

## NONLINEARLY PRECONDITIONED INEXACT NEWTON ALGORITHMS\*

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**Abstract.** Inexact Newton algorithms are commonly used for solving large sparse nonlinear system of equations  $F(u^*) = 0$  arising, for example, from the discretization of partial differential equations. Even with global strategies such as linesearch or trust region, the methods often stagnate at local minima of  $\|F\|$ , especially for problems with unbalanced nonlinearities, because the methods do not have built-in machinery to deal with the unbalanced nonlinearities. To find the same solution  $u^*$ , one may want to solve instead an equivalent nonlinearly preconditioned system  $\mathcal{F}(u^*) = 0$  whose nonlinearities are more balanced. In this paper, we propose and study a nonlinear additive Schwarz-based parallel nonlinear preconditioner and show numerically that the new method converges well even for some difficult problems, such as high Reynolds number flows, where a traditional inexact Newton method fails.

**Key words.** nonlinear preconditioning, inexact Newton methods, Krylov subspace methods, nonlinear additive Schwarz, domain decomposition, nonlinear equations, parallel computing, incompressible flows

**AMS subject classifications.** 65F10, 65H10, 65H20, 65N06, 65N12, 65N22, 65N55, 65Y05, 76D05

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**1. Introduction.** Many computational engineering problems require the numerical solution of large sparse nonlinear system of equations, i.e., for a given nonlinear function  $F : R^n \rightarrow R^n$ , compute a vector  $u^* \in R^n$  such that

$$(1.1) \quad F(u^*) = 0,$$

starting from an initial guess  $u^{(0)} \in R^n$ . Here  $F = (F_1, \dots, F_n)^T$ ,  $F_i = F_i(u_1, \dots, u_n)$ , and  $u = (u_1, \dots, u_n)^T$ . Inexact Newton algorithms (INs) [8, 9, 12, 18] are commonly used for solving such systems 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.

ALGORITHM 1.1 (IN).

*Step 1. Find the inexact Newton direction  $p^{(k)}$  such that*

$$(1.2) \quad \|F(u^{(k)}) - F'(u^{(k)})p^{(k)}\| \leq \eta_k \|F(u^{(k)})\|.$$

*Step 2. Compute the new approximate solution*

$$(1.3) \quad u^{(k+1)} = u^{(k)} - \lambda^{(k)} p^{(k)}.$$

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Here  $\eta_k \in [0, 1)$  is a scalar that determines how accurately the Jacobian system needs to be solved using, for example, Krylov subspace methods [2, 3, 12, 13].  $\lambda^{(k)}$  is another scalar that determines how far one should go in the selected inexact Newton direction [8]. We comment on our strategy for selecting  $\lambda^{(k)}$  in section 4.

IN has two well-known features: (a) if the initial guess is close enough to the desired solution, then the convergence is very fast provided that the  $\eta_k$ 's are sufficiently small, and (b) such a good initial guess is generally very difficult to obtain, especially for nonlinear equations that have unbalanced nonlinearities [20]. The step length  $\lambda^{(k)}$  is often determined by the components with the strongest nonlinearities, and this may lead to an extended period of stagnation in the nonlinear residual curve; for a typical picture, see Figure 6.2 as well as figures in [5, 15, 17, 24, 28, 29]. We say that the nonlinearities are “unbalanced” when  $\lambda^{(k)}$  is, in effect, determined by a subset of the overall degrees of freedom.

In this paper, we develop some nonlinearly preconditioned inexact Newton algorithms (PINs): Find the solution  $u^* \in R^n$  of (1.1) by solving an equivalent nonlinear system

$$(1.4) \quad \mathcal{F}(u^*) = 0.$$

Systems (1.4) and (1.1) are said to be equivalent if they have the same solution. We solve (1.4) using the inexact Newton method in the following form.

ALGORITHM 1.2 (PIN).

*Step 1. Find the inexact Newton direction  $p^{(k)}$  such that*

$$(1.5) \quad \|\mathcal{F}(u^{(k)}) - \mathcal{F}'(u^{(k)})p^{(k)}\| \leq \eta_k \|\mathcal{F}(u^{(k)})\|.$$

*Step 2. Compute the new approximate solution*

$$(1.6) \quad u^{(k+1)} = u^{(k)} - \lambda^{(k)} p^{(k)}.$$

Here the step length parameter  $\lambda^{(k)}$  is determined with a linesearch procedure based on the new merit function  $1/2\|\mathcal{F}\|^2$ .

$\mathcal{F}$  and  $F$  may have completely different forms, but they must have the same solution. In general, the linear case being an exception,  $\mathcal{F}$  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

$$\mathcal{F}(u^*) \equiv G(F(u^*)) = 0,$$

which makes  $G$  look like a preconditioner if we use the language invented for linear systems of equations. In this case, some desirable properties of the preconditioner  $G : R^n \rightarrow R^n$  include the following:

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 (1.4), 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 [14], the definition of a preconditioner cannot 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 (1.4) has more uniform nonlinearities.  $G$  is ordinarily

not operationally useful, since it is defined only implicitly. This paper could be written without reference to  $G$  by defining  $\mathcal{F}$  directly. However, the concept of a nonlinear preconditioner seems expositoryly useful. Note that the Jacobian of the preconditioned function can be computed, at least in theory, using the chain rule, i.e.,

$$(1.7) \quad \mathcal{F}'(u) = \frac{\partial G}{\partial v} \frac{\partial F}{\partial u}.$$

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, Algorithm 1.2 converges in one iteration, or a few iterations, depending on how close  $G$  is to  $F^{-1}$ . In fact, the same thing happens as long as  $G(F(u)) \approx Au$ , where  $A$  is a constant matrix independent of  $u$ . On the other hand, if  $G$  is a linear function, then  $\frac{\partial G}{\partial v}$  would be a constant matrix independent of  $u$ . In this case the Newton equation of the preconditioned system

$$\mathcal{F}'(u^{(k)})p^{(k)} = \mathcal{F}(u^{(k)})$$

reduces to the Newton equation of the original system

$$F'(u^{(k)})p^{(k)} = F(u^{(k)})$$

and  $G$  does not affect the nonlinear convergence of the method, except for the stopping conditions. However,  $G$  does change the conditioning of the linear Jacobian system, and this forms the basis for the matrix-free Newton–Krylov methods.

