Commutation of Geometry-Grids and Fast Discrete PDE Eigen-Solver GPA*

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Abstract A geometric intrinsic pre-processing algorithm (GPA for short) for solving largescale discrete mathematical-physical PDE in 2-D and 3-D case has been presented by Sun (in 2022–2023). Different from traditional preconditioning, the authors apply the intrinsic geometric invariance, the Grid matrix G and the discrete PDE mass matrix B, stiff matrix A satisfies commutative operator BG = GB and AG = GA, where G satisfies $G^m = I, m \ll \dim(G)$. A large scale system solvers can be replaced to a more smaller block-solver as a pretreatment in real or complex domain.

In this paper, the authors expand their research to 2-D and 3-D mathematical physical equations over more wide polyhedron grids such as triangle, square, tetrahedron, cube, and so on. They give the general form of pre-processing matrix, theory and numerical test of GPA. The conclusion that "the parallelism of geometric mesh pre-transformation is mainly proportional to the number of faces of polyhedron" is obtained through research, and it is further found that "commutative of grid mesh matrix and mass matrix is an important basis for the feasibility and reliability of GPA algorithm".

Keywords Mathematical-physical discrete eigenvalue problems, Commutative operator, Geometric pre-processing algorithm, Eigen-polynomial factorization

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1 Introduction

Many discrete models on PDE solver are based on applying variable separation approach and variational principle, such as for solving PDE with initial-boundary value problem in three dimension.

By means of FEM discretization, we usually get three types of matrix representation, stiff matrix A, mass matrix B and basis matrix G endowed with supplemental structures. The basis matrix G usually originates from the so-called polar decomposition of mass matrix B = GR, which represents the process of an object's affine transformation such as rotation and reflection etc. According to bounded operators on Hilbert space, the polar decomposition of a square matrix B = GR always exists (see [14]).

In linear algebra and functional analysis, the basis matrix G can be given theoretically by intrinsic spectral-factorization over PDE's geometric domain such as grids, meshes or graphs. Suppose B is a compact self-adjoint operator on a (real or complex) Hilbert space H. Then

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there is an orthonormal basis of H consisting of eigenvectors of B. Each eigenvalue is real. The orthonormal basis of H gives the basis matrix G.

In mathematics, the so-called commutator gives an indication of the extent to which a certain binary operation [B, G] fails to be commutative, i.e. the metric of [B, G] is not zero. The commutator of two elements B and G of a ring is defined by [B, G] = BG - GB. It is zero if and only if B and G commute (see [10]).

In quantum mechanics, the commutation relation [A, G] and [B, G] acting on a Hilbert space H is a central concept, which is fundamental between the two conjugate quantities A and B (i.e., momentum and position, respectively), which are pairs of variables mathematically defined in such a way that they become Fourier transform duals. The duality relations lead naturally to an uncertainty relation between them. The uncertainty principle is ultimately a theorem about the commutator [A, B], by virtue of the Robertson-Schrodinger relation, it quantifies how well the two observables described by these operators can be measured simultaneously (see [12]). The conjugate variables A,B are related by Noether's theorem, which states that if the laws of physics are invariant with respect to a change in one of the conjugate variables, then the other conjugate variable will not change with time (see [29]).

In noncommutative geometry and related branches of mathematical physics, a spectral triple (A, H, G) is a set of data which encodes a geometric phenomenon in an analytic way (see [11]). The definition typically involves a Hilbert space H, an algebra of operators A on the Hilbert space and an unbounded self-adjoint operator G which is endowed with supplemental structures. We have two spectral triple (A, H, G) and (B, H, G), the former is used to depict the commutation relation [A, G], and the latter is used to depict the commutation relation [B, G] (see [8]).

In continuum mechanics, a change in the configuration of a continuum body results in a displacement which has two components: rigid-body displacement and deformation. The former consists of simultaneous translations and rotations without changing its shape or size, the latter implies the change in shape or size from undeformed configuration $\kappa_0(B)$ to deformed configuration $\kappa_t(B)$. The evolution of configurations throughout time can be depicted by means of a specific commutator [A, G], where A represents the physical and kinematic properties of a continuum, and G represents the motion of a continuum body (see [17]). Here, we can use commutation relation [B, G] = 0 to depict rigid-body displacement, and use noncommutation relation $[B, G] \neq 0$ to depict the deformation or distortion characteristic phenomenon.

In Geometric Deep Learning (GDL for short), an invariant is an object property that does not change as a result of some transformation, while an equivariant is a property or relationship that changes predictably under transformation. As a fundamental principles underlying Deep Learning architectures, a symmetry is depicted by means of geometry invariance and equivariance, which corresponds to a specific conservation law. The motivation behind GDL is to address some of the shortcomings of Convolutional Neural Networks (CNN for short). Traditional CNN fails to depicts effectively the symmetry of the practical physics problem. We need inject further assumptions about the geometry of through inductive biases, by means of restricting the functions or mappings in our hypothesis spaces to the destined Hilbert spaces that respect the geometry. By using of the commutator [B, G], we can get the geometry invariance and geometry equivariance affine transformation such as

> geometry – invariance : $f(GX, GBG^T) = f(X, B),$ geometry – equivariance : $f(GX, GBG^T) = Gf(X, B).$

Additionally, groups are the central object in the mathematical study of symmetry, it is natural to consider replacing convolution by group convolution in CNNs (see [3–4]). Consequently, in the process of developing generalized methods, many state-of-art algorithms occurs, such as Group-CNN, transformers, GNNS and Intrinsic CNNs etc..

In the early 1980s, the numerical analysis team in the Computer Science Department of Yale University proposed a preconditioned sub method for understanding linear equations (see [7, 9]). With the development of high-performance computing systems, the research on highperformance PDE eigenvalue algorithms is relatively slow and far from meeting the needs of E-level high-performance computing applications (see [1, 5–6, 13]). Relying solely on existing linear algebra software to efficiently solve large-scale PDE eigenvalue problems has emerged as a bottleneck (see [15–16, 18, 30]).

