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Algorithms for Spectral Methods**

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Schur Complement Domain Decomposition Algorithms for Spectral Methods

TONY F. CHAN¹
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Abstract. Spectral methods have been using a domain decomposition approach for handling irregular domains. The main focus has been on appropriate matching conditions for the solutions across the subdomain boundaries.

In this paper, we propose an efficient method for solving the discrete equations based on solving the Schur complement system for the interface variables. We consider both the Funaro-Maday-Patera weak C^1 matching of the solutions on the interfaces and Orszags exact C^1 matching. Numerical results for the model problem show that the condition number of the Schur Complement system is of order $O(n^2)$. We show how this can be improved to nearly $O(1)$ by a boundary probe preconditioner.

We also point out the relationship between our method and the alternating Neumann Dirichlet method of Funaro-Quarteroni-Zanolli.

1. Introduction

Spectral methods for partial differential equations are very attractive for their exponential accuracy. However, a drawback of these methods as compared to finite difference or finite element methods is that the matrices of the resulting algebraic equations are dense. For multi dimensional problems this has led to the use of tensor product polynomial basis functions. In this way, Fourier methods can be used for solving the discrete equations. This however restricts the applications of these methods to parallelotopes or deformed parallelotopes obtained by tensorization of 1 dimensional domains.

For more complex geometries, a domain decomposition approach is used. The computational domain is divided into the union of non overlapping parallelotopes. The solutions on each subdomain must satisfy appropriate matching conditions on the interfaces. In conforming methods, the gridpoints on the internal boundaries of adjacent subdomains must coincide while in non conforming methods this restriction does not apply. In the conforming methods, the patching method [11] imposes exact C^1 continuity of the solution on the interfaces, while the spectral element method [12] forces a weak C^1 continuity.

A domain decomposition approach can also be used in the solution of the algebraic equations resulting from these methods. In finite element or finite difference methods, a large class of domain decomposition methods are based on solving the Schur complement equations for the interface variables using the preconditioned conjugate gradient method. In this paper we propose using the same technique for conforming spectral methods. The outline of the paper is the following. In section 2 we derive the discrete equations for the model problem and show the structure of the matrix of the system of equations. In section 3 we introduce the Schur complement preconditioned conjugate gradient method and we show with numerical examples that the condition number of the Schur complement for the model problem, is $O(n^2)$, with n the order of the interface system. In section 4 we introduce the boundary probe preconditioner which improves the condition number to slowly increasing function of n . In section 5 we illustrate the relationship of the alternating Neumann Dirichlet iteration for the patching method [8] with the iteration on the Schur complement.

¹Department of Mathematics, UCLA.

²Department of Computer Science, K. U. Leuven. This research was done during a visit to the Department of Mathematics, UCLA, January 1988 - June 1988.

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2. Algebraic equations of the spectral element method.

We consider the 2 dimensional model problem :

$$(2-1) \quad -\Delta u = f \quad \text{on } \Omega \quad , u \in H^1(\Omega)$$

with Dirichlet boundary conditions :

$$(2-2) \quad u = 0 \quad \text{on } \partial\Omega$$

As domain Ω we take a rectangle, divided in two strips sharing the interface Γ :

$$\begin{aligned} \Omega &= [a, b] \otimes [c, d] \\ \Omega_1 &= [a, 0] \otimes [c, d] \\ \Omega_2 &= [0, b] \otimes [c, d] \end{aligned}$$

The problem (2-1), (2-2) can also be expressed in variational form :

$$(2-3) \quad \iint_{\Omega} \nabla u \nabla v = \iint_{\Omega} f v \quad u \in H_0^1(\Omega) \quad , \quad \forall v \in H_0^1(\Omega)$$

The integrals in (2-3) are splitted as the sum over the integrals over the 2 subdomains :

$$(2-4) \quad \iint_{\Omega_1} \nabla u \nabla v + \iint_{\Omega_2} \nabla u \nabla v = \iint_{\Omega_1} f v + \iint_{\Omega_2} f v \quad \forall v \in H_0^1(\Omega)$$

Writing the double integrals as repeted single integrals and expanding the gradients, the left hand side of (2-4) becomes :

$$(2-6) \quad \underbrace{\iint_{a \ c}^{0 \ d} \left(\frac{\partial u}{\partial x} \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \frac{\partial v}{\partial y} \right) dy dx}_{I_1} + \underbrace{\iint_{0 \ c}^{b \ d} \left(\frac{\partial u}{\partial x} \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \frac{\partial v}{\partial y} \right) dy dx}_{I_2} \quad ,$$

Let :

$$\begin{aligned} x_1^1 &= a \quad , \quad x_2^1 = 0 \\ x_1^2 &= 0 \quad , \quad x_2^2 = b \\ \Delta_x^i &= x_2^i - x_1^i \\ \Delta_y &= d - c \end{aligned}$$

We transform the subdomains to the squares $[-1, 1] \otimes [-1, 1]$ with the transformations :

$$\begin{aligned} \hat{x}^i &= -1 + 2 \frac{x - x_1^i}{\Delta_x^i} \\ \hat{y}^i &= -1 + 2 \frac{y - c}{\Delta_y} \end{aligned}$$

The integrals I_i , $i = 1, 2$ then are transformed into :

$$(2-7) \quad I_i = \sigma_i \int_{-1}^1 \int_{-1}^1 \frac{\partial u^i}{\partial \hat{x}^i} \frac{\partial v^i}{\partial \hat{x}^i} d\hat{x}^i d\hat{y}^i + 1/\sigma_i \int_{-1}^1 \int_{-1}^1 \frac{\partial u^i}{\partial \hat{y}^i} \frac{\partial v^i}{\partial \hat{y}^i} d\hat{x}^i d\hat{y}^i \quad ,$$

with σ_i the aspect ratio of the subdomains :

$$\sigma_i = \frac{\Delta_y}{\Delta_x^i}$$

and u^i and v^i the restrictions of u , respectively v to Ω_i . The weak formulation of the elliptic problem then is :

$$(2-5) \quad I_1 + I_2 = \frac{\Delta_x^1 \Delta_y}{4} \int_{-1}^1 \int_{-1}^1 f^1 v^1 d\hat{x}^1 d\hat{y}^1 + \frac{\Delta_x^2 \Delta_y}{4} \int_{-1}^1 \int_{-1}^1 f^2 v^2 d\hat{x}^2 d\hat{y}^2 \quad ,$$

with $f^i = f(\Delta_x^i(\hat{x}^i + 1)/2 + x_1^i, \Delta_y(\hat{y}^i + 1)/2 + c)$. In what follows we always refer to these transformed subdomains. We will drop the indices denoting the number of the subdomains when there is no danger for confusion, and we will denote the variables again by x and y .