Most of the current research has been on the case of linear  $G$ ; see, for example, [5, 25]. In this paper, we shall focus on the case when  $\mathcal{F}$  is obtained using the single-level nonlinear additive Schwarz method. As an example, we show the nonlinear iteration history, in Figure 6.2, for solving a two-dimensional flow problem with various Reynolds numbers using the standard IN (top figure) and the newly introduced PIN (bottom figure). It can be seen clearly that PIN is much less sensitive to the increase in Reynolds number than IN. Details of the numerical experiment will be given later in the paper. Nonlinear Schwarz algorithms have been studied extensively as *iterative methods* [4, 10, 21, 22, 23, 26, 27] and are known, at least experimentally, to be not very robust, in general, unless the problem is monotone. However, we show in this paper that nonlinear Schwarz can be an excellent *nonlinear preconditioner*.

We remark that nonlinear methods can also be used as linear preconditioners as described in [7], but we will not explore this issue here.

Nested linear and nonlinear solvers are often needed in the implementation of PIN, and as a consequence the software is much harder to develop than for the regular IN. Our target applications are these problems that are difficult to solve using traditional Newton-type methods. Those include (1) problems whose solutions have local singularities such as shocks or nonsmooth fronts, and (2) multiphysics problems with drastically different stiffness that require different nonlinear solvers based on a single physics submodel such as coupled fluid–structure interaction problems.

The rest of the paper is organized as follows. In section 2, we introduce the nonlinear additive Schwarz preconditioned system and show how it reduces in certain special cases to known methods. In section 3, we derive a formula for the Jacobian of the nonlinear preconditioned system and a readily computable approximation thereto. The details of the algorithm, with some practical comments about each step, are given in section 4. Section 5 contains a proof of the equivalence of the original nonlinear system and the preconditioned system, under some reasonable local assumptions. Some

numerical experiments motivating the value of the additive Schwarz preconditioned inexact Newton algorithm (ASPIN) appear in section 6. In section 7, we make further comments and discuss some future research topics in nonlinear preconditioning.

**2. A nonlinear additive Schwarz preconditioner.** In this section, we describe a nonlinear preconditioner based on the additive Schwarz method [4, 10]. Let

$$S = (1, \dots, n)$$

be an index set, i.e., one integer for each unknown  $u_i$  and  $F_i$ . We assume that  $S_1, \dots, S_N$  is a partition of  $S$  in the sense that

$$\bigcup_{i=1}^N S_i = S \quad \text{and} \quad S_i \subset S.$$

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

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

and an  $n \times n$  restriction (also extension) matrix  $I_{S_i}$  whose  $k$ th column is either the  $k$ th 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 operators. Many other forms of restriction/extension are available in the literature; however, we consider only 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 subspace nonlinear system

$$(2.1) \quad F_{S_i}(v - T_i(v)) = 0$$

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

$$(2.2) \quad \mathcal{F}(u) = \sum_{i=1}^N T_i(u),$$

which we will refer to as the nonlinearly preconditioned  $F(u)$ . The main contribution of this paper is the following algorithm.

**ALGORITHM 2.1.** *Find the solution  $u^*$  of (1.1) by solving the nonlinearly preconditioned system*

$$(2.3) \quad \mathcal{F}(u) = 0$$

with  $u^{(0)}$  as the initial guess.

*Remark 2.1.* In the linear case, this algorithm is the same as the additive Schwarz algorithm. Using the usual notation, if

$$F(u) = Au - b,$$

then

$$\mathcal{F}(u) = \left( \sum_{i=1}^N A_i^{-1} \right) (Au - b),$$

where  $A_i^{-1}$  is the subspace inverse of  $A_i = I_{S_i} A I_{S_i}$  in  $V_i$ .

*Remark 2.2.* The evaluation of the function  $\mathcal{F}(v)$ , for a given  $v$ , involves the calculation of the  $T_i$ , which in turn involves the solution of nonlinear systems on  $S_i$ .

*Remark 2.3.* If the overlap is zero, then this is simply a nonlinear block Jacobi preconditioner.

*Remark 2.4.* If (2.3) is solved with Picard iteration, or Richardson's method, then the algorithm is simply the nonlinear additive Schwarz method, which is not a robust algorithm, as is known from experience with linear and nonlinear problems.

**3. Basic properties of the Jacobian.** If (2.3) is solved using a Newton-type algorithm, then the Jacobian is needed in one form or another. Here we provide a computable form of it and discuss some of its basic properties. Let  $J$  be the Jacobian of the original nonlinear system, i.e.,

$$J = F' = \left( \frac{\partial F_i}{\partial u_j} \right)_{n \times n},$$

and let  $J_{S_i}$  be the Jacobian of the subdomain nonlinear system, i.e.,

$$J_{S_i} = (I_{S_i} J I_{S_i})_{n \times n},$$

for  $i = 1, \dots, N$ . Note that if  $F(\cdot)$  is a sparse nonlinear function, then  $J$  is a sparse matrix and so are the  $J_{S_i}$ . Unfortunately, the same thing cannot be said about the preconditioned function  $\mathcal{F}(\cdot)$ . Its Jacobian, generally speaking, is a dense matrix and is very expensive to compute and store, as one may imagine. In the following discussion, we denote by

$$(3.1) \quad \mathcal{J} = \mathcal{F}' = \left( \sum_{i=1}^N J_{S_i} \right)_{n \times n}$$

and

$$(3.2) \quad \mathcal{J}_{S_i} = \left( \frac{\partial T_i}{\partial u_j} \right)_{n \times n}$$

the Jacobian of the preconditioned whole system and the subsystems, respectively. Because of the definition of  $T_i$ ,  $\mathcal{J}_{S_i}$  is an  $n \times n$  matrix.  $T_i(u)$  has  $n_i$  nontrivial function components in  $S_i$  and  $n$  independent variables  $u_1, \dots, u_n$ ; its other  $n - n_i$  components are zeros.

