An Efficient and Exponentially Accurate Parallel *h-p* Spectral Element Method for Elliptic Problems on Polygonal Domains - The Dirichlet Case

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Abstract. For smooth problems spectral element methods (SEM) exhibit exponential convergence and have been very successfully used in practical problems. However, in many engineering and scientific applications we frequently encounter the numerical solutions of elliptic boundary value problems in non-smooth domains which give rise to singularities in the solution. In such cases the accuracy of the solution obtained by SEM deteriorates and they offer no advantages over low order methods. A new Parallel *h-p* Spectral Element Method is presented which resolves this form of singularity by employing a *geometric mesh* in the neighborhood of the corners and gives exponential convergence with asymptotically faster results than conventional methods. The normal equations are solved by the *Preconditioned Conjugate Gradient* (PCG) method. Except for the assemblage of the resulting solution vector, all computations are done on the element level and we don't need to compute and store *mass* and *stiffness* like matrices. The technique to compute the preconditioner is quite simple and very easy to implement. The method is based on a parallel computer with distributed memory and the library used for message passing is *MPI*. Load balancing issues are discussed and the communication involved among the processors is shown to be quite small.

1 Introduction

Many important real life problems, for example, shock waves in compressible flow or crack problems in structural mechanics, encounter irregular geometries which give rise to singularities in the solution. In such cases we require the solution of elliptic boundary value problems on non-smooth domains.

Current formulations of the spectral methods to solve elliptic boundary value problems on polygonal domains allow us to recover only algebraic convergence [4, 8]. Using conformal mapping of the form $z = \xi^{\alpha}$ relatively fast convergence

can be achieved but exponential convergence can not be fully recovered [8]. A method for obtaining a numerical solution with exponential accuracy to elliptic boundary value problems with analytic coefficients on curvilinear polygons with piecewise analytic boundary was first proposed by Babuska and Guo [1, 2] within the framework of the finite element method. They were able to resolve the singularities which arise at the corners by using a *geometric mesh.* The method we present here solves the same class of problems to exponential accuracy within the framework of spectral methods, and gives asymptotically faster results than conventional methods.

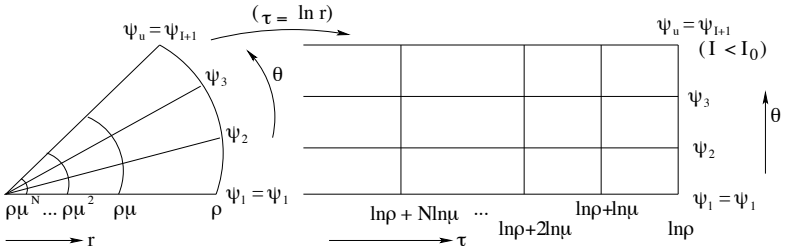

Fig. 1. Mapping $z = \ln \xi$

In a neighborhood of the corner A_k we also use a *geometric mesh,* but the important difference is the mapping, which is of the form $z = \ln \xi$ and this enables us to obtain the solution with exponential accuracy. In this neighborhood we switch to new variables (τ, θ) where $\tau = \ln r$ and (r, θ) are the usual polar coordinates with origin at A_k. In doing so the geometric mesh is reduced to a quasi-uniform mesh in a sectoral neighborhood of the corners. Away from these sectoral neighborhoods of the corners we retain (x, y) variables for our coordinate system.

With this mesh we seek a solution which minimizes a functional associated with the problem. *Differentiability estimates* and a *stability estimate* with respect to these new variables have been derived in [9]. A *Parallel preconditioner* and *error estimates* for the solution of the *minimization problem* are then obtained using the stability estimate.

The preconditioner is of block diagonal form and allows the solutions for different elements to *decouple* completely, which plays an important role in solving the problem *efficiently* on parallel computers. Moreover, the preconditioner is nearly optimal as the *condition number* of the preconditioned system is polylogarithmic in N, the number of elements in the radial direction.

The *normal equations* resulting from the minimization problem are then solved by a PCG method. Since we only need *matrix-vector products* in this procedure, the *assemblage* is to be performed *only* on the resulting vector. The matrix-vector product can be carried out at element level and hence we do not need to compute and store *mass* and *stiffness* matrices [7].