Spectral methods take as solution on the subdomains a polynomial approximation :

$$u^i \approx Q_{n_x^i n_y^i}(x, y) \quad ,$$

where $Q_{n_x n_y}(x, y)$ is a polynomial of maximum degree n_x in x and of maximum degree n_y in y . In conforming methods, $n_x^1 = n_x^2$. We will use the notation u^i also for this polynomial approximation.

The algebraic equations in the spectral element method are obtained by replacing the integrals in (2-5) by Gaussian quadrature rules and choosing an appropriate set of test functions v^i . Let :

$$-1 = \eta_0^n < \eta_1^n < \dots < \eta_{n-1}^n < \eta_n^n = 1 \quad ,$$

and

$$\rho_j, \quad j = 0, \dots, n \quad ,$$

be the Gauss Lobatto points and corresponding weights for a Gaussian quadrature rule with $n+1$ points for the Legendre weight function $w(x) \equiv 1$. The points η_i^n , $i = 1, \dots, n-1$ are the zeros of P_n' , where P_n is the Legendre polynomial of degree n . The Gauss Lobatto points define a grid on the subdomains :

$$\xi_{ki}^i = \left(\eta_k^{n_x^i}, \eta_l^{n_y^i} \right) \quad .$$

We denote the Lagrangian interpolating polynomials through the points η_j^n , $j = 0, \dots, n$ by L_k^n . They can be written as [10] :

$$L_k^n = -\frac{1}{n(n+1)P_n(x_k)} \frac{(1-x^2)P_n'(x)}{(x-x_k)} \quad .$$

The set of testfunctions corresponding to the interior grid points of the subdomains, is :

$$\begin{aligned} v^1 &= L_k^{n_x^1}(x) L_l^{n_y}(y) & k = 1, \dots, n_x^1 - 1, \quad l = 1, \dots, n_y - 1 \\ v^2 &= 0 \end{aligned} \quad ;$$

and

$$\begin{aligned} v^1 &= 0 \\ v^2 &= L_k^{n_x^2}(x) L_l^{n_y}(y) & k = 1, \dots, n_x^2 - 1, \quad l = 1, \dots, n_y - 1 \end{aligned} \quad .$$

This then leads to a collocation method for the interior points :

$$(2-6) \quad -\sigma_i \frac{\partial^2 u^i(\xi_{kl}^i)}{\partial x^2} - 1/\sigma_i \frac{\partial^2 u^i(\xi_{kl}^i)}{\partial y^2} = \frac{\Delta_x^i \Delta_y}{4} f(\xi_{kl}^i) \quad .$$

For the points on the interface between the subdomains, we take the following test functions :

$$\begin{aligned} v^1 &= L_{n_x^1}^{n_x^1}(x) L_l^{n_y}(y) \\ v^2 &= L_0^{n_x^2}(x) L_l^{n_y}(y) \end{aligned} \quad l = 1, \dots, n_y - 1$$

This gives the following equations :

$$\begin{aligned} (2-7) \quad & -\sigma_1 \frac{\partial^2 u^1(\xi_{n_x^1 l}^1)}{\partial x^2} - 1/\sigma_1 \frac{\partial^2 u^1(\xi_{n_x^1 l}^1)}{\partial y^2} + \sigma_1 \frac{\partial u^1(\xi_{n_x^1 l}^1)}{\partial x} / \rho_{n_x^1} \\ & - \sigma_2 \frac{\partial^2 u^2(\xi_{0l}^2)}{\partial x^2} - 1/\sigma_2 \frac{\partial^2 u^2(\xi_{0l}^2)}{\partial y^2} - \sigma_2 \frac{\partial u^2(\xi_{0l}^2)}{\partial x} / \rho_0 \\ & = \frac{\Delta_x^1 \Delta_y}{4} f^1(\xi_{n_x^1 l}^1) + \frac{\Delta_x^2 \Delta_y}{4} f^2(\xi_{0l}^2) \end{aligned}$$

From the equations (2-6) and (2-7) it can be seen that the spectral element method is an exact pseudo-spectral collocation method inside each subdomain (2-6) with a weak C^1 continuity on the interface. Patching methods [11] impose an exact C^1 matching of the subsolutions in the gridpoints on the interface :

$$\frac{\partial u^1(\xi_{n_x^1 l}^1)}{\partial x} - \frac{\partial u^2(\xi_{0l}^2)}{\partial x} = 0$$

The solution on a subdomain can be expressed as :

$$u^i = \sum_{k=0}^{n_x^i} \sum_{l=0}^{n_y} u_{kl}^i L_k^{n_x^i}(x) L_l^{n_y}(y)$$

We then have :

$$\begin{aligned} \frac{\partial u^i(\xi_{mn}^i)}{\partial x} &= \sum_{k=0}^{n_x^i} u_{kn}^i \left(L_k^{n_x^i} \right)' (\eta_m^{n_x^i}) \\ \frac{\partial^2 u^i(\xi_{mn}^i)}{\partial x^2} &= \sum_{k=0}^{n_x^i} u_{kn}^i \left(L_k^{n_x^i} \right)'' (\eta_m^{n_x^i}) \\ \frac{\partial u^i(\xi_{mn}^i)}{\partial y} &= \sum_{l=0}^{n_y} u_{ml}^i \left(L_l^{n_y} \right)' (\eta_n^{n_y}) \\ \frac{\partial^2 u^i(\xi_{mn}^i)}{\partial y^2} &= \sum_{l=0}^{n_y} u_{ml}^i \left(L_l^{n_y} \right)'' (\eta_n^{n_y}) \end{aligned}$$

