Parallel-in-time methods for fluid dynamics problems

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In collaboration with

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Antoine Rousseau (Inria)
Vincent Guinot (Univ. Montpellier)

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Full Outline

- Introduction
- Parallel-in-time methods
  - Parareal
  - MGRIT
- Some ideas for improving PinT
- Applications
  - Urban floods
  - Atmospheric circulation models

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- Accuracy and time-to-solution requirements in several applications
  - Weather forecast and climate modelling
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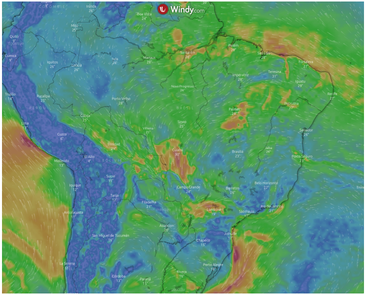
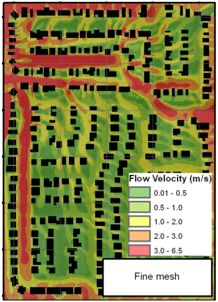
  - Real-time forecast and risk assessment



[ECMWF, windy.com]



[Guinot, Sanders, and Schubert (2017)]

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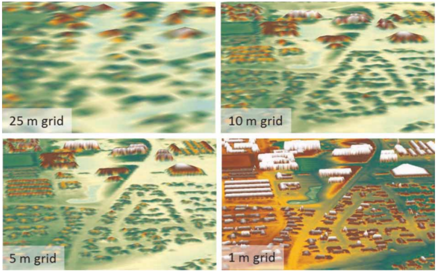

[Hénonin et al. (2013)]

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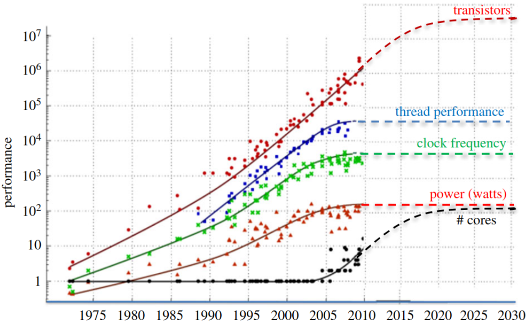

[Shalf (2020)]

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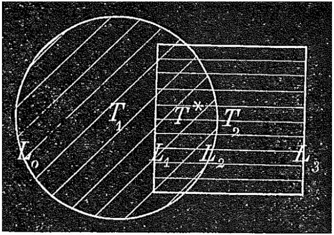
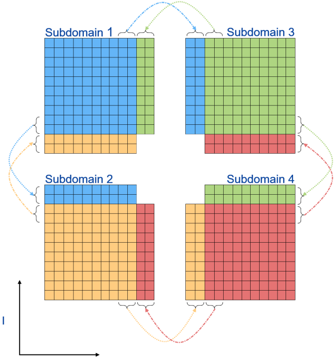


[Schwarz (1870)]



[Craig and Tien Lam (2022)]

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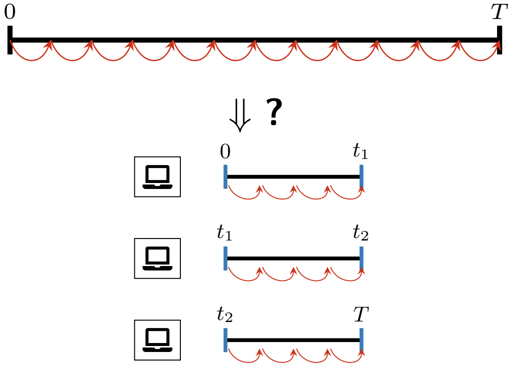

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  - Use of fine and coarse timestepping schemes
  - Simultaneous computation of several time steps
  - **Objective:** fast convergence to the fine solution

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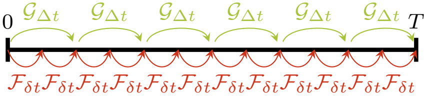

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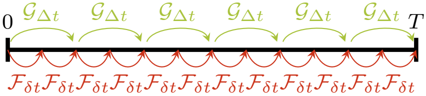

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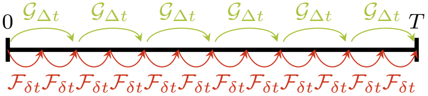

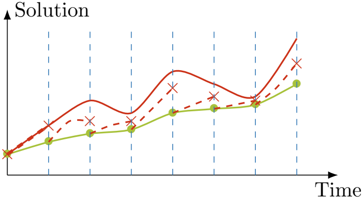

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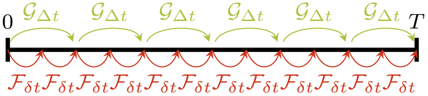

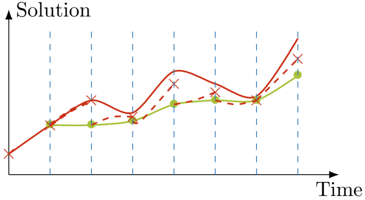

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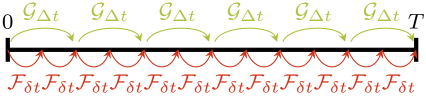

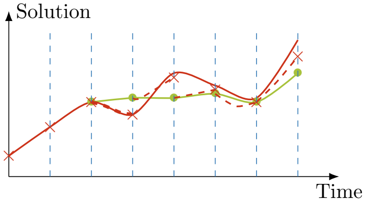

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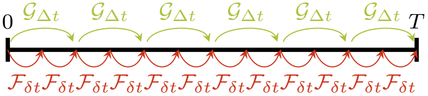