How to find the "approximate inverse" of the estimation matrix for PDE discrete eigenvalue problems physically reflects spectral distribution (see [20]). In classical computational mathematics, how to accurately estimate the multiplicity and separation of higher-order eigenvalues has always been an essential difficulty in computational mathematics (see [19]). However, based on the mathematical principles of elliptic partial differential equation eigenvalue problems (see [2]), it is possible to construct efficient parallel algorithms with distinctive characteristics to meet the needs of high-performance computing applications

Based on our research experience in efficient solvers such as preconditioners and domain decomposition (see [21-24]), we analyze the coupling relationship between the subspaces represented by block matrices, decouple the eigenvalue problems between large matrices into a group of lower order matrix eigenvalue problems through factorization, and then solve them asynchronously in parallel to achieve efficient parallel computing as a whole. Based on the study of geometric invariance of planar polygon meshes (triangles, quadrangles, hexagons, and general m-regular polygons), we proposed asynchronous parallel algorithms with corresponding nature (see [25-28]).

In Section 2, we introduce some lemmas on commutative among Grid matrix G, mass matrix B and stiff matrix A over various partitions, such as triangle, square in 2-D and tetrahedron, cube in 3-D.

Geometric Preprocessing Algorithm on discrete PDE Eigen-problems is studied on Section 3, such as discrete 2-D Laplace equation over polygon partition. In Section 4 and in Section 5, we investigate the GPA on 2-D hexagon and 3-D hexahedron partitions in detail. And numerical tests are listed to show the efficiency, for example, Table 1 shows the sequence speedup around 5 when dim(m) = 1 + 3m(m+1), 50 < m < 100 for hexagon partition, and Table 2 shows the sequence speedup around 4 for dim $(n) = n^3 = 8000$ for unit cube partition. The experiments have been done with MATLAB on Desktop recently and can be optimized further. Moreover, parallel speedup will be approximate, even exceed its theoretical value 6 in near future on parallel machines.

2 Basic Lemmas on Commutative Operator

 A^\prime, A^*, A^H denote the transpose, conjugate and transpose conjugate of matrix A, respectively.

2.1 Definition

Definition 2.1 Two complex matrices A and G are called to be commutative if AG = GA.

Lemma 2.1 Assume A and G are commutative and there are two different eigenvalues λ_1 and λ_2 such that

$$Gu_1 = \lambda_1 u_1, \quad Gu_2 = \lambda_2 u_2, \quad \lambda_1 \neq \lambda_2,$$

$$(2.1)$$

then u_1 and u_2 are orthogonal in the following triple sense

$$(u_1, u_2) = 0, \quad (u_1, Gu_2) = 0, \quad (u_1, Au_2) = 0.$$
 (2.2)

Proof There is trivial for the first argument of (2.2). By using AG = GA, we have

$$\lambda_2 (u_1, A^* u_2) = (u_1, A^* \overline{\lambda}_2 u_2) = (u_1, A^* G^* u_2) = (u_1, G^* A^* u_2)$$

= (Gu_1, A^* u_2) = \lambda_1 (u_1, A^* u_2). (2.3)

Thus,

$$(\lambda_2 - \lambda_1)(u_1, Au_2) = 0. (2.4)$$

Similarly, $(\lambda_2 - \lambda_1)(u_1, Gu_2) = 0$, the basic lemma has been proved.

Corollary 2.1 If A and G are commutative, then their eigen-decomposition block shape are the same.

Corollary 2.2 If AG = GA and the computational complexity for G is much less than A, then one may derive the eigen-decomposition block of A by using the block of G.

2.2 Commutativity between mass matrix and stiff matrix

As an example, suppose A_h is a stiff matrix based on an approximation (such as Finite Element and so on) around a geometric grid G_h (such as polygon in 2-D and polyhedron in 3-D and so on) and B_h is the corresponding mass matrix. If there we may find some relationship between A_h , B_h and G_h , it would be potential to reduce the cost to deal with A_h and B_h , because it would be more cheaper to deal with the geometry grid G_h .

Proposition 2.1 For 1-D two-point boundary problem

$$-u'' = f, \quad u(0) = u(1) = 0 \tag{2.5}$$

over a partition :

$$\Delta : 0 = x_0 < x_1 < \dots < x_n = 1.$$
(2.6)

Based on linear element, the mass matrix $B(\Delta)$ and the stiff matrix $A(\Delta)$ are called to be commutative if the partition Δ is symmetry along the center $\frac{1}{2}$ of the interval :

$$x_j + x_{n-j} = 1, \quad j = 1, \cdots, \left[\frac{n+1}{2}\right].$$
 (2.7)

Proof By using linear elements over the partition (2.7), the mass quadratic functional can be written as

$$LB_2 = \sum_{j=0}^{n-1} (Lf_{j+1,j}(x))^2 dx = \frac{1}{3} \sum_{j=1}^{n-1} (f_j^2 x_{j+1} + f_j f_{j+1}(x_{j+1} - x_j))$$
(2.8)

and the corresponding mass matrix $B(\Delta)$ becomes

$$BL_{2}(\Delta) = \begin{pmatrix} 2x_{2} & x_{2} - x_{1} & 0 & \cdots & 0 & 0 & 0 \\ x_{2} - x_{1} & 2(x_{3} - x_{1}) & x_{3} - x_{2} & \cdots & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & 2(x_{n-2} - x_{n-3}) & x_{n-1} - x_{n-2} \\ 0 & \cdots & 0 & \cdots & 0 & x_{n-1} - x_{n-2} & 2(1 - x_{n-2}) \end{pmatrix}.$$
 (2.9)

