CHAPTER 2

On the Discretization of Interdomain Coupling in Elliptic Boundary-value Problems*

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Abstract. In this article, we consider the discretization of the interdomain coupling of solutions of elliptic boundary-value problems on decomposed domains without overlaps. Our approach employs Lagrange multipliers to enforce compatibility constraints between adjacent domains. The multipliers explicitly appear as auxiliary dependent variables in continuous and discrete variational formulations of the elliptic problem. As a result, the interdomain coupling is included at a higher level of the discretization than in approaches yielding standard Schur complement systems. Our primary focus is on the convergence of such methods as determined by the choice of multiplier spaces on the interfaces. The main conclusion drawn is that an appropriate selection of the multipliers, based on well-known regularity properties of solutions of elliptic boundary-value problems, yields good resolution of the interdomain coupling in finite-dimensional spaces of very low dimension. This has some important practical advantages, which we demonstrate with some numerical examples.

1. Introduction. In solving an elliptic boundary-value problem on a decomposed domain without overlaps, a typical approach is to apply block elimination to a standard finite-element or finite-difference discretization of the problem. This yields a *Schur complement*, or *reduced*, system to be solved for the unknowns on the interfaces between adjacent subdomains. Much attention has been given (see [18] for a good survey) to the problem of solving these Schur complement systems, which are generally large, dense, and ill-conditioned. Iterative techniques with judiciously-chosen preconditioners are the usual methods of choice.

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Since the Schur complement system can be viewed as the linear system resulting from a discretization of a global coupling problem among the subdomains, it is natural to ask the following questions. What are the regularity properties of the global coupling problem? How efficiently does the discretization yielding the Schur complement system resolve the interdomain coupling? What advantage can be taken of any information which may be known *a priori* about the interdomain coupling? The fact that the usual Schur complement system may not represent the best discretization of the coupling problem can be illustrated by simple examples in which very fine meshes are required to resolve the solution on each of the subdomains, yet the coupling between subdomains can be approximated very accurately in a subspace of much smaller dimension than the number of unknowns imposed on the interfaces by the subdomain meshes. The basic problem in such cases is that the need to efficiently discretize the interdomain coupling was not considered early enough in the discretization process. Hence, although the meshes on each subdomain are presumably chosen to sufficiently resolve some desired solution features, the resulting dimension of the Schur complement system may be much greater than is necessary to resolve the components of the solution which are more naturally related to the interdomain coupling.

Rather than obtaining the Schur complement system as a by-product of block elimination applied to a standard finite-difference or finite-element discretization of the problem, one might instead choose to include explicitly in the initial continuous formulation the quantity which will ultimately be approximated by the solution of the interface system. Since this quantity would then be present during the discretization process along with the subdomain variables, a more effective discretization of both the subdomain and interface problems could presumably be obtained. In this paper, we summarize the results of [13], which describe the use of Lagrange multipliers in achieving this goal. The Lagrange multipliers, which are functions defined on the interface between adjacent subdomains, allow the interdomain coupling to be explicitly included in continuous and discrete variational formulations. Since the subdomain basis functions and interface Lagrange multipliers are independently represented in these formulations, there is the opportunity to choose the multipliers in such a way as to resolve the interdomain coupling in finite-dimensional interface spaces of very low dimension.

The utility of Lagrange multipliers specifically for domain decomposition has been recognized by other investigators, e.g., [10]. To our knowledge, in these approaches the Lagrange multipliers are assumed to belong to the reduced space of functions spanned by the traces of the finite-dimensional subdomain basis functions, which represents only one possible choice for the Lagrange multiplier space. In this case, the number of Lagrange multipliers is again equivalent to the number of unknowns L associated with the interface. Since the construction of the dense interface problems to be solved for the Lagrange multipliers requires L linear system solves on each subdomain, iterative procedures are proposed which avoid the otherwise costly construction of the Schur complements. As shown in [13] and the present article, by choosing the Lagrange multiplier space in a more general fashion, the number L of Lagrange multipliers on an interface can be so dramatically reduced that for many problems it is entirely feasible to construct the dense interface problem and solve it directly. Moreover, all of the subdomain solves required to compute the interface matrix can be done in parallel assuming that a sufficient number of processors are available. This provides some important flexibility in achieving load-balanced calculations.

As in [13], the following development will consider only the case of two subdomains separated by a single interface. The results obtained for the two-domain case readily

generalize to multidomain cases without crosspoints (e.g., stripwise decompositions). The application of the method described here in the general case with crosspoints will be the subject of a forthcoming paper. Also, although we are considering only self-adjoint problems here, there is nothing preventing the extension of our results to non-self-adjoint problems as well.

2. Lagrange Multipliers and Poincaré-Steklov Operators. In this section, we describe the method of Lagrange multipliers in the context of domain decomposition. We then show how the interface problems obtained by the Lagrange multiplier approach are related to certain dual interface formulations involving Poincaré-Steklov operators. As mentioned in the introduction, we will restrict our attention to the case of only two subdomains. Also, since we intend to focus on the use of Lagrange multipliers to enforce interface rather than boundary conditions, we will assume only homogeneous Dirichlet conditions on the boundary of the given domain.

Let Ω denote a two-dimensional Lipshitz domain whose boundary $\partial\Omega$ is the union of smooth (at least continuously differentiable) arcs. A polygon is an example of such a domain. Consider the following second-order, self-adjoint elliptic problem in Ω:

$$-\sum_{i,j=1}^{2} \frac{\partial}{\partial x_i}\left[a_{ij}(x)\frac{\partial u(x)}{\partial x_j} \right] + c(x)u(x) = f(x) \qquad \text{on } \Omega, \tag{2.1a}$$

with the homogeneous, Dirichlet boundary conditions

$$u = 0 \qquad \text{on } \partial\Omega. \tag{2.1b}$$

Here, the coefficients a_{ij} and c are assumed to belong to $L^\infty(\Omega)$ and satisfy the ellipticity condition

$$\sum_{i,j=1}^{2} a_{ij}\xi_i\xi_j \geq \beta \sum_{i=1}^{2} \xi_i^2, \qquad \text{for all } \xi_1, \xi_2, \quad \text{a.e. on } \Omega,$$

for some constant $\beta > 0$.

Next suppose that Ω is partitioned into two subdomains Ω_1 and Ω_2 by an interface Γ. We assume that Γ is at least continuously differentiable and subdivides Ω in such a way that the boundaries $\partial\Omega_k$ of the resulting subdomains are Lipschitz. For example, Γ might be a line segment partitioning a polygonal Ω.

For each k=1,2, let $H^1(\Omega_k)$ be the usual Sobolev space of functions with square-integrable first derivatives on Ω_k, and let $H_D^1(\Omega_k)$ be the subspace of $H^1(\Omega_k)$ consisting of the those functions which vanish on $\partial\Omega_k \cap \partial\Omega$. Let $H_D^{-1}(\Omega_k)$ be the dual of $H_D^1(\Omega_k)$. We denote by γ_k the operator mapping functions in $H_D^1(\Omega_k)$ to their traces on Γ. Let $H_{00}^{1/2}(\Gamma)$ denote the fractional-order Sobolev space on Γ consisting of all traces on Γ of functions in $H_D^1(\Omega_k)$ equipped with the norm

$$\|g\|_{H_{00}^{1/2}(\Gamma)} \equiv \inf_{u_k \in H_D^1(\Omega_k): g = \gamma_k u_k} \|u_k\|_{H^1(\Omega_k)},$$

and let $H_{00}^{-1/2}(\Gamma)$ denote its dual. With these definitions, it is clear that γ_k maps $H_D^1(\Omega_k)$ onto $H_{00}^{1/2}(\Gamma)$, and it can be shown [14] that γ_k has a continuous right inverse γ_k^{-1}.