We define the matrices D_n^1 and D_n^2 :

$$\begin{aligned} (D_n^1)_{kl} &= (L_l^n)'(\eta_k^n) \\ (D_n^2)_{kl} &= (L_l^n)''(\eta_k^n) \end{aligned}$$

Straightforward calculus and dropping the index n , gives [10] :

$$\begin{aligned} (D^1)_{kl} &= \frac{P_n(\eta_k)}{P_n(\eta_l)(\eta_k - \eta_l)} \quad , \quad k \neq l \\ (D^1)_{00} &= -\frac{\alpha_n}{4} \quad , \\ (D^1)_{kk} &= 0 \quad , \quad k = 1, \dots, n-1 \quad , \\ (D^1)_{nn} &= \frac{\alpha_n}{4} \quad , \end{aligned}$$

with $\alpha_n = n(n+1)$, and :

$$\begin{aligned}
(D^2)_{00} &= \frac{\alpha_n(\alpha_n - 2)}{24} , \\
(D^2)_{0l} &= -\frac{P_n(\eta_0)(2 + \alpha_n(\eta_0 - \eta_l)/2)}{P_n(\eta_l)(\eta_0 - \eta_l)^2} , \quad l \neq 0 , \\
(D^2)_{kl} &= -2\frac{P_n(\eta_k)}{P_n(\eta_l)(\eta_k - \eta_l)^2} , \quad \begin{array}{l} k = 1, \dots, n-1 , \\ l = 0, \dots, n , \end{array} \quad k \neq l , \\
(D^2)_{kk} &= -\frac{\alpha_n}{3(1 - \eta_k^2)} , \quad k = 1, \dots, n-1 , \\
(D^2)_{nn} &= \frac{\alpha_n(\alpha_n - 2)}{24} , \\
(D^2)_{nl} &= -\frac{P_n(\eta_n)(2 - \alpha_n(\eta_n - \eta_l)/2)}{P_n(\eta_l)(\eta_n - \eta_l)^2} , \quad l \neq n .
\end{aligned}$$

Let :

$$(2-8) \quad u_1 = \left(u_{11}^1 \dots u_{1(n_v-1)}^1 \ u_{21}^1 \dots u_{2(n_v-1)}^1 \ \dots \ u_{(n_z^1-1)1}^1 \dots u_{(n_z^1-1)(n_v-1)}^1 \right)^T$$

$$(2-9) \quad u_2 = \left(u_{n_z^1 1}^1 \dots u_{n_z^1(n_v-1)}^1 \right)^T$$

$$(2-9) \quad = \left(u_{01}^2 \dots u_{0(n_v-1)}^2 \right)^T$$

$$u_3 = \left(u_{11}^2 \dots u_{1(n_v-1)}^2 \ u_{21}^2 \dots u_{2(n_v-1)}^2 \ \dots \ u_{(n_z^2-1)1}^2 \dots u_{(n_z^2-1)(n_v-1)}^2 \right)^T ,$$

and

$$u = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} .$$

The equality (2-8) (2-9) forces C^0 continuity of the solution on the interface. The discrete equations for (2-6) and (2-7) then can be written as :

$$(2-10) \quad Au = f$$

where f is a discrete vector corresponding to the right hand sides. The matrix A has the following structure :

$$A = \begin{pmatrix} A_{11} & A_{12} & \\ A_{21} & A_{22} & A_{23} \\ & A_{32} & A_{33} \end{pmatrix} .$$

The matrices A_{ij} can be expressed as direct products of the matrices D :

$$\begin{aligned}
A_{11} &= -\sigma_1 D_{n_x^1}^2(1 : n_x^1 - 1, 1 : n_x^1 - 1) \otimes I_{(n_y-1)} - I_{(n_x^1-1)} \otimes D_{n_y}^2(1 : n_y - 1, 1 : n_y - 1)/\sigma_1 \\
A_{12} &= -\sigma_1 D_{n_x^1}^2(1 : n_x^1 - 1, n_x^1) \otimes I_{(n_y-1)} \\
A_{21} &= -\sigma_1 D_{n_x^1}^2(n_x^1, 1 : n_x^1 - 1) \otimes I_{(n_y-1)} + \sigma_1 D_{n_x^1}^1(n_x^1, 1 : n_x^1 - 1)/\rho_{n_x^1} \otimes I_{(n_y-1)} \\
A_{22} &= A_{22}^1 + A_{22}^2 \\
A_{22}^1 &= -\sigma_1 D_{n_x^1}^2(n_x^1, n_x^1) I_{(n_y-1)} - D_{n_y}^2(1 : n_y - 1, 1 : n_y - 1)/\sigma_1 + \sigma_1 D_{n_x^1}^1(n_x^1, n_x^1)/\rho_{n_x^1} I_{(n_y-1)} \\
A_{22}^2 &= -\sigma_2 D_{n_x^2}^2(0, 0) I_{(n_y-1)} - D_{n_y}^2(1 : n_y - 1, 1 : n_y - 1)/\sigma_2 - \sigma_2 D_{n_x^2}^1(0, 0)/\rho_0 I_{(n_y-1)} \\
A_{23} &= -\sigma_2 D_{n_x^2}^2(0, 1 : n_x^2 - 1) \otimes I_{(n_y-1)} - \sigma_2 D_{n_x^2}^1(0, 1 : n_x^2 - 1)/\rho_0 \otimes I_{(n_y-1)} \\
A_{32} &= -\sigma_2 D_{n_x^2}^2(1 : n_x^2 - 1, 0) \otimes I_{(n_y-1)} \\
A_{33} &= -\sigma_2 D_{n_x^2}^2(1 : n_x^2 - 1, 1 : n_x^2 - 1) \otimes I_{(n_y-1)} - I_{(n_x^2-1)} \otimes D_{n_y}^2(1 : n_y - 1, 1 : n_y - 1)/\sigma_2 \quad ,
\end{aligned}$$

with I_n a unity matrix of dimension n . The matrices A_{11} , A_{22} and A_{33} are not symmetric. They can be symmetrized by the similarity transformation :

$$S^{-1}AS$$

with

$$S = \begin{pmatrix} S_{n_x^1} \otimes S_{n_y} & & \\ & S_{n_y} & \\ & & S_{n_x^2} \otimes S_{n_y} \end{pmatrix}$$

S_n is a diagonal matrix with entries :

$$(S_n)_{kk} = P_n(\eta_k^n) \quad , \quad k = 1, \dots, n-1$$

3. Schur complement conjugate gradient

In finite element or finite difference methods, the discrete system of equations is of the same block tridiagonal form as (2-10) but the blocks itself are banded. A large class of domain decomposition methods for these methods focusses on solving this system. We propose to use the same technique for spectral methods.