The expression of stiff matrix is little bit complicated. Without loss generality, we only list AL_2 for n = 4 below

$$AL_{2}(\Delta) = \begin{pmatrix} x_{2}(x_{3} - x_{2})(1 - x_{3}) & x_{1}(x_{2} - x_{3})(1 - x_{3}) & 0 \\ x_{1}(x_{2} - x_{3})(1 - x_{3}) & x_{1}(x_{3} - x_{1})(1 - x_{3}) & x_{1}(x_{1} - x_{2})(1 - x_{3}) \\ 0 & x_{1}(x_{1} - x_{2})(1 - x_{3}) & x_{1}(x_{2} - x_{1})(1 - x_{2}) \end{pmatrix}, \quad (2.10)$$

$$\{(x_3 - 1)(x_1^3 + x_1^2(x_2 - 3x_3) + x_1(x_2^2 - 2x_2x_3 + 2x_3^2) + x_2^2(x_2 - x_3)), - x_1(x_3 - 1)(x_1 - x_3)(x_1 - 2x_2 + x_3), x_1(2x_1^2(1 - x_3) + x_1(x_2^2 + 2x_2(x_3 - 2) + 3x_3^2 - 4x_3 + 2) - x_2^3 - x_2^2(x_3 - 3)) - x_2(x_3^2 - 2x_3 + 2) - (x_3 - 1)x_3^2) = 0, 0 < x_1 < x_2 < x_3 < 1\}.$$
(2.11)

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Proposition 2.2 For n = 4, the commutative matrix equation

$$AL_2(\Delta) BL_2(\Delta) = BL_2(\Delta) AL_2(\Delta)$$
(2.12)

has the following four solutions

$$\{x_1, x_2, x_3\} = \left\{ \left\{\frac{1}{7}, \frac{3}{7}, \frac{5}{7}\right\}, \left\{\frac{1}{6}, \frac{1}{2}, \frac{5}{6}\right\}, \left\{\frac{1}{4}, \frac{1}{2}, \frac{3}{4}\right\}, \left\{\frac{2}{7}, \frac{4}{7}, \frac{6}{7}\right\} \right\}.$$
(2.13)

Remark 2.1 Note that in geometry all four solutions in (2.12) are symmetry with respect to the mid point $x = \frac{1}{2}$.

In other words, we have proved the following proposition.

Proposition 2.3 For a given 1-D partition Δ_h the sufficient and necessary condition for (2.13) is the partition to be symmetry with the interval (0, 1).

2.3 2-D BG = GB over a square

The Grid and the new Grid after rotation 90^o on the square are shown in the following two frames,

$$\mathbb{G}_{40} = \begin{bmatrix}
11 & 12 & 13 & 14 \\
21 & 22 & 23 & 24 \\
31 & 32 & 33 & 34 \\
41 & 42 & 43 & 44
\end{bmatrix}, \quad
\mathbb{G}_{41} := \begin{bmatrix}
41 & 31 & 21 & 11 \\
42 & 32 & 22 & 12 \\
43 & 33 & 23 & 13 \\
44 & 34 & 24 & 14
\end{bmatrix},$$
(2.14)

there is a mapping from Grid \mathbb{G}_{40} to Grid \mathbb{G}_{41} ,

Lemma 2.2

$$B_{16}G_{16} = G_{16}B_{16}, (2.16)$$

where

$$B_{16} = \begin{pmatrix} bdd & bd9 & bd5 & bd1 & bde & bda & bd6 & bd2 & bdf & bdb & bd7 & bd3 & bdg & bdc & bd8 & bd4 \\ bfg & bff & bfe & bfd & bfc & bfb & bfa & bf9 & bf8 & bf7 & bf6 & bf5 & bf4 & bf3 & bf2 & bf1 \\ bc4 & bc8 & bcc & bcg & bc3 & bc7 & bcb & bcf & bc2 & bc6 & bca & bce & bc1 & bc5 & bc9 & bcd \\ bdg & bdf & bde & bdd & bdc & bdb & bda & bd9 & bd8 & bd7 & bd6 & bd5 & bd4 & bd3 & bd2 & bd1 \\ bcg & bcf & bce & bcd & bcc & bcb & bca & bc9 & bc8 & bc7 & bc6 & bc5 & bc4 & bc3 & bc2 & bc1 \\ bbg & bbf & bbe & bbd & bbc & bbb & bba & bb9 & bb8 & bb7 & bb6 & bb5 & bb4 & bb3 & bb2 & bb1 \\ bb4 & b88 & bbc & bbg & bb3 & bb7 & bbb & bbf & bb2 & bb6 & bba & bbe & bb1 & bb5 & bb9 & bbd \\ bf4 & bf8 & bfc & bfg & bf3 & bf7 & bfb & bff & bf2 & bf6 & bfa & bfe & bf1 & bf5 & bf9 & bfd \\ bfd & bf9 & bf5 & bf1 & bfe & bfa & bf6 & bf2 & bff & bfb & bf7 & bf3 & bfg & bfc & bf8 & bb4 \\ bb1 & bb2 & bb3 & bb4 & bb5 & bb6 & bb7 & bb8 & bb0 & bba & bbb & bbc & bbd & bbe & bb1 & bb5 \\ bb1 & bb2 & bb3 & bb4 & bb5 & bd6 & bb7 & bk8 & bb9 & bba & bbb & bbc & bbd & bbe & bbf & bbg \\ bc1 & bc2 & bc3 & bc4 & bc5 & bc6 & bc7 & bc8 & bc9 & bca & bcb & bcd & bde & bdf & bdg \\ bc1 & bc2 & bc3 & bc4 & bc5 & bc6 & bc7 & bc8 & bc9 & bca & bcb & bcd & bde & bdf & bdg \\ bcd & bc9 & bc5 & bc1 & bce & bca & bc6 & bc2 & bcf & bcb & bc7 & bc3 & bcg & bcc & bc8 & bc4 \\ bf1 & bf2 & bf3 & bf4 & bf5 & bf6 & bf7 & bf8 & bf9 & bfa & bfb & bfc & bfd & bfe & bff & bfg \\ bd4 & bd8 & bdc & bdg & bd3 & bd7 & bdb & bdf & bd2 & bd6 & bda & bde & bd1 & bd5 & bd9 & bdd \end{pmatrix} \right)$$