Let $H \equiv H_D^1(\Omega_1) \times H_D^1(\Omega_2) \times H_{00}^{-1/2}(\Gamma)$. For each $(u_1,u_2,g^*) \in H$, we define

$$\Phi(u_1,u_2,g^*) \equiv \sum_{k=1}^{2} \int_{\Omega_k} \left[\sum_{i,j=1}^{2} a_{ij} \frac{\partial u_k}{\partial x_i} \frac{\partial u_k}{\partial x_j} + c u_k^2 - 2 f u_k \right] d\Omega \tag{2.2}$$

$$- 2 \int_{\Gamma} g^* (u_1 - u_2)\, d\Gamma.$$

In the last term of (2.2), the Lagrange multiplier g^* is integrated against the difference in the traces of the subdomain solutions u_k on Γ. The constraint that the u_k should agree on Γ is thereby incorporated into the usual quadratic functional to be minimized, which is the first term of (2.2). As a result of adding the Lagrange multiplier term, we have obtained a saddle-point problem, and the critical points (u_1,u_2,g^*) of Φ must satisfy the variational equality

$$B((u_1,u_2,g^*),(v_1,v_2,h^*)) = F((v_1,v_2,h^*)) \qquad \text{for all } (v_1,v_2,h^*) \in H\ , \tag{2.3}$$

where

$$B((u_1,u_2,g^*),(v_1,v_2,h^*)) \equiv \sum_{k=1}^{2} \int_{\Omega_k} \left[\sum_{i,j=1}^{2} a_{ij} \frac{\partial u_k}{\partial x_i} \frac{\partial v_k}{\partial x_j} + c u_k v_k \right] d\Omega$$

$$- \int_{\Gamma} \left[g^* (v_1 - v_2) + h^* (u_1 - u_2) \right] d\Gamma$$

and

$$F(v_1,v_2,h^*) \equiv \sum_{k=1}^{2} \int_{\Omega_k} f v_k\, d\Omega.$$

Let $\vec{n}$ denote the unit normal to Γ pointing from Ω_1 to Ω_2, and let A denote the 2×2 matrix whose entries are the coefficients a_{ij}. For any $u \in H^1(\Omega)$, we define the conormal derivative operator

$$\gamma^* u \equiv \gamma_k^* u_k \equiv \vec{n} \cdot (A \vec{\nabla} u). \tag{2.4}$$

We have the following result [13].

Theorem 2.1. *There exists a unique solution* (u_1,u_2,g^*) *of* (2.3) . *Moreover, if* f *is such that there exists a classical solution* u *of* (2.1), *then the element* (u_1,u_2,g^*) *of* H *given by*

$$u_k \equiv u \quad \text{on } \Omega_k, \quad k=1,2 \tag{2.5a}$$

$$g^* \equiv \gamma^* u, \tag{2.5b}$$

is the solution of (2.3).

For each k=1,2, let

$$B_k(u,v) \equiv \int_{\Omega_k} \left[\sum_{i,j=1}^{2} a_{ij} \frac{\partial u}{\partial x_i} \frac{\partial v}{\partial x_j} + cuv \right] d\Omega \tag{2.6}$$

on $H_D^1(\Omega_k) \times H_D^1(\Omega_k)$. Given g^* in $H_{00}^{-1/2}(\Gamma)$ and f_k in $H_D^{-1}(\Omega_k)$, we consider the variational problem of finding u_k in $H_D^1(\Omega_k)$ such that

$$B_k(u_k,v_k) = \int_\Gamma g^* v_k \, d\Gamma + \int_{\Omega_k} f_k v_k d\Omega, \quad \text{for all } v_k \in H_D^1(\Omega_k). \tag{2.7}$$

Lemma 2.1. *For k=1,2, given g^* in $H_{00}^{-1/2}(\Gamma)$ and f_k in $H_D^{-1}(\Omega_k)$, there exists a unique solution u_k of* (2.7) *and*

$$\|\gamma_k u_k\|_{H_{00}^{1/2}(\Gamma)} \le C \left[\|g^*\|_{H_{00}^{-1/2}(\Gamma)} + \|f_k\|_{H_D^{-1}(\Omega_k)} \right]$$

for some constant C.

We now define the *Poincaré-Steklov operator* (see, e.g., [1] and the references therein) $Q_k : H_{00}^{-1/2}(\Gamma) \to H_{00}^{1/2}(\Gamma)$ by

$$Q_k g^* = \gamma_k u_k, \tag{2.8}$$

where, for g^* in $H_{00}^{-1/2}(\Gamma)$, u_k is the solution of (2.7) with $f_k = 0$. Furthermore, let $R_k : H_D^{-1}(\Omega_k) \to H_{00}^{1/2}(\Gamma)$ be given by

$$R_k f_k = \gamma_k u_k \tag{2.9}$$

where, for f_k in $H_D^{-1}(\Omega_k)$, u_k is the solution of (2.7) with $g^* = 0$. From Lemma 2.1, whose simple proof is given in [13], we have that Q_k and R_k are bounded operators.

In terms of Q_k and R_k, the Lagrange multiplier g^* in $H_{00}^{-1/2}(\Gamma)$ obtained by solving (2.3) is the unique solution of

$$(Q_1 + Q_2) g^* = R_2 f_2 - R_1 f_1. \tag{2.10}$$

Equation (2.10) is a statement of the fact that solving the Lagrange multiplier formulation is equivalent to finding interface data g^* in $H_{00}^{-1/2}(\Gamma)$ such that, when (2.7) is solved, the traces on Γ of the resulting solutions u_k, k=1,2, have the same value g in $H_{00}^{1/2}(\Gamma)$. A dual formulation also exists in which one seeks Dirichlet data g on Γ such that when Dirichlet problems are solved on each subdomain Ω_k, the conormal derivatives $\gamma_k^* u_k$ of the resulting solutions have the same value g^* on Γ. In terms of the operators Q_k and R_k, this dual formulation can be written as

$$(Q_1^{-1} + Q_2^{-1})g = Q_1^{-1}R_1 f_1 + Q_2^{-1}R_2 f_2. \tag{2.11}$$

Equations (2.10) and (2.11) are compact expressions of the interdomain coupling problems to be discretized.

3. Discretization. Discrete analogs of the continuous formulations discussed in the previous section are obtained by the usual procedure of restriction to finite-dimensional subspaces.

