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34 A Nonlinear Additive Schwarz Preconditioned Inexact Newton Method for Shocked Duct Flows

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Introduction

A nonlinearly preconditioned inexact Newton algorithm (PIN) was recently introduced, in [CK00], for solving large sparse nonlinear system of equations arising from the discretization of nonlinear partial differential equations. In PIN the nonlinear system $F(u) = 0$ is transformed into a new nonlinear system $\mathcal{F}(u) = 0$, which has the same solution as the original system. For certain applications the nonlinearities of the new function $\mathcal{F}(u)$ are more balanced and, as a result, the inexact Newton method converges more rapidly. In this paper, we shall use the nonlinear additive Schwarz algorithm as the preconditioner and focus on the performance of PIN for a compressible shock tube problem, which is known to be a difficult test case for inexact Newton type algorithms.

A motivating problem

We consider a one-dimensional compressible flow problem described by the full potential equation in a variable-area duct [BBH+93]. The problem is to determine the solution potential $u(x)$ satisfying

$$(A\rho u_x)_x = 0, \tag{1}$$

for $0 < x < 2$ and $u(0) = 0$ and $u(2) = u_R$ given. The duct area

$$A = A(x) = 0.4 + 0.6(x-1)^2,$$

and the density ρ is given by

$$\rho = \rho(v) = (c^2)^{1/(\gamma-1)} = \left(1 + \frac{\gamma-1}{2}(1-v^2)\right)^{1/(\gamma-1)}.$$

Here $v = u_x$ is the velocity, $\gamma = 1.4$ is the ratio of specific heat and c is the speed of sound. The flow is supersonic at each point of the interval $(0, 2)$ where the Mach number $M = |v|/c$ exceeds 1. We use a standard finite difference method to discretize (1) on a uniform mesh

$$0 = x_0 < x_1 < \cdots < x_n < x_{n+1} = 2.$$

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Let $u^h = (u_1^h, \ldots, u_n^h)^T$ be the solution vector of the finite difference problem, and

$$v_i = (u_{i+1}^h - u_i^h)/(x_{i+1} - x_i).$$

The discrete nonlinear problem is of the form:

$$A_j \tilde{\rho}_j v_j = A_{j+1} \tilde{\rho}_{j+1} v_{j+1}, \quad j = 1, \ldots, n, \tag{2}$$

where A_j denotes the midpoint value $A((x_j + x_{j+1})/2)$, and $\tilde{\rho}_j$ is an approximation of $\rho_j = \rho(x_j)$ defined using the so-called first order density biasing [BBH+93, HMS78],

$$\tilde{\rho}_j = \rho_j - \mu_j \Delta_- \rho_j,$$

where Δ_- denotes the undivided upwind difference operator, i.e., $\Delta_- \rho_j = \rho_j - \rho_{j-1}$, and where the switching function μ_j is defined as

$$\mu_j = \max_{j-k<m<j+k} \max \left\{ 0, 1 - \frac{M_c^2}{M_j^2} \right\}. \tag{3}$$

In (3), M_j is the local Mach number at $(x_j + x_{j+1})/2$ and M_c is a given cutoff Mach number taken to be 0.95 in this paper. k is the level of the switching function, which is taken to be 2 in our numerical experiments. This means that μ_j is replaced by the maximum of the 5 values centered around x_j. The switching function μ_j controls the amount of artificial viscosity. At points where $M_j < M_c$, no upwinding is applied therefore $\tilde{\rho}_j = \rho_j$. As M_j increases above M_c, $\tilde{\rho}_j$ provides an increasing amount of upwinding. In the following discussion, we denote the nonlinear system (2) in the form of a standard equation:

$$F(u^*) = 0, \tag{4}$$

where $F = (F_1, \ldots, F_n)^T$, $F_i = F_i(u_1, \ldots, u_n)$, and we drop the superscript h and simply use $u = (u_1, \ldots, u_n)^T$ to denote vectors in the space R^n. The problem looks rather simple; however, it is quite a challenging equation for the inexact Newton algorithm (IN), which is commonly used for solving such systems ([DS83, DES82, EW94]), and can briefly be described here. Suppose $u^{(k)}$ is the current approximate solution; a new approximate solution $u^{(k+1)}$ can be computed through the following steps: Find the inexact Newton direction $p^{(k)}$ such that

