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On the Multiplicative Regularization of Graph Laplacians on Closed and Open Structures With Applications to Spectral Partitioning

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ABSTRACT A new regularization technique for graph Laplacians arising from triangular meshes of closed and open structures is presented. The new technique is based on the analysis of graph Laplacian spectrally equivalent operators in terms of Sobolev norms and on the appropriate selection of operators of opposite differential strength to achieve a multiplicative regularization. In addition, a new 3-D/2-D nested regularization strategy is presented to deal with open geometries. Numerical results show the advantages of the proposed regularization as well as its effectiveness when used in spectral partitioning applications.

INDEX TERMS Spectral partitioning, computational electromagnetics, integral equations, multiplicative preconditioners.

I. INTRODUCTION

Several integral equation formulations in Computational Electromagnetics require the partitioning of a surface into sub-manifolds or macro-cells. An incomplete list of examples includes domain decomposition integral equation methods [1], hierarchical quasi-Helmholtz decompositions [2], and characteristic or synthetic basis function methods [3], [4]. Standard approaches for partitioning a domain rely on the use of standard and adaptive octrees that became particularly popular for their use in fast integral equation algorithms [5]. Even though these partitioning algorithms are very effective when dealing with fast solvers, they are instead often inappropriate in hierarchical preconditioning or domain decomposition settings where connectivity constraints are present. In fact, for complex and non-convex geometries, octree based strategies often provide un-connected partitions that will require tedious and often hardly feasible post-processing.

An effective, although usually expensive, way of obtaining a partitioning of a meshed manifold into connected components is to rely on the spectral properties of the mesh associated graph Laplacian [6]. Such an approach, known in literature as spectral partitioning, has been widely applied to network design [7], VLSI layout [8], data mining [9], and parallel load balancing algorithms [10]. Spectral partitioning offers a robust partitioning strategy that works well even for very complex, folded, or non-simply connected geometries [6]. In many of these cases, partitioning techniques based on octree schemes fail dramatically, jeopardizing the performance of any subsequent method relying on the partitioning.

Lamentably, standard spectral partitioning methods are very expensive since they rely on the spectral analysis of the graph Laplacian matrix which is often severely ill-conditioned. Several schemes to regularize the Laplacian (like hierarchical bases approaches or geometric multi-grids) rely on domain partitions to achieve the regularization [11]–[14]. For this reason they cannot be used in this context since they would require the manifold partitioning which is instead the final goal of the procedure.

In this paper, we will introduce a different approach to the problem. The graph Laplacian will be regularized in a multiplicative way following a strategy similar to the one used in Calderón preconditioning the Electric Field Integral Equation (EFIE) [15]–[18]. The differential strength of the graph Laplacian will be regularized with operators of equal, but opposite strength by using single layer operators, suitably linked with Gram matrices [19]. In multiplicative preconditioning techniques a particular care should always be devoted when handling open structures. In this work,

we handle the issue by introducing a new preconditioning strategy based on two nested multiplicative preconditioners: one on the surface, and a nested one (of one dimension less) on the surface's boundary. The reader should notice that although this paper will use the regularized Laplacian for spectral partitioning applications, many numerical algorithms in computational electromagnetics [20]–[22] as well as in other branches of computational science (such as computational neuroscience [23], computational mechanics [24], machine learning [25], numerical linear algebra [26], high performance computing [27]) are based on inversion of graph Laplacians and, as such, can benefit from the contributions presented in this work.

This paper is organized as follows. Section II presents background material and introduces notation. Section III presents a new regularization of graph Laplacians for the close structure case. Section IV presents a new regularization of graph Laplacians for the open structure case. Section V presents numerical results that demonstrate the effectiveness of the proposed schemes. Section VI presents our conclusions and avenues for future research.

II. NOTATION AND BACKGROUND

The developments in this work apply to graph Laplacians arising from relatively general surface meshes and as such the treatment could stay general and independent of any particular implementation. This not with standing, mesh graph Laplacians arise naturally from boundary element formulations of electromagnetic integral equations. Given that integral operators will play a role in the regularization of the graph Laplacians presented in this work, we thus find useful to introduce here graph Laplacians from quasi-Helmholtz decompositions of discrete boundary elements electric currents.

Integral equations for electromagnetic perfect electrically conducting scatterers often aim at the determination of the induced electric current $\boldsymbol{J}(\boldsymbol{r})$ on an orientable manifold Γ discretized using a uniform mesh of triangular cells with an average length h. The electric current $\boldsymbol{J}(\boldsymbol{r})$ is approximated by

$$\boldsymbol{J}(\boldsymbol{r}) = \sum_{n=1}^{N} I_n f_n(\boldsymbol{r}) \tag{1}$$

where $f_n(\boldsymbol{r})$ are the Rao-Wilton-Glisson (RWG) basis functions and where N is the number of internal edges of the mesh. It is very well-known that the coefficient vector $\mathbf{I}$, with $\mathbf{I}_i = I_i$, can be decomposed into Loop and Start coefficients [21], [28]–[32]

$$\mathbf{I} = \mathbf{\Lambda}\lambda + \mathbf{\Sigma}\sigma \tag{2}$$

where, with the conventions of Fig. 1, the matrix $\mathbf{\Lambda}$ is defined as

$$\mathbf{\Lambda}_{i,j} = \begin{cases} 1 & \text{if the node } j \text{ equals } v_i^+ \\ -1 & \text{if the node } j \text{ equals } v_i^- \\ 0 & \text{otherwise} \end{cases} \tag{3}$$