For each k=1,2, let $P_{M_k}(\Omega_k)$ be a finite-dimensional subspace of $H_D^1(\Omega_k)$ with basis $\{\phi_{k\mu}, \mu=1,2,...,M_k\}$. We assume that, for some $m_k \geq 1$ and $t_k \geq 2$,

$$P_{M_k}(\Omega_k) \subset H^{m_k}(\Omega_k)\,, \tag{3.1}$$

and that for every $u_k \in H^{n_k}(\Omega_k)$, $n_k \geq 0$, and $0 \leq s \leq \min(m_k, n_k)$ there exists v_k in $P_{M_k}(\Omega_k)$, independent of s, such that

$$\|u_k - v_k\|_{H^s(\Omega_k)} \leq C M_k^{-\sigma_k/2} \|u_k\|_{H^{n_k}(\Omega_k)}\,, \qquad \sigma_k = \min(t_k - s, n_k - s)\,, \tag{3.2}$$

where C is independent of u_k, M_k, and s. An example of such a space is the subspace of $H_D^1(\Omega_k)$ consisting of continuous piecewise linear functions on a quasiuniform triangulation of Ω_k. In this case, $m_k = 1$, $t_k = 2$, and M_k is roughly proportional to h_k^{-2} where h_k is the mesh size.

Next, let $W_L(\Gamma)$ denote a finite-dimensional subspace of $H_{00}^{1/2}(\Gamma)$ with basis $\{w_\lambda, \lambda=1,...,L\}$ such that, for some $m_\gamma \geq -1/2$ and $t_\gamma \geq 2$,

$$W_L(\Gamma) \subset H^{m_\gamma}(\Gamma)\,, \tag{3.3}$$

and for every $g^* \in H^{n_\gamma}(\Gamma)$, $n_\gamma \geq -1/2$, and $-1/2 \leq s \leq \min(m_\gamma, n_\gamma)$ there exists μ^* in $W_L(\Gamma)$, independent of s, such that

$$\|g^* - \mu^*\|_{H^s(\Gamma)} \leq C L^{-\sigma_\gamma} \|g^*\|_{H^{n_\gamma}(\Gamma)}\,, \qquad \sigma_\gamma = \min(t_\gamma - s, n_\gamma - s)\,, \tag{3.4}$$

where C is independent of g^*, L, and s. In addition, we assume that $W_L(\Gamma)$ satisfies the inverse assumption

$$\|g^*\|_{H^s(\Gamma)} \leq C L^{s-q} \|g^*\|_{H^q(\Gamma)}\,, \qquad \text{for all } g^* \in W_L(\Gamma), \quad -1/2 \leq q \leq s \leq m_\gamma\,, \tag{3.5}$$

where C is independent of g^*, L, and s. For example, $W_L(\Gamma)$ could be the space of continuous piecewise linear functions on a quasiuniform partitioning of Γ, in which case $m_\gamma = 1$, $t_\gamma = 2$, and L is roughly proportional to the number of partition segments.

Let

$$H_{M,L} \equiv P_{M_1}(\Omega_1) \times P_{M_2}(\Omega_2) \times W_L(\Gamma), \quad M = (M_1, M_2) .$$

Since $H_{M,L}$ is contained in H, we may consider the discrete problem of finding $(\psi_1,\psi_2,\lambda^*)$ in $H_{M,L}$ satisfying

$$B((\psi_1,\psi_2,\lambda^*),(\phi_1,\phi_2,\mu^*)) = F((\phi_1,\phi_2,\mu^*)) \quad \text{for all } (\phi_1,\phi_2,\mu^*) \in H_{M,L} . \tag{3.6}$$

The following result is proved in [13]:

Theorem 3.1. *Assume that the solution u of (2.1) satisfies $u|_{\Omega_k} \in H^{n_k}(\Omega_k)$ for some $n_k \geq 1$, k=1,2, and that $\gamma^* u \in H^{n_\gamma}(\Gamma)$ for some $n_\gamma \geq -1/2$. Let K be a constant independent of M_k and L such that*

$$KL \leq M_k^{1/2}, \qquad k=1,2. \tag{3.7}$$

If K is sufficiently large, then there exists a unique $(\psi_1,\psi_2,\lambda^*)$ in $H_{M,L}$ satisfying (3.6). Moreover,

$$\sum_{k=1}^{2} \|u_k-\psi_k\|_{H^1(\Omega_k)} + \|\gamma^* u-\lambda^*\|_{H_{00}^{-1/2}(\Gamma)} \tag{3.8}$$

$$\leq C \left\{ \sum_{k=1}^{2} \inf_{v_k \in P_{M_k}(\Omega_k)} \|u_k-v_k\|_{H^1(\Omega_k)} + \inf_{\mu^* \in W_L(\Gamma)} \|\gamma^* u-\mu^*\|_{H_{00}^{-1/2}(\Gamma)} \right\}$$

$$\leq C \left\{ \sum_{k=1}^{2} M_k^{-\sigma_k/2} \|u\|_{H^{n_k}(\Omega_k)} + L^{-\sigma_\gamma} \|\gamma^* u\|_{H^{n_\gamma}(\Gamma)} \right\},$$

where

$$\sigma_k = \min(\, t_k, n_k \,) - 1, \quad k=1,2,$$

$$\sigma_\gamma = \min(\, t_\gamma, n_\gamma \,) + 1/2,$$

and C is independent of M_k and L.

Some error estimates obtainable from Theorem 3.1 for specific choices of $P_{M_k}(\Omega_k)$ and $W_L(\Gamma)$ are contained in the following results.

Corollary 3.1. *For k=1,2, let $P_{M_k}(\Omega_k)$ denote a subspace of $H_D^1(\Omega_k)$ consisting of continuous piecewise linear polynomials defined on a quasiuniform triangulation of Ω_k, and let $W_L(\Gamma)$ be*

a subspace of $H_{00}^{1/2}(\Gamma)$ *consisting of continuous piecewise linear polynomials defined on a quasiuniform partitioning of* Γ. *Then, under the hypothesis of Theorem 3.1, there exists a unique* $(\psi_1,\psi_2,\lambda^*)$ *in* $H_{M,L}$ *satisfying* (3.6) *and*

$$\sum_{k=1}^{2} \|u_k-\psi_k\|_{H^1(\Omega_k)} + \|\partial u/\partial\vec{n}-\lambda^*\|_{H_{00}^{-1/2}(\Gamma)} \tag{3.9}$$

$$\leq C\left[\sum_{k=1}^{2} M_k^{-[\min(n_k,2)-1]/2} + L^{-\min(n_\gamma,2)-1/2}\right],$$

where $C = C(u,n_k,n_\gamma)$ is independent of M_k and L.

Corollary 3.2. *For* k=1,2, *let* $P_{M_k}(\Omega_k)$ *denote a subspace of* $H_D^1(\Omega_k)$ *consisting of continuous piecewise linear polynomials defined on a quasiuniform triangulation of* Ω_k, *and let* $W_L(\Gamma)$ *be the subspace of* $H_{00}^{1/2}(\Gamma)$ *consisting of polynomials of degree* $\leq L+1$ *defined on* Γ. *Then, under the hypothesis of Theorem 3.1, there exists a unique* $(\psi_1,\psi_2,\lambda^*)$ *in* $H_{M,L}$ *satisfying* (3.6) *and*

$$\sum_{k=1}^{2} \|u_k-\psi_k\|_{H^1(\Omega_k)} + \|\partial u/\partial\vec{n}-\lambda^*\|_{H_{00}^{-1/2}(\Gamma)} \tag{3.10}$$

$$\leq C\left[\sum_{k=1}^{2} M_k^{-[\min(n_k,2)-1]/2} + L^{-n_\gamma-1/2}\right],$$

where $C = C(u,n_k,n_\gamma)$ is independent of M_k and L.

