CENTRE EUROPÉEN DE RECHERCHE ET DE FORMATION AVANCÉE EN CALCUL SCIENTIFIQUE

Optimised Runge-Kutta time integration for the Spectral Difference method

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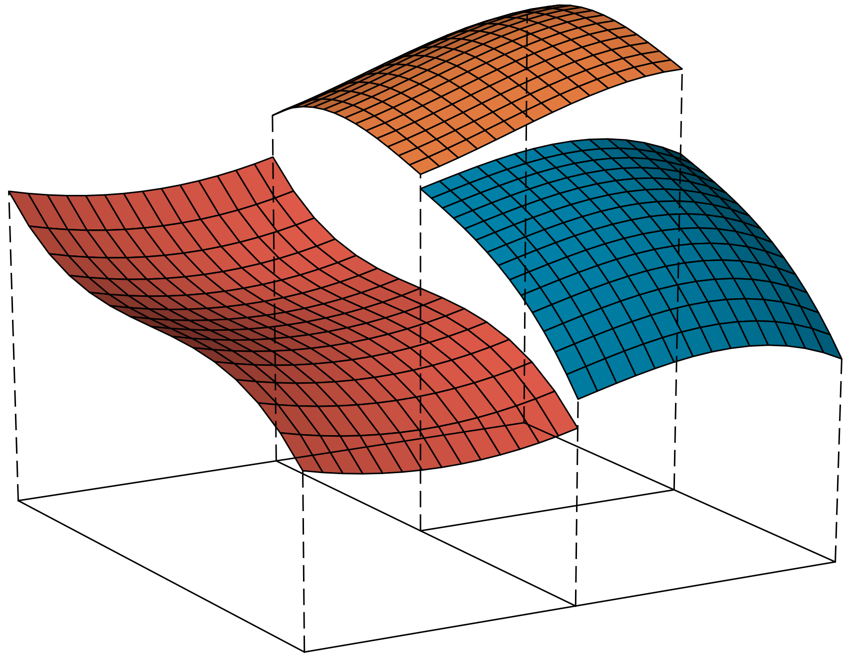
Context (1)

- High order spectral discontinuous methods are promising for LES and DNS
  - Accuracy
  - Good vectorisation
  - High parallel efficiency
  - Local treatment
- In addition, compatible with hp-adaptation



- *Within the TILDA project, we wish to <u>demonstrate the capability</u> of such methods <u>to perform massively parallel LES and DNS</u>, far from the capability of current LES solvers.*

Context (2)

- Basic ingredients:
  - Polynomial representation of unknowns per mesh cell
  - Discontinuity => flux given by a Riemann solver, as in Finite Volume

- At the present time:
  - Many efforts done to perform such simulations, focusing on spatial scheme (many versions of DG, SD, FR, HDG schemes…)
  - Much less attention paid on the analysis of the time integration technique.

Context (3)

- For LES/DNS, the standard time integration schemes are the Runge-Kutta schemes
  - Explicit time integration with controls on 1- the number of steps, 2- the scheme accuracy and 3 - its mathematical properties (TVD)

- Our experience with our solver based on the Spectral Difference method shows that ***the CFL constraint is stronger with SD than with FV, leading to smaller time steps***
  - ***More iterations to perform!***

Context (4)

- Two solutions to recover the same computational time for the spectral discontinuous methods and high-order FV:
  1. ***Make many efforts on CPU optimisation*** in order to perform more iterations than FV for the same physical time
  2. ***Optimise the time integration technique*** in order to allow larger stable time steps

- ***In this context, choice to focus our attention on the optimisation of the time integration technique.***

Context (5)

- In which points are our approach different with the previous ones?
  1. ***Coupled space/time analysis***, using results published recently in *J. Comput. Phys* [1].
  2. Dedicated to the ***Spectral Difference Method***
  3. ***Based on the 6 step RK scheme*** (the 6-step 2nd order RK DRP scheme of Bogey and Bailly [2] is our reference for aeroacoustic simulations)

