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Domain Decomposition Methods for Model Parallelization

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This paper is devoted to presenting a brief overview of domain decomposition methods. Overlapping and nonoverlapping procedures are discussed. For this latter kind of method, Poincaré-Steklov operators are presented and a maximum principle is introduced. Conjugated gradient and preconditioned conjugated gradient are considered. Also Schwarz's alternating method is briefly discussed.

1. Introduction

Domain decompositon methods for the numerical solution of partial differential equations have received much attention in recent years [Chan *et al.*, 1989a, 1989b; Glowinski *et al.*, 1988, 1990; Keyes *et al.*, 1991; Quarteroni *et al.*, 1992]. At present, this is mainly due to the fact that they constitute a very effective manner of parallelizing numerical models of continuous systems. Parallel computing is already a very important resource in supercomputing and it is expected to be even more important in the future.

There are additional reasons for the interest in domain decomposition methods, such as the following: domains of irregular shape can be decomposed into subdomains of regular shape and regions of relative nonuniformity of the differential operator or roughness of the solutions can be isolated into different subdomains. This paper is devoted to presenting a brief overview of domain decomposition methods.

2. General Discussion

One approach to domain decomposition deals with the systems that are obtained after the differential equations have been discretized, but it is also possible to formulate domain decomposition procedures treating the differential equations before discretization. In this paper this latter approach will be applied because it is more elegant and has the advantage of permitting use of the known properties of partial differential equations in a more direct manner. In addition, it is always possible afterward to give discretized versions of the results so obtained.

In the exposition that follows the different methods will be derived from a unified perspective, which is based on the experience and clarity that have been gained through the considerable amount of work that has been done in recent years. This manner of presenting matters has clear expository advantages, although it does not correspond to the way in which, historically, the methods were developed.

In domain decomposition methods, the region in which the problem is formulated is split into several – usually many – subregions. Given a differential equation, consider its set of solutions at each of the subregions. Then, the main objective of domain decomposition methods is to select a solution at each subregion in such a way that some

matching conditions are satisfied. Generally, the methods may be classified into two broad categories, depending on whether such subregions do not overlap – nonoverlapping methods – or do overlap – overlapping methods. The main difference between these two kinds of procedures is the matching conditions. For elliptic equations of second order, for example, the nonoverlapping procedures require that the solution, together with its normal derivative across the common boundaries of the nonoverlapping subregions, be continuous. On the other hand, for the same kind of equations, when the procedure is overlapping, the smoothness conditions are relaxed, since only the solution itself is required to be continuous.

For elliptic differential equations of second order [Keyes and Gropp, 1987], which are the only ones to be considered in some detail in what follows, independently of the kind of domain decomposition that is applied – overlapping or nonoverlapping – knowing the restriction of the solution to the boundaries of the subregions determines uniquely the solution at the interior of the subregions, and the process of extending such restriction from the boundaries to the interior involves solving local problems only. Therefore, domain decomposition procedures frequently aim to obtain that restriction and the problem of obtaining the solution at the boundaries of the subregions may be referred as the "domain decomposition problem."

Time-dependent problems of parabolic type, when time discretization is applied, give rise to elliptic problems at each time step and the discussion presented in this paper applies to them in this manner. Some special methods for this kind of equation profit from the local behavior of the responses [Israeli and Vozovoi, 1993], but even if the methodology is not specialized, when iterative procedures are applied, the locality of the responses for this kind of equation produces rapid convergence.

3. Nonoverlapping Procedures

Consider the most general elliptic equation of second order, in any number of dimensions, written in conservative form

$$\mathcal{L}u \equiv -\nabla \cdot (\underline{\underline{a}} \cdot \nabla u) + \nabla \cdot \underline{b} u + cu = f_\Omega \tag{3.1}$$

To apply domain decomposition methods, the region Ω in which the problem is formulated is partitioned into a collection of disjoint subregions $\{\Omega_1, \ldots, \Omega_N\}$ and solutions are constructed separately in each. However, when putting such local solutions together, adequate "matching conditions" must be satisfied. They usually derive from physical requirements of the models. For Eq. (3.1), one is usually led to

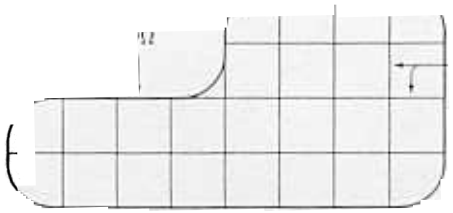
$$[u] = 0 \qquad \text{and} \qquad \left[\frac{\partial u}{\partial n}\right] = 0 \quad \text{on } \Sigma \tag{3.2}$$

where Σ is the union of the intersections of the boundaries of the subregions (see Figure 1), and the square brackets stand for the jump – across Σ – of the function contained inside.