$$\|F(u^{(k)}) - F'(u^{(k)}) p^{(k)}\| \leq \eta_k \|F(u^{(k)})\|, \tag{5}$$

and then the new approximate solution

$$u^{(k+1)} = u^{(k)} - \lambda^{(k)} p^{(k)}.$$

Here η_k is a scalar that determines how accurately the Jacobian system needs to be solved using, for example, Krylov subspace methods [BS90, BS94, EW94, EW96]. $\lambda^{(k)}$ is another scalar that determines how far one should go in the selected inexact Newton direction [DS83]. IN has two well-known properties. First, if the initial guess is close enough to the desired solution then the convergence is very fast. Second, such a good initial guess is generally very difficult to obtain, especially for nonlinear equations that have unbalanced nonlinearities [LRW96]. The step length $\lambda^{(k)}$ is often determined by the components with the worst nonlinearities, and this may lead to an extended period of stagnation in the nonlinear residual curve; see Fig.2 for a typical picture and more in the references [CGK+98, GKM+00, JF95, PCS+99, YMB+90, YMB+91].

Descriptions of algorithms

Let us recall the nonlinearly preconditioned inexact Newton algorithms [CK00]: Find the solution $u^* \in R^n$ of (4) by solving a preconditioned system

$$\mathcal{F}(u^*) = 0. \tag{6}$$

Note that $\mathcal{F}$ and F may have different forms, but we require that they have the same solution. In general, $\mathcal{F}$ is a function of both F and u, and we do not expect to know explicitly how $\mathcal{F}$ depends on F or u. As an example, $\mathcal{F}$ may take the form of a composite function

$$\mathcal{F}(u^*) \equiv G(F(u^*)),$$

which makes G look like a preconditioner and some desirable properties of G include:

1. If $G(x) = 0$, then $x = 0$.
2. $G \approx F^{-1}$ in some sense.
3. $G(F(w))$ is easily computable for $w \in R^n$.
4. If a Newton-Krylov type method is used for solving (6), then the matrix-vector product $(G(F(w)))'v$ should also be easily computable for $w, v \in R^n$.

As in the linear equation case, the definition of a preconditioner can not be given precisely, nor is it necessary. Also as in the linear equation case, preconditioning can greatly improve the robustness of the iterative methods, since the preconditioner is designed so that the new system (6) has more uniform nonlinearities. Note that the Jacobian of the preconditioned function can be computed, at least in theory, using the chain rule; i.e.,

$$\mathcal{F}'(u) = \frac{\partial G}{\partial v}\frac{\partial F}{\partial u}. \tag{7}$$

If G is close to F^{-1} in the sense that $G(F(u)) \approx u$, then $\frac{\partial G}{\partial v}\frac{\partial F}{\partial u} \approx I$, i.e., $\mathcal{F}'(u) \approx I$. In this case, the algorithm converges in one iteration, or few iterations, depending on how close is G to F^{-1}. Most of the current research has been on the case of linear G; see, for example, [CGK+98, GKM+00, PW98]. In this paper, we shall focus on the case when G is the single-level nonlinear additive Schwarz method [CD94, DH97].

Let $S = (1, \ldots, n)$ be an index set; i.e., one integer for each unknown u_i and F_i. We assume that $S_1, \ldots, S_N$ is a partition of S in the sense that

$$\cup_{i=1}^{N} S_i = S, \text{ and } S_i \subset S.$$

Here we allow the subsets to have overlap. Let n_i be the dimension of S_i; then, in general, $\sum_{i=1}^{N} n_i \geq n$. Using the partition of S, we introduce subspaces of R^n and the corresponding restriction and extension matrices. For each S_i we define $V_i \subset R^n$ as

$$V_i = \{v | v = (v_1, \ldots, v_n)^T \in R^n, v_k = 0, \text{ if } k \notin S_i\}$$

and a $n \times n$ restriction (also extension) matrix I_{S_i} whose kth column is either the kth column of the $n \times n$ identity matrix $I_{n\times n}$ if $k \in S_i$ or zero if $k \notin S_i$. Similarly, let s be a subset

of S; we denote by I_s the restriction on s. Note that the matrix I_s is always symmetric and the same matrix can be used as both restriction and extension operator. Many other forms of restriction/extension are available in the literature; however, we only consider the simplest form in this paper.

