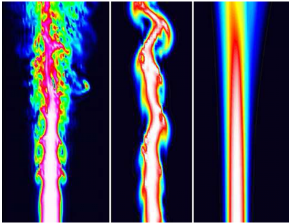
Stable time-parallel integration of advection dominated problems using Parareal with space coarsening.

Julien Bodart – *ISAE-SUPAERO*
Serge Gratton – *Toulouse-INP-IRIT*
Xavier Vasseur – *ISAE-SUPAERO*
Thibaut Lunet – *University of Geneva*

May 4, 2018

Larger and larger problems for research and industrial applications with Computational Fluid Dynamics

- Higher complexity
  → Turbulence, Acoustics, Combustion ...
- High fidelity simulation
  → High Order Discretization, LES, DNS, ...



From right to left: RANS, LES, DNS

Massively parallel supercomputer for tomorrow

- Supercomputer speed rather based on **number of cores** than *processor speed*
- Largest one today:
  - $\sim 10 \times 10^6$ cores
  - ~ 100 PetaFlop/s
- Highlights the limits of exclusive space-parallelization

Sunway TaihuLight (2016) ©www.dailymail.co.uk

⇒ Space-time parallelism could be an interesting alternative to enhance efficiency on exascale supercomputers

Actual solutions for time-parallelization

- Space-Time Multigrid - The first born
- Parareal - The famous cadet
- PFASST - When complexity serves efficiency
- MGRIT - Toward an universal solution
- And many others ...

How to convince the HPC-CFD community ?

- Proof of concept on representative test-cases
  1. Accuracy of the time-parallel integration
  2. Efficiency gain compared to exclusive space-parallelization
- Solution that can be easily integrated into (huge) pre-existent CFD codes
  - Explicit time-stepping solvers
  - Temporal evolution of variables (*e.g.* pressure sensor for acoustics simulation)
  - ...

$\Rightarrow$ **First step : investigations of Parareal[R1] with space coarsening[R2]**

[R1] Lions et al., *"A "Parareal" in time discretization of PDE's"* (2001)

[R2] Fischer et al., *"A Parareal in time semi-implicit approximation of the Navier-Stokes equations"* (2005)

What was done so far

PhD Thesis - "Space-time parallel strategies for the numerical simulation of turbulent flows" (Defended January 9, 2018)

- What could be the best solution from today's algorithms ? (Chap. 2)
- Can we understand theoretically the behavior of explicit forms of PARAREAL? (Chap. 3)
- What about large scale turbulent flow problems ? (Chap. 4)
  - Space-time parallel efficiency ?
  - Accuracy on two representative test case (Homogeneous Isotropic Turbulence, Turbulent Channel Flow)

Part of the work was accepted for publication [R1]

But there was a major issue at the beginning ...

[R1] Lunet et al., *"Time-parallel simulation of the decay of homogeneous turbulence using Parareal with spatial coarsening"* (2017)

Parareal VS Advective Problems

Many studies underlined the difficulties of Parareal on

$$\frac{\partial U}{\partial t} + c\frac{\partial U}{\partial x} = 0$$

- Numerical instabilities[R1] and slow convergence for some setting[R2]
- PARAREAL looses its contraction factor on periodic domains (*cf.* M. Gander's talk)

Difficulty to prove with such problem if it would work on CFD problems

1. PARAREAL does not define a unique algorithm
2. Molecular viscosity and Reynolds number
   - *"The convergence of Parareal deteriorates as the viscosity parameter becomes smaller and the flow becomes more and more dominated by convection."* [R3]
   - **But : the Reynolds number does not have a unique definition !**
     Low influence of the Re_λ number increase compared to other parameters for Homogeneous Isotropic Turbulence (*cf.* PhD manuscript)
3. In most CFD problem, space resolution and Reynolds number increase simultaneously
4. Space coarsening implies to choose an interpolation method (Linear, High Order, Fourier, ...)

[R1] Ruprecht and Krause, *"Explicit parallel-in-time integration of a linear acoustic-advection system"* (2012)
[R2] Gander, *"Analysis of the Parareal algorithm applied to hyperbolic problems using characteristics"* (2008)
[R3] Steiner et al., *"Convergence of Parareal for the Navier-Stokes equations depending on the Reynolds number"* (2015)

Main object of this talk

- Starts from the 1D linear advection problem with low diffusion
- Focus on one particular PARAREAL form
    1. Space coarsening for $\mathcal{G}$ (one point out of two)
    2. High order explicit time-integration (RK4)
    3. Highly accurate space discretization (Centered 6^{th} order)
- Change several parameters that can influence PARAREAL convergence (Reynolds, space resolution, interpolation method, ...)
- Increase problem complexity (non-linearity, ...)
- Try to answer the following questions :

What are the most influent parameters for this version of PARAREAL ?