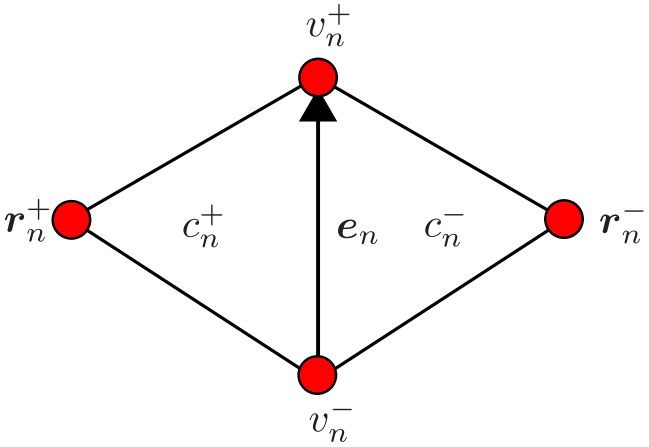

FIGURE 1. Symbols used in the definition of RWG, Loop, and Star functions based on edge e_n, vertices v_n^- & v_n^+, and triangles c_n^+ & c_n^-.

and the matrix $\mathbf{\Sigma}$ is defined as

$$\mathbf{\Sigma}_{i,j} = \begin{cases} 1 & \text{if the cell } j \text{ equals } c_i^+ \\ -1 & \text{if the cell } j \text{ equals } c_i^- \\ 0 & \text{otherwise} \end{cases} \tag{4}$$

In writing (2) we have assumed for simplicity that Γ is simply connected. With the definitions above we can immediately obtain the two vertex-based and cell-based graph Laplacians associated with the mesh as

$$\mathbf{\Lambda}^T\mathbf{\Lambda} \quad \text{and} \quad \mathbf{\Sigma}^T\mathbf{\Sigma} \tag{5}$$

respectively (see [21] and references therein). Using these graph Laplacians, the connected partitions of the manifold Γ can be obtained using spectral partitioning (refer to Appendix A).

The spectral properties of the graph Laplacian can be understood from their mapping properties between Sobolev spaces. The space of square integrable functions $L^2(\Omega)$ is defined as

$$L^2(\Omega) = \{f : \Omega \to \mathbb{R} \mid \|f\|_{L^2(\Omega)} < \infty\}, \tag{6}$$

with L^2-norm of a function f given by $\|f\|_{L^2(\Omega)} = \left(\int_\Omega |f(x)|^2 d\Omega\right)^{1/2}$. The space of square integrable functions (defined on Ω) whose gradient is also a square integrable function is known as Sobolev space $H^1(\Omega)$ and it is given by

$$H^1(\Omega) = \{f : \Omega \to \mathbb{R} \mid f \in L^2(\Omega) \wedge \nabla f \in (L^2(\Omega))^3\}. \tag{7}$$

Using this space, we can define the space $H^{1/2}(\Gamma)$ as

$$H^{1/2}(\Gamma) = \{f : \Gamma \to \mathbb{R} \mid \exists\, g \in H^1(\Omega) \text{ such that } f = g|_\Gamma\} \tag{8}$$

The space $H^{1/2}(\Gamma)$ and its dual space $H^{-1/2}(\Gamma)$ (set of continuous functionals $f : H^{1/2}(\Gamma) \to \mathbb{R}$ [33]) can be used to define the mapping properties of some relevant static operators that will be defined and used in what follows.

The static operators which we will use in our analysis are the single layer operator $\mathcal{S}$, given by

$$\mathcal{S}(w(\boldsymbol{r})) = \int_{\partial\Gamma} \frac{1}{4\pi\,|\boldsymbol{r}-\boldsymbol{r}'|} w(\boldsymbol{r}')d\boldsymbol{r}' \tag{9}$$

and hypersingular operator $\mathcal{N}$ defined as

$$\mathcal{N}(w(\boldsymbol{r})) = \partial_{\boldsymbol{n}} \int_{\partial\Gamma} \partial'_{\boldsymbol{n}'} \frac{1}{4\pi\,|\boldsymbol{r}-\boldsymbol{r}'|} w(\boldsymbol{r}')d\boldsymbol{r}' \tag{10}$$

where $\partial_{\boldsymbol{n}} = \boldsymbol{n}\cdot\nabla$ and $\boldsymbol{n}$ is Γ's surface normal at a given location. The single layer operator and hypersingular operator, when restricted to Γ, have the following mapping properties $\mathcal{S} : H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma)$ and $\mathcal{N} : H^{1/2}(\Gamma) \to H^{-1/2}(\Gamma)$ [34]. Using these operators, we can define the equivalent norms in $H^{-1/2}$ and $H^{1/2}$ as [35]

$$\langle w, \mathcal{S}(w)\rangle \asymp \|w\|_{H^{-1/2}(\Gamma)} \forall w \in H^{-1/2} \tag{11}$$

$$\langle w, \mathcal{N}(w)\rangle \asymp \|w\|_{H^{1/2}(\Gamma)} \forall w \in H^{1/2}, \int_\Gamma w d\Gamma = 0. \tag{12}$$

The equivalence relationship $a \asymp b$ between a and b means there exists two positive real numbers c_1 and c_2 such that $c_1 b \le a \le c_2 b$.

III. PROPOSED REGULARIZATION: THE CLOSED STRUCTURE CASE

This section will deal with the regularization of the graph Laplacian in case of a closed manifold. We will perform the analysis explicitly for the case of $\mathbf{\Lambda}^T\mathbf{\Lambda}$ and then we will explain how its dual regularization for $\mathbf{\Sigma}^T\mathbf{\Sigma}$ follows. This will require a propaedeutic definition of some relevant basis functions introduced in [36].

On each inner vertex i of the original mesh, a pyramid basis function λ_i can be defined. The function λ_i is equal to 1 on the i^{th} vertex and goes linearly to 0 on the adjacent vertices. The patch basis functions ϕ_i is defined on i^{th} triangular cells of original mesh with constant value of $1/\sqrt{A}$ (A being area of the triangular cell) and 0 everywhere else.

