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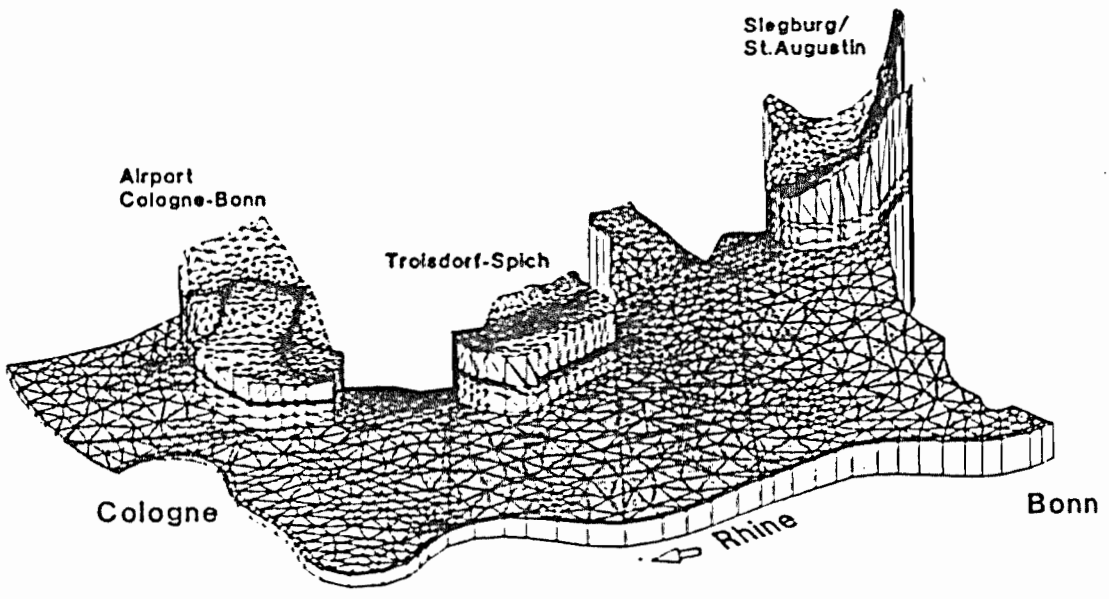

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DOMAIN DECOMPOSITION METHOD FOR COLLOCATION PROCEDURES

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ABSTRACT

Combining collocation procedures with domain decomposition methods presents complications that must be overcome in order to profit from the advantages of parallel computing. Recently, Herrera supplied formulations which effectively combine these methods. In this paper such formulations an their implementations are presented and discussed. In a companion paper, also presented in this conference, the application of this method to nonlinear flow and transport of a multiphase system is discussed.

1. INTRODUCTION

Domain decomposition techniques have received much attention in recent years. They constitute a natural route to parallelism. Using them it is possible to transform large discrete systems into smaller ones. Also, domains of irregular shape can be decomposed into regular subdomains in which tensor-product discretizations can be applied. In addition, domain decomposition techniques are quite suitable for carrying out grid refinements in regions where they are required, as where the coefficient variability is high.

For elliptic problems, domain decomposition methodologies are well developed (see, for example [1-5]). In many instances time dependent problems of parabolic type can be treated in the same manner, because for usual time discretizations, they give rise to an elliptic problem at each time-step. In this case, the grid Green function has a rapid exponential decay and this property can be exploited to minimize the amount of work that is required for applying the domain decomposition method [6-8]. Also, domain decomposition methods are frequently applied by means of a preconditioned conjugate gradient iteration. When this is done, the type of preconditioner to be used is case dependent (see for example [1]).

In this paper and a companion one [9], we address the problem of

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combining collocation (see, for example [10]), with domain decomposition methods. In the present paper, the procedure we propose and its foundations, are explained and in the companion one [9], the numerical implementation is illustrated and discussed in connection with flow and transport problems. Actually, the method here presented has considerable generality and its applicability is no restricted, by any means, to cases where the discretization procedure used is collocation.

