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Time-adaptive methods for the incompressible Navier-Stokes equations

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Contents

- Introduction
- Diagonally implicit Runge–Kutta methods
- Results with OpenFOAM
- Summary and Outlook

Semi-Discretisation in space

- Discretise incompressible Navier–Stokes equations in space with Finite differences, volumes or elements.
- MOL-DAE:**

$$\begin{pmatrix} M & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \dot{\mathbf{u}} \\ \dot{\mathbf{p}} \end{pmatrix} = \begin{pmatrix} \mathbf{f} \\ 0 \end{pmatrix} - \begin{pmatrix} A(\mathbf{u}) & B \\ B^\top & 0 \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{p} \end{pmatrix}$$

with M ... mass matrix (regular) and A stiffness matrix

- Assumption:** $B^\top M^{-1} B$ is regular
- Then:** MOL-DAE has differentiation index 2.

Initial pressure

Semi-discretised problem:

$$M\dot{\mathbf{u}} = \mathbf{f} - A(\mathbf{u})\mathbf{u} - B\mathbf{p}$$

$$B^T \mathbf{u} = 0$$

Differentiation: $B^T \dot{\mathbf{u}} = 0$

It follows

$$B^T \dot{\mathbf{u}} = B^T M^{-1}(\mathbf{f} - A(\mathbf{u})\mathbf{u} - B\mathbf{p}) = 0$$

and for $\mathbf{u} = \mathbf{u}_0$ and $\mathbf{p} = \mathbf{p}_0$

$$B^T M^{-1}(\mathbf{f} - A(\mathbf{u}_0)\mathbf{u}_0) = B^T M^{-1} B\mathbf{p}_0$$

Properties

- problems to be solved: stiff ODEs, PDEs, DAEs
- sufficiently high order
- no order reduction for the Prothero–Robinson example
- good stability properties (at least strongly A-stable)
- adaptive timestep control without further computations
- “low” costs for the linear algebra

Examples:

- Diagonally implicit Runge–Kutta methods (special cases: Euler, CN, FS)
- linear implicit Runge–Kutta methods (Rosenbrock–Wanner methods)
- fully implicit Runge–Kutta methods with a regular coefficient matrix (for example Radau-IIA methods)

Motivating example

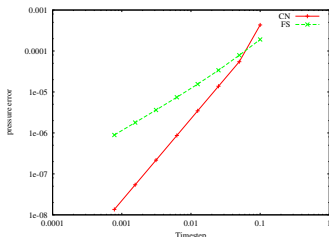
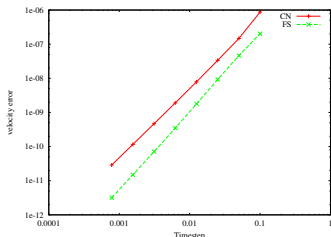
Let $T = 1$, $\Omega = (0, 1)^2$ and $Re = 1$.

Exact solution of NSE:

$$u_1(t, x, y) = (y^2 + x) \sin t, \quad u_2(t, x, y) = (x^2 - y) \sin t,$$

$$p(t, x, y) = e^{-t}(x + y - 1).$$

$\tau = \frac{1}{10 \cdot 2^N}$ with $N = 0, 1, \dots, 8$

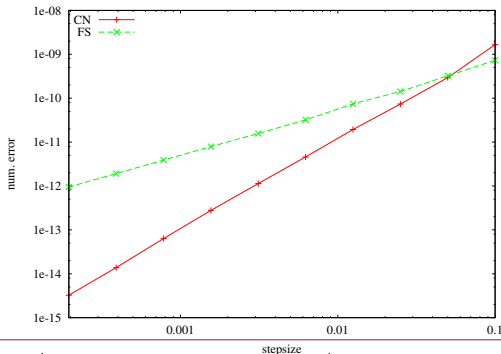


Example of Prothero and Robinson

$$\dot{u} = \lambda(u(t) - \varphi(t)) + \dot{\varphi}(t), \quad u(0) = \varphi(0), \quad \lambda = -10^6, t \in (0, 1/10)$$

with

$$\varphi(t) = \sin\left(t + \frac{\pi}{4}\right).$$



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- Introduction
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- Summary and Outlook

