On Nonlinear Preconditioners in Newton-Krylov-Methods for Unsteady Flows

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October 14, 2008

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Abstract

The application of nonlinear schemes like dual time stepping as preconditioners in matrix-free Newton-Krylov-solvers is considered and analyzed. We provide a novel formulation of the left preconditioned operator that says it is in fact linear in the matrix-free sense, but changes the Newton scheme. This allows to get some insight in the convergence properties of these schemes which are demonstrated through numerical results.

Keywords: Unsteady flows, Preconditioning, Newton-Krylov

1 Introduction

As was shown by Jameson and Caughey in [2], the solution of steady Euler flows is today possible in three to five multigrid steps. Thus, two dimensional flows around airfoils can be solved on a PC in a matter of seconds. The solution of the steady RANS equations is more difficult and takes about fifty steps. Nevertheless this means that adequate methods for steady flows exist and the next big challenge for computational fluid dynamics is the computation of unsteady problems. Now, for a lot of applications, the interesting flow phenomena are not on the scale of the fast acoustic eigenvalues, but on the scale of the convective eigenvalues. This makes implicit schemes for time integration much more interesting than explicit schemes, which are then severely restrained by the CFL condition. Usually, A-stable methods like BDF-2 are employed. For implicit schemes, their applicability is determined by the availability of fast solvers for the arising large nonlinear equation systems.

Using dual time stepping, the above mentioned multigrid method can be used for unsteady flows. This results in a good method for Euler flows, but for the Navier-Stokes equations, dual time stepping was observed to be very slow for some cases, in particular for turbulent flows on high aspect ratio grids. The alternative to this is to use Newton's method, which requires the solution of large sparse linear equation systems, usually by preconditioned Krylov subspace methods like GMRES or BiCGSTAB. Due to the excessive memory requirements for Navier-Stokes flows in three dimensions, matrix-free methods that circumvent computation and storage of the jacobian are an attractive alternative, see the overview paper by Knoll and Keyes [5]. Newton's method suffers from the problem that convergence is guaranteed only in a neighborhood of the solution and that the linear equation systems become more difficult to solve, the larger the chosen time step is. All in all it must be said that currently, no fast solver exists for this type of nonlinear equation systems.

To improve upon the existing methods, a few approaches have been tried. Jameson and Hsu suggest in [3] to use one step of the ADI method, followed by few multigrid steps for the dual time problem, which is similar to using one Newton step, followed by dual time stepping. Bijl and Carpenter on the other hand use k_1 dual time stepping up front, followed by k_2 steps of Newton's methods, see [1]. Both report an improvement in comparison to the base pure dual time stepping scheme.

In this paper, we will explore the techniques of blending dual time stepping with Newton's method further. In particular, the idea of using dual time stepping as nonlinear preconditioner for the linear solver will be examined. This was first tried by Wigton, Yu and Young in 1985 [10], lately by Mavriplis [6] and Bijl and Carpenter [1]. Here, we provide a novel formulation for the nonlinearly left preconditioned operator in the matrix-free case that gives new insight into those methods.

2 The governing equations

The Navier-Stokes equations are a second order system of conservation laws (mass, momentum, energy) modeling viscid compressible flow. We consider the two dimensional case, written in conservative variables density ρ, momentum $\mathbf{m} = \rho\mathbf{v}$ and energy per unit volume ρE:

$$\begin{aligned}
\partial_t \rho + \nabla \cdot \mathbf{m} &= 0, \\
\partial_t m_i + \sum_{j=1}^{2} \partial_{x_j}(m_i v_j + p\delta_{ij}) &= \frac{1}{Re}\sum_{j=1}^{2} \partial_{x_j} S_{ij}, \qquad i = 1, 2, \\
\partial_t(\rho E) + \nabla \cdot (H\mathbf{m}) &= \frac{1}{Re}\sum_{j=1}^{2} \partial_{x_j} \left(\sum_{i=1}^{2} S_{ij} v_i - \frac{1}{Pr} W_j \right).
\end{aligned}$$

Here, $\mathbf{S}$ represents the viscous shear stress tensor and W the heat flux. As the equation are dimensionless, the Reynoldsnumber Re and the Prandtlnumber Pr appear. The equations are closed by the equation of state for the pressure $p = (\gamma - 1)\rho e$.

