Energy conserving time integration methods for the incompressible Navier-Stokes equations

B. Sanderse

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Introduction

• Accurate and efficient numerical simulation of turbulence with Large Eddy Simulation

• Requirements for discretization:
  • low numerical diffusion
  • high order spatial discretization
  • stable long-term integration

• Energy conserving discretizations\(^1\):
  • Correctly capture the turbulence energy spectrum and cascade
  • Non-linear stability bound

Discretization of fluid flows

The incompressible Navier-Stokes equations describe fluid flow:

\[ \nabla \cdot \mathbf{u} = 0, \]
\[
\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \nu \nabla^2 \mathbf{u}. \]

To compute flows of practical interest, we need:

- A numerical approximation to the NS equations
- A turbulence model
Energy properties of incompressible NS

The incompressible Navier-Stokes equations:

\[
\begin{align*}
\nabla \cdot \mathbf{u} &= 0, \\
\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} &= -\nabla p + \nu \nabla^2 \mathbf{u}.
\end{align*}
\]

possess a number of mathematical properties, e.g.

- The convective operator is skew-symmetric
- The diffusive operator is symmetric
- The divergence and gradient operator are related
Energy properties of incompressible NS

• In inviscid flow energy is an invariant:

\[
\frac{dk}{dt} = -\nu(\nabla u, \nabla u) \leq 0, \quad k = \frac{1}{2}\|u\|^2
\]

• The NS equations are then time-reversible

• Time-reversibility has been proposed as test for energy conservation\(^1\)

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1: Duponcheel et al. (2008), Time reversibility of the Euler equations as benchmark for energy conserving schemes, JCP
Spatial discretization

- Finite volume method on staggered Cartesian grid
- Exact conservation of mass
- Compatible divergence and gradient operator, no pressure-velocity decoupling
- Skew-symmetric convective operator
- Energy is conserved: a stable discretization on any grid!

- Fourth order accuracy: Verstappen & Veldman, JCP 2003
Spatial discretization

- Method of lines gives non-autonomous semi-discrete DAE system of index 2:

\[ \Omega \frac{du}{dt} + C(u, u) - \nu Du + Gp = g_2(t) \]

\[ Mu = g_1(t) \]

\[ 0 = g(y, t) \]

\[ y' = f(y, z, t) \]

- Continuous properties are mimicked in a discrete sense:

\[ (Gp, u) = -(Mu, p) \]

\[ (C(u, v), w) = -(v, C(u, w)) \quad \rightarrow \quad (C(u, u), u) = 0 \]
Temporal discretization

• Current practice: multistep or multistage methods with pressure correction and explicit convection
• Not energy conserving, not time-reversible

• Research questions:
  • Energy conservation and/or time reversibility with Runge-Kutta methods?
  • Order reduction when applying Runge-Kutta methods to the incompressible NS equations?
  • Can implicit methods be more efficient than explicit methods?
Runge-Kutta methods

• General implicit/explicit Runge-Kutta method:

\[ U_i = u^n + \Delta t \sum_{j=1}^{s} a_{ij} F(U_j, p_j, t_j) \quad u^{n+1} = u^n + \Delta t \sum_{i=1}^{s} b_i F(U_i, p_i, t_i) \]

\[ MU_i = g_1(t_i) \quad M u^{n+1} = g_1(t^{n+1}) \]

• supplemented with consistent initial conditions:

\[ Mu^0 = g_1(t^0) \]

\[ Lp^0 = M(-C(u^0) + \nu Du^0 + g_2(t^0)) - \dot{g}_1(t^0) \]

where \( L = MG \) is the Laplacian; \( L^{-1} \) should be bounded.
Explicit methods

• In literature there is confusion on how to handle the pressure
• The theory on DAEs gives a guideline: half-explicit methods
• Equations for the stages:

\[ U_i = u^n + \Delta t \sum_{j=1}^{i-1} a_{ij} F(U_j, p_j, t_j) \]

\[ MU_i = g_1(t_i) \]

\[ F(U_i, p_i, t_i) = -C(U_i) + \nu DU_i - Gp_i + g_2(t_i) \]

\[ \tilde{F}(U_i, t_i) = -C(U_i) + \nu DU_i + g_2(t_i) \]

1: Hairer et al. (1989), The numerical solution of differential-algebraic systems by Runge-Kutta methods
Explicit methods