Observe, in particular, that when the coefficients are continuous, Eq. (3.2) implies that "diffusive flux" $(\underline{\underline{a}} \cdot \nabla u) \cdot \underline{n}$ and "total flux" $(\underline{\underline{a}} \cdot \nabla u - \underline{b} u) \cdot \underline{n}$ are continuous.

Consider first the one-dimensional case, for which the region Ω will be the interval $(0, l)$ and the subregions Ω_i will be subintervals (x_{i-1}, x_i), where $i = 1, \ldots, N$. At each subinterval Ω_i, let $\overset{i}{u}$ be a function defined on Ω_i and satisfying Eq. (3.1) there. The boundary values which are relevant in Ω_i, constitute a 4-D vector

$$\overset{i}{\underline{S}} = \left(\overset{i}{U}_{i-1}, \overset{i}{V}_{i-1}, \overset{i}{U}_i, \overset{i}{V}_i\right) \tag{3.3}$$



where $\overset{i}{U} = \overset{i}{u}(x_j)$, $\overset{i}{V}_j = d\overset{i}{u}/dx(x_j)$. Observe that the four components of such a vector are not independent; indeed, there is a 2×4 matrix $\overset{i}{\underline{\underline{R}}}$ and a 2-D vector $\overset{i}{\underline{F}}$ such that

$$\overset{i}{\underline{\underline{R}}} \cdot \overset{i}{\underline{S}} = \overset{i}{\underline{F}}; \quad i = 1, \ldots, N \tag{3.4}$$

This is a system of $2N$ equations in $4N$ unknowns. Introducing the notation $\overset{i}{\underline{S}}_- = (\overset{i}{U}_{i-1}, \overset{i}{V}_{i-1})$ and $\overset{i}{\underline{S}}_+ = (\overset{i}{U}_i, \overset{i}{V}_i)$ allows decomposition of the matrix $\overset{i}{\underline{\underline{R}}}$ into two 2×2 submatrices $\overset{i}{\underline{\underline{R}}}_-$ and $\overset{i}{\underline{\underline{R}}}_+$, so that Eq. (3.4) becomes

$$\overset{i}{\underline{\underline{R}}} \cdot \overset{i}{\underline{S}} = \overset{i}{\underline{\underline{R}}}_- \cdot \overset{i}{\underline{S}}_- + \overset{i}{\underline{\underline{R}}}_+ \cdot \overset{i}{\underline{S}}_+ = \overset{i}{\underline{F}}; \qquad i = 1, \ldots, N \tag{3.5}$$

while Eq. (3.2) is

$$\overset{i}{\underline{S}}_+ = \overset{i+1}{\underline{S}}_- \tag{3.6}$$

Generally, Eqs. (3.5) and (3.6), together with two boundary conditions, constitute a determined system for the $4N$ components of the vectors $\{\overset{1}{\underline{S}}, \ldots, \overset{N}{\underline{S}}\}$. This is the basic system of equations of nonoverlapping methods.

Different methods with nonoverlapping subdomains derive from different approaches to solving this system of equations. A first option is to set, making use of Eq. (3.6),

$$\overset{i}{\underline{S}} = \left(\overset{i}{U}_i, \overset{i}{V}_i\right) = \overset{i}{\underline{S}}_+ = \overset{i+1}{\underline{S}}_-; \qquad i = 1, \ldots N-1 \tag{3.7}$$

Substituting into Eq. (3.5) one obtains

$$\overset{i}{\underline{\underline{R}}}_- \cdot \overset{i-1}{\underline{S}} + \overset{i}{\underline{\underline{R}}}_+ \cdot \overset{i}{\underline{S}} = \overset{i}{\underline{F}}; \qquad i = 1, \ldots, N \tag{3.8}$$

Equations (3.8), together with two boundary conditions, usually determine the value of the function and its derivative at the $N+1$ nodes of the partition. The system (3.8) is a 2×2 block bidiagonal system and is the basis for application of direct methods of solution.