Dual basis functions can be defined by using a barycentrically refined mesh as shown in Fig. 2. The original mesh is shown with thick blue lines and the barycentric refined mesh is shown with the thin red color lines. The dual pyramid function λ_i^{bar} is the weighted sum of pyramid functions defined on each vertex of barycentric refined mesh which lies on the i^{th} triangular cell of original mesh. If N_b is the number of barycentric refined mesh edges connected to each such vertex then the coefficient of each pyramid functions is given by $2/N_b$. For example, in Fig. 2b the vertex with coefficient $1/5$ has 10 barycentric edges connected to it. The coefficient of the pyramid function on the barycenter of the original triangular cell is 1. The dual patch basis functions ϕ_i^{bar} shown in Fig. 2a is defined on the barycentric refined triangular cells connected to the i^{th} vertex with constant value of $1/\sqrt{A^{bar}}$ (A^{bar} being the total area of these triangular cells) over them and 0 everywhere else.

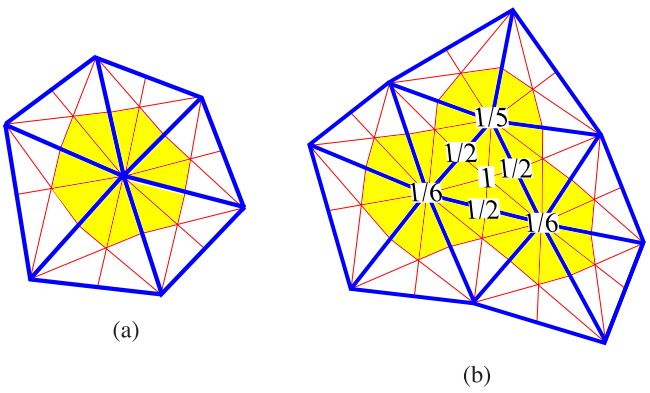

FIGURE 2. Basis functions defined on the dual mesh based on vertex and cell of the original mesh. (a) Dual patch. (b) Dual Pyramid.

From the definition of Loop functions, it can be easily seen that

$$\mathbf{x}^T\mathbf{\Lambda}^T\mathbf{\Lambda}\mathbf{x} \asymp \mathbf{x}^T\mathbf{\Lambda}^T\mathbf{G}\mathbf{\Lambda}\mathbf{x} = \langle\nabla_s\lambda_{\mathbf{x}}, \nabla_s\lambda_{\mathbf{x}}\rangle = \|\lambda_{\mathbf{x}}\|_{H^1(\Gamma)} \tag{13}$$

where $\lambda_{\mathbf{x}} = \sum_i \mathbf{x}_i\lambda_i$, and the first passage follows from the well-conditioning of the RWG Gram matrix $\mathbf{G}$. The previous expression makes evident that graph Laplacian is ill conditioned, since it is spectrally equivalent to the discretization of an operator of differential order 2 and thus gives rise to matrices with condition number growing as $O(h^2)$ (see also the treatment in [21]). Our aim is to find a multiplicative preconditioner $\mathbf{P}^\Lambda$ such that

$$\mathbf{x}^T(\mathbf{P}^\Lambda)^T\mathbf{\Lambda}^T\mathbf{\Lambda}\mathbf{P}^\Lambda\mathbf{x} \asymp \mathbf{x}^T\mathbf{x} \tag{14}$$

by using operators of opposite order. More specifically, for the hypersingular operator $\mathcal{N}$ it is known that

$$\langle\lambda_{\mathbf{x}}, \mathcal{N}(\lambda_{\mathbf{x}})\rangle = \mathbf{x}^T\mathbf{N}\mathbf{x} \asymp \|\lambda_{\mathbf{x}}\|_{H^{\frac{1}{2}}(\Gamma)}. \tag{15}$$

Since both direct and inverse inequalities are satisfied by the functions λ [37] we get

$$\mathbf{x}^T\mathbf{\Lambda}^T\mathbf{\Lambda}\mathbf{x} \asymp \mathbf{x}^T\mathbf{N}^T\mathbf{N}\mathbf{x}. \tag{16}$$

The left hand side of the well-known scalar Calderón identity

$$\mathcal{N}\mathcal{S} = -\frac{\mathcal{I}}{4} + \mathcal{K} \tag{17}$$

where $\mathcal{K}$ is a compact operator, can be stably discretized as

$$\mathbf{N}\mathbf{G}_{mix}^{-1}\mathbf{S} \tag{18}$$

where the mixed Gram matrix is defined as $(\mathbf{G}_{mix})_{i,j} = \langle\phi_i^{bar}, \lambda_j\rangle$ and where the single layer operator is discretized using dual patch basis functions, i.e. $(\mathbf{S})_{i,j} = \left\langle\phi_i^{bar}, \mathcal{S}(\phi_j^{bar})\right\rangle$. The identity (17) ensures the well-conditioning of (18) and thus the spectral equivalency

$$\mathbf{x}^T\mathbf{S}^T(\mathbf{G}_{mix}^{-1})^T\mathbf{N}^T\mathbf{N}\mathbf{G}_{mix}^{-1}\mathbf{S}\mathbf{x} \asymp \mathbf{x}^T\mathbf{x} \tag{19}$$

holds. Using equation (16) and (19) we get

$$\mathbf{x}^T\mathbf{S}^T(\mathbf{G}_{mix}^{-1})^T\mathbf{\Lambda}^T\mathbf{\Lambda}\mathbf{G}_{mix}^{-1}\mathbf{S}\mathbf{x} \asymp \tag{20}$$

$$\mathbf{x}^T\mathbf{S}^T(\mathbf{G}_{mix}^{-1})^T\mathbf{N}^T\mathbf{N}\mathbf{G}_{mix}^{-1}\mathbf{S}\mathbf{x} \asymp \mathbf{x}^T\mathbf{x}. \tag{21}$$

The overall regularized vertex based graph Laplacian is given by

$$\mathbf{S}^T(\mathbf{G}_{mix}^{-1})^T\boldsymbol{\Lambda}^T\boldsymbol{\Lambda}\mathbf{G}_{mix}^{-1}\mathbf{S} \tag{22}$$

from which it follows that

$$\mathbf{P}^{\Lambda} = \mathbf{G}_{mix}^{-1}\mathbf{S} \tag{23}$$

is a valid preconditioner for $\boldsymbol{\Lambda}^T\boldsymbol{\Lambda}$, i.e. $(\mathbf{P}^{\Lambda})^T\boldsymbol{\Lambda}^T\boldsymbol{\Lambda}\mathbf{P}^{\Lambda}$ is a well conditioned matrix.