How to set them to enhance convergence for a more complex case ?

Definition of a baseline test case

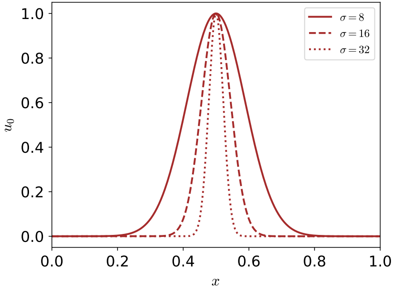
- Advection with small diffusion

$$\frac{\partial u}{\partial t} = -c\frac{\partial u}{\partial x} + \nu\frac{\partial^2 u}{\partial x^2}, \quad \nu << c$$

- Periodic 1D mesh with $x \in [0, 1[$
- Gaussian initial solution with varying width

$$u_0(x) = e^{-\dfrac{(x-1/2)^2}{\sigma^2}}$$

- $CFL = 1$ for both fine and coarse solvers
- Final time $T = 64\delta_t$ ($\sim T_{period}/7$)
- Time domain decomposition in 4 time-slices



Error criterion based on fine solution comparison

$$E^k_{T,L_2} = \frac{\left\|U^k_{\mathcal{P}}(T) - U_{\mathcal{F}}(T)\right\|_2}{\left\|U_{\mathcal{F}}(T)\right\|_2}, \quad \text{for } k \in \{0, 1, 2, 3\}$$

Definition of a baseline test case

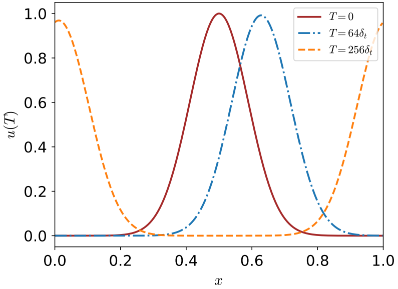
- Advection with small diffusion

$$\frac{\partial u}{\partial t} = -c\frac{\partial u}{\partial x} + \nu\frac{\partial^2 u}{\partial x^2}, \quad \nu << c$$

- Periodic 1D mesh with $x \in [0, 1[$
- Gaussian initial solution with varying width

$$u_0(x) = e^{-\frac{(x-1/2)^2}{\sigma^2}}$$

- $CFL = 1$ for both fine and coarse solvers
- Final time $T = 64\delta_t$ ($\sim T_{period}/7$)
- Time domain decomposition in 4 time-slices



Error criterion based on fine solution comparison

$$E^k_{T,L_2} = \frac{\left\| U^k_{\mathcal{P}}(T) - U_{\mathcal{F}}(T) \right\|_2}{\left\| U_{\mathcal{F}}(T) \right\|_2}, \quad \text{for } k \in \{0, 1, 2, 3\}$$

What will vary in the next graphs

Main parameters

- Interpolation method
  1. Linear ($o_I = 1$, blue-circle)
  2. Cubic ($o_I = 3$, orange-square)
  3. 7^{th} order ($o_I = 7$, green-triangle)
- Space mesh resolution
  1. Fine (left side)
  2. Coarse (right side)

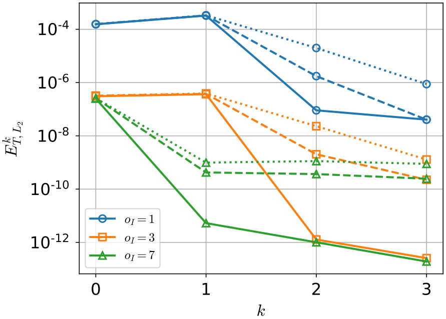
Secondary parameters (lines - dashes - dots)

1. Reynolds number
2. Time slice length
3. Regularity of the solution
4. Non-linearity of the advection term

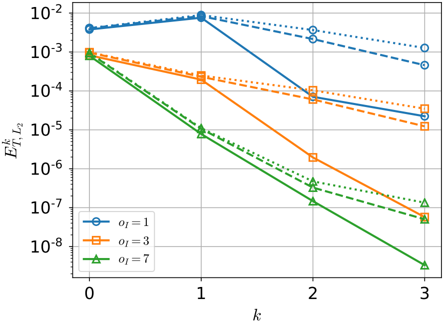
Linear case - influence of the Reynolds number

