Time matters: perspectives on time integration in CFD

Francesco Capuano

Department of Fluid Mechanics
Universitat Politècnica de Catalunya · BarcelonaTech
francesco.capuano@upc.edu

NUM-SCARS Workshop
CWI, Amsterdam
22-23 January 2026

Time integration in CFD

False (?) myths and common choices

> "Time integration is not so important: spatial and modeling errors dominate over temporal errors."

Time integration in CFD

False (?) myths and common choices

High-Order CFD Methods: Current Status and Perspective

Z.J. Wang, Krzysztof Fidkowski*, Rémi Abgrall, Francesco Bassi, Doru Caraeni, Andrew Cary, Herman Deconinck, Ralf Hartmann, Koen Hillewaert, H.T. Huynh, Norbert Kroll, Georg May, Per-Olof Persson, Bram van Leer, Miguel Visbal

> "[...] these results have focused on spatial errors. Temporal errors are also of concern in unsteady simulations, and for efficiency purposes high-order time-integration schemes should be used with spatially high-order methods. There are several choices of high-order time-integration schemes, and this topic will be explored in future workshops"
>
> — Wang et al., 2012

Time integration in CFD

False (?) myths and common choices

“Classical” methods are the still the common choice in many **open-source codes** and in **scale-resolving simulations** of turbulent flows

- Wray’s low-storage third-order Runge-Kutta (RK3)
- Lower-order multi-step methods (e.g., 2-step Adams-Bashforth)
- RK3/AB2 in combination with Crank-Nicolson
- Implicit-explicit Runge-Kutta schemes up to third order
- Strong Stability Preserving (SSP)-RK3

F. Capuano, A. Palha, H. Ranocha and X. Trias, ERCOFTAC Bulletin 142

Time integration in CFD

False (?) myths and common choices

- **Resolution** constraints — representation of smallest time scale τ_η
- **Stability** constraints, due to
  - *convective* terms

$$\mathrm{CFL} = \frac{U_{\max}\Delta t}{\Delta x} \le \sigma^c \qquad \rightarrow \qquad \frac{\Delta t}{\tau_\eta} \le \frac{U}{U_{\max}} \mathrm{Re}^{-\frac{1}{4}} \frac{\Delta x}{\eta}$$

  - viscous terms

$$\frac{\nu \Delta t}{(\Delta x)^2} \le \sigma^d \qquad \rightarrow \qquad \frac{\Delta t}{\tau_\eta} \le \left(\frac{\Delta x}{\eta}\right)^2$$

- In LES $\Delta x/\eta$ is typically large $\Longrightarrow$ *convective* stability limits the Δt

Time integration in CFD

False (?) myths and common choices

- **Resolution** constraints — representation of smallest time scale τ_η
- **Stability** constraints, due to
  - *convective* terms

$$\mathrm{CFL} = \frac{U_{\mathrm{max}}\Delta t}{\Delta x} \le \sigma^{\mathrm{c}} \qquad \rightarrow \qquad \frac{\Delta t}{\tau_\eta} \le \frac{U}{U_{\mathrm{max}}} \mathrm{Re}^{-\frac{1}{4}} \frac{\Delta x}{\eta}$$

  - *viscous* terms

$$\frac{\nu \Delta t}{(\Delta x)^2} \le \sigma^{\mathrm{d}} \qquad \rightarrow \qquad \frac{\Delta t}{\tau_\eta} \le \left(\frac{\Delta x}{\eta}\right)^2$$

- In LES $\Delta x/\eta$ is typically large $\Longrightarrow$ *convective* stability limits the Δt

Time integration in CFD

False (?) myths and common choices

- **Resolution** constraints — representation of smallest time scale τ_η
- **Stability** constraints, due to
  - *convective* terms

$$\mathrm{CFL} = \frac{U_{\mathrm{max}}\Delta t}{\Delta x} \le \sigma^{\mathrm{c}} \qquad \rightarrow \qquad \frac{\Delta t}{\tau_\eta} \le \frac{U}{U_{\mathrm{max}}}\mathrm{Re}^{-\frac{1}{4}}\frac{\Delta x}{\eta}$$

  - *viscous* terms

$$\frac{\nu\Delta t}{(\Delta x)^2} \le \sigma^{\mathrm{d}} \qquad \rightarrow \qquad \frac{\Delta t}{\tau_\eta} \le \left(\frac{\Delta x}{\eta}\right)^2$$

- In LES $\Delta x/\eta$ is typically large $\Longrightarrow$ *convective* stability limits the Δt

Time integration in CFD

False (?) myths and common choices

- **Resolution** constraints — representation of smallest time scale τ_η
- **Stability** constraints, due to
  - *convective* terms

$$\mathrm{CFL} = \frac{U_{\mathrm{max}} \Delta t}{\Delta x} \le \sigma^{\mathrm{c}} \qquad \rightarrow \qquad \frac{\Delta t}{\tau_\eta} \le \frac{U}{U_{\mathrm{max}}} \mathrm{Re}^{-\frac{1}{4}} \frac{\Delta x}{\eta}$$