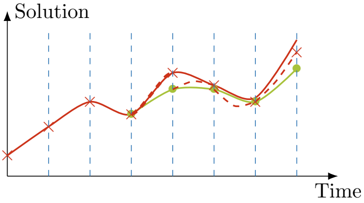

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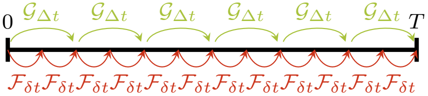

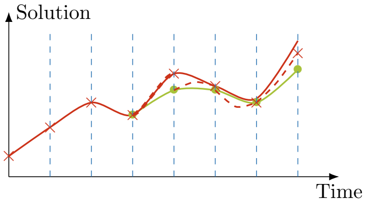

The parareal method

Jacques-Louis Lions, Yvon Maday, and Gabriel Turinici, “Résolution d'EDP par un schéma en temps “pararéel””, *Comptes Rendus de l'Académie des Sciences - Series I - Mathematics* (2001)

- Solve $\frac{du}{dt}(t) = F(u(t)), \quad u(0) = u_0$
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$N_{\Delta T}$

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$\mathcal{G}_{\Delta t}$ and $\mathcal{F}_{\delta t}$: user-defined schemes

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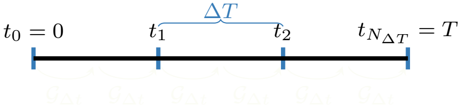

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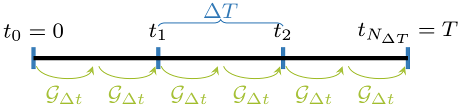

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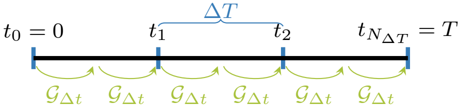

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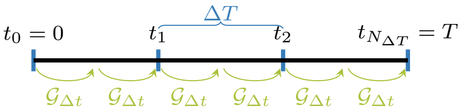

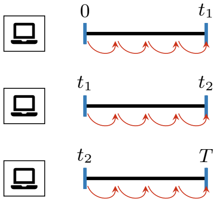

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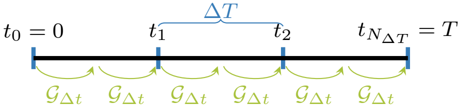

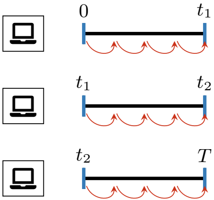

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S. Friedhoff et al., "A Multigrid-in-Time Algorithm for Solving Evolution Equations in Parallel", *Presented at: Sixteenth Copper Mountain Conference on Multigrid Methods* (2013)

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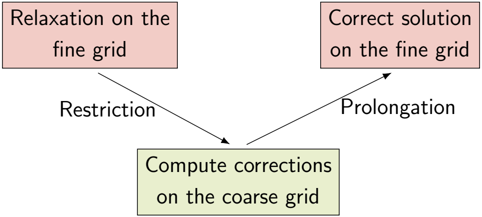

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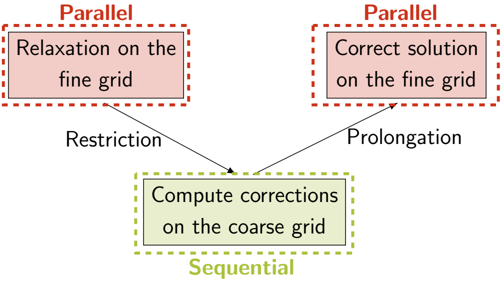

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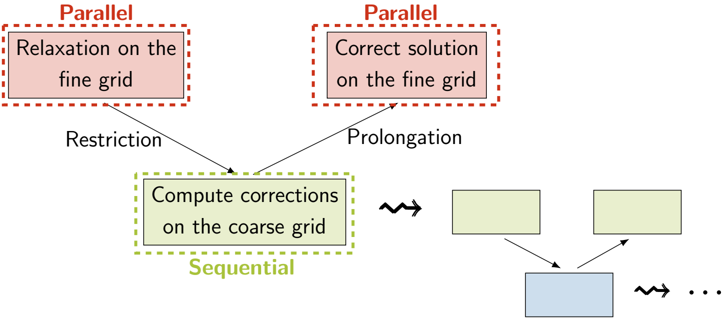

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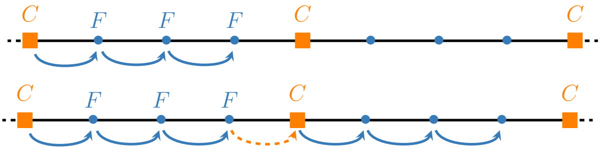

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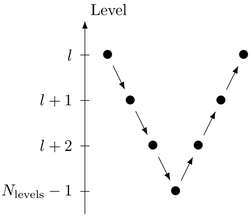

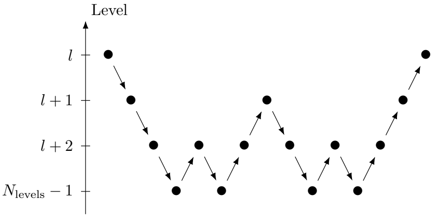

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Daniel Ruprecht, "Wave propagation characteristics of Parareal", *Computing and Visualization in Science* (2018)

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- Successful application to parabolic, diffusive problems;
- Hyperbolic problems: instabilities and slow convergence;
- Causes:
  - Mismatch of coarse and fine discrete phase speeds;
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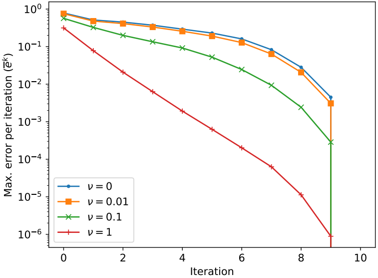

