Cost-vs-accuracy analysis of self-adaptive time-integration methods

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Introduction

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$$\frac{du}{dt} + u\frac{du}{dx} = 0$$

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$$\left(\frac{u\Delta t}{\Delta x}\right)_{max} \leq 1$$

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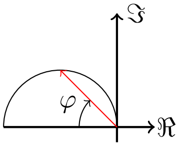
Computation of the eigenbounds in the predictor velocity step to set the maximum stable Δt



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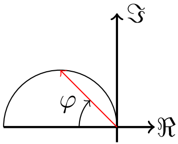

And now?

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Runge-Kutta applied to Navier-Stokes

Starting point...

$$M\mathrm{u}_s = 0_c$$

$$\Omega \frac{d\mathrm{u}_c}{dt} + C(\mathrm{u}_s)\mathrm{u}_c - D\mathrm{u}_c + \Omega G_c \mathrm{p}_c = 0_c$$

- Putting together both expressions...

$$\frac{d\mathrm{u}_c}{dt} = \underbrace{(I_n - GL^{-1}M)}_{\text{Projection operator}, P} F(\mathrm{u}_s)\mathrm{u}_c$$

- Hard to compute $PF(\mathrm{u}_s)$, thus projection method is used.

According to Sanderse and Koren [3],

$$\mathrm{u}_i^* = \mathrm{u}_n + \Delta t \sum_{j=1}^{i-1} a_{ij}\mathrm{F}_j \qquad \mathrm{u}_{n+1}^* = \mathrm{u}_n + \Delta t \sum_{i=1}^{s} b_i \mathrm{F}_i$$

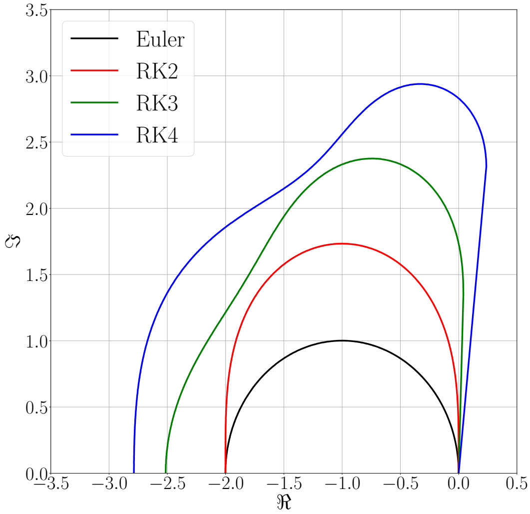
$$L\Psi_i = \frac{1}{\Delta t} D\mathrm{u}_i^* \qquad L\Psi_{n+1} = \frac{1}{\Delta t} D\mathrm{u}_{n+1}^*$$

$$\mathrm{u}_i = \mathrm{u}_i^* - \Delta t G\Psi_i \qquad \mathrm{u}_{n+1} = \mathrm{u}_{n+1}^* - \Delta t G\Psi_{n+1}$$

[3] Sanderse, B., Koren, B. (2012), "Accuracy analysis of explicit Runge-Kutta methods applied to the incompressible Navier-Stokes equations", Journal of Computational Physics 231 (8), pp. 3041-3063

Stability region of Runge-Kutta

- Coefficients a_{ij}, b_i from the method: Butcher tableau, $A = [a_{ij}]_{i=1,\ldots,s; j=1,\ldots,s}$, $b = (b_1 \; b_2 \; \ldots \; b_s)$
- In general, $R(z) = 1 + zb^T(I_s - zA)^{-1}1_s$, yet for $p = s$, $R(z) = 1 + \sum_{p=1}^{s} \frac{1}{p!} z^p$



Computation of eigenbounds

- Need to compute the eigenbounds of $F(\mathrm{u}_s) = D - C(\mathrm{u}_s)$
- If D and $C(\mathrm{u}_s)$ are discretized with a symmetry-preserving scheme[2],

$$\lambda_F \leq -|\lambda_D| + i\lambda_C$$

- λ_D and λ_C can be computed independently with Gershgorin circle theorem

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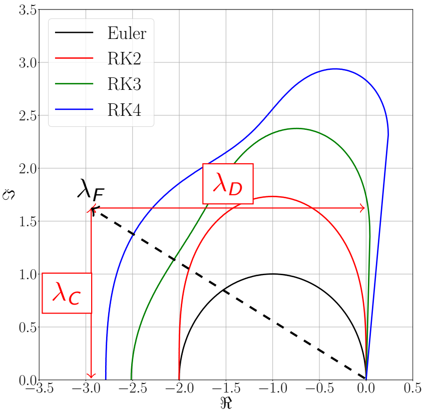