• Poisson equation for the pressure:

\[ a_{i+1,i} \Delta t L p_i = M \left( u^n + \Delta t \sum_{j=1}^{i-1} a_{i+1,j} F(U_j, p_j, t_j) + \Delta t a_{i+1,i} \tilde{F}(U_i, t_i) \right) - g_1(t_{i+1}) \]

\[ L p_i = M \tilde{F}(U_i, t_i) - \sum_{j=1}^{i} f(A) \frac{g_1(t_{i+1}) - g_1(t^n)}{\Delta t} \quad 1 \leq i \leq s \]

• Similar to pressure correction
• Butcher array and \( \Delta t \) only appear for unsteady BCs
Explicit methods

- Example: classical RK4

\[ L_{p1} = M \tilde{F}_1 - \frac{g_1(t^{n+1/2}) - g_1(t^n)}{\frac{1}{2} \Delta t} \]
\[ L_{p2} = M \tilde{F}_2 - \frac{g_1(t^{n+1/2}) - g_1(t^n)}{\frac{1}{2} \Delta t} \]
\[ L_{p3} = M \tilde{F}_3 - \frac{g_1(t^{n+1/2}) - g_1(t^n)}{\Delta t} \]
\[ L_{p4} = M \tilde{F}_4 - 4 \frac{g_1(t^{n+1}) - g_1(t^n)}{\Delta t} + 3 \frac{g_1(t^{n+1/2}) - g_1(t^n)}{\frac{1}{2} \Delta t} \]
Explicit methods

• No equation for $p^{n+1}$; $p_s$ is not of the expected order
• Higher order accurate with additional Poisson equation:

$$Lp^{n+1} = M\tilde{F}^{n+1} - \dot{g}_1(t^{n+1})$$

• This does not increase computational costs: solution of $p^{n+1}$ is the same as $p_1$.

• $p^{n+1}$ does not influence $u^{n+1}$ and can be computed as post-processing step
Implicit Runge-Kutta methods

- Recall the general form:

\[
U_i = u^n + \Delta t \sum_{j=1}^{s} a_{ij} F(U_j, p_j, t_j)
\]

\[
MU_i = g_1(t_i)
\]

\[
u^{n+1} = u^n + \Delta t \sum_{i=1}^{s} b_i F(U_i, p_i, t_i)
\]

\[
Mu^{n+1} = g_1(t^{n+1})
\]
Implicit Runge-Kutta methods

- **Energy conservation** (periodic BC, $\nu = 0$):

\[
(u^{n+1}, u^{n+1}) = (u^n, u^n) + 2\Delta t \sum_{i=1}^{s} b_i (F_i, U_i) + \ldots
\]

\[
\Delta t^2 \sum_{i,j=1}^{s} m_{ij} (F_i, F_j).
\]

- $$(F_i, U_i) = 0 : MU_i = 0, \quad (C(U_i, U_i), U_i) = 0, \quad M = -G^*$$
- $$m_{ij} = b_i b_j - b_i a_{ij} - b_j a_{ji} : \quad m_{ij} = -m_{ji}$$
Implicit Runge-Kutta methods

- Time reversibility
  \[ u^{n+c_i} \rightarrow -u^{n+1-c_i} \]
- Conditions for coefficients:
  \[ a_{ij} + a_{s+1-i,s+1-j} = b_j, \]
  \[ b_i = b_{s+1-i}, \]
  \[ c_i = 1 - c_{s+1-i} \]
- Time reversibility and energy conservation conditions are satisfied by **Gauss methods**
Implicit Runge-Kutta methods: Gauss

- Butcher tableaus:

\[
\begin{array}{c|c}
\frac{1}{2} & \frac{1}{2} \\
\hline
\frac{1}{2} & 1
\end{array}
\]

(a) \( s = 1 \)

\[
\begin{array}{c|c|c}
\frac{1}{2} - \frac{\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4} - \frac{\sqrt{3}}{6} \\
\hline
\frac{1}{2} + \frac{\sqrt{3}}{6} & \frac{1}{4} + \frac{\sqrt{3}}{6} & \frac{1}{2}
\end{array}
\]

(b) \( s = 2 \)

- \( m_{ij} = 0 \): algebraic stability

- Convergence order\(^1\):

| \( s \) odd | ODE | \( s + 1 \) | DAE \( p \) |
| \( s \) even | \( 2s \) | \( s - 2 \) |
| \( s \) odd | \( 2s \) | \( s - 1 \) |

\(^1\): Hairer et al. (1989), The numerical solution of differential-algebraic systems by Runge-Kutta methods
Implicit Runge-Kutta methods

