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Overlapping Schwarz preconditioned eigensolvers for spectral element discretizations

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ABSTRACT

Model generalized eigenproblems associated with self-adjoint differential operators in nonstandard homogeneous or heterogeneous domains are considered. Their numerical approximation is based on Gauss–Lobatto–Legendre conforming spectral elements defined by Gordon–Hall transfinite mappings. The resulting discrete eigenproblems are solved iteratively with a Locally Optimal Block Preconditioned Conjugate Gradient (LOBPCG) method, accelerated by an overlapping Schwarz preconditioner. Several numerical tests show the good convergence properties of the proposed preconditioned eigensolver, such as its scalability and quasi-optimality in the discretization parameters, which are analogous to those obtained for overlapping Schwarz preconditioners for linear systems.

1. Introduction

Many interesting scientific applications require the accurate evaluation of the smallest eigenpairs of large sparse matrices. In recent years, several iterative methods have been proposed for this task, trying to extend to eigenproblems the promising results obtained by the research community on preconditioned iterative methods for linear systems, see e.g. [22, Ch. 16] and the references therein.

In this paper, we consider a model generalized eigenproblem $A\mathbf{u} = \lambda B\mathbf{u}$ associated with a self-adjoint differential operator, in nonstandard homogeneous or heterogeneous domains. The problem is discretized by the standard conforming Spectral Element Method (SEM) based on quadrilateral elements and Gauss–Lobatto–Legendre (GLL) quadrature points, so the method can be viewed as a nodal version of *hp* Finite Element Methods (FEM); see, e.g., [5,2,8,17,29]. One difficulty in the implementation of the SEM is the approximation of problems in complex-shaped domains, arising in several branches of applied sciences. We shall address this point by using transfinite interpolation, or Gordon–Hall maps [15], in order to build very flexible maps from the reference square domain to a generic spectral element with quadrilateral shape and, in the general case, with curvilinear edges. In our previous work [16] on preconditioned iterative solvers for SEM–GLL linear systems, we showed that the good convergence properties (with respect to the discretization parameters h and p) of Schwarz preconditioners for standard rectangular elements are retained for SEM–GLL elements with Gordon–Hall maps. This previous study is here extended to eigenproblems arising from SEM–GLL discretizations.

In the FEM framework, several large mesh eigenproblems arising from mathematical physics have been addressed by means of preconditioned eigensolvers; see, e.g. [1,3,4,12,9,21,7,20,22]. Here, we consider the Locally Optimal Block Preconditioned Conjugate Gradient (LOBPCG) method [20,19] that has been proposed for the numerical solution of large-scale, generalized symmetric positive definite eigenvalue problems. The SEM discrete systems arising at each LOBPCG iteration are

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preconditioned by the overlapping Schwarz (OS) method. The latter is based on partitioning the domain of the given problem into overlapping subdomains, solving parallel independent local problems on the subdomains, and solving a coarse problem on a coarse mesh, in order to ensure scalability; see, e.g., [11,32] for a general introduction to OS methods, and [6,13,14,16,25] for OS applications to SEM discretizations.

The outline of this paper is as follows. We introduce the model eigenvalue problem and its SEM approximation in Section 2. In order to deal with nonstandard geometries, Gordon–Hall transfinite interpolation is introduced in Section 3. In Section 4, we recall a family of preconditioned, iterative eigensolvers including the LOBPCG method. In Section 5, the classical domain decomposition overlapping Schwarz preconditioner is applied to the LOBPCG eigensolver. The paper is concluded, in Section 6, by several numerical test problems showing the convergence properties of the LOBPCG-OS preconditioner with respect to the discretization parameters H, h, p.

2. Eigenvalue problem and spectral elements

Let $\Omega \in \mathbb{R}^d,\ d = 2, 3$, be a bounded Lipschitz domain with piecewise smooth boundary $\partial\Omega$. For simplicity, we consider a model eigenvalue problem associated with an elliptic problem in the plane ($d = 2$): Find eigenvalues $\lambda \in \mathbb{C}$ and suitably regular eigenfunctions u such that

$$-\text{div}(\alpha\, \mathbf{grad}\, u) = \lambda\beta u \text{ in } \Omega \tag{1}$$

with Dirichlet boundary conditions $u = 0$ on $\Gamma = \partial\Omega$. The coefficients $\alpha > 0$ and $\beta > 0$ are piecewise constant functions in Ω. Let V be the space $V := \{v \in H^1(\Omega) : v = 0 \text{ on } \Gamma\}$, where $H^1(\Omega)$ is the usual Sobolev space of functions in $L^2(\Omega)$ whose gradient is in $[L^2(\Omega)]^2$. In case of boundary conditions of Neumann or mixed type, the space V must be modified accordingly. The weak formulation of (1) reads (see e.g. [28]): Find eigenvalues $\lambda \in \mathbb{C}$ and eigenfunctions $u \in V$ such that

$$a(u, v) = \lambda b(u, v), \quad \forall v \in V \tag{2}$$

with $a(u, v) := \int_\Omega (\alpha\, \mathbf{grad} u \cdot \mathbf{grad}\, v)\, d\mathbf{x}, b(u, v) := \int_\Omega \beta\, u\, v\, d\mathbf{x}$. Owing to the symmetry of the differential operator and the positivity of β, the eigenvalues are actually real, and the eigenfunctions can always be chosen to be real valued.