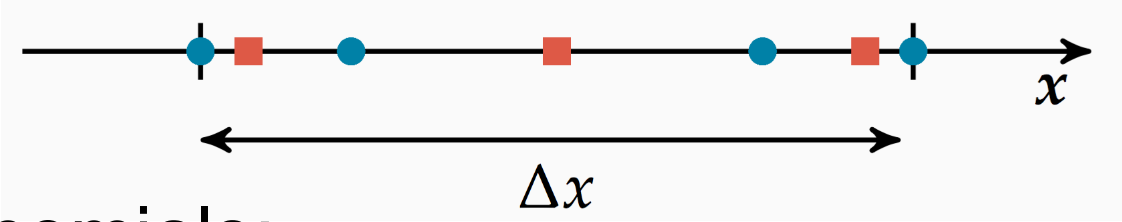
[1] Revisiting the spectral analysis for high-order spectral discontinuous methods, J. Vanharen, G. Puigt, X. Vasseur, J-F. Boussuge and P. Sagaut, *J. Comput. Phys.* 337 (2017) 379–402.
[2] C. Bogey, C. Bailly, A family of low dispersive and low dissipative explicit schemes for flow and noise computations, *J. Comput. Phys.* 194 (1) (2004) 194–214,

Outline

- Spatial Discretisation
- Time Discretisation
- Optimization
- Numerical Verification

The Spectral Difference Method

- Solves the strong form of the NS Eq. (as FD).



- Two sets of polynomials:
  - Degree ***p*** for the ***solution <=> p+1 fields in SP***
  - Degree ***p+1*** for the ***flux <=> p+2 fields in FP***

  In order to recover the solution polynomial degree when computing the flux divergence.

- *Staggered approach* and *directional treatment* suitable for meshes composed of unstructured hexa

Principle of the spatial discretisation

- Algorithm:
  1. Interpolate solution from SP to FP
  2. Compute the flux from solution (for internal FP) or using a Riemann solver (for FP on cell interface).
  3. Define the flux polynomial and compute the divergence in SP
  4. Update in time

- For the definition of optimised RK schemes, let's apply the algorithm to the advection equation.

Spatial Discretisation (1)

- 1D linear advection equation: $\dfrac{\partial u}{\partial t} + a\dfrac{\partial u}{\partial x} = 0$

- Mesh composed of regular elements of length Δx
- General definition of the exact Riemann solver:

$$f^R(u_l, u_r) = \frac{(a + \phi|a|)}{2}u_l + \frac{(a - \phi|a|)}{2}u_r$$

- Step 1: define the SD formulation in matrix form:

$$\frac{\partial u_i}{\partial t} + \frac{a}{\Delta x}D(M^{-1}u_{i-1} + M^0 u_i + M^{+1}u_{i+1}) = 0$$

where *M* represents both extrapolation and flux, index refers cell index and D is the derivation matrix.

Spatial Discretisation (2)

- Insert a spatial Fourier mode

$$u_i(x,t) = \tilde{u}_i(t) \cdot exp(jki\Delta x)$$

- With the dimensionless wave number, one gets

$$\frac{\partial \tilde{u}_i}{\partial t} + \frac{a}{\Delta x} D(M^{-1}e^{-jk} + M^0 + M^{+1}e^{jk})\tilde{u}_i = 0$$

- This can be written as

$$\frac{\partial \tilde{u}_i}{\partial t} = \frac{a}{\Delta x} A(k) \cdot \tilde{u}_i$$

Time integration

- Time integrate $$\frac{\partial \tilde{u}_i}{\partial t} = \frac{a}{\Delta x} A(k) \cdot \tilde{u}_i$$

- With low-storage 6-stage RK method:

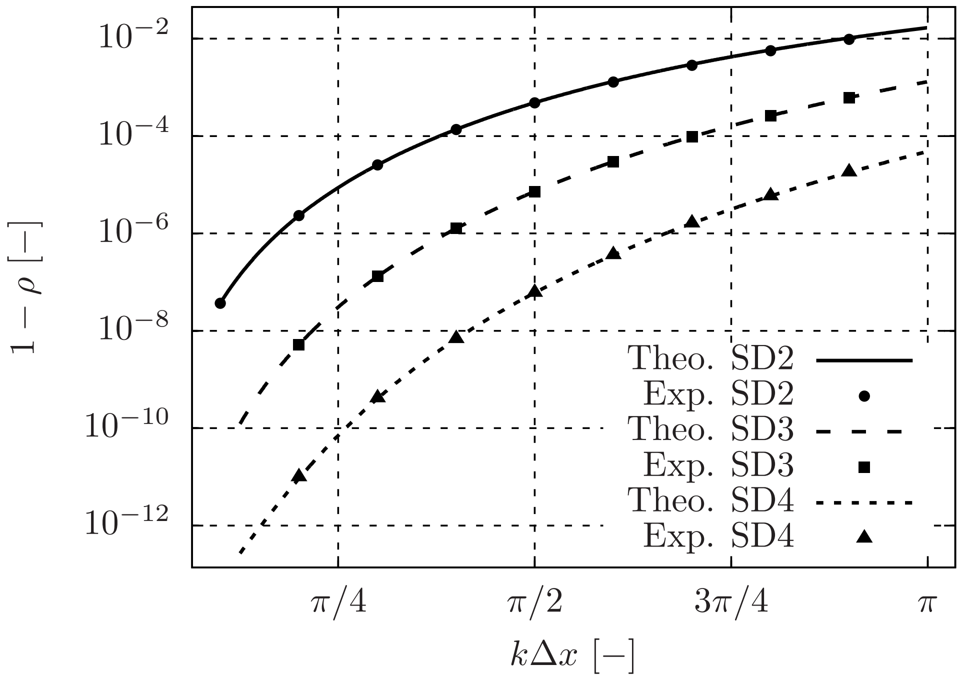
$$\tilde{u}_i^{n+1} = \tilde{u}_i^n + \sum_{\alpha=1}^{6} \gamma_\alpha \mathrm{CFL}^\alpha A^\alpha \tilde{u}_i^n \qquad \tilde{u}_i^{n+1} = G(k, \mathrm{CFL}) \tilde{u}_i^n$$