Suppose we want to compute the Jacobian  $\mathcal{J}$  at a given point  $u \in R^n$ . Consider one subdomain  $S_i$ . Let  $S_i^c = S \setminus S_i$  be the complement of  $S_i$  in  $S$ . We can write  $u =$

$(u_{S_i}, u_{S_i^c})$ , which is correct up to a reordering of the independent variables  $u_{S_i} = I_{S_i}u$  and  $u_{S_i^c} = I_{S_i^c}u$ . Using the definition of  $T_i(u)$ , we have that

$$(3.3) \quad F_{S_i}(u_{S_i} - T_i(u_{S_i}, u_{S_i^c}), u_{S_i^c}) = 0.$$

Taking the derivative of the above function with respect to  $u_{S_i}$ , we obtain

$$(3.4) \quad \left( \frac{\partial F_{S_i}}{\partial v_{S_i}} \right) \left( I_{S_i} - \frac{\partial T_i(u)}{\partial u_{S_i}} \right) = 0.$$

Here  $v_{S_i} \equiv u_{S_i} - T_i(u_{S_i}, u_{S_i^c})$ . Equation (3.4) implies that

$$(3.5) \quad \frac{\partial T_i(u)}{\partial u_{S_i}} = I_{S_i},$$

assuming the subsystem Jacobian matrix  $\frac{\partial F_{S_i}}{\partial v_{S_i}}$  is nonsingular in the subspace  $V_i$ . Next, we take the derivative of (3.3) with respect to  $u_{S_i^c}$ ,

$$(3.6) \quad -\frac{\partial F_{S_i}}{\partial v_{S_i}} \frac{\partial T_i(u)}{\partial u_{S_i^c}} + \frac{\partial F_{S_i}}{\partial u_{S_i^c}} = 0,$$

which is equivalent to

$$(3.7) \quad \frac{\partial T_i(u)}{\partial u_{S_i^c}} = \left( \frac{\partial F_{S_i}}{\partial v_{S_i}} \right)^{-1} \frac{\partial F_{S_i}}{\partial u_{S_i^c}}.$$

Note that

$$\frac{\partial T_i(u)}{\partial u} = \frac{\partial T_i(u)}{\partial u_{S_i}} + \frac{\partial T_i(u)}{\partial u_{S_i^c}}$$

since the sets  $S_i$  and  $S_i^c$  do not overlap each other. Combining (3.4) and (3.5), we obtain

$$(3.8) \quad \frac{\partial T_i(u)}{\partial u} = \left( \frac{\partial F_{S_i}}{\partial v_{S_i}} \right)^{-1} \frac{\partial F}{\partial u}.$$

Although (3.8) is computable, it is more convenient and cheaper in practice to use the following approximation:

$$(3.9) \quad \frac{\partial T_i(u)}{\partial u} \approx J_{S_i}^{-1} J.$$

Summing up (3.9) for all subdomains, we have a formula for the Jacobian of the preconditioned nonlinear system in the form

$$(3.10) \quad \tilde{J} \equiv \sum_{i=1}^N J_{S_i}^{-1} J.$$

We shall use (3.10) in numerical experiments presented later in this paper. Equation (3.10) is an interesting formula since it corresponds to the additive Schwarz preconditioned linear Jacobian system of the original unpreconditioned 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 partly well-conditioned. In other words, nonlinear preconditioning automatically offers a linear preconditioning for the corresponding Jacobian system.

**4. Additive Schwarz preconditioned inexact Newton algorithm.** We describe a nonlinear additive Schwarz preconditioned inexact Newton algorithm (ASPIN). Suppose  $u^{(0)}$  is a given initial guess, and  $u^{(k)}$  is the current approximate solution; a new approximate solution  $u^{(k+1)}$  can be computed through the following steps.

ALGORITHM 4.1 (ASPIN).

Step 1. Compute the nonlinear residual  $g^{(k)} = \mathcal{F}(u^{(k)})$  through the following steps:

(a) Find  $g_i^{(k)} = T_{S_i}u^{(k)}$ ,  $i = 1, \dots, N$ , by solving the local subdomain nonlinear systems

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

with a starting point  $g_i^{(k)} = 0$ .

(b) Form the global residual

$$g^{(k)} = \sum_{i=1}^N g_i^{(k)}.$$

(c) Check stopping conditions on  $g^{(k)}$ .

Step 2. Find the inexact Newton direction  $p^{(k)}$  by solving the Jacobian system approximately,

$$\sum_{i=1}^N J_{S_i}^{-1} J p^{(k)} = g^{(k)},$$

in the sense that

$$\left\| g^{(k)} - \sum_{i=1}^N J_{S_i}^{-1} J p^{(k)} \right\| \leq \eta_k \|g^{(k)}\|$$

for some  $\eta_k \in [0, 1)$ . Various approximations to the matrix elements of the Jacobian may be used in forming the preconditioned Jacobian vector products required in the inexact solution process.

Step 3. Compute the new approximate solution

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

where  $\lambda^{(k)}$  is a damping parameter.

ASPIN may look a bit complicated, but as a matter of fact, the required user input is the same as that for the regular IN Algorithm 1.1, i.e., the user needs to supply only two routines for each subdomain:

(1) The evaluation of the original function  $F_{S_i}(w)$ . This is needed in both Step 1(a) and Step 2 if the Jacobian is to be computed using finite-difference methods. It is also needed in Step 3 in the linesearch steps.

(2) The Jacobian of the original function  $J_{S_i}$  in terms of a matrix-vector multiplication. This is needed in both Step 1(a) and Step 2.

We now briefly discuss the basic steps of the algorithm. In Step 1(a) of Algorithm 4.1,  $N$  subdomain nonlinear systems have to be solved in order to evaluate the preconditioned function  $\mathcal{F}$  at a given point. More explicitly, we solve

$$(4.1) \quad G_{S_i} \left( g_i^{(k)} \right) \equiv F_{S_i} \left( u_{S_i}^{(k)} - g_i^{(k)}, u_{S_i^c}^{(k)} \right) = 0,$$

which has  $n_i$  equations and  $n_i$  unknowns, using Algorithm 1.1 with a starting value 0 for  $i = 1, \dots, N$ . Note that the vector  $u_{S_i^c}^{(k)} \notin V_i$  is needed to evaluate  $G_{S_i}(\xi)$  for  $\xi \in V_i$ , and this requires the ghost points in a mesh-based software implementation. In a parallel implementation, the ghost values often belong to several neighboring processors, and communication is required to obtain their current values. We note, however, that the ghost values do not change during the solution of the subdomain nonlinear system.