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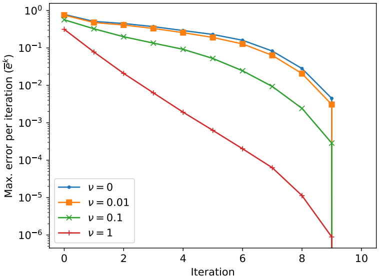

$$u_t + u_x = 0$$
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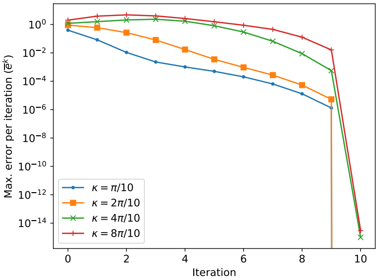

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- Introduction
- Parallel-in-time methods
  - Parareal
  - MGRIT
- Some ideas for improving PinT
- Applications
  - Urban floods
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PInT using semi-Lagrangian methods

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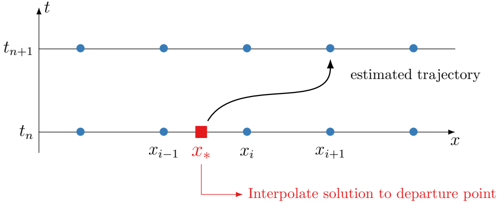
- Semi-Lagrangian treatment of advection: follow characteristics and interpolate solution from Eulerian grid
  - Improved stability $\Longrightarrow$ large time steps



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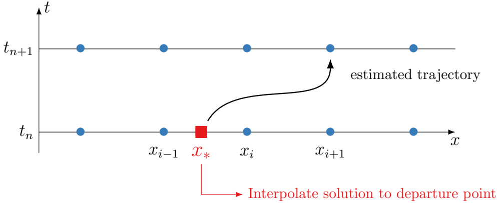

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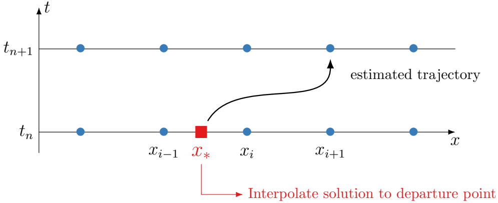

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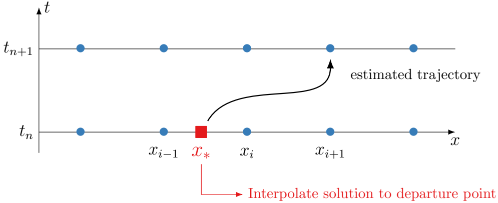

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ROM-based parareal methods

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- Replace coarse timestepping scheme by a reduced-order model (ROM):
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$$m \ll M$$

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- Shallow water equations on the plane
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$$\frac{\partial}{\partial t}\left(\boldsymbol{U}(t)\right) + \frac{\partial}{\partial x}\left(\boldsymbol{F}(\boldsymbol{U}(t))\right) + \frac{\partial}{\partial y}\left(\boldsymbol{G}(\boldsymbol{U}(t))\right) = \boldsymbol{S}(\boldsymbol{U}(t))$$

$$\boldsymbol{U} = \begin{pmatrix} h \\ hu_x \\ hu_y \end{pmatrix}, \qquad \boldsymbol{F}(\boldsymbol{U}) = \begin{pmatrix} hu_x \\ hu_x^2 + gh^2/2 \\ hu_x u_y \end{pmatrix},$$

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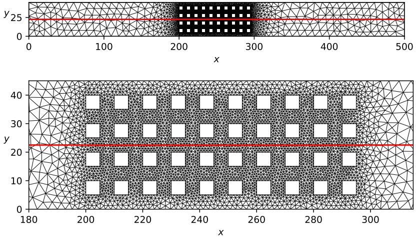

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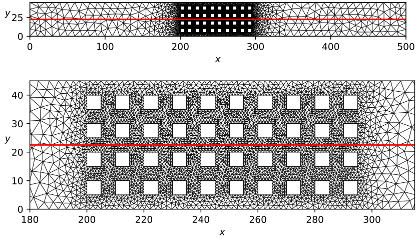

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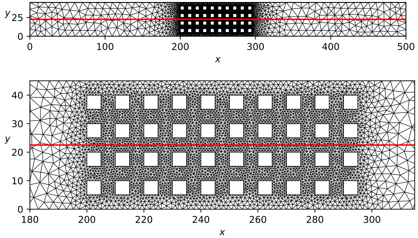

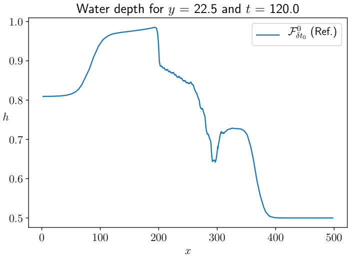

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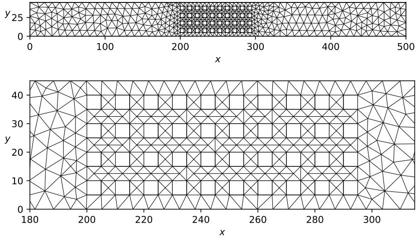

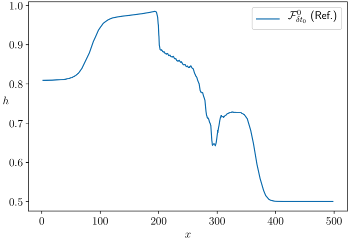

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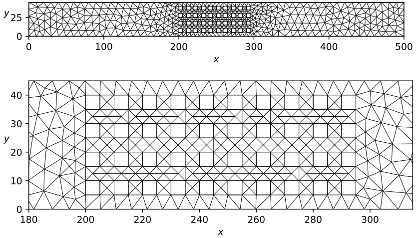

