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LU-SGS preconditioned Newton-Krylov solver applied to industrial relevant test cases

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DLR-TAU is a compressible flow solver based on finite volume methods on unstructured grids. Over the last years, this CFD code has matured and is now regularly employed on industrial applications. The working horse in TAU is the Lower Upper Symmetric Gauss-Seidel (LU-SGS) scheme [2] which is used as (single grid) solver or as smoother in an agglomeration multigrid. Including inviscid flux Jacobians, eigenvalues and an (implicit) local time step size this LU-SGS relaxation scheme was shown to be stronger than the traditionally used explicit Runge-Kutta iteration schemes. Nevertheless, these explicit and slightly implicit relaxation schemes are too weak to solve some of the more complex flow problems causing the flow solver to stall or even to diverge.
Given our previous experience on implicit solvers developed in other flow solvers (cf. [4] in the context of Discontinuous Galerkin methods and [3] in the context of FV methods), we now present the development of a new fully implicit solver in the DLR-TAU code. It is based on the Backward Euler method which replaces the LU-SGS iteration as single grid solver or multigrid smoother. Applied to nonlinear steady state problems, this implicit time integration method iterates in pseudo-time and recovers Newton's method when the CFL number and thus the local time-step size tends to infinity. Each Backward Euler step involves a linear problem which is solved using the preconditioned Generalized Minimum Residual (GMRes) method. This Krylov solver is right preconditioned with a single forward and backward sweep of the LU-SGS scheme. By increasing the number of LU-SGS sweeps within one GMRes iteration step, the condition number of the linear problems can be further reduced making the iterated LU-SGS scheme a stronger preconditioner for the GMRes method allowing the use of fewer Krylov iterations and vectors (with reduced memory requirements). Each GMRes iteration requires multiplication of the system matrix with a vector. This matrix includes the mass matrix divided by the local time step size and the (complete) Jacobian matrix which is given by the derivative of the residual vector with respect to conservative variables. This matrix-vector multiplication is implemented matrix-free by approximating it with a (one-sided or symmetric) difference quotient of residual vector evaluations. Also the LU-SGS preconditioner is matrix-free such that the resulting overall LU-SGS preconditioned Newton-Krylov method is realized matrix-free. The related memory requirements are significantly lower than using an assembled (and stored) system matrix and/or matrix-based preconditioners like an Incomplete Lower-Upper (ILU) decomposition of the system matrix. Newton's method provides a very fast (ideally quadratic) convergence once the solution iterate is sufficiently close to the solution. Starting with any initial solution (e.g. with free-stream quantities), one of the main challenges is to find a solution iterate which is in the region of attraction of Newton's method. Four (so-called globalization) techniques are implemented to address this issue:

- Full multigrid is used as the primary solver for the computations. The solution process is started on an agglomerated coarse grid level. This coarse grid solution is then interpolated to the next finer grid level where it serves as a start solution of the implicit solver. On all but the coarsest grid level a V-cycle is applied.
- The Backward Euler can be viewed as a relaxation of Newton's method.
- The Switched Evolution Relaxation (SER) method is employed to start the solution with a small CFL number CFL_{init}, and subsequently increase it according to $CFL_{new} = CFL_{init}*(||R_{freestream}||_{L2}/||R_{current}||_{L2})^{\alpha}$, where α is 0.4 for 3D turbulent cases.

- Some of the Backward Euler steps may still diverge. This is treated by a 'solver recovery' method which repeats divergent steps with half the CFL number for increased stability.

The SA-negative version [1] of the Spalart-Allmaras one equation turbulence model is used for all computations. The developments have been applied to 2D and 3D test cases. In the following, the results of two 3D test cases are shown:

Case 1: *Delta wing with attached sting* at M = 0.869, Re = 59.6×10^6 and an angle of attack of 24.7°. On an unstructured grid with 4.6×10^6 points this flow problem is solved using a full multigrid V5 cycle. Figure 1 (left) shows the resulting convergence history of the density residual. Here, we compare the performance of the baseline solver (pure LU-SGS) with that of the Newton-Krylov solver. The latter is employed with different numbers of Krylov vectors. As can be seen, the use of 20 Krylov vectors is sufficient to reach convergence below 10^{-10} and outperforms the baseline solver in terms of computing time. Figure 1 (right) shows flow streamlines indicating a large wing tip vortex on the upper side of the wing.

Case 2: *High-lift wing with installed missile* at M = 0.15, Re = 3.4×10^6 and an angle of attack of 20°. On an unstructured grid with 23×10^6 points this flow problem is solved using again a full multigrid V5 cycle. Figure 2 (left) shows the resulting convergence history of the density residual. For this test case, the baseline solver stalls. Also the GMRes solver with 50 Krylov vectors stalls due to the linear problems not being solved sufficiently. By increasing the number of Krylov vectors to 100, the solutions to the linear problems are improved and the Newton-Krylov solver converges with the density residual being reduced by 11 orders of magnitude. Furthermore, by keeping 50 Krylov vectors and strengthening the preconditioner helps to converge the problem, as can be seen, when using 3 sweeps of LU-SGS preconditioner (blue line in Figure 2 (left)). In Figure 2 (right), we see the pressure distribution over the geometry surface and the streamlines indicating the complexity of the flow. Given that the baseline solver stalls for this test case, we see that the proposed Newton-Krylov solver is more robust and more efficient than the baseline solver.

Figure 1: Delta wing with attached sting: ***(Left)*** *Convergence history of density residual vs. real time in hours,* ***(right)*** *pressure distribution on wing and streamlines.*

Figure 2: High-lift wing with installed missile: ***(Left)*** *Convergence history of density residual vs. real time in hours,* ***(right)*** *pressure distribution on wing and streamlines.*

References

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