$$G = 1 + \sum_{\alpha=1}^{6} \gamma_\alpha \mathrm{CFL}^\alpha A^\alpha$$

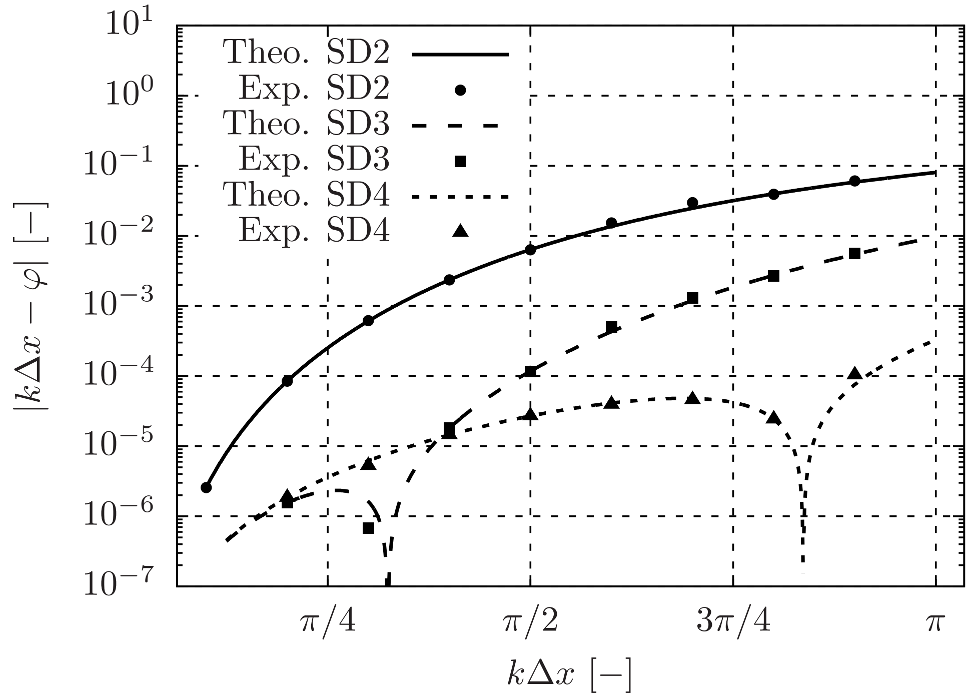
- The coefficients γ_α define the accuracy of the RK method

Key points (1)

Dissipation



Dispersion



Comparison of theoretical results and numerical simulations

- Details in *Revisiting the spectral analysis for high-order spectral discontinuous methods, J. Comput. Phys.* 337 (2017) 379–402.

Key points (2)

- High accuracy of the method
- Error in dissipation and dispersion increases with the wavenumber
- It seems possible to control error in dissipation and dispersion by optimising the behaviour in π

Optimisation

- The algorithm is stable if

$$|\rho(G(k, \mathrm{CFL}))| \leq 1, \quad \forall k \in [0, \pi]$$

- When the CFL is increased, the first value of k for which the spectral radius is equal to one is π

$$|\rho(G(\pi, \mathrm{CFL}))| \leq 1,$$

- To get 4th order RK scheme for linear advection, the first four coefficients are imposed.