When interpreting the error estimates (3.8-3.10), some care must be taken not to overlook (3.7). This assumed condition must be maintained in the asymptotic limit of increasing M_k and L to ensure that the constants C in (3.8-3.10) are independent of M_k and L. Essentially, (3.7) stipulates that one may not "over-resolve" the interface problem for a given level of subdomain discretization. Thus, in spite of the fact that there are two asymptotic parameters in (3.8), they are not totally independent. A discussion of why (3.7) cannot be removed in general can be found in [2, page 214], and some special cases in which (3.7) can be eliminated are discussed in [4]. For practical reasons which will be discussed later, L will be limited to a finite range of relatively small values, in which case there always exists a constant K such that (3.7) holds for sufficiently large M_k. In the numerical results of the next section, we will see that the need to satisfy (3.7) does not present any difficulties for the problems considered.

In general, the subdomain components ψ_k of the solution of (3.6) will not agree on Γ. If the traces on Γ of all functions in $P_{M_k}(\Omega_k)$, k=1,2, span the same space, then continuity of the approximate solution can be recovered by a simple patching procedure. Consider the interface jump function

$$\Delta \equiv \gamma_2\psi_2 - \gamma_1\psi_1 \in H_{00}^{1/2}(\Gamma).$$

For each k=1,2, let $\phi_k \in P_{M_k}(\Omega_k)$ be the solution of the Dirichlet problem

$$\int_{\Omega_k} \left[\sum_{i,j=1}^{2} a_{ij} \frac{\partial \phi_k}{\partial x_i} \frac{\partial \chi_k}{\partial x_j} + c\,\phi_k \chi_k \right] d\Omega = 0 \tag{3.11a}$$

for all $\chi_k \in P_{M_k}(\Omega_k) \cap H_0^1(\Omega_k)$,

$$\phi_k = (-1)^{k+1} \frac{\Delta}{2} \qquad \text{on } \Gamma, \tag{3.11b}$$

and define

$$\tilde{\psi}_k = \psi_k + \phi_k \qquad \text{on } \Omega_k. \tag{3.12}$$

The corrected approximations $\tilde{\psi}_1$ and $\tilde{\psi}_2$ then agree on Γ. Moreover, since

$$\|\phi_k\|_{H^1(\Omega_k)} \le C \|\Delta\|_{H_{00}^{1/2}(\Gamma)},$$

it follows that

$$\begin{aligned} \|u - \tilde{\psi}_k\|_{H^1(\Omega_k)} &\le \|u - \psi_k\|_{H^1(\Omega_k)} + C \|\psi_2 - \psi_1\|_{H_{00}^{1/2}(\Gamma)} \\ &\le \|u - \psi_k\|_{H^1(\Omega_k)} + C \sum_{k'=1}^{2} \|u - \psi_{k'}\|_{H_{00}^{1/2}(\Gamma)} \\ &\le C \sum_{k'=1}^{2} \|u - \psi_{k'}\|_{H^1(\Omega_{k'})}. \end{aligned}$$

Thus, the patching procedure does not degrade the asymptotic convergence rate of the approximate subdomain solutions.

The algebraic system resulting from (3.6) is

$$S_k \theta_k + (-1)^k U_k \eta^* = T_k, \qquad k=1,2, \tag{3.13a}$$

$$U_2^T \theta_2 - U_1^T \theta_1 = 0, \tag{3.13b}$$

where

$$(S_k)_{\mu,\nu} \equiv \int_{\Omega_k} \left\{ \sum_{i,j=1}^{2} a_{ij} \frac{\partial \phi_{k\mu}}{\partial x_i} \frac{\partial \phi_{k\nu}}{\partial x_j} + c\,\phi_{k\mu} \phi_{k\nu} \right\} d\Omega,$$

$$(T_k)_\mu \equiv \int_{\Omega_k} f\,\phi_{k\mu}\,d\Omega,$$

$$(U_k)_{\mu,\lambda} \equiv \int_{\Gamma} \phi_{k\mu} w_\lambda\,d\Gamma,$$

and the entries of the unknown vectors θ_k and η^* are the coefficients of the approximate solution components ψ_k and λ^* with respect to the bases $\{\phi_{k\mu}\}$ and $\{w_\lambda\}$, respectively. Solving (3.13a) for θ_k, one obtains, for k=1,2,

$$\theta_k = S_k^{-1}((-1)^{k+1}U_k\eta^* + T_k) \tag{3.14}$$

which, upon substitution in (3.13b) yields the following system to be solved for the discrete Lagrange multiplier η^*:

$$(\sum_{k=1}^{2} U_k^T S_k^{-1} U_k)\eta^* = U_2^T S_2^{-1} T_2 - U_1^T S_1^{-1} T_1. \tag{3.15}$$

Once η^* is determined from (3.15), the θ_k are obtained from (3.14). System (3.15) is the discrete analog of (2.10).

The discrete formulation of (2.11) is

$$[\sum_{k=1}^{2} (U_k^T S_k^{-1} U_k)^{-1}]\eta = \sum_{k=1}^{2} (U_k^T S_k^{-1} U_k)^{-1} U_k^T S_k^{-1} T_k, \tag{3.16}$$

where the entries of η are the coefficients with respect to $\{w_\lambda\}$ of the discrete Dirichlet data to be determined on Γ. After solving (3.16) for η, the subdomain solutions are obtained from

$$\theta_k = S_k^{-1}[U_k(U_k^T S_k^{-1} U_k)^{-1}(\eta - U_k^T S_k^{-1} T_k) + T_k], \qquad k=1,2. \tag{3.17}$$

We refer to (3.16) as a *Generalized Schur Complement (GSC)* system. The motivation for this terminology is the following. Consider the special case in which the finite-dimensional Lagrange multiplier space $W_L(\Gamma)$ is given by

$$W_L(\Gamma) = \left\{ w : w = \gamma_1 v_1 \text{ for some } v_1 \in P_{M_1}(\Omega_1) \right\} \tag{3.18}$$

$$= \left\{ w : w = \gamma_2 v_2 \text{ for some } v_2 \in P_{M_2}(\Omega_2) \right\}$$

where we have implicitly assumed that $P_{M_k}(\Omega_k)$, k=1,2, have the same traces on Γ. We can arrange the unknown vectors θ_k in such a way that the entries $\theta_{k\mu}$ which couple to Γ (i.e., have indices μ such that $(U_k)_{\mu,\lambda} \neq 0$ for some λ) are listed last. Then S_k, T_k, U_k, and θ_k

may be partitioned as

$$S_k = \begin{bmatrix} S_{11}^k & S_{21}^k \\ S_{12}^k & S_{22}^k \end{bmatrix}, \quad T_k = \begin{bmatrix} T_1^k \\ T_2^k \end{bmatrix}, \quad U_k = \begin{bmatrix} 0 \\ \tilde{U} \end{bmatrix}, \quad \theta_k = \begin{bmatrix} \theta_1^k \\ \theta_2^k \end{bmatrix}$$

where $\tilde{U}$ is a nonsingular $L \times L$ matrix. Straightforward matrix algebra yields that (3.16) can then be written as

$$\sum_{k=1}^{2} \left[S_{22}^k - S_{21}^k (S_{11}^k)^{-1} S_{12}^k \right] \tilde{\theta} = \sum_{k=1}^{2} \left[T_2^k - S_{21} (S_{11}^k)^{-1} T_1^k \right] \tag{3.19}$$

where $\tilde{\theta} = \tilde{U}^{-T} \eta = \theta_2^k$, k=1,2. Thus, in the special case defined by (3.18), the system (3.16) is equivalent to the usual Schur complement system, modulo the transformation of the interface unknowns effected by the matrix $\tilde{U}$.