$Re = c/\nu$: from low to high

2000 (line) $\rightarrow$ 10000 (dashes) $\rightarrow$ 20000 (dots)



High space resolution ($N_x = 500$)



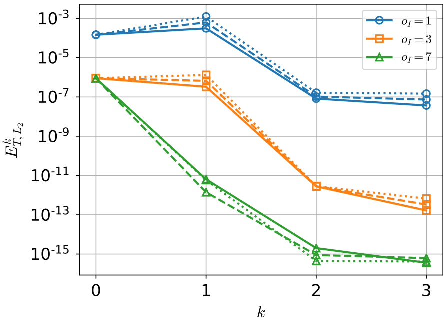
Low space resolution ($N_x = 100$)

Main observations

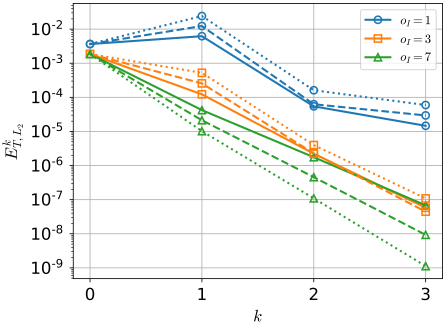
- Staggered benefit of interpolation order increase (first on $\mathcal{G}$, then on Parareal convergence)
- Few influence of *Re* for the 1^{st} iteration with low order interpolation or low space resolution

Linear case - influence of the time-slice length

Number of δ_t per time-slice: from large to small
64 (line) $\rightarrow$ 32 (dashes) $\rightarrow$ 16 (dots)



High space resolution ($N_x = 500$)



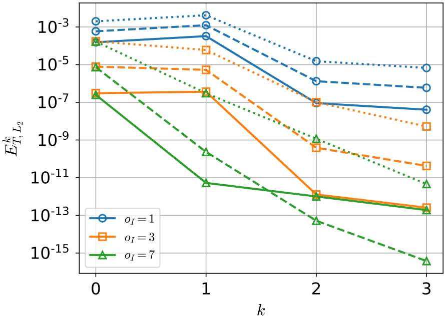
Low space resolution ($N_x = 100$)

Main observations

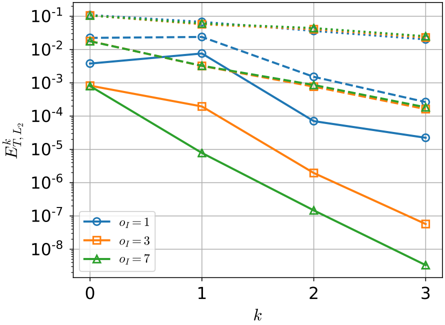
- Small impact on the convergence
- Effect is "inverted" when going to high order interpolation

Linear case - influence of the solution regularity

Width of the initial Gaussian: from large to small
$\sigma = 8$ (line) $\rightarrow \sigma = 16$ (dashes) $\rightarrow \sigma = 32$ (dots)



High space resolution ($N_x = 500$)



Low space resolution ($N_x = 100$)

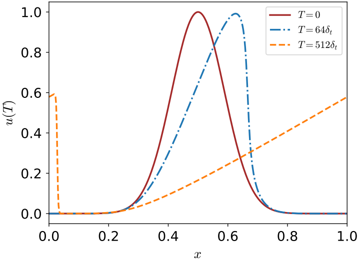
Main observations

- Mainly influence the coarse solver error, less the convergence
- A too low space resolution cancels the beneficial impact of high order interpolation

The new problem

- Non-linear advection term

$$\frac{\partial u}{\partial t} = -u\frac{\partial u}{\partial x} + \nu\frac{\partial^2 u}{\partial x^2}, \quad \nu << \max_x(u_0)$$

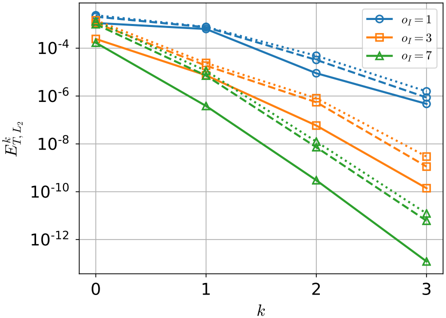


- Centered scheme applied to $\frac{1}{2}\frac{\partial u^2}{\partial x}$

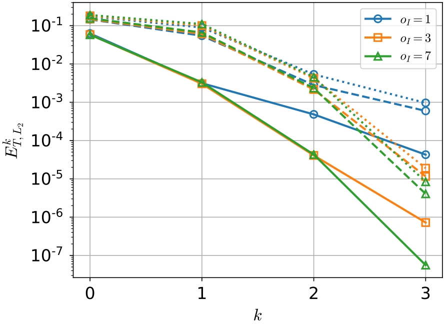
Non linear case - influence of the Reynolds number