  - *viscous* terms

$$\frac{\nu \Delta t}{(\Delta x)^2} \le \sigma^{\mathrm{d}} \qquad \rightarrow \qquad \frac{\Delta t}{\tau_\eta} \le \left(\frac{\Delta x}{\eta} \right)^2$$

- In LES $\Delta x/\eta$ is typically large $\Longrightarrow$ *convective* stability limits the Δt

Time integration in CFD

False (?) myths and common choices

- **Resolution** constraints — representation of smallest time scale τ_η
- **Stability** constraints, due to
  - *convective* terms

$$\mathrm{CFL} = \frac{U_{\mathrm{max}}\Delta t}{\Delta x} \le \sigma^{\mathrm{c}} \qquad \to \qquad \frac{\Delta t}{\tau_\eta} \le \frac{U}{U_{\mathrm{max}}} \mathrm{Re}^{-\frac{1}{4}} \frac{\Delta x}{\eta}$$

  - *viscous* terms

$$\frac{\nu \Delta t}{(\Delta x)^2} \le \sigma^{\mathrm{d}} \qquad \to \qquad \frac{\Delta t}{\tau_\eta} \le \left(\frac{\Delta x}{\eta}\right)^2$$

- In LES $\Delta x/\eta$ is typically large $\Longrightarrow$ *convective* stability limits the Δt

Common practice: use Δt close to the stability limit to minimize computational effort

Time integration in CFD

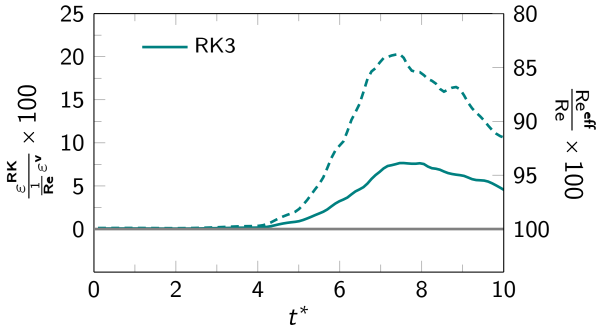
False (?) myths and common choices

… is this safe?
What about accuracy and physical fidelity?

Potential damages of time integration

Alteration of *effective* Reynolds number (no model LES)

$$\frac{\Delta E}{\Delta t} = \frac{1}{\mathrm{Re}}\varepsilon^{\mathrm{v}} + \varepsilon^{\mathrm{RK}} \overset{\mathrm{def}}{=} \frac{1}{\mathrm{Re}^{\mathrm{eff}}}\varepsilon^{\mathrm{v}}$$

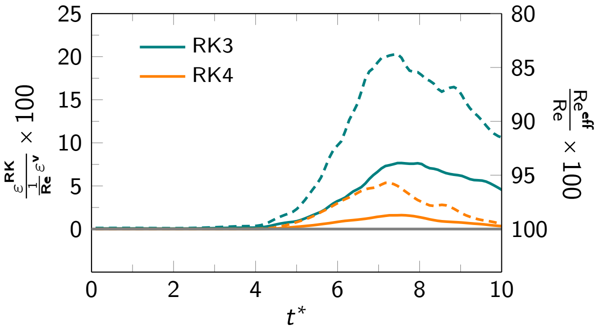


3D Taylor-Green vortex at Re = 1600 (solid lines) and Re = 3000 (dashed lines) on a 64^3 mesh using a fourth-order skew-symmetric Padé scheme and CFL = 1.0

Potential damages of time integration

Alteration of *effective* Reynolds number (no model LES)

$$\frac{\Delta E}{\Delta t} = \frac{1}{\mathrm{Re}}\varepsilon^{\mathrm{v}} + \varepsilon^{\mathrm{RK}} \overset{\mathrm{def}}{=} \frac{1}{\mathrm{Re}^{\mathrm{eff}}}\varepsilon^{\mathrm{v}}$$

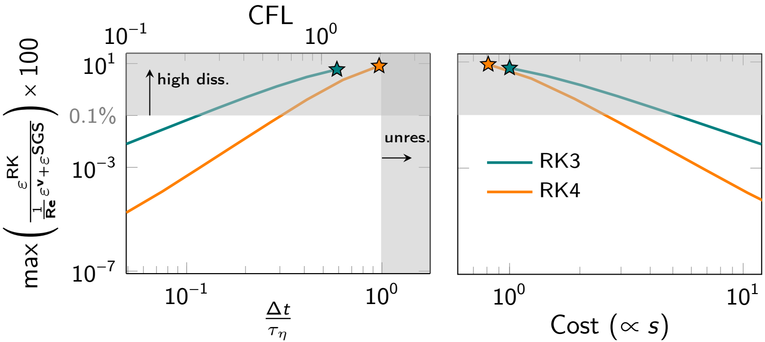


3D Taylor-Green vortex at $\mathrm{Re} = 1600$ (solid lines) and $\mathrm{Re} = 3000$ (dashed lines) on a 64^3 mesh using a fourth-order skew-symmetric Padé scheme and $\mathrm{CFL} = 1.0$

