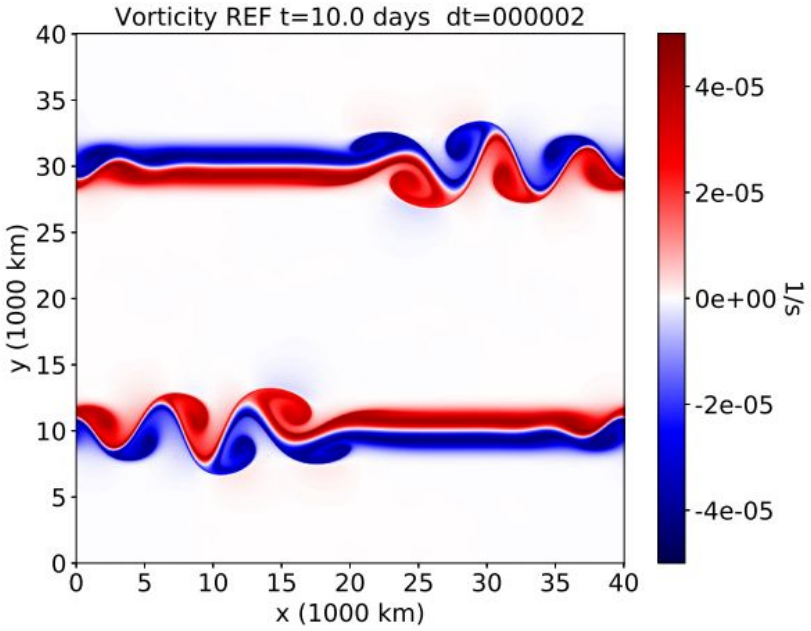
$$\omega_f(\vec{k}) = 0, \quad \omega_g(\vec{k}) = \pm i\sqrt{f^2 + g\bar{\eta}\,\vec{k}\cdot\vec{k}}$$

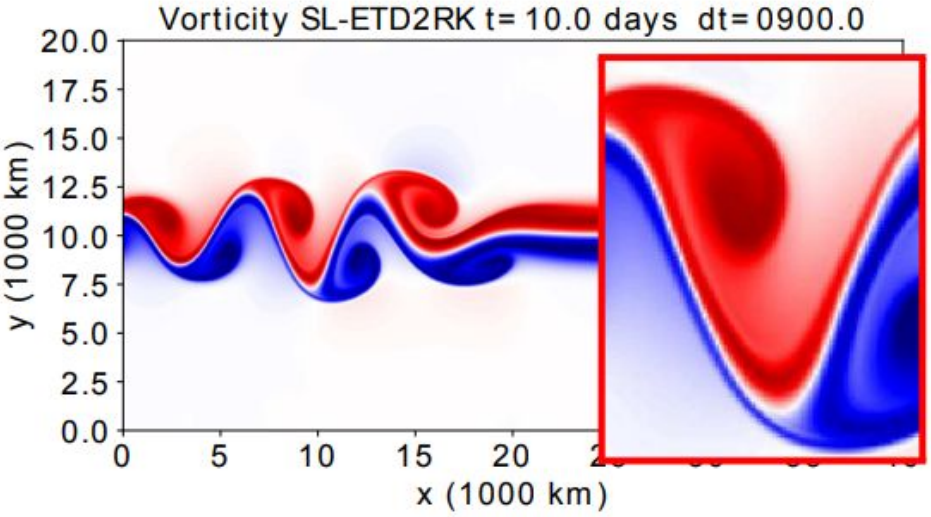
Exponential functions:

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

Planar SWE - 2019 results

2D planar **unstable jet test case**





Planar SWE - 2019 results

At day 1 of integration (dominance of linear waves)