$$\gamma_1 = 1 \qquad \gamma_3 = 1/6$$
$$\gamma_2 = 1/2 \qquad \gamma_4 = 1/24$$

Optimisation

- The last two coefficients are optimised.
- Maximize CFL subject to

$$|\rho(G(\pi, \mathrm{CFL}, \gamma_5, \gamma_6))| \leq 1$$

- Solve the equation for a given set of (γ_5, γ_6)

$$|\rho(G(\pi, \mathrm{CFL}, \gamma_5, \gamma_6))| = 1$$

- Use dichotomy to define the surface

$$|\rho(G(\pi, \mathrm{CFL}, \gamma_5, \gamma_6))| = 1$$

- Optimization is done using Nelder-Mead method

Remarks on the optimisation process

- At present, optimisation is in CFL in order to allow greater time steps
- Possible to define optimised RK schemes in dissipation and dispersion (DRP) by a coupled space / time analysis
- The spectral properties change with *p* and as a consequence, ***one optimised RK scheme is associated with one value of p***

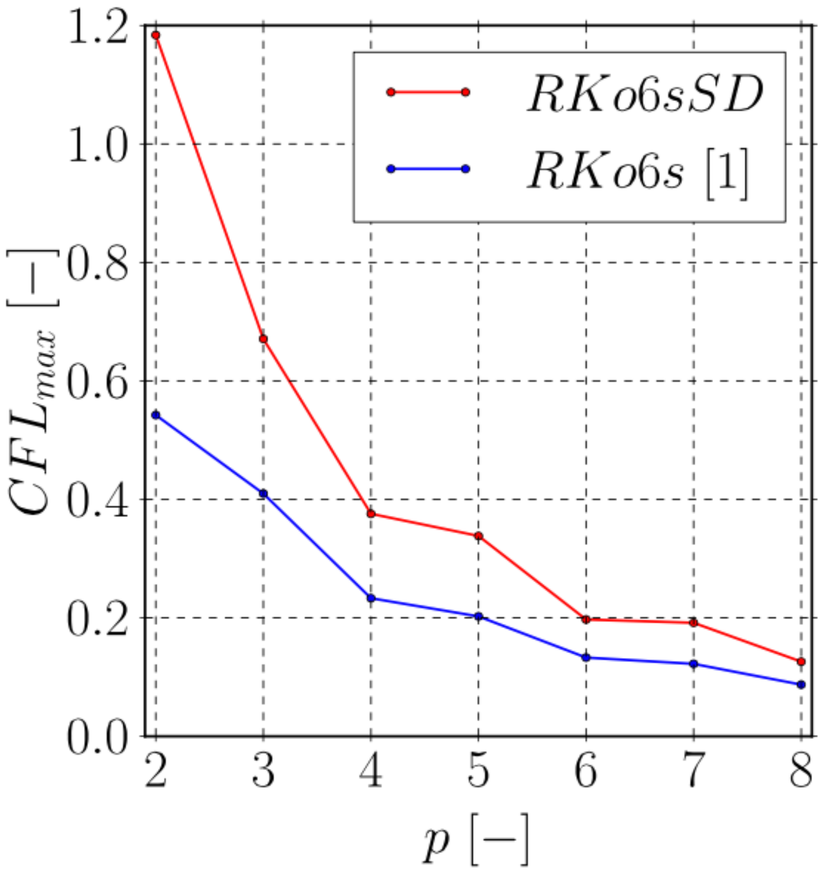
Optimisation results (1)

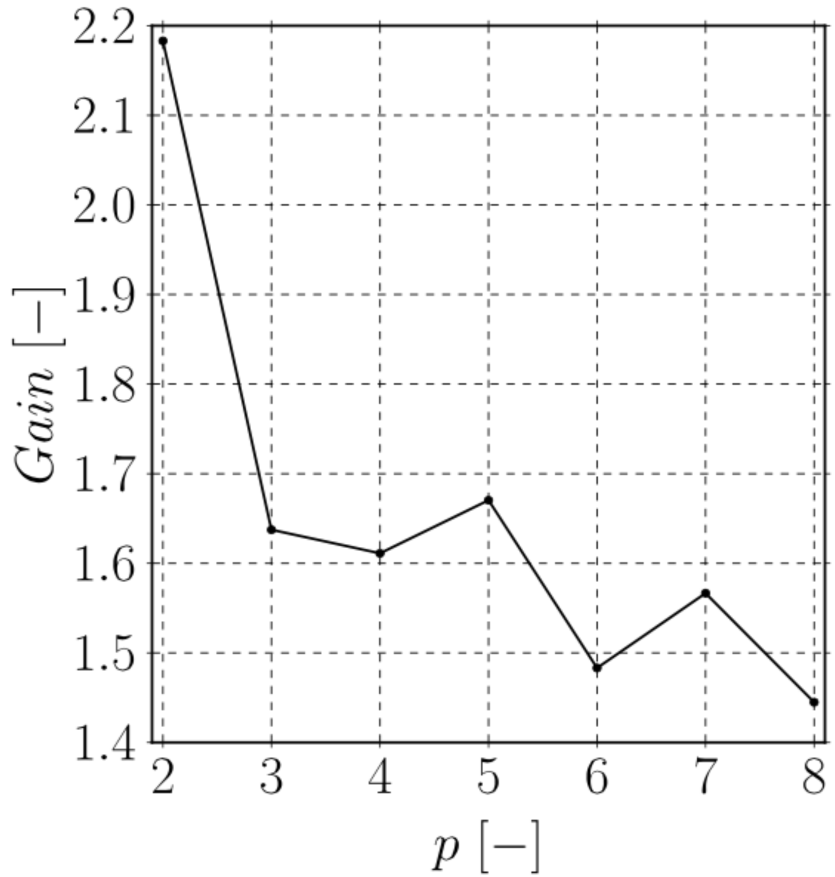
- Optimised coefficients and corresponding CFL numbers