Potential damages of time integration

Interaction with SGS modeling in LES

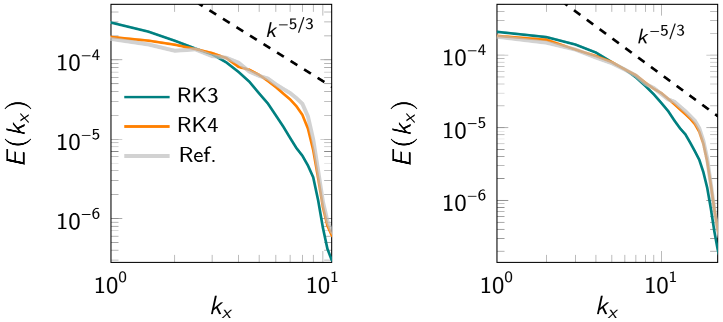
$$\boxed{\frac{\Delta E}{\Delta t} = \frac{1}{\mathrm{Re}}\varepsilon^{\mathrm{v}} + \varepsilon^{\mathrm{RK}} + \varepsilon^{\mathrm{SGS}}}$$



Large-eddy simulation of Taylor-Green vortex at $\mathrm{Re} = 1600$ on a 64^3 mesh using a fourth-order skew-symmetric scheme and the dynamic Smagorinsky model

Potential damages of time integration

Energy spectrum distortion in implicit large eddy simulation

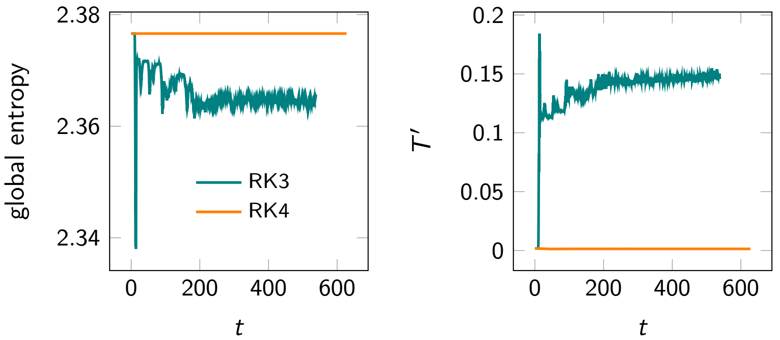


Time-averaged streamwise energy spectra of a turbulent channel flow at the centerline for $\mathrm{Re}_\tau = 180$ (left) and $\mathrm{Re}_\tau = 395$ (right) at CFL = 0.7. Implicit large-eddy simulation performed using a sixth-order skew-symmetric Padé scheme (Xcompact3d)

M. Artiano et al., Flow Turb. and Combust. **115**:389–403, 2025

Potential damages of time integration

Entropy drift in compressible flows



Inviscid compressible Taylor-Green vortex at $\mathrm{M} = 0.1$ on a 32^3 mesh using a second-order kinetic-energy and entropy-preserving scheme, using $\mathrm{CFL} = 0.8$; performed using the open-source code STREAmS

Courtesy of A. Aiello (Università degli Studi di Napoli Federico II)

Some pathways for improvement

1. Structure-preserving time integrators
2. Error control / adaptivity

Some pathways for improvement

1. Structure-preserving time integrators
2. Error control / adaptivity

- Semi-discrete Navier-Stokes equations:

$$\begin{cases} \dfrac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \mathbf{f}\left(t, \mathbf{u}(t)\right) \\ \mathbf{u}(t_0) = \mathbf{u}_0 \end{cases}$$

- The semi-discretized equations possess quantities η such that

$$\eta(\mathbf{u}^{n+1}) \leq \eta(\mathbf{u}^{n}) \text{ for a } \textit{dissipative} \text{ system}$$

$$\eta(\mathbf{u}^{n+1}) = \eta(\mathbf{u}_0) \text{ for a } \textit{conservative} \text{ system}$$

- Examples: inner products or *quadratic* invariants (e.g. kinetic energy, helicity for incompressible flow); entropy for compressible flow

- Semi-discrete Navier-Stokes equations:

$$\begin{cases} \dfrac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \mathbf{f}\left(t, \mathbf{u}(t)\right) \\ \mathbf{u}(t_0) = \mathbf{u}_0 \end{cases}$$