Runge-Kutta-methods

$$M\dot{\mathbf{u}} = \mathbf{F}(t, \mathbf{u}), \quad \mathbf{u}(0) = \mathbf{u}_0, \quad (1)$$

M ... mass-matrix. Let $s \in \mathbb{N}$. The one-step-method

$$M\mathbf{k}_i = \mathbf{F} \left(t_m + c_i\tau, \mathbf{u}_m + \tau \sum_{j=1}^s a_{ij}\mathbf{k}_j \right)$$

$$\mathbf{u}_{m+1} = \mathbf{u}_m + \tau \sum_{i=1}^s b_i\mathbf{k}_i$$

is called **s-stage Runge-Kutta-method** (RK-method).

- a_{ij} , b_i and c_i ... coefficients of the method
- **one nonlinear system of dimension ns**

Adaptive timestep control

- 1. RK method (order p):

$$\mathbf{u}_{m+1} = \mathbf{u}_m + \tau \sum_{i=1}^s b_i \mathbf{k}_i$$

- 2. RK method (order $p - 1$):

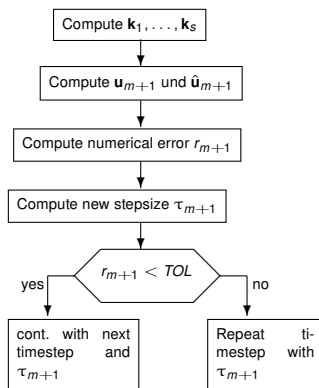
$$\hat{\mathbf{u}}_{m+1} = \mathbf{u}_m + \tau \sum_{i=1}^s \hat{b}_i \mathbf{k}_i$$

- TOL ... given tolerance

- PI-controller:

$$\tau_{m+1} = \rho \frac{\tau_m^2}{\tau_{m-1}} \left(\frac{TOL \cdot r_m}{r_{m+1}^2} \right)^{1/p}, \text{ with}$$

$$r_m = \|\mathbf{u}_m - \hat{\mathbf{u}}_m\|$$



Simplifying conditions

$$B(p) : \quad \sum_{i=1}^s b_i c_i^{k-1} = 1/k \quad k = 1, \dots, p,$$

$$C(q) : \quad \sum_{j=1}^s a_{ij} c_j^{k-1} = c_i^k / k \quad i = 1, \dots, s, k = 1, \dots, q,$$

$$D(r) : \quad \sum_{i=1}^s b_i c_i^{k-1} a_{ij} = b_j (1 - c_j^k) / k \quad j = 1, \dots, s, k = 1, \dots, r.$$

An RK-method with s internal stages has convergence order p , if the simplifying conditions $B(p)$, $C(l)$, and $D(m)$ with

$$p \leq \min\{l + m + 1, 2l + 2\}$$

are satisfied.

DIRK methods

diagonally implicit Runge–Kutta (DIRK) method: $a_{ij} = 0$ for $i < j$ and $a_{ii} \neq 0$ for $i = 2, \dots, s$

Advantage: "only" s nonlinear system of dimension n instead of one nonlinear system of dimension ns

But:

- DIRK method with $a_{11} \neq 0$: maximal stage order 1
- DIRK method with $a_{11} = 0$: maximal stage order 2

