



Towards Exponential Semi-Lagrangian Parallel-in-Time Methods for the Shallow Water Equations on the Rotating Sphere

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Process n. 2021/03777-2, 2021/06176-0

PinT
July 2023

Full Outline

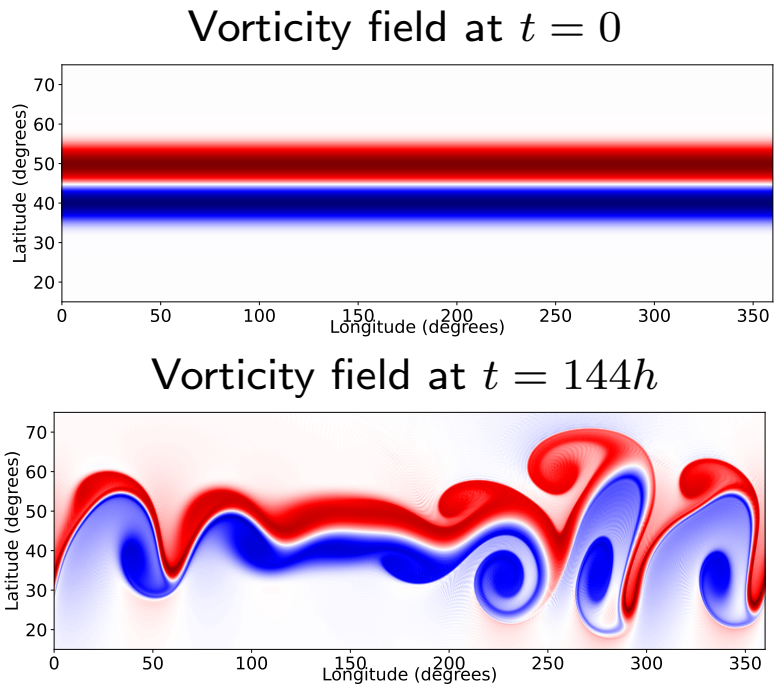
- Introduction
- Coarse time stepping methods
- MGRIT
- Numerical tests

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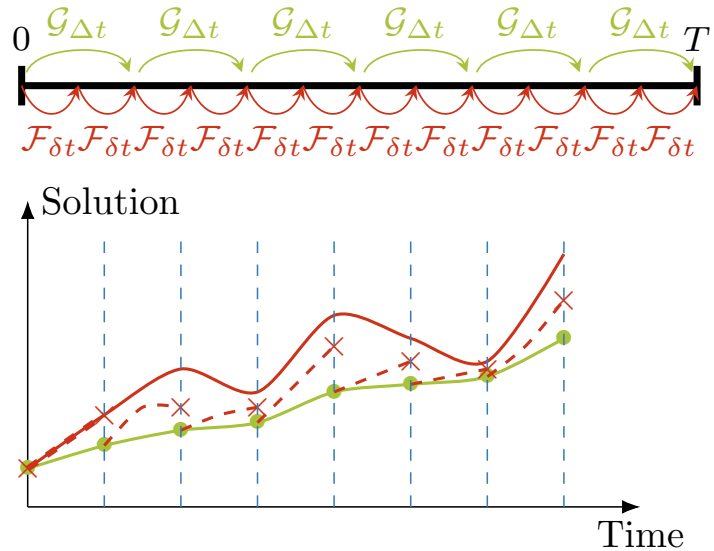
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PinT in atmospheric modelling

- Challenges:
  - Hyperbolic nature, nonlinear multiscale in time-space;
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- Choice of coarse time stepping method?
- Important dynamical charactistics?

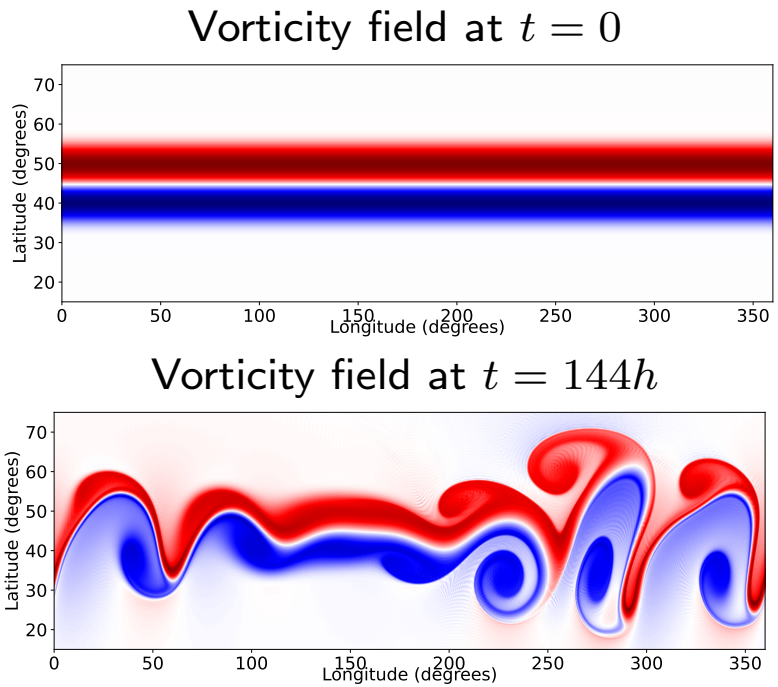


[Galewsky, Scott, and Polvani (2004)]

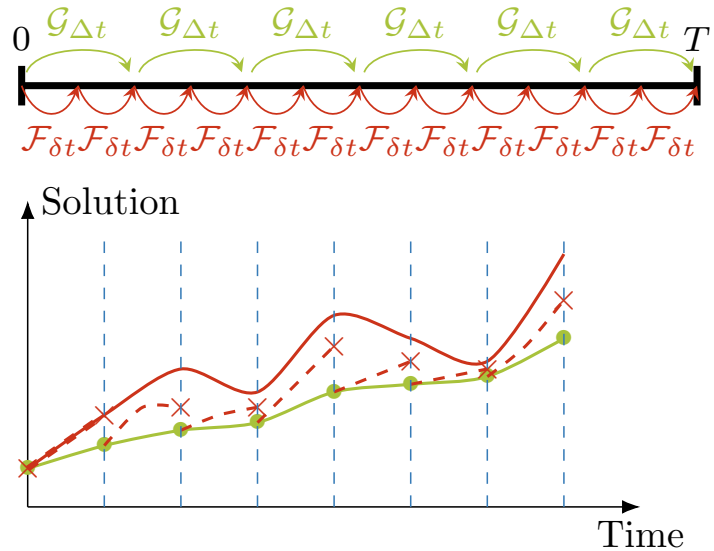


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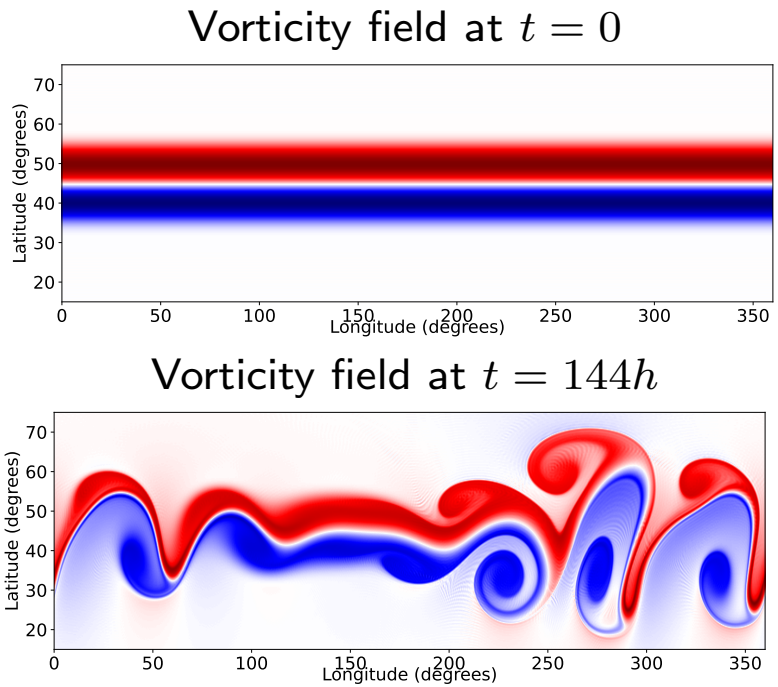


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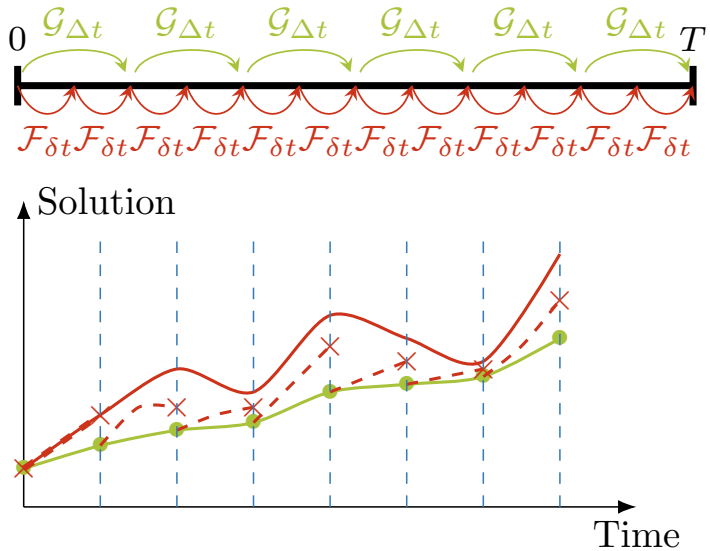


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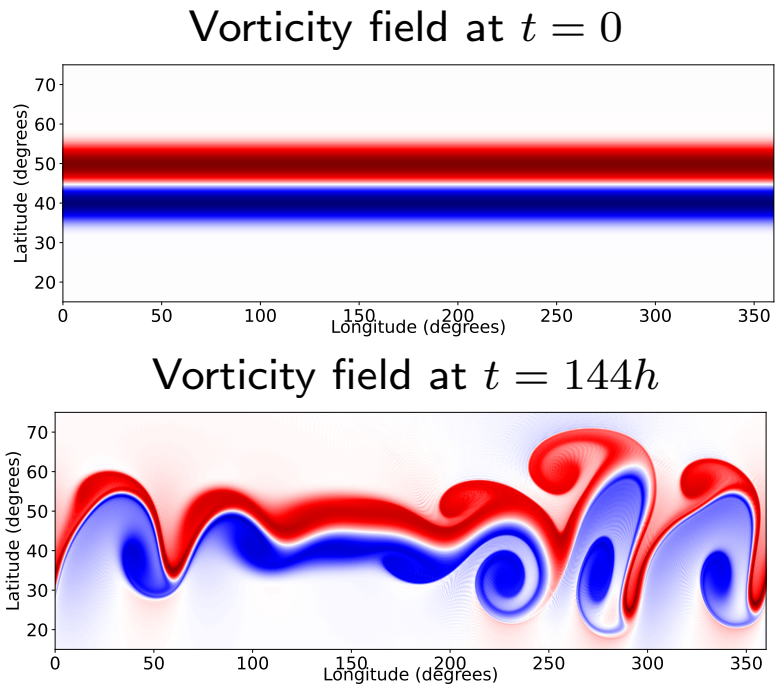


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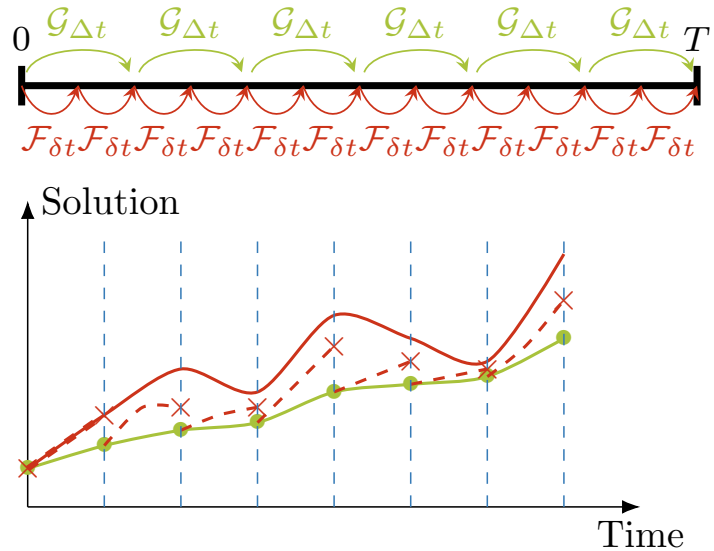


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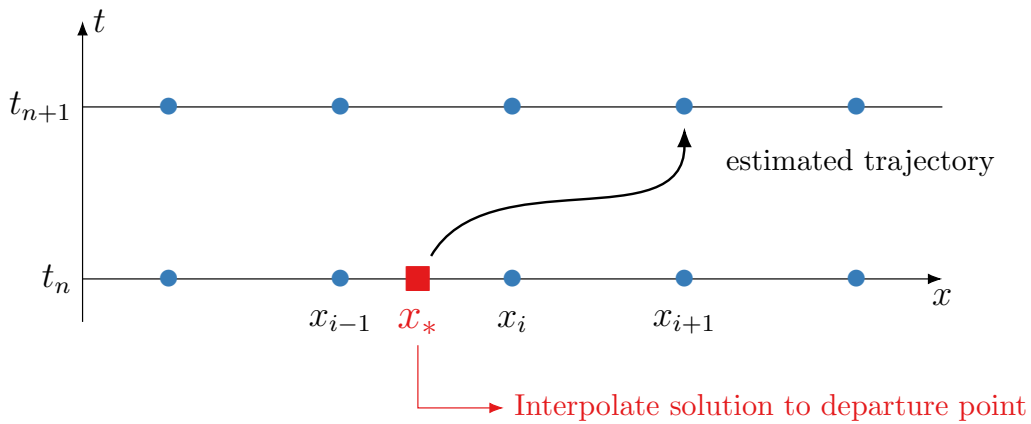
Some possibilites of coarse time stepping method

