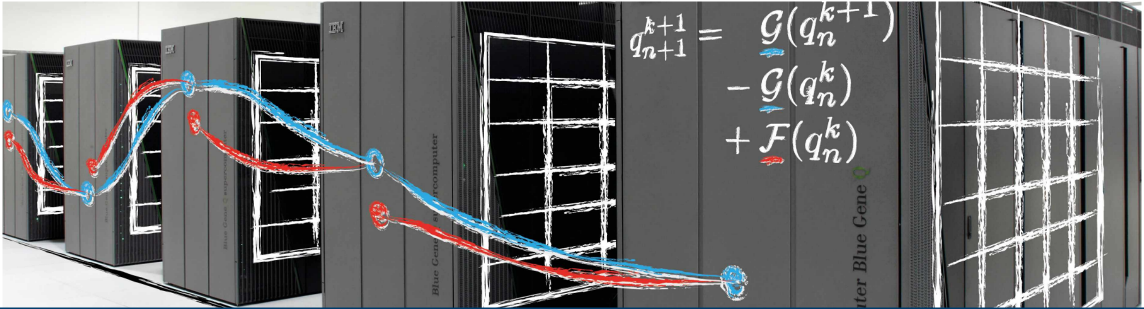


A PARALLEL-IN-TIME SPECTRAL DEFERRED CORRECTIONS METHOD FOR THE INCOMPRESSIBLE NAVIER-STOKES EQUATIONS

September 4th, 2024 | Abdelouahed Ouardghi, Robert Speck | Jülich Supercomputing Centre, Forschungszentrum Jülich

Acknowledgment

Federal Ministry of Education and Research

Novel Exascale-Architectures with Heterogeneous Hardware Components for CFD Simulations

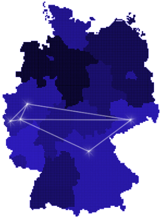
STROEMUNGSRAUM
SCALEXA HPC DEEPTECH

Project goals

- Enhance scalability and efficiency of FEATFLOW
- Develop exascale-ready methods
- Provide IANUS customers with access to methods, codes, and knowledge.

Project partners

- IANUS Simulation GmbH
- TU Dortmund University - Coordinator
- Jülich Supercomputing Centre
- University of Cologne
- Friedrich Alexander University Erlangen -Nuremberg
- Freiberg University of Technology



Outline

1. Collocation problem
2. Spectral deferred correction method (SDC)
3. Semi-implicit spectral deferred correction method (SISDC)
4. Diagonal Preconditioners for SDC
5. Software: pySDC and FEniCS
6. Numerical results
7. Summary

The Collocation Problem

Consider the classical initial value problem

$$\frac{du}{dt} = f(t, u), \qquad u \in \mathbb{R}^d, \quad t \in [t_0, t_0 + \Delta t].$$

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$$u(t) = u_0 + \int_{t_0}^{t} f(s, u(s))ds, \qquad t_0 \leq t \leq t_0 + \Delta t$$

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Discretize $[t_0, t_0 + \Delta t]$ using M quadrature nodes, then approximate f using Lagrange polynomials $l_j(t)$:

$$f(t, u) \approx \sum_{j=1}^{M} f(\tau_j, u(\tau_j))l_j(t), \qquad t_0 \leq \tau_1 \leq \cdots \leq \tau_m \leq \cdots \leq \tau_M \leq t_0 + \Delta t$$

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Approximate the integral on given quadrature nodes

$$u(\tau_m) \approx u_m = u_0 + \Delta t \sum_{j=1}^{M} q_{m,j} f(\tau_j, u_j), \qquad q_{m,j} = \int_{t_0}^{\tau_m} l_j(s)ds.$$

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Approximate the integral on given quadrature nodes

$$\vec{u} = \vec{u}_0 + \Delta t Q F(\vec{u})$$

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Spectral Deferred Corrections

- Consider the fully implicit collocation method

$$(I - \Delta t Q F)(\vec{u}) = \vec{u}_0$$

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$$P\vec{u}^{k+1} = P\vec{u}^{k} + \left[\vec{u}_0 - (I - \Delta t Q F)(\vec{u}^{k})\right]$$

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- Use the preconditioner $P = (I - \Delta t Q_\Delta F)$ with $Q_\Delta \approx Q$ is a lower triangular approximation of Q

$$(I - \Delta t Q_\Delta F)(\vec{u}^{k+1}) = (I - \Delta t Q_\Delta F)(\vec{u}^k) + \left(\vec{u}_0 - (I - \Delta t Q F)(\vec{u}^k)\right)$$