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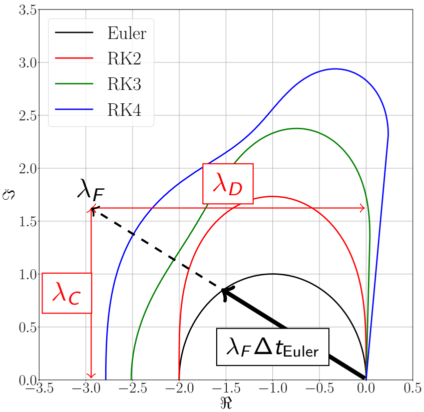

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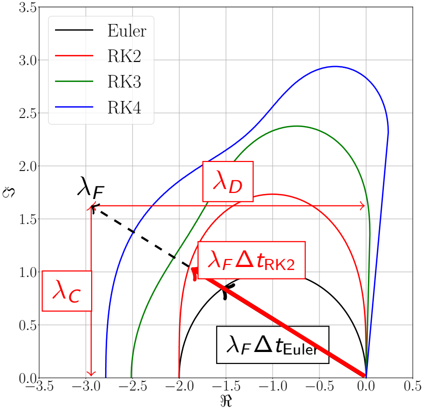

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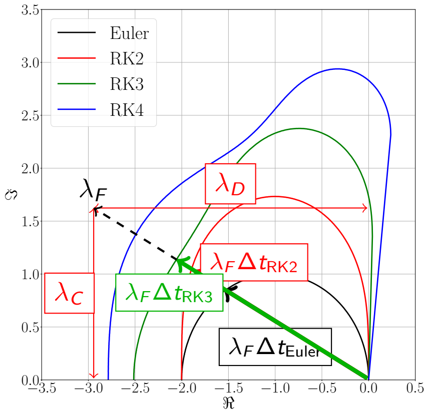

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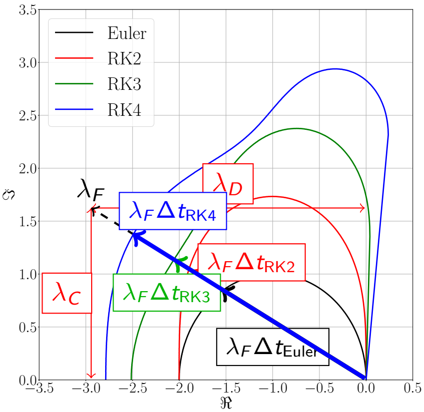

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From stability to efficiency regions

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Computational efficiency region

Combination of a set of stability regions normalized by the ratio of wall clock times per iteration between the current scheme and Euler scheme, τ_{Method}.

With the generalized implementation in our in-house CFD&HT code...

$$T_{\Delta t}(s) = sT_{SLAE} + 33sT_{SpMV} + s\left(24 + 3\frac{s-1}{2}\right)T_{axpy} + 10sT_{axty}$$

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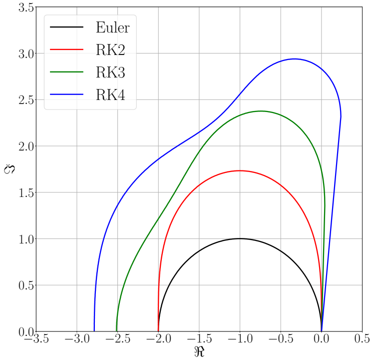
$$\tau_{\mathrm{Method}}(s) = \frac{T_{\Delta t}(s)}{T_{\Delta t}(1)} = s\left(1 + \frac{3}{2}(s-1)\frac{T_{axpy}}{T_{\Delta t}(1)}\right) \approx s$$

From stability to efficiency regions



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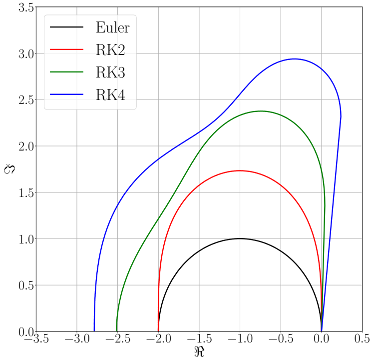

