Experiences with Domain Decomposition in Three Dimensions: Overlapping Schwarz Methods

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ABSTRACT. We have implemented the two-level overlapping Schwarz methods of Dryja and Widlund for coupled elliptic systems in three dimensions. After discretizing the PDE using the finite element method, the resulting linear system is solved by the preconditioned conjugate gradient method. The preconditioner consists of two parts, a global coarse solver and local solvers associated with overlapping regions of the domain. Numerical results on the Intel iPSC/860 on a convection-diffusion problem and linear and nonlinear elasticity problems are presented.

1. Introduction

The two–level overlapping Schwarz methods, in their additive form, were introduced by Dryja and Widlund in 1987 [**12**]. Several sets of numerical experiments have been performed using these algorithms for scalar problems in two dimensions, e.g., Greenbaum [**16**], Cai [**5**], and Bjørstad and Skogen [**2**]. The analysis was extended to non–self–adjoint problems by Cai [**5**]. Around the same time, Mathew developed the algorithms in the case of mixed methods [**20**]. Extensions of the theory to many levels have been developed more recently by Dryja and Widlund [**15**] and Zhang [**26**].

In this paper we report on numerical experiments using two-level overlapping Schwarz algorithms for coupled elliptic systems in three dimensions. We have found the convergence rates to be very good and believe that overlapping Schwarz methods with small overlap offer great potential for the numerical solution of nontrivial partial differential equations on massively parallel computers.

This paper is organized as follows. In Section 2, we introduce the types of problem we propose to solve. In Section 3, we introduce the overlapping Schwarz methods and briefly review the analysis associated with them. This is followed in Section 4 by a short discussion of practical issues related to implementing these algorithms on parallel MIMD architectures. Section 5 is devoted to numerical experiments on a scalar self-adjoint PDE, the equations of linear elasticity on curved domains, a slightly nonlinear model of a vibrating piezoelectric quartz crystal used in electronic products, and a non-self-adjoint convection-diffusion problem.

2. Elliptic Problems

We are interested in nearly optimal algorithms for the solution of general, uniformly-elliptic systems of PDEs that arise in an industrial context. We assume that the nonlinear problems will be solved by solving a sequence of linear problems. Therefore we focus in this paper on the fast solution of linear elliptic problems, the equations of linear elasticity being a particular example. We also restrict our attention to second-order problems. The overlapping Schwarz methods apply equally well to self-adjoint and non-self-adjoint (subject to some restrictions; cf. Cai [7]).

Consider the partial differential equation

$$-\sum_j \sum_k \sum_l \frac{\partial}{\partial x_j} \beta_{ijkl}(x) \frac{\partial u_k}{\partial x_l} + \alpha_i u_i = f_i, \qquad \text{in } \Omega,$$

$$u = 0, \qquad\qquad\qquad \text{on } \Gamma_0 \subset \partial\Omega,$$

$$\sum_j \sum_k \sum_l \beta_{ijkl}(x) \frac{\partial u_k}{\partial n} = g_i, \qquad \text{on } \Gamma_1 = \partial\Omega \setminus \Gamma_0.$$

Using a Green's formula for each component of u separately, we obtain the variational problem

(2.1) $a_\Omega(u, v) = f(v), \quad u \in V, \ \forall v \in V,$

where

$$a_\Omega(u, v) = \int_\Omega \sum_i \sum_j \sum_k \sum_l \beta_{ijkl}(x) \frac{\partial v_i}{\partial x_j} \frac{\partial u_k}{\partial x_l},$$

$$f(v) = \int_\Omega \sum_i f_i v_i + \int_{\Gamma_1} \sum_i g_i v_i,$$

and $V = \{v \in (H^1(\Omega))^q : v|_{\Gamma_0} = 0\}$.

We solve (2.1) using conforming finite elements; cf. [11]. This provides the projection of the solution of (2.1) onto a subspace $V^h \subset V$. This procedure results in a large, sparse linear system of equations, $A\bar{u} = \bar{f}$.