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$$(I - \Delta t Q_\Delta F)(\vec{u}^{k+1}) = \vec{u}_0 + \Delta t \,(Q - Q_\Delta)\, F(\vec{u}^k)$$

Spectral Deferred correction Sweep

Implicit SDC: $$Q_\Delta^{LU} = \begin{pmatrix} q_{1,1}^\Delta & & & \\ q_{1,2}^\Delta & q_{2,2}^\Delta & & \\ \vdots & & \ddots & \\ q_{1,M}^\Delta & \cdots & \cdots & q_{M,M}^\Delta \end{pmatrix}$$ with $Q_\Delta^{LU} = U^T$ for $Q^T = LU$.

$$u_m^{k+1} = u_0 + \Delta t \sum_{j=1}^{M} q_{m,j} f(\tau_j, u_j^k) + \Delta t \sum_{j=1}^{m} q_{m,j}^\Delta \left[f(\tau_j, u_j^{k+1}) - f(\tau_j, u_j^k) \right]$$

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Explicit SDC:
$$Q_\Delta^{EE} = \begin{pmatrix} 0 & & & \\ q_{2,1}^\Delta & 0 & & \\ \vdots & & \ddots & \\ q_{M,1}^\Delta & \dots & q_{M-1,M-1}^\Delta & 0 \end{pmatrix}$$

$$u_m^{k+1} = u_0 + \Delta t \sum_{j=1}^{M} q_{m,j} f(\tau_j, u_j^k) + \Delta t \sum_{j=1}^{m-1} q_{m,j}^\Delta \left[f(\tau_j, u_j^{k+1}) - f(\tau_j, u_j^k) \right]$$

Semi-implicit spectral deferred correction method (SISDC)

Consider the case when the initial value problem given previously can be cast in the form

$$\frac{du}{dt} = f(t, u(t)) = f_E(t, u(t)) + f_I(t, u(t)), \qquad u \in \mathbb{R}^d, \quad t \in [t_0, t_0 + \Delta t].$$

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Replace $Q_\Delta F$ with $Q_{\Delta,E} F_E + Q_{\Delta,I} F_I$ in SDC iteration

$$(I - \Delta t Q_{\Delta,E} F_E - \Delta t Q_{\Delta,I} F_I)(\vec{u}^{k+1}) = (I - \Delta t Q_{\Delta,E} F_E - \Delta t Q_{\Delta,I} F_I)(\vec{u}^k) + \left(\vec{u}_0 - (I - \Delta t Q F)(\vec{u}^k)\right)$$

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Choose $Q_{\Delta,I}$ lower triangular and $Q_{\Delta,E}$ strictly lower triangular for explicit integration

$$\begin{aligned} u_m^{k+1} \quad &= \quad u_0 + \Delta t \sum_{j=1}^{M} q_{m,j} f(\tau_j, u_j^k) \\ &\quad + \Delta t \sum_{j=1}^{m-1} q_{m,j}^{\Delta,E} \left[f_E(\tau_j, u_j^{k+1}) - f_E(\tau_j, u_j^k) \right] + \Delta t \sum_{j=1}^{m} q_{m,j}^{\Delta,I} \left[f_I(\tau_j, u_j^{k+1}) - f_I(\tau_j, u_j^k) \right] \end{aligned}$$

Parallel SDC: Diagonal Preconditioners

G. Čaklović et al., Improving Efficiency of Parallel Across the Method Spectral Deferred Corrections. *Preprint in arXiv*

Diagonal SDC: $Q_\Delta^{diag} = diag\left(d_1, \cdots, d_M\right)$

$$u_m^{k+1} = u_0 + \Delta t \sum_{j=1}^{M} q_{m,j} f(\tau_m, u_j^k) + \Delta t d_m \left[f(\tau_m, u_m^{k+1}) - f(\tau_m, u_m^k)\right]$$

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1 **Diagonal implicit Euler (IEpar)**

$$Q_\Delta^{IEpar} = diag(\tau_i - t_0),$$

with τ_i the nodes of the quadrature rule.

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1. **Diagonal implicit Euler (IEpar)**

$$Q_\Delta^{IEpar} = diag(\tau_i - t_0),$$

with τ_i the nodes of the quadrature rule.