Although it is the GSC system (3.16) which generalizes the well-known and much-studied Schur complement formulation, the presence of the matrices U_k in cases where (3.18) does not hold makes the GSC system more expensive to implement than system (3.15). This is consistent with conclusion that it is better to use the natural interface data represented by the Lagrange multipliers as the unknown quantity to be solved for on the interfaces rather than the Dirichlet data determined by the solution of the GSC system. We note that the estimates of Theorem 3.1 were obtained for system (3.15), since this was the discrete problem directly obtained from the continuous Lagrange multiplier formulation.

It is apparent that the predominant cost in implementing (3.15) is the construction of its coefficient matrix. In each subdomain, it is necessary to solve L linear systems to compute each subdomain's contribution to this matrix with an additional subdomain solve required to obtain the $S_k^{-1} T_k$ contribution to the right-hand side of (3.15). The feasibility of the explicit construction of (3.15) is therefore heavily dependent upon the size of L. In the discretization scheme described above, the space $W_L(\Gamma)$ was chosen independently of the discretizations on the subdomains (i.e., the $P_{M_k}(\Omega_k)$) subject only to the condition (3.7). This implies that we are essentially free to choose $W_L(\Gamma)$ in such a way as to approximate well the natural interface data $\gamma^* u$ on Γ. As can be seen from (3.8), if this is effectively done, then the error on each subdomain Ω_k will be dominated by the usual best-approximation errors on the subdomains. Since we are solving an elliptic partial differential equation, we know that for real problems the natural interface data $\gamma^* u$ will generally be very smooth, except perhaps for singularities of well-known functional form at the endpoints of Γ. Because of this smoothness, it is logical to choose the space $W_L(\Gamma)$ to contain either algebraic or trigonometric polynomials on Γ, since the smooth data $\gamma^* u$ can be approximated well by small numbers of such functions. Even if singularities exist, as the approximation theory [5-8,11,12,15-17] for the p-version of the finite element method demonstrates, on quasiuniform meshes high-order polynomials are superior to the usual low-order piecewise polynomials one is effectively using when the space $W_L(\Gamma)$ is given by (3.18). Therefore, by using such multipliers L should be very small. This means that only a small number of subdomain solves are required to construct the system (3.15), which may even be of sufficiently low dimension for solution via direct methods.

It should be observed that the $M_k \times L$ matrices U_k depend only upon the spaces $P_{M_k}(\Omega_k)$ and $W_L(\Gamma)$. In particular, the U_k are independent of the elliptic operator giving rise to the matrices S_k and therefore could be precomputed. Depending upon the choice of the spaces $P_{M_k}(\Omega_k)$ and $W_L(\Gamma)$, the U_k can also be quite sparse. Such sparsity can therefore be exploited both in the construction of the U_k and in the computations involved in setting up (3.15). For example, if $P_{M_k}(\Omega_k)$ consists of continuous piecewise-linear functions on a fine gridding of Ω_k, only a relatively small number of basis functions $\phi_{k\mu}$ have support meeting the interface Γ. This yields matrices U_k with many zero entries. On the other hand, if $P_{M_k}(\Omega_k)$ consists of globally-defined polynomials, such as in the p-version of the finite element method, then the U_k will necessarily be less sparse, although M_k will generally be much smaller in this case due to the superior approximation properties of such spaces.

We note that in iterative substructuring techniques which use methods such as preconditioned conjugate gradient (PCG) to solve the Schur complement system (3.19), it is necessary to do at least one subdomain solve in each iteration in order to evaluate the action of the Schur complement matrix on a vector. The approach described above in which the system (3.15) is explicitly formed also requires a number of subdomain solves. Here, the subdomain solves are needed to construct the quantities $S_k^{-1}U_k$ and $S_k^{-1}T_k$. Since all of the right-hand sides of the subdomain problems (namely, the columns of U_k and the vector T_k) are available at the same time, these subdomain solves can easily be performed in parallel. This is in contrast to iterative methods where the inherent sequential nature of the PCG iteration precludes exploitation of this extra level of parallelism on each subdomain. Furthermore, if, on a shared-memory multiprocessor, we consider as a pool of tasks the subdomain solves needed in the computation of $S_k^{-1}U_k$ and $S_k^{-1}T_k$, k=1,2, then any subdomain solve can be assigned to any available processor with no synchronization required until all subdomain solves have been performed (except for the solves needed to perform the patching procedure). In this way, load-balancing is enhanced and the granularity of the parallel work remains at the level of the subdomain solves.

Another advantage of explicitly forming (3.15) in contrast to iterative approaches is that if many problems involving the same elliptic operator are to be solved (for example in a time-dependent calculation in which S_k and U_k do not change) then the matrix of (3.15) can simply be constructed once, factored and stored.

4. Numerical Results. As our first example, we consider the problem

$$-\Delta u + u = f \qquad \text{in } \Omega, \tag{4.1a}$$

$$u = g \qquad \text{on } \partial\Omega, \tag{4.1b}$$

where Ω is the domain pictured in Figure 4.1, and f and g are such that the solution of (4.1) is

$$u(x, y) = e^{2x+y}\sin(\pi y). \tag{4.2}$$

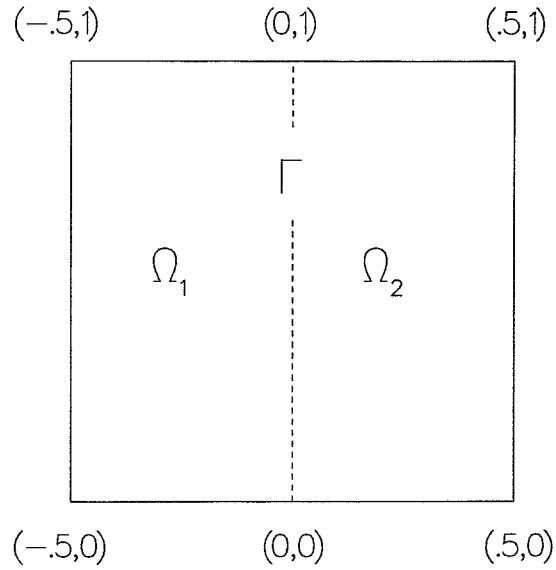

Figure 4.1. *Domain for problem* (4.1).

