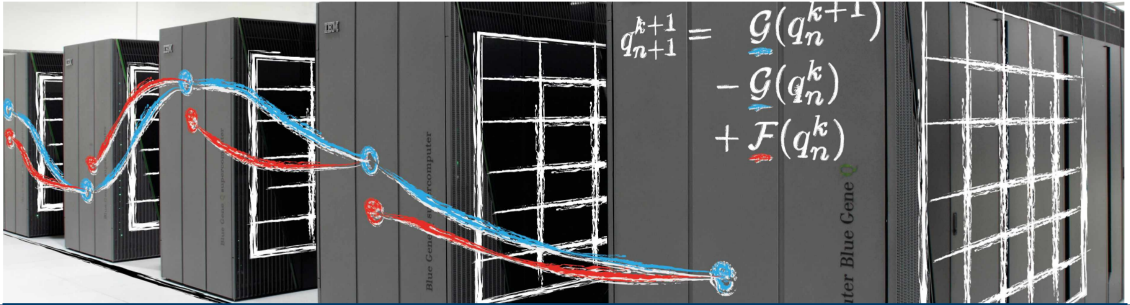


A PARALLEL-IN-TIME SPECTRAL DEFERRED CORRECTION FINITE ELEMENT METHOD FOR UNSTEADY INCOMPRESSIBLE VISCOUS FLOW PROBLEMS

March 8th, 2024 | Abdelouahed Ouardghi, Robert Speck | Jülich Supercomputing Centre, Forschungszentrum Jülich

Acknowledgment

Novel Exascale-Architectures with Heterogeneous Hardware Components for CFD Simulations

Federal Ministry
of Education
and Research

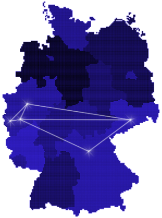
STROEMUNGSRAUM
SCALEXA HPC DEEPTECH

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

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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- Consider fully implicit collocation (linear form)

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

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

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

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

Spectral Deferred correction Sweep

Implicit SDC:

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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:

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

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

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

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

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

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

Parallel SDC: Diagonal Preconditioners

Robert Speck, Parallelizing spectral deferred corrections across the method. *Comput. Visual Sci*. **19, 75-83 (2018).**

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. **Minimize the spectral radius (MIN)**
   - Dahlquist equation: $u_t = \lambda u$ (linear ODE)
   - SDC iteration matrix: $K = \lambda \Delta t Q_\Delta (I - \lambda \Delta t Q_\Delta)^{-1} \left(Q_\Delta^{-1} Q - I\right) \rightarrow \vec{u}^{k+1} = K \vec{u}^k$
   - Stiff limit: $|\lambda \Delta t| \rightarrow \infty$: $K \rightarrow I - Q_\Delta^{-1} Q := k_\infty$ independent of λ
   - non-stiff limit: $|\lambda \Delta t| \rightarrow 0$: $K/(\lambda \Delta t) \rightarrow Q - Q_\Delta := K_0$ independent of λ
   - Minimize spectral radius $\rho\left(K_\infty\right)$ by choice of diagonal Q_Δ using scipy

Parallel SDC: Diagonal Preconditioners

Thibaut Lunet et al. in prep

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

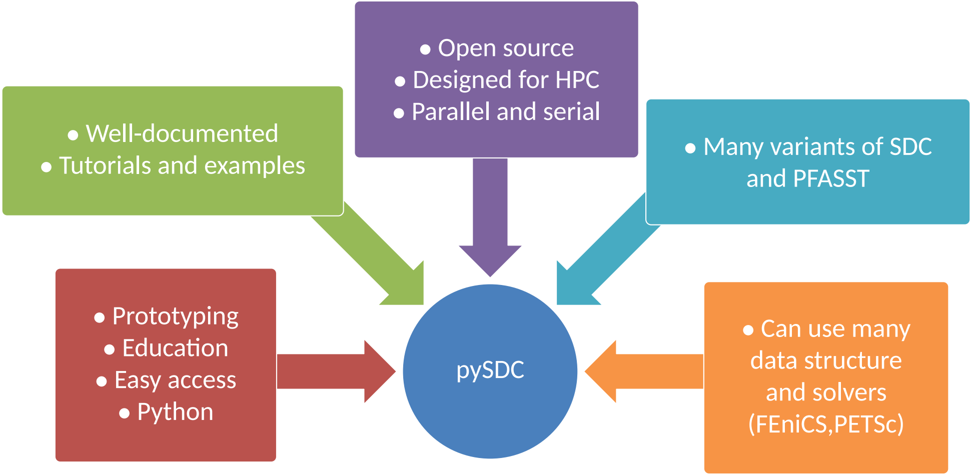
$$Q_\Delta = diag\left(\frac{\tau_1}{M}, \cdots, \frac{\tau_M}{M}\right)$$