- Implicit-explicit (IMEX)

$$\boldsymbol{U}^{n+1} = \boldsymbol{F}_I^{\Delta t/2}\left(\boldsymbol{F}_E^{\Delta t}\left(\boldsymbol{F}_I^{\Delta t/2}\left(\boldsymbol{U}^n\right)\right)\right)$$

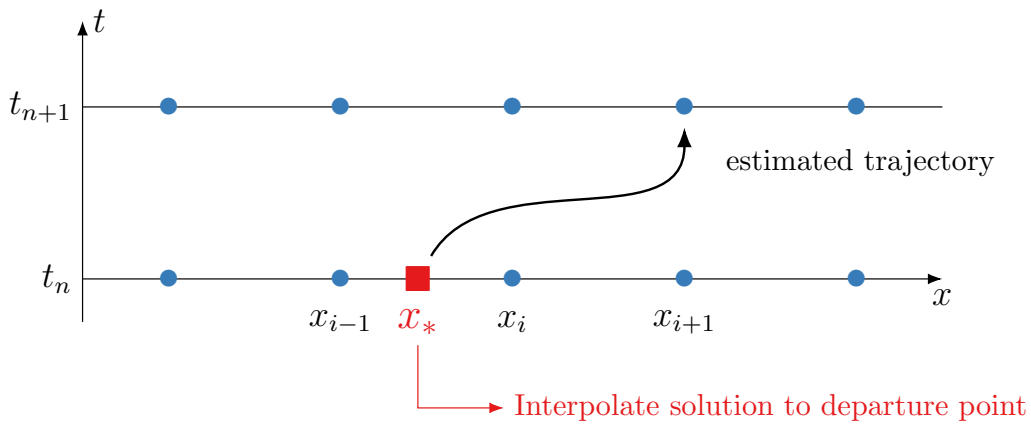
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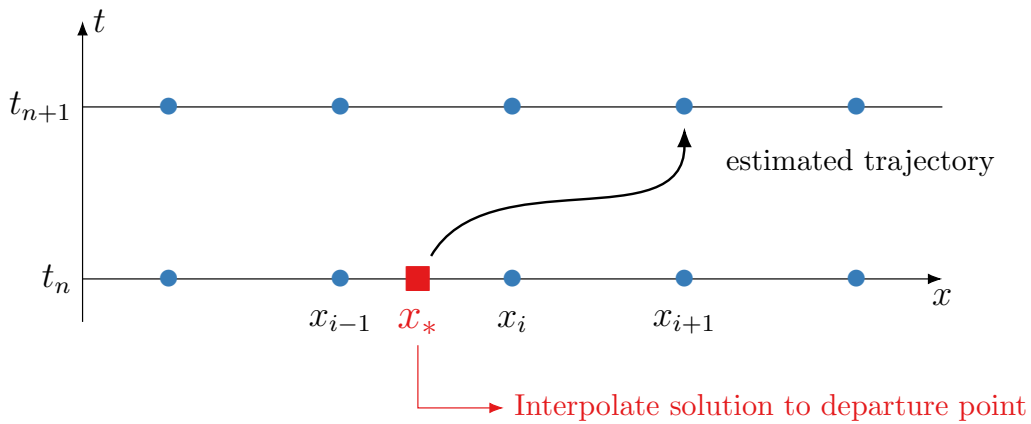
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  - Exact integration of linear terms
  - *e.g.* ETD2RK [Cox and Matthews (2002)]

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$$\begin{cases} \boldsymbol{U}^{n+1}_{\text{ETD1RK}} = \varphi_0(\Delta t \boldsymbol{L})\boldsymbol{U}^n + \Delta t \varphi_1(\Delta t L)\boldsymbol{N}(\boldsymbol{U}^n) \\ \boldsymbol{U}^{n+1}_{\text{EDT2RK}} = \boldsymbol{U}^{n+1}_{\text{ETD1RK}} + \Delta t \varphi_2(\Delta t L)\left[\boldsymbol{N}(\boldsymbol{U}^{n+1}_{\text{ETD1RK}}) - \boldsymbol{N}(\boldsymbol{U}^n)\right] \end{cases}$$

φ_k: matrix exponential functions (SWE $\implies$ for "free")

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- **Semi-Lagrangian exponential integration methods** [Peixoto and Schreiber (2019)]

$$\begin{cases} \boldsymbol{U}^{n+1}_{\text{SL-ETD1RK}} = \varphi_0(\Delta t L)\left[\boldsymbol{U}^n + \Delta t \psi_1(\Delta t \boldsymbol{L})\tilde{\boldsymbol{N}}(\boldsymbol{U}^n)\right]^n_* \\ \boldsymbol{U}^{n+1}_{\text{SL-ETD2RK}} = \boldsymbol{U}^{n+1}_{\text{SL-ETD1RK}} + \Delta t \varphi_0(\Delta t L)\left[\psi_2(\Delta t L)\tilde{\boldsymbol{N}}(\boldsymbol{U}^{n+1}_{\text{SL-ETD1RK}}) - \left(\psi_2(\Delta t \boldsymbol{L})\tilde{\boldsymbol{N}}(\boldsymbol{U}^n)\right)^n_*\right] \end{cases}$$

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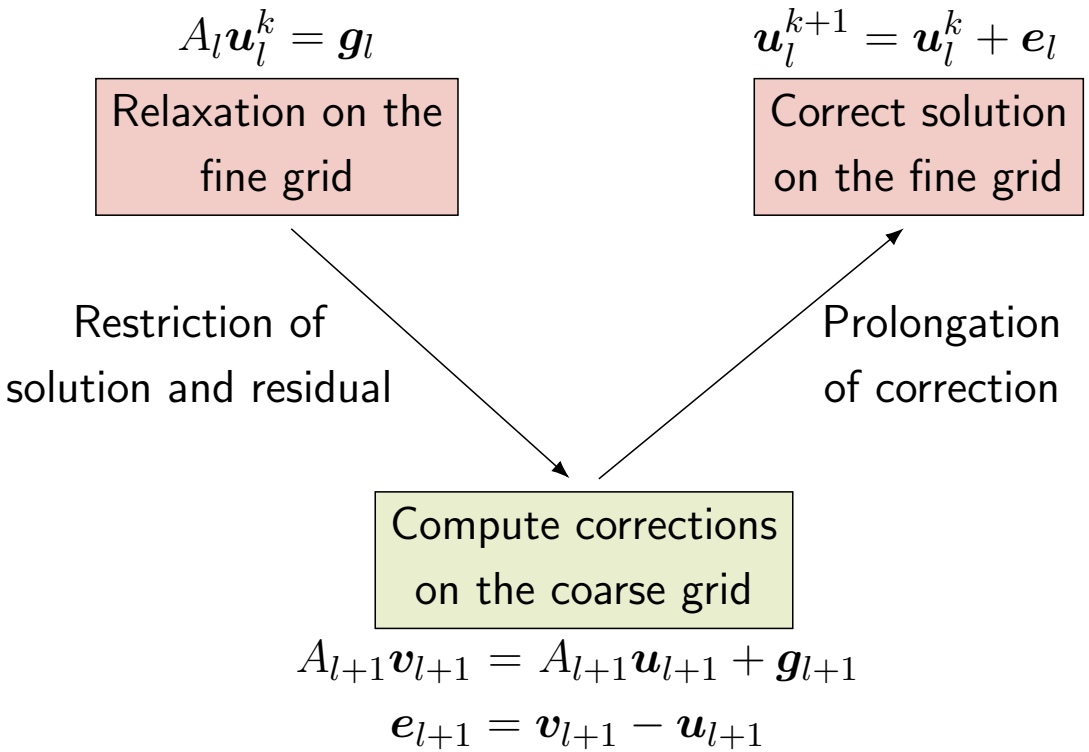
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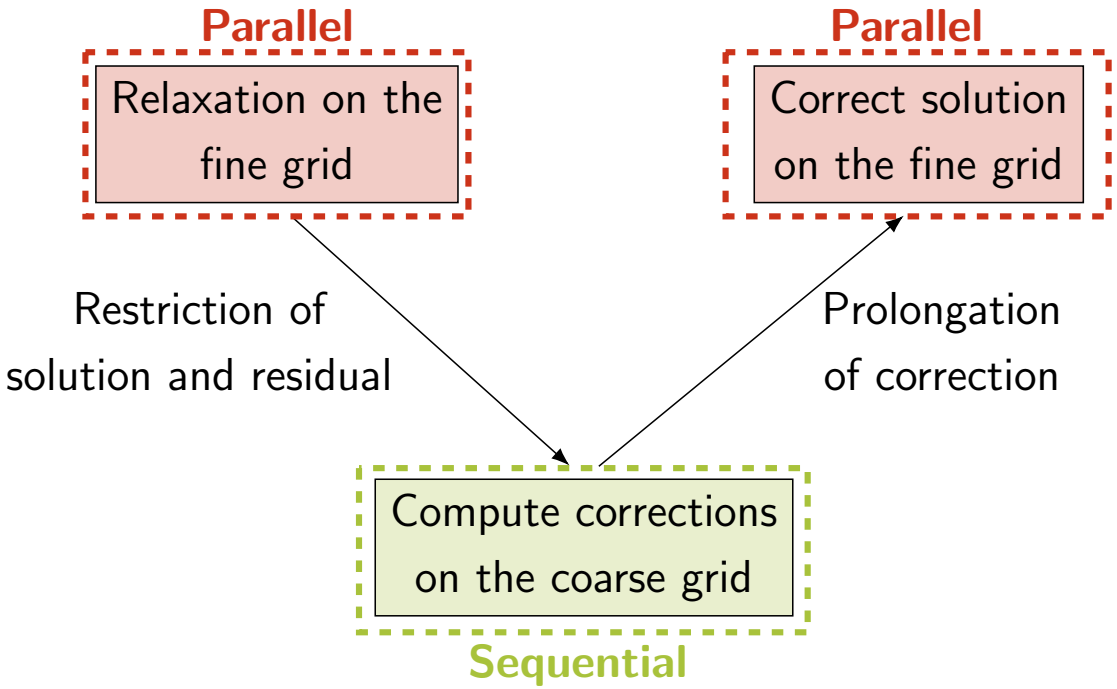
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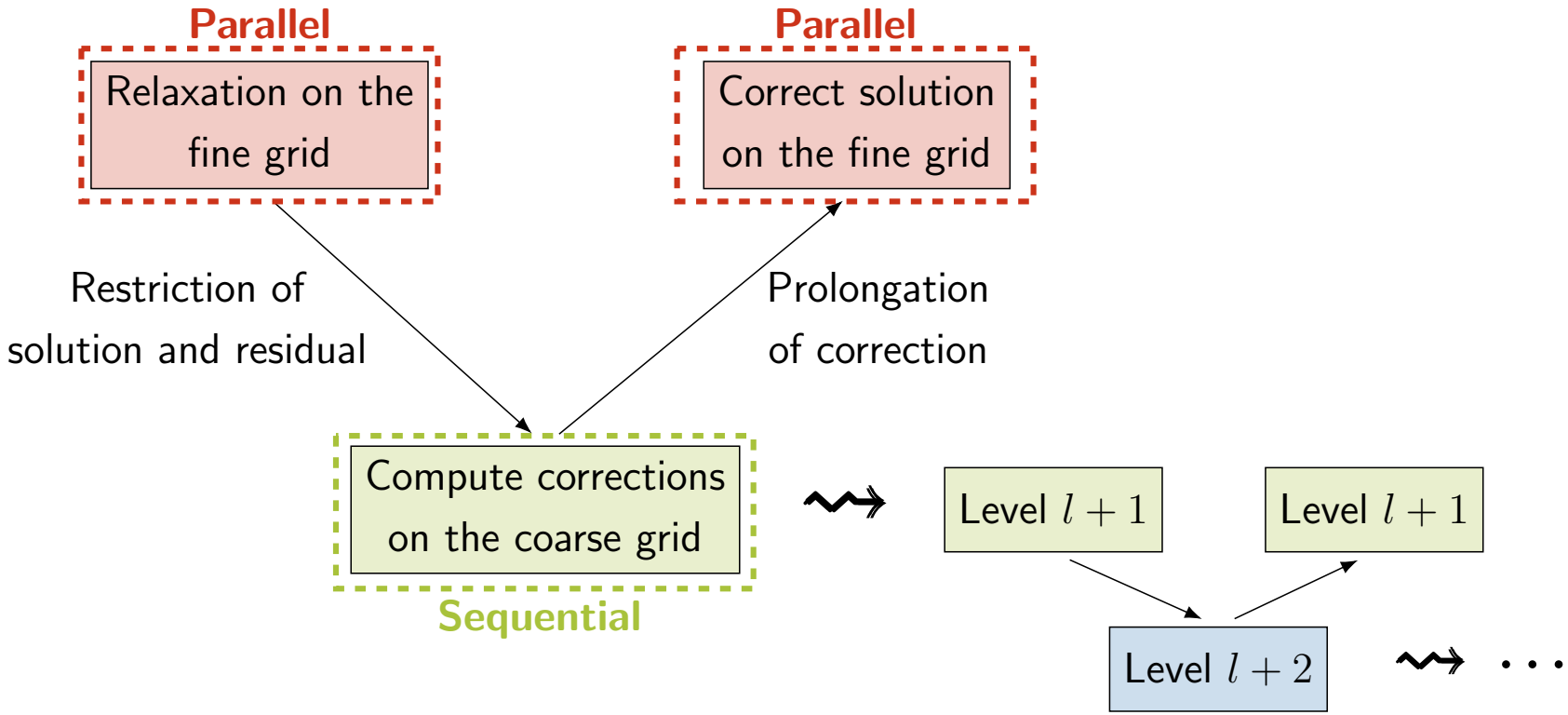
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- Solution of $A\boldsymbol{u} = \boldsymbol{g}$ is iteratively improved using the Full Approximation Scheme (FAS):
- Several parameters to be set, *e.g.* :
  - Number of levels;
  - Coarsening factor between levels: $\Delta t_{l+1} = m\Delta t_l$
  - Relaxation strategy: F, FCF, FCFCF, ..., F(CF)$^{N_{\text{relax}}}$