On the interface Γ separating the two subdomains Ω_1 and Ω_2, the solution conormal derivative, or "flux", is

$$\partial u/\partial \vec{n} = 2e^{y}\sin(\pi y), \tag{4.3}$$

where $\vec{n}$ is the unit normal to Γ pointing into Ω_2. Let Ω_k, k=1,2, be uniformly triangulated, and let h_k denote the maximum diameter of any mesh triangle. Similarly, let Γ be uniformly partitioned such that $(L+1)^{-1}$ is the length of any mesh segment. Let $P_{M_k}(\Omega_k)$ and $W_L(\Gamma)$ be the corresponding continuous piecewise linear spaces satisfying the appropriate boundary conditions. We see that the restictions u_k, k=1,2, of the exact solution (4.2) belong to $C^{\infty}(\overline{\Omega}_k)$ and that $\partial u/\partial \vec{n}$ belongs to $C^{\infty}(\overline{\Gamma})$. If $(\psi_1,\psi_2,\lambda^*)$ is the solution of the discrete problem (3.6) corresponding to (4.1), then, provided that (3.7) holds, it follows from Corollary 3.1 that

$$\sum_{k=1}^{2}\|u_k-\psi_k\|_{H^1(\Omega_k)} + \|\partial u/\partial \vec{n}-\lambda^*\|_{H_{00}^{-1/2}(\Gamma)} \le C(u)\left[\sum_{k=1}^{2} h_k + L^{-5/2}\right], \tag{4.4}$$

where $C(u)$ is independent of h_k and L. In (4.4), we have used the fact that, for a uniform triangulation of Ω_k, $h_k = O(M_k^{-1/2})$.

As a second option for $W_L(\Gamma)$, we consider the space of globally-defined (i.e., not piecewise) polynomials of degree $\le L+1$ on Γ which vanish at the endpoints of Γ. In this case, again assuming (3.7), it follows from Corollary 3.2 that

$$\sum_{k=1}^{2} \|u_k - \psi_k\|_{H^1(\Omega_k)} + \|\partial u/\partial \vec{n} - \lambda^*\|_{H_{00}^{-1/2}(\Gamma)} \tag{4.5}$$

$$\leq C(u, n_\gamma) \left[\sum_{k=1}^{2} h_k + L^{-(n_\gamma + 1/2)} \right],$$

for arbitrarily large n_γ, where $C(u, n_\gamma)$ is independent of h_k and L.

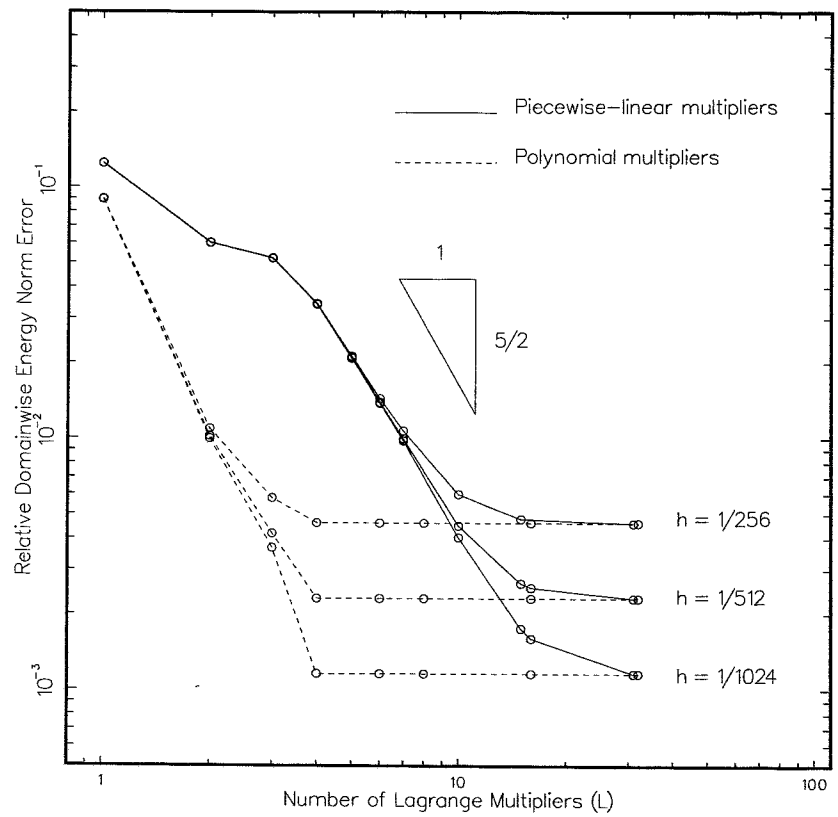

Figure 4.2. *Convergence of the domainwise relative energy norm error with respect to the number of piecewise-linear and polynomial multipliers in the solution of problem* (4.1).

Since the exact solution (4.2) of (4.1) is known, we can calculate the subdomain error terms in the left-hand sides of (4.4) and (4.5) to experimentally observe the convergence rates predicted by the above theory. We cannot directly compute the interface error involving the $H_{00}^{-1/2}(\Gamma)$ norm, but this can be estimated as described in [13]. Figure 4.2 shows some results obtained using the piecewise-linear and polynomial Lagrange multiplier spaces $W_L(\Gamma)$ together

with uniform subdomain partitionings corresponding to $h^{-1} = 256, 512$, and 1024, with $h_1 = h_2 = h$. Plotted against the number of Lagrange multipliers L is the relative domainwise energy norm error

$$\frac{\left[\sum_{k=1}^{2} \|u_k - \psi_k\|^2_{H^1(\Omega_k)}\right]^{1/2}}{\|u\|_{H^1(\Omega)}}. \tag{4.6}$$

Since a log-log scale is used in Figure 4.2, the predicted 5/2 convergence rate with respect to L^{-1} for the case of piecewise-linear multipliers is easy to see. On the other hand, the prediction that the errors using polynomial multipliers are decreasing faster than any polynomial rate with respect to L^{-1} is difficult to verify from the few data points which precede the bottoming out of the error curves. The fact that the errors do not decrease past a certain point for large L is to be expected since the subdomain errors will ultimately predominate as more multipliers are used on Γ. Hence the curve asymptotes represent the errors which would be obtained by a standard finite-element or finite-difference method applied to the original problem (4.1). We note that it was necessary to take a ridiculously fine gridding of the subdomains in order to reduce the subdomain errors enough to even see the convergence rates of the errors introduced by the Lagrange multipliers. This is partially due to the relatively poor approximation properties of the piecewise linear functions used on the subdomains, but it is also an indication of the rapid convergence of the discrete Lagrange multipliers. Using piecewise-linear $W_L(\Gamma)$, 4 multipliers were required to reduce the relative domainwise energy norm error to less than 5%, whereas for polynomial $W_L(\Gamma)$, only 2 multipliers were needed to reach this tolerance. In the latter case, this means that only 2 subdomain solves are required on each subdomain to construct system (3.15), and that the cost of a direct solution of this 2×2 system is negligible.

Since no patching was performed in obtaining the results presented above, the computed solutions of (4.1) are discontinuous at Γ. This discontinuity at Γ can nevertheless be removed using the patching procedure described in Section 3. The quantity (4.6) will then represent the true relative energy norm error on Ω. In Figure 4.3, the error curves obtained using polynomial Lagrange multipliers with patching are plotted against the corresponding unpatched error curves taken from Figure 4.2. Although we showed in Section 3 that the patching procedure will not degrade the rate of convergence of the subdomain solutions with respect to the number of Lagrange multipliers, we cannot observe this in Figure 4.3 since, for all three subdomain mesh sizes, the patching has reduced the interface error below the level of the subdomain error. This means the error obtained using 1, 2, and 3 polynomial Lagrange multipliers in the unpatched version of the algorithm is entirely due to nonsatisfaction of exact continuity at the interface, even though the energy norm error was only computed in a domainwise sense (i.e., discontinuities at the interface do not directly contribute to the errors). It should again be noted that we are using very fine subdomain grids, and from Figure 4.3 we see that if coarser subdomain grids had been used then the difference between the unpatched and patched errors might not be seen. Nevertheless, this example shows that the use of the patching procedure not only recovers the continuity of the computed solutions at the interface, but in fact can even further reduce the errors on the subdomains.