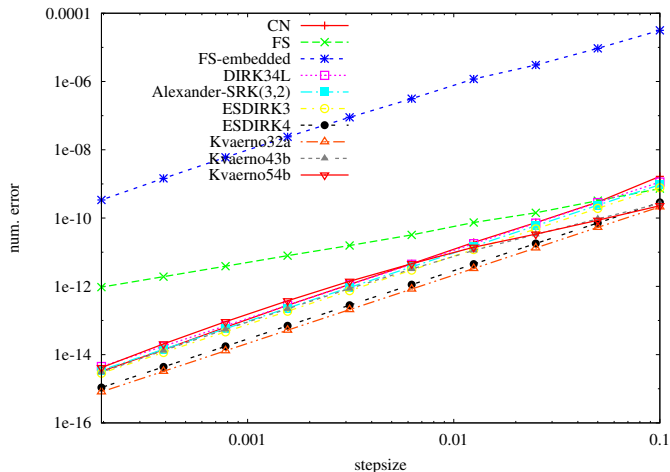
stiffly accurate: $a_{si} = b_i$, $i = 1, \dots, s$, $c_s = 1$

Consider only stiffly accurate methods with $q = 2$ and $\gamma := a_{ij}$, $i = 1, \dots, s \implies$ **ESDIRK methods**

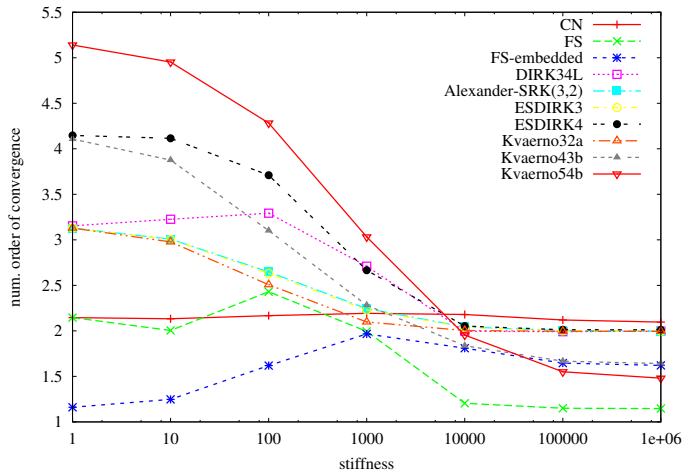
Studied methods

- **CN**: $s = p = q = 2$, A-stable
- **FS**: $s = 4, p = 2, q = 1$, strongly A-stable
- **DIRK34L**: $s = 4, p = 3, q = 2$, L-stable
- **Alexander-SRK(3,2)**: $s = 4, p = 3, q = 2$, L-stable (Alexander 2003)
- **ESDIRK3**: $s = 4, p = 3, q = 2$, L-stable (Bijl, Carpenter, Vatsa, and Kennedy 2002)
- **ESDIRK4**: $s = 6, p = 4, q = 2$, L-stable (Bijl, Carpenter, Vatsa, and Kennedy 2002)
- **Kvaerno32a**: $s = 4, p = 3, q = 2$, L-stable (Kværnø 2004)
- **Kvaerno43b**: $s = 5, p = 4, q = 2$, L-stable (Kværnø 2004)
- **Kvaerno54b**: $s = 7, p = 5, q = 2$, L-stable (Kværnø 2004)

Example of Prothero and Robinson



Numerical order of convergence



Local error

- Apply an ESDIRK method to the ODE of Prothero–Robinson
- Local error:

$$\begin{aligned}
 \delta_\tau(t_{m+1}) &= \tau[b_1 + \tilde{\mathbf{b}}^\top \tilde{\mathbf{A}}^{-1}(\tilde{\mathbf{c}} - \mathbf{a}_1) - 1] \dot{\phi}_m \\
 &+ \sum_{k=2}^p \left[\tilde{\mathbf{b}}^\top \tilde{\mathbf{A}}^{-1} \tilde{\mathbf{c}}^k - 1 \right] \varphi_m^{(k)} \frac{\tau^k}{k!} + \mathcal{O}(\tau^{p+1}) \\
 &+ \sum_{k=2}^{\infty} \tilde{\mathbf{b}}^\top \left[\tilde{\mathbf{A}}^{-k}(\tilde{\mathbf{c}} - \mathbf{a}_1) - \tilde{\mathbf{A}}^{-k+1} \tilde{\mathbf{e}} \right] \dot{\phi}_m \frac{\tau}{z^{k-1}} \\
 &- \sum_{k=2}^{\infty} \tilde{\mathbf{b}}^\top \sum_{l=1}^{k-2} \tilde{\mathbf{A}}^{-l} \left[\tilde{\mathbf{A}}^{-1} \tilde{\mathbf{c}}^{k-l} - (k-l) \tilde{\mathbf{c}}^{k-l-1} \right] \varphi_m^{(k-l)} \frac{\tau^{k-l}}{(k-l)! z^l}.
 \end{aligned}$$