If a direct approach is used, one solves for the function and its derivative at each of the nodes. However, to develop domain decomposition methods, most frequently a trial and error, or search, approach is applied. To this end, observe that the Dirichlet problem at each one of the subintervals is well posed and the values of the derivative at the end points of the subintervals are determined in this manner; the essential process may be

described as follows: Choose a collection of values $\{U^1, \ldots, U^{N-1}\}$, set $\overset{i}{U}_i =$ solve for $\overset{i}{V}_{i-1}$ *and* $\overset{i}{V}_i$ each one of the equations of system (3.5), and compute

$$J_i = V_i - \tag{3.9}$$

Re oosing new lues $\{U = 0.$

Extension of the previous discussion to more dimensions is relatively straightforward. If one defines again the function $J(x, y)$ by $J \equiv [\partial u/\partial n]$, on Σ, and assumes the Dirichlet problem is well posed in each of the subregions, then J is a functional of the values of the function $u(x, y)$ on Σ. When a direct approach is used, the resulting matrices are generally sparse because the value of J at a given point has a localized domain of dependence. Thus, for example, consider two neighboring subregions, Ω_i and Ω_j, in Figure 2, then at any point of the common boundary $\Sigma_{i,j} = \partial\Omega_i \cap \partial\Omega_j$, the normal derivative on one side is a functional of the values of u on $\partial\Omega_i$, while on the other side it is a functional of the values on $\partial\Omega_j$.

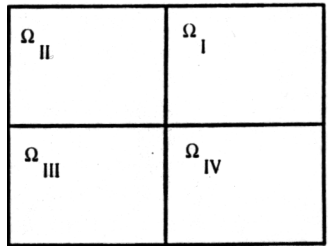


FIGURE 2. The elemental subregions.

Hence, the domain of dependence of J at that point is $\partial\Omega_i \cup \partial\Omega_j$. This would lead to a block heptadiagonal structure of the matrix when a direct aproach is used. However, the number of significant diagonals may be increased by the continuity conditions at corners (Figuré 1).

When a search approach is used, as when iterative procedures are applied, one searches for a function $U(x, y)$, defined on Σ, for which $J \equiv 0$. The search approach is the basis of all iterative methods. The different strategies that are followed by the iterative procedures are intended to make the search more efficient. Maybe the most elemental iterative procedure is the Jacobi method [Allen *et al.*, 1988] and more sophisticated methods frequently were derived with the intention of improving efficiency. One which has been very successful is the conjugate gradient method [Hestens and Stiefel, 1952], which in its original form can be applied to positive definite matrices only.

In the case of elliptic differential operators of second order, it is possible to associate positive quadratic forms to nonoverlapping domain decompositions, when the differential operator is symmetric and positive: $b = 0$, $c \geq 0$, in Eq. (3.1). Indeed, this becomes possible by introducing Poincaré–Steklov operators [Agoshkov, 1987]. A method for doing this, which is more direct and simple and was introduced in Herrera *et al.* [1994], is explained next in a revised form.

For simplicity Dirichlet boundary conditions will be considered exclusively, but the procedure has more general validity. Let D_H be the subspace of functions of D, which are continuous, vanish on the boundary, and satisfy the homogeneous differential equation

in Ω. Then, given $\hat{u}_H$ and $\hat{v}_H \in D_H$, the following identity holds:

$$-\int_\Sigma \hat{v}_H[\underline{\underline{a}}\cdot\nabla\hat{u}_H]\cdot\underline{n}\,d\underline{x} = \int_\Omega(\nabla\hat{u}_H\cdot\underline{\underline{a}}\cdot\nabla\hat{v}_H + c u_H\hat{v}_H)d\underline{x} \qquad (3.10a)$$

which exhibits the symmetry of the expressions involved. In addition

$$-\int_\Sigma u_H[\underline{\underline{a}}\cdot\nabla\hat{u}_H]\cdot\underline{n}\,d\underline{x} = \int_\Omega(\nabla\hat{u}_H\cdot\underline{\underline{a}}\cdot\nabla\hat{u}_H + c\hat{u}_H^2)d\underline{x} \geq 0 \qquad (3.10b)$$

and the equality holds, if and only if $\hat{u}_H \equiv 0$ in Ω. If $u \in D$ is a solution of the boundary value problem then