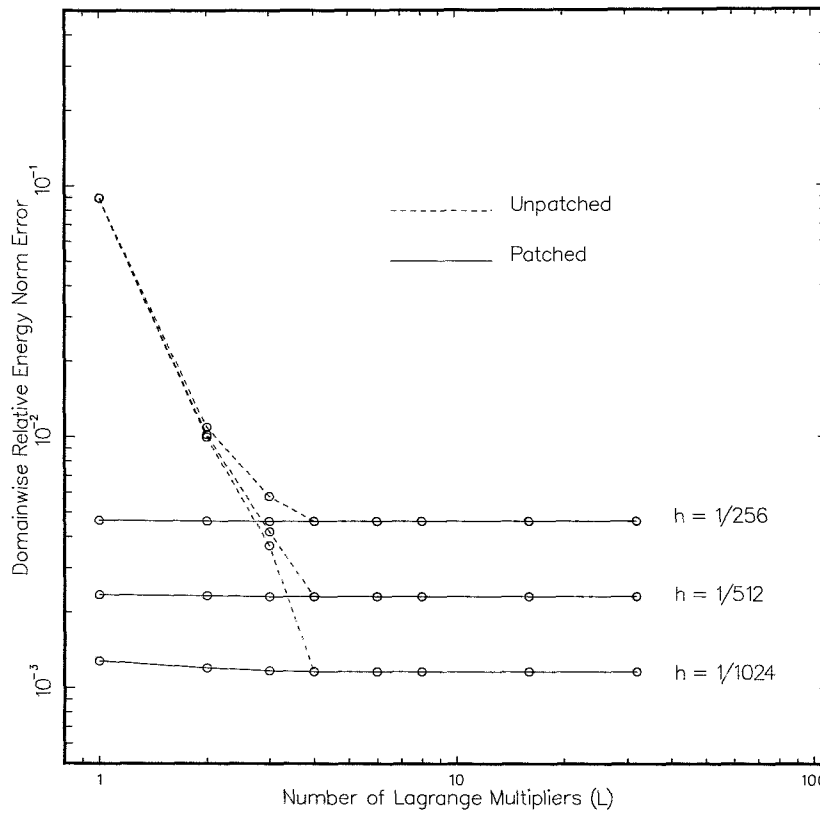

Figure 4.3. *Comparison of the convergence rates of the domainwise relative energy norm error with respect to the number of polynomial Lagrange multipliers before and after application of the patching procedure.*

As an example of a nonsmooth problem, we consider

$$-\Delta u + u = f \qquad \text{in } \Omega, \tag{4.7a}$$

$$u = 0 \qquad \text{on } \partial\Omega, \tag{4.7b}$$

where Ω is the L-shaped domain shown in Figure 4.4. We assume that f is such that the solution of (4.7) is

$$u(x,y) = (1-x^2)(1-y^2)r^{2/3}\sin((2\theta + \pi)/3) \tag{4.8}$$

where r and θ are the usual polar coordinates based at the origin. The singularity in the derivatives of (4.8) at the origin is representative of the singularity existing in all problems with reentrant corner angles of measure $3\pi/2$ and homogeneous Dirichlet conditions on the sides of the domain meeting at such corners [14].

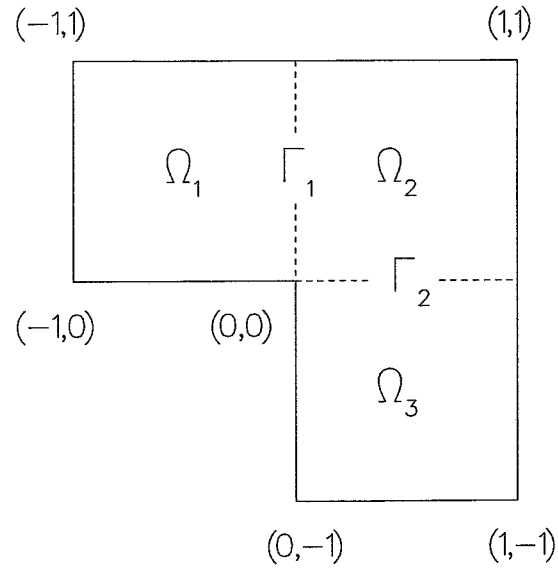

Figure 4.4. *Domain for problem* (4.7).

Figure 4.4 also indicates a very natural domain decomposition of Ω via the introduction of interfaces Γ_1 and Γ_2. Although three subdomains are shown, we observe that the problem is actually symmetric with respect to the line $y = x$ and therefore can be treated as a two-domain problem with one interface. The decomposition shown in Figure 4.4 has the advantage of yielding geometrically simple subdomains, yet both interfaces contain the reentrant corner and therefore also contain the singularity. Letting s denote the arc length along either Γ_1 or Γ_2 as measured from the origin, we have that the solution flux on Γ_j, j=1,2, is given by

$$\partial u/\partial \vec{n}_j = \frac{1}{3}(1-s^2)s^{-1/3} \tag{4.9}$$

modulo a sign depending on the direction of the unit vector $\vec{n}_j$ normal to Γ_j. Letting $P_{M_k}(\Omega_k)$, k=1,2, be the same piecewise linear subdomain space used in the previous example, and taking the Lagrange multiplier spaces $W_L(\Gamma_j)$ to be the spaces of all continuous piecewise linear functions on uniform partitionings of Γ_j, it follows from Corollary 3.1 and the regularity properities of (4.8,4.9) that if (3.7) is satisfied and $(\psi_1,\psi_2,\psi_3,\lambda_1^*,\lambda_2^*)$ is the solution of the discrete problem (3.6) (trivially generalized to the case of three subdomains and two interfaces) corresponding to (4.7), then

$$\sum_{k=1}^{3}\|u_k-\psi_k\|_{H^1(\Omega_k)} + \sum_{j=1}^{2}\|\partial u/\partial \vec{n}_j-\lambda_j^*\|_{H_{00}^{-1/2}(\Gamma_j)} \tag{4.10}$$

$$\leq C(u)\left[\sum_{k=1}^{2} h_k^{2/3} + L^{-2/3}\right].$$

Furthermore, letting $W_L(\Gamma_j)$ be the space of all polynomials of degree $\leq L+1$ which vanish at the endpoints of Γ_j, then

$$\sum_{k=1}^{3} \|u_k - \psi_k\|_{H^1(\Omega_k)} + \sum_{j=1}^{2} \|\partial u/\partial \vec{n}_j - \lambda_j^*\|_{H_{00}^{-1/2}(\Gamma_j)} \tag{4.11}$$

$$\leq C(u) \left[\sum_{k=1}^{2} h_k^{2/3} + L^{-5/6} \right].$$

Figures 4.5 and 4.6 are the analogs of Figures 4.2 and 4.3 for problem (4.7). Uniform triangulations of the subdomains Ω_k corresponding to mesh sizes of h^{-1}=16, 32 and 64, $h_1=h_2=h_3=h$, were used together with L=1,2,4,8, and 16 multipliers on each of the interfaces Γ_j. Comparing these results with Figures 4.2 and 4.3, the negative effects of the reduced interface flux regularity are evident. Considering Figure 4.5, we see that for h=1/64, at least 10 polynomial multipliers were required to reduce the error to the point at which the subdomain errors are dominant, and the error using 16 piecewise-linear multipliers had not yet