2.4 General solution GB = BG over triangle domain partition

For $h = \frac{1}{7}$, we give two different ordering of the triangle partition with barycentric coordinates

$$T_{\rm old} = \begin{bmatrix} * & * & * & * & 511 & * & * & * & * & * \\ * & * & * & 421 & * & 412 & * & * & * & * \\ * & * & 331 & * & 322 & * & 313 & * & * & * \\ * & 241 & * & 232 & * & 223 & * & 214 & * \\ 151 & * & 142 & * & 133 & * & 124 & * & 115 \end{bmatrix},$$
(2.18)
$$T_{\rm new} = \begin{bmatrix} * & * & * & * & 151 & * & * & * & * \\ * & * & * & 142 & * & 241 & * & * & * \\ * & * & 133 & * & 232 & * & 331 & * & * \\ * & 124 & * & 223 & * & 322 & * & 421 & * \\ * & 124 & * & 223 & * & 322 & * & 421 & * \\ 115 & * & 214 & * & 313 & * & 412 & * & 511 \end{bmatrix},$$
(2.19)

there is a mapping from $T_{\rm new}$ to $T_{\rm old},$

Lemma 2.3

$$B_{15}G_{15} = G_{15}B_{15}, (2.21)$$

where

$$B_{15} = \begin{pmatrix} b_{11} & b_{12} & b_{13} & b_{14} & b_{15} & b_{16} & b_{17} & b_{18} & b_{19} & b_{1a} & b_{1b} & b_{1c} & b_{1d} & b_{1e} & b_{1f} \\ b_{21} & b_{22} & b_{23} & b_{24} & b_{25} & b_{26} & b_{27} & b_{28} & b_{29} & b_{2a} & b_{2b} & b_{2c} & b_{2d} & b_{2e} & b_{2f} \\ b_{31} & b_{32} & b_{33} & b_{34} & b_{35} & b_{36} & b_{37} & b_{38} & b_{39} & b_{3a} & b_{3b} & b_{3c} & b_{3d} & b_{3e} & b_{3f} \\ b_{41} & b_{42} & b_{43} & b_{44} & b_{45} & b_{46} & b_{47} & b_{48} & b_{49} & b_{4a} & b_{4b} & b_{4c} & b_{4d} & b_{4e} & b_{4f} \\ b_{51} & b_{52} & b_{53} & b_{54} & b_{55} & b_{56} & b_{57} & b_{58} & b_{59} & b_{5a} & b_{5c} & b_{5d} & b_{5e} & b_{5f} \\ b_{4b} & b_{4c} & b_{47} & b_{4d} & b_{48} & b_{44} & b_{4e} & b_{49} & b_{45} & b_{42} & b_{4f} & b_{4a} & b_{46} & b_{43} & b_{41} \\ b_{3f} & b_{3a} & b_{3e} & b_{36} & b_{39} & b_{3d} & b_{33} & b_{35} & b_{38} & b_{3c} & b_{31} & b_{32} & b_{34} & b_{37} & b_{3b} \\ b_{5f} & b_{5a} & b_{5e} & b_{56} & b_{59} & b_{5d} & b_{53} & b_{55} & b_{52} & b_{5f} & b_{5a} & b_{56} & b_{53} & b_{51} \\ b_{2b} & b_{2c} & b_{27} & b_{2d} & b_{28} & b_{24} & b_{2e} & b_{29} & b_{25} & b_{22} & b_{2f} & b_{2a} & b_{26} & b_{23} & b_{21} \\ b_{1f} & b_{1a} & b_{1e} & b_{16} & b_{19} & b_{1d} & b_{13} & b_{15} & b_{18} & b_{1c} & b_{11} & b_{12} & b_{14} & b_{17} & b_{1b} \\ b_{2f} & b_{2a} & b_{2e} & b_{26} & b_{29} & b_{2d} & b_{23} & b_{25} & b_{28} & b_{2c} & b_{21} & b_{22} & b_{24} & b_{27} & b_{2b} \\ b_{4f} & b_{4a} & b_{4e} & b_{46} & b_{49} & b_{4d} & b_{43} & b_{45} & b_{48} & b_{4c} & b_{41} & b_{42} & b_{44} & b_{47} & b_{4b} \\ b_{3b} & b_{3c} & b_{37} & b_{3d} & b_{38} & b_{34} & b_{3e} & b_{39} & b_{35} & b_{32} & b_{3f} & b_{3a} & b_{36} & b_{33} & b_{31} \\ b_{1b} & b_{1c} & b_{17} & b_{1d} & b_{18} & b_{14} & b_{19} & b_{15} & b_{12} & b_{1f} & b_{1a} & b_{16} & b_{13} & b_{11} \end{pmatrix}$$

2.5 3-D BG = GB over a tetrahedron

For $h = \frac{1}{6}, n = 10$, we give two different ordering of the tetrahedron partition with homogeneous coordinates

