Computer aided analysis of preconditioned multistage Runge-Kutta methods applied to solve the compressible Reynolds averaged Navier-Stokes equations

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Munich, 2014, November 5th

Goal: Design of a robust solution method

Apply multistage Runge-Kutta method to (approximately) solve the Reynolds averaged Navier Stokes equations:

$$\frac{d}{dt}\int_{\Omega} \mathrm{W}\,dx + \int_{\partial\Omega} \big(\underbrace{\mathrm{F_c}}_{\text{Convection}} - \underbrace{\mathrm{F_v}}_{\text{Diffusion}} \big) \bullet \mathrm{n}\,ds = \underbrace{\int_{\Omega} Q\,dx}_{\substack{\text{Source terms}\\ \text{(Turbulence model)}}}$$

$$\overbrace{\Leftrightarrow}^{\substack{\text{Finite volume}\\ \text{Discretization}}} \qquad \frac{d\mathrm{W}}{dt} = -\mathrm{M}^{-1}\mathrm{R}(\mathrm{W})$$

Implicit Multistage Runge-Kutta method

$$\mathrm{W}^{(0)} := \mathrm{W}^{(n)}$$

$$\mathrm{W}^{(j)} := \mathrm{W}^{(0)} - \alpha_{j+1,j}\mathrm{P}_j^{-1,\mathrm{app}}\mathrm{R}\left(\mathrm{W}^{(j-1)}\right), \quad j = 1,\ldots,s$$

$$\mathrm{W}^{(n+1)} := \mathrm{W}^{(s)}$$

$$\mathrm{P}_j := \frac{1}{CFL\Delta t} + \frac{\partial \mathrm{R}^{\mathrm{app}}}{\partial \mathrm{W}}$$

- How to choose number of stages?
- How to choose stage coefficients?
- How to choose CFL number?
- How to construct preconditioner?

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Analysis tool is required

Rough explanation of parameters: Heuristic

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- Number of stages: 1
- Stage coefficient: $\alpha_{2,1} = 1$
- CFL = ∞
- Preconditioner: Exact Derivative

Newton's method

$$W^{(n+1)} := W^{(n)} - \left(\frac{\partial R}{\partial W}\right)^{-1} R\left(W^{(j-1)}\right)$$

Requires (at least)

1. Good initial guess
2. Solution of linear system $\frac{\partial R}{\partial W} \Delta W = R\left(W^{(n)}\right)$

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Sol. not available

→ Newton‘s method in general not realizable, because

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Stabilization term (Linear systems are easier to solve)

Necessity ? Hope of additional stability!

- Number of stages: 1,…,s → Multistage
- Stage coefficient: $\alpha_{2,1}$, …, $\alpha_{s+1,s}$
- CFL < ∞

Prec tioner: Exact Derivative

Newton's method

Not available

$$W^{(n+1)} := W^{(n)} - \left(\frac{\partial R}{\partial W}\right) R($$

Requires (at least)

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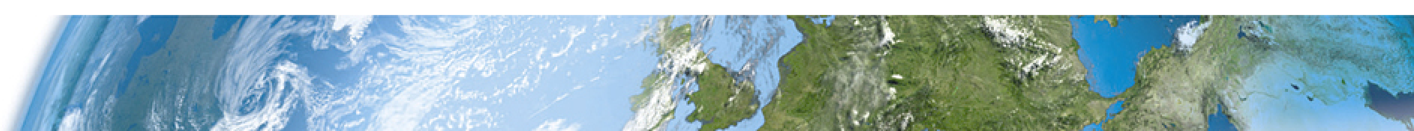

Simplifications and Stabilizations

$$1)\quad \text{Stabilize linear system}: \frac{\partial R}{\partial W} h = R(W) \Rightarrow \left(\frac{1}{CFL\Delta t} I + \frac{\partial R}{\partial W} \right) h = R(W)$$

$$2)\ \text{Simplify linear system}: \left(\frac{1}{CFL\Delta t} I + \frac{\partial R}{\partial W} \right) h = R(W) \Rightarrow \left(\frac{1}{CFL\Delta t} I + \frac{\partial R^{app}}{\partial W} \right) h = R(W)$$

$$3)\ \text{Solve approximately}: h = \left(\frac{1}{CFL\Delta t} I + \frac{\partial R^{app}}{\partial W} \right)^{-1} R(W) \Rightarrow h = \left(\frac{1}{CFL\Delta t} I + \frac{\partial R^{app}}{\partial W} \right)^{-1,\ app} R(W)$$

$$4)\ \text{Stabilize}: \text{Embed in a multistage method}$$

Simplification of $\frac{\partial R}{\partial W}$ and choice of

linear solution methods determines method:

→ Newton, First order prec., LU-SGS, Line-implicit, Point-implicit, expl. Runge-Kutta + local time stepping (all well known methods in CFD literature)

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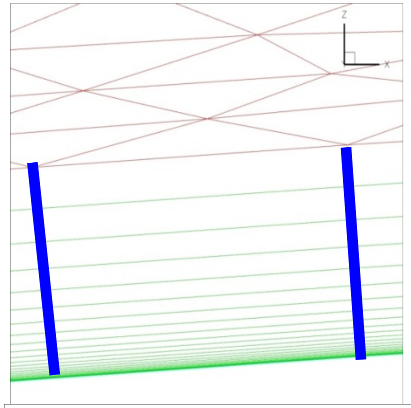
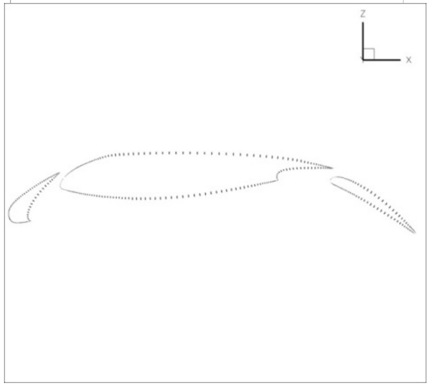
Iterative solution methods

Jacobi method:



$$x_i^{(m+1)} = D_i^{-1}\left(b_i - \sum_{j=1,\, j\neq i}^{N} A_{ij}\, x_j^{(m)}\right), \quad i = 1, \ldots, N$$

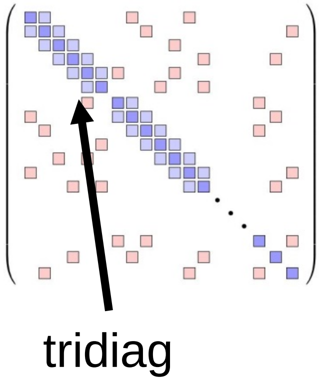
Gauss-Seidel method:



$$x_i^{(m+1)} = D_i^{-1}\left(b_i - \sum_{j=1}^{i-1} A_{ij}\, x_j^{(m+1)} - \sum_{j=i+1}^{N} A_{ij}\, x_j^{(m)}\right), \quad i = 1, \ldots, N$$

(Symmetric) Line Gauss-Seidel method:

$$x_{L_i}^{(m+1)} = \mathrm{tridiag}\left(D_{L_i}\right)^{-1}\left(b_{L_i} - \sum_{j\in L_1,\ldots,L_{i-1},\, j\notin L_i} A_{L_i j}\, x_j^{(m+1)} - \sum_{j\notin L_1,\ldots,L_{i-1},\, j\notin L_i} A_{L_i j}\, x_j^{(m)}\right)$$



Point implicit: Apply 1 Jacobi sweep
Line implicit: Apply 1 line Jacobi sweep

Construction of investigation tool: Idea

Nonlinear Problem:

$$\frac{\mathrm{dW}}{\mathrm{dt}} = \mathrm{R}(\mathrm{W})$$

$$\mathrm{W}^{(0)} := \mathrm{W}^{(n)}$$

$$\mathrm{W}^{(j)} := \mathrm{W}^{(0)} - \alpha_{j+1,j} \mathrm{P}_j^{-1,\mathrm{app}} \mathrm{R}\left(\mathrm{W}^{(j-1)}\right), \quad j = 1,\ldots,s$$

$$\mathrm{W}^{(n+1)} := \mathrm{W}^{(s)}$$

$$\mathrm{P}_j := \frac{1}{CFL\Delta t} + \frac{\partial \mathrm{R}^{\mathrm{app}}}{\partial \mathrm{W}}$$

Influence of CFL and choice of $\dfrac{\partial \mathrm{R}^{\mathrm{app}}}{\partial \mathrm{W}}$