System (2-10) can be solved by Block Gaussian Elimination which gives the equations for the interface variables u_2 :

$$(3-1) \quad Su_2 = \hat{f}_2 \quad ,$$

with

$$S = A_{22} - A_{21}A_{11}^{-1}A_{12} - A_{23}A_{33}^{-1}A_{32}$$

and

$$\hat{f}_2 = f_2 - A_{21}A_{11}^{-1}f_1 - A_{23}A_{33}^{-1}f_3 \quad .$$

The matrix S is the Schur complement of A_{22} in the matrix A . It corresponds to the reduction of the operator L on Ω to an operator on the internal boundary Γ . Constructing the Schur complement would require the solution on n_y elliptic problems on each subdomain. Furthermore it is dense, so that factoring would be expensive.

Instead of solving the system (3-1) directly, iterative methods such as preconditioned conjugate gradient (PCG) can be applied. The PCG algorithm is the following :

$$\begin{aligned} & \text{choose} \quad u_2^0 \\ & r^0 = \hat{f}_2 - Su_2^0 \\ & p^{-1} \text{arbitrary} \\ & \text{for } k = 0, 1, \dots \\ & \quad \text{solve} \quad Mz^k = r^k \\ & \quad \left\{ \begin{array}{l} \beta_0 = 0 \\ \beta_k = \frac{(z^k)^T r^k}{(z^{k-1})^T r^{k-1}} \quad , \quad k \neq 0 \end{array} \right. \\ & \quad p^k = z^k + \beta^k p^{k-1} \\ & \quad q^k = Sp^k \\ & \quad \alpha_k = \frac{(z^k)^T r^k}{(p^k)^T q^k} \\ & \quad u_2^{k+1} = u_2^k + \alpha_k p^k \\ & \quad r^{k+1} = r^k - \alpha_k q^k \end{aligned}$$

where M is the preconditioning matrix. This only requires the matrix S in the matrix vector product Sy . This product can be computed by one solve on each subdomain with boundary condition on the interface determined by y .

The convergence of PCG is determined by the eigenvalue distribution of $M^{-1}A$. Let :

$$\kappa = \lambda_{max}(M^{-1}A) / \lambda_{min}(M^{-1}A)$$

A very well known result about PCG is [5] :

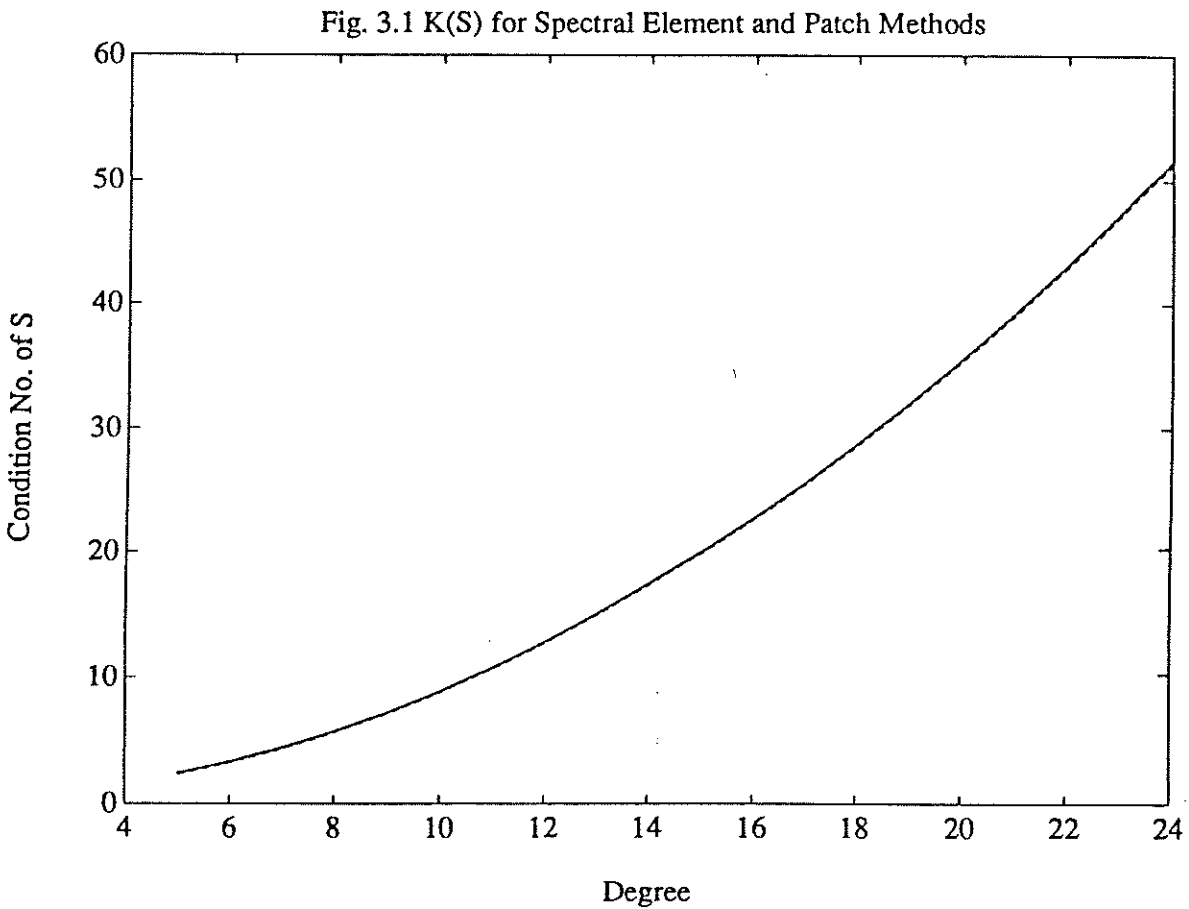
$$\frac{(u_2^k - u_2)^T A (u_2^k - u_2)}{(u_2^0 - u_2)^T A (u_2^0 - u_2)} \leq 4 \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^{2k}$$