$$\begin{aligned}-\int_\Sigma \hat{u}_H[\underline{\underline{a}}\cdot\nabla\hat{u}_H]\cdot\underline{n}\,d\underline{x} &= \int_\Omega \hat{u}_H\mathcal{L}u\,d\underline{x} - \int_{\partial\Omega} u(\underline{\underline{a}}\cdot\nabla\hat{u}_H)\cdot\underline{n}\,d\underline{x}\\ &= \int_\Omega \hat{u}_H f_\Omega\,d\underline{x} - \int_{\partial\Omega} u_\partial(\underline{\underline{a}}\cdot\nabla\hat{u}_H)\cdot\underline{n}\,d\underline{x} \qquad (3.11)\end{aligned}$$

where u_∂ is the boundary value of u. Observe that when $\hat{u}_H \in D_H$ is given, evaluation of the last two integrals is possible because both f_Ω and u_∂ are data of the problem.

Assume for the time being that there is a function $u_H \in D_H$, such that $u_H = u$ on Σ; then for any $\hat{u}_H \in D_H$, one has

$$-\int_\Sigma \hat{u}_H[\underline{\underline{a}}\cdot\nabla\hat{u}_H]\cdot\underline{n}\,d\underline{x} + 2\int_\Sigma u_H[\underline{\underline{a}}\cdot\nabla\hat{u}_H]\cdot\underline{n}\,d\underline{x} \geq \int_\Sigma u_H[\underline{\underline{a}}\cdot\nabla u_H]\cdot\underline{n}\,d\underline{x} \qquad (3.12)$$

and the minimum of the left-hand side is attained if and only if $\hat{u}_H = u_H = u$ on Σ. It is finally observed that the left-hand member of (3.12) can be expressed by means of any of the two following functionals

$$\Im_1(\hat{u}_H) \equiv \int_\Omega\{\nabla\hat{u}_H\cdot\underline{\underline{a}}\cdot\nabla\hat{u}_H + c\hat{u}_H^2\}d\underline{x} - 2\left\{\int_\Omega \hat{u}_H f_\Omega\,d\underline{x} - \int_{\partial\Omega} u_\partial(\underline{\underline{a}}\cdot\nabla\hat{u}_H)\cdot\underline{n}\,d\underline{x}\right\} \qquad (3.13a)$$

and

$$\Im_2(\hat{u}_H) \equiv -\int_\Sigma \hat{u}_H[\underline{\underline{a}}\cdot\nabla\hat{u}_H]\cdot\underline{n}\,d\underline{x} - 2\left\{\int_\Omega \hat{u}_H f_\Omega\,d\underline{x} - \int_{\partial\Omega} u_\partial(\underline{\underline{a}}\cdot\nabla\hat{u}_H)\cdot\underline{n}\,d\underline{x}\right\} \qquad (3.13b)$$

Our conclusion is that a function $u_H \in D_H$ satisfies the condition $u_H = u$, on Σ – here, $u \in D$ is a solution of the boundary value problem – if and only if the functionals $\Im_1$ and $\Im_2$, which are identical, attain their minimum.

Taking the variation of these functionals two variational formulations follow; the first

$$\int_\Omega(\nabla\hat{u}_H\cdot\underline{\underline{a}}\cdot\nabla v_H + c\hat{u}_H v_H)d\underline{x} = \int_\Omega f_\Omega v_H\,d\underline{x} - \int_{\partial\Omega} u_\partial(\underline{\underline{a}}\cdot\nabla v_H)\cdot\underline{n}\,d\underline{x} \qquad (3.14a)$$

characterizes any function $u \in D$ which takes, on Σ, the values of the solution u of the boundary value problem, while the second one

$$-\int_\Sigma u_H[\underline{\underline{a}}\cdot\nabla v_H]\cdot\underline{n}\,d\underline{x} = \int_\Omega v_H f_\Omega\,d\underline{x} - \int_{\partial\Omega} u_\partial(\underline{\underline{a}}\cdot\nabla v_H)\cdot\underline{n}\,d\underline{x} \qquad (3.14b)$$

characterizes directly the values of u on Σ. Of course, the full statement of these variational principles requires that Eqs. (3.14) be satisfied for every $v_H \in D_H$.