3. Overlapping Schwarz Methods

The overlapping Schwarz methods are generalizations and alternatives to the alternating Schwarz method [21]. The linear system that arises from the application of the finite element method to problem (2.1) is solved by a preconditioned iterative method such as the conjugate gradient method or GMRES. (The use of an accelerator is not absolutely necessary; it does, however, improve convergence greatly at very little additional cost and therefore is always recommended.)

For Schwarz methods (cf. Dryja and Widlund [14] and Xu [25]) the preconditioner is constructed by solving a sequence of subproblems of the form: Find $T_i e \in V_i^h \subset V^h$ such that

$$a_i(T_i e, v) = a(e, v), \qquad \forall v \in V_i^h.$$

In the case $a_i(\cdot, \cdot) = a(\cdot, \cdot)$, $T_i e$ is a projection of the error e onto the subspace V_i^h. The two most common preconditioners constructed in this manner are the additive (Jacobi-like) and multiplicative (Gauss–Seidel-like) Schwarz preconditioners. However, alternative approaches are possible; see, for instance, Cai and Xu [9].

For the additive Schwarz preconditioner, the preconditioned system can be written as

$$B_A^{-1} A \bar{u} = \sum T_i \bar{u} = \bar{f},$$

where B_A^{-1} is defined implicitly by the above relationship. We note that each of the terms $T_i \bar{u}$ can be computed simultaneously in parallel.

The preconditioned system for multiplicative Schwarz can be written as

$$B_M^{-1} A \bar{u} = (I - (I - T_N) \cdots (I - T_0)) \bar{u} = \bar{f}.$$

The subspaces are treated in a serial manner. This approach seems to suggest less potential for parallel execution. In many cases, however, this need not be a problem. We color the subspaces V_i^h so that subspaces of the same color do not overlap, then update on all the subspaces of the same color in parallel.

In overlapping Schwarz methods the subspaces $V_i^h \subset V^h$ are chosen in the following manner. Assume that the domain is of diameter $O(1)$ and the elements are of diameter $O(h)$. The domain Ω is divided into N overlapping subdomains Ω_i of diameter $O(H)$. We assume that the overlap is uniformly of diameter $O(\beta)$, where $\beta > 0$. The subspaces are $V_i^h = V^h \cap W_0(\Omega_i)$, where $W_0(\Omega_i) = \{v \in (H^1(\Omega))^q : v = 0 \text{ on } \partial\Omega_i \setminus \Gamma_1\}$, i.e., we impose homogeneous Dirichlet boundary conditions on the artificial boundaries and inherit the original boundary conditions on the true boundary.

This is a one-level algorithm; as the number of subdomains, Ω_i, is increased, the convergence rate deteriorates rapidly; cf. Widlund [23]. We therefore introduce one more subspace, V_0^h, which will provide for global communication of information at each iteration. We triangulate the domain with large elements

of diameter $O(H)$ and define V_0^h to be the finite element subspace of V defined by these large elements. To get a multi-level algorithm, we simply apply the algorithm recursively to solve the coarse problem.

We are now prepared to give the convergence rates for the overlapping Schwarz methods. For the proofs we refer the reader to Dryja and Widlund [13], Widlund [24], and Bramble, Pasciak, Wang, and Xu [3].

THEOREM 3.1. *The number of iterations required for a fixed relative reduction in the energy norm of the error is bounded by* $C\sqrt{H/\beta}$. *In particular, if the overlap is of order H, then the number of iterations is bounded independent of h and H.*

We note that the matrix representation of T_i can be expressed as $T_i = R_i^T A_i^{-1} R_i A$. The restriction matrix R_i is a rectangular matrix that maps from a global vector to a local vector that represents a function in the subspace. Its transpose, R_i^T, represents interpolation from the coefficients of a function on the subspace to the coefficients of the function on the global solution space. For the local spaces, R_i simply selects those coefficients associated with the nodes that lie in Ω_i. For the coarse space V_0^h, R_i has the same structure as the restriction operator that appears in multigrid.