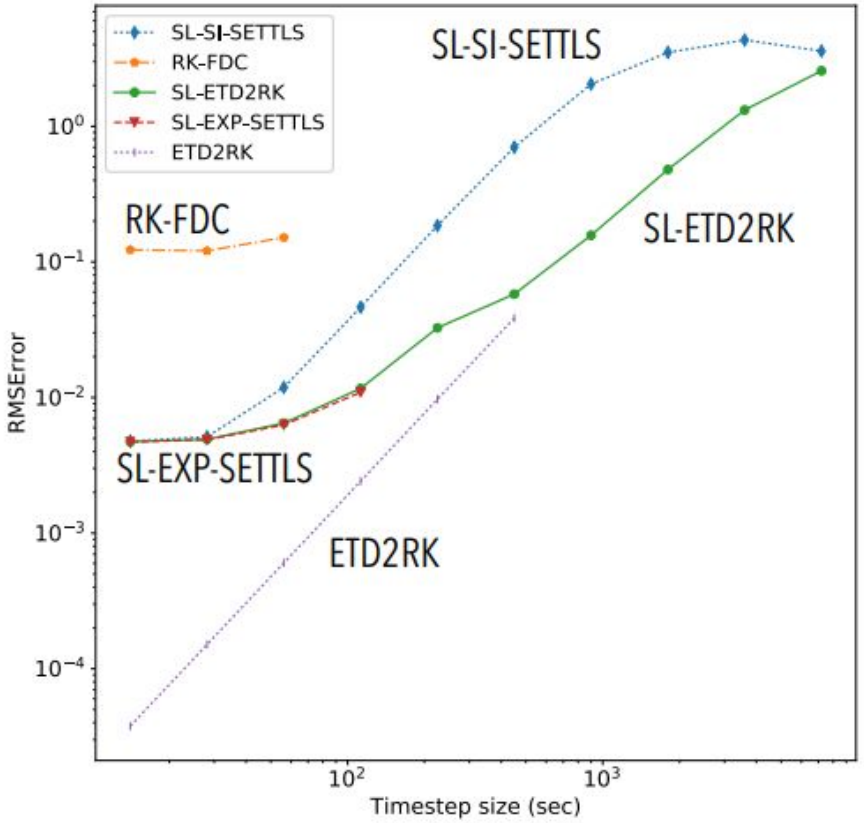
PROS

Improves accuracy of Semi-Lag-Semi-implicit

Extends stability of Exponential Integrators (ETD)

CONS

First order accurate in time



Model Problem - Shallow Water Eq. Sphere

$$\frac{\partial}{\partial t}\boldsymbol{U} = \boldsymbol{L_G}(\boldsymbol{U}) + \boldsymbol{L_C}(\boldsymbol{U}) + \boldsymbol{N_A}(\boldsymbol{U}) + \boldsymbol{N_R}(\boldsymbol{U}) + \boldsymbol{L_\nu}(\boldsymbol{U}) + \boldsymbol{b}$$

$$\boldsymbol{U} = (\Phi,\ \xi,\ \delta)^T$$

geopotential $\Phi = \overline{\Phi} + \Phi' = gh$

vorticity $\xi := \boldsymbol{z} \cdot (\nabla \times \boldsymbol{V})$

divergence $\delta := \nabla \cdot \boldsymbol{V}$

$$\boldsymbol{L_G}(\boldsymbol{U}) = \begin{pmatrix} 0 & 0 & -\overline{\Phi} \\ 0 & 0 & 0 \\ -\nabla^2 & 0 & 0 \end{pmatrix} \boldsymbol{U}$$

$$\boldsymbol{L_C}(\boldsymbol{U}) = \begin{pmatrix} 0 \\ -\nabla \cdot (f\boldsymbol{V}) \\ \boldsymbol{z} \cdot \nabla \times (f\boldsymbol{V}) \end{pmatrix}$$

$$\boldsymbol{N_A}(\boldsymbol{U}) = \begin{pmatrix} -\boldsymbol{V} \cdot \nabla\Phi \\ -\nabla \cdot (\xi \boldsymbol{V}) \\ -\nabla^2 \left(\frac{\boldsymbol{V}\cdot\boldsymbol{V}}{2}\right) + \boldsymbol{z} \cdot \nabla \times (\xi \boldsymbol{V}) \end{pmatrix}$$

$$\boldsymbol{N_R}(\boldsymbol{U}) = \begin{pmatrix} -\Phi'\delta \\ 0 \\ 0 \end{pmatrix}$$

Exponential - Spherical Harmonics

$$\mathcal{L} = \begin{pmatrix} 0 & 0 & -\overline{\Phi} \\ 0 & 0 & 0 \\ -D_n & 0 & 0 \end{pmatrix}$$

$$D_n := -n(n+1)/a^2$$

Eigenvalues

$$\pm\sqrt{-D_n\overline{\Phi}}$$

$$\varphi_k(z) = Q\varphi_k(\Lambda)Q^{-1}$$

Coriolis term is treated as a nonlinearity

$$\boldsymbol{N := L_C + N_A + N_R + b}$$

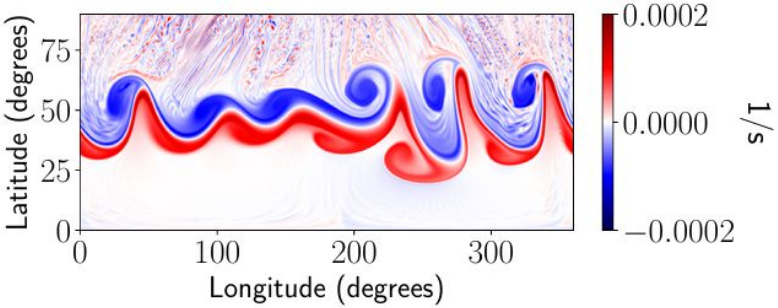
(Hough harmonics would be required to have Coriolis within the exponentials - reducing computational efficiency)