In Step 2, pieces of the Jacobian matrix are computed. The full Jacobian matrix  $\mathcal{J}$  never needs to be formed. In our distributed memory parallel implementation, the submatrices  $J_{S_i}$  are formed and saved, and the multiplication of  $J$  with a given vector is carried out using the submatrices  $J_{S_i}$ . Therefore the global  $J$  matrix is never needed. Several techniques are available for computing the  $J_{S_i}$ , for example, using an analytic formula, multicolored finite differencing, or automatic differentiation. A triangular factorization of  $J_{S_i}$  is also performed at this step, in our implementation, and the resulting matrices are stored.

Note that the matrix

$$\sum_{i=1}^N J_{S_i}^{-1}$$

should not be considered as a linear preconditioner since it does not appear on the right-hand side of the linear system. However, using the additive Schwarz preconditioning theory, we know that for many applications the matrix  $\sum_{i=1}^N J_{S_i}^{-1} J$  is well-conditioned, under certain conditions. We also note that if an inexact solver is used to compute  $\sum_{i=1}^N J_{S_i}^{-1} w$  in Step 2, the Newton search direction would be changed and, as a result, the algorithm becomes more inexact than a regular inexact Newton algorithm, in which the matrix is assumed to be exact but the linear system is not solved exactly.

As noted above the Jacobian system in Step 2 does not have the standard form of a preconditioned sparse linear system

$$M^{-1}Ax = M^{-1}b.$$

However, standard linear solver software packages can still be used with some slight modification, such as removing the line that performs

$$b := M^{-1}b.$$

Since the explicit sparse format of  $\sum_{i=1}^N J_{S_i}^{-1} J$  is often not available, further preconditioning of the Jacobian system using sparse matrix-based techniques, such as ILU, is difficult.

A particular interesting case is when the overlap is zero; then the diagonal blocks of  $\sum_{i=1}^N J_{S_i}^{-1} J$  are all identities and therefore do not involve any computations when multiplied with vectors. Let us take a two-subdomain case, for example,

$$J = \begin{pmatrix} J_{11} & J_{12} \\ J_{21} & J_{22} \end{pmatrix}$$

and  $J_{S_i} = J_{ii}$ ; then

$$\sum_{i=1}^2 J_{S_i}^{-1} J = \begin{pmatrix} I & J_{11}^{-1} J_{12} \\ J_{22}^{-1} J_{21} & I \end{pmatrix}.$$



The same thing can also be done for the overlapping case. This is a small savings when there are many small subspaces. However, the savings can be big if there are relatively few subspaces and the sizes are large. For example, in the case of a coupled fluid-structure interaction simulation, there could be only two subdomains: one for the fluid flow and one for the structure.

In Step 3, the step length  $\lambda^{(k)}$  is determined using a standard linesearch technique [8] based on the function

$$f(u) = \frac{1}{2} \|\mathcal{F}(u)\|^2.$$

More precisely, we first compute the initial reduction

$$(4.2) \quad s^{(k)} = (g^{(k)})^T \sum_{i=1}^N J_{S_i}^{-1} J p^{(k)}.$$

Then,  $\lambda^{(k)}$  is picked such that

$$f(u^{(k)} - \lambda^{(k)} p^{(k)}) \leq f(u^{(k)}) - \alpha \lambda^{(k)} s^{(k)}.$$

Here  $\alpha$  is a preselected parameter (use  $\alpha = 10^{-4}$ ). The standard cubic backtracking algorithm [8] is used in our computations.

**5. Some analysis of ASPIN.** In this section we provide some preliminary analysis of ASPIN. We show that, under certain conditions, the original nonlinear system (1.1) and the nonlinearly preconditioned system (2.3) have the same solution. Such analysis is trivial for the case of linear preconditioning, but not so for the case of nonlinear preconditioning. Our analysis will be based mostly on the results of [4, 10].

We consider the nonlinear problem (1.1). Let  $D$  be a neighborhood of the exact solution  $u^*$ . We assume that the function  $F(u)$  is well-defined in  $D$ , and in addition we assume the following.

ASSUMPTION 5.1.  *$F'(u)$  is continuous in  $D$  and the matrix  $F'(u^*)$  is nonsingular.*

These assumptions are satisfied, for example, for the class of monotone elliptic partial differential equations [4, 10]. Following the nonlinear additive Schwarz theory of [10], we have the following.

LEMMA 5.1 (Dryja and Hackbusch). *The subproblems (2.1) are all uniquely solvable in a neighborhood of  $u^*$  in  $D$ .*

LEMMA 5.2 (Dryja and Hackbusch). *The matrix  $\tilde{\mathcal{J}} = \sum_{i=1}^N J_{S_i}^{-1} J$  is nonsingular for any  $u$  in a neighborhood of  $u^*$  in  $D$ .*

The difference between  $\tilde{\mathcal{J}}$  and  $\mathcal{J}$  is that, in the latter case, the subdomain derivatives are taken at the point  $v_{S_i} = u_{S_i} - T_i(u_{S_i}, u_{S_i^c})$  instead of  $u_{S_i}$ . Due to the continuity assumption on  $F$ , we know that  $T_i(u) \rightarrow 0$  as  $u \rightarrow u^*$ . Therefore using Assumption 5.1, Lemma 5.1, and Lemma 5.2, it is clear that there exists a subdomain  $D'$  satisfying  $u^* \in D' \subset D$  such that the following hold.