Remark: Multilevel Schwarz methods are conceptually not much different from multigrid methods. The multigrid "smoothing" is replaced by "local solvers"; in anisotropic, multicomponent problems where smoothing is ineffectual, solving small overlapping blocks exactly appears to make the method very robust. However, for model problems a few sweeps of Gauss-Seidel are effective enough; see Table 5. Thus the local solvers should be tuned to the particular problem being solved.

4. Implementation

We have implemented the algorithms on the Intel iPSC/860 and on networks of workstations using the p4 message passing package [4]. Most of the code is completely portable across Unix machines, and only a few library routines must be changed to run it under a different message–passing system.

To ensure maximum flexibility and code reuse, we have constructed a suite of independent libraries including a communications library, a sparse matrix library, and an iterative solvers library. In all cases, the data structures for the individual pieces are hidden. In this way, individual libraries can be changed or optimized for a particular architecture without changing the application program. The results reported in this paper were obtained by using a prototype domain decomposition code built on top of the libraries. We plan to make the libraries available via anonymous ftp.

In the prototype code the coarse problem is solved in a very naive manner; it is solved simultaneously on all of the processors. As the number of processors is increased, the coarse problem becomes too large to be solved in this way. At

this point, we will solve the coarse problem in parallel, probably by applying the code recursively.

We have implemented the parallel communications in a semi-portable manner by layering the software. On the lowest level, there is the machine–dependent communication method, whether it be via special software/hardware or via Unix IP/TCP sockets. At the next level are our generic message–passing macros, which are automatically compiled into the appropriate machine–dependent form. Above that is the BlockComm package of Gropp [17], which is a programmable communications package. The user need give only the locations of the data and when during the calculations the data is to be transferred. The details of sending and receiving the actual message packets are all hidden from the application programmer. The copies between domains in the serial version of the code simply become calls to the BlockComm package in the parallel version.

On each processor, we store the vectors and pieces of the matrices associated with from one to a small number of subdomains. For the additive variant, one subdomain per processor is fine. For the multiplicative, we generally would like to have a subdomain of each color on each processor. The size of the subdomains is then determined by the amount of memory available to an individual processor. At the present time, 16 megabytes are available per processor on the Intel iPSC/860. Modern workstations generally have around 32 megabytes of memory. For coupled systems in three dimensions this means that the subdomains must be rather small, containing only on the order of a few thousand unknowns. We find for such problems that using an overlap of one element width provides excellent convergence rates. This had previously been observed for scalar problems in two dimensions by Bjørstad, Moe, and Skogen [1], Bjørstad and Skogen [2], Cai [5], [6], and Cai, Gropp, and Keyes [8].

5. Experimental Results

We present convergence and timing results on four different elliptic PDEs. The first is a scalar example modeled on the Ellpack test problems. The second is the equations of linear elasticity on a curved domain. The third is a slightly nonlinear problem of a vibrating crystal. The fourth is a convection-diffusion equation with recirculating flow. In all examples we use an overlap of one element. We make the first problem trivial, to demonstrate that the condition numbers and convergence rates behave remarkably similarly for the simple and more difficult problems. The stopping criteria for determining iteration counts was a relative decrease in the 2–norm of the residual of 10^{-5}.

5.1. Model Problem. We consider the scalar problem

$$(e^{2xyz}u_x)_x + (e^{-yz}u_y)_y + ((1 + e^{-x}sin(y))u_z)_z = g,$$

on a rectangular parallelepiped with homogeneous boundary conditions. We use piecewise trilinear elements. In Table 1, we give some sample results as

the number of subdomains is increased. In this example the subdomains are simply cubes. The column labeled "% Co." gives the percentage of the solution time devoted to constructing and solving the coarse problem, for a multilevel implementation this time would be significantly reduced.

Remark: The condition numbers in Table 1 are not monotone because the aspect ratio of the domain changes slightly as we add additional subdomains.