p	γ_5	γ_6	CFL_{max}
2	0.00576453257856	0.00029485511654	1.183
3	0.00539500786873	0.00042341598334	0.670
4	0.00641025285761	0.00040879950330	0.375
5	0.00552476535973	0.00038479937257	0.338
6	0.00657464711078	0.00044773200057	0.197
7	0.00584100342617	0.00040660871984	0.191
8	0.00675819809625	0.00048326301743	0.125

Optimisation results (2)

- Comparison with reference RK scheme RK06s of Bogey and Bailly





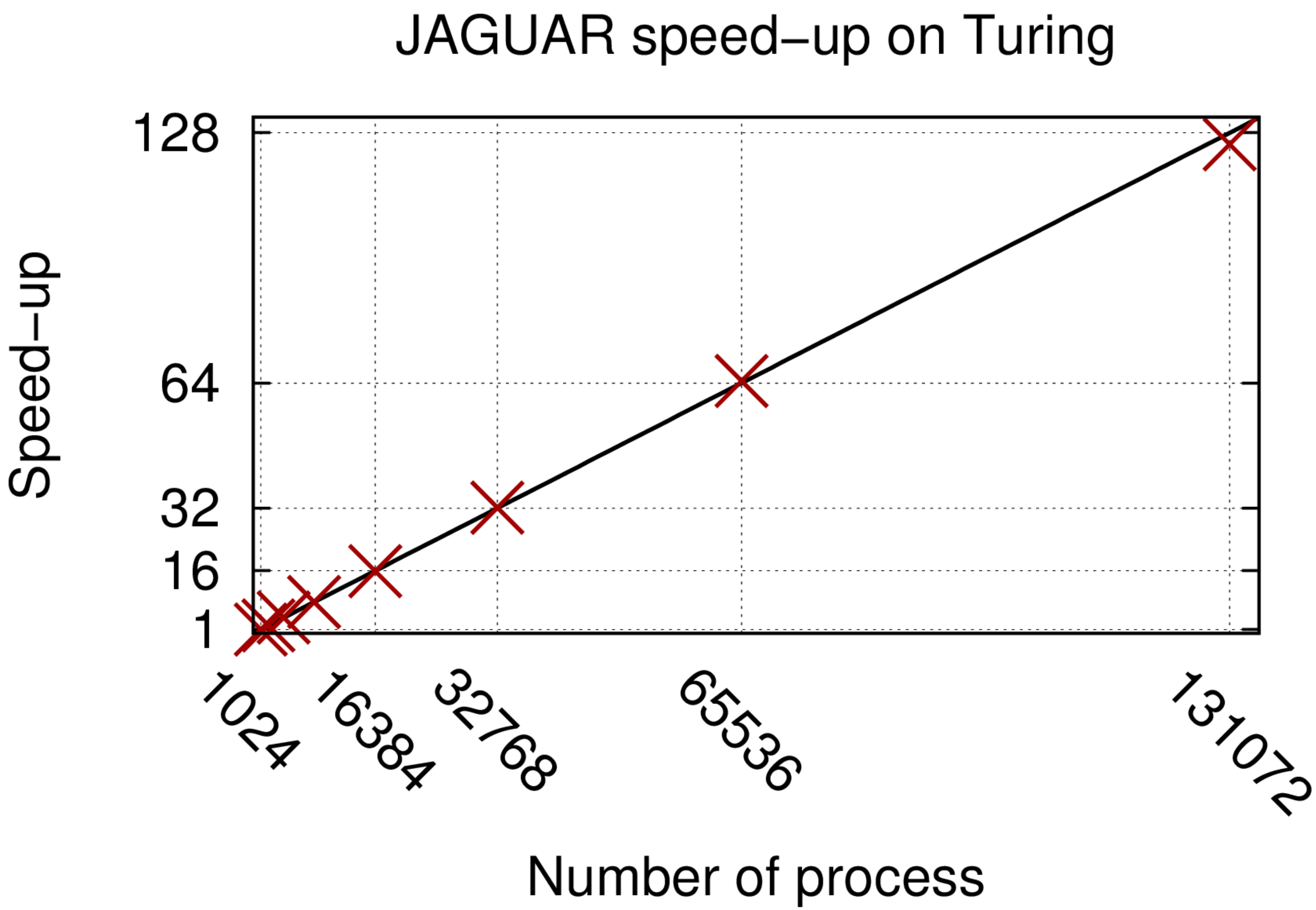
Same CPU cost but larger stability!