- Solution of non-linear system with Newton linearization

\[
\begin{bmatrix}
I + a_{11} \Delta t J(U_1) & G \\
\frac{\Delta F_1}{a_{11} \Delta t M} & 0
\end{bmatrix}
\begin{bmatrix}
\Delta F_1 \\
\Delta p_1
\end{bmatrix} = R
\]

\[
\begin{bmatrix}
I + a_{11} \Delta t J(U_1) & a_{12} \Delta t J(U_1) & G & 0 \\
a_{21} \Delta t J(U_2) & I + a_{22} \Delta t J(U_2) & 0 & G \\
a_{11} \Delta t M & a_{12} \Delta t M & 0 & 0 \\
a_{21} \Delta t M & a_{22} \Delta t M & 0 & 0
\end{bmatrix}
\begin{bmatrix}
\Delta F_1 \\
\Delta F_2 \\
\Delta p_1 \\
\Delta p_2
\end{bmatrix} = R
\]
Implicit Runge-Kutta methods

• For general \( g_1(t) \) there is no guarantee that \( M u^{n+1} = g_1(t^{n+1}) \)
• Additional projection\(^1\):

\[
\hat{u}^{n+1} = u^n + \Delta t \sum_{i=1}^{s} b_i F_i
\]

\[
u^{n+1} = \hat{u}^{n+1} - G\phi
\]

\[
L\phi = M\hat{u}^{n+1} - g_1(t^{n+1})
\]

• Alternative:
Stiffly accurate RK methods: \( a_{si} = b_i, c_s = 1 \), e.g. Radau IIA or Lobatto IIIA/C methods, not energy conserving

Implicit Runge-Kutta methods

- Pressure can be solved as for explicit methods

- Alternatively:

\[ p_i = p^n + \Delta t \sum_{j=1}^{s} a_{ij} Z_j \]

\[ Z_i = \frac{1}{\Delta t} \sum_{j=1}^{s} \omega_{ij} (p_j - p_n) \]

\[ p^{n+1} = p^n + \Delta t \sum_{i=1}^{s} b_i Z_i \]

- Order reduction expected
Implicit Runge-Kutta methods - PC

- Sacrificing energy conservation: pressure correction
- Provisional velocity:

\[
\frac{u^* - u^n}{\Delta t} = \tilde{F}(\frac{u^n + u^*}{2}) - Gp^n
\]

- Pressure solve:

\[
\frac{1}{2}L\Delta p = \frac{1}{\Delta t}(Mu^* - g_1(t^{n+1}))
\]

- Velocity update:

\[
\frac{u^{n+1} - u^*}{\Delta t} = -\frac{1}{2}G\Delta p
\]
Implicit Runge-Kutta methods - PC

- An energy error is introduced since $M u^* \neq g_1(t^{n+1})$
- The scheme remains unconditionally stable, but only in a linear sense

$$\| u^{n+1} \|^2 + \frac{\Delta t^2}{8} \| Gp^{n+1} \|^2 \leq \| u^n \|^2 + \frac{\Delta t^2}{8} \| Gp^n \|^2.$$

- Time reversibility is unaffected

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Implicit Runge-Kutta methods - linear

- Sacrificing time-reversibility: *extrapolated convecting velocity*

- \((C(u, u), u) = 0\): independent of the time level of the convecting velocity

- First order: \(C(u^n, u^{n+1/2})\)

- Second order: \(C\left(\frac{3}{2}u^n - \frac{1}{2}u^{n-1}, u^{n+1/2}\right)\)

- Still unconditionally stable

- **Linear** system

- Not time reversible
Summary

- Energy conservation and time reversibility

<table>
<thead>
<tr>
<th>Energy conserving</th>
<th>Time reversible</th>
</tr>
</thead>
<tbody>
<tr>
<td>y</td>
<td>n</td>
</tr>
<tr>
<td>IRK</td>
<td>IRK - linear (ERK-cons)</td>
</tr>
</tbody>
</table>

- Computational cost

<table>
<thead>
<tr>
<th>Method</th>
<th>Nonlinear SP</th>
<th>Linear SP</th>
<th>Nonlinear</th>
<th>Laplace</th>
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<tbody>
<tr>
<td>ERK s</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>s</td>
</tr>
<tr>
<td>IRK - steady BC</td>
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<td>0</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>IRK - unsteady BC</td>
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<td>0</td>
<td>0</td>
<td>2</td>
</tr>
<tr>
<td>IRK - linear</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>2</td>
</tr>
<tr>
<td>IRK - PC</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>2</td>
</tr>
</tbody>
</table>
Summary

Table 4: Overview of energy conservation and time reversibility.