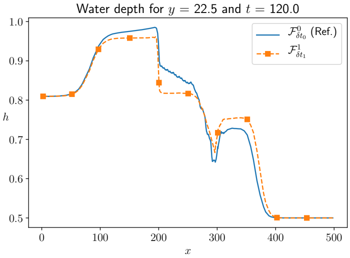

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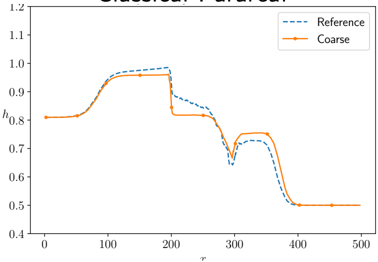

Speedup after 3 iterations: 1.66

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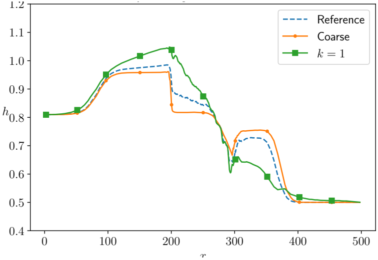

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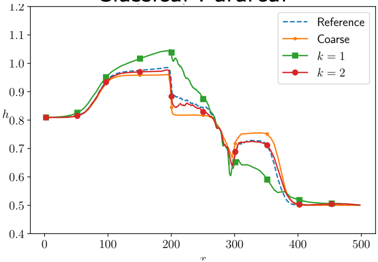

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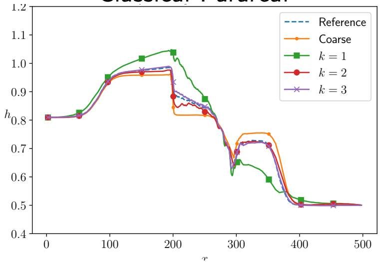

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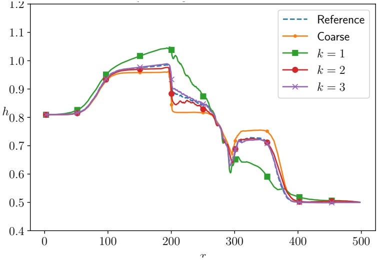

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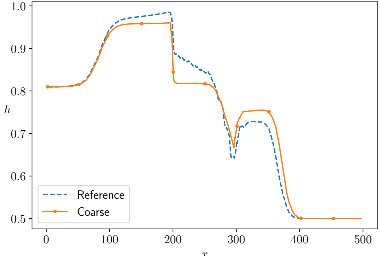

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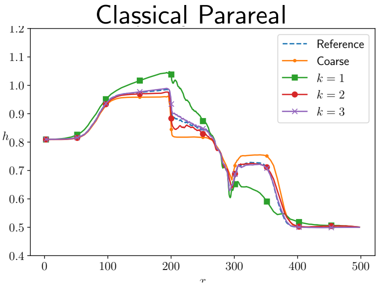

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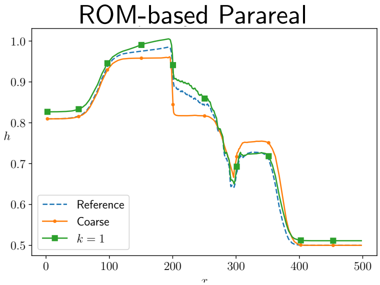

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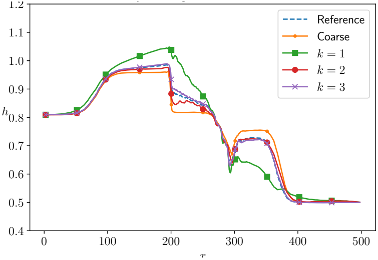
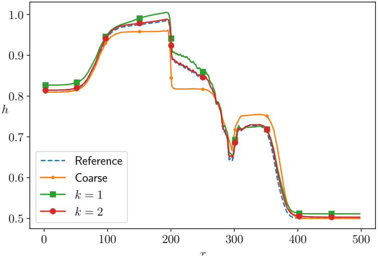


Speedup after 3 iterations: 1.66

ROM-based Parareal



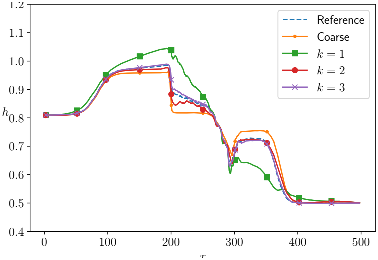
Speedup after 2 iterations: 1.28

Application: urban floods

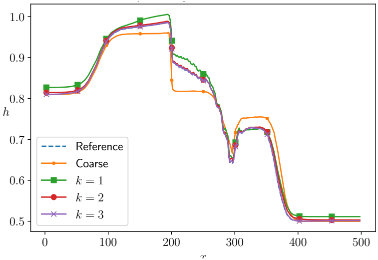
Joao Guilherme Caldas Steinstraesser, "Coupling large and small scale shallow water models with porosity in the presence of anisotropy", PhD thesis (2021). Developed with Antoine Rousseau and Vincent Guinot.