Order conditions

Finally we get the new order conditions

$$b_1 + \tilde{\mathbf{b}}^\top \tilde{\mathbf{A}}^{-1}(\tilde{\mathbf{c}} - \mathbf{a}_1) = 1$$

$$\tilde{\mathbf{b}}^\top \tilde{\mathbf{A}}^{-1} \tilde{\mathbf{c}}^k = 1, \quad k = 2, \dots, p,$$

$$\tilde{\mathbf{b}}^\top [\tilde{\mathbf{A}}^{-k}(\tilde{\mathbf{c}} - \mathbf{a}_1) - \tilde{\mathbf{A}}^{-k+1} \tilde{\mathbf{e}}] = 0, \quad k = 2, \dots, p,$$

$$\tilde{\mathbf{b}}^\top \tilde{\mathbf{A}}^{-l} [\tilde{\mathbf{A}}^{-1} \tilde{\mathbf{c}}^{k-l} - (k-l) \tilde{\mathbf{c}}^{k-l-1}] = 0,$$

for $k = 2, \dots, \infty$ and $l = \max\{1, k - p\}, \dots, k - 1$.

Remarks

- If the ESDIRK method is stiffly accurate conditions the first two conditions are automatically satisfied.
- If the ESDIRK method is consistent and satisfies $C(q)$ the third condition is automatically satisfied for $k = 2, \dots, \infty$ and $l = \max\{1, k - q\}, \dots, k - 1$.

New methods

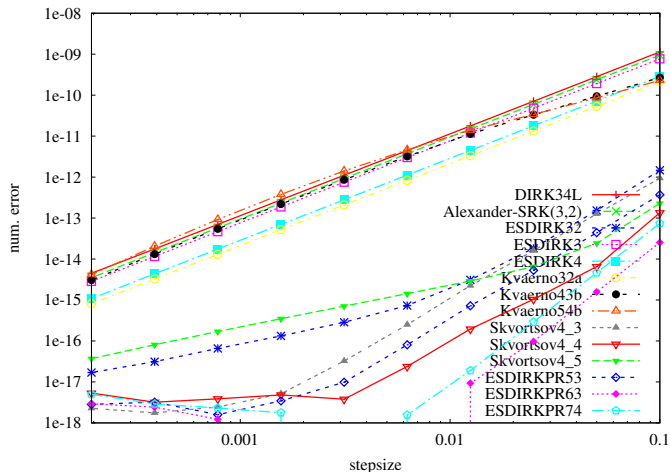
Methods for index-2 DAEs

- ESDIRK32: $s = 4, p = 2$
(Williams, Burrage,
Cameron and Kerr, 2002)
- Skvortsov4-3: $s = 6, p = 4$
(Skvortsov, 2010)
- Skvortsov4-4: $s = 6, p = 4$
(Skvortsov, 2010)
- Skvortsov4-5: $s = 8, p = 5$
(Skvortsov, 2010)