As a matter of fact, the method is to a large extent independent of the discretization procedure applied to the basic equations, because it is based on general properties of elliptic partial differential equations which are symmetric and positive definite. Given a decomposition of a region into subdomains, the problem is transformed into one which exclusively involves the internal boundaries (Γ) separating the subdomains from each other. Then, a positive definite transformation is associated with this latter problem. Up to this point the discussion refers to the continuous problem. Then, a discretization is introduced in an abstract manner, by means of a finite dimensional subspace of functions defined on Γ. It is shown that the restriction of the transformation previously introduced to such subspace, also possesses the positive-definiteness property and it is suitable for applying the Conjugate Gradient Method. The use of preconditioners, in conjunction with our method, is also possible and it is being the subject of ongoing research [11].

Here the method is explained for elliptic equations but it can also be applied to a large class of parabolic equations when a step by step procedure, for integration of time is used, either by means of a θ-scheme fixed in space or an Eulerian-Lagrangian approach (see for example [12,13]). In such case, an elliptic problem has to be solved at each time-step, and domain decomposition methods converge rapidly, because of the radius of influence of fundamental solutions in such situations are usually small, the radius decreasing with decreasing time-step (see, for example [6]).

2.- DOMAIN DECOMPOSITION FORMULATION

In this Section and the following one, we outline the general ideas of the method, leaving aside some technical details. Later, in Section 4, the method is presented in a more systematic and rigorous manner. In addition a more thorough analysis is being prepared [11].

Consider the boundary value problem (BVP), defined in Ω (Fig. 1a), which consists in satisfying

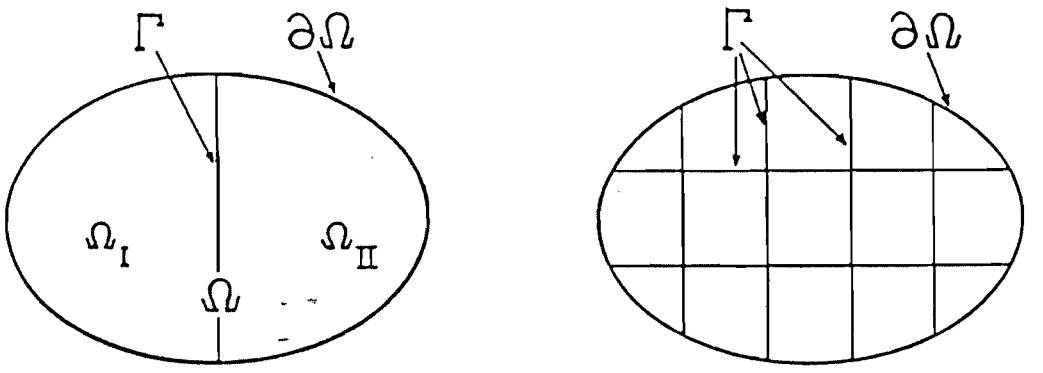
$$\mathcal{L}u \equiv -\nabla\cdot(K\cdot\nabla u) + Ru = f_{\Omega}, \qquad \text{in } \Omega \qquad (2.1)$$

together with Dirichlet boundary conditions:

$$u(\underline{x}) = u_{\partial}(\underline{x}), \quad \text{in } \partial\Omega \qquad (2.2)$$

It will be assumed that for every $\underline{x}$ of Ω, the matrix K is positive definite and $R\geq 0$. In addition, suitable smoothness conditions for the coefficients in Eq. (2.1) are assumed, so that the general existence theorems for partial differential equations (see for example [14]) grant the existence of a unique solution of the BVP.