3 The Method

The standard method to solve this type of equations are finite volume methods. We consider some general finite volume space discretization, which is represented by the grid function $R(w)$, which acts on the vector of all conserved variables w:

$$(Vw)_t + R(w) = 0,$$

where the diagonal matrix V represents the volume of the cells of the grid. As time integrator we use BDF-2 which results for a nonmoving grid and a fixed timestep Δt in the equation

$$\frac{V}{\Delta t}(\frac{3}{2}w^{n+1} - \frac{4}{2}w^n + \frac{1}{2}w^{n-1}) + R(w^{n+1}) = 0.$$

Multiplying by two, we define the function $F(w)$ to obtain the nonlinear equation system for the unknown $w = w^{n+1}$

$$F(w) = \frac{V}{\Delta t}(3w - 4w^n + w^{n-1}) + 2R(w) = 0. \tag{1}$$

3.1 Newton-Krylov-Method

The numerical solution of the above nonlinear equation system can be done using Newton's method. One Newton step is given by:

$$(\frac{3}{\Delta t}V + 2\frac{\partial R(w)}{\partial w})|_{w^{(k)}} \Delta w = -F(w^{(k)})$$

$$w^{(k+1)} = w^{(k)} + \Delta w.$$

We solve this linear equation system with system matrix $A = (\frac{3}{\Delta t}V + 2\frac{\partial R(w)}{\partial w})|_{w^{(k)}}$ using matrix free Krylov subspace methods. These approximate the solution to the linear system in the Krylov subspace

$$x_0 + \text{span}\{r_0, Ar_0, A^2r_0, ..., A^{m-1}r_0\}.$$

Since Krylov subspace methods never need the matrix A explicitely, but only matrix-vector products, we circumvent the expensive computation of the Jacobian to obtain a matrix-free method. This is done by approximating all matrix vector products by finite difference approximations of directional derivatives:

$$Aq \approx \frac{F(w^{(k)} + \epsilon q) - F(w^{(k)})}{\epsilon} = \frac{3V}{\Delta t}q + 2\frac{R(w^{(k)} + \epsilon q) - R(w^{(k)})}{\epsilon}$$

For epsilon, we use $\epsilon = \sqrt{\frac{\epsilon_{machine}}{\|q\|_2}}$ following [7]. As reported by several authors, GMRES-like methods that have an optimality property are more suitable for this approach than methods like BiCGSTAB with short recurrences. The GMRES algorithm is iterated until the relative linear residual has dropped by some factor, whereby we restart after a fixed number of iterations to bound the memory needed. Newton is iterated until a maximal number of steps has been performed or the norm of $F(w^{(k)})$ is below some threshhold.

3.2 Dual Time stepping

The dual time stepping scheme solves the equation system (1) by adding a pseudo time derivative and computing the steady state of the following equation system:

$$\frac{\partial w}{\partial t^*} + F(w) = 0.$$

This is done using the nonlinear multigrid method for the computation of steady flows of Jameson et al. [4]. There, two special Runge-Kutta schemes for the convective and the dissipative fluxes, which have large stability regions, are used as a smoother. The prolongation Q is done using bilinear interpolation and the restriction by using volume-weighted averages of the entries of w. Convergence is accelerated by local time stepping and residual averaging. Then, a W-cycle with four or five grid levels is performed.

This results in a very fast method for Euler flows, which needs only three to five multigrid steps per time step [2]. For Navier-Stokes flows, this is significantly slower, in particular for high aspect ratio grids and turbulent flows, where sometimes more than a hundred steps are needed for convergence.

3.3 Preconditioning

The convergence speed of Krylov subspace methods can and has to be significantly improved using preconditioners. A preconditioner P^{-1} is usually a linear operator that is an approximation of A^{-1}. First, we have left preconditioning:

$$P^{-1}Ax = P^{-1}b,$$

and the Krylov subspace is changed to

$$x_0 + \text{span}\{P^{-1}r_0, P^{-1}AP^{-1}r_0, (P^{-1}A)^2P^{-1}r_0, ..., (P^{-1}A)^{m-1}P^{-1}r_0\}.$$

On the other hand, right preconditioning corresponds to

$$AP^{-1}y, \quad x = P^{-1}y,$$

so that the Krylov subspace is unchanged. Right preconditioning in the matrix-free case becomes

$$AP^{-1}q \approx \frac{F(w^{(k)} + \epsilon P^{-1}q) - F(w^{(k)})}{\epsilon} = \frac{3V}{\Delta t}P^{-1}q + 2\frac{R(w^{(k)} + \epsilon P^{-1}q) - R(w^{(k)})}{\epsilon},$$

which means that before applying A, we have to apply the preconditioner to q.