TABLE 1. Convergence for the Model Problem

Number of Processors	Number of Unknowns	Additive				Multiplicative			
		κ	Its.	Time	% Co.	κ	Its.	Time	% Co.
1	3,150	16.7	17	14.1	27	1.4	6	13.1	26
2	6,090	15.5	18	15.6	30	1.3	6	14.1	29
4	12,180	17.4	20	19.2	32	1.4	6	16.8	31
8	23,548	23.4	23	22.6	34	1.7	7	19.4	34
16	46,284	17.2	19	23.9	39	1.4	6	21.6	32
32	92,568	21.2	21	30.6	40	1.6	7	26.1	40

5.2. Equations of Linear Elasticity. We refer the reader to Smith [22], and Zienkiewicz and Taylor [27] for a discussion of the equations of linear elasticity and their solution using the finite element method. We have chosen to use the 20 node, isoparametric serendipity elements for this set of experiments. In this section and the next, we concentrate on the additive form of the overlapping Schwarz method since this requires us to store only one subdomain per processor.
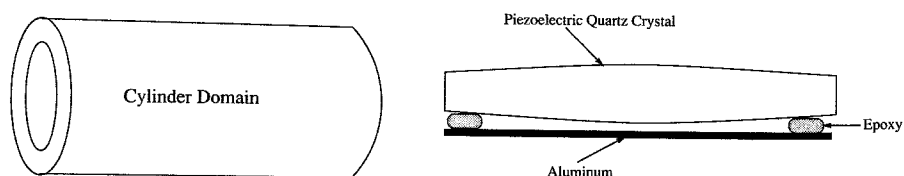

FIGURE 1. The Domains for the Test Problems

We consider the cylindrical domain as given in Fig. 1[1]. The cylinder is sliced into cylindrical rings, and each subdomain is a quarter of one of the cylindrical rings. It takes four colors to color the subdomains for multiplicative Schwarz. In Table 2 we list some convergence results for a cylinder of internal diameter 2, external diameter 3, and length 4. In the second set of columns, labeled "compressed cylinder", the length is .4, but the number of elements used is the same as in the first set of columns. This is done to observe the effect of changing the aspect ratio of the domains and elements on the convergence rate. The numbers in parenthesis indicate the number of iterations required for multiplicative Schwarz.

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[1] Figure of crystal reprinted, with permission, from Jones, Plassmann [19]

In Table 3, for a cylinder problem with $7,824$ unknowns and eight processors, we examine the behavior as Poisson's ration, ν, approaches the incompressible limit. For the row labeled $.3/.49$, we alternated the values of ν between .3 and .49 on different subdomains.

TABLE 2. Convergence in the Cylinder Problem

Number of Domains	Number of Unknowns	Cylinder			Compressed Cylinder		
		κ	Its.	Time	κ	Its.	Time
4	5,040	22	26 (10)	34.8	95	51 (20)	43.9
8	9,576	21	27 (10)	35.2	92	51 (20)	44.3
16	19,152	31	33 (12)	43.0	263	86 (34)	67.2
32	38,304	38	34 (13)	51.4	~ 813	152 (60)	111.9

TABLE 3. Convergence for Different ν in the Cylinder Problem

ν	κ	Its.	Time
.3	14.8	22	26.7
.45	26.2	27	30.0
.49	~ 50	39	34.2
$.3/.49$	46.4	37	31.4

5.3. Anisotropic Vibrating Piezoelectric Crystal Problem. Piezoelectric crystals (see Fig. 1) play an important role in most modern electronic equipment. Their mathematical and numerical modeling is important in the design of smaller and more accurate oscillators. Let Ω be an anisotropic dielectric crystal and $u(x)$ be the displacement of any point in the crystal and $\phi(x)$ be the electric potential in the crystal. We use a large displacement model of the crystal. The full strain tensor is given by

$$\epsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} + \sum_k \frac{\partial u_k}{\partial x_i}\frac{\partial u_k}{\partial x_j}\right).$$