Linearized Problem

$$\frac{\mathrm{dW}}{\mathrm{dt}} = \mathrm{R}(\mathrm{W}) \approx \underbrace{\mathrm{R}\left(\mathrm{W}^*\right)}_{=0;\,\text{Steady state}} - \frac{\partial \mathrm{R}}{\partial \mathrm{W}}\left[\mathrm{W}^*\right]\Delta \mathrm{W}$$

$$\mathrm{W}^{(0)} := \mathrm{W}^{(n)}$$

$$\mathrm{W}^{(j)} := \mathrm{W}^{(0)} - \alpha_{j+1,j} \mathrm{P}_j^{-1,\mathrm{app}} \frac{\partial \mathrm{R}}{\partial \mathrm{W}} \mathrm{W}^{(j-1)}$$

$$\mathrm{W}^{(n+1)} := \mathrm{W}^{(s)} \Leftrightarrow \mathrm{W}^{(n+1)} = q_s\left(\mathrm{P}_j^{-1,\mathrm{app}} \frac{\partial \mathrm{R}}{\partial \mathrm{W}}\right) \mathrm{W}^{(j-1)}$$

$$q_s(z) = 1 + \sum_{j=1}^{s} \beta_j z^j$$

Convergence $\Leftrightarrow \rho\left(q_s\left(\mathrm{P}_j^{-1,\mathrm{app}} \dfrac{\partial \mathrm{R}}{\partial \mathrm{W}}\right)\right) < 1$

Approximation to eigenvalues can be computed exploiting Arnoldi‘s method

Computation of spectrum: Prec. (GmRes) with inner Arnoldi iteration

Given initial guess $x^{(0)}, r^{(0)} = b - \mathrm{P}^{-1,app} \frac{\partial \mathrm{R}}{\partial \mathrm{W}} x^{(0)}, \beta = \left\| r^{(0)} \right\|, \mathrm{z}^{(1)} = \frac{1}{\beta} r^{(0)}$

Approximate by finite difference

$$\frac{\partial \mathrm{R}}{\partial \mathrm{W}} \Delta \mathrm{W} \approx \frac{\mathrm{R}(\mathrm{W} + \varepsilon \Delta \mathrm{W}) - \mathrm{R}(\mathrm{W} - \varepsilon \Delta \mathrm{W})}{2\varepsilon}$$

for $j = 1, 2, \ldots, m$

$$w^{(j)} := \mathrm{P}^{-1,app} \frac{\partial \mathrm{R}}{\partial \mathrm{W}} \mathrm{z}^{(j)}$$

for $i = 1, \ldots, j$

$$h^{(i,j)} := \left(w^{(j)}, \mathrm{z}^{(i)} \right)$$

$$w^{(j)} := w^{(j)} - h^{(i,j)} \mathrm{z}^{(i)}$$

$$h^{(j,j+1)} := \left\| w^{(j)} \right\|_2$$

$$\mathrm{z}^{(j+1)} := \frac{1}{h^{(j,j+1)}} w^{(j)}$$

Solve $\min \left(\left\| \beta e_1 - H^{(m)} y \right\|_2 \right)$ e.g. by Givens rotation,

Approximate solution : $x^{(m)} = x^{(0)} + V^{(m)} y$

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$$\left.\begin{aligned}
&\text{for } j = 1,2,\ldots,m \\
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\end{aligned}\right\}$$

Inner Arnoldi process:

- Constructs orthonormal basis of Krylov subspace via Gram Schmidt
- Coefficient matrix is upper Hessenberg matrix

$$\mathrm{H}_m = \begin{pmatrix} h^{(1,1)} & h^{(1,2)} & \cdots & \cdots & h^{(1,m)} \\ h^{(2,1)} & h^{(2,2)} & \cdots & \cdots & h^{(2,m)} \\ & h^{(3,2)} & h^{(3,3)} & & h^{(3,m)} \\ & & \ddots & & \vdots \\ & & & h^{(m,m-1)} & h^{(m,m)} \end{pmatrix}$$

- Eigenvalues of Hessenberg matrix approximate eigenvalues of original matrix on Krylov subspace:

$$\mathrm{eig}\left(\mathrm{P}^{-1,app} \frac{\partial \mathrm{R}}{\partial \mathrm{W}} \right) = \mathrm{eig}\left(\mathrm{H}_m \right) + \text{computable error bound}$$