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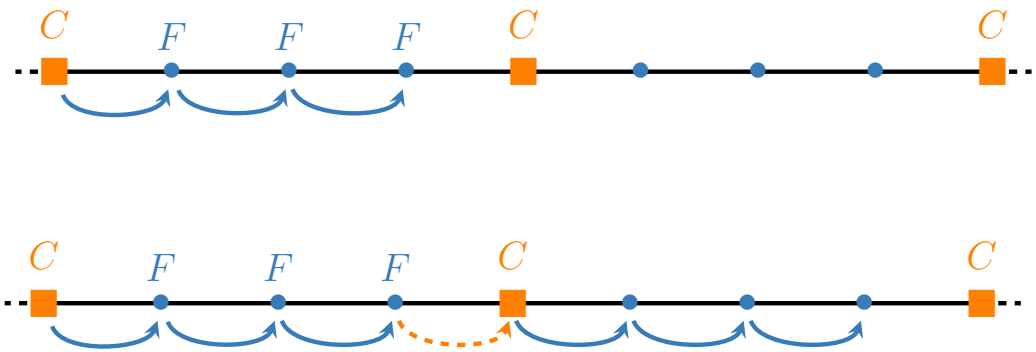
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Stability analysis of MGRIT

- Extension of stability analysis of Parareal [Staff and Rønquist (2005)]
- Linearized ODE:

$$\frac{\partial u}{\partial t} = \lambda_{\boldsymbol{L}} u + \boldsymbol{N}(u) \implies \frac{\partial u}{\partial t} = \lambda_{\boldsymbol{L}} u + \lambda_{\boldsymbol{N}} u$$

- Stability as a function of $\xi_{\boldsymbol{N}} := \lambda_{\boldsymbol{N}} \Delta t \in \mathbb{C}$:

$$|A_{\text{scheme}}(Re(\xi_{\boldsymbol{N}}), Im(\xi_{\boldsymbol{N}}))| \leq 1, \qquad u^{n+1} = A_{\text{scheme}} u^n$$

  for fixed
  - $\xi_{\boldsymbol{L}} = \lambda_{\boldsymbol{L}} \Delta t \in i\mathbb{R}$ (inertia-gravity modes) or
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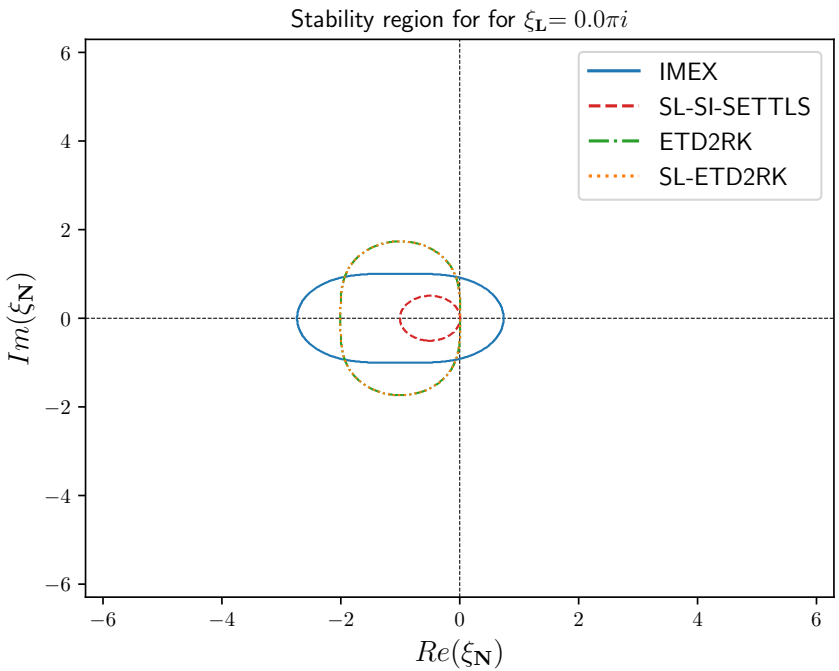
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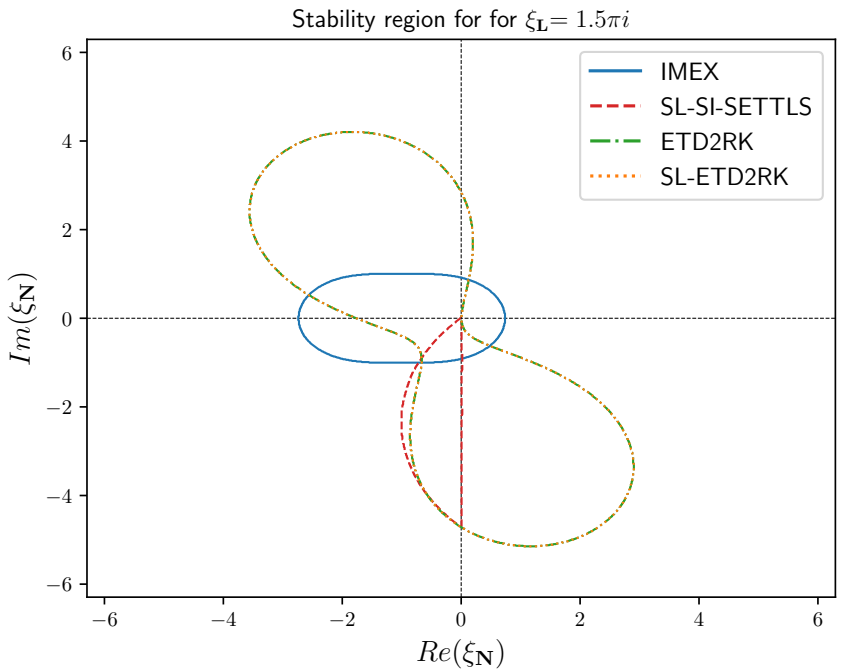
Stability analysis of MGRIT

- Stability of the serial schemes:

$\xi_L = 0$



$\xi_L = 1.5\pi i$



Stability analysis of MGRIT

- Two-level MGRIT with F(CF)$^{N_{\text{relax}}}$ relaxation:
  - equivalent to Parareal with overlapping [Gander, Kwok, and Zhang (2018)]

$$u_n^k = \phi_c(u_{n-1}^k) + \phi_f{}^{N_{\text{relax}}+1}\left(u_{n-(N_{\text{relax}}+1)}^{k-1}\right) - \phi_c\phi_f{}^{N_{\text{relax}}}\left(u_{n-(N_{\text{relax}}+1)}^{k-1}\right)$$

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- Which coarse time stepping scheme?

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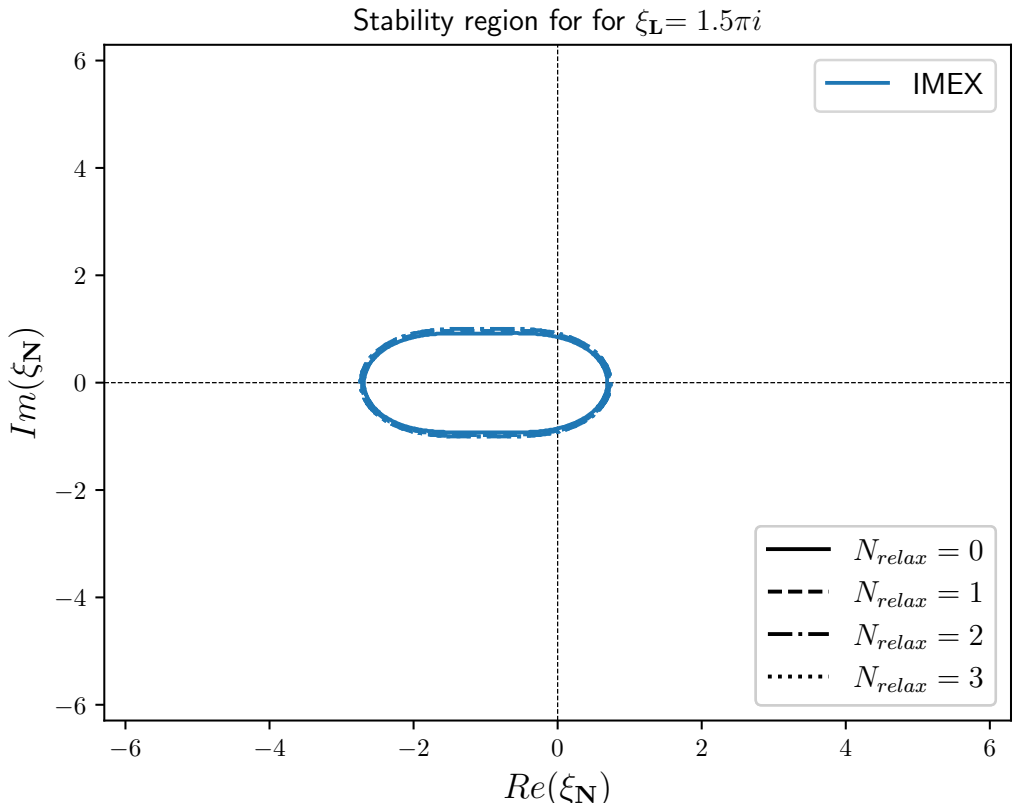
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- **Which coarse time stepping scheme?**
  - IMEX
  - SL-SI-SETTLS
  - ETD2RK
  - SL-ETD2RK

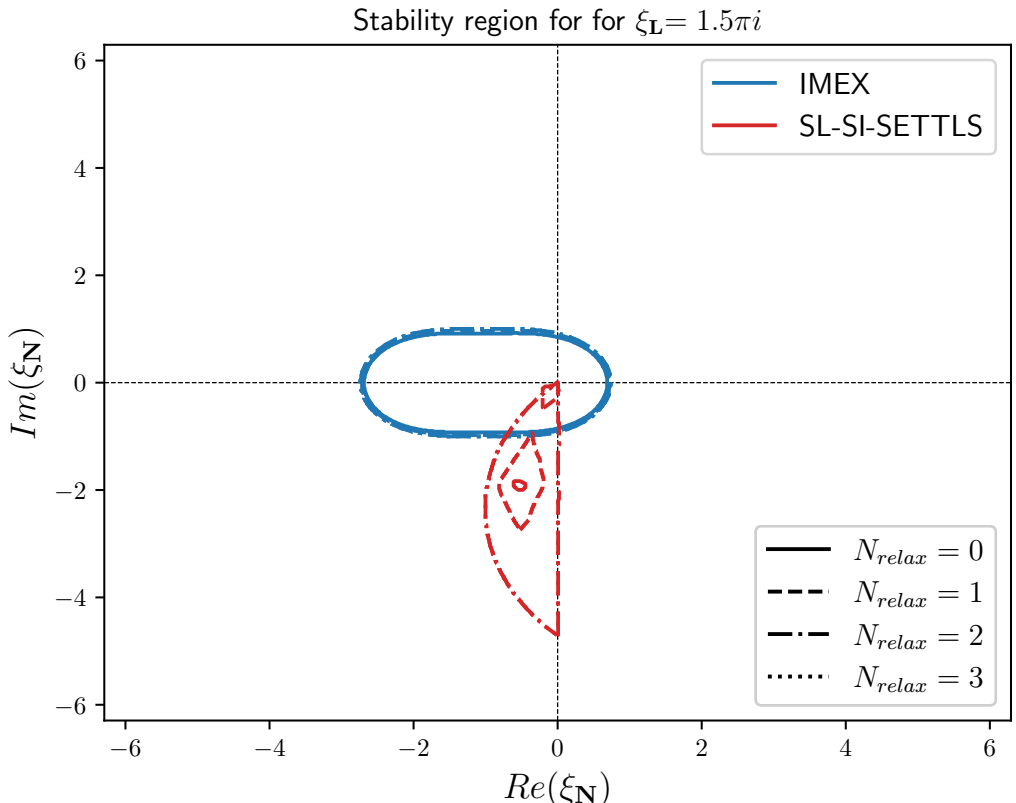
Stability analysis of MGRIT

- Stability in function of the coarse time stepping method and N_{relax}
  - Fine scheme: IMEX
  - Coarse scheme: IMEX , SL-SI-SETTLS , ETD2RK , SL-ETD2RK
  - $k = 2$, $n = 2$, $m = 100$, $\xi_{\boldsymbol{L}} = \frac{3\pi}{2} i$