The problem is nonlinear because we retain the cross–product terms above, rather than dropping them as is done for the linearized strain tensor. The stress tensor, σ_{ij}, and electric displacement, D_i, are given by

$$\sigma_{ij} = \sum_{kl} c_{ijkl}\epsilon_{kl} + \sum_k e_{kij}\frac{\partial \phi}{\partial x_k}, \qquad D_i = \sum_{jk} e_{ijk}\epsilon_{jk} + \sum_k d_{ik}\frac{\partial \phi}{\partial x_k}.$$

The tensors c_{ijkl}, e_{kij}, and d_{ij} are the elastic stiffness coefficient, the piezoelectric strain constant, and the dielectric permittivity, respectively. The PDEs are given by Newton's law and Gauss's law for dielectrics,

$$\sum_j \frac{\partial \sigma_{ij}}{\partial x_j} = f_i, \qquad \sum_i \frac{\partial D_i}{\partial x_i} = 0, \text{ in } \Omega.$$

Natural boundary conditions are imposed except on a small portion of $\partial\Omega$ where the crystal is fixed. Lagrangian P_2 finite elements are used to approximately solve the variational formulation of the above equations. The derivation of the variational formulation is given in Canfield, Tang, and Foster [10].

TABLE 4. Convergence for the Crystal Problem

Number of Processors	Number of Unknowns	κ	Its.	Time	% Coarse
4	4,320	44.8	25	23.0	14
8	8,460	46.8	18	24.5	25
16	17,100	203	24	35.0	37

In Table 4 we list some convergence results as we increase the number of subdomains used in modeling the crystal. The column labeled "% Coarse" gives the percentage of the total solution time devoted to constructing the coarse system contribution to the preconditioner. As was stated above, at the moment this is done in a naive serial manner, the time devoted to this when it is fully parallelized will be smaller.

In the next table, Table 5, we compare the use of a few sweeps of SSOR-CG as an approximate solver for both the model problem and the crystal problem. For the model problems the mesh on the subdomain was 6 by 6 by 6; for the crystal problem it was 4 by 5 by 3. We observe that the smoothing is very effective for the model problem but essentially useless for the crystal problem.

TABLE 5. Convergence with Local Smoothing Vs Exact Solvers

	Poisson	Model	Crystal
Number of Unknowns	8,820	8,820	8,460
Exact Local Solvers	17	21	18
2 iterations SSOR-CG	18	21	No Convergence
5 iterations SSOR-CG	21	26	320

5.4. Convection-Diffusion Problem. For our final problem we consider,

$$-\triangle u + \nu(\cos(x)\sin(y)u_x - \sin(x)\cos(y)u_y - u_z) = g,$$

on a unit cube with mixed Dirichlet and Neumann boundary conditions. The PDE is discretized with trilinear finite elements using streamline diffusion, see eg. Johnson [18]. The preconditioner is multiplicative Schwarz with eight colors. In Table 6, we report on numerical experiments with 8 processors and 64 subdomains, using several accelerators; GMRES, transpose free QMR (TFQMR), BiCG-stab, conjugate gradient squared (CGS). Since some of the the accelerators require a different number of applications of the operator per iteration we report normalized iterations (Norm. Its.); which is the number of actions of the

operator on a vector that were required for convergence. In this problem there are $22,707$ unknowns, $H = 1/4$ and $h = 1/28$.

TABLE 6. Convergence for Recirculating Flow

	$\nu = 10$		$\nu = 1000$	
Method	Norm. Its.	Time	Norm. Its.	Time
GMRES	7	16.7	30	30.9
TFQMR	10	18.6	42	35.2
CGS	10	18.5	42	35.0
BiCG-stab	10	18.5	38	32.8

6. Conclusions

Overlapping Schwarz methods have very good convergence properties for difficult coupled elliptic systems in three dimensions. Unfortunately, given the present programming languages and software tools, developing parallel, portable, and flexible codes that apply Schwarz methods for particular problems is difficult, error prone, and expensive. We hope that the tools we have developed will make the transition easier.

Acknowledgments. We thank Mark Jones and Paul Plassmann for their assistance with the piezoelectric crystal problem. We also thank Xiao-Chuan Cai for his advice and suggestions on this project.

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