The preconditioner is obtained in the same way as the residuals in the normal equations but with homogenous boundary data and the homogenous form of the partial differential equation. Hence the technique to compute the preconditioner is quite simple and easy to implement with minimal effort. This is particularly effective when solving such problems on a parallel computer with distributed memory.

Since the number of elements of the mesh in the neighborhood of the corner are to be increased for increasing accuracy, the model problem is demonstrated on a parallel computer with distributed memory using *MPI* library. Every element in our computational domain is mapped to a separate processor and since the dimension of every element is chosen to be the same on each element, the load on individual processors is perfectly balanced. The communication involved is also shown to be quite small [9].

For the purely Dirichlet problem our spectral element functions are fully non-conforming and hence there are no *common boundary values* to solve for. This turns out to be computationally more efficient than conventional methods [9]. The spectral element functions for the mixed Dirichlet and Neumann case are discussed in [9]. If the data is analytic then the error is shown to be exponentially small in N [9].

The outline of the paper is as follows. In Section 2 we describe the mesh strategy and the *stability estimate*. The numerical scheme based on this stability estimate is then presented. In Section 3 we have discussed the computation of a parallel preconditioner and the load balancing issues together with the overall complexity of the method. Finally, in Section 4 computational results are provided which verify the asymptotic estimates we have obtained.

2 The Problem and the Numerical Scheme

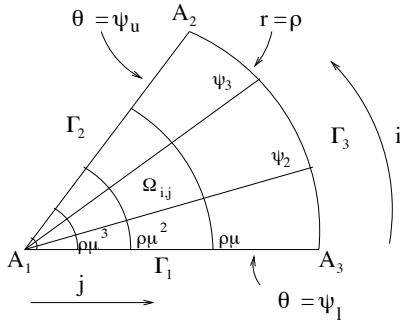

Fig. 2. The mesh at sectoral domain

Here we examine the solution of the problem

$$Lu = f \qquad \text{for } (x, y) \in \Omega, \tag{1}$$

with Dirichlet boundary conditions $u = g_j$ for $(x,y) \in \Gamma_j$ where $\partial\Omega = \bigcup \Gamma_j$. Here L denotes the Laplacian operator.

For simplicity we present here only the sectoral domain case which consists of only one vertex, namely A_1 and its sectoral neighborhood. For the treatment of a polygonal domain, as well as the mixed Dirichlet and Neumann boundary conditions case, the reader is referred to [9].

On a sectoral domain with vertex A_1, as shown in Fig. 2, we define a geometric mesh with ratio $0 < \mu < 1$, as has been done in [2]. Let (r,θ) denote polar coordinates with center at A_1 and $\tau = \ln r$. The sector S_ρ (in this case Ω itself), may be represented as $S_\rho = \{(x,y) : 0 < r < \rho, \psi_l < \theta < \psi_u\}$.

- Let $\{\psi_i\}_{i=1,\ldots,I+1}$ be an increasing sequence of points such that $\psi_1 = \psi_l$ and $\psi_{I+1} = \psi_u$. Let $\Delta\psi_i = \psi_{i+1} - \psi_i$. Let $\sigma_1 = 0$, and $\sigma_j = \rho(\mu)^{N+1-j}$ for $2 \le j \le N+1$. Finally we define $\eta_j = \ln \sigma_j$ for $1 \le j \le N+1$.
- Let us denote the index sets $\mathcal{I} = \{i | 1 \le i \le I\}$ and $\mathcal{J} = \{j | 1 \le j \le N\}$. Let $\Omega_{i,j} = \{(x,y) : \sigma_j < r < \sigma_{j+1}, \psi_i < \theta < \psi_{i+1}\}$ for $i \in \mathcal{I}$ and $j \in \mathcal{J}$. Let B_ρ is the circular arc which bounds Ω.
- Now let $\tau = \ln r$. Define $\widetilde{\Omega}_{i,j} = \{(\tau,\theta) : \eta_j < \tau < \eta_{j+1},\ \psi_i < \theta < \psi_{i+1}\}$ for $i \in \mathcal{I}$ and $j \in \mathcal{J}$. Also let $\widetilde{B}_\rho$ denotes the representation of B_ρ in (τ,θ) coordinates, i.e. $\widetilde{B}_\rho = \{(\tau,\theta) :\ \tau = \ln\rho,\ \psi_l < \theta < \psi_u\}$. Similarly let $\widetilde{\Gamma}_k, \widetilde{\Gamma}_{k+1}$ denote the representation of the sides Γ_k and Γ_{k+1} in (τ,θ) coordinates. Let γ_l be a side of $\Omega_{i,j}$ for some i and j and let $\widetilde{\gamma}_l$ denotes its representation in (τ,θ) coordinates.