- Error = 0 $\Leftrightarrow$ GmRes stops with exact solution

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Linearized Problem

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Influence of CFL and choice of $\frac{\partial R^{\text{app}}}{\partial W}$

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$$q_s(z) = 1 + \sum_{j=1}^{s} \beta_j z^j$$

Convergence $\Leftrightarrow \rho\left(q_s\left(P_j^{-1,\text{app}} \frac{\partial R}{\partial W}\right)\right) < 1$

Evaluate complex valued polynomial

$$P^{-1,app} \frac{\partial R}{\partial W} = \underbrace{V \Lambda V^{-1}}_{\text{Eigendecomposition}} \Rightarrow \rho\left(q_s\left(P^{-1,app} \frac{\partial R}{\partial W}\right)\right) = \rho\left(V q_s(\Lambda) V^{-1}\right) = \rho(q_s(\Lambda))$$

Approach to check correspondence of theory and applicaton

1. Compute steady state solution of nonlinear problem (density residual reduced 1e-14)

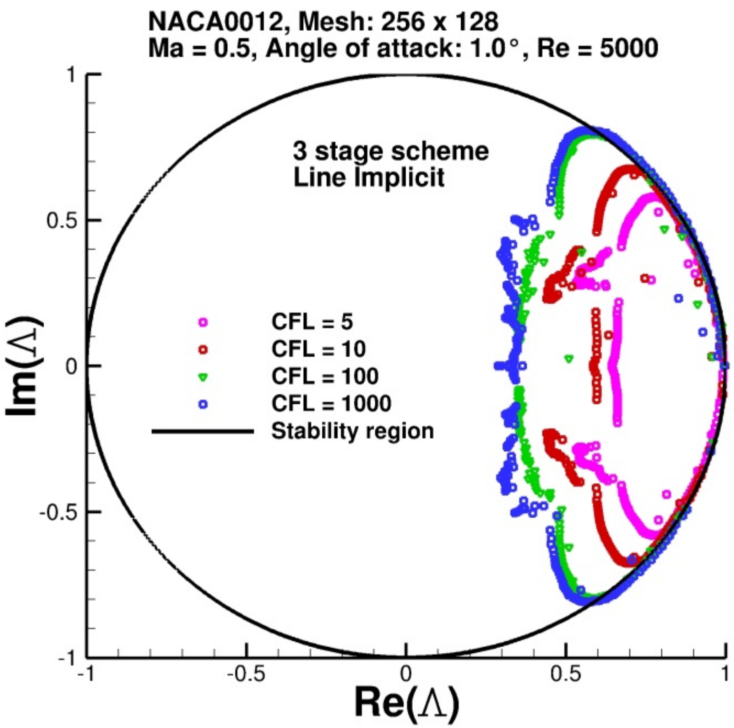
2. Determine approximate spectrum of linearized operator at steady state

3. Transform spectral data by polynomial describing the multistage solution method

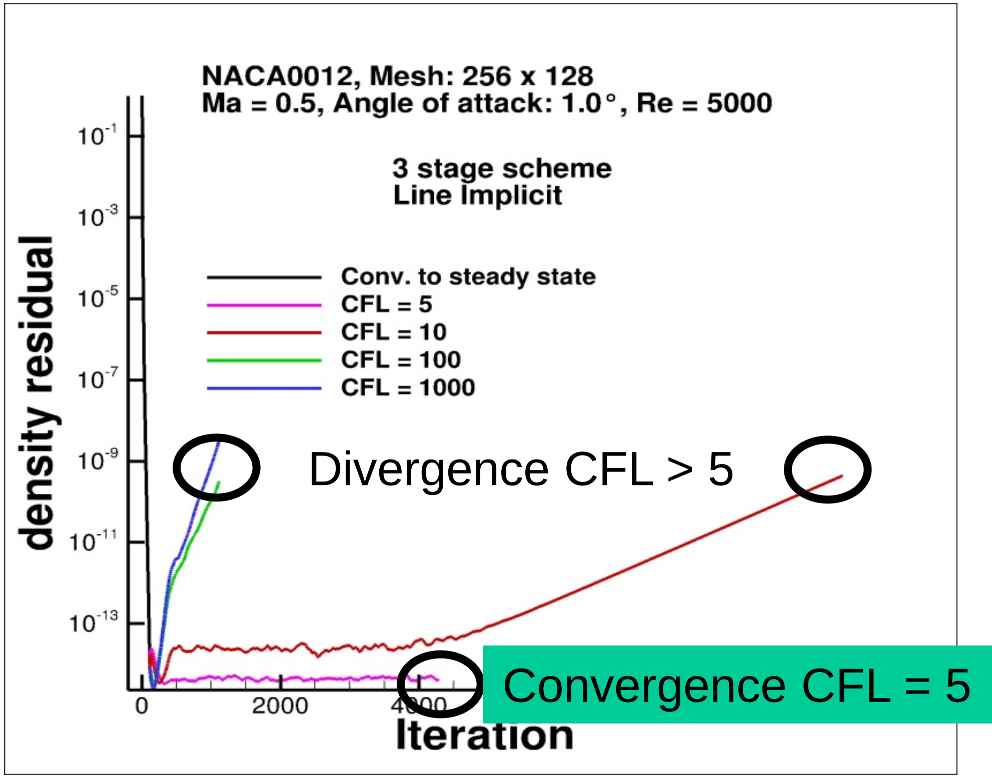
4. Determine largest absolute value of approximate eigenvalues

