Blending Dual Time Stepping and Newton-Krylov Methods for Unsteady Flows

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We explore the idea of using nonlinear schemes as preconditioners in Newton-Krylov schemes for unsteady flow computations. Analysis shows that left preconditioning changes the Newton scheme in a non equivalent way, leading to a stall in Newton convergence, whereas right preconditioning leads to a sound method.

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1 Finite Volume Scheme

We consider a general finite volume discretization on a nonmoving grid, which is represented by the grid function $\mathbf{R}(\mathbf{w})$, which acts on the vector of all conserved variables w:

$$(\mathbf{V}\mathbf{w})_t + \mathbf{R}(\mathbf{w}) = \mathbf{0}.$$

The diagonal matrix V represents the volume of the cells of the grid. As an exemplary implicit time integrator we use BDF-2 which results for a fixed timestep Δt in the nonlinear equation system for the unknown $\mathbf{w} = \mathbf{w}^{n+1}$

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

which we use to define the function F(w).

1.1 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:

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

This is done using the nonlinear multigrid method for the computation of steady flows of Jameson et al [1]. For Euler flows, this needs only three to five multigrid steps per time step, whereas for Navier-Stokes flows, this is significantly slower and sometimes more than a hundred steps are needed for convergence.

1.2 Newton-Krylov-Method

The numerical solution of system (1) can also be done using Newton's method. One Newton step is given by:

$$\left(\frac{3}{\Delta t}\mathbf{V} + 2\frac{\partial \mathbf{R}(\mathbf{w})}{\partial \mathbf{w}}\right)|_{\mathbf{w}^{(k)}} \Delta \mathbf{w} = -\mathbf{F}(\mathbf{w}^{(k)}), \quad \mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} + \Delta \mathbf{w}.$$

We solve this linear equation system with system matrix $\mathbf{A} = \left(\frac{3}{\Delta t}\mathbf{V} + 2\frac{\partial \mathbf{R}(\mathbf{w})}{\partial \mathbf{w}}\right)|_{\mathbf{w}^{(k)}}$ using matrix free Krylov subspace methods. 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, using a suitable epsilon:

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

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. We will use GMRES and GCR.

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



Fig. 2 Nonlinear Res. vs. Iter. for one time step for unsteady viscous flow

1.3 Preconditioning

The convergence speed of Krylov subspace methods is improved using preconditioners. Here, we will use nonlinear schemes like dual time stepping as preconditioners, represented by N, instead of the typical linear ones. This was first tried in [2] and lately for example by Bijl and Carpenter [3]. Following these, we define the nonlinear preconditioner for the matrixfree method via

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

As was shown in [4] for the left preconditioned case, this actually corresponds in the matrix free sense to the linear operator

$$\mathbf{P}^{-1}\mathbf{A} = (\mathbf{I} - \frac{\partial \mathbf{N}}{\partial \mathbf{w}})|_{\mathbf{w}^{(k)}} \Leftrightarrow \mathbf{P}^{-1} = (\mathbf{I} - \frac{\partial \mathbf{N}}{\partial \mathbf{w}})|_{\mathbf{w}^{(k)}}\mathbf{A}^{-1}.$$
(3)

As for the right hand side, using $-\mathbf{A}^{-1}\mathbf{F}(\mathbf{x}^k) = \Delta \mathbf{w}^k$, we obtain

$$-(\mathbf{I} - \frac{\partial \mathbf{N}}{\partial \mathbf{w}})\mathbf{A}^{-1}\mathbf{F}(\mathbf{w}^{(k)}) = (\mathbf{I} - \frac{\partial \mathbf{N}}{\partial \mathbf{w}})\Delta\mathbf{w}^{(k)} = \mathbf{w}^{(k+1)} - \mathbf{w}^{(k)} - \frac{\partial \mathbf{N}}{\partial \mathbf{w}}\Delta\mathbf{w}^{(k)} \neq \mathbf{N}(\mathbf{w}^{(k)}) - \mathbf{w}^{(k)},$$
(4)

which is what the preconditioner does and thus the left preconditioned right hand side is changed in a nonequivalent way. By contrast, the right preconditioned method is truly nonlinear and does not have the presented problem of the left preconditioner of changing the right hand side of the Newton scheme. Note that unmodified GMRES cannot be used in this context, since it uses an inappropriate space of basis vectors, but GMRES-* can, see [5].

2 Numerical Results

We consider viscous flow around a cylinder at Reynolds number 100.000 and freestream Mach number 0.25, before the onset of turbulence. A 512×64 mesh was used. In figure 1, you can see the linear residual for the first system, whereas in figure 2, you can see the nonlinear residual for the first time step. As we can see, if left preconditioning is used, the nonlinear residual stalls. If we use the right preconditioned method, however, no significant improvement in convergence speed is attained and thus, different preconditioners should be employed.

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