- Shallow water equations on the plane
- Explicit-in-time finite volume scheme
- Challenges: large spatial and temporal domains, discontinuous solutions
- PInT with Parareal and ROM-based Parareal

Classical Parareal



ROM-based Parareal



Speedup after 3 iterations: 1.66

Speedup after 2 iterations: 1.28

Application: atmospheric circulation models

Ongoing work with Pedro Peixoto and Martin Schreiber

- Climate modelling and numerical weather prediction
- Shallow water equations on the rotating sphere
- Spatial discretization using spherical harmonics
- Challenges: large domains, development of small-scale spatial features

Application: atmospheric circulation models

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- Climate modelling and numerical weather prediction
- Shallow water equations on the rotating sphere
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- Challenges: large domains, development of small-scale spatial features

$$\begin{aligned}\frac{\partial}{\partial t}\boldsymbol{U} &= \boldsymbol{L_G U} + \boldsymbol{L_C U} + \boldsymbol{N_A}(\boldsymbol{U}) + \boldsymbol{N_R}(\boldsymbol{U}) \\ &= \boldsymbol{LU} + \boldsymbol{N}(\boldsymbol{U})\end{aligned}$$

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

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

Application: atmospheric circulation models

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$$
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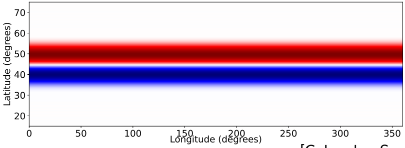
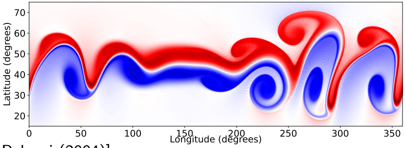
&= \boldsymbol{LU} + \boldsymbol{N}(\boldsymbol{U})
\end{aligned}
$$

Vorticity field at $t = 0$



Vorticity field at $t = 144h$



[Galewsky, Scott, and Polvani (2004)]

Application: atmospheric circulation models

Ongoing work with Pedro Peixoto and Martin Schreiber

- Two- and multilevel PinT (Parareal and MGRIT)

$$\frac{\partial \boldsymbol{U}}{\partial t} = \boldsymbol{L}\boldsymbol{U} + \boldsymbol{N}(\boldsymbol{U})$$

- Which coarse time integration method?

Application: atmospheric circulation models

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Application: atmospheric circulation models

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$$\frac{\partial \boldsymbol{U}}{\partial t} = \boldsymbol{L}\boldsymbol{U} + \boldsymbol{N}(\boldsymbol{U})$$

- Which coarse time integration method?
  - **Implicit-Explicit (IMEX)**

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

    - Linear term: implicit
    - Nonlinear term: explicit

Application: atmospheric circulation models

Ongoing work with Pedro Peixoto and Martin Schreiber

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$$\frac{\partial \boldsymbol{U}}{\partial t} = \boldsymbol{L}\boldsymbol{U} + \boldsymbol{N}(\boldsymbol{U})$$

- Which coarse time integration method?
  - Implicit-Explicit (IMEX)
  - **SL-SI-SETTLS [Hortal (2002)]**

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

    - Semi-Lagrangian + semi-implicit
    - Operational use in IFS-ECMWF

Application: atmospheric circulation models

Ongoing work with Pedro Peixoto and Martin Schreiber

- Two- and multilevel PinT (Parareal and MGRIT)

$$\frac{\partial \boldsymbol{U}}{\partial t} = \boldsymbol{L}\boldsymbol{U} + \boldsymbol{N}(\boldsymbol{U})$$

- Which coarse time integration method?
  - Implicit-Explicit (IMEX)
  - SL-SI-SETTLS [Hortal (2002)]
  - **Exponential integration: ETDRK [Cox and Matthews (2002)]**

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

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

- Linear term solved exactly
- Approximation for the nonlinear term
- φ_k: matrix exponential functions

Application: atmospheric circulation models

Ongoing work with Pedro Peixoto and Martin Schreiber

- Two- and multilevel PinT (Parareal and MGRIT)

$$\frac{\partial \boldsymbol{U}}{\partial t} = \boldsymbol{L}\boldsymbol{U} + \boldsymbol{N}(\boldsymbol{U})$$

- Which coarse time integration method?
  - Implicit-Explicit (IMEX)
  - SL-SI-SETTLS [Hortal (2002)]
  - Exponential integration: ETDRK [Cox and Matthews (2002)]
  - **SL - Exponential integration: SL-ETDRK [Peixoto and Schreiber (2019)]**

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

    - SL-version of ETDRK
    - Improved stability

Application: atmospheric circulation models

Ongoing work with Pedro Peixoto and Martin Schreiber

- Stability analysis:
  - Consider the ODE (*e.g.* spectral discretization) and its linearization:

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

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

$$|A_{\text{scheme}}(\xi_{\boldsymbol{L}}, \xi_{\boldsymbol{N}})| \leq 1$$

    where

$$u^{n+1} = A_{\text{scheme}} u^n$$

  - Plot stability regions in function of $Re(\xi_{\boldsymbol{N}})$ and $Im(\xi_{\boldsymbol{N}})$ for fixed $\xi_{\boldsymbol{L}} = 0$ (geostrophic mode) and $\xi_{\boldsymbol{L}} \in i\mathbb{R}^*$ (inertia-gravity modes)

Application: atmospheric circulation models

Ongoing work with Pedro Peixoto and Martin Schreiber

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Application: atmospheric circulation models

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Application: atmospheric circulation models

Ongoing work with Pedro Peixoto and Martin Schreiber

- Stability of Parareal [Staff and Rønquist (2005)]
  - Fine scheme: timestep δt and stability function A_f
  - Coarse scheme: timestep $\Delta t = m\delta t$ and stability function A_c

$$u_n^k = \mathcal{G}_{\Delta t}(u_{n-1}^k) + \mathcal{F}_{\delta t}(u_{n-1}^{k-1}) - \mathcal{G}_{\Delta t}(u_{n-1}^{k-1})$$

$$\implies u_n^k = A_c u_{n-1}^k + (A_f^m - A_c) u_{n+1}^{k-1}$$

  - Recurrence relation:

$$u_n^k = \underbrace{\left(\sum_{i=0}^{k} \begin{pmatrix} n \\ i \end{pmatrix} \left(A_f^m - A_c\right)^i (A_c)^{n-i} \right)}_{A_{\text{parareal}}} u_0$$