- The semi-discretized equations possess quantities η such that

$$\eta(\mathbf{u}^{n+1}) \leq \eta(\mathbf{u}^{n}) \text{ for a } \textit{dissipative} \text{ system}$$

$$\eta(\mathbf{u}^{n+1}) = \eta(\mathbf{u}_0) \text{ for a } \textit{conservative} \text{ system}$$

- Examples: inner products or *quadratic* invariants (e.g. kinetic energy, helicity for incompressible flow); entropy for compressible flow

- Semi-discrete Navier-Stokes equations:

$$\begin{cases} \dfrac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \mathbf{f}\left(t, \mathbf{u}(t)\right) \\ \mathbf{u}(t_0) = \mathbf{u}_0 \end{cases}$$

- The semi-discretized equations possess quantities η such that

$$\eta(\mathbf{u}^{n+1}) \leq \eta(\mathbf{u}^{n}) \text{ for a } \textit{dissipative} \text{ system}$$

$$\eta(\mathbf{u}^{n+1}) = \eta(\mathbf{u}_0) \text{ for a } \textit{conservative} \text{ system}$$

- Examples: inner products or *quadratic* invariants (e.g. kinetic energy, helicity for incompressible flow); entropy for compressible flow

- Time integration: only **Runge-Kutta (RK)** schemes preserve linear invariants and can potentially preserve quadratic ones

$$\begin{cases} \mathbf{u}_i = \mathbf{u}^n + \Delta t \sum_{j=1}^{s} a_{ij}\mathbf{f}_j, & i = 1, \dots, s \\ \mathbf{u}^{n+1} = \mathbf{u}^n + \Delta t \sum_{i=1}^{s} b_i\mathbf{f}_i, & \end{cases}$$

- If η is the *energy* of the system $\eta = E = \mathbf{u}^T\mathbf{u}$, its discrete evolution reads

$$\boxed{\frac{\Delta E}{\Delta t} = 2\sum_{i}^{s} b_i \mathbf{u}_i^T \mathbf{f}_i - \Delta t \sum_{i,j}^{s} \left(b_i a_{ij} + b_j a_{ji} - b_i b_j\right) \mathbf{f}_i^T \mathbf{f}_j}$$

- Only implicit schemes satisfy: $b_i a_{ij} + b_j a_{ji} - b_i b_j \stackrel{\text{def}}{=} g_{ij} = 0$
- Invariant-preserving and *symplectic* coincide for irreducible RK

Gauss ($p = 2$) Radau IIB ($p = 3$)

$$
\begin{array}{c|c}
\frac{1}{2} & \frac{1}{2} \\
\hline
 & 1
\end{array}
\qquad
\begin{array}{c|cc}
\frac{1}{3} & \frac{3}{8} & -\frac{1}{24} \\
1 & \frac{7}{8} & -\frac{1}{8} \\
\hline
 & \frac{3}{4} & \frac{1}{4}
\end{array}
$$

☺ Full space/time conservation: no dissipation and solutions *cannot blow up*!

☹ Difficult implementation and high computational cost

B. Sanderse. *J. Comput. Phys.* **233**: 100–131 (2013)

1. Expand temporal error in Taylor series

$$\frac{\Delta E}{\Delta t} = -\Delta t \sum_{i,j=1}^{s} g_{ij}\mathbf{f}_i^T\mathbf{f}_j \approx \Delta t C_2 \sum_{ij} g_{ij} + \Delta t^2 C_3 \sum_{ijk} g_{ij} a_{jk} + \\ + \Delta t^3 \left(C_{4,1} \sum_{ijkl} g_{ij} a_{ik} a_{kl} + C_{4,2} \sum_{ijkl} g_{ij} a_{ik} a_{jl} \right) + \dots$$

2. Get *pseudo-symplectic conditions* for conservation of E up to order q
3. Couple order and pseudo-symplectic conditions to get **explicit** schemes of order p that preserve energy to order q, with $q > p$
4. Solve the nonlinear system (when possible) to obtain RK coefficients