$T_{\rm old} =$	* * *	* * *	* * *	* * 2121	3113 2211	* * 2112	* * *	* * *	* * * .	, (2.23)
	* * *	* * *	* * 1131	* 1221 *	* 1122	* 1212 *	* * 1113	* * *	* * *	
$T_{\rm new} =$	* * * * *	* * * * *	* * * * 1113	* 1212 * 1122 *	1311 1221 1131 * 2112	* 2211 * 2121 *	* * * 3111	* * * * *	* * * * *	, (2.24)

there is a mapping from $T_{\rm new}$ to $T_{\rm old},$

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$$BT_{10} = \begin{pmatrix} b_{11} & b_{12} & b_{13} & b_{14} & b_{15} & b_{16} & b_{17} & b_{18} & b_{19} & b_{1a} \\ b_{21} & b_{22} & b_{23} & b_{24} & b_{25} & b_{26} & b_{27} & b_{28} & b_{29} & b_{2a} \\ b_{31} & b_{32} & b_{33} & b_{34} & b_{35} & b_{36} & b_{37} & b_{38} & b_{39} & b_{3a} \\ b_{41} & b_{42} & b_{43} & b_{44} & b_{45} & b_{46} & b_{47} & b_{48} & b_{49} & b_{4a} \\ b_{51} & b_{52} & b_{53} & b_{54} & b_{55} & b_{56} & b_{57} & b_{58} & b_{59} & b_{5a} \\ b_{5a} & b_{59} & b_{58} & b_{57} & b_{56} & b_{55} & b_{54} & b_{53} & b_{52} & b_{51} \\ b_{4a} & b_{49} & b_{48} & b_{47} & b_{46} & b_{45} & b_{44} & b_{43} & b_{42} & b_{41} \\ b_{3a} & b_{39} & b_{38} & b_{37} & b_{36} & b_{35} & b_{34} & b_{33} & b_{32} & b_{31} \\ b_{2a} & b_{29} & b_{28} & b_{27} & b_{26} & b_{25} & b_{24} & b_{23} & b_{22} & b_{21} \\ b_{1a} & b_{19} & b_{18} & b_{17} & b_{16} & b_{15} & b_{14} & b_{13} & b_{12} & b_{11} \end{pmatrix},$$

3 Geometric Preprocessing Algorithm on Discrete PDE Eigen-Problems

3.1 2-D Laplace equation over a polygon domain

Consider the Laplace eigen-problem with Dirichlet zero boundary over a polygon domain Ω :

$$Lf(x,y) := -\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) f(x,y) = \lambda f(x,y), \quad f(x,y)|_{\partial\Omega} = 0.$$
(3.1)

For a unit square Ω , with so-called separation variable approach, we know

$$\phi_{j,k}[x,y] := \sin j\pi x \sin k\pi y := f_j[x] f_k[y]$$
(3.2)

is a class of eigen-function with zero boundary condition and the corresponding eigenvalues equal to

$$\lambda_{j,k} = (j^2 + k^2)\pi^2. \tag{3.3}$$

In general, one may define the corresponding eigen-functions family as

$$f_{jk}(x,y) = \sum_{j,k} \alpha_{j,k} f_j[x] f_k[y],$$
(3.4)

and a general eigenfunctions can be written as

$$Lf(x,y) = \sum_{j,k} (j^2 + k^2) \pi^2 \alpha_{j,k} f_j[x] f_k[y] = \sum_{j,k} \lambda_{j,k} \alpha_{j,k} f_j[x] f_k[y].$$
(3.5)

Now we turn to deal with the discrete eigen-problem by traditional 5-point scheme or bilinear FEM. As an example, suppose the step size $h = \frac{1}{6}$.

The corresponding mass matrices in 1-D and 2-D become

$$B_{51} = \begin{pmatrix} 2 & 1 & 0 & 0 & 0 \\ 1 & 2 & 1 & 0 & 0 \\ 0 & 1 & 2 & 1 & 0 \\ 0 & 0 & 1 & 2 & 1 \\ 0 & 0 & 0 & 1 & 2 \end{pmatrix}, \quad B_{52} = \operatorname{kron}(B_{51}, I_5) + \operatorname{kron}(I_5, B_{51}), \tag{3.6}$$

where notation kron denotes so-called Kronecker product.

Similarly we may write the stiff matrices A_{51} and A_{52} .

The Grid and the new Grid after rotation 90° are shown in the following two frames:

	$= \begin{bmatrix} 51 & 41 & 31 & 21 & 11 \\ 52 & 42 & 32 & 22 & 12 \\ 53 & 43 & 33 & 23 & 13 \\ 54 & 44 & 34 & 24 & 14 \\ 55 & 45 & 35 & 25 & 15 \end{bmatrix}.$ (3.7)
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It is clear, the Grid is just back to the original after four times rotations. Moreover, there is a mapping from Grid \mathbb{G}_{50} to Grid \mathbb{G}_{51} ,

Lemma 3.1 The Grid matrix G_{25} is periodic with four cycles $G_{25}^4 = I_{25}$. Moreover, matrix G_{25}, A_{25}, B_{25} are commutative interchange each other

$$G_{25}B_{52} = B_{52}G_{25}, \quad G_{25}A_{52} = A_{52}G_{25}, \quad A_{25}B_{52} = A_{52}G_{25}. \tag{3.9}$$

Denote

$$P_{725} = \text{NullSpace}(I_{25} - G_{25}), \quad J_{625} = \text{NullSpace}(I_{25} + G_{25}),$$

$$FI_{625} = \text{NullSpace}(i I_{25} - G_{25}), \quad FII_{625} = \text{NullSpace}(i I_{25} + G_{25}).$$
(3.10)

The 25 entries can be divided into 6 subsets according to the symmetry, as an example

$$\begin{bmatrix} 11 & 12 & 13 & 14 & 22 & 23 \\ 15 & 25 & 35 & 45 & 24 & 34 \\ 55 & 54 & 53 & 52 & 44 & 43 \\ 51 & 41 & 31 & 21 & 42 & 32 \end{bmatrix}$$
 (3.11)