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Application: atmospheric circulation models

Ongoing work with Pedro Peixoto and Martin Schreiber

- Stability of Parareal along iterations
  - Fine scheme: IMEX
  - Coarse scheme: IMEX, SL-SI-SETTLS, ETD2RK, SL-ETD2RK
  - $n = 2$, $m = 100$

Application: atmospheric circulation models

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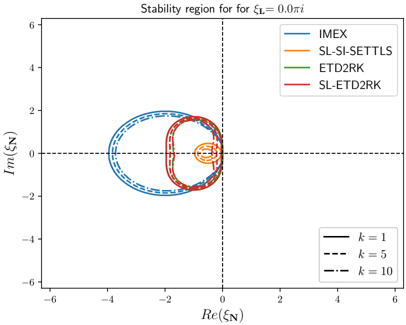
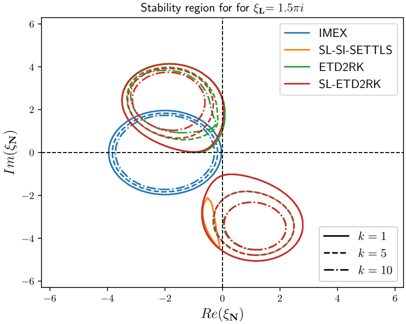
$\xi_L = 0$



$\xi_L = \frac{3\pi}{2} i$



Application: atmospheric circulation models

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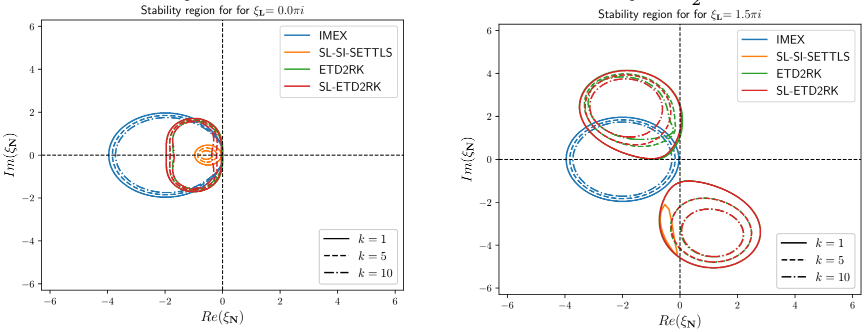
  - $n = 2$, $m = 100$
- **Loss of stability with SL-SI-SETTLS**

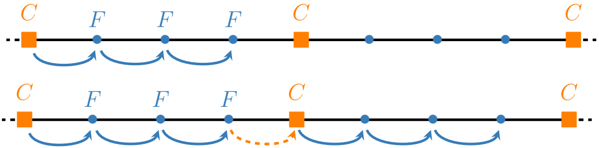
$\xi_L = 0$ $\qquad\qquad$ $\xi_L = \frac{3\pi}{2} i$



Application: atmospheric circulation models

Ongoing work with Pedro Peixoto and Martin Schreiber

- Stability of MGRIT (two levels with $\text{F(CF)}^{N_{\text{relax}}}$)



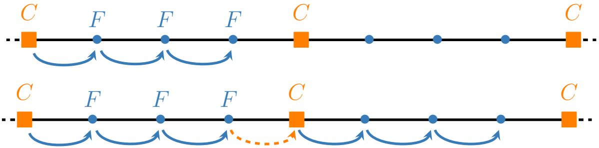
- Recurrence relation:

$$u_n^k = \underbrace{\left(\sum_{i=0}^{\lfloor k/(N_{\text{relax}}+1) \rfloor} \binom{n - iN_{\text{relax}}}{i} A_f^{mN_{\text{relax}}} \left(A_f^m - A_c\right)^i A_c^{n-i(N_{\text{relax}}+1)} \right)}_{A_{\text{MGRIT}}} u_0$$

Application: atmospheric circulation models

Ongoing work with Pedro Peixoto and Martin Schreiber

- Stability of MGRIT (two levels with F(CF)$^{N_{\text{relax}}}$)



  - Recurrence relation:

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Application: atmospheric circulation models

Ongoing work with Pedro Peixoto and Martin Schreiber

- Stability of MGRIT (two levels with F(CF)$^{N_{\text{relax}}}$)
  - Fine scheme: IMEX
  - Coarse scheme: IMEX, SL-SI-SETTLS, ETD2RK, SL-ETD2RK
  - $n = 2$, $m = 100$, $k = 5$

Application: atmospheric circulation models

Ongoing work with Pedro Peixoto and Martin Schreiber

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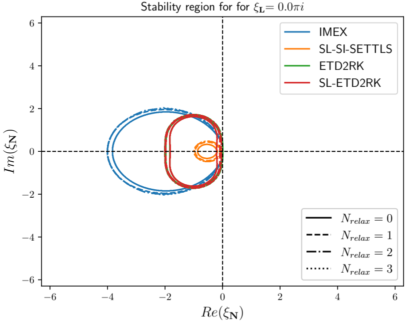
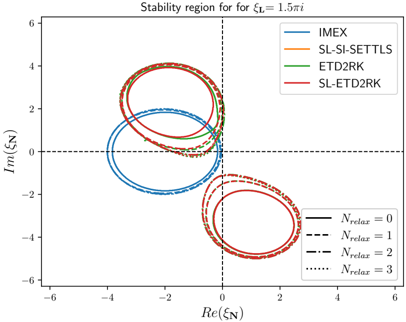
  - $n = 2,\ m = 100,\ k = 5$