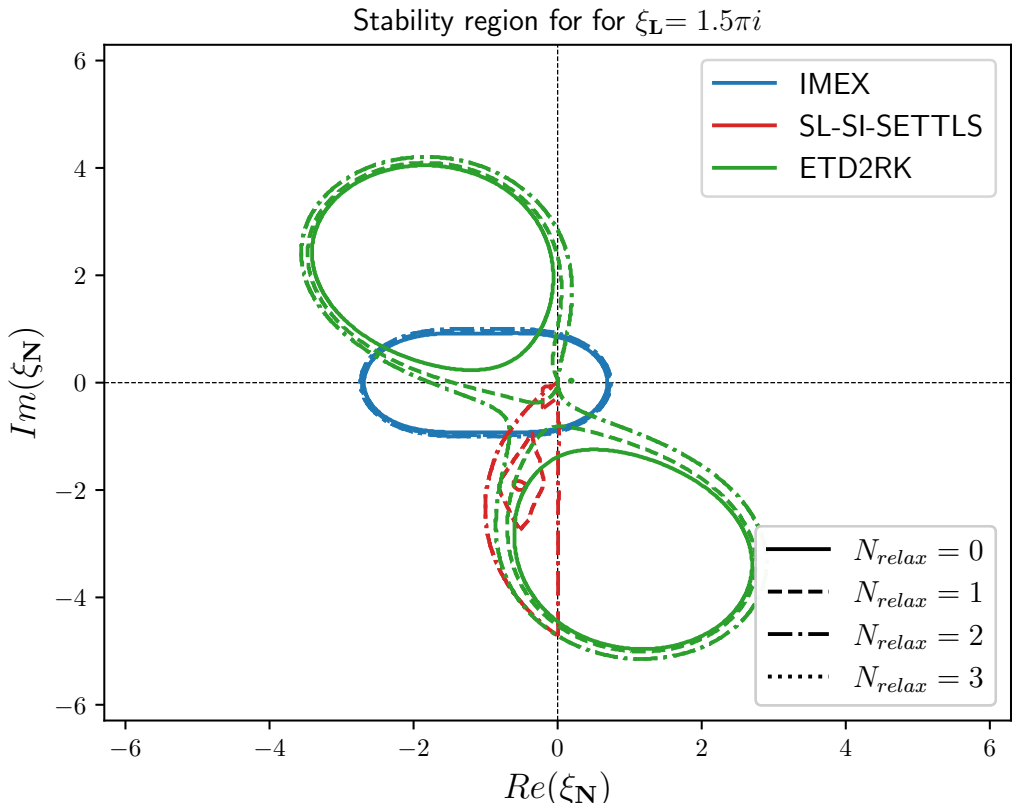
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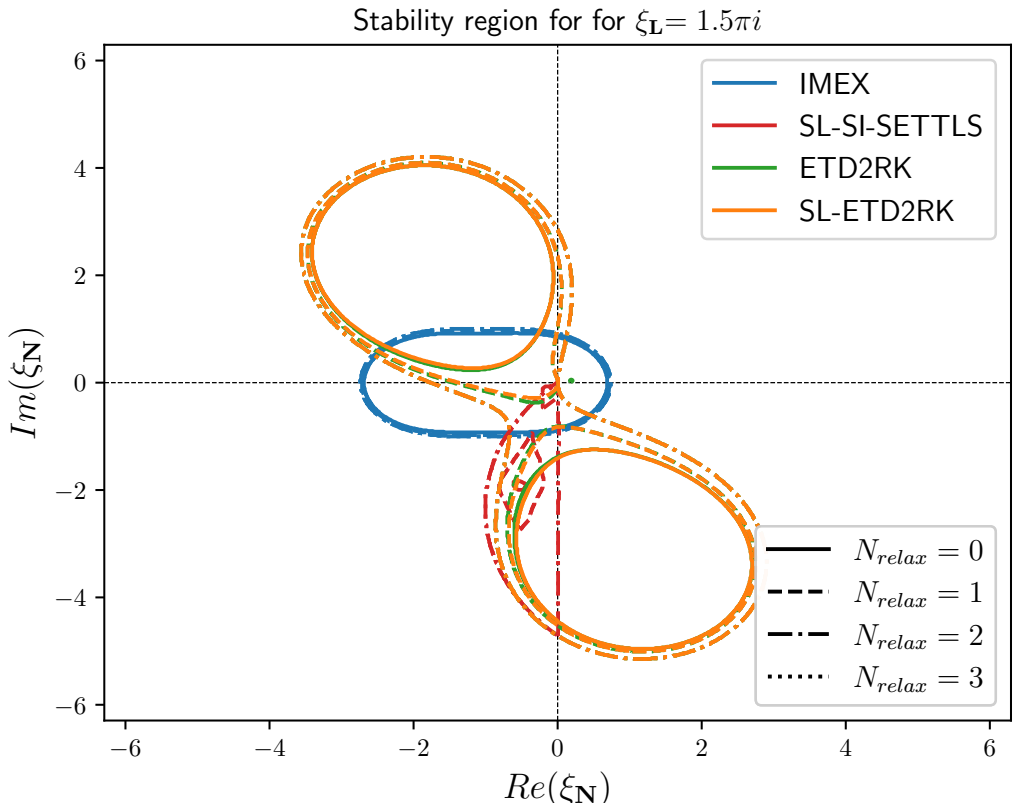
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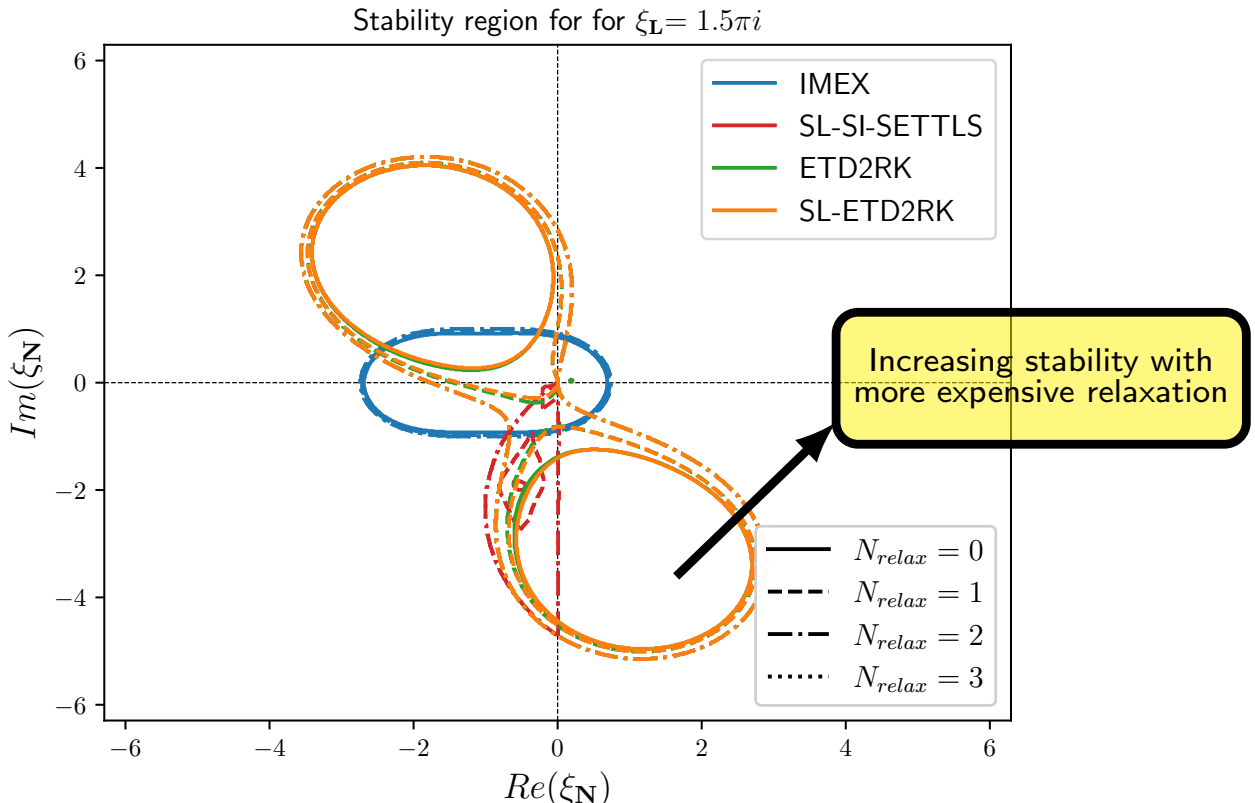
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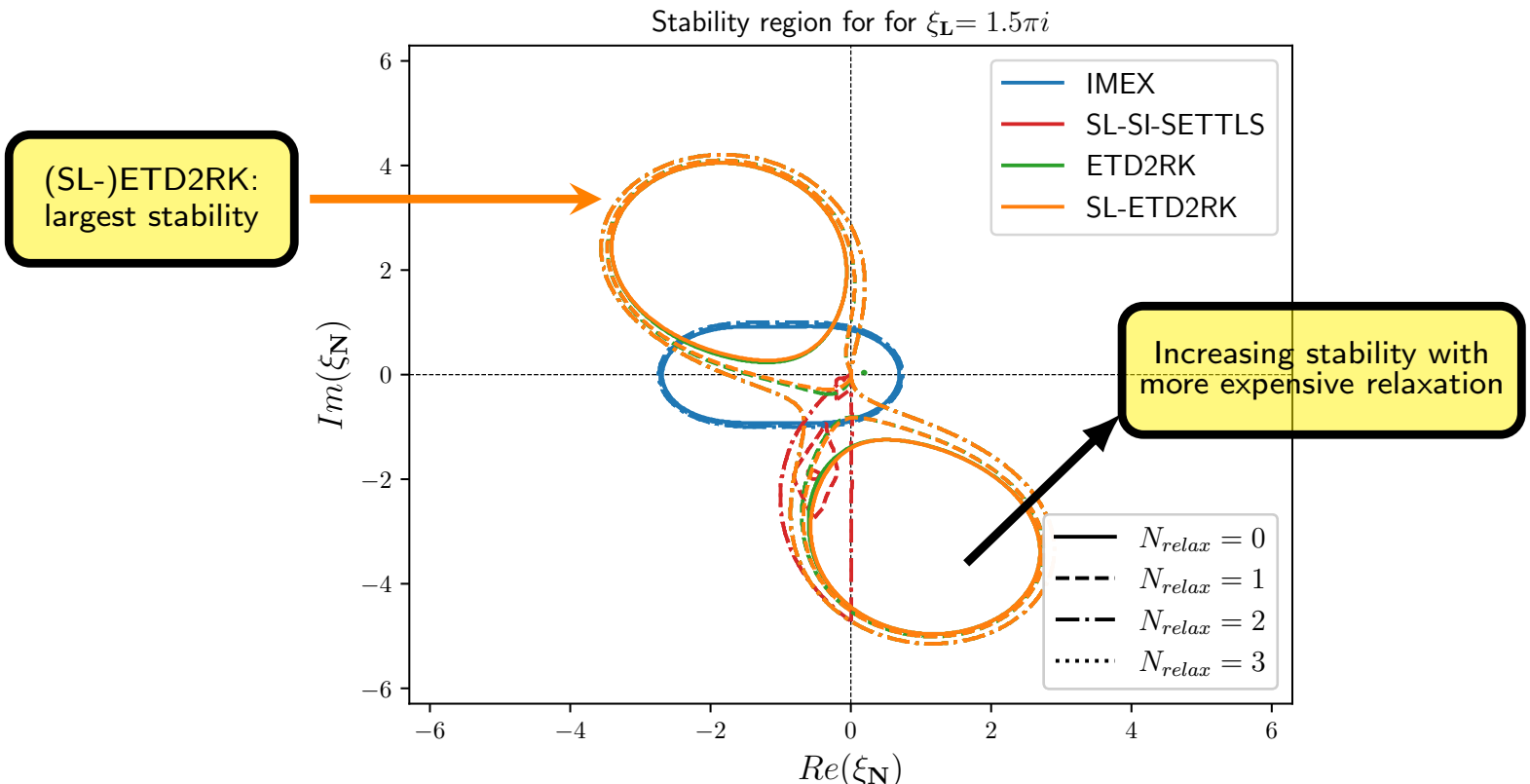
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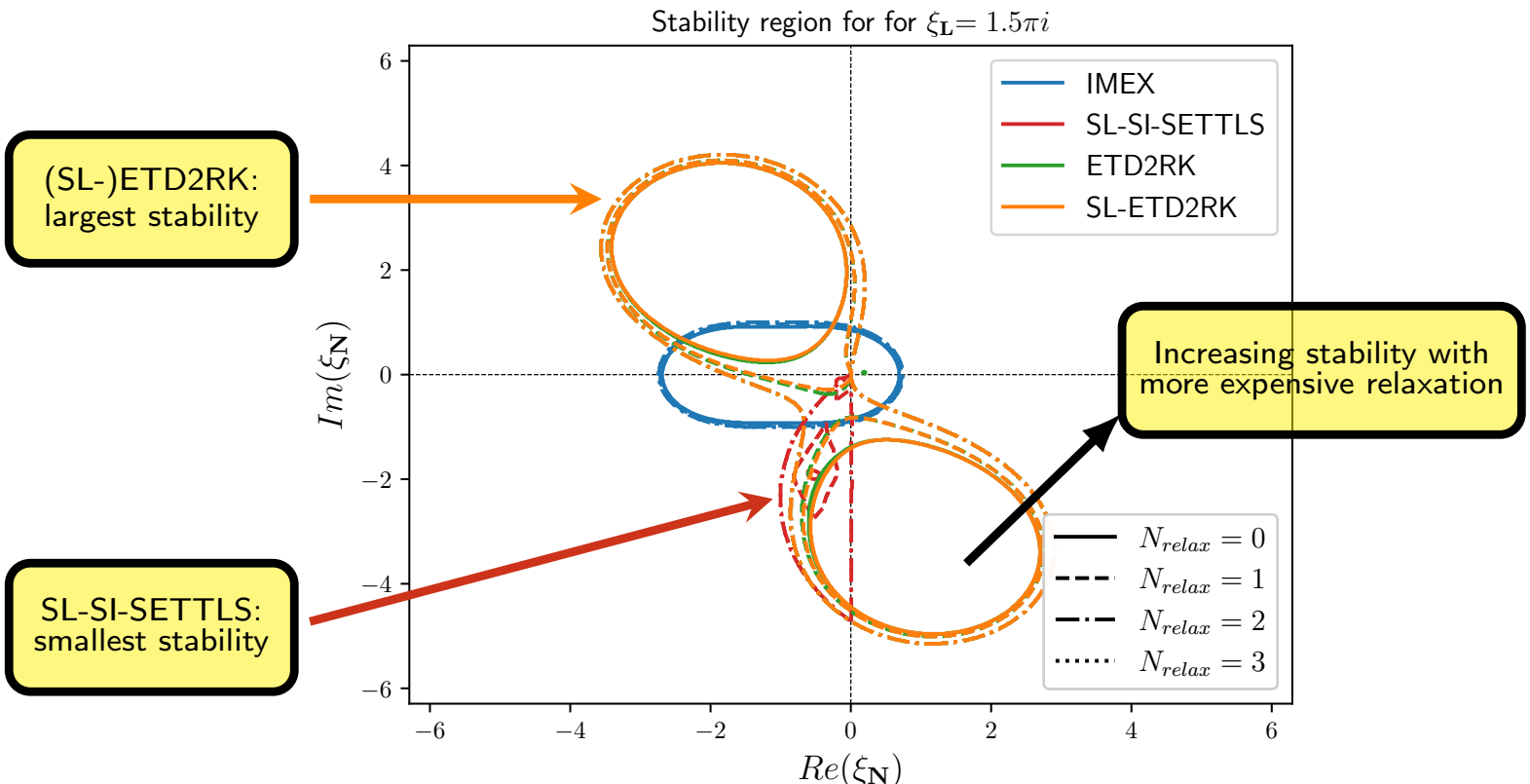
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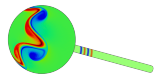
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Outline

