On self-adaptive Runge-Kutta Schemes with Improved Energy-Conservation Properties

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Introduction

CFL[1]

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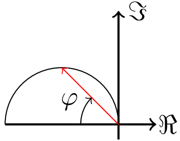
Computation of the eigenbounds in the predictor velocity step to set the maximum stable Δt



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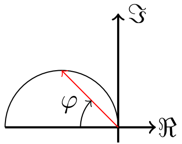

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Introduction

Energy-preserving simulations

- Conservation in space has been widely studied, by Verstappen and Veldman[3] and Trias et al.[4].
  - Sets how operators have to be constructed.
- But... conservation in time?
  - Sanderse[5] applied symplectic Runge-Kutta schemes → implicit integrators
  - Capuano et al.[6] used pseudo-symplectic schemes: explcit, conservation of energy up until a certain order q

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[3] Verstappen, R.W.C.P, Veldman, A.E.P. (2003), "Symmetry-preserving discretization of turbulent flow". Journal of Computational Physics 187 (1), pp. 343-368

[4] Trias, F.X. et al. (2014), "Symmetry-preserving discretization of Navier-Stokes equations on collocated unstructured grids". Journal of Computational Physics 258, pp. 24-267

[5] Sanderse, B. (2013), "Energy-conserving Runge-Kutta methods for the incompressible Navier-Stokes equations". Journal of Computational Physics 233 (1), pp. 100-131

[6] Capuano, F. et al. (2016), "Explicit Runge-Kutta schemes for incompressible flow with improved energy-conservation properties". Journal of Computational Physics 328, pp. 86-94

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.

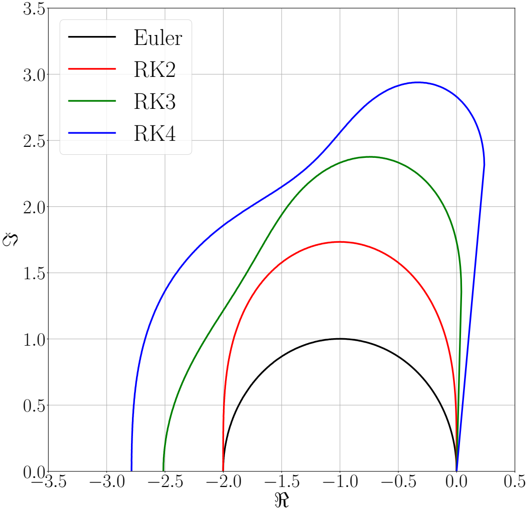
According to Sanderse and Koren [5],

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

[5] 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, $A = [a_{ij}]_{i=1,\dots,s; j=1,\dots,s}$, $b = (b_1 \ b_2 \ \dots \ b_s)$
- 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 $F(u_s) = D - C(u_s)$
- If D and $C(u_s)$ are discretized with a symmetry-preserving scheme[2],

$$\lambda_F \leq -|\rho(D)| + i\rho(C)$$

- $\rho(D)$ and $\rho(C)$ can be computed independently with Gershgorin circle theorem

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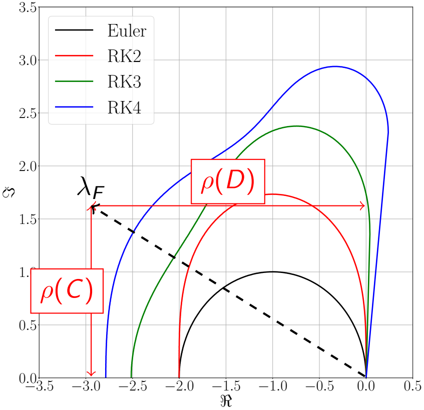

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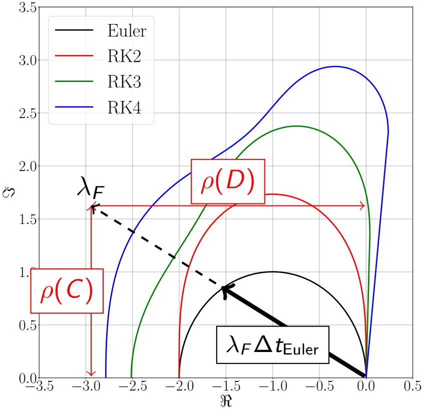

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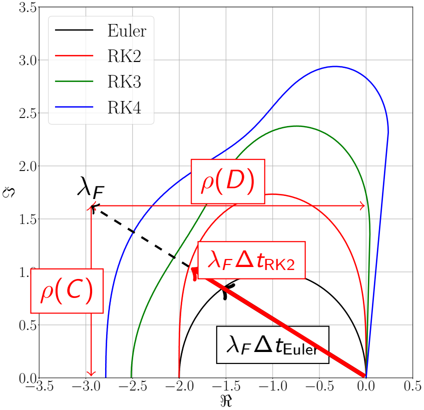