5. Start from steady state with chosen multistage solution method and observe behavior

Numerical example 1: Laminar flow over NACA 0012 airfoil



Eigenvalue distribution



$$\mathrm{CFL} = 5: \ \max\left|\lambda_j\right| = 0.997975$$

$$\mathrm{CFL} = 10: \ \max\left|\lambda_j\right| = 1.000179$$

$$\mathrm{CFL} = 100: \ \max\left|\lambda_j\right| = 1.013867$$

$$\mathrm{CFL} = 1000: \ \max\left|\lambda_j\right| = 1.01767$$

Weak Preconditioner:
Significant reduction of CFL number necessary

Numerical example 1: Laminar flow over NACA 0012 airfoil

Better clustering of eigenvalues when stronger linear solvers are used.

Dependency on number of sweeps and linear solver:

Line Jacobi:

$$\text{Sweeps} = 1: \ \max|\lambda_j| = 1.01760$$

$$\text{Sweeps} = 3: \ \max|\lambda_j| = 1.003566$$

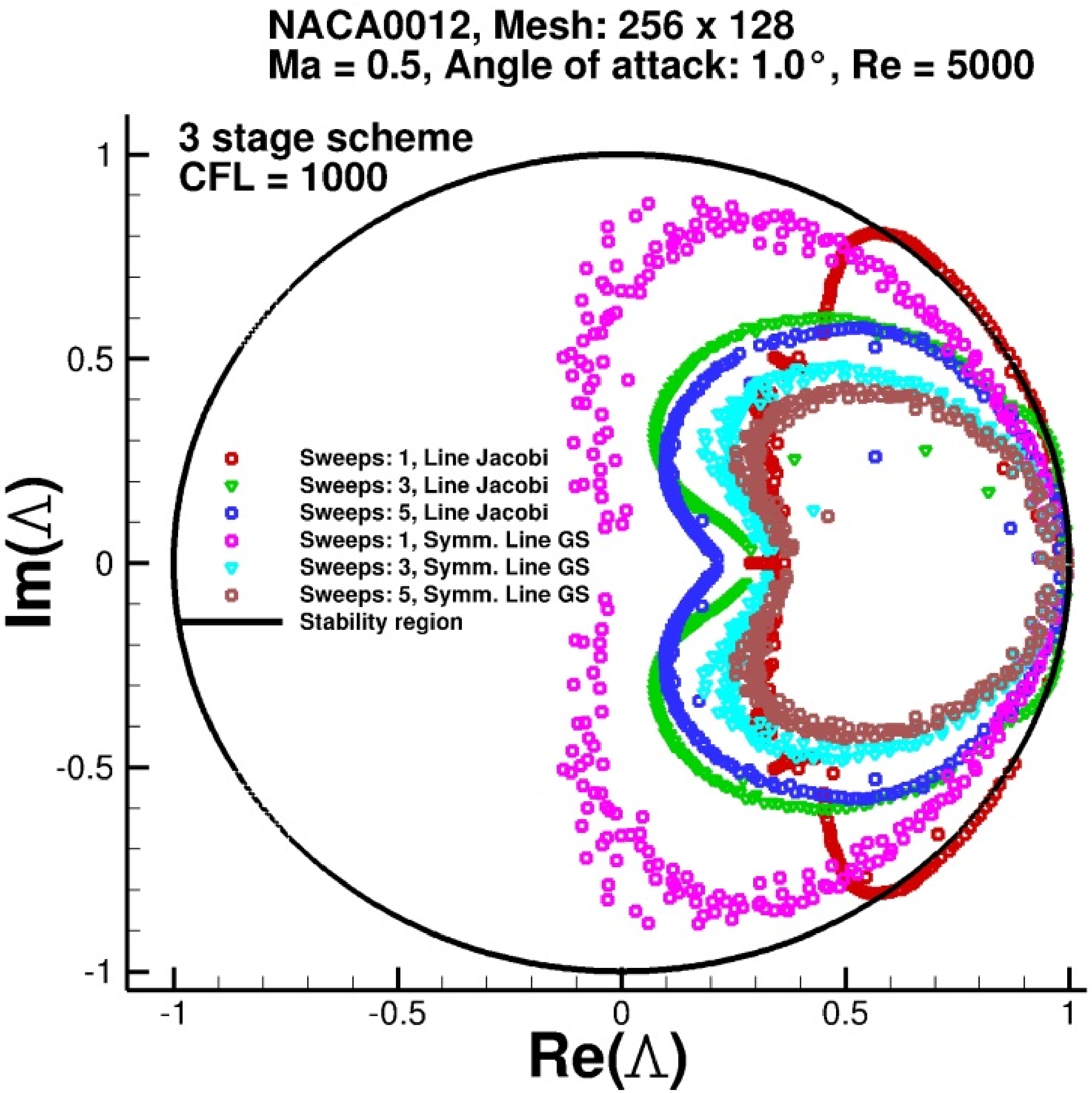
$$\text{Sweeps} = 5: \ \max|\lambda_j| = 0.989747$$