$\xi_L = 0$



$\xi_L = \frac{3\pi}{2} i$



Application: atmospheric circulation models

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  - Fine scheme: IMEX
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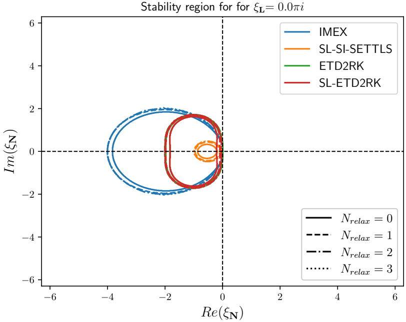
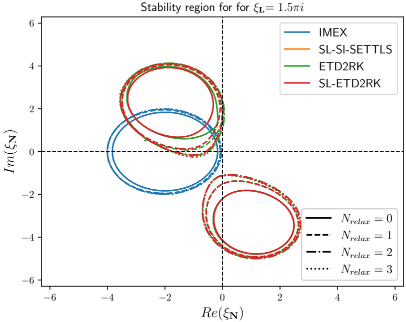
  - $n = 2,\ m = 100,\ k = 5$
- **Increasing stability with more expensive relaxation**

$\xi_{\boldsymbol{L}} = 0$



$\xi_{\boldsymbol{L}} = \frac{3\pi}{2} i$



Application: atmospheric circulation models

Ongoing work with Pedro Peixoto and Martin Schreiber

- **Test case: Gaussian bump**
  - T = 102400
  - Reference solution: $\delta t = 60$, spectral resolution $M = 256$
  - Coarse levels: coarsening factor m, spectral resolution $M_{\text{coarse}} = 128$
  - Artificial diffusion
  - Reference solution (geopotential field Φ):

Application: atmospheric circulation models

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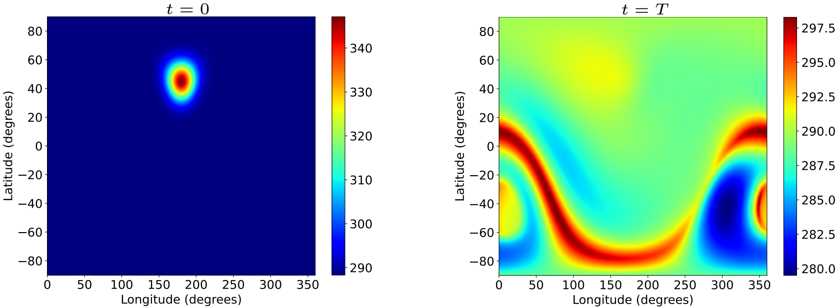


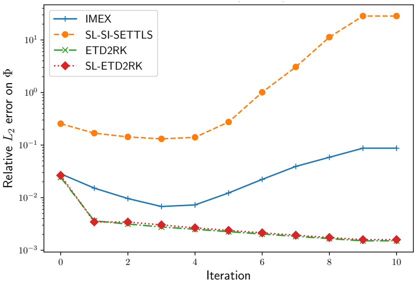
Application: atmospheric circulation models

Ongoing work with Pedro Peixoto and Martin Schreiber

- **Test case: Gaussian bump**

Errors in function of the coarse time stepping method

$$N_{\text{levels}} = 2,\ m = 2,\ N_{\text{relax}} = 4$$



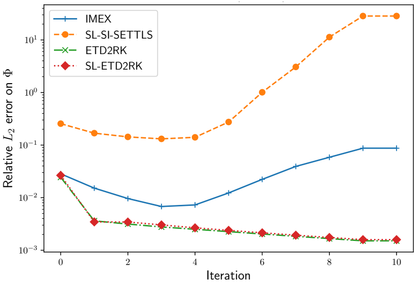
Application: atmospheric circulation models

Ongoing work with Pedro Peixoto and Martin Schreiber

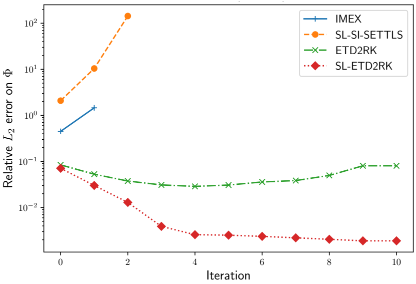
- **Test case: Gaussian bump**

Errors in function of the coarse time stepping method

$N_{\text{levels}} = 2,\ m = 2,\ N_{\text{relax}} = 4$



$N_{\text{levels}} = 3,\ m = 4,\ N_{\text{relax}} = 1$



- More levels $\implies$ larger timestep in coarsest level $\implies$ stability issues
- More convergence and stability with exponential methods, mainly SL

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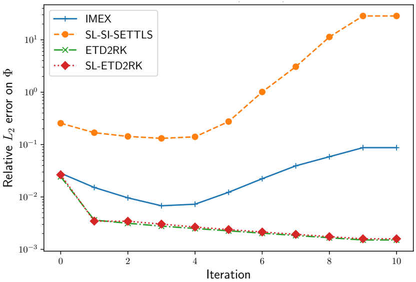
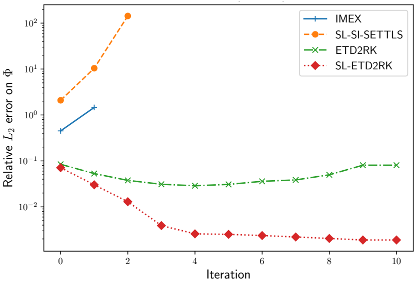