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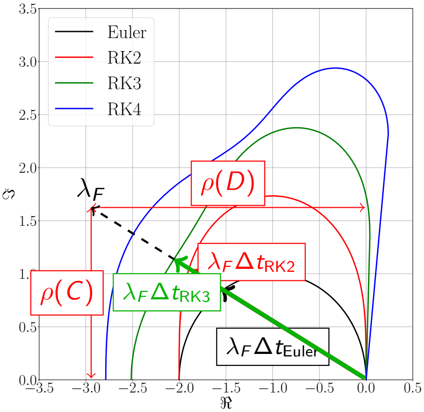

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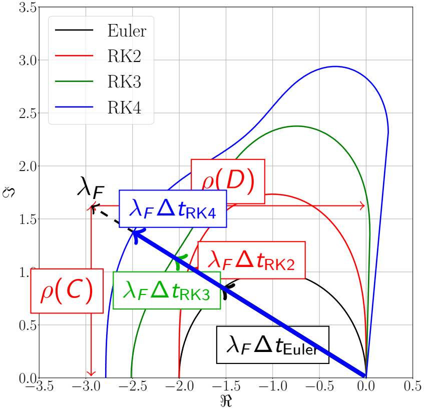

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Computation of eigenbounds

Construction of operators

$$D_c(\alpha_s) = -T_{sc} A_s \Lambda_s \Delta_s^{-1} T_{cs} = -T_{sc} \tilde{\Lambda}_s T_{cs}$$

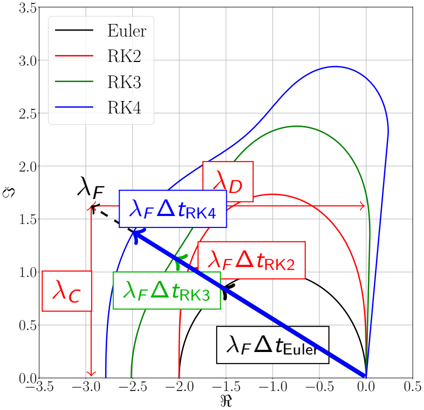
$$C_c(\mathrm{u}_s) = T_{sc} A_s U_s \underbrace{\Pi_{c\to s} =}_{SP} \frac{1}{2} A_s U_s |T_{cs}|$$

By knowing $\rho(AB) = \rho(A^T B^T)$

$$\rho(D_c) = \rho(-\tilde{\Lambda}^{\alpha} T_{cs} T_{cs}^T \tilde{\Lambda}^{1-\alpha})$$

$$4\rho(C_c(\mathrm{u}_s)) \leq \rho(|F_s|^{\alpha} |T_{cs} T_{cs}^T| |F_s|^{1-\alpha})$$

- Allows recomputing the eigenbounds without the reconstruction of D_c, C_c



Kinetic energy budget for the Navier-Stokes equations

- Conservation of energy is a **requirement** for a physics-compatible solver

Semi-discrete Kinetic energy equation

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

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So... integrated in time with Runge-Kutta...

$$\frac{\Delta E}{\Delta t} = -\sum_{i=1}^{s} b_i \mathrm{u}_i^T C_i \mathrm{u}_i - \sum_{i=1}^{s} b_i \mathrm{u}_i^T G_c \mathrm{p}_i + \sum_{i=1}^{s} b_i \mathrm{u}_i^T D \mathrm{u}_i + \varepsilon_{RK}$$

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- $\sum_{i=1}^{s} b_i \mathrm{u}_i^T C_i \mathrm{u}_i = 0$ if C is skew-symmetric
- $\sum_{i=1}^{s} b_i \mathrm{u}_i^T G_c \mathrm{p}_i = 0$ if $M\mathrm{u}_i = 0$ and mesh is staggered

Effective Reynolds number

Definition

First introduced by Capuano et al.[6],

$$\mathrm{Re}_{eff} = \frac{\sum_{i=1}^{s} b_i \mathrm{u}_i^T L \mathrm{u}_i}{\Delta E / \Delta t}$$

- $D = \frac{1}{\mathrm{Re}} L$

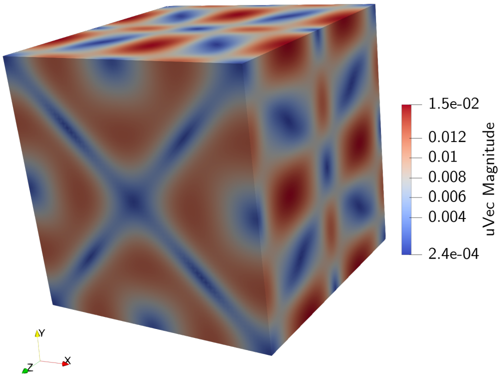
[6] Capuano, F. et al. (2016), "Explicit Runge-Kutta schemes for incompressible flow with improved energy-conservation properties". Journal of Computational Physics 328, pp. 86-94

Numerical experiments

Three-dimensional Taylor-Green vortex

- $2\pi \times 2\pi \times 2\pi$ domain, 32^3 grid
- $f_{\Delta t} = [0.15, 0.25, 0.35, 0.45, 0.5]$
- Re=1500
- TermoFluids Algebraic