The region Ω will be divided in two subregions, Ω_I and Ω_{II}, with internal boundary Γ (Fig. 1a). Let $\partial\Omega_I$ and $\partial\Omega_{II}$, be the boundaries of Ω_I



a) b)

Figure 1.- Illustration of domain decompositions.

and Ω_{II}, respectively and define

$$\partial_I\Omega=\partial\Omega\cap\partial\Omega_I \quad \& \quad \partial_{II}\Omega=\partial\Omega\cap\partial\Omega_{II} \tag{2.3}$$

Observe that $\partial\Omega_I=\Gamma\cup\partial\Omega_I$ and $\partial_{II}\Omega=\Gamma\cup\partial\Omega_{II}$. In what follows a procedure is presented for constructing the solution (u) of the BVP, by exclusively solving boundary value problems in Ω_I and Ω_{II}, separately. Such procedure will be the "domain decomposition" method. It must be mentioned that although in order to make the explanations that follow simpler, the region Ω is divided into two subregions only, the results to be presented remain valid even if the region Ω is divided into many subdomains, as long as Γ is interpreted as the union of all the internal boundaries separating the subdomains from each other (Fig. 1b).

To this end define the function v_I, in Ω_I, as the unique solution of the boundary value problem

$$\mathcal{L}v_I = f_\Omega, \quad \text{in } \Omega_I \tag{2.4}$$

subject to the boundary conditions

$$v_I(\underline{x}) = u_\partial(\underline{x}), \text{ in } \partial_I\Omega \text{ and } v_I(\underline{x}) = V(\underline{x}), \text{ in } \Gamma, \tag{2.5}$$

where $V(\underline{x})$ is a suitably chosen function, defined on Γ. In particular, $V(\underline{x})$ can be chosen to be identically zero on Γ, and for simplicity we assume this in what follows. The function v_{II} is defined similarly, replacing I by II, above. Having v_I and v_{II} at hand, the function $v(\underline{x})$ is defined in Ω by

$$v(\underline{x}) = \begin{cases} v_I(\underline{x}), & \underline{x}\in\Omega_I \\ v_{II}(\underline{x}), & \underline{x}\in\Omega_{II} \end{cases} \tag{2.6}$$

Observe that the function $v(\underline{x})$, so defined, is continuous in Ω. However, the normal derivative of v may be discontinuous across Γ. In addition, observe that the construction of $v(\underline{x})$ only requires solving boundary value problems formulated in Ω_I and Ω_{II}, separately.

Proposition 1

Let the function $u(\underline{x})$, be the solution of the BVP in Ω. Then, the function $w(\underline{x})$, defined in Ω by $w \equiv u-v$, is the unique solution of the boundary value problem with prescribed jumps (BVPJ) on Γ, defined by the following conditions:

"The differential equation $\mathcal{L}w=0$ *is satisfied in* Ω_I *and* Ω_{II}, *separately,* $w(\underline{x})=0$ *for every* $\underline{x}\in\partial\Omega$, w *is continuous across* Γ *and its first order partial derivatives have jump discontinuities across* Γ, *which satisfy the jump condition*

$$\left[K\cdot\nabla w\right]\cdot\underline{n} = -\left[K\cdot\nabla v\right]\cdot\underline{n}\ , \qquad \text{on } \Gamma" \qquad (2.7)$$

Here, the square-bracket stands for the value of the "jump" across Γ (value on the "positive" side minus value on the "negative" one) and $\underline{n}$ is taken pointing towards the positive side.

Proof.- Because $\mathcal{L}w=\mathcal{L}u-\mathcal{L}v=0$ in Ω_I and Ω_{II}, and $w = u-v=o$, in $\partial\Omega$ Also,

$$\left[K\cdot\nabla w\right]\cdot\underline{n} = \left[K\cdot\nabla u\right]\cdot\underline{n} - \left[K\cdot\nabla v\right]\cdot\underline{n} = -\left[K\cdot\nabla v\right]\cdot\underline{n} \quad \text{on } \Gamma \qquad (2.8)$$

since the function u, has first order continuous derivatives.