F. Capuano et al. *J. Comput. Phys.* **328**:86–94, 2017

Structure-preserving time integrators

Pseudo-symplectic methods - order conditions

q	Summation	Vector
1	$\sum_i b_i = 1$	$\mathbf{b}^T\mathbf{e} = 1$
2	$\sum_{ij} g_{ij} = 0$	$\mathbf{b}^T\mathbf{A}\mathbf{e} + \mathbf{b}^T\mathbf{c} = \mathbf{b}^T\mathbf{e}$
3	$\sum_{ijk} g_{ij}a_{jk} = 0$	$\mathbf{b}^T\mathbf{A}\mathbf{c} + \mathbf{b}^T\mathbf{c}^2 = \mathbf{b}^T\mathbf{c} = 0$
4	$\sum_{ijkl} g_{ij}a_{ik}a_{kl} = 0$	$\mathbf{b}^T\mathbf{A}^2\mathbf{c} + \mathbf{b}^T(\mathbf{c}.\mathbf{A}\mathbf{c}) = \mathbf{b}^T\mathbf{A}\mathbf{c}$
	$\sum_{ijkl} g_{ij}a_{ik}a_{jl} = 0$	$\mathbf{b}^T(\mathbf{c}.\mathbf{A}\mathbf{c}) = \frac{1}{2}\left(\mathbf{b}^T\mathbf{c}\right)^2$
5	$\sum_{ijklm} g_{ij}a_{jk}a_{kl}a_{lm} = 0$	$\mathbf{b}^T\mathbf{A}^3\mathbf{c} + \mathbf{b}^T\left(\mathbf{c}.\mathbf{A}^2\mathbf{c}\right) = \mathbf{b}^T\mathbf{A}^2\mathbf{c}$
	$\sum_{ijklm} g_{ij}a_{jk}a_{kl}a_{km} = 0$	$\mathbf{b}^T\mathbf{A}^2\mathbf{c}^2 + \mathbf{b}^T\left(\mathbf{c}.\mathbf{A}\mathbf{c}^2\right) = \mathbf{b}^T\mathbf{A}\mathbf{c}^2$
	$\sum_{ijklm} g_{ij}a_{jk}a_{kl}a_{jm} = 0$	$\mathbf{b}^T\mathbf{A}(\mathbf{c}.\mathbf{A}\mathbf{c}) + \mathbf{b}^T\left(\mathbf{c}^2.\mathbf{A}\mathbf{c}\right) = \mathbf{b}^T(\mathbf{c}.\mathbf{A}\mathbf{c})$
	$\sum_{ijklm} g_{ij}a_{jk}a_{kl}a_{im} = 0$	$\mathbf{b}^T\left(\mathbf{c}.\mathbf{A}^2\mathbf{c}\right) + \mathbf{b}^T(\mathbf{A}\mathbf{c})^2 = \left(\mathbf{b}^T\mathbf{c}\right)\left(\mathbf{b}^T\mathbf{A}\mathbf{c}\right)$
	$\sum_{ijklm} g_{ij}a_{ik}a_{jl}a_{jm} = 0$	$\mathbf{b}^T\left(\mathbf{c}.\mathbf{A}\mathbf{c}^2\right) + \mathbf{b}^T\left(\mathbf{c}^2.\mathbf{A}\mathbf{c}\right) = \left(\mathbf{b}^T\mathbf{c}^2\right)\left(\mathbf{b}^T\mathbf{c}\right)$

$$\mathbf{e} = (1,\dots,1) \in \mathbb{R}^s,\ \mathbf{b} = b_i, \mathbf{A} = a_{ij}, \mathbf{c} = \mathbf{A}\mathbf{e},\ g_{ij} = \left(b_i a_{ij} + b_j a_{ji} - b_i b_j\right)$$

Structure-preserving time integrators

Pseudo-symplectic methods - examples (1/2)

- Construction of a four-stage method with $p = 3$ and $q = 5$: 3p5q(4)

$$\left\{\begin{aligned} \mathbf{b}^T\mathbf{e} &= 1 \\ \mathbf{b}^T\mathbf{c} &= 1/2 \\ \mathbf{b}^T\mathbf{c}^2 &= 1/3 \\ \mathbf{b}^T\mathbf{A}\mathbf{c} &= 1/6 \end{aligned}\right. \quad \cap \quad \left\{\begin{aligned} \mathbf{b}^T\left(\mathbf{c}.\mathbf{A}\mathbf{c}\right) &= 1/8 \\ \mathbf{b}^T\left(\mathbf{A}\mathbf{c}\right)^2 &= 1/24 \\ \mathbf{b}^T\left(\mathbf{c}.\mathbf{A}\mathbf{c}^2\right) + \mathbf{b}^T\left(\mathbf{c}^2.\mathbf{A}\mathbf{c}\right) &= 1/6 \\ \mathbf{b}^T\mathbf{A}^2\mathbf{c} &= 1/24 \\ \mathbf{b}^T\left(\mathbf{c}.\mathbf{A}^2\mathbf{c}\right) &= 1/24 \end{aligned}\right.$$

- Solution of the nonlinear system

$$\begin{array}{c|cccc}
0 & 0 & & & \\
\dfrac{c_3-1}{4c_3-3} & \dfrac{c_3-1}{4c_3-3} & 0 & & \\
c_3 & c_3 - \dfrac{(2c_3-1)(4c_3-3)}{2(c_3-1)} & \dfrac{(2c_3-1)(4c_3-3)}{2(c_3-1)} & 0 & \\
1 & -\dfrac{(2c_3-1)^2}{2(c_3-1)(4c_3-3)} & \dfrac{6c_3^2-8c_3+3}{2(c_3-1)(2c_3-1)} & \dfrac{c_3-1}{(2c_3-1)(4c_3-3)} & 0 \\
\hline
 & -\dfrac{1}{12(c_3-1)} & \dfrac{(4c_3-3)^2}{12(c_3-1)(2c_3-1)} & -\dfrac{1}{12(c_3-1)(2c_3-1)} & \dfrac{4c_3-3}{12(c_3-1)}
\end{array}$$