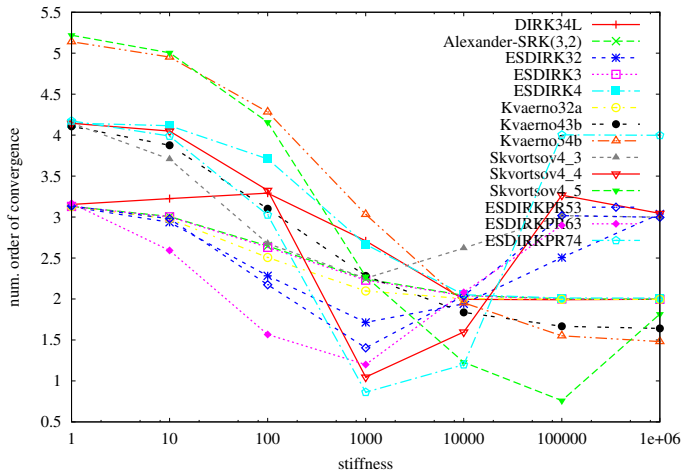
Methods for PR

- ESDIRKPR53: $s = 5, p = 3$
- ESDIRKPR63: $s = 6, p = 3$
- ESDIRKPR74: $s = 7, p = 4$

Example of Prothero and Robinson ($\lambda = -10^6$)



Numerical order of convergence



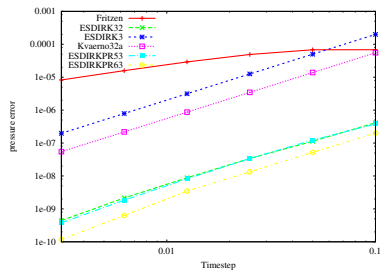
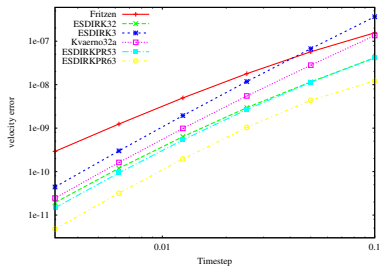
Navier–Stokes equations (3rd order methods)

Exact solution:

$$u_1(t, x, y) = t^3 y^2,$$

$$u_2(t, x, y) = t^2 x,$$

$$p(t, x, y) = tx + y - (t + 1)/2$$



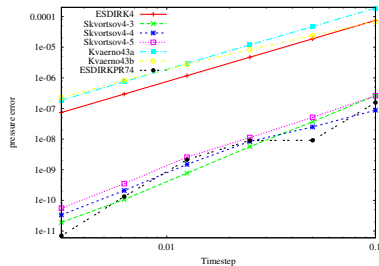
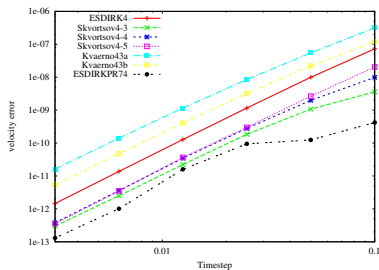
Navier–Stokes equations (4th order methods)

Exact solution:

$$u_1(t, x, y) = t^3 y^2,$$

$$u_2(t, x, y) = t^2 x,$$

$$p(t, x, y) = tx + y - (t + 1)/2$$



2D Benchmark problem

$$J = (0, 8)$$

Problem:

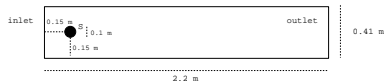
$$\begin{cases} \dot{u} - Re^{-1} \Delta u \\ + (u \cdot \nabla) u + \nabla p = f \\ \nabla \cdot u = 0 \end{cases}$$

boundary conditions:

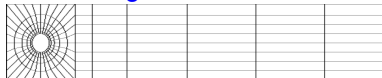
$$u(t, 0, y) = u(t, 2.2, y) = 0.41^{-2} \sin(\pi t / 8) (6y(0.41 - y), 0) \text{ m s}^{-1}, \quad 0 \leq y \leq 0.41.$$

On all other boundaries: $u = 0$

Domain:



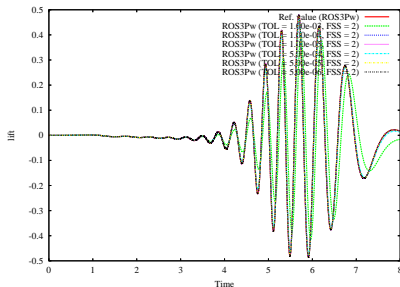
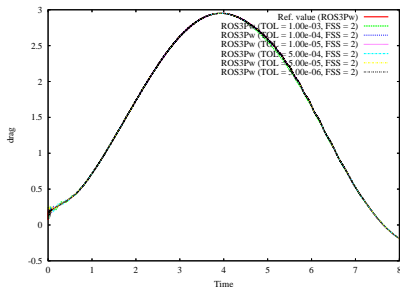
Coarsest grid:



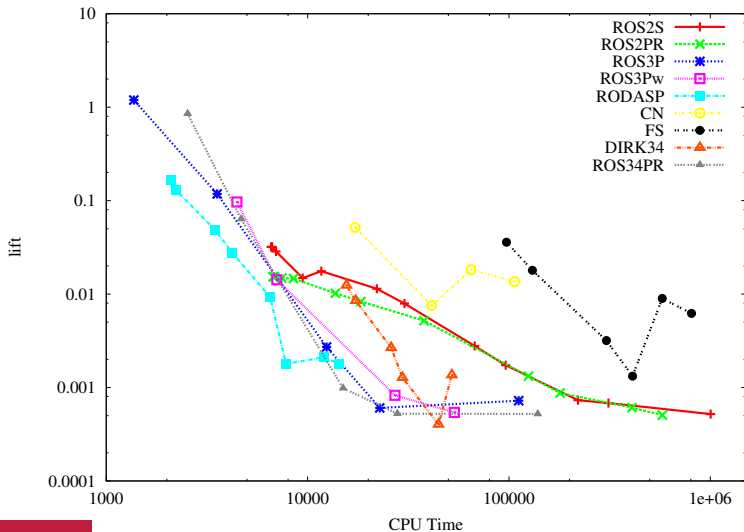
Drag and lift coefficient

$$c_d(t) = -20 [(\mathbf{u}_t, \mathbf{v}_d) + (\nu \nabla \mathbf{u}, \nabla \mathbf{v}_d) + ((\mathbf{u} \cdot \nabla) \mathbf{u}, \mathbf{v}_d) - (p, \nabla \cdot \mathbf{v}_d)],$$

$$c_l(t) = -20 [(\mathbf{u}_t, \mathbf{v}_l) + (\nu \nabla \mathbf{u}, \nabla \mathbf{v}_l) + ((\mathbf{u} \cdot \nabla) \mathbf{u}, \mathbf{v}_l) - (p, \nabla \cdot \mathbf{v}_l)]$$



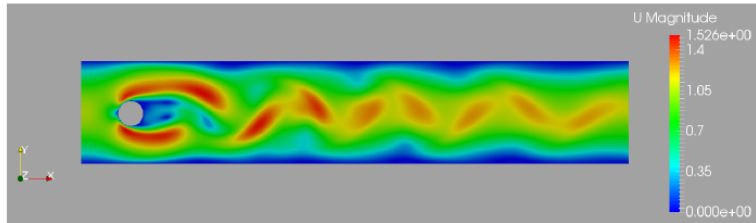
The lift coefficient



Contents

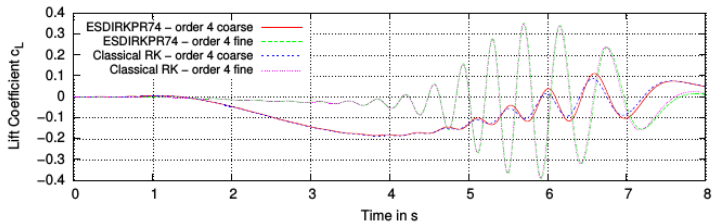
- Introduction
- Diagonally implicit Runge–Kutta methods
- Results with OpenFOAM
- Summary and Outlook