The JAGUAR solver

- JAGUAR is CERFACS' CFD code using the SD method.
- New solver developed for 5 years.
- Dedicated today to LES / DNS on unstructured hexa grids
- Mesh splitters: Metis, ParMetis, Manual splitting
- Many efforts for HPC
  - Serial optimisation, vectorisation
  - MPI, OpenMP, hybrid MPI/OpenMP

Strong scaling on Blue Gene

- #99 for TOP500



Numerical verification

- Transport of an isentropic vortex solution of Euler equations in a periodic box.
- Test case from the High Order Workshop
- Input data: initialisation of a mean flow + superposition of the vortex

$$
\begin{aligned}
M_\infty &= 0.05 \\
\beta &= 1/5 \\
R &= 0.005 \\
(X_c, Y_c) &= (0.05, 0.05)
\end{aligned}
$$

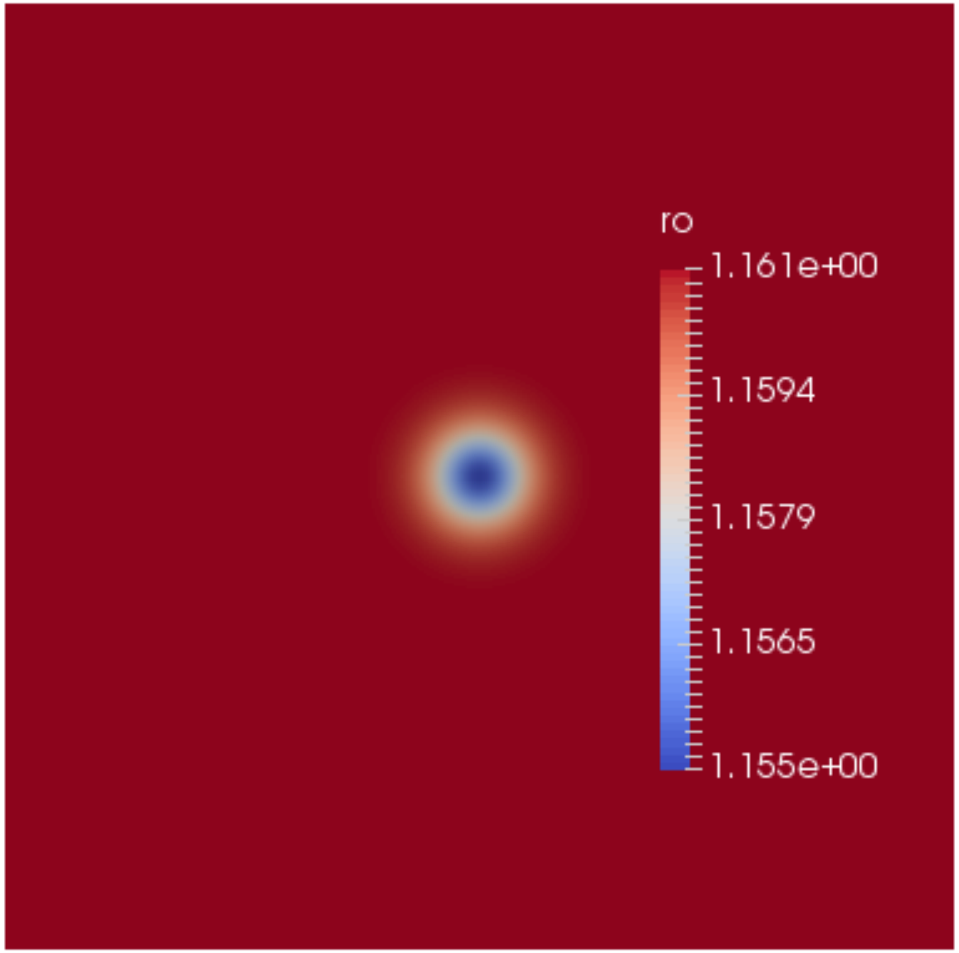
$$\delta u = -U_\infty \beta \frac{y - Y_c}{R} exp\left(\frac{-r^2}{2}\right)$$