Carrying the same analysis for the cell based graph Laplacian $\boldsymbol{\Sigma}^T\boldsymbol{\Sigma}$ accounts at finding the multiplicative preconditioner $\mathbf{P}^{\Sigma}$ such that

$$\mathbf{x}^T(\mathbf{P}^{\Sigma})^T\boldsymbol{\Sigma}^T\boldsymbol{\Sigma}\mathbf{P}^{\Sigma}\mathbf{x} \asymp \mathbf{x}^T\mathbf{x}. \tag{24}$$

Here we will use the fact that $\mathbf{x}^T\boldsymbol{\Sigma}^T\boldsymbol{\Sigma}\mathbf{x} \asymp \mathbf{x}^T\boldsymbol{\Sigma}^T\mathbf{G}_{BC}\boldsymbol{\Sigma}\mathbf{x} = \langle\nabla_s\lambda_{\mathbf{x}}^{bar}, \nabla_s\lambda_{\mathbf{x}}^{bar}\rangle = \|\lambda_{\mathbf{x}}^{bar}\|_{H^1(\Gamma)}$ (refer [21]) where $\lambda_{\mathbf{x}}^{bar} = \sum_i \mathbf{x}_i\lambda_i^{bar}$. The gram matrix $(\mathbf{G}_{BC})_{i,j} = \left\langle f_i^{BC}, f_j^{BC}\right\rangle$ is defined using Buffa-Christiansen basis functions [16], [36], [38]. The steps from equation (15) to (21) can be repeated to get the overall regularized cell based graph Laplacian given by

$$\tilde{\mathbf{S}}^T(\tilde{\mathbf{G}}_{mix}^{-1})^T\boldsymbol{\Sigma}^T\boldsymbol{\Sigma}\tilde{\mathbf{G}}_{mix}^{-1}\tilde{\mathbf{S}} \tag{25}$$

where the mixed Gram matrix is $(\tilde{\mathbf{G}}_{mix})_{i,j} = \left\langle\phi_i, \lambda_j^{bar}\right\rangle$ and single layer operator matrix is $(\tilde{\mathbf{S}})_{i,j} = \langle\phi_i, \mathcal{S}(\phi_j)\rangle$. Therefore, the preconditioning matrix

$$\mathbf{P}^{\Sigma} = \tilde{\mathbf{G}}_{mix}^{-1}\tilde{\mathbf{S}} \tag{26}$$

is a valid preconditioner for $\boldsymbol{\Sigma}^T\boldsymbol{\Sigma}$, i.e. $(\mathbf{P}^{\Sigma})^T\boldsymbol{\Sigma}^T\boldsymbol{\Sigma}\mathbf{P}^{\Sigma}$ is a well conditioned matrix.

Either of the graph Laplacians with their respective preconditioner matrices can be used in the spectral partitioning algorithm described in Appendix A to obtain connected partitions.

IV. PROPOSED REGULARIZATION: THE OPEN STRUCTURE CASE

When the structure Γ is open, the regularization above can be sub-optimal since (17) does not hold. A strategy to solve this issue is presented next.

The main idea for doing this is to bring back the problem of preconditioning the graph Laplacian on an open geometry to two subsequent closed geometry preconditioning problems, the second of which is one dimension less. More specifically, consider an open domain Γ which needs to be partitioned using a graph Laplacian matrix $\boldsymbol{\Lambda}_o^T\boldsymbol{\Lambda}_o$ (the subscript o is used to indicate that it is a graph Laplacian of an open geometry). The matrix is spectrally equivalent to $(\boldsymbol{\Lambda}_o^T\mathbf{G}\boldsymbol{\Lambda}_o)$, where $\mathbf{G}$ is the Gram matrix of RWG basis functions, which is well conditioned. Therefore $(\boldsymbol{\Lambda}_o^T\mathbf{G}\boldsymbol{\Lambda}_o)^{-1}\boldsymbol{\Lambda}_o^T\boldsymbol{\Lambda}_o$ can be inverted with few iterations of an iterative solver. This accounts for the need of performing efficiently the following inversion

$$\mathbf{u}_o = (\boldsymbol{\Lambda}_o^T\mathbf{G}\boldsymbol{\Lambda}_o)^{-1}\mathbf{f}_o, \tag{27}$$

for any given $\mathbf{f}_o$. We will now assume that $\mathbf{G}$ in $\boldsymbol{\Lambda}_o^T\mathbf{G}\boldsymbol{\Lambda}_o$ is defined on a plane, given that since Γ comes out of known geometry, if this is not the case a pull back (based on NURBS [39] for example) can always be used without recurring to mesh parameterization algorithms. Moreover, we easily and efficiently find a closed domain Ω such that $\Gamma \subset \Omega$ by cylindrical extrusion for example see Fig. 3. Solving (27) accounts of solving the Laplace-Beltrami operator [40] on a planar face of Γ with Dirichlet boundary conditions. We can then invert the Laplace-Beltrami operator on the entire close object Γ (where we can use the preconditioner developed above) and then correct the boundary conditions with the 2D single layer potential

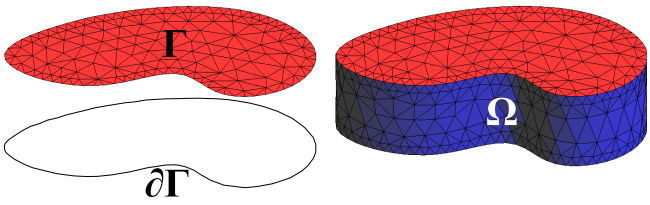

FIGURE 3. Domains used in the nested approach for open structures: a surface Γ with its corresponding closed domain Ω and its boudary $\partial\Gamma$.