In figure 3.1 we plot the condition number κ of S of the spectral element method, versus n for the following problem :

$$\begin{aligned} \Omega &= [0, 1] \otimes [0, 1] \\ \Omega_1 &= [0, 0.5] \otimes [0, 1] \\ \Omega_2 &= [0.5, 1] \otimes [0, 1] \end{aligned} ,$$

and

$$n_{x1} = n_x^2 = n_y = n$$



Numerical datafitting gives that $\kappa(S) = O(n^2)$. The results for the patching collocation method are very similar.

4. Boundary probe preconditioner for the Schur complement

In the finite element and finite difference case, several preconditioners have been proposed for the Schur complement S . A large class of preconditioners have been derived for the splitting of a rectangle and are intimately related to the underlying properties of the differential operator [7], [9], [2], or are based on symmetry properties of the operator and of the domain [1].

Another preconditioner is the boundary probe preconditioner [4]. The main motivation for this approach is the observation that, in the finite difference case for the Laplace operator, the elements of the matrix S decay rapidly away from the main diagonal [9]. This is inherently related to the fact that the operator S is predominantly local. In spectral element and patching methods, this operator is even more local. In figure 4.1, 4.2, we plot the elements of S for the spectral element method, respectively the patching collocation method, for a geometry with $\sigma_1 = \sigma_2 = 2$ and $n_x^1 = n_x^2 = n_y = 10$.

Fig. 4.1. Interface Operator for Spectral Element Method

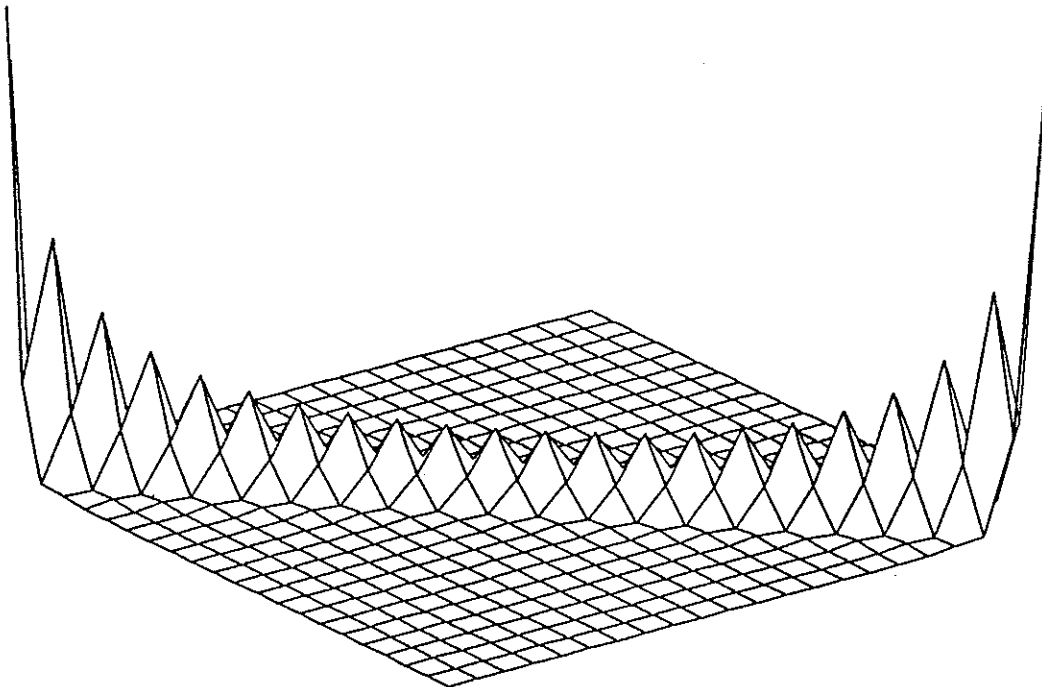
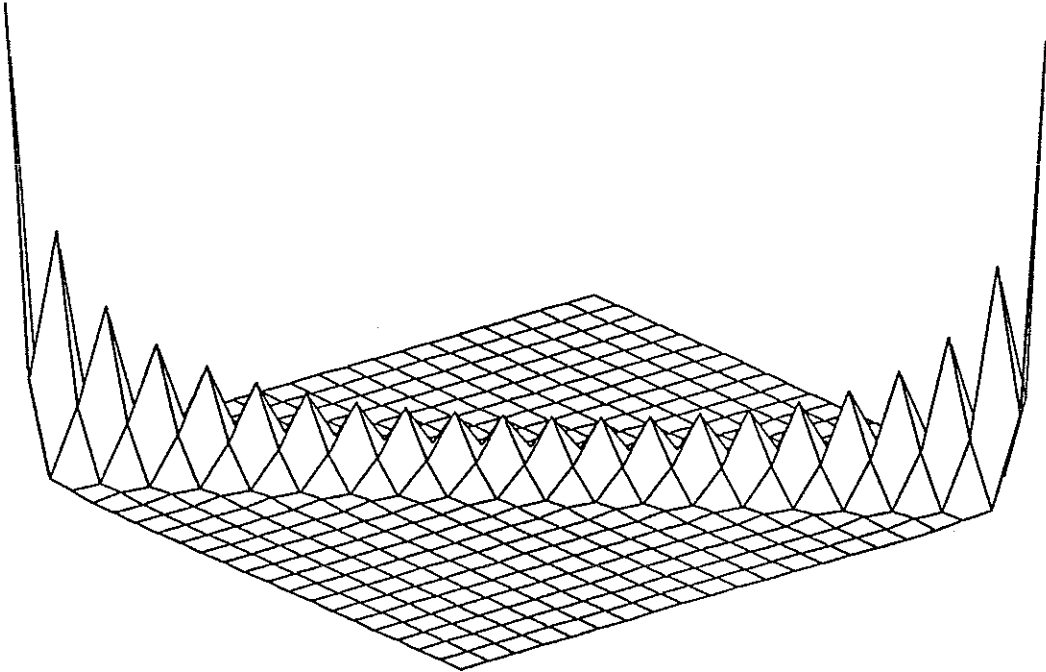