4. Overlapping Procedures

Going back to the one-dimensional case of Section 3, the domain decomposition of the interval may be defined as the collection of subintervals $\Omega_i = (x_{i-1}, x_{i+1})$, where

$i = 1, \ldots, N-1$. These subintervals are not disjoint. Again, the domain decomposition problem may be transformed into finding the values of the solution of the problem at $\{x_1, \ldots, x_{N-1}\}$, which in turn may be formulated as a search problem. Let $\{U_1, \ldots, U_{N-1}\}$ be a collection of values which are being tested as possible solutions of this problem. Consider the Dirichlet problem in Ω_i, with boundary values U_{i-1} and U_{i+1}, at x_{i-1} and x_{i+1}, respectively. The value of the solution of this problem at x_i is linear in U_{i-1}, U_{i+1} and f_Ω. Thus, it can be written as $L_-^i U_{i-1} + L_+^i U_{i+1} + \mathcal{G}^i(f_\Omega)$, and the condition that characterizes the solution is

$$L_-^i U_{i-1} - U_i + L_+^i U_{i+1} = -\mathcal{G}^i(f_\Omega) \qquad (4.1)$$

This is a tridiagonal system. A first point to be observed is that only the values of the function occur in the system and the derivatives are not involved. This is typical of overlapping procedures.

Let Σ_{ij} be the set of internal boundaries contained in Ω_{ij} and $\Sigma = \bigcup_{ij}\Sigma_{ij}$. Then $\Sigma = (\bigcup_{ij}\partial\Omega_{ij}) - \partial\Omega$. When $U(x, y)$ is a function defined on Σ, the symbols $U_{\Sigma_{ij}}$ and $U_{\partial_{ij}}$ will be used to represent the restrictions of such a function to Σ_{ij} and $\partial\Omega_{ij}$, respectively. On every Ω_{ij}, consider the Dirichlet problem for which the boundary data is $U_{\partial_{ij}}$. Then the restriction of the solution of this problem to Σ_{ij} is linear on $U_{\partial_{ij}}$ and on f_Ω, and can be written as $\mathcal{L}(U_{\partial_{ij}}) + \mathcal{G}(f_\Omega)$. Any function U defined on Σ is a solution of the domain decomposition problem if and only if

$$U_{\Sigma_{ij}} = \mathcal{L}(U_{\partial_{ij}}) + \mathcal{G}(f_\Omega) \qquad \text{on} \quad \Sigma \qquad (4.2)$$

and the resulting system of equations is at most nine-diagonal. The size of the blocks depends on the kind of discretization applied.

5. Conjugate Gradient Method

If the search space is a linear space, a basis for it can be constructed and the solution be found by successively trying each of the members of the basis. If the dimension of the space is N, this process would involve N steps: one for each new search direction. The computations required are simplified if an orthogonal basis is available. However, when N is large, construction of such a basis is generally quite expensive, since each new element has to be orthogonalized with respect to each of the previous ones. A fundamental advantage of the conjugate gradient method (CGM, or simply CG) is that it supplies a simple manner of constructing new search directions which are orthogonal to all those that have already been tried, except the very last one. Consider the equation

$$\underline{\underline{A}}\,\underline{U} = \underline{b} \qquad (5.1)$$

where $\underline{\underline{A}}$ is positive definite and symmetric with respect to an inner product and write $\underline{U}_*$ for the unique solution of (5.1). The procedure for constructing an orthogonal basis may be described as follows:

(a) Choose $\underline{U}^0$ arbitrarily.

(b) Define the error $\underline{e}^k = \underline{U}_* - \underline{U}^0$.

(c) Choose the first search direction $\underline{p}^1 = \underline{\underline{A}}\,\underline{e}^0 = \underline{b} - \underline{\underline{A}}\,\underline{U}^0$.

(d) In the space spanned by $\{\underline{p}^1, \ldots, \underline{p}^k\}$, where the system $\{\underline{p}^1, \ldots, \underline{p}^k\}$ is orthogonal, choose $\underline{U}^k$ so that $\underline{e}^k \perp$ span $\{\underline{p}^1, \ldots, \underline{p}^k\}$.
Note: This requires $\underline{U}^k = \underline{U}^{k-1} + \alpha^k\underline{p}^k$ with $\alpha^k = (\underline{e}^k, \underline{p}^k)/(\underline{p}^k, \underline{p}^k)$.

(e) Incorporate $\underline{\underline{A}}\,\underline{e}^k$ in the search space.