$$\mathcal{V}_p(w(\boldsymbol{r})) = \int_{\partial\Gamma}\frac{-1}{2\pi}\log|\boldsymbol{r}-\boldsymbol{r}'|w(\boldsymbol{r}')d\boldsymbol{r}' \tag{28}$$

which is harmonic in Γ. An advantage of solving the Laplace-Beltrami operator over the close object rather than using the infinite solution as it is usually done in solving 2D integral equations is that $\mathbf{f}_o$ is naturally extended to be the right-hand-side of the overall problem and no further interpolation is necessary. In fact, define the sparse transformation matrices $\mathbf{T}$ as the map from vertices of closed structure to the non-boundary vertices of open structure

$$\mathbf{T}_{i,j} = \begin{cases} 1 & \text{if open structure non-boundary vertex } j \\ & \text{coincides with closed structure vertex } i, \\ 0 & \text{otherwise,} \end{cases} \tag{29}$$

and $\mathbf{B}$ as the map from vertices of closed structure to the boundary vertices of open structure

$$\mathbf{B}_{i,j} = \begin{cases} 1 & \text{if open structure boundary vertex } i \\ & \text{coincides with closed structure vertex } j \\ 0 & \text{otherwise} \end{cases} \tag{30}$$

The basis functions needed to discretize the 2D single layer operator and to define the Gram matrices are pulse and triangular basis functions. Each pulse basis function p_i is defined by

$$p_i(\boldsymbol{r}) = \begin{cases} 1 & \boldsymbol{r} \in \alpha\boldsymbol{r}_i + (1-\alpha)\boldsymbol{r}_{i+1} : \alpha \in (0,1) \\ 0 & \text{otherwise} \end{cases} \tag{31}$$

on the adjacent pair of vertices with coordinates $\boldsymbol{r}_i$ and $\boldsymbol{r}_{i+1}$. The triangular basis function t_i at a vertex with coordinates $\boldsymbol{r}_i$

is given by

$$t_i(\boldsymbol{r}) = \begin{cases} \frac{|\boldsymbol{r}_{i+1}-\boldsymbol{r}|}{|\boldsymbol{r}_{i+1}-\boldsymbol{r}_i|} & \boldsymbol{r} \in \alpha \boldsymbol{r_i} + (1-\alpha)\boldsymbol{r}_{i+1} : \alpha \in [0,1] \\ \frac{|\boldsymbol{r}_{i-1}-\boldsymbol{r}|}{|\boldsymbol{r}_{i-1}-\boldsymbol{r}_i|} & \boldsymbol{r} \in \alpha \boldsymbol{r}_{i-1} + (1-\alpha)\boldsymbol{r}_i : \alpha \in [0,1] \\ 0 & \text{otherwise} \end{cases} \quad (32)$$

where $\boldsymbol{r_i}$ is the vertex adjacent to both $\boldsymbol{r}_{i-1}$ and $\boldsymbol{r}_{i+1}$. The single layer operator equation (28) on $\partial\Gamma$ when discretized using pulse basis functions gives $(\mathbf{V}_p)_{i,j} = \langle p_i, \mathcal{V}_p(p_j)\rangle$. The operator matrix $(\mathbf{V}_{\delta p})_{i,j} = \langle \delta_i, \mathcal{V}_p(p_j)\rangle$ brings the correction of boundary conditions on Γ. δ is the delta function defined on the inner vertices of Γ. The mixed pulse-triangular basis Gram matrix $(\mathbf{G}_{p,t})_{i,j} = \langle p_i, t_j\rangle$ is obtained using pulse basis p and triangular basis t defined on the boundary vertices of open structure.

The overall RHS $\mathbf{f}_c$ over the closed domain will be $\mathbf{f}_c = (\mathbf{T} - \mathbf{1e}_i)^T \mathbf{f}_o$ where $\mathbf{e}_i$ is the canonical basis element in the row vector space of $\mathbf{T}$ such that $\mathbf{T}(:, i) = \mathbf{0}$. Moreover, up to the discretization precision, the inverse in (27) can be computed as

$$\mathbf{u}_o = \mathbf{T}\mathbf{u}_c - \mathbf{u}_H \quad (33)$$

where $\mathbf{u}_c = (\mathbf{\Lambda}^T \mathbf{G} \mathbf{\Lambda})^+ \mathbf{f}_c$ and where $\mathbf{u}_H = \mathbf{V}_{\delta p}\mathbf{V}_p^{-1}\mathbf{G}_{p,t}\mathbf{B}\mathbf{u}_c$ is a harmonic correction. Overall

$$\mathbf{u}_o = \left(\mathbf{T} - \mathbf{V}_{\delta p}\mathbf{V}_p^{-1}\mathbf{G}_{p,t}\mathbf{B}\right)(\mathbf{\Lambda}^T \mathbf{G} \mathbf{\Lambda})^+ (\mathbf{T} - \mathbf{1e}_i)^T \mathbf{f}_o \quad (34)$$

so that the preconditioning matrix is selected as

$$\mathbf{P}_o = \left(\mathbf{T} - \mathbf{V}_{\delta p}\mathbf{V}_p^{-1}\mathbf{G}_{p,t}\mathbf{B}\right)(\mathbf{\Lambda}^T \mathbf{G} \mathbf{\Lambda})^+ (\mathbf{T} - \mathbf{1e}_i)^T \quad (35)$$

note that $\mathbf{P}_o$ is never formed explicitly, it is instead always applied multiplicatively and, in particular, the two (pseudo) inverses $(\mathbf{\Lambda}^T \mathbf{G} \mathbf{\Lambda})^+$ and $\mathbf{V}_p^{-1}$ are always preconditioned.