Structure-preserving time integrators

Pseudo-symplectic methods - examples (2/2)

- $3p6q(5)$

$$
\begin{array}{ccc}
a_{21} = 0.13502027922909 & a_{31} = -0.47268213605237 & a_{32} = 1.05980250415419 \\
a_{41} = -1.21650460595689 & a_{42} = 2.16217630216753 & a_{43} = -0.37234592426536 \\
a_{51} = 0.33274443036387 & a_{52} = -0.20882668296587 & a_{53} = 1.87865617737921 \\
a_{54} = -1.00257392477721 & b_1 = 0.04113894457092 & b_2 = 0.26732123194414 \\
b_3 = 0.86700906289955 & b_4 = -0.30547139552036 & b_5 = 0.13000215610576
\end{array}
$$

- $4p7q(6)$

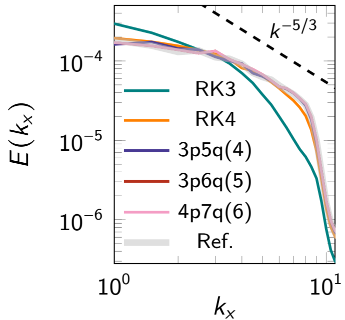
$$
\begin{array}{ccc}
a_{21} = 0.23593376536652 & a_{31} = 0.34750735658424 & a_{32} = -0.13561935398346 \\
a_{41} = -0.20592852403227 & a_{42} = 1.89179076622108 & a_{43} = -0.89775024478958 \\
a_{51} = -0.09435493281455 & a_{52} = 1.75617141223762 & a_{53} = -0.96707850476948 \\
a_{54} = 0.06932825997989 & a_{61} = 0.14157883255197 & a_{62} = -1.17039696277833 \\
a_{63} = 1.30579112376331 & a_{64} = -2.20354136855289 & a_{65} = 2.926568375015948 \\
b_{1,6} = 0.07078941627598 & b_{2,5} = 0.87808570611881 & b_{3,4} = -0.44887512239479
\end{array}
$$

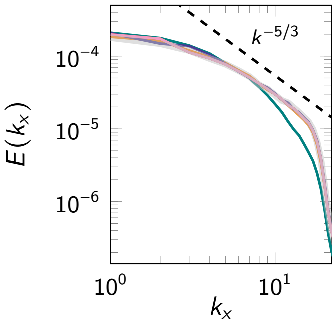
F. Aubry and P. Chartier *BIT* **38**:439–461, 1998

F. Capuano et al. *JCP* **328**:86–94, 2017

Structure-preserving time integrators

Numerical results (1)

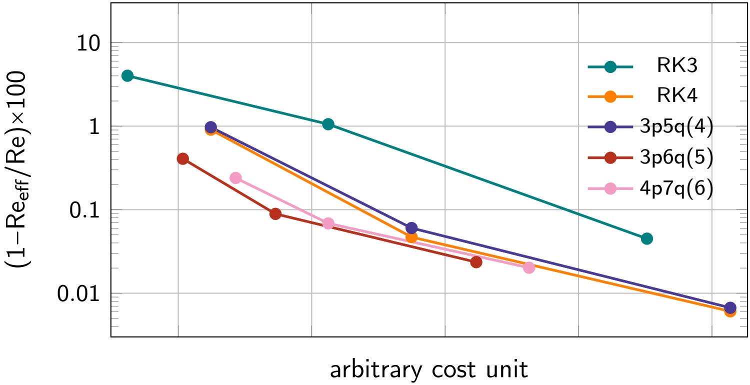




Time-averaged streamwise energy spectra of a turbulent channel flow at the centerline for $Re_\tau = 180$ (left) and $Re_\tau = 395$ (right) at CFL $= 0.7$. Implicit large-eddy simulation performed using the open-source code Xcompact3d

Structure-preserving time integrators

Numerical results (2)



Accuracy Vs. cost for $Re_\tau = 180$ (left). Implicit large-eddy simulation performed using the open-source code Xcompact3d

- Kinetic energy in compressible flows is a cubic quantity: no RK preservation

$$\rho k = \frac{(\rho u_i)^2}{\rho}$$

- Previous attempts based on *square-root* formulation

$$\mathbf{u} = \begin{bmatrix} \sqrt{\rho} \\ \sqrt{\rho}\boldsymbol{u}/\sqrt{2} \\ \sqrt{\rho e} \end{bmatrix}$$

- Kinetic energy becomes a quadratic quantity!