3. REDUCTION TO A PROBLEM FORMULATED ON Γ

For the sake of clarity, we introduce the following notation. Given any function $s(\underline{x})$ defined in Ω, we write $S:\Gamma\longrightarrow R^1$, for the restriction of $s(\underline{x})$ to Γ, which is defined for every $\underline{x}\in\Gamma$ by $S(\underline{x})\equiv s(\underline{x})$. In particular, $W:\Gamma\longrightarrow R^1$ will be the restriction to Γ of the function $w(\underline{x})$ introduced in Proposition 1. It will be shown that when $W(\underline{x})$ is known on Γ, the construction of $w(\underline{x})$ in Ω only requires solving two boundary value problems: one in Ω_I and the other one in Ω_{II}.

Proposition 2

Let $w_I(\underline{x})$ be defined for every $\underline{x}\in\Omega_I$, as the unique solution of the boundary value problem

$$\mathcal{L}w_I=0, \qquad \text{in } \Omega_I \qquad (3.1)$$

subject to the boundary conditions in $\partial\Omega_I$, given by

$$w_I(\underline{x}) = 0, \quad \text{in } \partial_I\Omega \text{ and } w_I(\underline{x}) = W(\underline{x}) \text{ in } \Gamma, \qquad (3.2)$$

In addition, define $w_{II}(\underline{x})$ for every $\underline{x}\in\Omega_{II}$, replacing I by II in the definition of w_I, given above. Then

$$w(\underline{x})=w_I(\underline{x}), \text{ for every } \underline{x}\in\Omega_I \text{ and } w(\underline{x})=w_{II}(\underline{x}), \text{ for every } \underline{x}\in\Omega_{II} \qquad (3.3)$$

Proof.- According to Proposition 1, the restrictions of $w(\underline{x})$ to Ω_I and Ω_{II}, are solutions of the first and second of these boundary value problems, respectively. Thus, Eqs. (3.3) follow from the uniqueness of solution properties of these problems.

The mapping A

In view of Proposition 2, the key to obtain a domain decomposition method is to develop a procedure for constructing the function $W(\underline{x})$, which is restriction of $w(\underline{x})$ to Γ. In what follows, we develop such procedure using exclusively solutions of boundary value problems

formulated in Ω_I and in Ω_{II}, separately. In view of Propositions 1 and 2, this will complete the outline of the domain decomposition method we propose in this paper. The following auxiliary mapping, will be useful in the sequel.

Given a function $S\epsilon L^2(\Gamma)\equiv H^0(\Gamma)$, construct the function s_I, defined in Ω_I, as the unique solution of the boundary value problem

$$\mathcal{L}s_I=0, \qquad \text{in } \Omega_I \tag{3.4}$$

subject to the boundary conditions in $\partial\Omega_I$, given by

$$s_I(\underline{x}) = 0, \quad \text{in } \partial_I\Omega \text{ and } s_I(\underline{x}) = S(\underline{x}) \text{ in } \Gamma, \tag{3.5}$$

In addition, define $s_{II}(\underline{x})$ for every $\underline{x}\epsilon\Omega_{II}$, replacing I by II in the definition of s_I. The function $s(\underline{x})$ is then defined in Ω, by

$$s(\underline{x}) = \begin{cases} s_I(\underline{x}), & \underline{x}\epsilon\Omega_I \\ s_{II}(\underline{x}), & \underline{x}\epsilon\Omega_{II} \end{cases} \tag{3.6}$$

The function $AS:\Gamma\longrightarrow R^1$, is defined by:

$$AS(\underline{x}) = -\left[K\cdot\nabla s\right]\cdot\underline{n}, \qquad \underline{x}\epsilon\Gamma \tag{3.7}$$

Formulation of the problem on Γ

Define the function J on Γ by:

$$J \equiv \left[K\cdot\nabla v\right]\cdot\underline{n}, \qquad \textit{on } \Gamma \tag{3.8}$$

Where $v(\underline{x})$ is given by Eq. (2.6). Then, using the mapping A and in view of Eq. (2.7), the problem can be stated as follows:

"*Find* $W(\underline{x})$ *on* Γ, *such that*

$$AW = J, \qquad \textit{on } \Gamma" \tag{3.9}$$

In the next Section, it will be shown that after discretization, the solution of Eq. (3.9), can be constructed applying the Conjugate Gradient (C-G) procedure. This is because the mapping A is positive definite, as it is shown next.