- Introduction
- Coarse time stepping methods
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- Numerical tests

SWEET 

Shallow Water Equation Environment for Tests
C++ optimized code

Time discretizations:

- Explicit RK
- Implicit RK
- Leapfrog
- Crank-Nicolson
- Semi-Lagrangian
- Exponential integrators

Parallel-in-time

- Parareal
- PFASST
- Rational approximation of exponential integrators (REXI)
- Parallel Spectral Deferred Corrections
- MGRIT (XBRAID)

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

Test case

- Shallow water equations on the rotating sphere
- Gaussian bump perturbations in geopotential field Φ
- $T = 36$h
- Reference (fine) solution: $\delta t = 60s$, IMEX
- Coarse levels: coarsening factor m
- Artificial (hyper)viscosity only on the coarse levels: $\nu \nabla^q \boldsymbol{U}$
- Reference solution (geopotential field Φ):

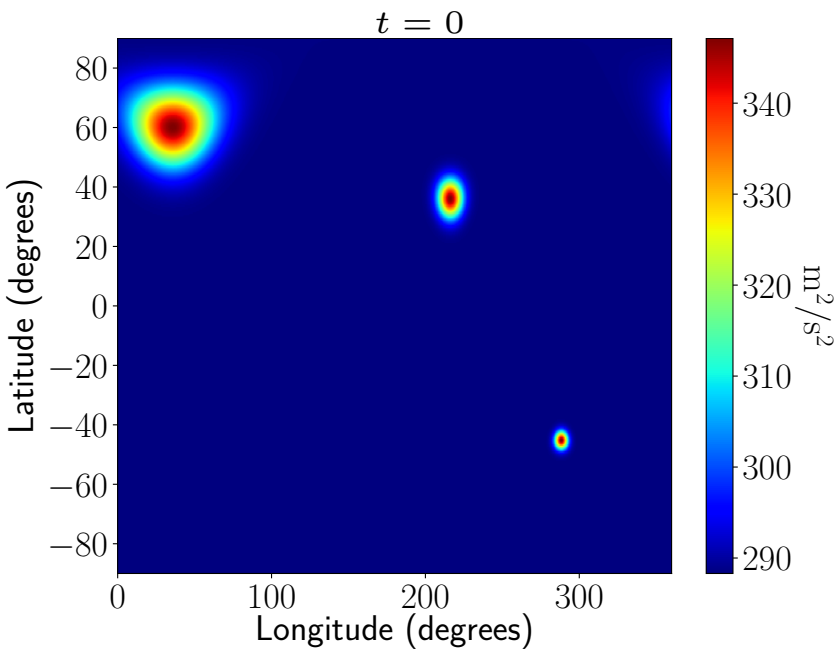
$$\frac{\partial}{\partial t}\boldsymbol{U} = \boldsymbol{L_G U} + \boldsymbol{L_C U} + \boldsymbol{N_A}(\boldsymbol{U}) + \boldsymbol{N_R}(\boldsymbol{U})$$

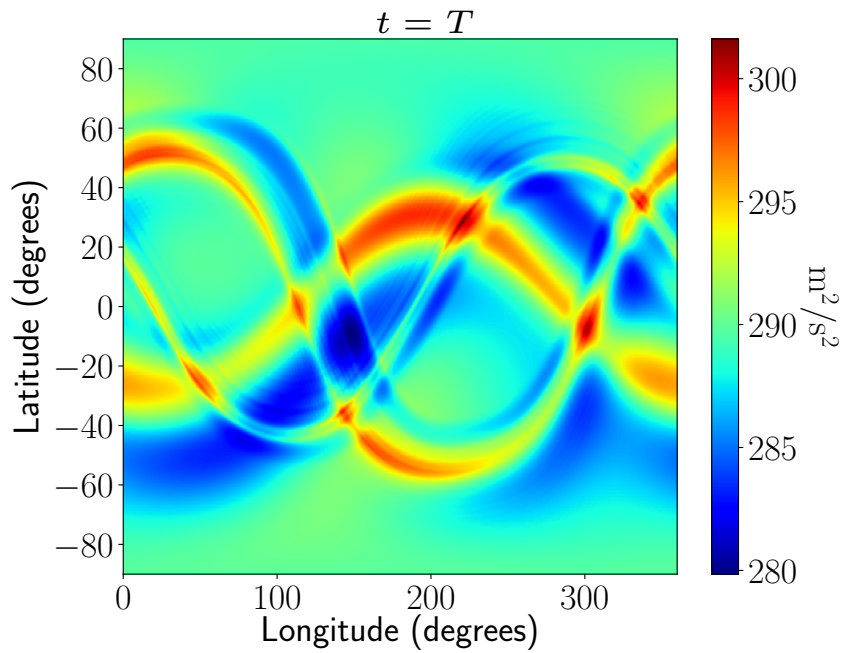
$$\boldsymbol{U} = \begin{pmatrix} \Phi \\ \xi \\ \delta \end{pmatrix}, \qquad \boldsymbol{L_G}(\boldsymbol{U}) = \begin{pmatrix} \overline{\Phi}\delta \\ 0 \\ -\nabla^2\Phi \end{pmatrix}, \qquad \boldsymbol{L_C}(\boldsymbol{U}) = \begin{pmatrix} 0 \\ -\nabla\cdot(f\boldsymbol{V}) \\ -\boldsymbol{k}\cdot\nabla\times(f\boldsymbol{V}) \end{pmatrix}$$

$$\boldsymbol{N_A}(\boldsymbol{U}) = \begin{pmatrix} -\boldsymbol{V}\cdot\nabla\Phi \\ -\nabla\cdot(\xi\boldsymbol{V}) \\ \nabla^2\left(\frac{\boldsymbol{V}\cdot\boldsymbol{V}}{2}\right) + \boldsymbol{k}\cdot\nabla\times(\xi\boldsymbol{V}) \end{pmatrix}, \qquad \boldsymbol{N_R}(\boldsymbol{U}) = \begin{pmatrix} -\Phi'\delta \\ 0 \\ 0 \end{pmatrix}$$

Test case

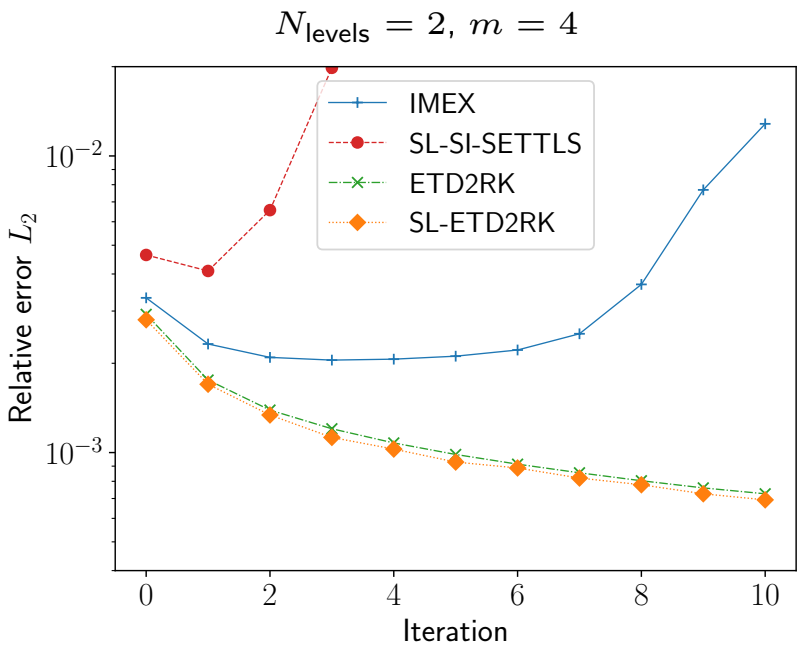
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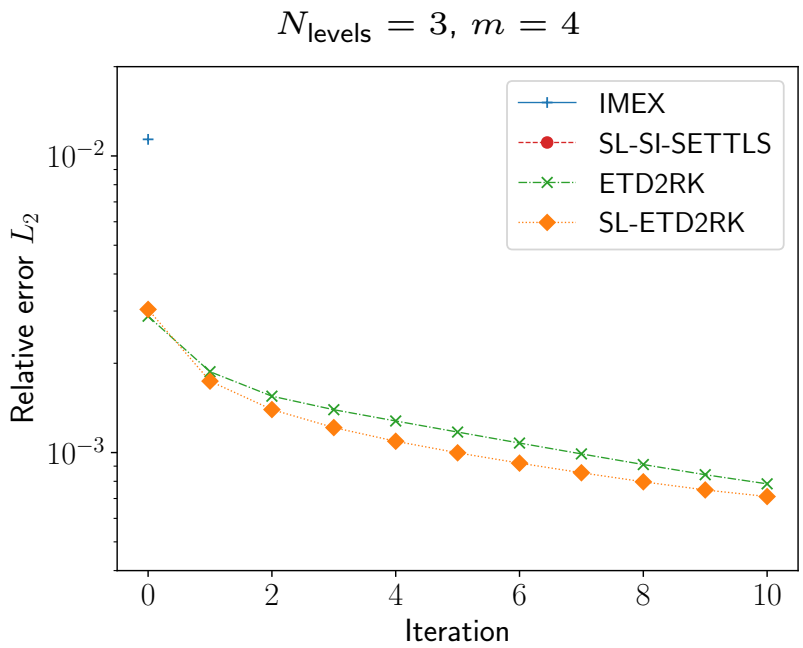




Test case: choice of coarse scheme

Errors along iterations in function of the coarse time stepping method:

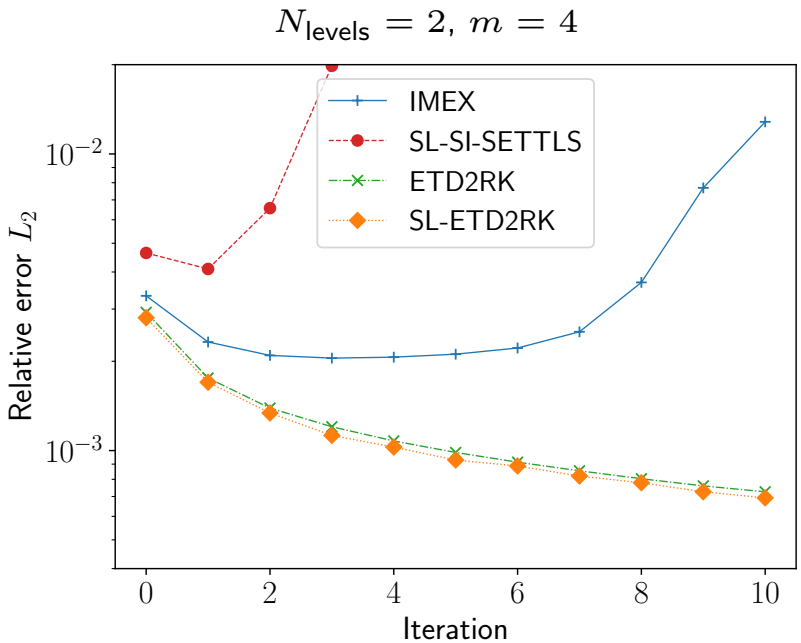


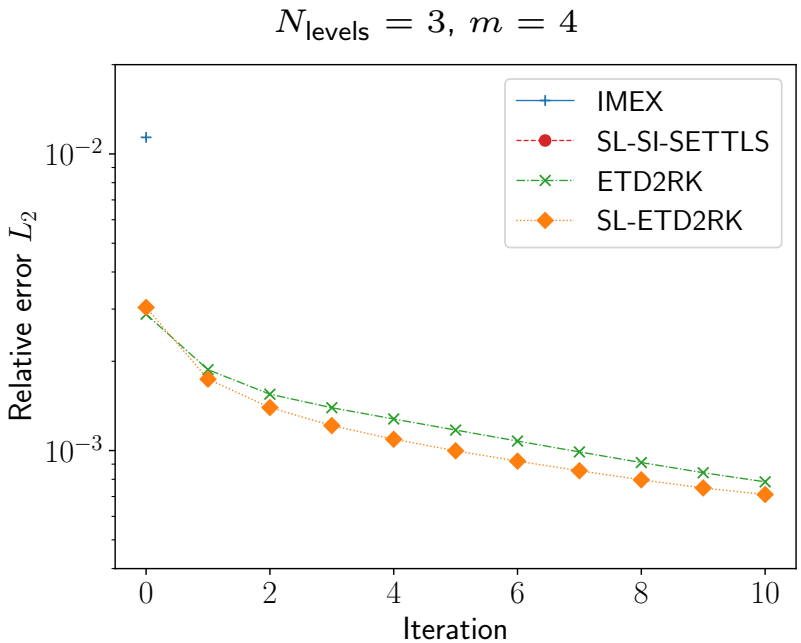


- Results with $N_{\text{relax}} = 0$. In practice: larger $N_{\text{relax}} \implies$ only small improvements
- More levels $\implies$ larger timestep in coarsest level $\implies$ stability issues
- Faster convergence and more stability with exponential methods