Nonlinear advection is treated in Semi-Lagrangian in SL-EXP and SL-SI

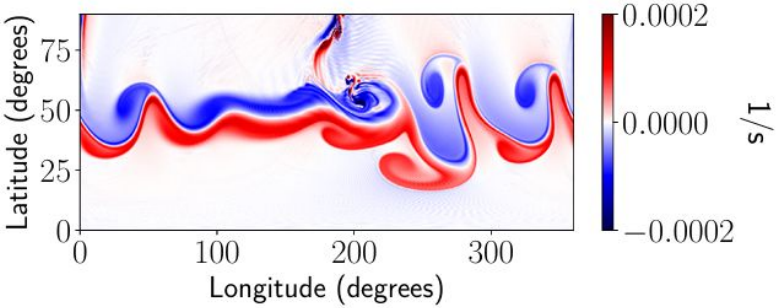
$\boldsymbol{N_A}$ Advection

$\boldsymbol{\tilde{N} := N_R + L_C + b}$ Other nonlinear terms

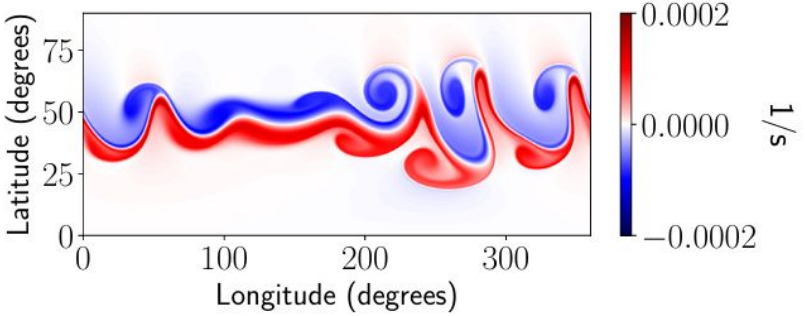
Unstable Jet (Galewsky et al) - 10 days



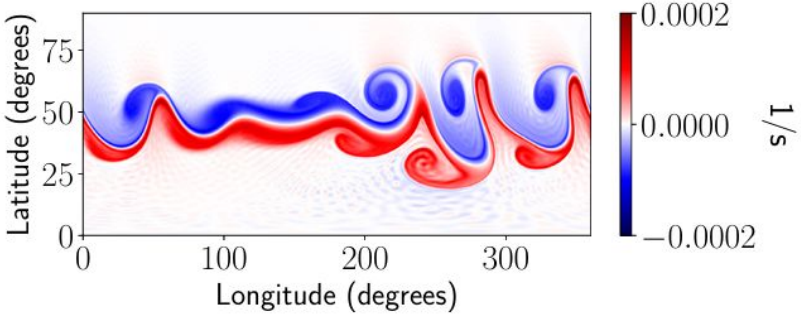
(b) SL-SI-SETTLS, $\Delta t = 120$s



(c) SL-SI-SETTLS, $\Delta t = 960$s



(f) SE22, $\Delta t = 120$s



(g) SE22, $\Delta t = 960$s

Improves accuracy of SL-semi-implicit - Reaches large time steps

SWE - Sphere

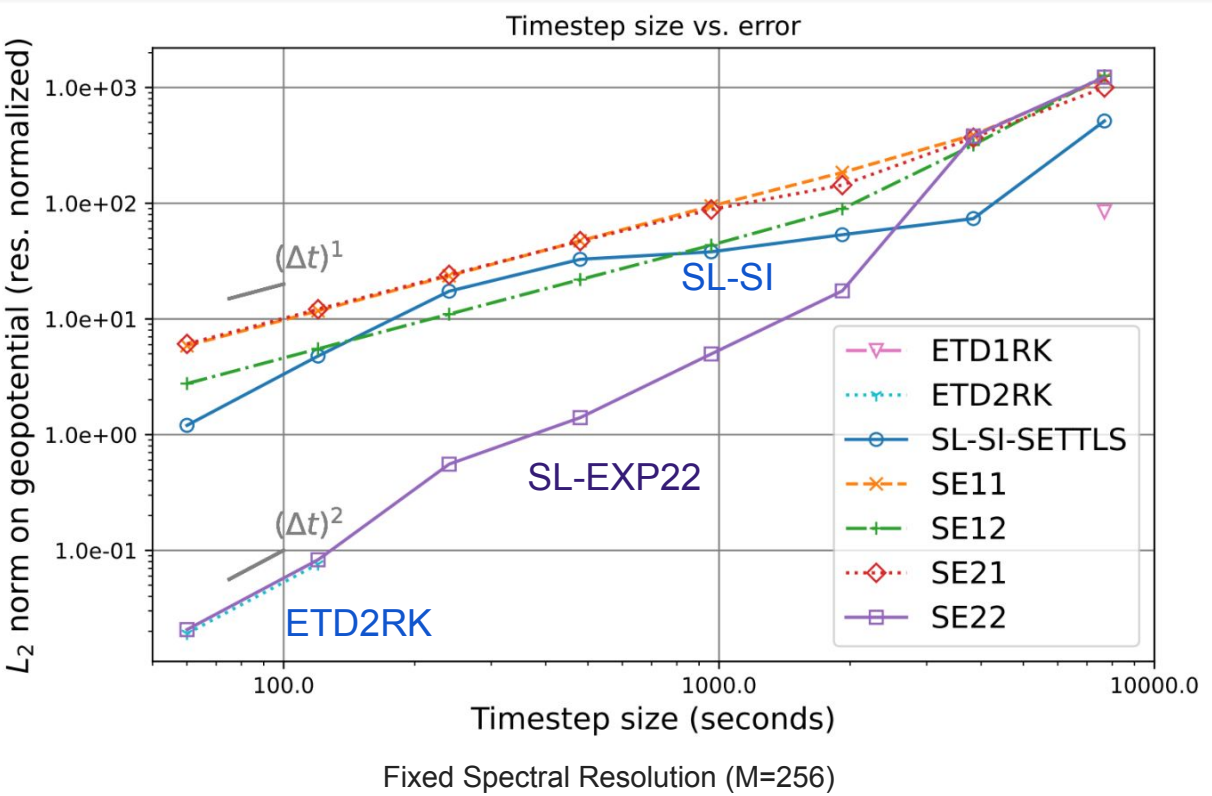
Unstable Jet (Galewsky) - 1 day

PROS

Improves accuracy of Semi-Lag-Semi-implicit

Extends stability of Exponential Integrators (ETD)