$Re = \max(u_0)/\nu$: from low to high

2000 (line) $\rightarrow$ 10000 (dashes) $\rightarrow$ 20000 (dots)



High space resolution ($N_x = 500$)



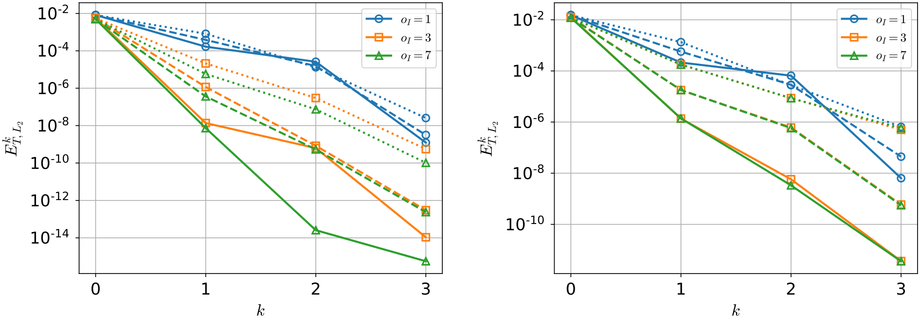
Low space resolution ($N_x = 250$)

Main observations

- Similar behavior as the linear case, except for deterioration of the coarse solver accuracy
- Bad space resolution quickly cancels high order interpolation benefits

Non linear case - influence of the time-slice length

Number of δ_t per time-slice: from large to small
128 (line) $\rightarrow$ 64 (dashes) $\rightarrow$ 32 (dots)



High space resolution ($N_x = 500$) | Low space resolution ($N_x = 250$)

Main observation

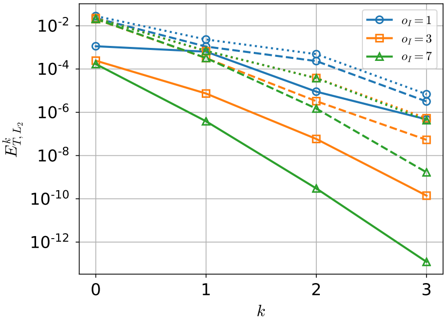
- Increasing the time-slice length enhances the convergence (for each resolutions)

$\neq$ **linear case**

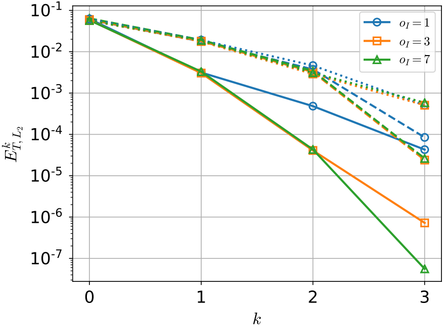
Non linear case - influence of the solution regularity

Width of the initial Gaussian: from large to small

$\sigma = 8$ (line) $\rightarrow \sigma = 16$ (dashes) $\rightarrow \sigma = 32$ (dots)



High space resolution ($N_x = 500$)



Low space resolution ($N_x = 250$)

Main observation

- Increasing sharpness of the solution $\simeq$ increasing the Reynolds number

Conclusions from this study

General conclusion for Parareal with space coarsening on advection problem

- Reasonably good convergence obtained for some cases
- Advection is not the only player to blame, there is also
  1. Low order interpolation (**PLEASE do not use linear interpolation !**)
  2. Space mesh resolution not adapted to a sharp initial solution
  3. ...
- Non-linearity can change everything
  1. Increasing the time-slice can enhance the convergence
  2. More sensitivity to the tuple: (mesh resolution, solution form)

Perspectives

- Numerical experiments done with the Casper Python code
  1. Not open-source yet but can be shared at demand
  2. Could be used to conduct many other tests
- Theoretical Fourier analysis of the algorithm to understand its main behavior (DD25 + draft)
- Complete convergence theory for the advection-diffusion problem (contraction factor, ...)

Thanks a lot for your attention,

I would be glad to answer if you have

Any questions ?