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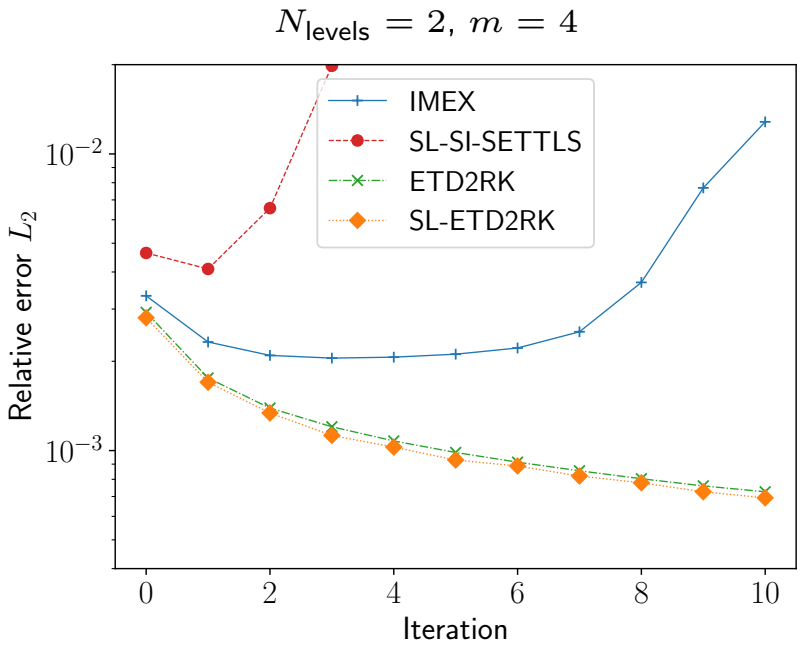


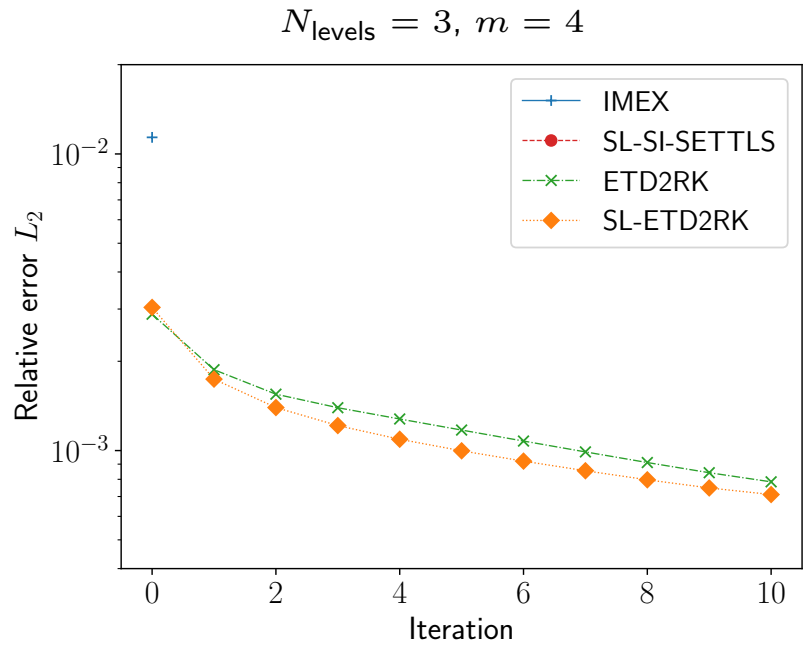


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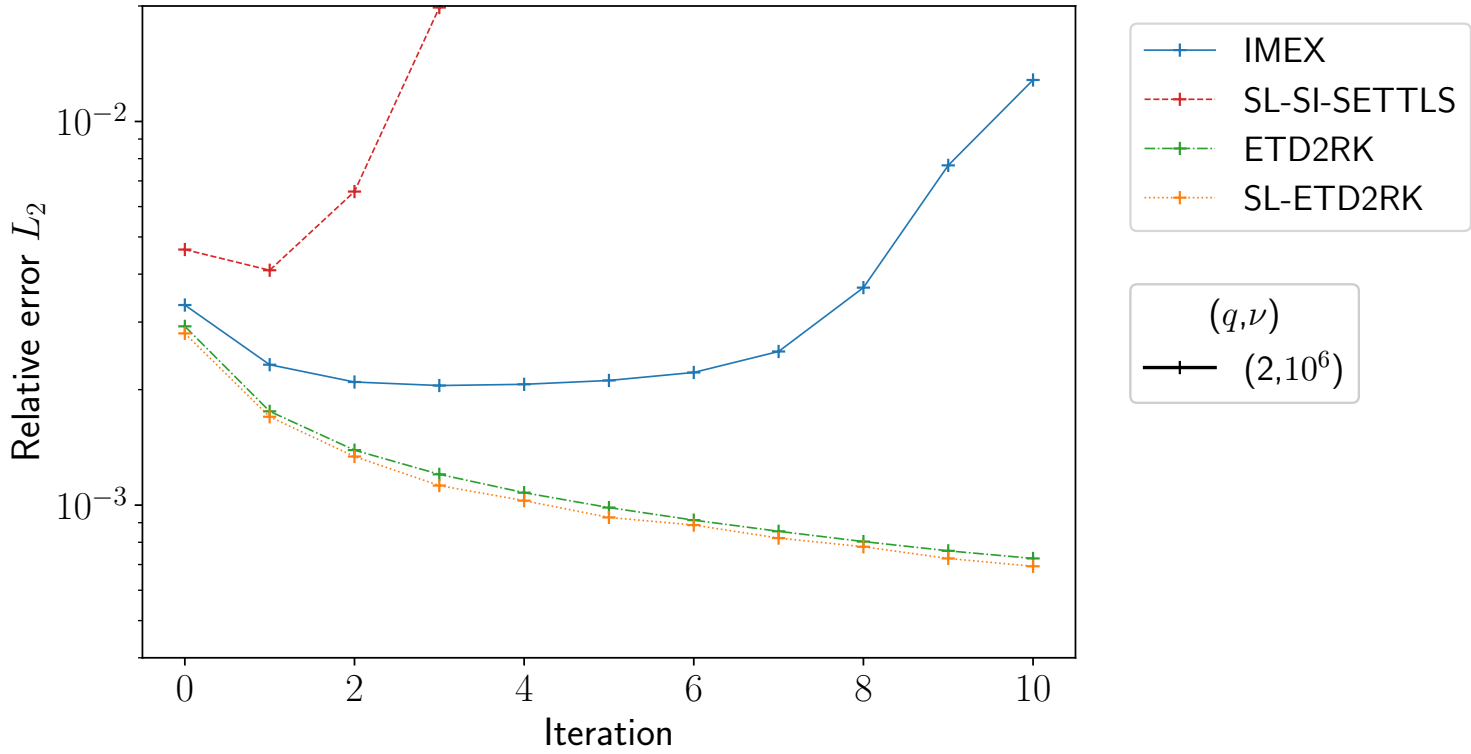




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Test case: influence of artificial viscosity

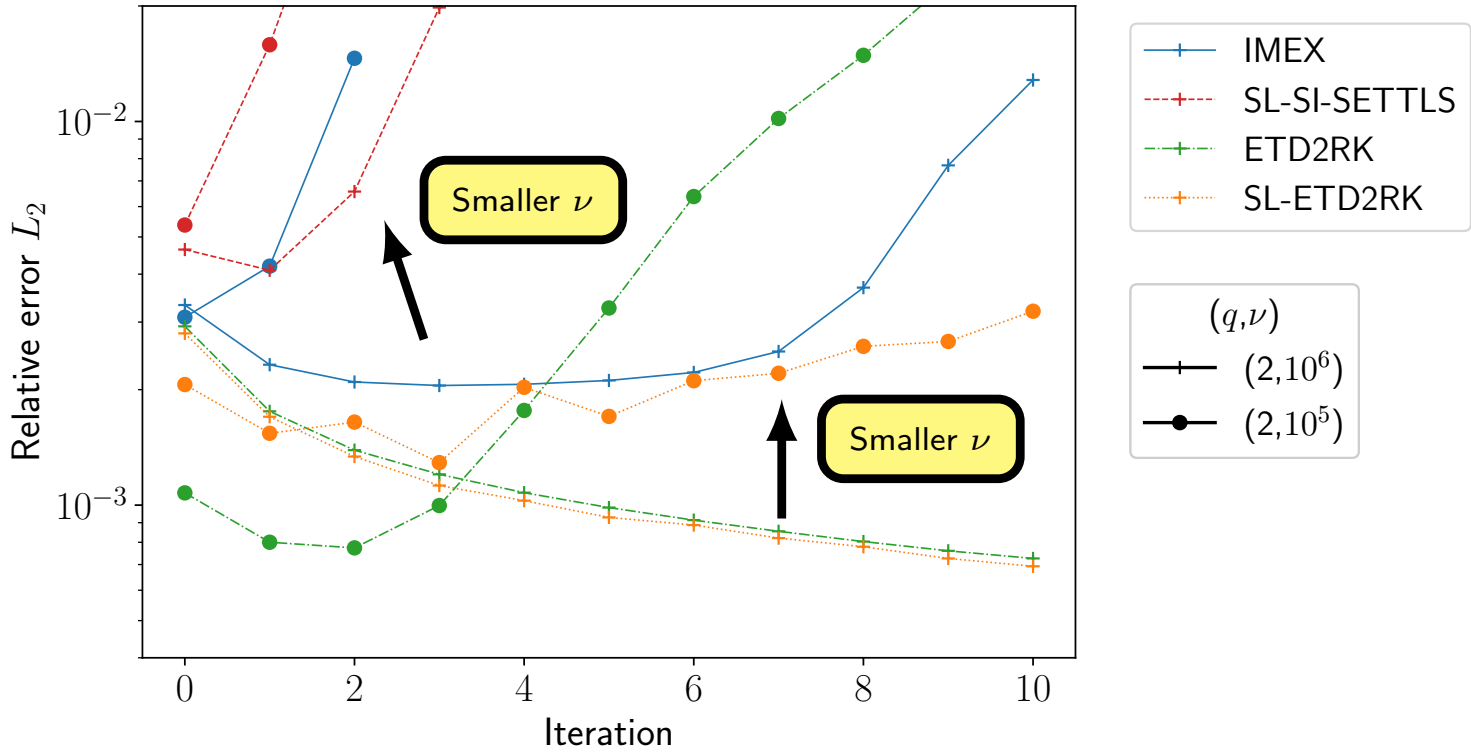
Influence of viscosity coefficient



- Choice of viscosity order and coefficient
  - Damping of smaller or larger wavenumbers $\Longrightarrow$ stability vs convergence
  - Optimal choice depends on coarse scheme