A. Iserles and A. Zanna. *JCAM* **125**:69–81, 2000
W. Rozema et al. *J. Turbul.* **15**:386–410, 2014

Structure-preserving time integrators

Beyond quadratic invariants: relaxation RK (RRK)

- For general convex quantities (e.g., entropy): no way!
- Introduction of a relaxation factor at the last RK step

$$\begin{cases} \mathbf{u}_i = \mathbf{u}^n + \Delta t \sum_{j=1}^{s} a_{ij}\mathbf{f}_j, \quad i = 1, \dots, s \\ \mathbf{u}_\gamma^{n+1} = \mathbf{u}^n + \gamma_n \Delta t \sum_{i=1}^{s} b_i \mathbf{f}_i \end{cases}$$

- Find γ_n as a root of:

$$r(\gamma) = \eta(\mathbf{u}_\gamma^{n+1}) - \eta(\mathbf{u}^n) - \gamma \Delta t \sum_{i=1}^{s} b_i \boldsymbol{\eta}'^T \mathbf{f}$$

- For quadratic invariants, γ_n has a closed form expression

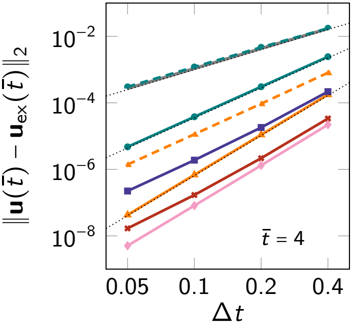
$$\gamma_n = \frac{2 \sum_{i,j=1}^{s} b_i a_{ij} \mathbf{f}_i^T \mathbf{f}_j}{\sum_{i,j=1}^{s} b_i b_j \mathbf{f}_i^T \mathbf{f}_j}$$

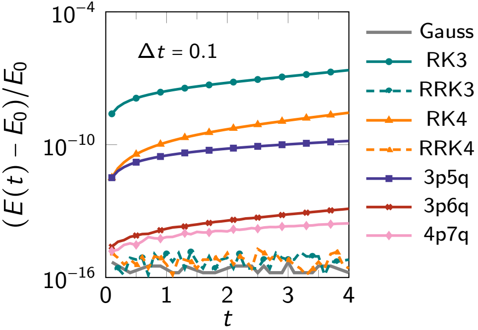
D. Ketcheson *SIAM JNA* **57**:2850–2870, 2019

H. Ranocha et al. *SIAM J. Sci. Comput.* **42**:A612–A638, 2020

Structure-preserving time integrators

Numerical results (3)





Error on solution (left) and on energy conservation (right) for an inviscid double mixing layer on a 20^2 mesh, using a second-order centred scheme for spatial discretization. The three dotted lines on the left denote the Δt^2, Δt^3 and Δt^4 trends

Some pathways for improvement

1. Structure-preserving time integrators
2. Error control / adaptivity

- Most common: CFL-based control (stability-driven)
- Less common: error-based control (accuracy-driven), e.g., embedded RK
- **Idea**: entropy-preserving adaptive time stepping

$$\boxed{\frac{\Delta\eta}{\Delta t} = \varepsilon^{\mathsf{v}} + \varepsilon^{\mathsf{SGS}} + \varepsilon^{\mathsf{RK}}}$$

- Adapt time step to ensure conservation through a proportional controller

$$\xi = \left|\frac{\varepsilon^{\mathsf{RK}}}{\varepsilon^{\mathsf{v}} + \varepsilon^{\mathsf{SGS}}}\right| < \delta^E \quad \rightarrow \quad \Delta t^{n+1} = \Delta t^n \left|\frac{\delta^E}{\xi^{n+1}}\right|^{1/q}$$

F. Capuano et al. AIMETA Proceedings, pp. 2311-2323, 2017
A. Aiello et al., in preparation

- Most common: CFL-based control (stability-driven)
- Less common: error-based control (accuracy-driven), e.g., embedded RK
- **Idea**: entropy-preserving adaptive time stepping

$$\boxed{\frac{\Delta\eta}{\Delta t} = \varepsilon^{\mathrm{v}} + \varepsilon^{\mathrm{SGS}} + \varepsilon^{\mathrm{RK}}}$$

- Adapt time step to ensure conservation through a proportional controller

$$\xi = \left|\frac{\varepsilon^{\mathrm{RK}}}{\varepsilon^{\mathrm{v}} + \varepsilon^{\mathrm{SGS}}}\right| < \delta^{E} \quad \rightarrow \quad \Delta t^{n+1} = \Delta t^{n}\left|\frac{\delta^{E}}{\xi^{n+1}}\right|^{1/q}$$

F. Capuano et al. AIMETA Proceedings, pp. 2311-2323, 2017

A. Aiello et al., in preparation

Error control / adaptivity

Entropy-preserving adaptive time stepping

- Most common: CFL-based control (stability-driven)
- Less common: error-based control (accuracy-driven), e.g., embedded RK
- **Idea**: entropy-preserving adaptive time stepping

$$\boxed{\frac{\Delta\eta}{\Delta t} = \varepsilon^{\mathsf{v}} + \varepsilon^{\mathsf{SGS}} + \varepsilon^{\mathsf{RK}}}$$