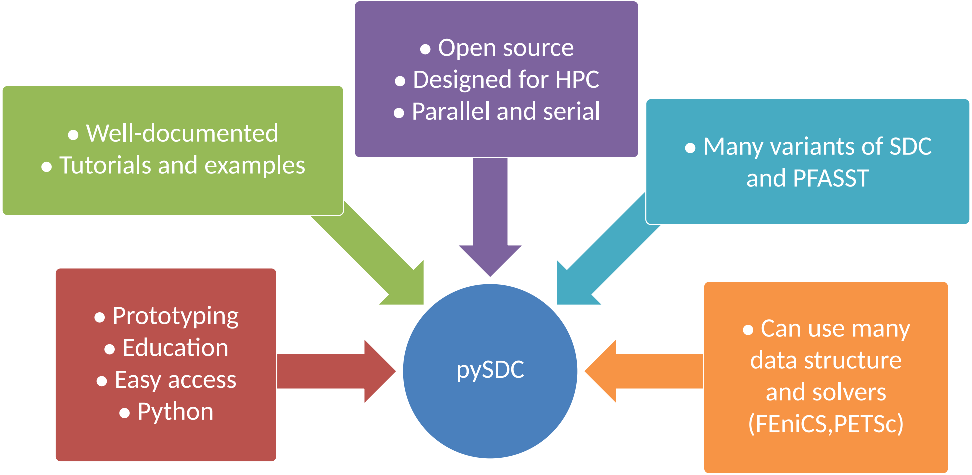
2. **MIN-SR-NS diagonal coefficients**
For any collocation method on M distinct nodes, then $\rho(Q - Q_\Delta) = 0$ for

$$Q_\Delta = diag\left(\frac{\tau_1}{M}, \cdots, \frac{\tau_M}{M}\right)$$

3. **MIN-SR-S diagonal coefficients**
We minimize $\rho(I - Q_\Delta^{-1}Q)$ by choosing diagonal coefficients such that

$$det\left((1-z)I + zQ_\Delta^{-1}Q\right) = 1, \qquad z \in \{\tau_1, \cdots, \tau_M\}$$

pySDC prototyping



`https://parallel-in-time.org/pySDC`

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IMEX SDC (SISDC) for advection-diffusion equations

Advection-diffusion of a Gaussian hill problem

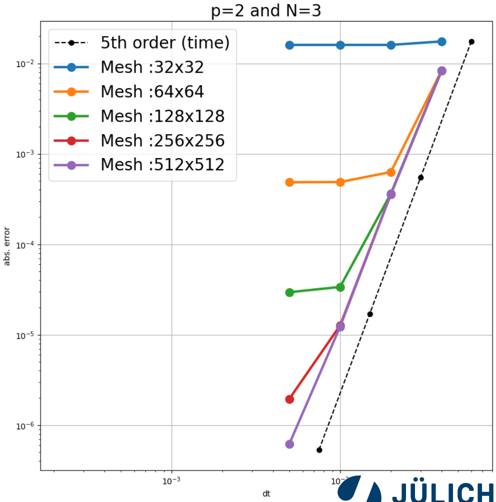
1 Mathematical model

$$\begin{cases} \frac{\partial c}{\partial t} + \mathbf{v} \cdot \nabla c - \nu \Delta c = f & \text{in} \quad \Omega \times [0, T] \\ c = g & \text{on} \quad \partial\Omega \times [0, T] \\ c(x, y, 0) = c_0(x, y) & \text{in} \quad \Omega \end{cases}$$

2 Problem setup

$$c(x, y, t) = \frac{5}{7\sqrt{1 + \frac{4\nu t}{l^2}}} exp \left\{ - \left(\frac{x - x_0 - t}{l\sqrt{1 + \frac{4\nu t}{l^2}}} \right)^2 \right\}$$

with $l = 7\frac{\sqrt{2}}{300}$, $x_0 = \frac{2}{15}$ and $\Omega = [0, 1] \times [0, 1]$