Let $u_{i,j}(\tau,\theta)$ be a set of nonconforming elements, defined on $\widetilde{\Omega}_{i,j}$, given by

$$u_{i,j}(\tau,\theta) = \sum_{n=0}^{N}\sum_{m=0}^{N} a_{m,n}\tau^m\theta^n$$

for $j > 1$. Since we are assuming that the data g is analytic and compatible at the vertex A_1, the value of u at the vertex A_1 is well defined. Thus if we subtract from u an analytic function which assumes this value at the vertex A_1 then the difference would satisfy (1) with a modified set of analytic data and the Dirichlet boundary data would assume the value zero at A_1. Hence without loss of generality we may assume $g(A_1) = 0$. We shall thus choose $u_{i,1} \equiv 0$ for all i. Let us denote the jump in u across inter-element boundaries as follows

$$[u_{i,j}](\eta_{j+1},\theta) := (u_{i,j+1} - u_{i,j})(\eta_{j+1},\theta),$$
$$[u_{i,j}](\tau,\psi_{i+1}) := (u_{i+1,j} - u_{i,j})(\tau,\psi_{i+1}).$$

We now state the stability result on which our numerical scheme and preconditioner are based. For the proof the reader is referred to [9].

Theorem 1. *For the sectoral domain $\widetilde{\Omega}$ the following stability estimate holds.*

$$\sum_{j=2}^{N}\sum_{i=1}^{I} \|u_{i,j}(\tau,\theta)\|^2_{2,\widetilde{\Omega}_{i,j}} \tag{2}$$

$$
\begin{aligned}
&\leq C\left(\ln N\right)^2 \left\{ \sum_{j=2}^{N} \sum_{i=1}^{I} \left|\left|Lu_{i,j}\left(\tau,\theta\right)\right|\right|^2_{0,\widetilde{\Omega}_{i,j}} \right. \\
&\quad + \sum_{\widetilde{\gamma}_l \subseteq \widetilde{\Omega}} \left(\left|\left|\left[u\right]\right|\right|^2_{0,\widetilde{\gamma}_l} + \left|\left|\left[u_\tau\right]\right|\right|^2_{1/2,\widetilde{\gamma}_l} + \left|\left|\left[u_\theta\right]\right|\right|^2_{1/2,\widetilde{\gamma}_l} \right) \\
&\quad + \sum_{\widetilde{\gamma}_l \subseteq \widetilde{B}_\rho} \left(\left|\left|u\right|\right|^2_{0,\widetilde{\gamma}_l} + \left|\left|u_\theta\right|\right|^2_{1/2,\widetilde{\gamma}_l} \right) \\
&\quad \left. + \sum_{m=1}^{2} \sum_{\widetilde{\gamma}_l \subseteq \partial\widetilde{\Omega} \bigcap \widetilde{\Gamma}_m} \left(\left|\left|u\right|\right|^2_{0,\widetilde{\gamma}_l} + \left|\left|u_\tau\right|\right|^2_{1/2,\widetilde{\gamma}_l} \right) \right\}.
\end{aligned}
$$

Here $u_\tau = \frac{\partial u}{\partial \tau}$, $u_\theta = \frac{\partial u}{\partial \theta}$, *and* $\left|\left|.\right|\right|_{s,\widetilde{\gamma}_l}$ *denotes the fractional Sobolev norm when* s *is not an integer.*

In [9] it has been shown that an exponentially accurate solution in the $H^1\left(\Omega\right)$ norm is obtained by using the above estimate and trace theorems for Sobolev spaces.