More specifically, if the operator $\mathcal{W}_p$ represents 2D hyper-singular operator given by

$$\mathcal{W}_p(w(\boldsymbol{r})) = \partial_{\boldsymbol{n}} \int_{\partial\Gamma} \partial'_{\boldsymbol{n}'} \frac{-1}{2\pi} \log|\boldsymbol{r} - \boldsymbol{r}'| w(\boldsymbol{r}') d\boldsymbol{r}' \quad (36)$$

where $\partial_{\boldsymbol{n}} = \boldsymbol{n} \cdot \frac{\partial}{\partial \boldsymbol{r}}$ then the a 2D counterpart [40] of the Calderón identity (17) reads

$$\mathcal{W}_p \mathcal{V}_p = -\frac{\mathcal{I}}{4} + \mathcal{D} \quad (37)$$

and it can be used to apply the regularization of the discretized matrix $(\mathbf{V}_p)$. In fact, the discretization of the 2D hyper-singular operator needs dual triangular basis functions like those proposed in [41]. The domain of this triangular basis can be seen in Fig. 4 where the crosses are placed at the midpoint of the edge connecting the nodes. If the original mesh consists of nodes represented by $\boldsymbol{r}$ and the dual mesh consists of cross represented by $\boldsymbol{d}$, then let $\boldsymbol{r}_{i-1}$, $\boldsymbol{d}_{i-1}$, $\boldsymbol{r}_i$, $\boldsymbol{d}_i$, $\boldsymbol{r}_{i+1}$, $\boldsymbol{d}_{i+1}$ and $\boldsymbol{r}_{i+2}$ be the coordinates of the vertices moving from left to right through the boundary mesh. The dual triangular function

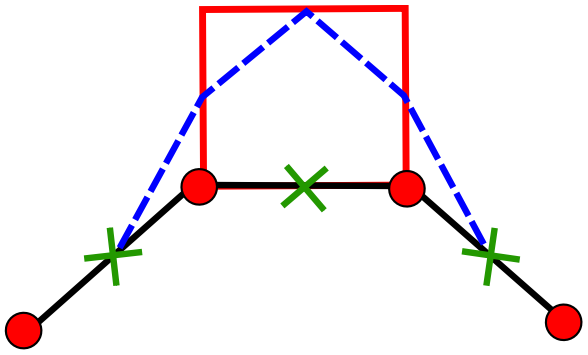

FIGURE 4. Triangular basis functions on the dual mesh (dashed blue line) and constant basis function on the standard mesh (red line).

(refer also to Fig. 4) is defined as

$$t_i^*(\boldsymbol{r}) = \begin{cases} \frac{|\boldsymbol{d}_{i+1}-\boldsymbol{r}|}{2|\boldsymbol{d}_{i+1}-\boldsymbol{r}_{i+1}|} & \boldsymbol{r} \in \alpha r_i + 1 + (1-\alpha)\boldsymbol{d}_{i+1} : \\ & \alpha \in [0,1] \\ \frac{1}{2} + \frac{|\boldsymbol{r}_{i+1}-\boldsymbol{r}|}{2|\boldsymbol{r}_{i+1}-\boldsymbol{d}_i|} & \boldsymbol{r} \in \alpha \boldsymbol{d_i} + (1-\alpha)\boldsymbol{r}_{i+1} : \alpha \in [0,1] \\ \frac{1}{2} + \frac{|\boldsymbol{r}_i-\boldsymbol{r}|}{2|\boldsymbol{r}_i-\boldsymbol{d}_i|} & \boldsymbol{r} \in \alpha \boldsymbol{r}_i + (1-\alpha)\boldsymbol{d}_i : \alpha \in [0,1] \\ \frac{|\boldsymbol{d}_{i-1}-\boldsymbol{r}|}{2|\boldsymbol{d}_{i-1}-\boldsymbol{r}_i|} & \boldsymbol{r} \in \alpha \boldsymbol{d}_{i-1} + (1-\alpha)\boldsymbol{r}_i : \alpha \in [0,1] \\ 0 & \text{otherwise} \end{cases} \quad (38)$$

The left hand side of equation (37) results in the following well conditioned matrix $\mathbf{W}_p\mathbf{G}_{p,t^*}^{-1}\mathbf{V}_p$ where the discretized 2D hyper-singular operator matrix $(\mathbf{W}_p)_{i,j} = \langle t_i^*, \mathcal{W}_p(t_j^*)\rangle$ is linked with the mix Gram matrix $(\mathbf{G}_{p,t^*})_{i,j} = \langle p_i, t_j^*\rangle$ defined using pulse basis function and the dual triangular basis function. So $\mathbf{P}_t = \mathbf{W}_p\mathbf{G}_{p,t^*}^{-1}$ is a left preconditioner for $\mathbf{V}_p$, i.e. $\mathbf{P}_t\mathbf{V}_p$ is a well conditioned matrix.

V. NUMERICAL RESULTS

The effect of the proposed regularization scheme for the graph Laplacian is firstly tested on a sphere of radius 1m. In Fig. 5,

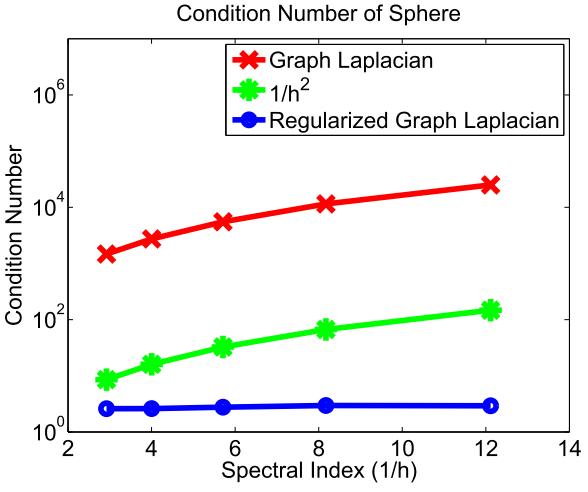

FIGURE 5. Condition number (closed structure).

the condition number of the graph Laplacian $\mathbf{\Sigma}^T\mathbf{\Sigma}$ is plotted for different values of the spectral index $1/h$ and compared with the condition number of the regularized operator. It is clear that the condition number of the graph Laplacian grows quadratically as a function of the spectral index, while the regularized operator shows a constant conditioning as expected from the theory. The impact of this on the iterative inversion of the graph Laplacian is shown in Fig. 6 where the number of iterations are plotted against the number of unknowns for both standard and regularized graph Laplacian. The relative error for the iterative solver is 10^{-5} and the number of unknowns is varied between 250 and 1 million. An ACA algorithm [42] is used for compressing the regularizer, with compression precision of 10^{-6}. It is clear that the regularized graph Laplacian can be iteratively inverted in a constant number of iterations, independently of the number of unknowns, while an increasingly high number of iterations are required for inverting the standard graph Laplacian, as expected from the theory.