IMEX SDC (SISDC) using projection-based splitting scheme

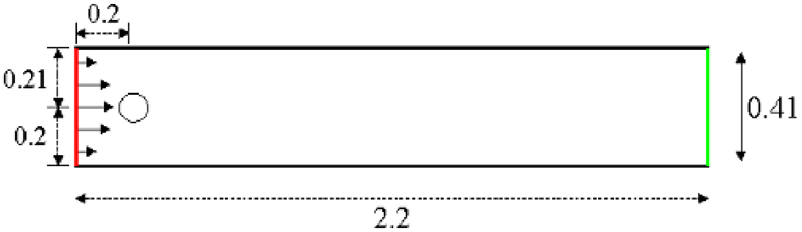
DFG flow around cylinder: Benchmark 2D-3

$$
\begin{cases}
\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u} + \nabla p - \nu\Delta\mathbf{u} = f & \text{in} \quad \Omega \times [0,T] \\
\nabla\cdot\mathbf{u} = 0 & \text{in} \quad \Omega \times [0,T] \\
\mathbf{u} = \mathbf{u}_{in} & \text{on} \quad \Gamma_1 \times [0,T] \\
\mathbf{u} = 0 & \text{on} \quad \Gamma_2 \times [0,T] \\
\nu\partial_{\mathbf{n}}\mathbf{u} - p\mathbf{n} = 0 & \text{on} \quad \Gamma_3 \times [0,T]
\end{cases}
$$

with

$$\mathbf{u}_{in} = \frac{(4Uy(0.41-y)}{0.41^2}, 0),$$

$$U = U(t) = 1.5 sin(\pi t/8)$$



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IMEX SDC (SISDC) using projection-based splitting scheme

DFG Flow around cylinder: Chorin's projection method

1. **Step 1: Predictor Step:**

$$\frac{\mathbf{u}^* - \mathbf{u}^n}{\Delta t} + (\mathbf{u}^n \cdot \nabla)\mathbf{u}^n = \nu \Delta \mathbf{u}^*$$

2. **Step 2: Corrector Step:**

$$\Delta p^{n+1} = \frac{1}{\Delta t} \nabla \cdot \mathbf{u}^*$$

$$\mathbf{u}^{n+1} = \mathbf{u}^* - \Delta t \nabla p^{n+1}$$

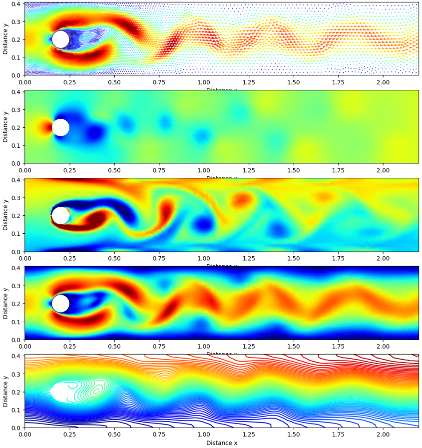

Figure: Velocity, pressure, vorticity, magnitude and streamlines at time $t = 5.5s$

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IMEX SDC (SISDC) using projection-based splitting scheme

Lift coefficient using different SDC

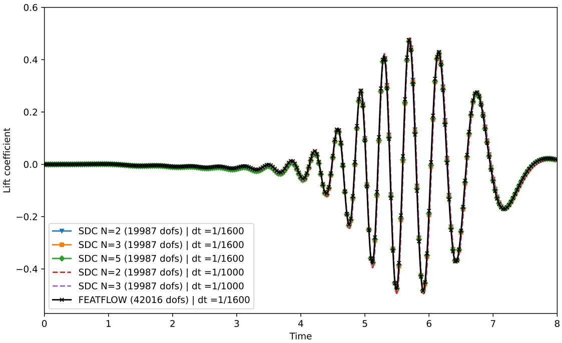

Figure: Lift coefficient using different SDC setups and time steps

IMEX SDC (SISDC) using projection-based splitting scheme

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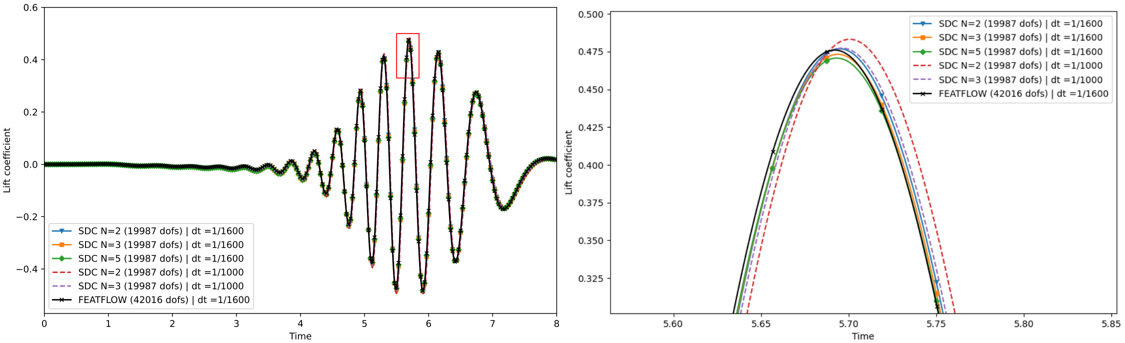