Symm. Line Gauss-Seidel:

$$\text{Sweeps} = 1: \ \max|\lambda_j| = 0.994866$$

$$\text{Sweeps} = 3: \ \max|\lambda_j| = 0.981674$$

$$\text{Sweeps} = 5: \ \max|\lambda_j| = 0.976196$$



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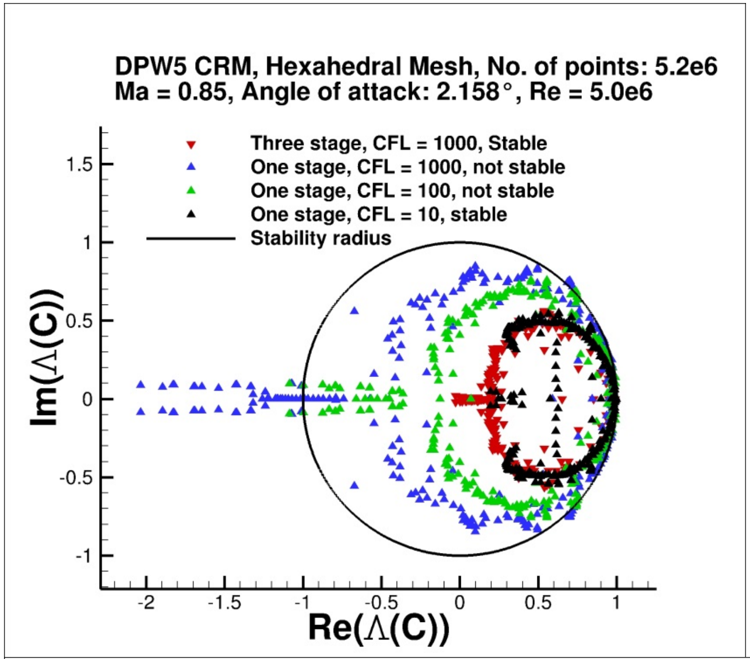
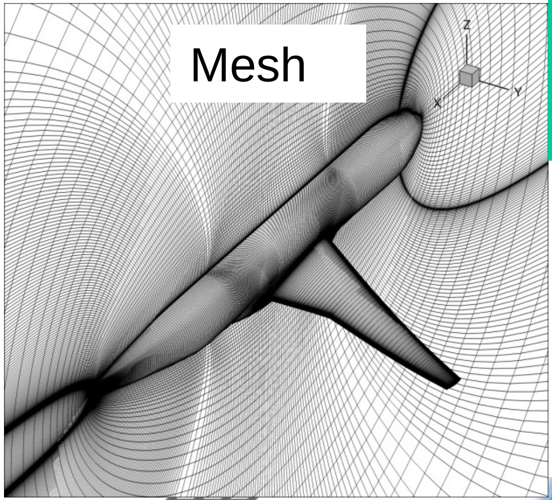
Numerical example 2: Turbulent flow over DPW 5 CRM