Thus, it is easy to find four unitary eigen-subspaces of G_{25} according to (3.11).

and

are real and other two subspaces are complex with conjugate each other:

Proposition 3.1

$$\frac{P7UAB\lambda \times J6UAB\lambda \times (FI6A\lambda)^2}{\det(A_{52} - \lambda B_{52})} = 1,$$
(3.15)

where

$$P7UAB\lambda = \det(P_{725}A_{52}P'_{725} - \lambda P_{725}B_{52}P'_{725})$$

= $-4(\lambda - 4)(\lambda - 1)(3\lambda - 4)(\lambda^2 - 104\lambda + 4)(4\lambda^2 - 44\lambda + 13),$
 $J6UAB\lambda = \det(J_{625}A_{52}J'_{625} - \lambda J_{625}B_{52}J'_{625})$
= $(\lambda - 6)(\lambda - 4)(3\lambda - 4)(9\lambda - 2)(4\lambda^2 - 44\lambda + 13),$
 $FI6AB\lambda = \det(FI_{625}A_{52}FI^H_{625} - \lambda FI_{625}B_{52}FI^H_{625})$
= $9(2\lambda - 5)(2\lambda - 1)(\lambda^2 - 26\lambda + 22)(3\lambda^2 - 18\lambda + 2).$

In general for n = 2m + 1, the GPA algorithm on square partition can be listed below (see [25]).

For a given square, the only four non-zero entries in the following four sparse matrices

$$PMm(n,k,j), JMm(n,k,j), FIMm(n,k,j), FIIMm(n,k,j)$$

locate on the column as follows

$$PMm(n,k,j) = n(k-1) + j, n(j-1) + n + 1 - k, n(n-j) + k, n(n-k) + n + 1 - j,$$

$$JMm(n,k,j) = n(k-1) + j, n(j-1) + n + 1 - k, n(n-j) + k, n(n-k) + n + 1 - j,$$

$$FIMm(n,k,j) = -(n(k-1) + j), i(n(j-1) + n + 1 - k), -i(n(n-j) + k),$$

$$n(n-k) + n + 1 - j,$$

$$FIIMm(n,k,j) = FIMm(n,k,j)^*.$$

(3.16)

Remark: Notation i is the unit of imaginary number, * denotes complex conjugate.

4 The GPA on Regular Hexagon Grid

It is trivial that for a regular hexagon $\dim(S_m^6) = 1 + 3m(m+1)$. Denote $\omega = e^{\frac{i\pi}{3}}$ for m = 1, $\dim(S_1^6) = 7$, the preprocessing matrix is

$$PG_{7} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & -1 & 1 & -1 & 1 & -1 & 1 \\ 0 & -\omega & -\omega^{-1} & 1 & -\omega & -\omega^{-1} & 1 \\ 0 & -\omega^{-1} & -\omega & 1 & -\omega^{-1} & -\omega & 1 \\ 0 & \omega & -\omega^{-1} & -1 & -\omega & \omega^{-1} & 1 \\ 0 & \omega^{-1} & -\omega & -1 & -\omega^{-1} & \omega & 1 \end{pmatrix}$$
(4.1)

and

$$PG_7PG_7' = \text{Diag}\{1, 6, 6, 6, 6, 6, 6\}.$$
(4.2)

Define geometry preprocess matrix with $6k \ (k = 2, 3, \cdots)$ order as follows

$$PG_{k} = \frac{1}{\sqrt{6}} \begin{pmatrix} J_{k} & J_{k} & J_{k} & J_{k} & J_{k} & J_{k} & J_{k} \\ -J_{k} & J_{k} & -J_{k} & J_{k} & -J_{k} & J_{k} \\ -\omega J_{k} & -\omega^{-1} J_{k} & J_{k} & -\omega J_{k} & -\omega^{-1} J_{k} & J_{k} \\ -\omega^{-1} J_{k} & -\omega J_{k} & J_{k} & -\omega^{-1} J_{k} & -\omega J_{k} & J_{k} \\ \omega J_{k} & -\omega^{-1} J_{k} & -J_{k} & -\omega J_{k} & \omega^{-1} J_{k} & J_{k} \\ \omega^{-1} J_{k} & -\omega J_{k} & -J_{k} & -\omega^{-1} J_{k} & \omega J_{k} & J_{k} \end{pmatrix},$$
(4.3)

where J_k is the unit sub-diagonal matrix

$$J_k = \begin{pmatrix} 0 & 0 & \dots & 0 & 0 & 1 \\ 0 & 0 & \dots & 0 & 1 & 0 \\ 0 & 0 & \dots & 1 & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 1 & \dots & 0 & 0 & 0 \\ 1 & 0 & \dots & 0 & 0 & 0 \end{pmatrix}$$

Lemma 4.1 PG_k is unitary :

$$PG_k PG_k^H = PG_k^H PG_k = I_{6k}.$$
(4.4)

 $\dim(S_m^6) = 1 + 3m(m+1) = 1 + \sum_{k=1}^m 6k$, PG_7 and PG_k form the preprocessing matrix for arbitrary partition m.

Proposition 4.1 For an arbitrary index m, the discrete Laplace eigen-problem can asynchronously be solved by eigen-polynomial factorization into six eigen-subproblems.