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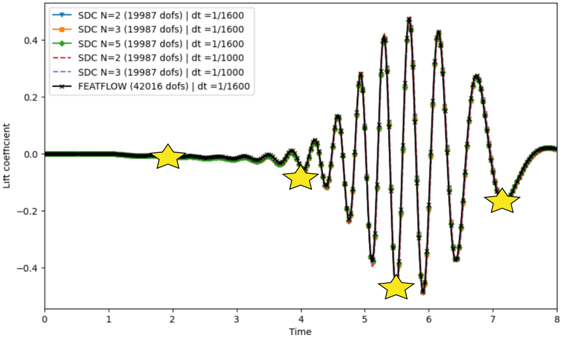

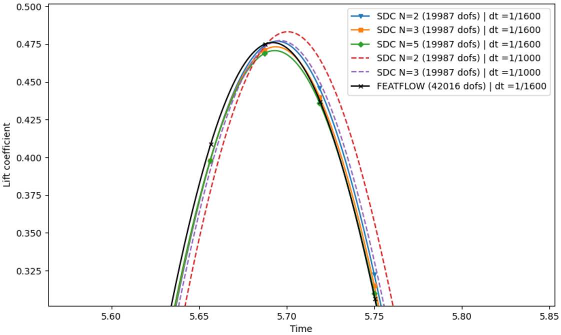

Figure: Lift coefficient using different SDC setups and time steps

IMEX SDC (SISDC) using projection-based splitting scheme

Comparison of different preconditioners

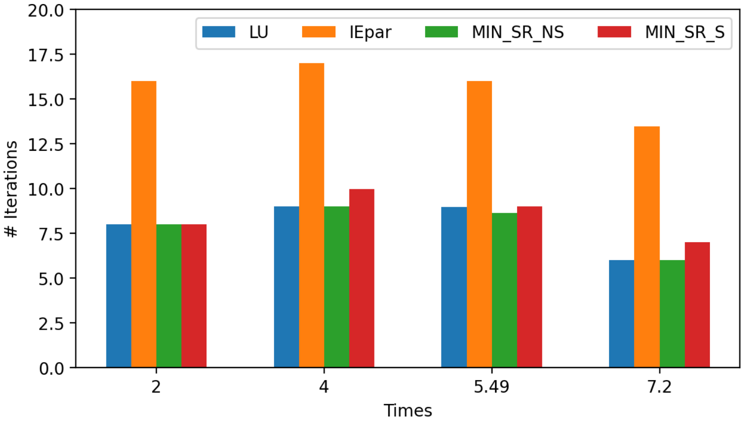

Figure: Average number of iterations needed by various preconditioners after 50 timesteps at four different time points throughout the simulation

Fully implicit SDC using the monolithic approach

- Semi-discrete form of the Navier-Stokes equations.

$$
\begin{aligned}
[\mathtt{M}]\frac{d\mathbf{u}}{dt} &= -[\mathtt{C}_{\mathbf{u}}]\mathbf{u} - [\mathtt{k}]\mathbf{u} + [\mathtt{B}]p + [\mathtt{M}]\mathbf{g}, \\
\mathbf{0} &= [\mathtt{B}^T]\mathbf{u}
\end{aligned}
$$

- Differential algebraic equation (DAEs)

$$
\begin{aligned}
[\mathtt{M}]\frac{d\mathbf{u}}{dt} &= \mathcal{F}\left(\mathbf{u}, p, t\right), \\
0 &= \mathcal{G}\left(\mathbf{u}, t\right).
\end{aligned}
$$

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\end{aligned}
$$

- Matrix-vector form of the semi-discrete form

$$
\begin{pmatrix} [\mathtt{M}] & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}
\begin{pmatrix} \frac{d\mathbf{u}}{dt} \\ \frac{dp}{dt} \end{pmatrix}
=
\begin{pmatrix} -[\mathtt{C}_{\mathbf{u}}] - [\mathtt{k}] & [\mathtt{B}] \\ [\mathtt{B}^T] & \mathbf{0} \end{pmatrix}
\begin{pmatrix} \mathbf{u} \\ p \end{pmatrix}
+
\begin{pmatrix} [\mathtt{M}]\mathbf{g} \\ 0 \end{pmatrix}.
$$