Now to find $\left\{u_{i,j}\left(\tau,\theta\right)\right\}_{i\in\mathcal{I},j\in\mathcal{J}}$ which minimizes a functional

$$
\mathfrak{R}^N\left(\left\{v_{i,j}\left(\tau,\theta\right)\right\}_{i\in\mathcal{I},j\in\mathcal{J}}\right)
$$

closely related to the right hand side of the stability estimate stated above, we need to solve the normal equations of the least-squares problem corresponding to collocating the partial differential equation and boundary conditions at an over-determined set of collocation points [5,6]. We can then obtain a solution by using PCG techniques for solving the normal equations.

Now

$$
\mathfrak{R}^N\left(U+\varepsilon V\right) = \mathfrak{R}^N\left(U\right) + 2\varepsilon V^t\left(SU-TG\right) + O\left(\varepsilon^2\right)
$$

for all V, where U is a vector assembled from the values of

$$
\left\{ \left\{ u_{i,j}\left(\tau_{j,l}^{N_j}, \theta_{i,m}^{N_j}\right) \right\}_{0\leq l,m\leq N_j} \right\}_{2\leq j\leq N, i\in\mathcal{I}}.
$$

The vector V is similarly assembled and G is assembled from the data. Here S and T denote matrices. For the least-squares discretization we now need to solve the linear system $SU-TG=0$; which is symmetric and positive definite and hence the solution can be obtained efficiently by the PCG method. This requires an efficient computation of $SV-TG$ during the iterative process.

For the details of element wise computations and how to solve the corresponding linear system without having to compute and store mass and stiffness matrices, the reader can refer to [9].

3 Parallel Computations

3.1 Preconditioner

We define the quadratic form $\mathcal{W}^N\left(\{v_{i,j}(\tau,\theta)\}_{i,j}\right)$ as:

$$\mathcal{W}^N = \sum_{j=2}^{N}\sum_{i=1}^{I} ||v_{i,j}(\tau,\theta)||^2_{2,\widetilde{\Omega}_{i,j}}. \tag{3}$$

In the same way we may define the quadratic form $\mathcal{V}^N\left(\{v_{i,j}(\tau,\theta)\}_{i,j}\right)$ as the right hand side of the Theorem 1. Then, using the stability estimate (2) and the trace theorems for Sobolev spaces it can be been shown that the two quadratic forms $\mathcal{W}^N$ and $\mathcal{V}^N$ are spectrally equivalent and the constant of equivalence is $O(\ln N)^2$ [9]. Hence, if we use $\mathcal{W}^N$ as a preconditioner the condition number of the preconditioned system is $O(\ln N)^2$.

Now since $\mathcal{W}^N$ is of block diagonal form, this is an important benefit for computations on a parallel computer. Each block can be computed and stored on a respective element and the computation of $\mathcal{W}^N$ for each element is completely decoupled from other elements. Here each block corresponds to the H^2 norm of the spectral element function defined on a particular element which is mapped onto the master square S $([-1,1]\times[-1,1])$. Next we show how this can be computed.

Let $v_{i,j}(\xi,\eta)$ be the spectral element function defined on the square S to which the domain $\overline{\Omega}_{i,j}$ is mapped. Then $v_{i,j}(\xi,\eta)$ is determined by its values at the points $\{\xi_l,\eta_m\}_{0\le l\le N, 0\le m\le N}$. Dropping sub and superscripts we order the values of $v(\xi_l,\eta_m)$ in lexicographic order and denote them as v_n for $1\le n\le (N+1)^2$. Now consider the bilinear form $\mathcal{S}^N(u,v)$ induced by the H^2 norm on S, i.e. $\mathcal{S}^N(u,u) = ||u||^2_{H^2(S)}$. Then there is a matrix A such that

$$\mathcal{S}^N(u,v) = \sum_{i=1}^{(N+1)^2}\left(\sum_{j=1}^{(N+1)^2} A_{i,j}u_i\right)v_j.$$

The matrix A can be determined by its columns Ae_i where e_i is a unit vector with a one in its i^{th} place and zero everywhere else.