Using the restriction operator, we define the subdomain nonlinear function as

$$F_{S_i} = I_{S_i} F.$$

We next define the major component of the algorithm, namely the nonlinearly preconditioned function. For any given $v \in R^n$, define $T_i(v) \in V_i$ as the solution of the following subspace nonlinear system

$$F_{S_i}(v - T_i(v)) = 0,$$

for $i = 1, \ldots, N$. We introduce a new function

$$\mathcal{F}(u) = \sum_{i=1}^{N} T_i(u), \tag{8}$$

which we will refer to as the nonlinearly preconditioned $F(u)$ and the corresponding algorithm additive Schwarz preconditioned inexact Newton method (ASPIN).

We remark that the evaluation of the function $\mathcal{F}(v)$, for a given v, involves the calculation of T_i, which in turn involves the solution of nonlinear systems on S_i. If the overlap is zero, then this is simply a block nonlinear Jacobi preconditioner. Assuming that all the subdomain problems are uniquely solvable, it is proved in [CK00] that the nonlinear systems (4) and (6) are equivalent in the sense that they have the same solution.

If (6) is solved using a Newton type algorithm, then the Jacobian is needed in one form or another. Let

$$J = F' = \left(\frac{\partial F_i}{\partial u_j}\right)_{n \times n} \text{ and } J_{S_i} = (I_{S_i} J I_{S_i})_{n \times n}$$

be the Jacobians of the original nonlinear system and subdomain nonlinear system, respectively. Then, as shown in [CK00], the Jacobian of the preconditioned nonlinear system can be approximated by

$$\mathcal{J} \approx \sum_{i=1}^{N} J_{S_i}^{-1} J. \tag{9}$$

(9) is an extremely interesting formula since it corresponds exactly to the additive Schwarz preconditioned linear Jacobian system of the original un-preconditioned equation. This fact implies that, first of all, we know how to solve the Jacobian system of the preconditioned nonlinear system, and second, the Jacobian itself is already well-conditioned. In other words, nonlinear preconditioning automatically offers a linear preconditioning for the corresponding Jacobian system.

Numerical experiments

We show a few numerical experiments in this section using ASPIN. In all the experiments, the subdomain Jacobian matrices J_{S_i} are formed using a finite difference scheme. The implementation is done using PETSc [BGM+01] on a cluster of workstations. In the tests, we always set $u_R = 1.15$ and the corresponding Mach distribution of the solution is given in Fig.1. The level number k in the switching function is set to 2.

We stop the global ASPIN iterations if

$$\|\mathcal{F}(u^{(k)})\| \leq 10^{-10}\|\mathcal{F}(u^{(0)})\|.$$

The global linear iteration for solving the global Jacobian system is stopped if

$$\|\mathcal{F}(u^{(k)}) - \mathcal{F}'(u^{(k)})p^{(k)}\| \leq 10^{-3}\|\mathcal{F}(u^{(k)})\|.$$

At the kth global nonlinear iteration, nonlinear subsystems

$$F_{S_i}(g_i^{(k)}) = 0,$$

have to be solved. We use the standard inexact Newton with a cubic line search for such systems with initial guess $g_{i,0}^{(k)} = 0$. The local nonlinear iteration in subdomain S_i is stopped if $\|F_{S_i}(g_{i,l}^{(k)})\| \leq 10^{-2}\|F_{S_i}(g_{i,0}^{(k)})\|$.

For comparison purposes, we first solve the problem using the regular inexact Newton's method. The Jacobian problems are solved with GMRES, and the nonlinear residual history are shown in Fig.2 for two mesh sizes $h = 1/128$ and $h = 1/256$. It can be seen clearly the convergence degenerates as the mesh is refined. In general, The finer the mesh, the longer the plateau period lasts. This happens no matter how accurately one solves the Jacobian problems. We next solve the same discrete nonlinear systems using ASPIN. We use 8 subdomains with the overlapping size equals to $5h$. The numbers of ASPIN iterations are shown in Fig.1. The iteration numbers are much smaller than that of the regular inexact Newton's method (Fig.2), and the nonlinear iteration numbers do not change that much as we refine the mesh from $h = 1/128$ to $h = 1/256$ to get a better resolution of the shock wave.