Analysis for mesh with 5.2e6 points:

Investigation of number of stages
With respect to symmetric Line Gauss-Seidel method and different CFL numbers:
Sweeps: 5

One stage: CFL = 1000 → unstable
One stage: CFL = 100 → unstable
One stage: CFL = 10 → stable
Three stage: CFL = 1000 → stable

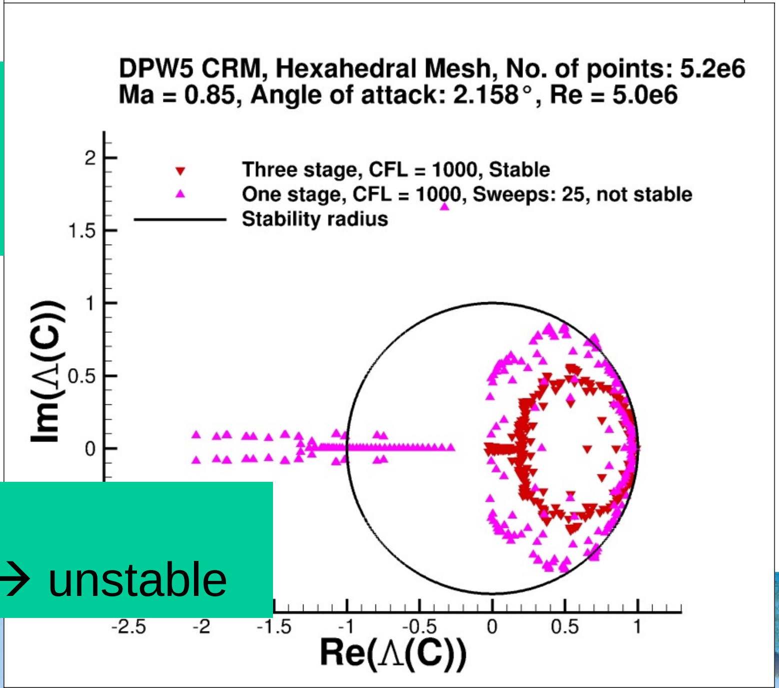




Significant reduction of CFL necessary for one stage schemes

Additional effort does not pay of

Sweeps: 25
One stage: CFL = 1000 → unstable



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Numerical example 3: Turbulent flow over DPW 5 CRM

Analysis for mesh with 41.2e6 points:

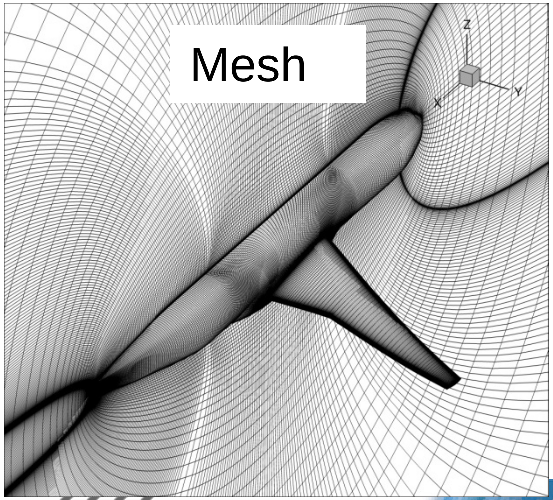
Investigation of number of stages With respect to symmetric Line Gauss-Seidel method:

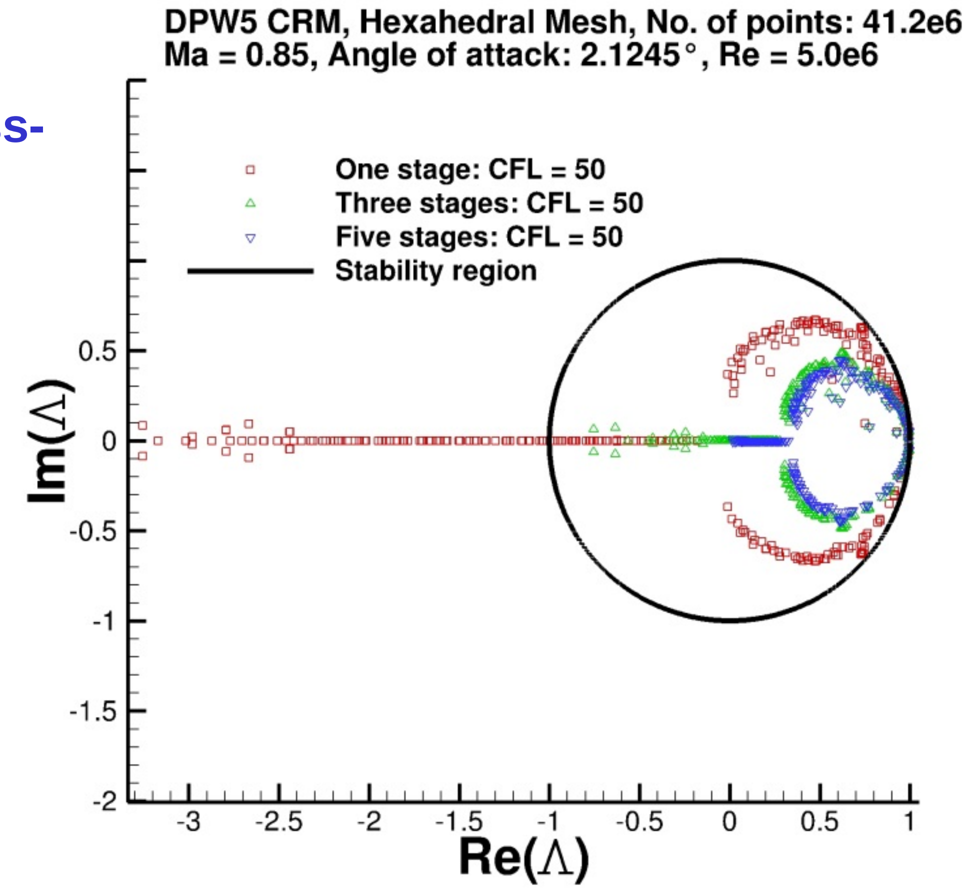
CFL = 50, Sweeps: 5

$$\text{Stages} = 1:\ \max\left|\lambda_j\right| = 3.390514$$

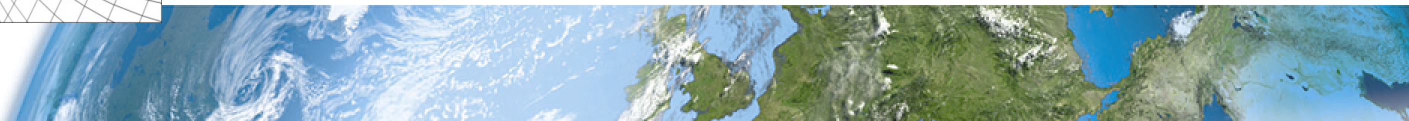
$$\text{Stages} = 3:\ \max\left|\lambda_j\right| = 0.997233$$

$$\text{Stages} = 5:\ \max\left|\lambda_j\right| = 0.996946$$





Only three and five stage method are stable



Conclusion 1: Evaluation of analysis tool

- Analyis shows good correlation of theory and application
    - if instability is predicted by method, this instability was also observed in application
- Analysis tool comprises the actual flow solver including boundary conditions and all other terms, **no severe simplifications** such as in classical Fourier analysis are assumed
- Analysis tool only deals with approximate spectral data
- Multigrid is not included
- a-posteriori tool (steady state solution required)

Conclusion 2: Evaluation of solution methods

- Analyis shows good correspondence to the heuristic expectations
- Weak solution methods (point/line implicit) show stability only for small CFL numbers already for basic testcases
- Improving the linear solvers (including lines, Gauss-Seidel instead of Jacobi, symmetric sweeps) allows for larger CFL numbers and gives additional stability
- Use of multistage methods has an additional stabilizing effect, in particular for large scale three dimensional flows

Future work

- Use analysis tool to optimize stage coefficients of multistage methods
- Include multigrid into the analysis tool
- In principle one can compute at any state spectral data → Computation diverges, compute spectral data and analyze

→ Development of tool which can be used in daily engineer‘s work to help better understand the behavior of CFD codes

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Questions?