LEMMA 5.3. *The matrix  $\mathcal{J}$ , defined by (3.1), (3.2), and (3.8), is nonsingular for any  $u \in D'$ .*

THEOREM 5.4. *Under Assumption 5.1, the nonlinear systems (1.1) and (2.3) are equivalent in the sense that they have the same solution in a neighborhood of  $u^*$  in  $D$ .*

*Proof.* Let us first assume that  $u^*$  is the solution of (1.1), i.e.,  $F(u^*) = 0$ , which immediately implies that

$$(5.1) \quad F_{S_i}(u^*) = 0.$$

By definition,  $T_i$  satisfies

$$(5.2) \quad F_{S_i}(u^* - T_i(u^*)) = 0.$$

Comparing (5.1) and (5.2), and using the local unique solvability Lemma 5.1, we must have

$$T_i(u^*) = 0$$

for  $i = 1, \dots, N$ . Therefore,  $u^*$  is a solution of (2.3); i.e.,

$$(5.3) \quad \sum_{i=1}^N T_i(u^*) = 0.$$

This proves not only that the solution of (1.1) is a solution of (2.3) but also that (2.3) has at least one solution. Next, we show that (2.3) has *only* one solution in the common neighborhood of Lemmas 5.1 and 5.2, which will then imply that the solution must be  $u^*$ .

Using Lemma 5.3, we have that  $\mathcal{F}'$  is nonsingular in a neighborhood of  $u^*$  in  $D$ ; therefore, according to the inverse function theorem of calculus, the solution is unique. This concludes the proof.  $\square$

We remark that the theorem implies that any isolated solution of the nonlinear system (1.1) in a relatively smooth region can be captured by solving the preconditioned nonlinear system. We also remark that our analysis is local, and it does not require that the nonlinear problem (1.1) have a global unique solution. As long as the solution is locally isolated, our analysis should apply.

**6. Numerical experiments.** We show a few numerical experiments in this section using ASPIN and compare with the results obtained using a standard inexact Newton's algorithm. We are mostly interested in the kind of problems on which the regular inexact Newton-type algorithm does not work well. The application of ASPIN for a full potential equation can be found in the report [6], and in this paper we shall focus our discussion on the following two-dimensional driven cavity flow problem [16] using the velocity-vorticity formulation in terms of the velocity  $u, v$  and the vorticity  $\omega$ , defined on the unit square  $\Omega = (0, 1) \times (0, 1)$ ,

$$(6.1) \quad \begin{cases} -\Delta u - \frac{\partial \omega}{\partial y} = 0, \\ -\Delta v + \frac{\partial \omega}{\partial x} = 0, \\ -\frac{1}{Re} \Delta \omega + u \frac{\partial \omega}{\partial x} + v \frac{\partial \omega}{\partial y} = 0. \end{cases}$$

Here  $Re$  is the Reynolds number. The boundary conditions are

- bottom, left, and right:  $u = v = 0$ ,
- top:  $u = 1, v = 0$ .

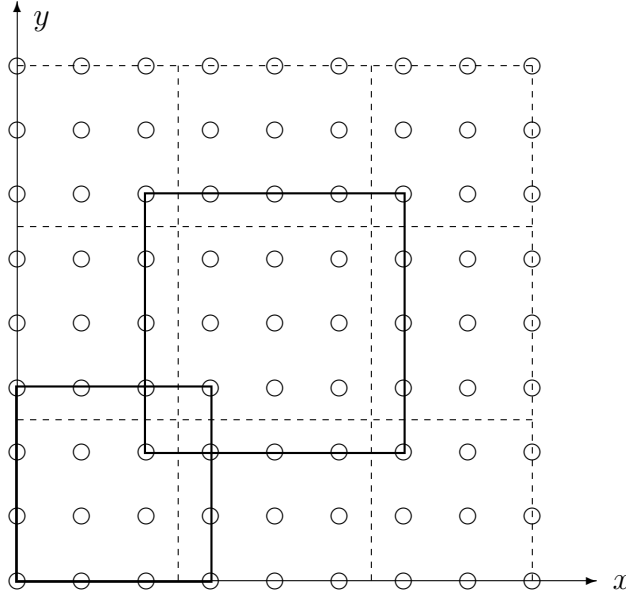


FIG. 6.1. A  $9 \times 9$  fine mesh with  $3 \times 3$  subdomain partition. The “o” are the mesh points. The dashed lines indicate a  $3 \times 3 = 9$  subdomain nonoverlapping partitioning. The solid lines indicate the “overlapping = 1” subdomains.

We vary the Reynolds number in the experiments. The boundary condition on  $\omega$  is given by its definition:

$$(6.2) \quad \omega(x, y) = -\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}.$$

The usual uniform mesh finite difference approximation with the 5-point stencil is used to discretize the boundary value problem. Upwinding is used for the divergence (convective) terms and central differencing for the gradient (source) terms. To obtain a nonlinear algebraic system of equations  $F$ , we use natural ordering for the mesh points, and at each mesh point, we arrange the knowns in the order of  $u$ ,  $v$ , and  $\omega$ . The partitioning of  $F$  is through the partitioning of the mesh points. In other words, the partition is neither physics-based nor element-based. Figure 6.1 shows a typical mesh, together with an overlapping partition. The subdomains may have different sizes depending on whether they touch the boundary of  $\Omega$ . The size of the overlap is as indicated in Figure 6.1. Note that since this is mesh-point-based partition, the zero overlap case in fact corresponds to the half-cell overlap case of the element-based partition, which is used more often in the literature on domain decomposition methods for finite element problems [11].

The subdomain Jacobian matrices  $J_{S_i}$  are formed using a multicolored finite difference scheme.

The implementation is done using PETSc [1], and the results are obtained on a cluster of DEC workstations. Double precision is used throughout the computations. The initial iterate is zero for  $u$ ,  $v$ , and  $\omega$ . Either  $2 \times 2$  or  $4 \times 4$  processor decompositions are used in all experiments reported here. We report here only the machine-independent properties of the algorithms.

**6.1. Parameter definitions.** We stop the global PIN iterations if

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

$\epsilon_{global-nonlinear} = 10^{-10}$  is used for all the tests. The global linear iteration for solving the global Jacobian system is stopped if the relative tolerance

$$\left\| \mathcal{F}(u^{(k)}) - \sum_{i=1}^N J_{S_i}^{-1} J(u^{(k)}) p^{(k)} \right\| \leq \epsilon_{global-linear-rtol} \|\mathcal{F}(u^{(k)})\|$$

is satisfied. In fact we pick  $\eta_k = \epsilon_{global-linear-rtol}$  independent of  $k$  throughout the nonlinear iterations. Several different values of  $\epsilon_{global-linear-rtol}$  are used as given in the tables found near the end of this section.