Note: Since $\underline{\underline{A}}\,\underline{e}^k$ is orthogonal to $\{\underline{p}^1, \ldots, \underline{p}^k\}$, the only requirement for the new search direction $\underline{p}^{k+1}$ is that it be orthogonal to $\underline{p}^k$. Thus, $\underline{p}^{k+1} = \underline{\underline{A}}\underline{e}^k - \beta^{k+1}\underline{p}^k$, with $\beta = (\underline{\underline{A}}\underline{e}^k, \underline{p}^k)/(\underline{p}^k, \underline{p}^k)$.

Final note: The term $\alpha^k = (\underline{e}^k, \underline{p}^k)/(\underline{p}^k, \underline{p}^k)$ is not computable for an arbitrary inner product since $\underline{e}^k$ is not known. A suitable inner product is $(\underline{e}^k, \underline{p}^k) \equiv \underline{e}^k \cdot \underline{\underline{A}}\underline{p}^k = \underline{p}^k \cdot \underline{\underline{A}}\underline{e}^k = \underline{p}^k \cdot \underline{r}^k = \underline{p}^k \cdot (\underline{b} - \underline{\underline{A}}\underline{U}^k)$, where the dot stands for the standard Euclidean inner product. For an algorithm derived in this manner, suitable for numerical implementation, see, for example, Allen [1988].

6. Preconditioners

Another important property of CGM is that the manner of generating the new search directions is not random; on the contrary, it is related to the solution of the problem since $\underline{\underline{A}}\,\underline{e}^k$ is incorporated at every step. Indeed, the angle between $\underline{e}^k$ and $\underline{\underline{A}}\,\underline{e}^k$ is controlled by properties of the matrix $\underline{\underline{A}}$; more specifically, it has to be small if the condition number is small. In other words, the selection of the search direction is very good when the condition number is small. It can be shown [Golub and Van Loan, 1983, Section 10.2] that

$$\|u - \underline{U}^k\| \leq \|u - \underline{U}^0\| \left[\frac{\rho - 1}{\rho + 1}\right]^{2k} \tag{6.1}$$

where ρ is the square root of the condition number of $\underline{\underline{A}}$. Also, $\|\,\|$ is used to indicate the energy norm associated with $\underline{\underline{A}}$. From this relation it may be concluded that CGM converges rapidly when the condition number is not large. However, if ρ is large, then $(\rho - 1)/(\rho + 1)$ is close to 1 and the performance of CG may be poor. When applying the conjugate gradient method, the domain decomposition procedure may involve many subdomains, and frequently this leads to systems of equations which are poorly conditioned. In such cases means of diminishing the condition number of the system have to be sought. One way of achieving such a reduction is by the use of "preconditioners."

Before proceeding to discuss the *preconditioned* conjugate gradient (PCG) method, some comments are in order, in particular, when a condition number must be considered large. If we are dealing with a system of 1000 equations, then a condition number such that 100 iterations are required for convergence is pretty large, but probably satisfactory, since it reduces by a factor of 1/10 the number of search directions required to find the solution.

PCG consists in choosing a preconditioner – i.e., a matrix $\underline{\underline{B}}$, positive-definite and symmetric – and writing the equivalent system

$$\underline{\underline{B}}^{-1}\underline{\underline{A}}\,\underline{U} = \underline{\underline{B}}^{-1}\underline{b} \tag{6.2}$$

This system is symmetric in the inner product $(\underline{U}, \underline{V}) = \underline{U} \cdot \underline{\underline{B}}\underline{V}$ and CGM will converge faster when applied to (6.2) than when applied to the original system, if ρ', the square root of the condition number of the modified system, is smaller than ρ: the closer to 1, the faster.

Because of the importance of reducing the condition number effectively, a lot of work has been done to develop efficient preconditioners. Noticing that the only matrix with condition number equal to 1 is the identity matrix, preconditioners may be thought of as approximate inverses of the original matrix $\underline{\underline{A}}$. Considerable progress has been made in the understanding of the problems associated with the construction of preconditioners for systems occurring in domain decomposition methods (see, for example, Bramble *et al.* [1986, 1987]).

Actually, the best strategy in the construction of such preconditioners depends on many factors related not only to the nature of the system considered but also to the frequency with which the same system will have to be solved (several accounts of the matters involved may be found in Glowinski *et al.* [1988, 1990], Chan *et al.* [1989a, 1989b] and Keyes *et al.* [1991]).

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