Now using integration by parts Ae_i can be computed in $O\left(N^3\right)$ operations in exactly the same way as we compute the residual in the normal equations. For this we need to consider homogenous form of the partial differential equation and boundary data. Hence it requires minimal extra effort to compute and store the preconditioner.

If we distribute the $(N+1)^2$ columns among the N_B processors then the matrix A can be computed in $O\left(N^4\right)$ operations on a parallel computer since $N_B = O(N)$. Moreover the L-U factorization of A can be performed in $O\left(N^5\right)$ operations and stored on every processor. Once this has been done the *action of the inverse* of the matrix on different right hand sides can be computed in $O\left(N^4\right)$ operations on every processor.

3.2 Load Balancing

The dimension of our spectral element function is $(N_j+1)^2$ for $2 \leq j \leq N$ where $\alpha j \leq N_j \leq N$, α is a positive constant. We choose an upper bound i.e. $N_j = N$ for all $j \geq 2$ defined on $\widetilde{\Omega}_{i,j}$ and map each $u_{i,j}(\tau,\theta)$ onto separate processor. By doing so we are able to achieve perfect load balancing among individual processors, but at the cost of making some of the processors do extra computational work which would not increase the accuracy of the numerical solution substantially. Alternatively, if we were to assign each $u_{i,j}(\tau,\theta)$ with varying N_j onto different processors this would cause a severe imbalance in the loads assigned to different processors and we will additionally need to employ the load balancing techniques. We should also point out that the latter strategy has the drawback that the degree of the polynomials $N_j \sim \alpha j$ is data dependent since α is determined by the data. The strategy of choosing a uniform N as an upper bound for N_j for every element is thus more robust and hence is to be preferred as it would apply to the most general class of data. The numerical results with this upper bound perfectly match with the theoretical estimates. This affirms the robustness of the proposed method.

Further, to compute the residuals in the normal equations we need to enforce continuity across inter-element boundaries. In doing so we only need to exchange the function and its derivative's values at inter-element boundaries between neighboring processors. During the PCG steps we also need to compute two global scalars to update the approximate solution and the search direction which can be achieved by a simple *MPI_ALLREDUCE* call with *MPI_SUM* operation. The inter-processor communication is thus quite small.

Finally, since we would need to perform $O(N \log N)$ iterations to obtain the solution to exponential accuracy and every iteration requires $O\left(N^4\right)$ operations, the total operations required to compute the solution would be $O\left(N^5 \log N\right)$, which for the same class of problems and on a parallel computer with N processors requires $O\left(N^6 \log N\right)$ operations with an *h-p* finite element method.

4 Computational Results

We consider Poisson equation as a model problem with Dirichlet boundary conditions. We consider only a sectoral domain as shown in Fig. 3 and show that the geometric mesh with Dirichlet boundary data gives exponential convergence. We choose our data so that there is a singularity only at the vertex O and hence we need to impose a geometric mesh only for the vertex O, as has been done in [2].

The solution thus obtained is nonconforming and we can make a correction to the solution so that the corrected solution is conforming. The error between the exact solution and the corrected solution in the $H^1(\Omega)$ norm is exponentially small in N. The details of how to do this can be found in [9].

We present the results of our numerical simulations for a sector with sectoral angle $\omega = \frac{3\pi}{2}$ and radius $\rho = 1$. We choose our data so that the solution has

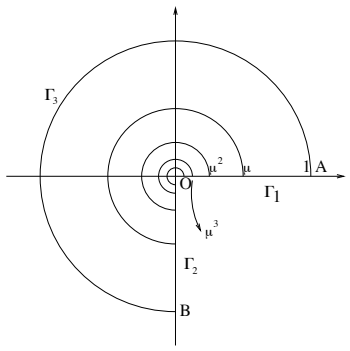

Fig. 3. The Geometric mesh at sector

the form of the leading singular solution $u = r^{\alpha} \sin(\alpha\theta)$ where $\alpha = \frac{\pi}{\omega}$. Then u vanishes along the sides OA and OB and is analytic along the curvilinear side AB. Hence the Dirichlet data is analytic and continuous at the vertices and moreover $\Delta u = 0$ in Ω. The solution of this problem is analytic in Ω except that it has a singularity at the vertex O. We divide the sector into three equal subsectors and choose the geometric ratio $\mu = .15$, which gives optimal convergence [3]. Let N be the number of spectral elements in the radial direction and the number of degrees of freedom of each variable in every element. The total degrees of freedom thus will be $3N^3$. Table 1 shows the relative error $||e||_{ER}$ against degrees of freedom, where the relative error $||e||_{ER}$ is defined as $||e||_{ER} = ||e||_E / ||u||_E$ and $||.||_E$ stands for the energy norm. Fig. 4 shows the