Velocity field

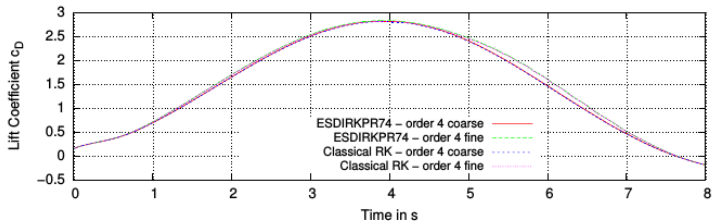


Drag and lift coefficient

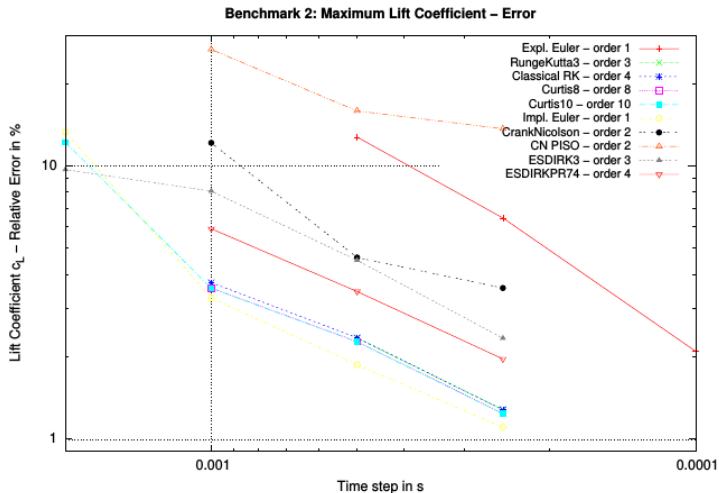
Lift Coefficient Benchmark 2 – Comparison coarse/fine mesh



Drag Coefficient Benchmark 2 – Comparison coarse/fine mesh



Performance



Contents

- **Introduction**
- **Diagonally implicit Runge–Kutta methods**
- **Results with OpenFOAM**
- **Summary and Outlook**

Summary and Outlook

- DIRK methods have stages order $\leq 2 \implies$ order reduction for the Prothero–Robinson example and NSE
- Error analysis for the Prothero–Robinson example \implies further order conditions
- Solution of the nonlinear systems is expensive \implies use linear implicit RK methods, i.e. Rosenbrock–Wanner methods
- Again further order conditions must be satisfied to avoid order reduction
- For higher order ($p > 4$) fully implicit RK methods can be applied. If the simplified Newton method and a transformation of the coefficient matrix A is used, the linear systems split and can be solved in parallel.

Literature

- **Student work:** J. Wiegmann: On the Implementation of Explicit Runge-Kutta and ESDIRK Methods for Laminar Incompressible Transient Flows Using OpenFOAM, Student work, TU Braunschweig, 2016.
- **Papers:**
 - An analysis of the Prothero-Robinson example for constructing new DIRK and ROW methods. *Journal of Computational and Applied Mathematics* (262), pp. 105-114, 2012
 - Adaptive timestep control for fully implicit Runge-Kutta methods of higher order. *Informatik-Bericht 2014-03*, TU BS, 2014
 - The Prothero and Robinson example: Convergence studies for Runge-Kutta and Rosenbrock-Wanner methods *Informatik-Bericht 2014-08*, TU BS, 2014
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 - An analysis of the Prothero-Robinson example for constructing new adaptive ESDIRK methods of order 3 and 4. *Applied Numerical Mathematics*, volume 94, pages 75-87, 2015
 - A component framework for the parallel solution of the incompressible Navier-Stokes equations with Radau-IIA methods (with R. Niekamp), *Int. J. Numer. Meth. Fluids*, DOI: 10.1002/fld.4018, 2015