We give the numerical results for the hexagon. DOF: Degree of freedom, t_s : The computational time of the initial problem, t_p : The computational time of the preprocessing problems, SP: The speed up ratio which equals to $\frac{t_s}{t_p}$.

m	DOF	$t_s(s)$	$t_p(s)$	SP
40	4921	7.224	1.526	4.73
50	7651	29.611	5.66	5.23
60	10981	95.991	16.926	5.67
80	19441	547.144	99.158	5.52
90	24571	1114.36	212.24	5.25
100	30301	1997.51	400.01	4.99

Table 1 The GPA of hexagon

5 The GPA on Regular Hexahedron Grid

5.1 Model problem: Mesh size $h = \frac{1}{5}$

For $h = \frac{1}{5}$, the degree of freedom is 64. We can define two sorts of the hexahedron grid. Sort I Sort II (5.1)

Between the two sorts there is a permutation matrix $G = \{g_{ij}\}$, the sixty-four row indexes for non-zero elements (both are 1) according to column 1–64 can be compressed expressed by (5.2),

1	4	8	12	16	20	24	28	32	36	40	44	48	52	56	60	64	١	
	3	7	11	15	19	23	27	31	35	39	43	47	51	55	59	63		(5.0)
	2	6	10	14	18	22	26	30	34	38	42	46	50	54	58	62	,	(0.2)
	1	5	9	13	17	21	25	29	33	37	41	45	49	53	57	61	/	

we have $g_{41} = 1$, $g_{82} = 1$, $g_{12,3} = 1$, \cdots , $g_{57,63} = 1$, $g_{61,64} = 1$.

Define $\omega = e^{\frac{2i\pi}{3}}$, $\overline{\omega} = e^{-\frac{2i\pi}{3}}$, I_{64} is the 64 × 64 identity matrix. It is easy to verify that $I_{64} - G^6 = 0$, we have the following factorization in real field and complex field.

Lemma 5.1

$$I_{64} - G^6 = (I_{64} - G)(I_{64} + G)(I_{64} + G + G^2)(I_{64} - G + G^2),$$
(5.3)

$$I_{64} - G^6 = (I_{64} - G)(I_{64} + G)(I_{64} - \omega G)(I_{64} + \omega G)(I_{64} - \overline{\omega} G)(I_{64} + \overline{\omega} G), \qquad (5.4)$$

the factorization is the basis of the GPA.

The null space $P = \{p_{ij}\}$ of $I_{64} - G$ is a sparse 12×64 matrix, the column indexes for non-zero elements (both are 1) of every row can be expressed by the following matrix:

$$\begin{pmatrix} 1 & 4 & 16 & 49 & 61 & 64 \\ 2 & 8 & 32 & 33 & 57 & 63 \\ 3 & 12 & 17 & 48 & 53 & 62 \\ 5 & 15 & 20 & 45 & 50 & 60 \\ 6 & 24 & 31 & 34 & 41 & 59 \\ 7 & 18 & 28 & 37 & 47 & 58 \\ 9 & 14 & 29 & 36 & 51 & 56 \\ 10 & 25 & 30 & 35 & 40 & 55 \\ 11 & 15 & 20 & 45 & 50 & 60 \\ 13 & * & * & * & * & * & 52 \\ 22 & 23 & 27 & 38 & 42 & 43 \\ 26 & * & * & * & * & * & 29 \end{pmatrix},$$

$$(5.5)$$

we have $p_{11} = 1, p_{14} = 1, p_{1,16} = 1, p_{1,49} = 1, p_{1,61} = 1, p_{1,64} = 1, \dots, p_{12,26} = 1, p_{12,29} = 1.$

The null space J of $I_{64} + G$ is a sparse 12×64 matrix too, the column indexes for non-zero elements are the same with P. The non-zero elements of J are 1 and -1. The null spaces F_1 of $I_{64} - \omega G$, F_2 of $I_{64} + \omega G$, F_3 of $I_{64} - \overline{\omega}G$, F_4 of $I_{64} + \overline{\omega}G$ are both sparse 10×64 matrices, and the column indexes for non-zero elements are the same, the column indexes for non-zero elements of every row can be expressed by the following matrix:

$$\begin{pmatrix} 1 & 4 & 16 & 49 & 61 & 64 \\ 2 & 8 & 32 & 33 & 57 & 63 \\ 3 & 12 & 17 & 48 & 53 & 62 \\ 5 & 15 & 20 & 45 & 50 & 60 \\ 6 & 24 & 31 & 34 & 41 & 59 \\ 7 & 18 & 28 & 37 & 47 & 58 \\ 9 & 14 & 29 & 36 & 51 & 56 \\ 10 & 25 & 30 & 35 & 40 & 55 \\ 11 & 15 & 20 & 45 & 50 & 60 \\ 22 & 23 & 27 & 38 & 42 & 43 \end{pmatrix}.$$

$$(5.6)$$

And $F_3 = F_1^*$, $F_4 = F_2^*$, the non-zero elements are some of $1, -1, \omega, -\omega, \overline{\omega}, -\overline{\omega}$. The different column indexes between P, J and F_1 , F_2 , F_3 , F_4 are P, J have two additional rows with two non-zero elements. P, J, F_1 , F_2 , F_3 , F_4 form the preprocessing matrix. They have the following proposition.

Proposition 5.1 They are orthogonal to each other in the L_2 norm, that is

$$PJ' = \mathbf{0}_{12,12},\tag{5.7}$$

$$PF_i^H = \mathbf{0}_{12,10} \quad for \quad i = 1, 2, 3, 4, \tag{5.8}$$

$$JF_i^H = \mathbf{0}_{12,10} \quad for \quad i = 1, 2, 3, 4.$$
 (5.9)

For tri-linear element we have the stiff matrix A and mass matrix B, and they satisfy commutative operator AG = GA, BG = GB.

Proposition 5.2 The different preprocessing matrices are orthogonal to the stiff matrix A, mass matrix B in the L_2 norm, that is

$$PAJ' = \mathbf{0}_{12,12}, \quad PBJ' = \mathbf{0}_{12,12},$$
 (5.10)

$$PAF_i^H = \mathbf{0}_{12,10}, \quad PBF_i^H = \mathbf{0}_{12,10} \quad for \quad i = 1, 2, 3, 4,$$
 (5.11)

$$JAF_i^H = \mathbf{0}_{12,10}, \quad JBF_i^H = \mathbf{0}_{12,10} \quad for \quad i = 1, 2, 3, 4.$$
 (5.12)

So the initial eigenvalue problem $Au = \lambda Bu$ can be divided into six sub-problems.