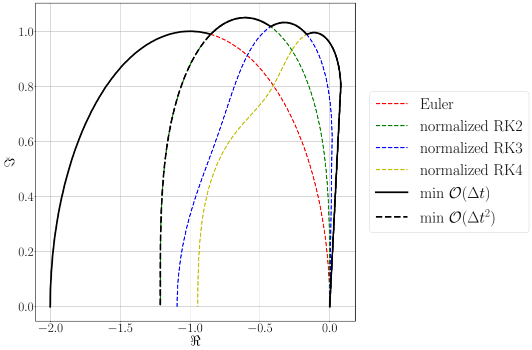

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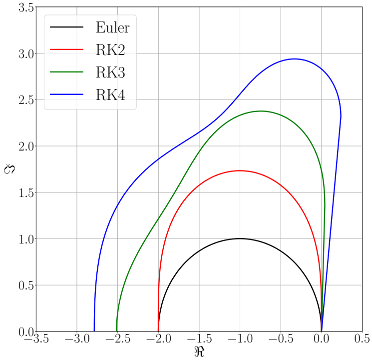
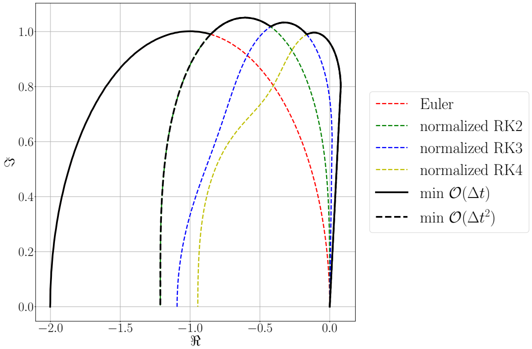




Additional conditions

Other possible conditions can be set to limit or handicap the proposed schemes in order to filter according to different categories.

From stability to efficiency regions

Algorithm 1: Self-adaptive efficiency time-step scheme

Data: *Pool* of schemes, (Scheme 1,Scheme 2,. . . ,Scheme n),Eigenbounds (λ_C, λ_D), Scale factor $f_{\Delta t}$

Result: Time-step, Δt

$i := 1;$

$i_s := i;$

$\Delta t_s := 0.0;$

while $i \leq n$ **do**

  $\Delta t_{s,i} = \Delta t_s(\text{Scheme}_i, \lambda_C, \lambda_D);$

  if $\Delta t_{s,i} / \tau_{Scheme_i} \geq \Delta t_s$ **then**

    $\Delta t_s = \Delta t_{s,i} / \tau_{\text{Scheme}_i};$

    $i_s := i;$

  end

end

return $\Delta t := f_{\Delta t} \Delta t_s(Scheme_{i_s}, \lambda_C, \lambda_D);$

Numerical experiments

Three-dimensional Taylor-Green vortex

- Initial conditions:

$$u_{x,0} = U_0 \frac{2}{\sqrt{3}} \sin(x)\cos(y)\cos(z)$$

$$u_{y,0} = U_0 \frac{2}{\sqrt{3}} \cos(x)\sin(y)\cos(z)$$

$$u_{z,0} = U_0 \frac{2}{\sqrt{3}} \cos(x)\cos(y)\sin(z)$$

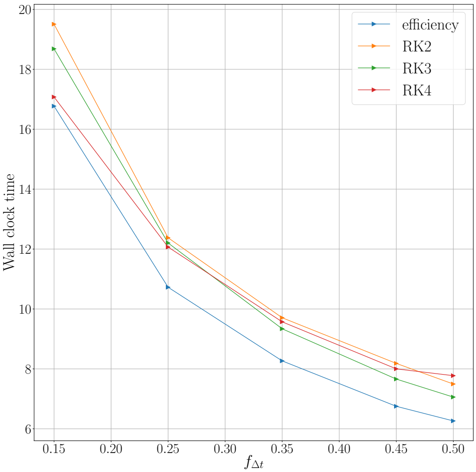
- Run until $t = 20\frac{2\pi}{U_0}$[4]
- $f_{\Delta t} = [0.15, 0.5]$, $\mathrm{Re} = 1500$
- $(32, 64)^3$ grid, cube with a side length of 2π