$$\delta v = U_\infty \beta \frac{x - X_c}{R} exp\left(\frac{-r^2}{2}\right)$$

$$\delta T = -\frac{1}{2C_p} \left(U_\infty \beta\right)^2 exp\left(-r^2\right)$$

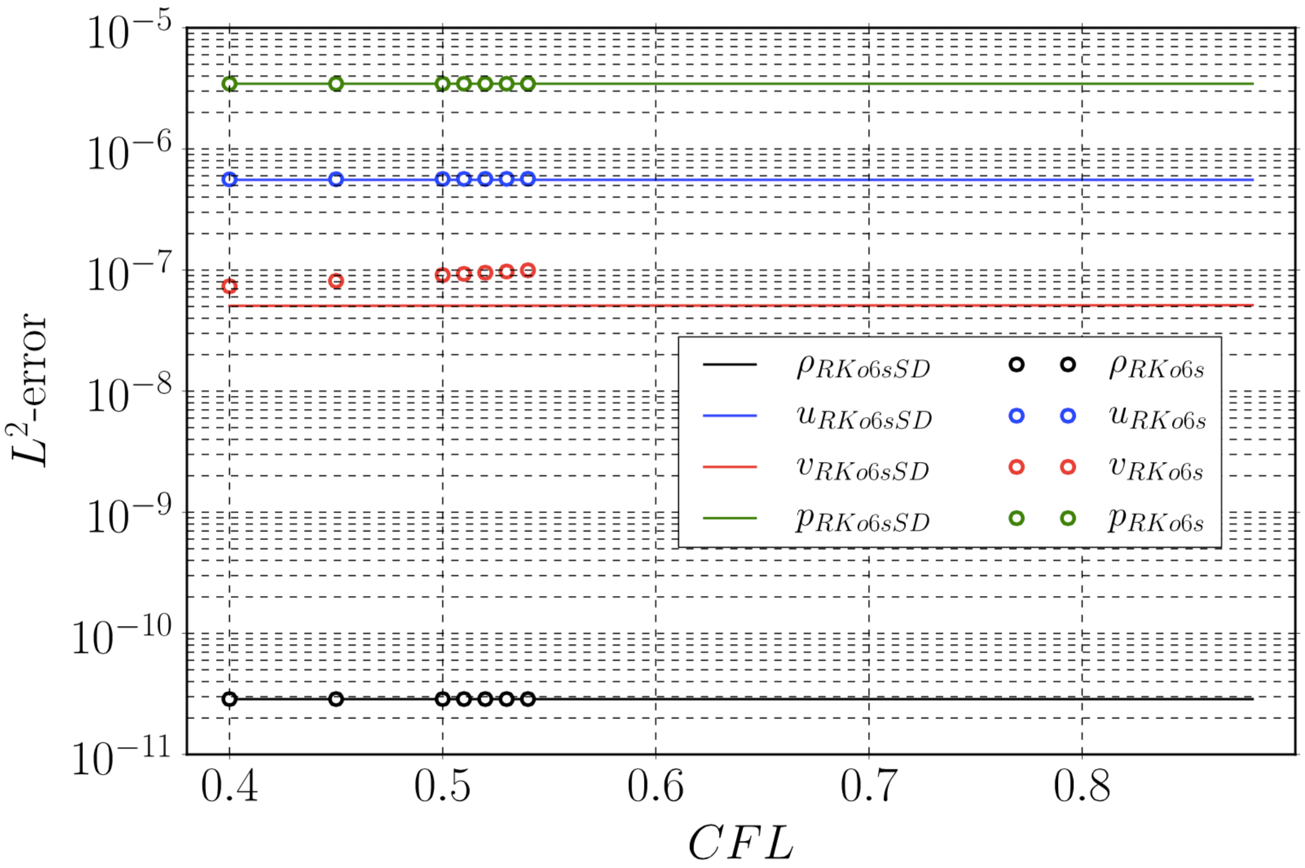
Numerical verification - 2D vortex

- Transport of an isentropic vortex solution of Euler equations in a periodic box.