At the  $k$ th global nonlinear iteration, nonlinear subsystems

$$F_{S_i} \left( u^{(k)} - g_i^{(k)} \right) = 0,$$

defined in Step 1(a) of Algorithm 4.1, have to be solved. We use the standard IN with a cubic linesearch for such systems with initial guess  $g_{i,0}^{(k)} = 0$ . The local nonlinear iteration in subdomain  $S_i$  is stopped if the following condition is satisfied:

$$\left\| F_{S_i} \left( g_{i,l}^{(k)} \right) \right\| \leq \epsilon_{local-nonlinear-rtol} \left\| F_{S_i} \left( g_{i,0}^{(k)} \right) \right\|.$$

The overall cost of the algorithm depends heavily on the choice of  $\epsilon_{local-nonlinear-rtol}$ . We report computational results using a few different values for it.

**6.2. Comparison with a Newton–Krylov–Schwarz algorithm.** We compare the newly developed algorithm ASPIN with a well-understood inexact Newton algorithm using a cubic backtracking linesearch as the global strategy, as described in [8]. At each IN iteration, the Newton direction  $p^{(k)}$  satisfies

$$(6.3) \quad \|F(u^{(k)}) - F'(u^{(k)})p^{(k)}\| \leq \eta_k \|F(u^{(k)})\|.$$

Several values of  $\eta_k$  were tested and the results are similar. The stagnation appears in all cases. Here we show the result with  $\eta_k = 10^{-10}$ . GMRES with a one-level additive Schwarz preconditioner is used as the linear solver with the same partition and overlap as in the corresponding ASPIN algorithm. The history of nonlinear residuals is shown in Figure 6.2 (top) with several different Reynolds numbers on a fixed fine mesh of size  $128 \times 128$ .

**6.3. Test results and observations.** As the Reynolds number increases, the nonlinear system becomes more and more difficult to solve. In this paper, the Reynolds number should be understood only as a parameter that controls the nonlinearity. We do not claim that the physics of the viscous boundary layer is resolved independently of Reynolds number for our fixed discretization. The Newton–Krylov–Schwarz algorithm fails to converge once the Reynolds number passes the value  $Re = 770.0$  on this  $128 \times 128$  mesh. Standard techniques for going further would employ pseudotime stepping [19], nonlinear continuation in  $h$  or  $Re$  [29], or mesh sequencing [29]. ASPIN converges for a much larger range of Reynolds numbers, as shown in Figure 6.2, without employing any of the standard tricks. Furthermore, the number of PIN iterations does not change much as we increase the Reynolds number. A key to the

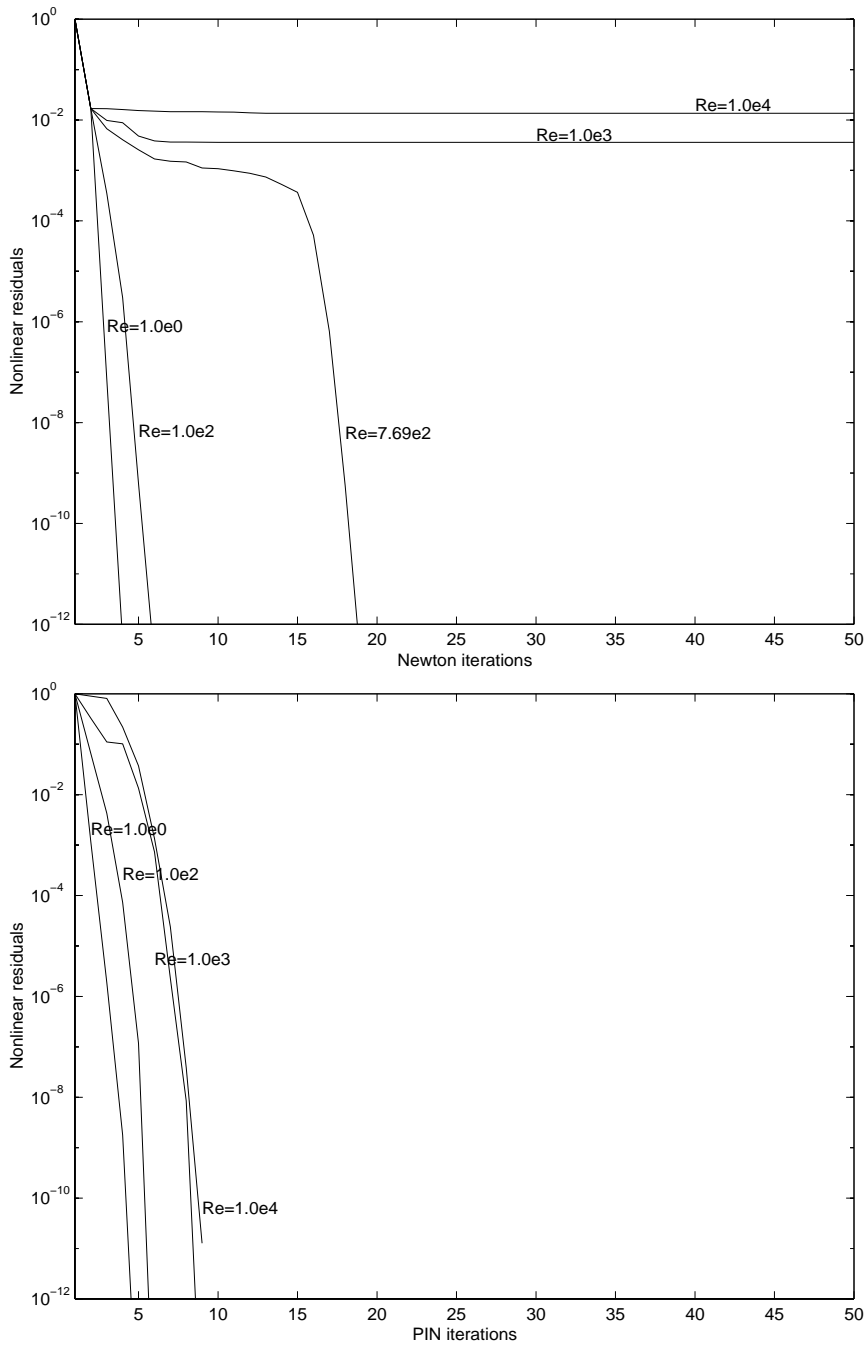


FIG. 6.2. Nonlinear residual history for the flow problem with different Reynolds numbers.

success of the method is that the subdomain nonlinear problems are well solved, which helps balance the nonlinearities of the outer Newton iterations.