2nd order accurate!



Fixed Spectral Resolution (M=256)

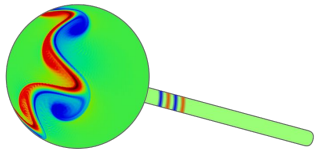
Computational Cost

Approximate wall clock times (in seconds) for the integration of the unstable jet test case (10 days of simulation)

	SL-SI-SETTLS	SE11	SE21	SE12	SE22
$\Delta t = 120$s	1378	757	1051	1244	1538
$\Delta t = 960$s	178	97	132	149	190

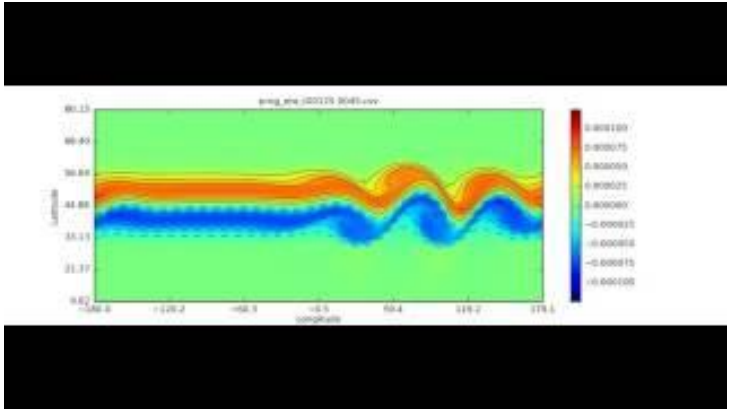
Marginal increase in computational cost for SL-EXP22

SWEET!



Shallow Water Equation Environment for Tests

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



https://sweet.gitlabpages.inria.fr/sweet-www/

"All models are wrong, but some are useful"

— George Box

Thanks!

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