Proposition 3

In the <u>linear subspace</u> of $L^2(\Gamma)$ for which $AS\epsilon L^2(\Gamma)\equiv H^0(\Gamma)$, the mapping A, is symmetric and positive definite.

Proof.- In view of the fact that $\mathcal{L}s=0$ in Ω, except on Γ where a jump discontinuity of the first order derivatives occurs. Application of the generalized divergence theorem [15], yields:

$$-\int_\Omega s\nabla\cdot(K\cdot\nabla s)d\underline{x} = -\int_{\partial\Omega} s(K\cdot\nabla s)\cdot\underline{n}\, d\underline{x} + \int_\Gamma s\left[K\cdot\nabla s\right]\cdot\underline{n}\, d\underline{x} + \int_\Omega (K\cdot\nabla s)\cdot\nabla s\, d\underline{x} \tag{3.10}$$

Observe that

$$\int_\Omega s\nabla\cdot(K\cdot\nabla s)d\underline{x} = \int_\Omega Rs^2\, d\underline{x};\ \int_{\partial\Omega} s(K\cdot\nabla s)\cdot\underline{n}\, d\underline{x} = 0 \tag{3.11a}$$

and

$$-\int_\Gamma s \left[K\cdot\nabla s\right]\cdot\underline{n}\, d\underline{x} = \int_\Gamma (AS)S\, d\underline{x} \qquad (3.11b)$$

by virtue of the conditions imposed on $s(\underline{x})$ and the definition of the mapping A. Therefore

$$(AS^*S) = \int_\Gamma (AS)S\, d\underline{x} = \int_\Omega \left\{(K\cdot\nabla s)\cdot\nabla s + Rs^2\right\} d\underline{x} \geq 0 \qquad (3.12)$$

Where, the inner product operation in $L^2(\Gamma)$ is denoted by $(^*)$. Finally, observe that the equality in relation (3.12) holds when the function $s(\underline{x})$ is identically zero, exclusively, in which case so is $S(\underline{x})$.

Remark 1.- Observe that the linear subspace of $H^0(\Gamma)$, we are referring to in Proposition 3, is $H^1(\Gamma)$. Indeed, the image of $H^1(\Gamma)$ under the mapping A, is $H^0(\Gamma)$ [14]. This is a linear subspace of $H^0(\Gamma)$, since $H^1(\Gamma)\subset H^0(\Gamma)$. However, $H^1(\Gamma)$ is not closed with respect to the metric of $H^0(\Gamma)=L^2(\Gamma)$.

4. DISCRETIZATION AND CONJUGATE GRADIENT FORMULATION

The fact that the transformation A introduced in the previous Section is positive definite, permits applying the conjugate gradient method (C-G) to the problem of obtaining the function $W(\underline{x})$, on Γ. However, it is necessary to discretize the problem before C-G can be applied. The procedure to be presented is independent of the actual set of approximating functions used to carry out the discretization. What is essential is that, after discretization, the problem is no longer formulated on the whole space $L^2(\Gamma)$, but instead, it is formulated in a finite dimensional subspace of $L^2(\Gamma)$.

Thus, let $\mathcal{G}\subset H^1(\Gamma)\subset H^0(\Gamma)=L^2(\Gamma)$ be such finite dimensional subspace which is necessarily closed in $L^2(\Gamma)$, since it is finite dimensional. Elements belonging to $\mathcal{G}$ will wear a hat. In particular, for any $S\in L^2(\Gamma)$, we write $\hat{S}$ for its projection on $\mathcal{G}$, with respect to the $L^2(\Gamma)$ inner product. In addition, for every $\hat{S}\in\mathcal{G}$, $\hat{A}\hat{S}\in\mathcal{G}$ is defined as the projection of $\hat{A}\hat{S}\in H^0(\Gamma)=L^2(\Gamma)$, on $\mathcal{G}$. Thus, in this manner a well defined mapping $\hat{A}$ of $\mathcal{G}$ into itself, is obtained $(\hat{A}:\mathcal{G}\longrightarrow\mathcal{G})$.