Scheme	p	q	s
Euler		1	
Heun RK2		2	
Heun RK3		3	
Standard RK4		4	
4p7q(6)[6]	4	7	6



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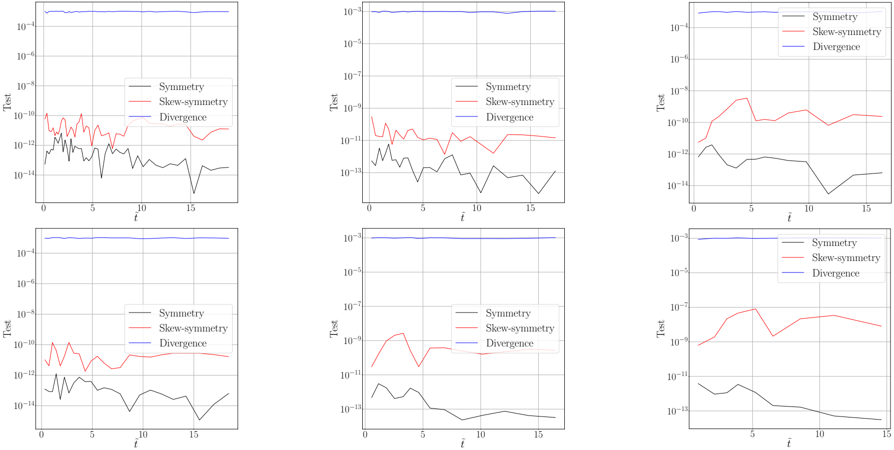
Numerical experiments

Symmetry-preserving discretization

Heun RK2

Standard RK4



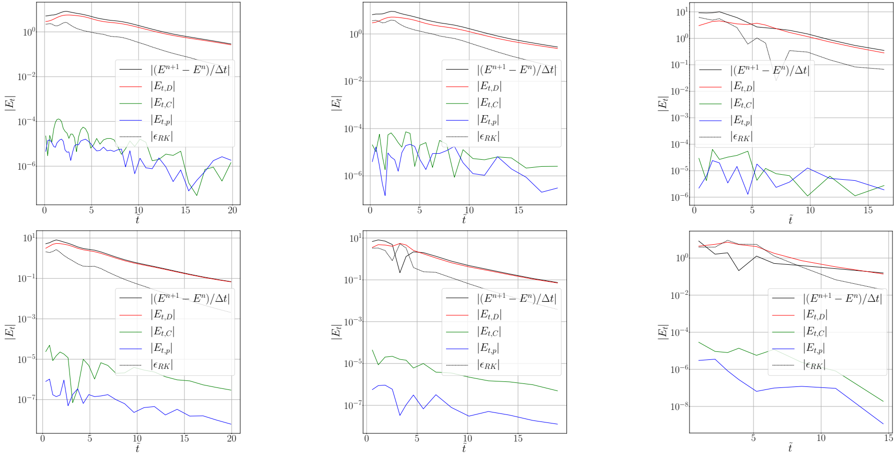
(a) $f_{\Delta t} = 0.15$ (b) $f_{\Delta t} = 0.25$ (c) $f_{\Delta t} = 0.45$

Numerical experiments

Energy budgets

Heun RK2

Standard RK4



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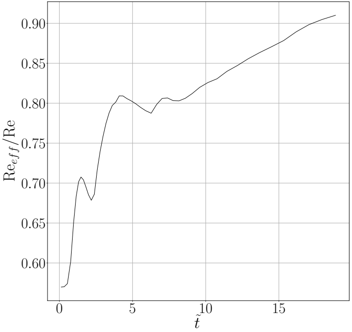
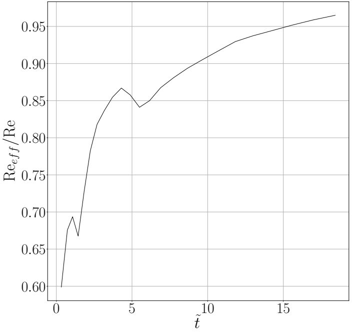
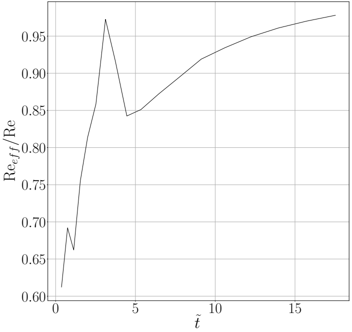


(a) Heun RK2



(b) Standard RK4



(c) 4p7q(6)

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- Evaluation of the different terms for the Kinetic energy budget
  - Only physical contribution has to be the diffusive
  - Which is the weight of the RK scheme?
    - For Re=1500, variation of ≈8% between RK2 and pseudo-symplectic (4p7q(6)), and ≈3% between RK4 and 4p7q(6)
    - Implementation shows negligible contributions of both pressure and convective terms
    - Re_{eff} should be maintained throughout the simulation, but it is not. Some implementation error? Notable variation of Δt throughout the simulation?

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  - Extra computational cost due to added stages in integration.