The variational problem (2) is discretized by the standard conforming Spectral Element Method (SEM) based on quadrilateral elements and Gauss–Lobatto–Legendre (GLL) quadrature points; see [2,8,17] for a general introduction and an analysis of the method. The method can also be viewed as a nodal version of *hp*-FEM that uses GLL points and employs a discrete space consisting of continuous piecewise polynomials of degree p in each variable within each quadrilateral. Let Q_{ref} be the reference square $(-1, 1)^2$ and let $\mathbb{Q}_p(Q_{\text{ref}})$ be the set of polynomials on Q_{ref} of degree $\leqslant p$ in each variable. We assume that the original domain Ω is decomposed into K quadrilateral elements Q_k as $\overline{\Omega} = \bigcup_{k=1}^K \overline{Q}_k$. This is a conforming finite element partition, since the intersection between two distinct elements Q_k is either the empty set or a common vertex or a common side. We denote by h the maximum diameter of the elements and by τ_h the associated finite element mesh. Each element Q_k is the image of the reference square Q_{ref} by means of a suitable mapping $\varphi_k,\ k = 1, \ldots, K$, i.e., $Q_k = \varphi_k(Q_{\text{ref}})$, to be defined in Section 3. Finally, the space V is discretized by the space $V_{K,p}$ of continuous functions whose restrictions to each Q_k are the images of polynomials of $\mathbb{Q}_p(Q_{\text{ref}})$.

The spectral element approximation of the variational eigenvalue problem (2) is obtained by replacing the L^2-inner product and the bilinear form with their approximations based on GLL quadrature formulae described below.

We denote by $\{\xi_j\}_{j=0}^p$ the set of GLL points of $[-1, 1]$, that are the $(p + 1)$ zeros of the polynomial $(1 - \xi^2)\frac{\partial L_p(\xi)}{\partial \xi}$, where L_p is the pth Legendre polynomial in $[-1, 1]$. It is well-known that these nodes cluster towards the endpoints of the interval, where the distance between GLL nodes is on the order of $1/p^2$, while in the middle of the interval $[-1, 1]$ the distance is on the order of $1/p$ (see [2]). Then we denote by $\sigma_j = \frac{2}{p(p+1)} \frac{1}{(L_p(\xi_j))^2}$ the quadrature weight associated with ξ_j. Let $l_{j,p}(\xi)$ be the Lagrange interpolating polynomial of degree $\leqslant p$ which vanishes at all the GLL nodes except ξ_j, where it equals one. The Lagrangian nodal basis functions on the reference square Q_{ref} are defined by building tensor products $l_{j,p}(\xi)l_{\ell,p}(\eta),\ 0 \leqslant j,\ \ell \leqslant p$, providing a tensor-product basis for $V_{K,p}$. Each function $u \in \mathbb{Q}_p(Q_{\text{ref}})$ can be expanded in this nodal basis through its values at GLL nodes $u(\xi_j,\ \xi_\ell),\ 0 \leqslant j,\ \ell \leqslant p$, as $u(\xi, \eta) = \sum_{j=0}^p \sum_{\ell=0}^p u(\xi_j, \xi_\ell) l_{j,p}(\xi) l_{\ell,p}(\eta)$. Then, on Q_{ref}, the discrete L^2-inner product is

$$(u, v)_{Q_{\text{ref}},p} = \sum_{j=0}^{p} \sum_{\ell=0}^{p} u(\xi_j, \xi_\ell) v(\xi_j, \xi_\ell) \sigma_j \sigma_\ell$$

and in general on Ω,

$$(u, v)_{K,p} = \sum_{k=1}^{K} \sum_{j,\ell=0}^{p} (u \circ \varphi_k)(\xi_j, \xi_\ell)(v \circ \varphi_k)(\xi_j, \xi_\ell) \mid J_k \mid \sigma_j \sigma_\ell, \tag{3}$$

where $\mid J_k \mid$ is the Jacobian of the mapping φ_k at $(\xi_j,\ \xi_\ell)$. The precise building of this mapping arising in the case of complex geometries has been developed in [16] and is recalled in Section 3.

We obtain the discrete variational eigenvalue problem: Find $u \in V_{K,p}$ such that

$$a_{K,p}(u, v) = \lambda b_{K,p}(u, v), \quad \forall v \in V_{K,p}, \tag{4}$$