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

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

Looks for nilpotency of $I - Q_\Delta^{-1}Q$.
Analytical solution for $M = 2$, very hard to find for larger M
Constrain on finding ordered coefficients

pySDC prototyping



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

SISDC for advection-diffusion equations

Advection-diffusion of a Gaussian hill problem

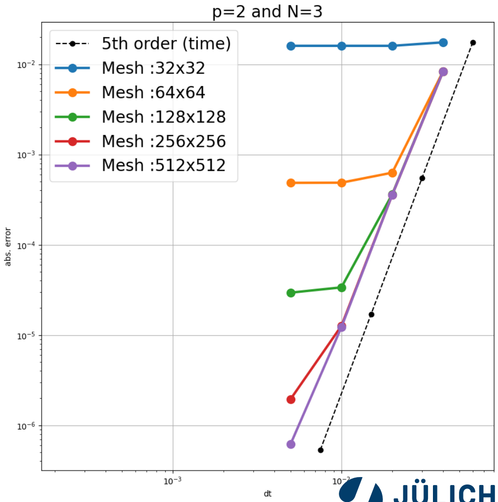
1. Mathematical model

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

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 $\Omega = [0, 1] \times [0, 1]$



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SISDC for icompressible Navier-Stokes equations

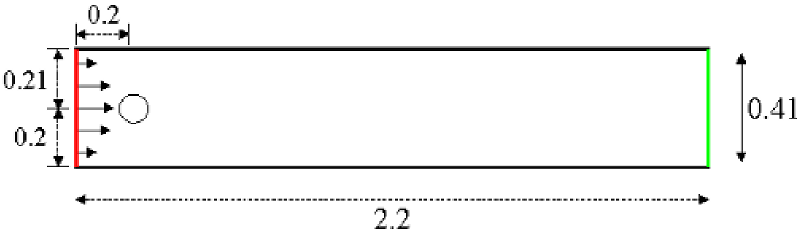
DFG flow around cylinder: Benchmark 2D-3

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

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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SISDC for incompressible Navier-Stokes Equations

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:**

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

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

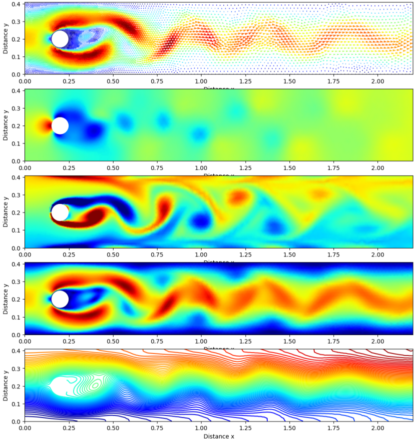

Figure: Velocity, pressure, vorticity, magnitude and streamlines at time $t = 5.5s$