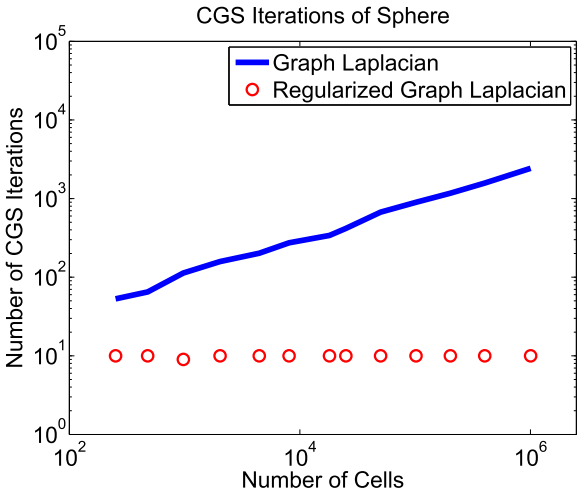

FIGURE 6. CGS iterations (closed structure).

We have applied our method to perform spectral partitioning of models of a space shuttle and of a ship. For both models, the tolerance error of subspace iteration, CGS iterations and ACA is set to 10^{-2}, 10^{-5} and 10^{-6} respectively. As expected, the spectral partitioning produces connected partitions (represented by different colors) as shown in the Fig. 7 and 8.

In the case of the space shuttle, the subspace method took 7 iterations to converge. The number of CGS iterations to invert graph Laplacian using regularization was brought down from 1167 to 50. The ship model partitioning algorithm took 12 subspace iterations to converge and the number of CGS iterations using regularization decreased from 1222 to 85. When comparing the spectrally obtained and a standard octree [5] obtained partitions produced for the ship model in Fig. 9 and 10, we see that spectral partitioning produces connected partitions whereas the octree partitions are disconnected. This exemplifies one of the advantages of using spectral partitioning over other techniques; connectivity

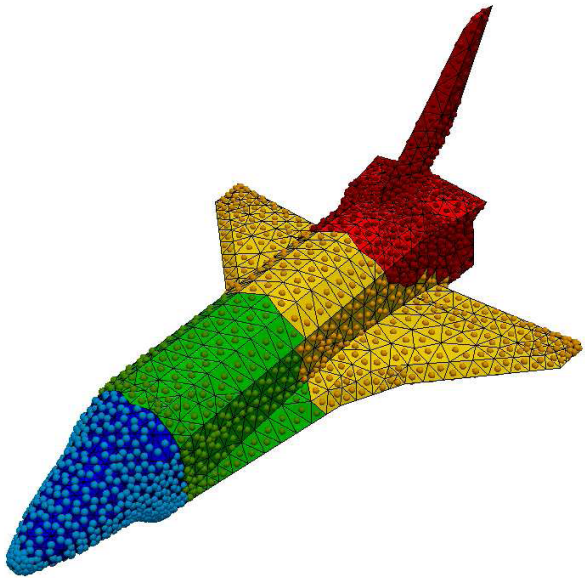

FIGURE 7. Spectral partitioning of a shuttle model.

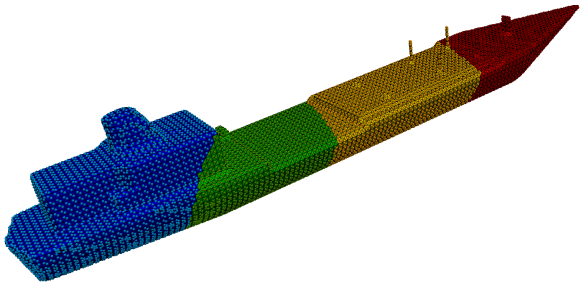

FIGURE 8. Spectral partitioning of a ship model.

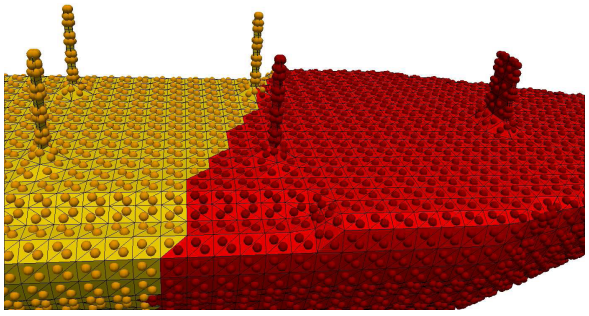

FIGURE 9. Spectral partitions of ship's deck.

in fact is required by many techniques requiring the partitioning of a domain.

The regularization approach for an open structure was tested on a square plate of dimension 1×1m. In this case we partitioned the vertex based mesh (thus we inverted the graph Laplacian $\mathbf{\Lambda}^T\mathbf{\Lambda}$). The number of iterative solver's iterations is shown in Fig. 11. It is clear that also in this case the regularization effect is indeed achieved as expected by the theory since the number of iterations stays constant irrespective of the dimension of the problem. If the closed structure regularization technique is applied to the square plate, we

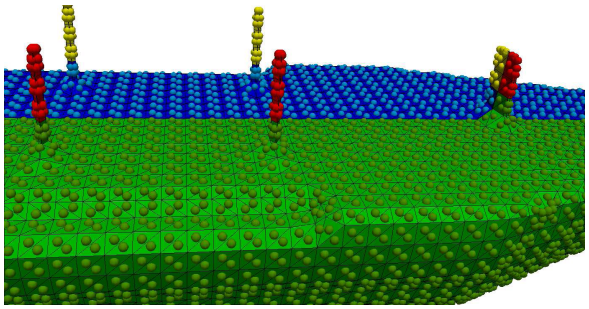

FIGURE 10. Octree partitions of ship's deck.