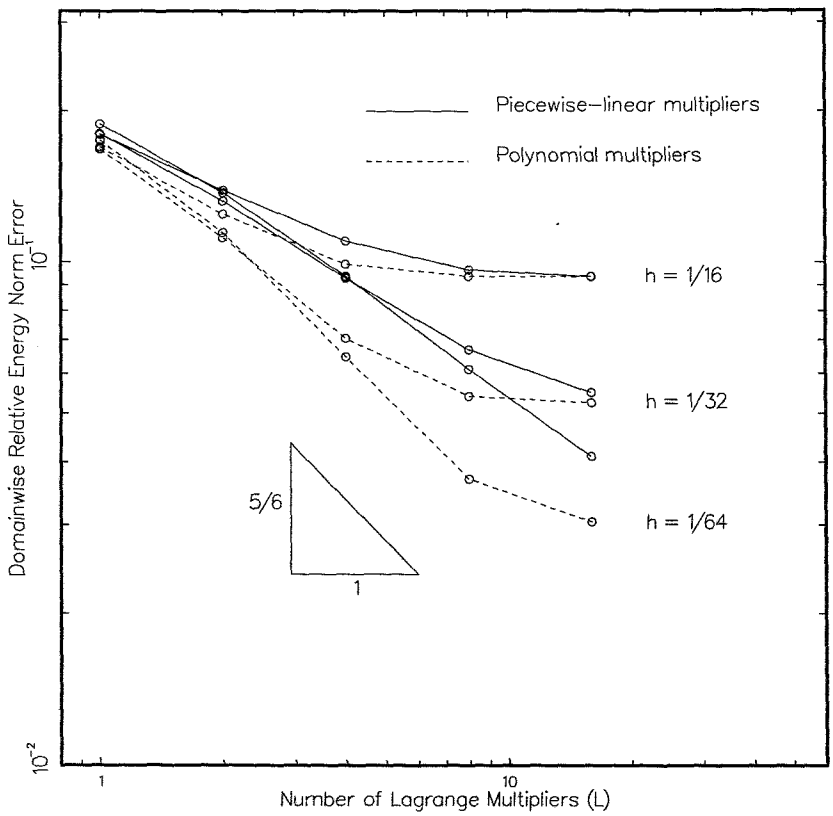

Figure 4.5. *Convergence of the domainwise relative energy norm error with respect to the number of piecewise-linear and polynomial multipliers in the solution of problem* (4.7).

reached this floor. Even 10 multipliers must be considered a rather large number since this would mean that 10 subdomain solves would be required in subdomains Ω_1 and Ω_3 and 20 solves in Ω_2 to construct the system (3.15). As Figure 4.6 shows, by applying the patching procedure the error can nevertheless be reduced to the subdomain error floor using 5 or 6 polynomial multipliers for the case h=1/64 and even fewer for the cases h=1/16 and h=1/32.

In the previous example, our principal concern was the convergence of the Lagrange multipliers. In obtaining our computed results, we therefore used simple uniform subdomain triangulations even though the problem has a singularity at the origin. Indeed, the subdomain approximations can be greatly improved by appropriate mesh refinement near the singularity. However, the same techniques may also be applied on the interface. We could generalize the spaces $W_L(\Gamma_j)$ to consist of arbitrary degree piecewise polynomials on a partitioning of Γ_j as is done in the h–p version of the finite element method [6,7,15-17]. Since we know the form of the singularity at the reentrant corner, we could appropriately grade the interface meshes near the singularity to improve the approximation properties of the Lagrange multiplier spaces $W_L(\Gamma_j)$. It seems clear that, from a practical point of view, it will always be easier to implement effective Lagrange multiplier spaces $W_L(\Gamma_j)$ on the one-dimensional interfaces in order to exploit known solution characteristics than it would be to make an equivalent change in the two-dimensional subdomain spaces $P_{M_k}(\Omega_k)$.

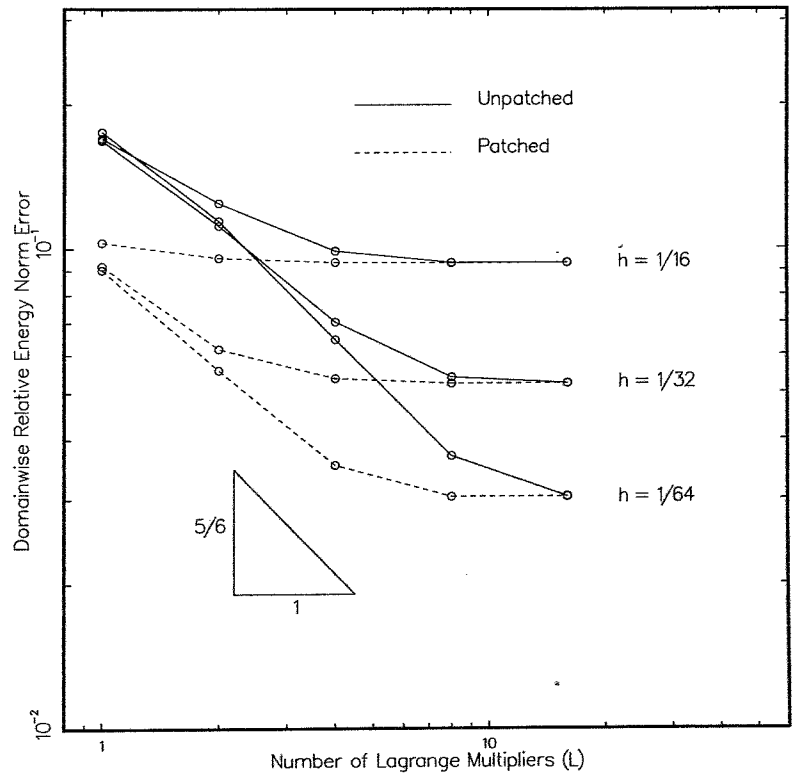

Figure 4.6. *Comparison of the convergence rates of the domainwise relative energy norm error with respect to the number of polynomial Lagrange multipliers before and after application of the patching procedure.*

Based on the results obtained for the smooth model problem (4.1) and the nonsmooth model problem (4.7), we conclude that the set of polynomials of degree $\leq L+1$ on Γ which vanish at the endpoints of Γ are a good general-purpose choice for the Lagrange multiplier space $W_L(\Gamma)$. Considering the fact that the Legendre polynomials mapped to Γ can be used to construct a hierarchical basis for such a space, there are other benefits of this choice as well. Furthermore, we have seen that it is generally a good idea to perform the patching procedure even if the application at hand does not strictly require continuity at the interfaces.

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