(a) ERK2
(b) ERK4
(c) IRK2
(d) IRK4

Figure 1: Stability regions.
Results

- Taylor vortex: Order of accuracy
- Shear-layer roll-up: Energy conservation and time reversibility
- Corner flow: Order of accuracy and efficiency
Taylor vortex

- Analytical solution on a domain of \([\frac{1}{4}, 2\frac{1}{4}] \times [\frac{1}{4}, 2\frac{1}{4}]\)

\[
\begin{align*}
  u(x, y, t) &= -\sin(\pi x) \cos(\pi y) e^{-2\pi^2 \nu t}, \\
  v(x, y, t) &= \cos(\pi x) \sin(\pi y) e^{-2\pi^2 \nu t}, \\
  p(x, y, t) &= \frac{1}{4}(\cos(2\pi x) + \cos(2\pi y)) e^{-4\pi^2 \nu t}
\end{align*}
\]

- Boundary conditions: periodic or unsteady Dirichlet

- Temporal error evaluated at \(t = 1\)
Taylor vortex; velocity field
Taylor vortex; periodic BC

\[ \nu = \frac{1}{100} \]

20x20 volumes

Energy error
Taylor vortex; periodic BC

\[ \nu = \frac{1}{100} \]

20x20 volumes

Pressure error
Taylor vortex; Dirichlet BC

\[ \nu = \frac{1}{100} \]

20x20 volumes

Energy error

\[ \epsilon \]
Taylor vortex; Dirichlet BC

\[ \nu = \frac{1}{100} \]

20x20 volumes

Pressure error
Shear-layer roll-up

• Analytical solution on a domain of \([0, 2\pi] \times [0, 2\pi]\)

\[
\begin{aligned}
u &= \begin{cases} 
\tanh \left( \frac{y-\pi/2}{\delta} \right) & y \leq \pi, \\
\tanh \left( \frac{3\pi/2-y}{\delta} \right) & y > \pi,
\end{cases} \\
v &= \varepsilon \sin(x), \\
p &= 0.
\end{aligned}
\]

• Boundary conditions: periodic

• Inviscid: \(\nu = 0\)

• Time reversal at \(t = 8\)
Shear-layer roll-up; time reversibility

- Implicit midpoint
- 100x100 volumes
- $\Delta t = 0.05$
Shear-layer roll-up; energy conservation
Shear-layer roll-up; energy conservation

\[ \Delta t \]

\[ \epsilon_k \]

IRK2 - PC
Shear-layer roll-up; time reversibility

- Implicit midpoint
- 10x10 volumes
- $\Delta t = 1$
Shear-layer roll-up; time reversibility

- Explicit RK 4
- 100x100 volumes
- $\Delta t = 0.05$
Shear-layer roll-up; energy conservation

\[
\Delta t \quad \epsilon_k
\]

\[
\times 10^{-7}
\]

ERK4
Shear-layer roll-up; time reversibility

- 2nd order Adams-Bashforth
- $\Delta t = 0.05$
- 100x100 volumes
Shear-layer roll-up; energy conservation

32x32 volumes

$t = 4$
Corner flow

- ‘stiff’ problem; boundary layers, $\nu = 1/10$
- domain $[0, 1] \times [0, 1]$
- 20x20 volumes
- simulation until $t = 1$

$$u = 0, v = -\sin(\pi(x^3 - 3x^2 + 3x))e^{1-1/t}$$

$$-p + \nu \frac{\partial u}{\partial x} = 0$$

$$\frac{\partial v}{\partial x} = 0$$
Corner flow
Corner flow

\[\epsilon_k \quad \Delta t\]

- IRK2
- IRK2-linear
- IRK2-PC
- AB-CN
Corner flow

\[ \Delta t \epsilon_k \]

- IRK4
- IRK4 - no projection
Corner flow

![Graph showing Corner flow](image)

- ERK2
- IRK2
- IRK2-linear
- IRK2-PC
- AB-CN
- ERK4
- IRK4
- IRK4-no projection

$\Delta t \epsilon_k$

Energy research Centre of the Netherlands  www.ecn.nl
Corner flow: computational time
Conclusions

• Time-reversible and energy conserving integration of the NS equations can be achieved with Gauss methods.

• Order reduction is observed for unsteady boundary conditions only, and can be cured with an extra projection step. Both the differential and algebraic variable obtain the classical order.

• Cheaper methods can be constructed by linearizing or splitting, leading to loss of time-reversibility or energy conservation properties.

• Optimization of matrix solvers and investigation of turbulent flow will shed more light on the usefulness of these properties.