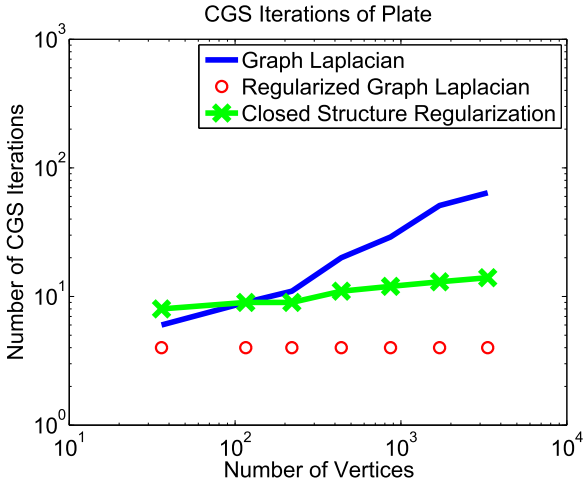

FIGURE 11. CGS iterations (open structure).

see that the number of iterations, although decreased, is still varying with the discretization density.

VI. CONCLUSION

A new regularization technique for graph Laplacians arising from triangular meshes of closed and open structures has been presented. The ill-conditioned behavior of graph Laplacian matrices is neutralized by exploiting scalar Calderón identities and operators of opposite differential strength. A new 3D/2D nested regularization strategy has been presented to deal with open geometries. Finally, numerical results have shown the effectiveness of the proposed regularization as well as its applicability to real case scenarios when used in spectral partitioning applications.

APPENDIX
SPECTRAL PARTITIONING

Given a Graph Laplacian with vertices indexed by $i = 1, \ldots, N$, Spectral Partitioning aims at dividing the vertices in two sets giving rise to two connected subgraphs. Spectral partitioning is based on the following strategy [6]:

1) Compute the singular vector $\mathbf{V}$ associated to the second smallest singular value of a graph Laplacian
2) Separate the indices of the Laplacian matrix in the two groups: $\mathbf{I}^+ = \{i : \mathbf{V}_i \geq 0\}$ and $\mathbf{I}^- = \{i : \mathbf{V}_i \leq 0\}$

Algorithm 1 Subspace Iteration Method for Graph Laplacian

$\mathbf{L}^T\mathbf{L} = \mathbf{L}^T\mathbf{L} + \frac{\mathbf{1}\mathbf{1}^T}{n^2}$
$\mathbf{X}_k = \mathbf{I}_{n\times p}$
$\mathbf{S}_k = 0$
while $tol < err$ **do**
  for $i = 0$ to p **do**
    $\mathbf{b} = \mathbf{P}^T\mathbf{X}_k(:, i)$
    $\mathbf{x} = \text{cgs}(\mathbf{P}^T\mathbf{L}^T\mathbf{L}\mathbf{P}, \mathbf{b})$
    $\mathbf{X}_{k+1}(:, i) = \mathbf{P}\mathbf{x}$
    $\mathbf{X}_{k+1}(:, i) = \frac{\mathbf{X}_{k+1}(:,i)}{\text{norm}(\mathbf{X}_{k+1}(:,i),2)}$
  end for
  $\mathbf{A}_{k+1} = \mathbf{X}_{k+1}^T\mathbf{L}^T\mathbf{L}\mathbf{X}_{k+1}$
  $\mathbf{I}_{k+1} = \mathbf{X}_{k+1}^T\mathbf{X}_{k+1}$
  $[\mathbf{V}_{k+1}, \mathbf{S}_{k+1}] = \text{eig}(\mathbf{A}_{k+1}, \mathbf{I}_{k+1})$
  $\text{err} = \frac{\text{norm}(\mathbf{S}_{k+1}-\mathbf{S}_k)}{\text{norm}(\mathbf{S}_k)}$
  $\mathbf{S}_k = \mathbf{S}_{k+1}$
  $\mathbf{X}_k = \mathbf{X}_{k+1}\mathbf{V}_{k+1}$
end while

for which it can be proved that the graphs associated to the two groups are connected [6]. In practice, one of the most common algorithms to obtain the required singular vector is the subspace iteration method [43], it represents a block generalization of the the simple inverse power method. The reason for using a block scheme is that the naive inverse power algorithm behaves very poorly in case of non unitary multiplicity of the eigenvalues. A 3-dimensional manifold can show multiplicities of the second-last eigenvalues up to 3, so that 4-block subspace iteration method must be used to ensure the convergence of the scheme.

In our case, we are interested in finding the $p = 3$ eigenvectors $(\mathbf{X})_{n\times p}$ corresponding to the p smallest eigenvalues of the graph Laplacian $\mathbf{L}^\mathbf{T}\mathbf{L}$ of dimension $n \times n$ where $\mathbf{L} = \mathbf{\Sigma}$ or $\mathbf{L} = \mathbf{\Lambda}$. Algorithm 1 presents a synthetic and implementation-oriented description of the subspace iteration method adapted to our case. In the algorithms the p smallest eigenvalues are stored stored in $\mathbf{S}_k$ and the corresponding eigenvectors are stored in $\mathbf{X}_k$ once a tolerance level has been achieved. The eigenvector $\mathbf{X}_k(:, p-1)$ corresponding to second smallest eigenvalue is selected and the cells of the mesh are partitioned in two sets $\mathbf{I}^+$ and $\mathbf{I}^-$. If $\mathbf{X}_k(i, p-1) > 0$ then the i^{th} cell is assigned to $\mathbf{I}^+$ otherwise it is assigned to $\mathbf{I}^-$ and we obtain connected graphs associated with two sets. Notice that the graph Laplacian is preconditioned with the matrix $\mathbf{P}$ whose choice depends on the type of graph Laplacian (see Section III).

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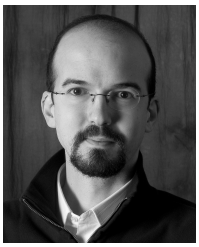

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