First we compute the sub-matrix by using the preprocessing matrix P,

similarly we get

$$J_A = JAJ', \qquad J_B = JBJ',$$

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$$\begin{split} F_{1A} &= F_1 A F_1^H, \quad F_{1B} = F_1 B F_1^H, \\ F_{2A} &= F_2 A F_2^H, \quad F_{2B} = F_2 B F_2^H, \\ F_{3A} &= F_3 A F_3^H, \quad F_{3B} = F_3 B F_3^H, \\ F_{4A} &= F_4 A F_4^H, \quad F_{4B} = F_4 B F_4^H. \end{split}$$

It is easy to verify $F_{1A} = F_{3A}^*$, $F_{1B} = F_{3B}^*$, $F_{2A} = F_{4A}^*$, $F_{2B} = F_{4B}^*$. Six sub-eigenvalue problems can be reduced to four sub-eigenvalue problems as follows

$$P_{\lambda} = \det(P_A - \lambda P_B),$$

$$J_{\lambda} = \det(J_A - \lambda J_B),$$

$$F_{1\lambda} = \det(F_{1A} - \lambda F_{1B}),$$

$$F_{2\lambda} = \det(F_{2A} - \lambda F_{2B}).$$

We have the following proposition.

Proposition 5.3

$$\frac{\det(A - \lambda B)}{P_{\lambda} \cdot J_{\lambda} \cdot (F_{1\lambda} \cdot F_{2\lambda})^2} = \text{Constant},$$
(5.13)

that means the eigen-computation of initial (A,B) can be gotten by the small eigen-problems, if we normalize the preprocessing matrix P, J, F_1, F_2, F_3, F_4 , the constant equals to 1.

5.2 Arbitrary mesh size h

Define $N = \frac{1}{h}$, n = N - 1, the degree of freedom $DOF = n^3$, we can get the preprocessing matrices P, J, F_1 , F_2 , F_3 , F_4 directly, they are only relevant to the geometry symmetry of the hexahedron. The number of columns for P, J, F_1 , F_2 , F_3 , F_4 equal to DOF, the number of rows for F_1 , F_2 , F_3 , F_4 are the same, the number of rows for P, J, F_1 are N_P , N_J , N_F which can be obtained by the following Algorithm 1:

Algorithm 1 The dimensions of P, J, F_1

```
thp

if \operatorname{mod}(n, 2) == 1 then

d = \operatorname{fix}\left(\frac{n}{2}\right)

N_P = \frac{DOF - 1 - 2*d}{6} + d + 1

N_J = \frac{DOF - 1 - 2*d}{6} + d

N_F = \frac{DOF - 1 - 2*d}{6}

else

d = \operatorname{fix}\left(\frac{n}{2}\right)

N_P = \frac{DOF - 2*d}{6} + d

N_J = \frac{DOF - 2*d}{6} + d

N_F = \frac{DOF - 2*d}{6}

end if
```

Matrices F_i , i = 1, 2, 3, 4 have six non-zero elements every row, and P, J have extra d rows with two non-zero elements, P has one row with one non-zero element if mod(n, 2) = 1. If we

get the column indexes for non-zero elements, then we obtain the preprocessing matrices. The indexes are relevant to the mesh of the hexahedron, we have Algorithm 2.

Algorithm 2 The indexes of P, J, F_1

```
thp
  set d = \operatorname{fix}\left(\frac{n}{2}\right), L = 0
  for k = 1 : d do
    for i = 1 : n - (2 * k - 1) do
      for j = 1 : n - (2 * k - 1) do
         L = L + 1;
         id(L,1) = (i-1) * n + j + (n^2 + n + 1) * (k-1)
         id(L,4) = DOF + 1 - id(L,1)
         id(L,5) = DOF + 1 - id(L,2)
         id(L,6) = DOF + 1 - id(L,3)
         P(L, id(L, 1)) = 1
         P(L, id(L, 2)) = 1
         P(L, id(L, 3)) = 1
         P(L, id(L, 4)) = 1
         P(L, id(L, 5)) = 1
         P(L, id(L, 6)) = 1
      end for
    end for
  end for
  for i = 1 : d do
    L = L + 1;
    id(L,1) = (n^2 - n + 1) * i
    id(L,2) = n^3 - n^2 + n - (n^2 - n + 1) * (i - 1)
    P(L, id(L, 1)) = 1
    P(L, id(L, 2)) = 1
    J(L, id(L, 1)) = -1
    J(L, id(L, 2)) = 1
  end for
  if mod(n, 2) == 1 then
    P\left(N_P, \frac{DOF+1}{2}\right) = 1
  end if
```

Following the step of Subsection 5.1 we divide the initial large eigenvalues problem into four sub eigenvalues problems which can be computed parallel.

5.3 Numerical results

The computational domain is a unit cube. N: The number of grid for x-direction, DOF: Degree of freedom, t_s : The computational time of the initial problem, t_p : The computational time of the preprocessing problems, SP: The speed up ratio which equals to $\frac{t_s}{t_p}$, err: The error of the eigenvalues of two methods.

N	DOF	$t_s(s)$	$t_p(s)$	SP	err
17	4096	4.876	0.896	5.44	1.17e - 13
19	5832	13.025	3.058	4.26	1.88e - 13
21	8000	33.587	8.231	4.08	2.88e - 13
25	13824	172.693	49.106	3.52	5.25e - 13
31	27000	1234.166	385.711	3.19	1.29e - 12

Table 2 The GPA of unit cube

Declarations

Conflicsts of interest The authors declare no conflicts of interest.

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