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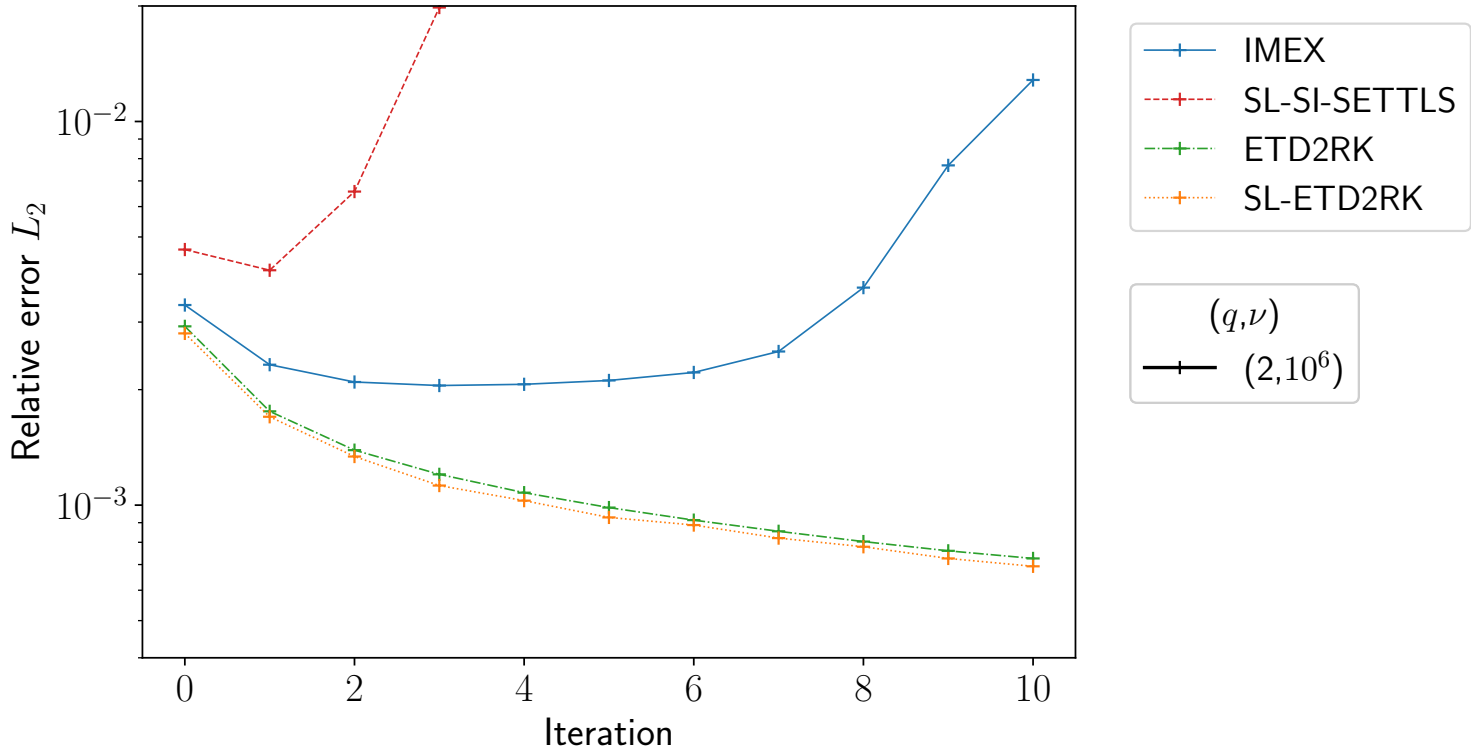
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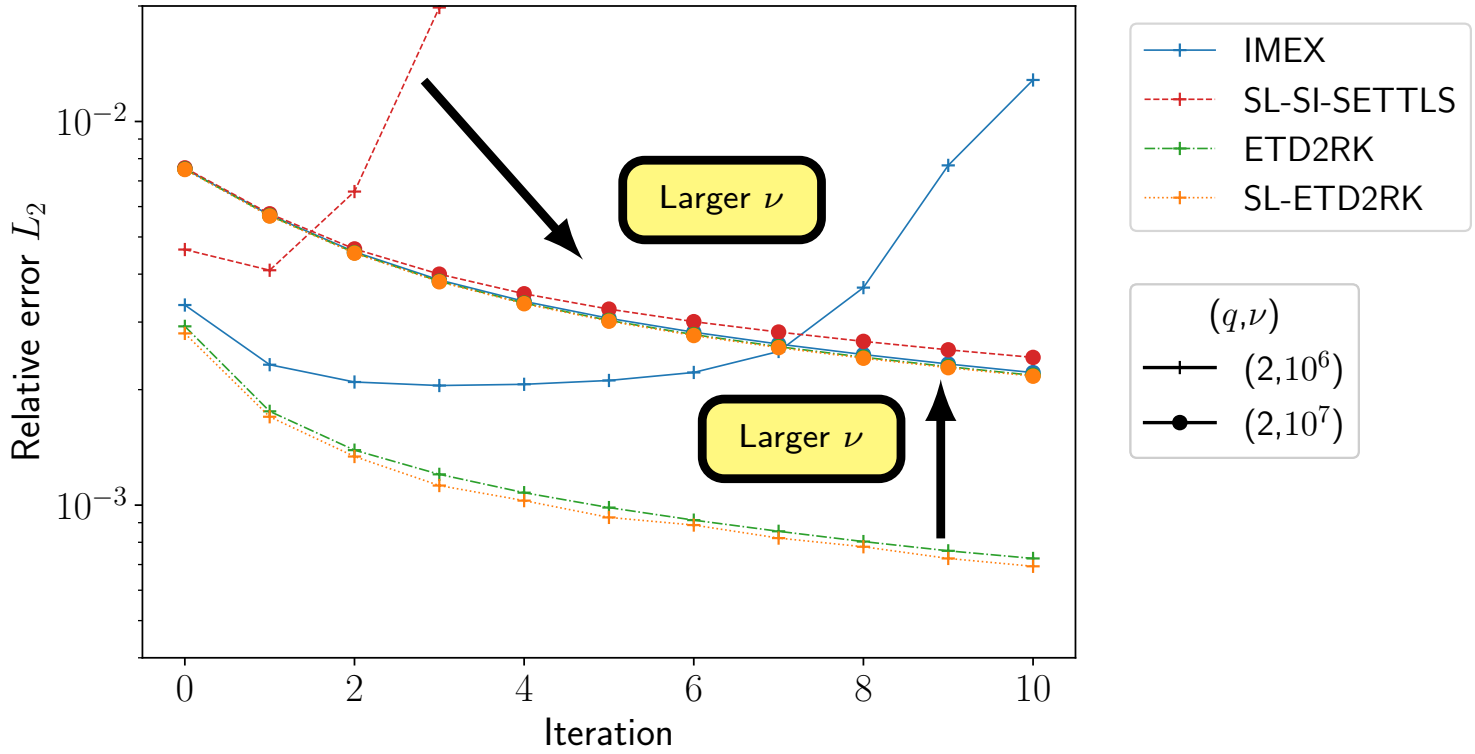
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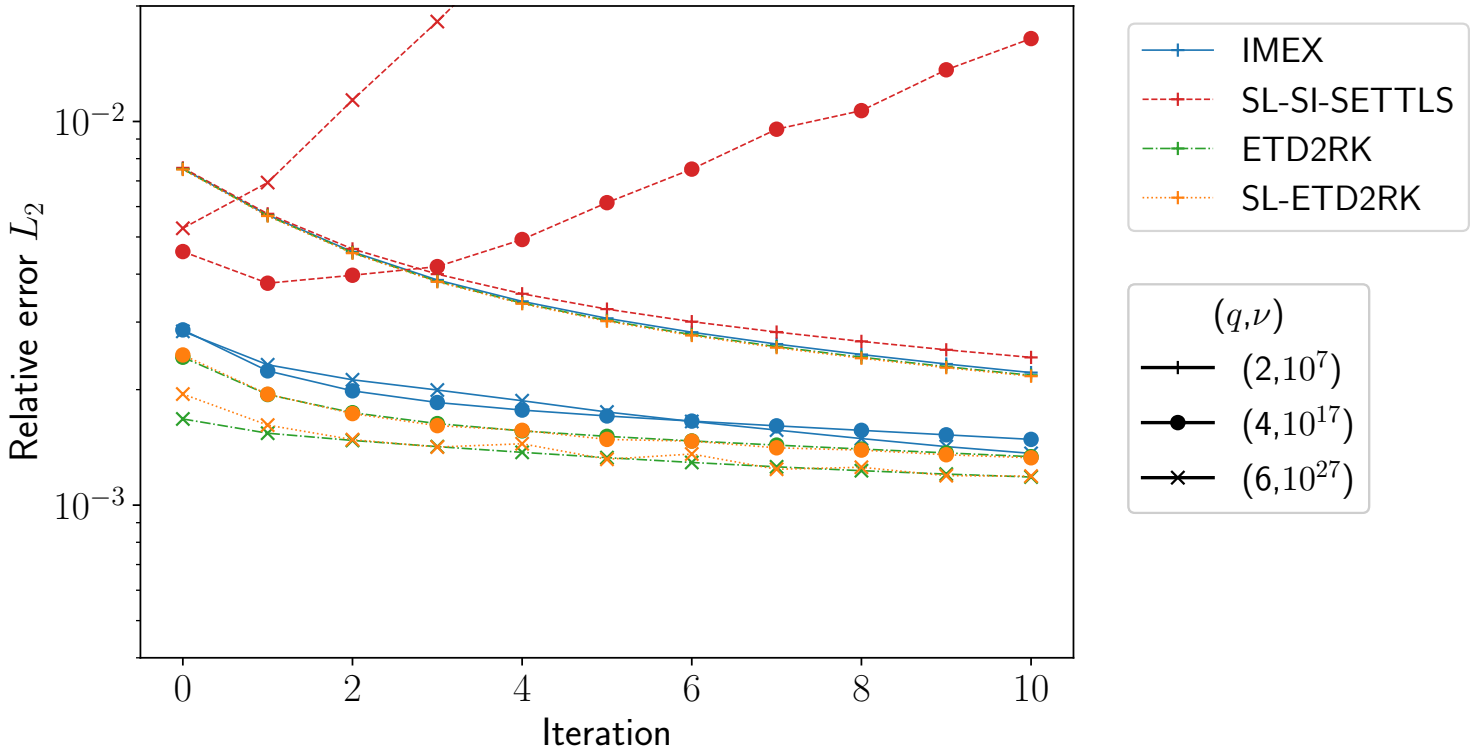
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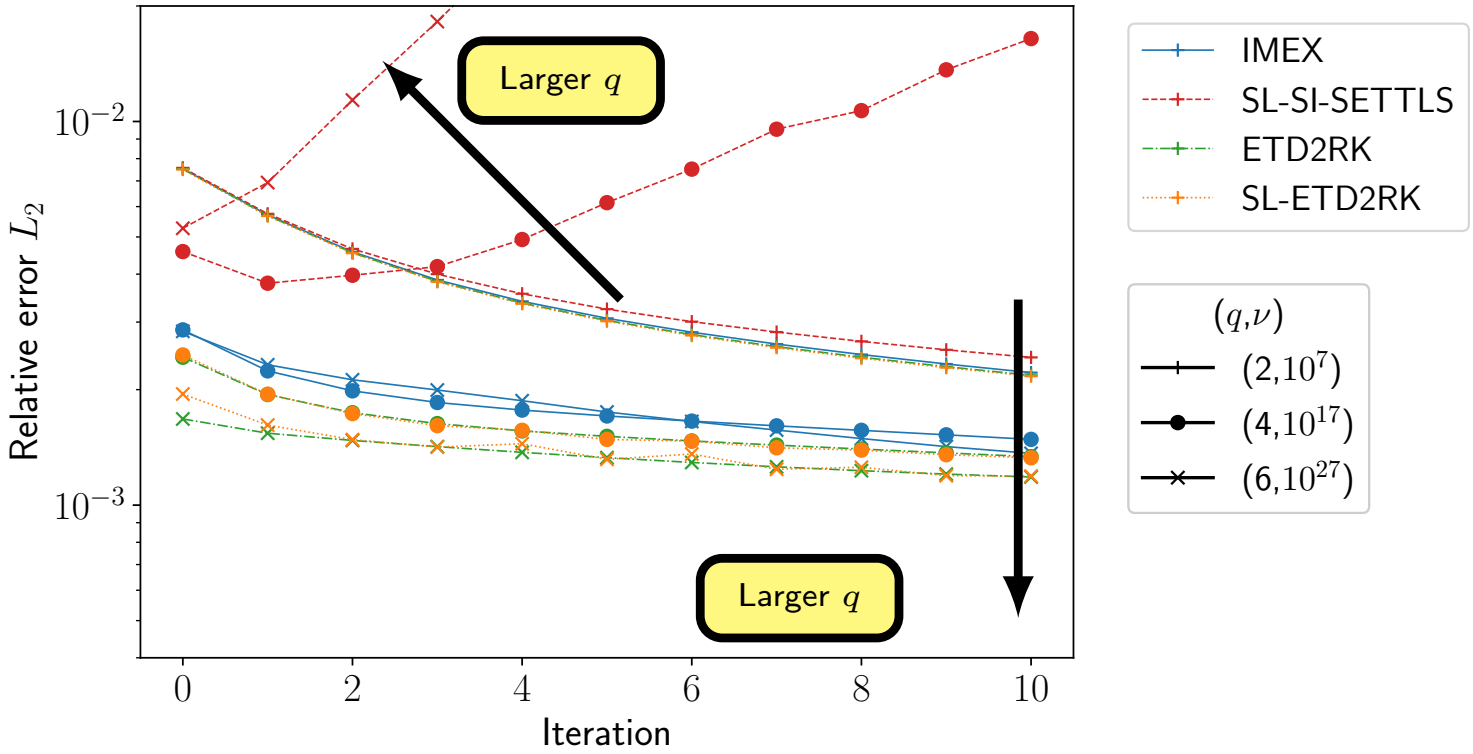
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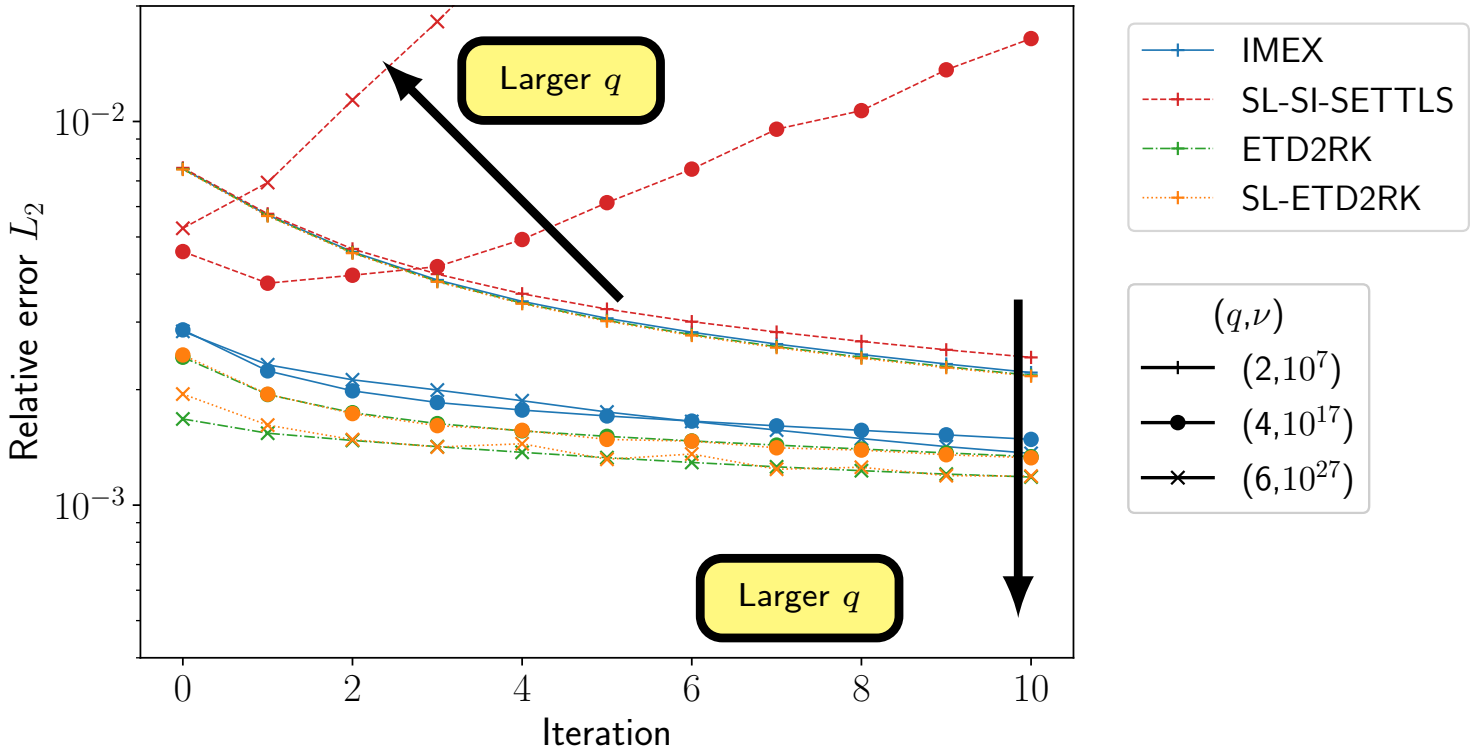
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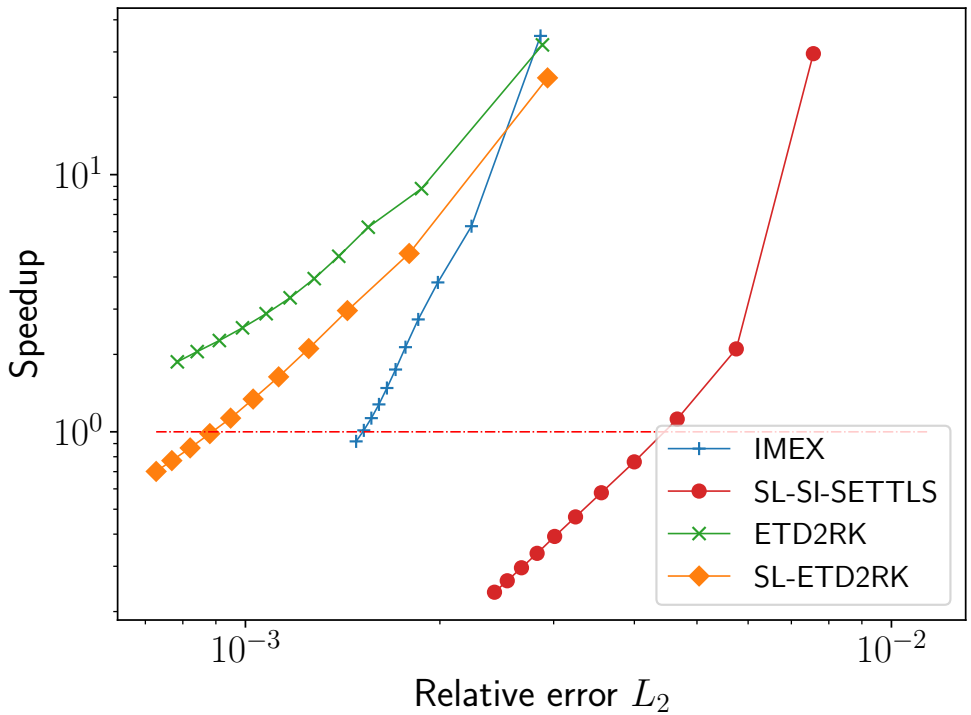
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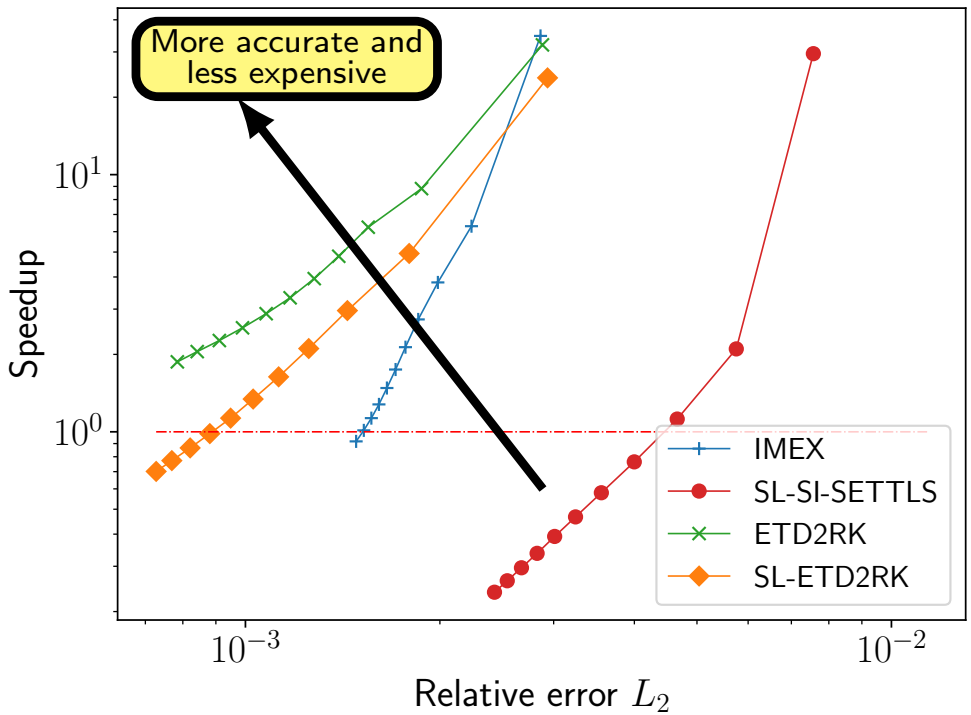
Test case: speedups