Here, we will use nonlinear schemes like dual time stepping as preconditioners. This was first tried by Wigton, Yu and Young in 1985 [10], lately by Mavriplis [6] and Bijl and Carpenter [1]. Following those, we define the nonlinear preconditioner for the matrixfree method via

$$-P^{-1}F(x) = N(x) - x. \tag{2}$$

4 Analysis of the Preconditioned Scheme

Let us first consider left preconditioning. Since N is nonlinear, we expect P^{-1} to be changing with every step, so the space in which the Krylov subspace method works would be

$$x_0 + \text{span}\{P_0^{-1}r_0, P_1^{-1}AP_0r_0, P_2^{-1}AP_1^{-1}AP_0^{-1}r_0, ...\}.$$

This is in general not a Krylov subspace. However, for the matrix-free method we have

$$P^{-1}Aq = \frac{P^{-1}F(w^{(k)} + \epsilon q) - P^{-1}F(w^{(k)})}{\epsilon}.$$

For the first term we have

$$-P^{-1}F(w^{(k)} + \epsilon q) = N(w^{(k)} + \epsilon q) - w^{(k)} - \epsilon q$$

and we obtain

$$P^{-1}Aq = \frac{-N(w^{(k)} + \epsilon q) + w^{(k)} + \epsilon q + N(w^{(k)}) - w^{(k)}}{\epsilon}.$$

Now, in the matrix free sense, this is nothing but

$$P^{-1}Aq = (I - \frac{\partial N}{\partial w})|_{w^{(k)}}q. \tag{3}$$

Thus this is not a nonlinear preconditioner, but a linear operator and may be applied to any Krylov subspace method without changes. We also obtain a representation of the preconditioner: $P^{-1} = (I - \frac{\partial N}{\partial w})|_{w^{(k)}}A^{-1}$.

The preconditioned right hand side is slightly off. In the current method, the definition of the preconditioner is applied when computing the preconditioned right hand side:

$$-P^{-1}F(w^{(k)}) = N(w^{(k)}) - w^{(k)}.$$

But, as we just saw, the correct thing would be to apply (3), resulting in

$$-(I - \frac{\partial N}{\partial w})A^{-1}F(w^{(k)}) = (I - \frac{\partial N}{\partial w})\Delta w^{(k)} = w^{(k+1)} - w^{(k)} - \frac{\partial N}{\partial w}\Delta w^{(k)}.$$

Note that this cannot be fixed easily since $w^{(k+1)}$ is an unknown. An approach would now be to approximate that, but the most reasonable approximation is $w^{(k)}$ and then we would end up with a zero right hand side and no update for Newton.

We will now use the novel formulation (3) to look more closely at the properties of the new method. In particular, it becomes clear that $I - \frac{\partial N}{\partial w}|_{w^{(k)}}$ is not necessarily better than A for convergence. For the special case of the dual time stepping method, the preconditioner is equal to the original value plus an update from the multigrid method: $N(w) = w + MG(w)$. We thus obtain

$$I - \frac{\partial N}{\partial w} = \frac{\partial MG}{\partial w}.$$

If the dual time stepping stalls, for example because we are close to a steady state, this is close to zero and may be ill conditioned and thus hinder convergence.

A more favorable approach is right preconditioning:

$$AP^{-1}y = b, \quad x = P^{-1}y.$$

This uses the same Krylov subspace, but after the iteration is finished, the solution has to be transformed back. Problems:

1. GMRES uses basisvectors of the solution space. We don't know how to apply multigrid to something like Δw.

2. Since P^{-1} might be variable, we do not really know what the proper backtransformation would be.

Problem 2 is solved by the flexible GMRES method [8], but not problem 1. Both problems are solved by GMRES-* [9], works with residualvectors. * represents the right preconditioner. For $* = I$, we obtain GCR, which is algebraically equivalent to GMRES.

Nonlinear right preconditioning is applied via:

$$P^{-1}r_m \approx P^{-1}F(w^{(k)} + x_m) = w^{(k)} + x_m - N(w^{(k)} + x_m).$$

This is a truly nonlinear method.

5 Numerical Experiments

Our basic multigrid solver is UFLO103 developed by Jameson et. al. As numerical flux function, we employ the central scheme of Jameson, Schmidt and Turkel (JST-scheme).

5.1 Effect on linear solver

At first we consider the effect of the nonlinear preconditioner on the linear iterative scheme. The first test case is the computation of the steady state around the NACA0012 airfoil at Mach 0.796 and zero angle of attack.

At first, we consider viscous flow on a 256×64 mesh. In an initial phase, perform 20 steps of the steady state solver. Then, we switch to the instationary solver, so that we are still in a phase of the computation where instationary effects are present. Shown is the convergence history of different solvers for the first linear system to be solved. We iterate until the norm of the residual has dropped by three orders of magnitude. In figure 1 we can see that the nonlinear preconditioner improves the convergence speed significantly, whereas the unpreconditioned solver stagnates.

As a second test case, we consider Euler flow on a 192×32 mesh. where we have computed the steady state already and the steady state multigrid solvers has slowed down (NACA0012, Mach 0.796). Again we show the convergence history for the first linear system to be solved. It can be seen in figure 2 that now, the preconditioned scheme is not an improvement over the unpreconditioned scheme. Apparently, $N(w)$ is close to the identity.