Table 1. Percent of relative error against $||e||_{ER}$ the number of degrees of freedom

DOF	$\|\|e\|\|_{ER}$ %
24	.7462E+01
81	.3709E+01
192	.1407E+01
375	.5151E+00
648	.1736E+00
1029	.5720E-01
1536	.1830E-01
2187	.5779E-02
3000	.1798E-02
3993	.5547E-03
5184	.1696E-03

error on the scale $\ln ||e||_{ER}$ against total degrees of freedom.

We next choose the angle of the sector as $\omega = \frac{3\pi}{8}$ (with no division in θ direction) so that the solution is sufficiently regular in the neighborhood of the

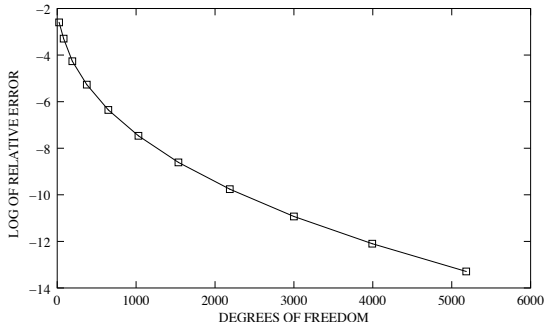

Fig. 4. Log of relative error in the energy norm $||e||_{ER}$ vs. the degrees of freedom

vertex O. We have achieved an accuracy of order e^{-10} in $H^1(\Omega)$ norm with 1350 degrees of freedom.

Table 2 shows how the relative error $||e||_{ER}$ depends on number of iterations. Fig. 5 shows the error on the scale $\ln ||e||_{ER}$ against the number of iterations and the relationship is almost linear.

Table 2. Relative error $||e||_{ER}$ in percent against the number of iterations

Iterations	$\|\|e\|\|_{ER}$ %
10	.7921E-01
20	.3121E-02
30	.1157E-03
40	.8448E-05
50	.2035E-06
61	.4187E-08

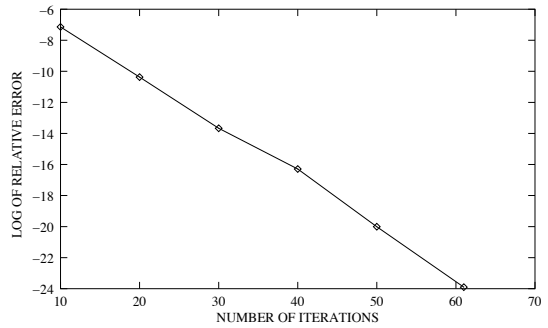

Fig. 5. Log of relative error in the energy norm $||e||_{ER}$ vs. the number of iterations

5 Conclusions

We have described a least-squares approach to solve elliptic boundary value problems on a sectoral domain with exponential convergence within the framework of spectral methods. The numerical scheme has a computational complexity which is less than that of finite element methods. Moreover, the construction of the preconditioner is simple and easy to implement with minimal effort. For the mesh strategy, various estimates, numerical scheme and parallelization strategies for the polygonal domain, the reader can refer to [9]. This includes additional terms on elements away from the sectoral neighborhood and is a straight forward extension of what has been presented here. The elliptic boundary value problems with mixed Dirichlet and Neumann boundary conditions on polygonal domains are solved in [9]. To solve the associated Schur Complement matrix the technique we have presented there is also computationally more efficient than h-p FEM. All these results are valid for elliptic problems with mixed boundary conditions on domains with curvilinear boundaries which satisfy the usual conditions [9].

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