In Table 6.1, we present the number of global nonlinear PIN iterations and the number of global GMRES iterations per PIN iteration for various Reynolds numbers

TABLE 6.1

Global PIN iterations. Fine mesh  $128 \times 128$ ,  $4 \times 4$  subdomain partition on 16 processors. Subdomain linear systems are solved exactly.  $\epsilon_{\text{global-linear-rtol}}$  is the stopping condition for the global GMRES iterations.  $\epsilon_{\text{local-nonlinear-rtol}}$  is the stopping condition for the local nonlinear iterations. The finite difference step size is  $10^{-8}$ .

Overlap	Number of PIN iterations				
	$Re = 10^0$	$Re = 10^1$	$Re = 10^2$	$Re = 10^3$	$Re = 10^4$
	$\epsilon_{\text{global-linear-rtol}} = 10^{-6}, \epsilon_{\text{local-nonlinear-rtol}} = 10^{-6}$				
0	2	3	4	8	7
1	2	3	4	7	7
	$\epsilon_{\text{global-linear-rtol}} = 10^{-6}, \epsilon_{\text{local-nonlinear-rtol}} = 10^{-3}$				
0	2	3	4	8	7
1	2	3	4	8	7
	$\epsilon_{\text{global-linear-rtol}} = 10^{-3}, \epsilon_{\text{local-nonlinear-rtol}} = 10^{-6}$				
0	4	4	5	7	8
1	3	3	4	7	7
	$\epsilon_{\text{global-linear-rtol}} = 10^{-3}, \epsilon_{\text{local-nonlinear-rtol}} = 10^{-3}$				
0	4	4	5	7	9
1	3	2	4	7	6
	Number of GMRES iterations per PIN				
	$\epsilon_{\text{global-linear-rtol}} = 10^{-6}, \epsilon_{\text{local-nonlinear-rtol}} = 10^{-6}$				
0	118	100	152	146	122
1	71	61	87	90	69
	$\epsilon_{\text{global-linear-rtol}} = 10^{-6}, \epsilon_{\text{local-nonlinear-rtol}} = 10^{-3}$				
0	118	100	153	141	130
1	71	62	87	80	69
	$\epsilon_{\text{global-linear-rtol}} = 10^{-3}, \epsilon_{\text{local-nonlinear-rtol}} = 10^{-6}$				
0	60	61	56	46	34
1	42	37	40	32	27
	$\epsilon_{\text{global-linear-rtol}} = 10^{-3}, \epsilon_{\text{local-nonlinear-rtol}} = 10^{-3}$				
0	60	61	56	45	37
1	42	37	40	31	26

and overlapping sizes. Two key stopping parameters are  $\epsilon_{\text{global-linear-rtol}}$  for the global linear Jacobian systems and  $\epsilon_{\text{local-nonlinear-rtol}}$  for the local nonlinear systems. We test several combinations of two values  $10^{-6}$  and  $10^{-3}$ . As shown in the table, the total number of PIN iterations does not change much as we change  $\epsilon_{\text{global-linear-rtol}}$  and  $\epsilon_{\text{local-nonlinear-rtol}}$ ; however, it does increase from 2 or 3 to 6 or 9 when the Reynolds number increases from 1 to  $10^4$ . The bottom part of Table 6.1 shows the corresponding number of GMRES iterations per PIN iteration. These linear iteration numbers change drastically as we switch to different stopping parameters. Solving the global Jacobian too accurately costs many GMRES iterations and does not result in corresponding savings in the total number of PIN iterations.

Table 6.1 also compares the results with two sizes of overlap. A small number of PIN iterations can be saved as one increases the overlapping size from 0 to 1 or more, as shown also in Table 6.2. The corresponding number of global linear iterations decreases considerably. We should mention that the size of subdomain nonlinear systems increases as one increases the overlap, especially for three-dimensional prob-

TABLE 6.2

Varying the overlapping size. Fine mesh  $128 \times 128$ ,  $4 \times 4$  subdomain partition on 16 processors. Subdomain linear systems are solved exactly.  $\epsilon_{\text{global-linear-rtol}} = 10^{-3}$  is the stopping condition for the global GMRES iterations.  $\epsilon_{\text{local-nonlinear-rtol}} = 10^{-3}$  is the stopping condition for the local nonlinear iterations. The finite difference step size is  $10^{-8}$ .

Overlap	0	1	2	3	4	5
PIN	7	7	6	6	4	6
GMRES/PIN	45	31	23	21	18	17

TABLE 6.3

Total number of subdomain nonlinear iterations. Fine mesh  $128 \times 128$ ,  $4 \times 4$  subdomain partition on 16 processors. Subdomains are naturally ordered. Subdomain linear systems are solved exactly.  $\epsilon_{\text{global-linear-rtol}} = 10^{-3}$  is the stopping condition for the global GMRES iterations.  $\epsilon_{\text{local-nonlinear-rtol}} = 10^{-3}$  is the stopping condition for the local nonlinear iterations. Overlap = 1. The finite difference step size is  $10^{-8}$ .

Subdomain #	$Re = 10^0$	$Re = 10^1$	$Re = 10^2$	$Re = 10^3$	$Re = 10^4$
$\Omega_1$	2	2	3	7	12
$\Omega_2$	2	2	3	6	8
$\Omega_3$	2	2	3	6	8
$\Omega_4$	2	2	3	7	9
$\Omega_5$	2	2	3	8	10
$\Omega_6$	2	2	3	7	10
$\Omega_7$	2	2	3	6	9
$\Omega_8$	2	2	3	9	10
$\Omega_9$	2	2	3	10	12
$\Omega_{10}$	2	2	3	9	10
$\Omega_{11}$	2	2	3	8	10
$\Omega_{12}$	2	2	3	10	10
$\Omega_{13}$	4	4	6	12	18
$\Omega_{14}$	4	4	6	13	19
$\Omega_{15}$	4	4	6	13	18
$\Omega_{16}$	4	4	7	15	19

lems. The communication cost in a distributed parallel implementation also increases as we increase the overlap. Recent experiments seem to indicate that small overlap, such as overlap = 1, is preferred when balancing the saving of the computational cost and the increase of the communication cost; see, for example, [11, 15]. Of course, the observation is highly machine- and network-dependent.