- Adapt time step to ensure conservation through a proportional controller

$$\xi = \left| \frac{\varepsilon^{\mathsf{RK}}}{\varepsilon^{\mathsf{v}} + \varepsilon^{\mathsf{SGS}}} \right| < \delta^{E} \quad \rightarrow \quad \Delta t^{n+1} = \Delta t^{n} \left| \frac{\delta^{E}}{\xi^{n+1}} \right|^{1/q}$$

F. Capuano et al. AIMETA Proceedings, pp. 2311-2323, 2017

A. Aiello et al., in preparation

Error control / adaptivity

Entropy-preserving adaptive time stepping

- Most common: CFL-based control (stability-driven)
- Less common: error-based control (accuracy-driven), e.g., embedded RK
- **Idea**: entropy-preserving adaptive time stepping

$$\boxed{\frac{\Delta\eta}{\Delta t} = \varepsilon^{\mathrm{v}} + \varepsilon^{\mathrm{SGS}} + \varepsilon^{\mathrm{RK}}}$$

- Adapt time step to ensure conservation through a proportional controller

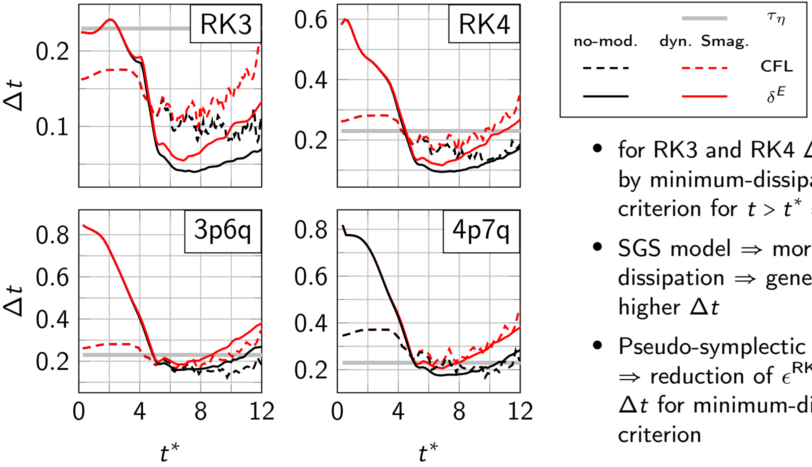
$$\xi = \left| \frac{\varepsilon^{\mathrm{RK}}}{\varepsilon^{\mathrm{v}} + \varepsilon^{\mathrm{SGS}}} \right| < \delta^{E} \quad \rightarrow \quad \Delta t^{n+1} = \Delta t^{n} \left| \frac{\delta^{E}}{\xi^{n+1}} \right|^{1/q}$$

F. Capuano et al. AIMETA Proceedings, pp. 2311-2323, 2017

A. Aiello et al., in preparation

Error control / adaptivity

Entropy-preserving adaptive time stepping



- for RK3 and RK4 Δt dictated by minimum-dissipation criterion for $t > t^* \approx 5$
- SGS model $\Rightarrow$ more dissipation $\Rightarrow$ generally higher Δt
- Pseudo-symplectic schemes $\Rightarrow$ reduction of ϵ^{RK} $\Rightarrow$ higher Δt for minimum-dissipation criterion

Incompressible Taylor-Green Vortex at Re = 1600 on a 64^3 mesh, using a second-order skew-symmetric scheme for spatial discretization

F. Capuano et al. AIMETA Proceedings, pp. 2311-2323, 2017

Conclusions

Lessons learnt

- Low-order time integrators operated at moderate-to-high CFL numbers **can introduce non-negligible temporal errors**, even when spatial discretization is highly accurate
- Temporal errors may interact non-trivially with LES modeling, effectively acting as **an *implicit* subgrid-scale contribution** whose impact is rarely quantified or controlled
- **Structure-preserving time integration can be more efficient overall**, as improved stability and long-time behavior may offset the higher per-step cost
- Accuracy-driven adaptivity in time offers a promising route to improved fidelity, **but remains largely underexploited in CFD practice**

Conclusions

Some questions for the community

- Should time integration be co-designed with spatial discretization, rather than treated as a modular, interchangeable component?
- Do scale-resolving simulations require structure-preserving time integrators, or are current practices sufficient in most practical LES settings?
- Are we benchmarking the right quantities, or are important temporal effects hidden by commonly used diagnostics?
- What is the practical impact of entropy drift and invariant violation in long-time under-resolved simulations?
- Is accuracy-driven time adaptivity underused in CFD, and if so, what are the real barriers to its adoption?