Fig. 4.2. Interface Operator for Patching Method



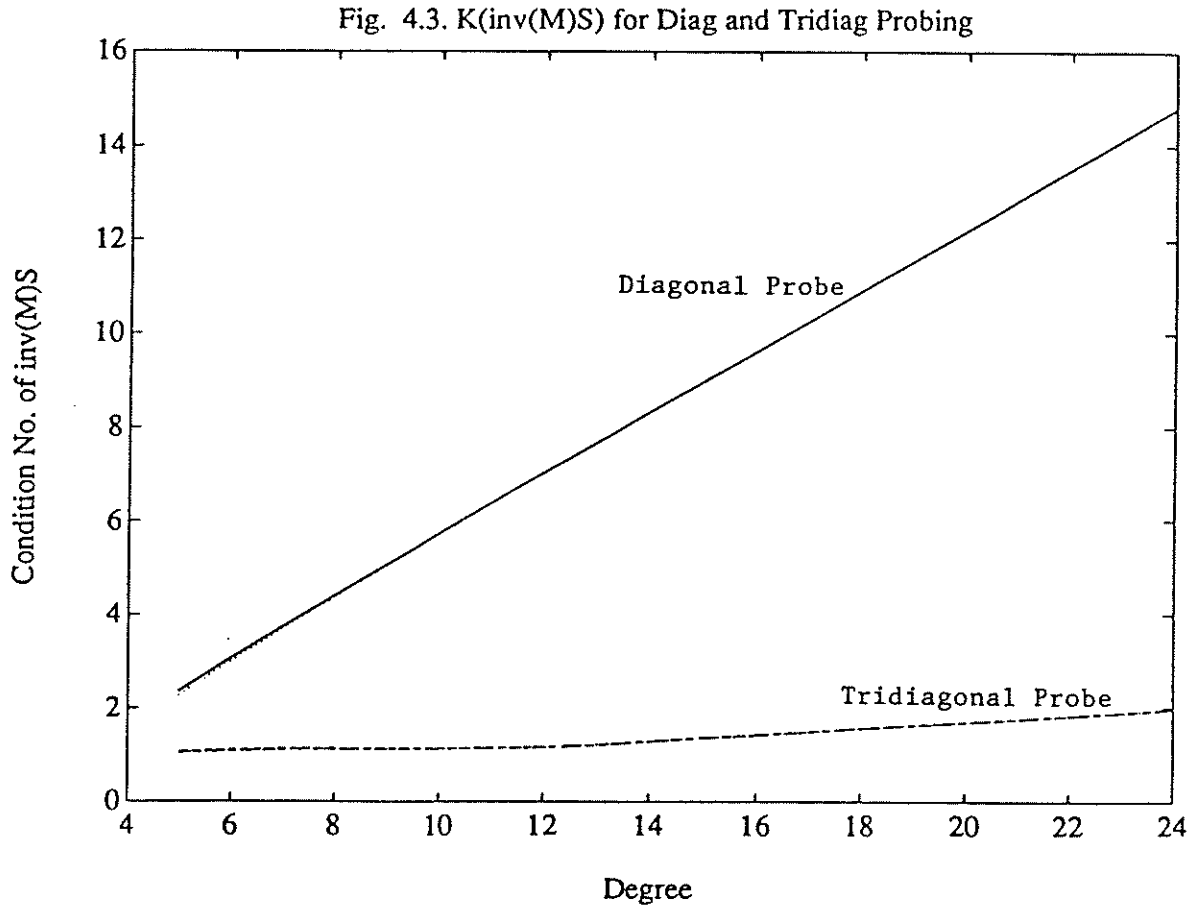
The (weak) C^1 continuity imposes merely a restriction in the direction orthogonal to the interface. The coupling along the interface is rather weak. In the patching method, A_{22} is diagonal and the coupling between the unknowns of the interface only comes from the terms $A_{21}A_{11}^{-1}A_{12}$ and $A_{23}A_{33}^{-1}A_{32}$.

It would not be efficient to calculate the elements of S in order to get a diagonal approximation. Instead, as proposed in [4], a $2k + 1$ diagonal approximation to S can be constructed by multiplying S by $2k + 1$ "probing" vectors $v_j, j = 1, \dots, 2k + 1$. The idea is motivated by sparse Jacobian evaluation techniques [6]. For the case $k = 0$ and $k = 1$ the probing vectors are the following :