Lift coefficient using different SDC

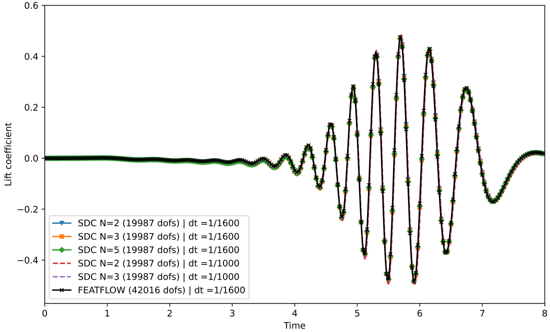

Figure: Lift coefficient using different SDC setups and time steps

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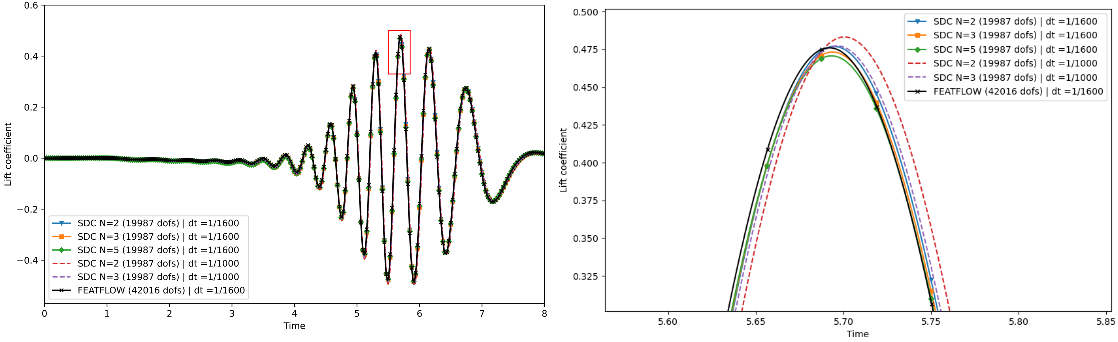

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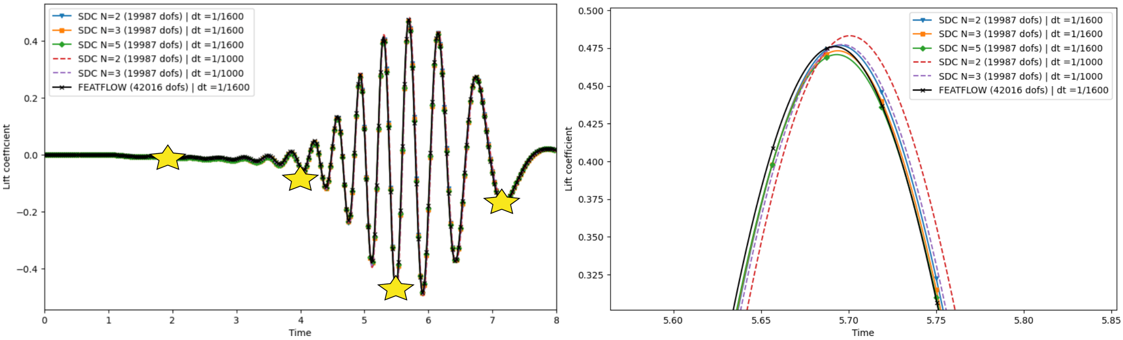

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Comparison of different preconditioners

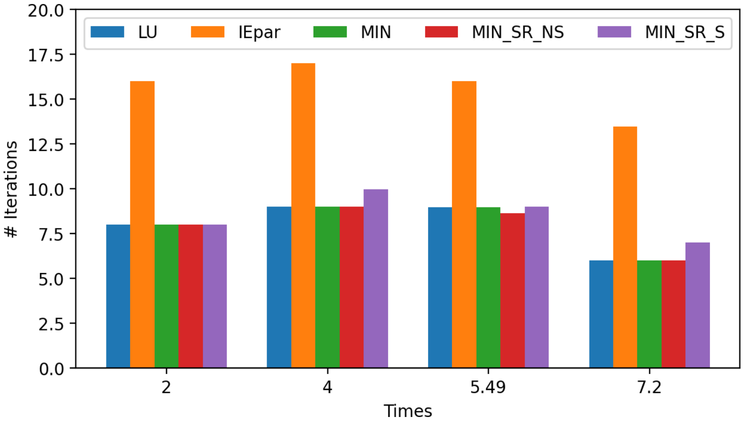

Figure: Average number of iterations needed by various preconditioners after 50 timesteps at four different time points throughout the simulation

Summary

- SDC method can use simple numerical method (even a first-order method) to compute a solution with higher-order accuracy.
- In this work, a simple first-order, semi-implicit method is used in the context of SDC to construct higher-order semi-implicit SDC methods (SISDC).
- parallelization can be done across the method (i.e. using diagonal preconditioners).

what's next?

- Adaptive time steps integration.
- Advanced projection schemes vs monolithic scheme.
- Parallel Speedup Enhancement.