$N_{\text{levels}} = 3,\ m = 4,\ N_{\text{relax}} = 1$



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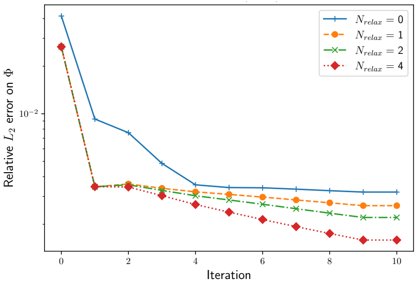
Test case: Gaussian bump

Errors in function of N_{relax}

$N_{\text{levels}} = 2$, $m = 2$, coarse time stepping method: SL-ETD2RK



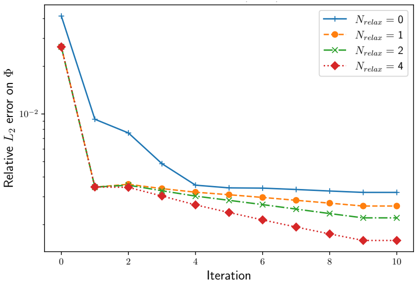
Application: atmospheric circulation models

Ongoing work with Pedro Peixoto and Martin Schreiber

- **Test case: Gaussian bump**

Errors in function of N_{relax}

$$N_{\text{levels}} = 2,\ m = 2,\ \text{coarse time stepping method: SL-ETD2RK}$$



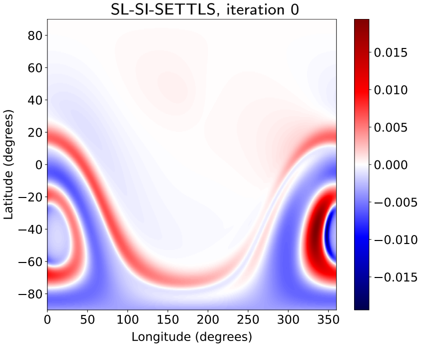
- Better convergence with more expensive relaxation;
- Convergence vs computational cost?

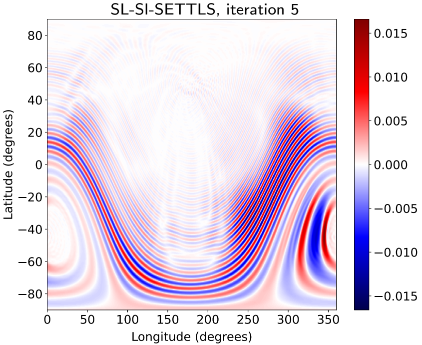
Application: atmospheric circulation models

Ongoing work with Pedro Peixoto and Martin Schreiber

Test case: Gaussian bump

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





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- **Test case: Gaussian bump**

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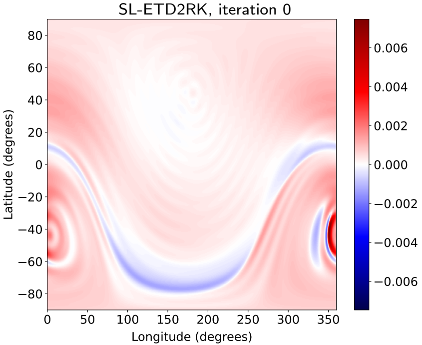

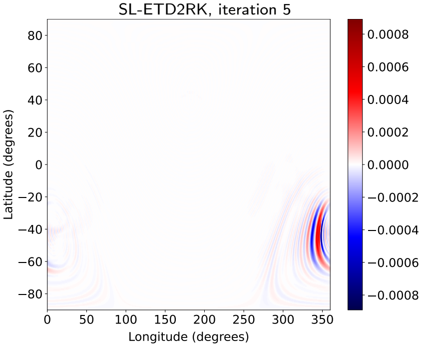

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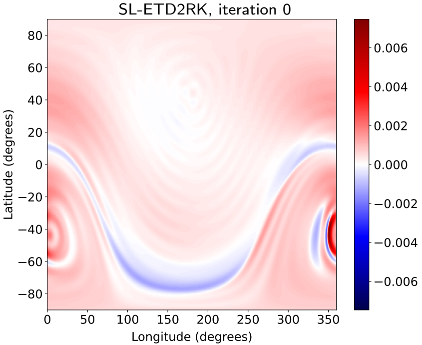

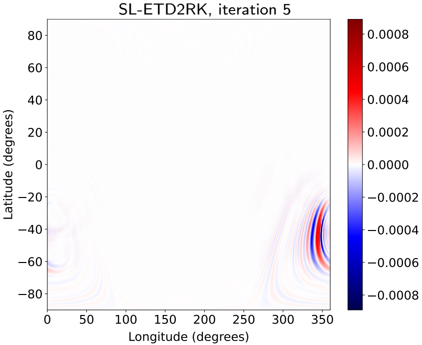

- Errors on small-scale spatial features

Conclusions and perspectives

- Parallel-in-time for fluid dynamics
  - Demands from operational applications
  - Challenges due to hyperbolic nature
  - Configurations for improving convergence and stability
    - Choice of coarse time stepping method
    - Multilevel and relaxation strategies
  - Trade-off with computational cost
- Application to atmospheric circulation models
  - Promising results using SL-EXP methods
  - More complex problems?
  - Convergence and stability of small-scale spatial features are still a bottleneck
  - Parallel implementation and evaluation of feasibility in practice
  - Evaluation of influence of artificial diffusion

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Thank you!

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Outline

- Introduction
- Parallel-in-time methods
  - Parareal
  - MGRIT
- Some ideas for improving PinT
- Applications
  - Urban floods
  - Atmospheric circulation models

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