In Table 6.3, we look at the number of Newton iterations for solving the subdomain nonlinear systems. In this test case, we partition the domain into 16 subdomains, 4 in each direction, and number them naturally from the bottom to top, and left to right. Four subdomains  $\Omega_{13}$ ,  $\Omega_{14}$ ,  $\Omega_{15}$ , and  $\Omega_{16}$  touch the moving lid. The solution of the problem is less smooth near the lid, especially when the Reynolds number is large. As expected, the subdomains near the lid need more iterations—two to three times more than what is needed in the smooth subdomains for the large Reynolds number cases.

We next show how the iteration numbers change as we change the number of subdomains with a fixed  $128 \times 128$  fine mesh. The results are displayed in Table 6.4. As we increase the number of subdomains from 4 to 16 the number of global PIN iterations does not change much—up or down by 1—and is most likely due to the last bits of the stopping conditions rather than to the change of the algorithm.

TABLE 6.4

Different subdomain partitions with the same fine mesh  $128 \times 128$ . Subdomain linear systems are solved exactly.  $\epsilon_{\text{global-linear-rtol}} = 10^{-3}$  is the stopping condition for the global GMRES iterations.  $\epsilon_{\text{local-nonlinear-rtol}} = 10^{-3}$  is the stopping condition for the local nonlinear iterations. Overlap = 1. The finite difference step size is  $10^{-8}$ .

Subdomain partition	Number of PIN iterations				
	$Re = 10^0$	$Re = 10^1$	$Re = 10^2$	$Re = 10^3$	$Re = 10^4$
$N = 2 \times 2 = 4$	3	3	4	6	7
$N = 4 \times 4 = 16$	3	2	4	7	6
Number of GMRES iterations per PIN					
$N = 2 \times 2 = 4$	22	21	23	20	15
$N = 4 \times 4 = 16$	42	37	40	31	26

TABLE 6.5

Different fine meshes on 16 processors. Subdomain linear systems are solved exactly.  $\epsilon_{\text{global-linear-rtol}} = 10^{-3}$  is the stopping condition for the global GMRES iterations.  $\epsilon_{\text{local-nonlinear-rtol}} = 10^{-3}$  is the stopping condition for the local nonlinear iterations. Overlap = 1. The finite difference step size is  $10^{-8}$ .

Fine mesh	Number of PIN iterations				
	$Re = 10^0$	$Re = 10^1$	$Re = 10^2$	$Re = 10^3$	$Re = 10^4$
$32 \times 32$	3	3	4	6	6
$64 \times 64$	3	3	4	6	7
$128 \times 128$	3	2	4	7	6
Number of GMRES iterations per PIN					
$32 \times 32$	16	16	18	15	16
$64 \times 64$	25	25	24	22	20
$128 \times 128$	42	37	40	31	26

Note that when we change the number of subdomains, the inexact Newton direction changes, and as a result the algorithm changes. As a matter of fact, we are comparing two mathematically different algorithms. The bottom part of Table 6.4 shows that the number of GMRES iterations per PIN increases quite a bit as we increase the number of subdomains. In a one-level Schwarz preconditioned linear solver, we would expect the condition number to deteriorate linearly in the number of partitions in each coordinate direction and the iteration count to go up as the square root of this.

In Table 6.5, both linear and nonlinear iteration numbers are given with a fixed  $4 \times 4$  subdomain partition. The fine mesh sizes change from  $32 \times 32$  to  $128 \times 128$ . The number of Newton iterations is not sensitive to the change of the fine mesh size, but the number of linear iterations increases as we refine the mesh. This is due to that fact that we fix the overlapping size to one mesh cell. In this case, the ratio of the overlap to the subdomain size becomes smaller as we refine the fine mesh without changing the number of subdomains.

**7. Some further comments.** We comment on a few important issues concerning the newly proposed algorithm, including parallel scalabilities and load balancing in parallel implementations.

Parallel scalability is a very important issue when using linear or nonlinear iterative methods for solving problems with a large number of unknowns on machines with a large number of processors. It usually involves two separate questions, namely, how the iteration numbers change with the number of processors and with the num-



ber of unknowns. From our limited experience, the number of ASPIN iterations is not sensitive at all to either the number of processors or the number of unknowns. In other words, the number of nonlinear PIN iterations is completely scalable, as is often seen with Newton's method on PDE problems. However, this cannot be carried over to the linear solver. To make the linear solver scalable, a coarse grid space is definitely needed. Our current software implementation is not capable of dealing with the coarse space; therefore no further discussion of this issue can be offered at this point.

Load balancing is another important issue for parallel performance that we do not address in the paper. As shown in Table 6.3, the computational cost is much higher in the subdomains near the lid than in the other subdomains, in particular for the large Reynolds number cases. To balance the computational load, ideally one should partition the domain such that these subdomains that require more linear/nonlinear iterations contain fewer mesh points. However, the solution-dependent cost information is not available until after a few iterations, and therefore the ideal partition has to be obtained dynamically as the computation is being carried out.

We discussed only one partitioning strategy based on the geometry of the mesh and the number of processors available in our computing system. Many other partitioning strategies need to be investigated. For example, physics-based partitions: all the velocity unknowns as  $\Omega_1$  and the vorticity unknowns as  $\Omega_2$ . In this case, the number of subdomains may have nothing to do with the number of processors. Further partitions may be needed on both  $\Omega_1$  and  $\Omega_2$  for the purpose of parallel processing. One possible advantage of this physics-based partition is that the nonlinearities between different physical quantities can be balanced.

An extreme case of a mesh-based partition would be that each subdomain contains only one grid point. Then, the dimension of the subdomain nonlinear system is the same as the number of variables associated with a grid point, 3 for our test case. In this situation, ASPIN becomes a pointwise nonlinear scaling algorithm. As noted in [8], linear scaling does not change the nonlinear convergence of Newton's method, but nonlinear scaling does. Further investigation should be of great interest.

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