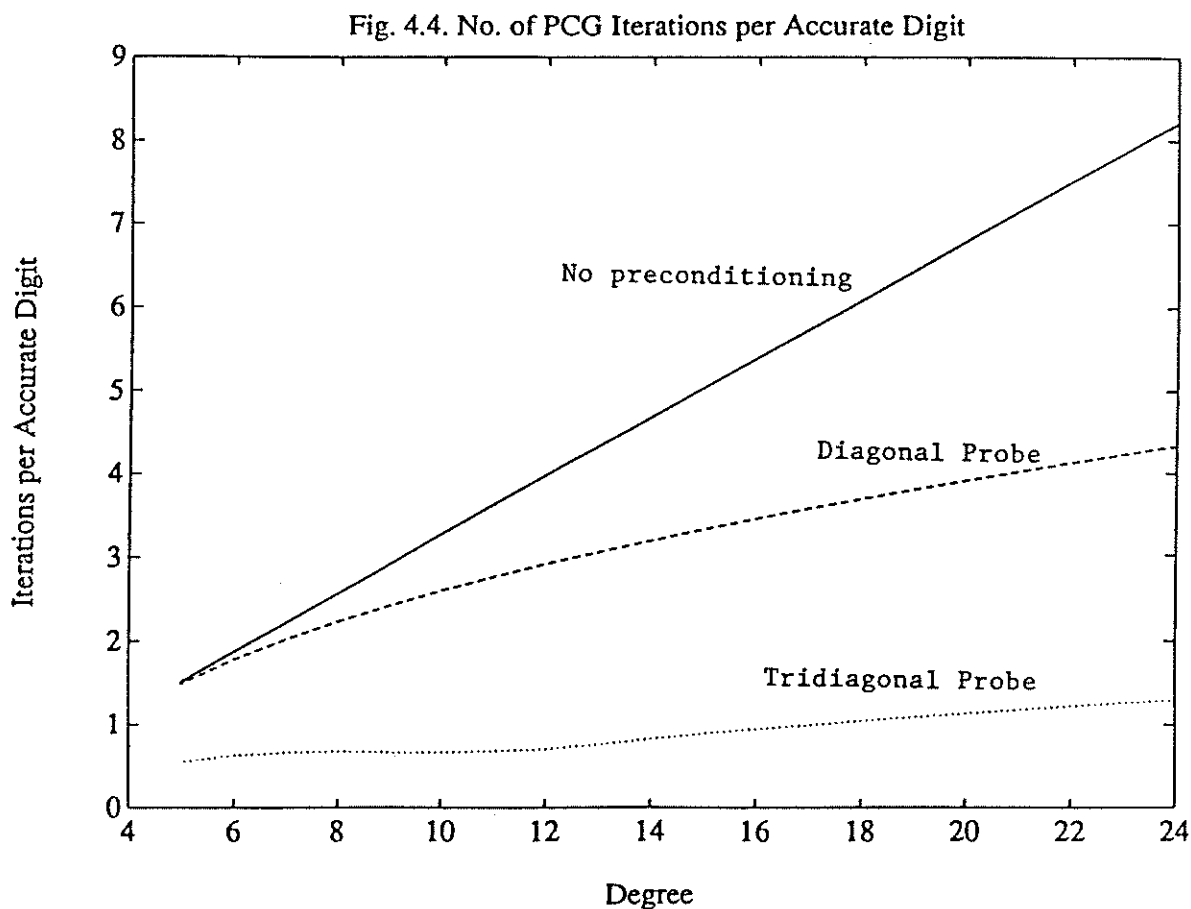
$$\begin{aligned} k = 0 : v_1 &= (1, 1, 1, 1, 1, 1, \dots)^T \\ k = 1 : v_1 &= (1, 0, 0, 1, 0, 0, \dots)^T \\ &v_2 = (0, 1, 0, 0, 1, 0, \dots)^T \\ &v_3 = (0, 0, 1, 0, 0, 1, \dots)^T \end{aligned}$$

The case $k = 0$ corresponds to a scaling of each row of the matrix S by the sum of the elements of the row. For $k = 1$, if S were indeed tridiagonal, all of its elements would be found in the vectors $Sv_j, j = 1, 2, 3$. For the more general case of $k > 1$, we refer to [4]. The probing technique asks for $2k + 1$ products Sv_j . This implies $(2k + 1)$ solves on each subdomain.

In figure 4.3, we show the condition number of $M^{-1}S$ for a one and a tridiagonal approximation for the spectral element, versus n for the same problem as in section 2. The curves for the patching collocation method coincide.



As can be seen, the boundary probe preconditioner yields a very good approximation to S . These numerical experiments indicate that for $k = 0$ the condition number is $O(n)$ and for $k = 1$, it is nearly constant. To construct the tridiagonal preconditioner, we have to make 3 matrix vector multiplications Sy , as opposed to just 1 in the diagonal case, and in each iteration step a tridiagonal system has to be solved. This however is amply compensated by the faster convergence. In figure 4.4, we plot the number of iteration steps per digit accuracy ($\frac{1}{-\log_{10}(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1)}}$) versus n for PCG iteration without preconditioning and with the diagonal and tridiagonal probing preconditioner.



Using a tridiagonal boundary probe preconditioner, the number of iteration steps to achieve a certain accuracy is independent of the order of S . This saving compensates greatly for the extra work for constructing the preconditioner and calculating the preconditioning step.

Since the boundary probe preconditioner senses the elements of the matrix S , it naturally adapts to the differential operator and to the type of discretization used [3].

5. Relation between Neumann Dirichlet alternating procedures for patching methods and Schur compl
Patching methods impose exact C^1 continuity on the internal boundary Γ :

$$(5-1) \quad \begin{cases} -\Delta u^1 = f & \text{on } \Omega_1 \\ u^1 = 0 & \text{on } \partial\Omega_1 \cap \partial\Omega \end{cases}$$

$$(5-2) \quad \frac{\partial u^1}{\partial x} = \frac{\partial u^2}{\partial x} \quad \text{on } \Gamma$$

$$(5-3) \quad \begin{cases} -\Delta u^2 = f & \text{on } \Omega_2 \\ u^2 = 0 & \text{on } \partial\Omega_2 \cap \partial\Omega \end{cases}$$

An analogous derivation as in section 2, but replacing the discrete equations for the grid points on the interface Γ by a discrete version of (5-2) leads to the set of equations :

$$\begin{pmatrix} A_{11} & A_{12} & \\ A_{21} & A_{22}^1 + A_{22}^2 & A_{23} \\ & A_{32} & A_{33} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = \begin{pmatrix} f_1 \\ 0 \\ f_3 \end{pmatrix}$$

with :

$$A_{21} = \sigma_1 D_{n_x^1}^1(n_x^1, 1 : n_x^1 - 1) \otimes I_{(n_y-1)}$$

$$A_{22}^1 = \sigma_1 D_{n_x^1}^1(n_x^1, n_x^1) I_{(n_y-1)}$$

$$A_{22}^2 = -\sigma_2 D_{n_x^2}^1(0, 0) I_{(n_y-1)}$$

$$A_{23} = -\sigma_2 D_{n_x^2}^1(0, 1 : n_x^2 - 1) \otimes I_{(n_y-1)}$$

Let :

$$\hat{A}^1 = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22}^1 \end{pmatrix} \quad \text{and} \quad \hat{A}^2 = \begin{pmatrix} A_{22}^2 & A_{23} \\ A_{32} & A_{33} \end{pmatrix}$$