Remark 2.- Observe that we could associate a square matrix with the mapping A, since it is a linear transformation of a finite dimensional space into itself. However, such matrix will not be used in what follows, because in applications it is too costly to construct.

The Conjugate Gradient formulation

Projecting Eq (3.9) on $\mathcal{G}$, the following "discrete" version of the problem is obtained:

"*Find* $\hat{W}\in\mathcal{G}$ *on* Γ, *such that*

$$\hat{A}\hat{W} = \hat{J}, \qquad \text{on } \Gamma" \qquad (4.1)$$

Here the function J is defined on Γ, by Eq (3.8). This problem is suitable to be solved by means of the C-G method. This is due to the

fact that $\hat{A}$ is finite dimensional and positive definite.

Proposition 4

The mapping $\hat{A}: \mathcal{G} \longrightarrow \mathcal{G}$, is (symmetric and) positive definite.

Proof.- This is a well known result of Linear Algebra. It can be easily derived from the fact that

$$(\hat{A}\hat{S}, \hat{W}) = (\hat{A}\hat{S}, \hat{W}) \qquad (4.2)$$

whenever $\hat{S}$ and $\hat{W}$ belong to $\mathcal{G}$.

The C-G algorithm

Because of the special character of the application of the Conjugate Gradient method, the corresponding algorithm is given in detail. Recall the notations that have been adopted and in particular, that when a low case letter is used for a function defined in Ω, the corresponding capital letter is reserved to denote the restriction of such function to Γ. The C-G algorithm follows:

Given a tolerance $\varepsilon>0$, *define* $w^0 \equiv 0$ *in* Ω.

$R^0 = J$

$\hat{P}^0 = \hat{R}^0$

$k=0$

@) Do

"*Construct* p^k *in* Ω, *satisfying* $\mathcal{L}p^k = 0$ *in* Ω_1 *and* Ω_2 *separately, homogeneous boundary conditions in* $\partial\Omega$ *and*

$p^k = \hat{P}^k$ *in* Γ"

(Recall in what follows that $A\hat{P}^k(\underline{x}) = -\left[K \cdot \nabla p^k\right] \cdot \underline{n}$, on Γ)

$\alpha^k = \hat{R}^k \cdot \hat{R}^k / \hat{P}^k \cdot A\hat{P}^k$

$w^{k+1} = w^k + \alpha^k p^k$

$R^{k+1} = \hat{R}^k - \alpha^k A\hat{P}^k$

If $\|\hat{R}^{k+1}\|_\infty \leq \varepsilon$, *set* $u = v + w^{k+1}$ *in* Ω, *and stop.*

$\beta^k = \hat{R}^{k+1} \cdot A\hat{P}^k / \hat{P}^k \cdot A\hat{P}^k$

$\hat{P}^{k+1} = \hat{R}^{k+1} - \beta^k \hat{P}^k$

$k=k+1$ go to (@)

5. EXTENSIONS

Firstly, it must be observed that in the preceding discussion nothing has been assumed about the dimension of the space in which the problem is defined. Thus, the domain decomposition method developed in this paper is applicable independently of the number of dimensions. Secondly, in addition to elliptic problems, it is applicable to time dependent problems, because many of them at each time step adopt the form of Eq (2.1), after the time discretization has been applied.

There are several options for treating differential operators which are not self-adjoint, such as those occurring in transport-diffusion problems. The most rigorous one, is to apply an extension of the theory and this is being developed at present. Another one, more direct and simple was successfully applied in the companion paper [9]. Another very interesting possible extension that should be studied, is combining the

method here presented with Eulerian-Lagrangian procedures, such as those developed in [12,13].

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