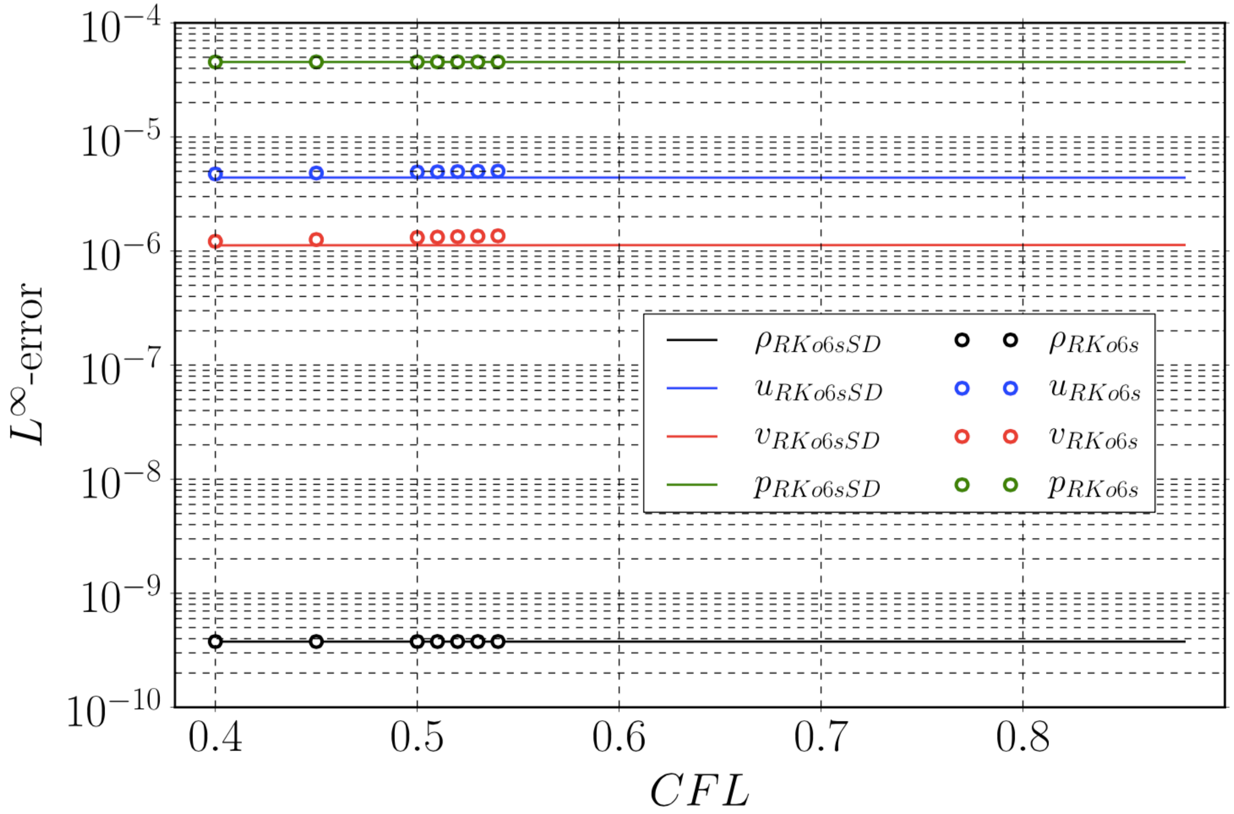
Numerical verification - 2D vortex

- Comparison with RK scheme of Bogey and Bailey, p=4
- L^2 error Vs. CFL number



Numerical verification - 2D vortex

- Comparison with RK scheme of Bogey and Bailey, p=4
- L^∞ error Vs. CFL number



$CFL_{max}^{RKo6s} = 0.54 \quad CFL_{max}^{RKo6sSD} = 0.88$ $Gain \approx 60\%$

Conclusion

- Our goal was to propose a new set of coefficients to enable larger time steps while keeping accuracy
- Using a revisited analysis, we have performed a spectral analysis
  - Coupled time and space discretisation
  - Using a 6 stage low-storage RK scheme
- Finally, a technique was proposed to increase the maximum stable CFL number for 4th-order 6-stage RK schemes for SD and polynomial degree from 2 to 8
- ***Time step increased by 60%!***

Future work

- The optimisation problem is today solved for wavenumber at π
- The procedure has to be extended to optimise on the whole spectral domain
  - Avoid any hypothesis on the shape of the dissipation / dispersion curves
- Another optimisation may consist using a DRP criteria on the time RK schemes.

Acknowledgements

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