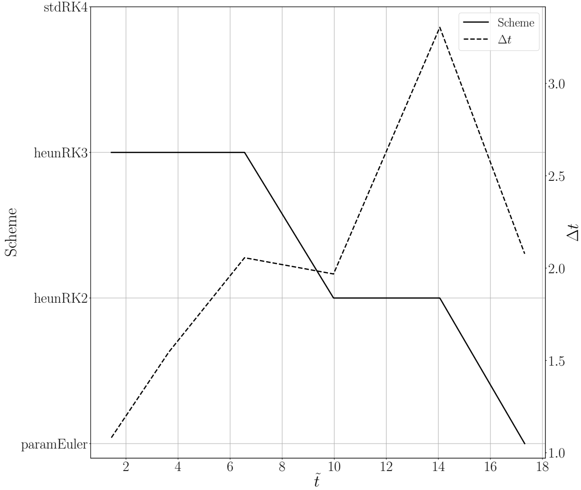
Method	Num. stag. s	Ord. acc. p
Euler	1	1
Heun RK2	2	2
Heun RK3	3	3
Standard RK4	4	4

[4] Capuano, F., Coppola, G., and de Luca, L. (2015), "An efficient time advancing strategy for energy-preserving simulations". Journal of Computational Physics 295, pp. 209-229

Numerical experiments

32^3 grid





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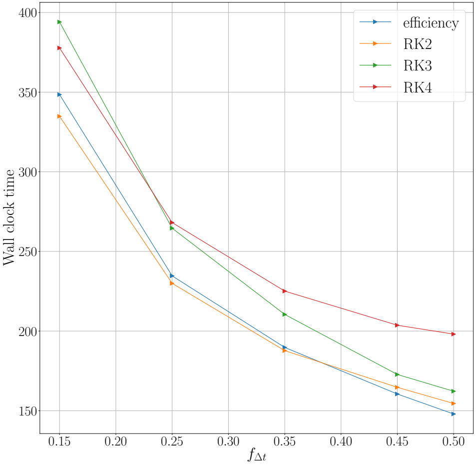
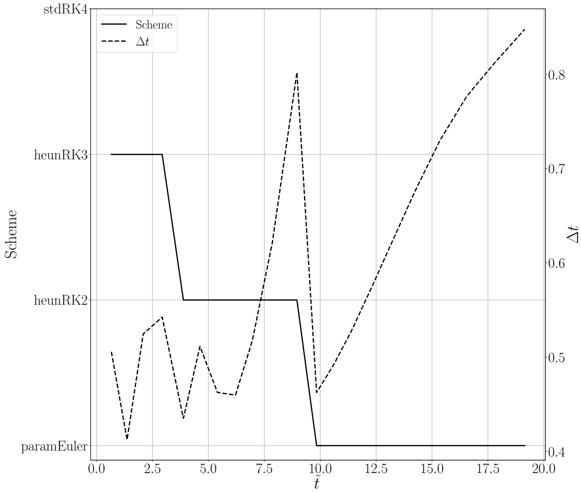
64^3 grid





Conclusion

Method

- Method is born as an evolution of self-adaptive strategies:
  - Pool of schemes chosen previous to the start of the simulation
  - Computational efficiency region allows addition of constraints or handicaps to methods to set other characteristics to just performance
  - Computation of eigenbounds might be swapped for a more efficient method

Conclusion

Numerical tests

- Numerical tests have provided improved performance vs the schemes presented on the pool.
- Starts simulation with higher order methods (RK4, RK3) to move to lower order with the evolution of the simulation (Euler).
- Could be tested with higher Re to check if the high order methods are more relevant in the solution.
- Method performance improves when cost per iteration is reduced, or for bigger $f_{\Delta t}$

Conclusion

Future perspectives

Can other properties from Runge-Kutta integration be exploited?

- Computation of Ψ only at the end of the stage, according to Le and Moin[5]:
  - Reduction of accuracy to second order
  - Stability region of the method is preserved

$$\tau_{\text{Method}^*} = 1 + (s-1)(1 - f_{SLAE})$$

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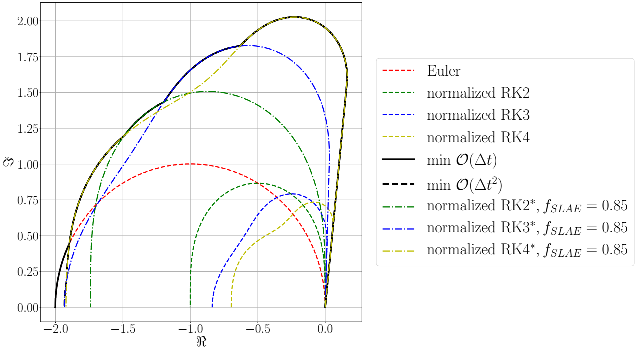

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