It can also be seen that after some iterations, GCR and GMRES, although being mathematically equivalent, start to deviate due to rounding errors.

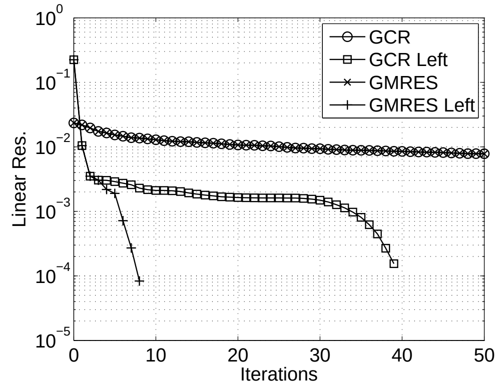

Figure 1: Linear Res. vs. Iter. for one system for unsteady viscous flow

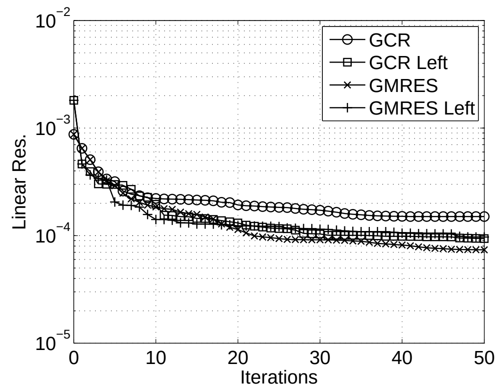

Figure 2: Linear Residual vs. Iterations for one system for stationary Euler flow

5.2 Effect on nonlinear solver

We now consider the effect of left preconditioning on Newton convergence. As we saw from the analysis, the nonlinear left preconditioner changes the right hand side of the linear system, so that the preconditioned system is no longer equivalent to the original one. While we saw in the first example that left preconditioning is beneficial for convergence of the linear solver in the relevant case of nonsteady flowfields, the question arises whether this affects Newton convergence. To test this, we consider one time step and look at the nonlinear residual to get an indication of the convergence of the Newton scheme.

The left picture shows one time step for the Euler flow around the NACA0012 profile from the last example, whereas the second picture shows one time step for viscous flow around a cylinder at Reylonds 100.000 and freestream Mach number 0.25, before the onset of turbulence. A 512×64 mesh was used for the second case.

As we can see, if left preconditioning is used, the residual curve stalls. This is only an indicator for the convergence of the Newton scheme, but cannot be considered good. However, it should be mentioned that for the cases we tested, the left preconditioned scheme did provide correct results.

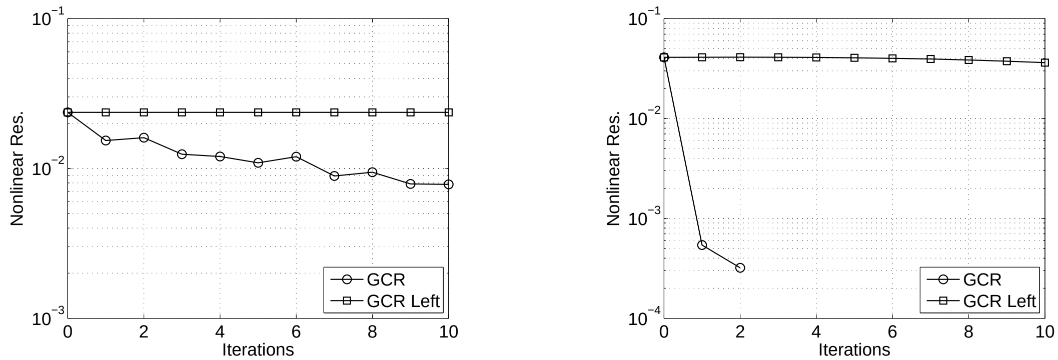

Figure 3: Convergence of Newton scheme for Euler flow (left) and for viscous flow around cylinder (right)

6 Conclusions

We found a novel formulation of the nonlinear preconditioned operator that allows to investigate the properties of such schemes better. In particular, it turns out that the left preconditioned scheme can be seen as a linear preconditioner in the matrix-free sense that changes the right hand side of the Newton scheme in a nonequivalent way. The analysis predicts specific convergence behavior for the linear and the nonlinear iterative solver which is confirmed by numerical experiments.

Acknowledgements

We'd like to thank Dr. Nawee Butsuntorn for his support in debugging the code and his helpful comments. The first author was funded by the Deutsche Forschungsgemeinschaft as part of the SFB TRR-30.

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