The matrices A_{11} and A_{22} are the discretization matrices for Dirichlet problems on the domains Ω_1 , respectively Ω_2 while the matrices \hat{A}^i describe Neumann Dirichlet problems on the subdomains, with the Neumann boundary condition on the interface. The Schur complement S can also be written as

$$(5-4) \quad S = S^1 + S^2 \quad ,$$

with :

$$S^1 = A_{22}^1 - A_{21} A_{11}^{-1} A_{12} \quad ,$$

and

$$S^2 = A_{22}^2 - A_{23} A_{33}^{-1} A_{32} \quad .$$

S^i is the Schur complement of A_{22}^i in \hat{A}^i [1].

A large class of iterative methods for solving a system of the form $Ax = b$ consists of (relaxed) preconditioned fixed point iterations. Let $A = S + R$.

$$\begin{aligned}
& \text{choose } x^0 \\
& r^0 = b - Ax^0 \\
& p^0 = S^{-1}r^0 \\
& x^1 = x^0 + p^0 \\
& \text{for } k = 1, 2, \dots \\
& \quad r^k = b - Ax^k \\
& \quad p^k = S^{-1}(r^k - R(\theta_k - 1)p^{k-1}) \\
& \quad x^{k+1} = x^k + p^k
\end{aligned}$$

with θ_k , $k = 1, 2, \dots$ a series of relaxation parameters. The updating can also be written as :

$$Sx^{k+1} = -R(\theta_k x^k + (1 - \theta_k)x^{k-1}) + b$$

Applying this method to the Schur complement system with the splitting (5-4), we get :

$$\begin{aligned}
(5-5) \quad S_2 u_2^{k+1} &= -S_1(\theta_k u_2^k + (1 - \theta_k)u_2^{k-1}) - A_{21}A_{11}^{-1}f_1 - A_{23}A_{33}^{-1}f_3 \\
&= -A_{21}A_{11}^{-1}(f_1 - A_{12}(\theta_k u_2^k + (1 - \theta_k)u_2^{k-1})) - A_{22}^1(\theta_k u_2^k + (1 - \theta_k)u_2^{k-1}) - A_{23}A_{33}^{-1}f_3
\end{aligned}$$

Funaro, Quarteroni and Zanolli [8] have proposed an efficient iterative technique for solving (5-1), (5-2), (5-3) :

$$\begin{aligned}
& (u^2)^{-1} \text{ arbitrary} \\
& \text{choose } (u^2)^0 \\
& \theta_0 = 1 \\
& \text{for } k = 0, 1, \dots \\
(5-6) \quad & \begin{cases} -\Delta (u^1)^{k+1} = f & \text{on } \Omega_1 \\ (u^1)^{k+1}|_{\Gamma} = \theta_k (u^2)^k|_{\Gamma} + (1 - \theta_k) (u^2)^{k-1}|_{\Gamma} \end{cases} \\
(5-7) \quad & \begin{cases} -\Delta (u^2)^{k+1} = f & \text{on } \Omega_2 \\ \frac{\partial (u^2)^{k+1}}{\partial x}|_{\Gamma} = \frac{\partial (u^1)^{k+1}}{\partial x}|_{\Gamma} \end{cases}
\end{aligned}$$

Using the same collocation technique to solve the differential equations (5-6) and (5-7) we get the following equations :

$$(5-8) \quad A_{11}u_1^{k+1} = f_1 - A_{12}(\theta_k u_2^k + (1 - \theta_k)u_2^{k-1})$$

$$(5-9) \quad \hat{A}^2 \begin{pmatrix} u_2^{k+1} \\ u_3^{k+1} \end{pmatrix} = \begin{pmatrix} -A_{21}u_1^{k+1} - A_{22}^1(\theta_k u_2^k + (1 - \theta_k)u_2^{k-1}) \\ f_3 \end{pmatrix}$$

Substituting the solution of (5-8) in (5-9) gives :

$$(5-10) \quad \begin{pmatrix} A_{22}^2 & A_{23} \\ A_{32} & A_{33} \end{pmatrix} \begin{pmatrix} u_2^{k+1} \\ u_3^{k+1} \end{pmatrix} = \begin{pmatrix} -A_{21}A_{11}^{-1}(f_1 - A_{12}(\theta_k u_2^k + (1 - \theta_k)u_2^{k-1})) - A_{22}^1(\theta_k u_2^k + (1 - \theta_k)u_2^{k-1}) \\ f_3 \end{pmatrix}$$

Solving the equations (5-10) for u_2^{k+1} using the Schur complement of A_{22}^2 in \hat{A}^2 gives :

$$(5-11) \quad S^2 u_2^{k+1} = -A_{21}A_{11}^{-1}(f_1 - A_{12}(\theta_k u_2^k + (1 - \theta_k)u_2^{k-1})) - A_{22}^1(\theta_k u_2^k + (1 - \theta_k)u_2^{k-1}) - A_{23}A_{33}^{-1}f_3$$

Equation (5-11) is the same as equation (5-5). The alternating Neumann Dirichlet iteration thus can be considered a dynamically relaxed preconditioned fixed point iteration on the Schur complement S , using S^2 as preconditioner.

With an appropriate choice of the relaxation parameter θ_k , the alternating Neumann Dirichlet procedure converges very fast [8]. As it is an alternating method, such as the Schwarz iterative procedure [13], it consists of two sequential steps. It also needs a Dirichlet and a Neumann solver. In the PCG iteration on the Schur complement, the subdomain solves can all be done simultaneously. Furthermore, they are all Dirichlet problems.

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