- Ordinary differential equation (ODE)

$$
[\alpha]\frac{d\mathbf{w}}{dt} = [\beta]\mathbf{w} + \gamma = f\left(\mathbf{w}, t\right),
$$

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Fully implicit SDC using the monolithic approach

Lift coefficient using different SDC

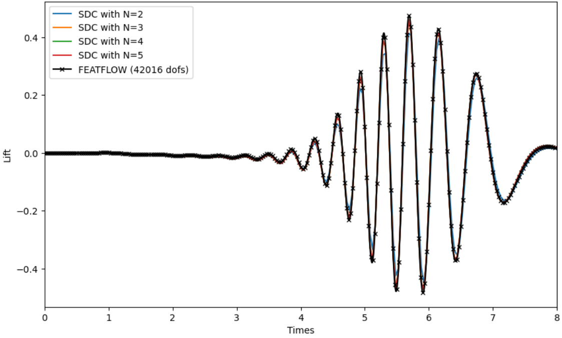
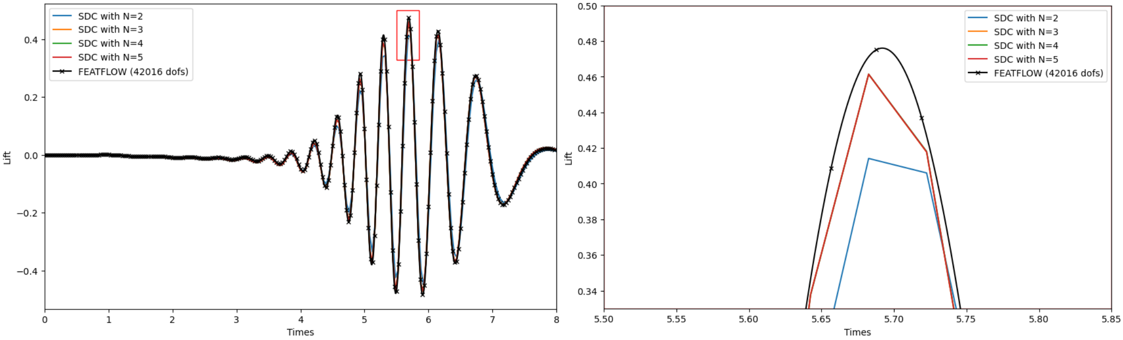


Figure: Lift coefficient using various SDC methods with $\Delta t = \frac{1}{25}$, compared to FEATFLOW reference data with $\Delta t = \frac{1}{1600}$

Fully implicit SDC using the monolithic approach

Lift coefficient using different SDC



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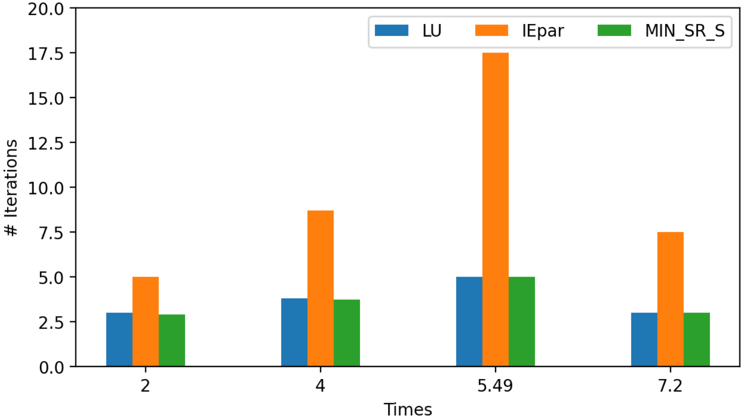

Figure: Average number of iterations needed by various preconditioners after 10 timesteps at four different time points throughout the simulation

Summary

- SDC method can use simple numerical method (even a first-order method) to compute a solution with higher-order accuracy.
- SDC can be used for various initial value problems, using explicit, implicit or implicit- explicit schemes.
- parallelization can be done across the method (i.e. using diagonal preconditioners).

what's next?

- Assess code performance with advanced numerical test cases to ensure robustness.
- Optimize parallel execution and analyze the speedup.
- Integrate pySDC with the FEAT3 toolbox to enable and evaluate space-time parallelization strategies.