- Speedups along iterations w.r.t. the fine solution
- 64 processors in time (in theory: ≈ 500 could be used!)



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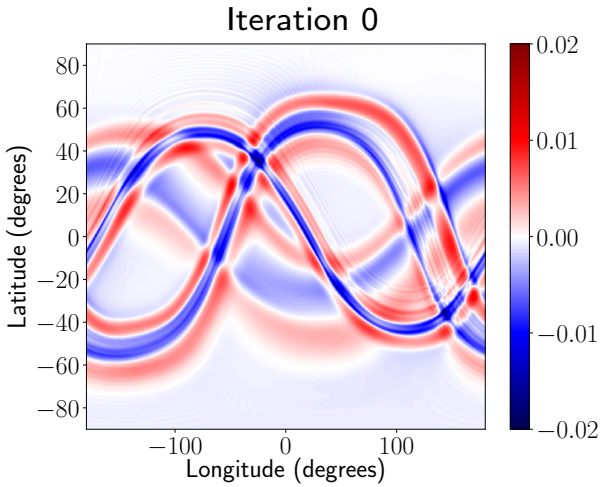
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- **(SL-)EXP:** coarser levels / larger q / smaller ν: better accuracy/cost
- **SL-EXP:** smaller errors but larger computing cost

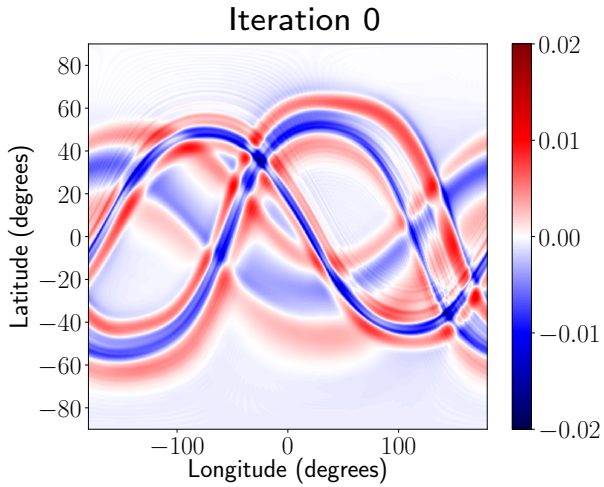
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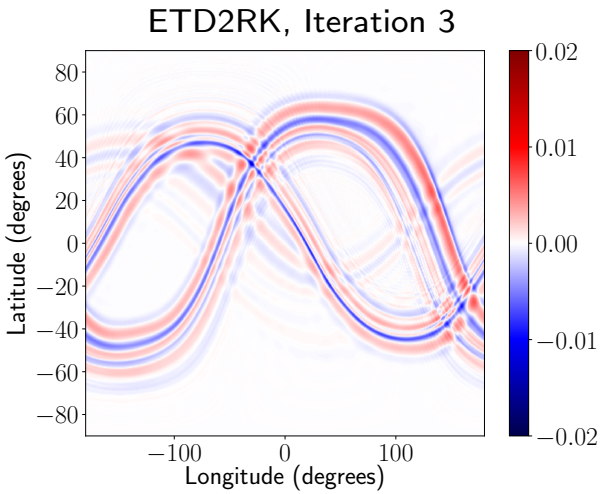
Relative error of geopotential Φ at $t = T$:

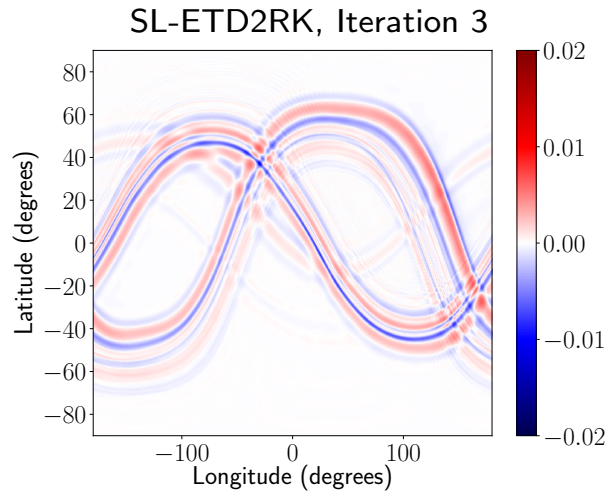


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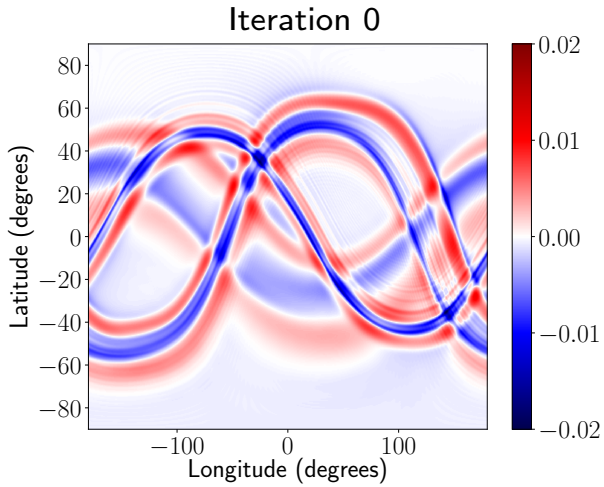


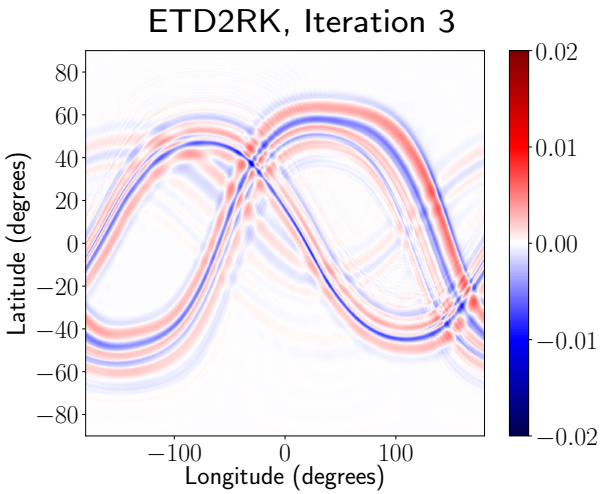




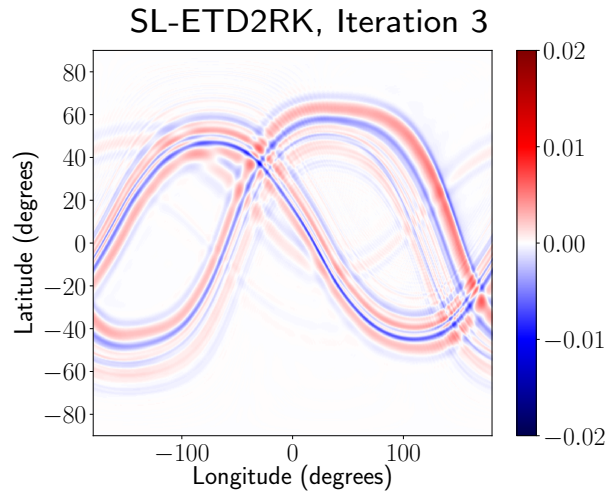
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Speedup = 4.8



Speedup = 2.1

Conclusions

- PinT for the SWE on the rotating sphere
- Choice of coarse time stepping method
- Poor stability properties using SL-SI-SETTLS in MGRIT
- Improved stability and convergence with ETD2RK and SL-ETD2RK
- Viscosity plays a role in MGRIT convergence.
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Perspectives

- Improve SL-EXP: "naturally" incorporates the nonlinear advection into EXP framework.
- Filtering approaches for MGRIT: Essential for adequate convergence.
- Nonlinear interaction effects and scale separation: Adequate dynamical treatment of multiscale.
- SWEET as framework for quick testing of ideas

- Paper with IMEX and SL-SI under review:
  Steinstraesser, Peixoto, Schreiber, 2023: Parallel-in-time integration of the shallow water equations on the rotating sphere using Parareal and MGRIT. `https://arxiv.org/abs/2306.09497`
- Paper with EXP and SL-EXP under preparation.

Thank you!

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Cox, S.M. and P.C. Matthews (2002). "Exponential Time Differencing for Stiff Systems". In: *Journal of Computational Physics* 176.2, pp. 430–455. ISSN: 0021-9991. DOI: https://doi.org/10.1006/jcph.2002.6995. URL: https://www.sciencedirect.com/science/article/pii/S0021999102969950.

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