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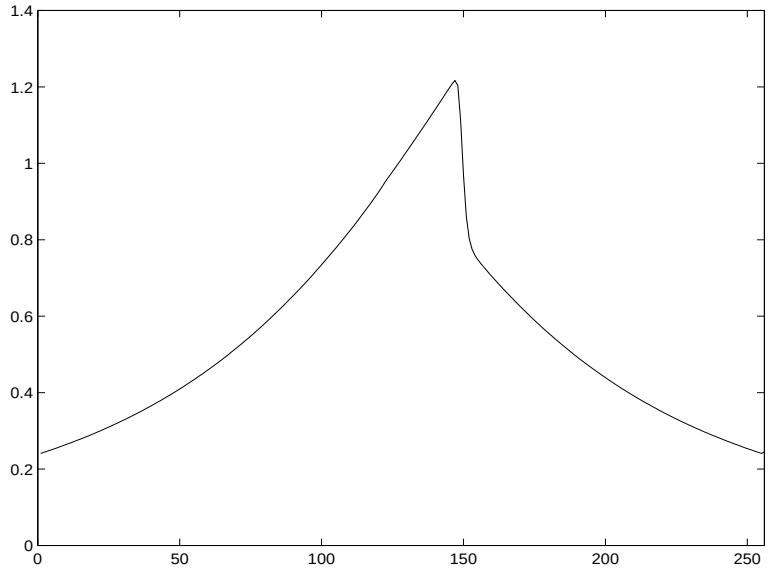

Figure 1: Mach distribution and the shock location.

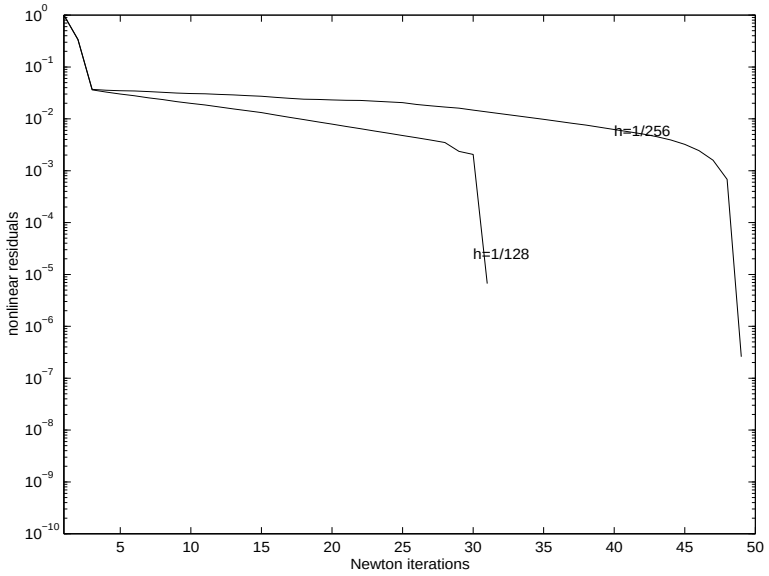

Figure 2: Nonlinear residual history of the inexact Newton's algorithm for the flow problem with mesh sizes $h = 1/128$ and $h = 1/256$.

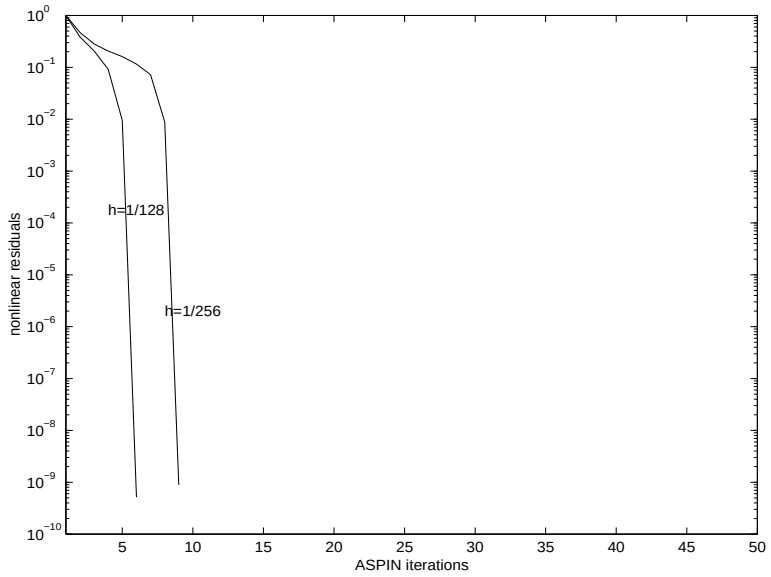

Figure 3: Nonlinear residual history of the additive Schwarz preconditioned inexact Newton's algorithm for the flow problem with mesh sizes $h = 1/128$ and $h = 1/256$.

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