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NUMERICAL SOLUTION OF BI-PERIODIC ELLIPTIC PROBLEMS IN UNBOUNDED DOMAINS*

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Abstract. This paper aims at an efficient numerical approach for bi-periodic elliptic problems with local defects in unbounded domains. We employ the methodology of artificial boundary methods and try to design an accurate boundary condition in the form of a Dirichlet-to-Neumann (DtN) map. The key issue is how to take advantage of periodicity as much as possible. We develop an approach of computing the DtN map based on the DtN gluing and homogenization techniques, and prove the unique solvability of the resulting discrete variational problem. Numerical evidence validates the effectiveness of the proposed method.

Key words. Periodic structure, DtN homogenization, DtN gluing, artificial boundary method.

AMS subject classifications. 35J55, 65N30.

1. Introduction

Periodic media play an important role in many applications such as optics and material science. When the number of periodic cells is huge, a domain-based discretization method directly using the details of each periodic cell could be too demanding and even hopeless. However, if the size of periodic cell is relatively small, one can apply the homogenization theory [2], either directly or indirectly, to develop a PDE solver which is asymptotically valid for the large scale homogenized equation. We say that this kind of numerical method is homogenization-based. So far, the validity of homogenization-based methods strongly relies on the scale separation of the exact solution. In more realistic applications, unfortunately, this precondition is generally violated since the media are not perfectly periodic and the defects appear in some local regions. In this case, a full continuous set of scales might get involved, which renders the homogenization-based methods either inaccurate or not applicable. New ideas should be developed for this kind of problem.

In this paper, we are concerned with the numerical strategy for a particular instance of the above defect problems: the exterior elliptic problem with bi-periodic variable coefficients of the form

$$-\nabla\cdot(\mathbf{A}(x)\nabla u)+a_0(x)u=0,\ \forall x\in\mathbb{R}^2\backslash\bar{D}, \tag{1.1}$$

$$u(x)=g(x),\ \forall x\in\partial D, \tag{1.2}$$

$$\int_{\mathbb{R}^2\backslash\bar{D}}|\nabla u|^2dx<\infty, \tag{1.3}$$

where $g\in H^{\frac{1}{2}}(\partial D)$, $a_0(x)$ is a nonnegative scalar function, and $\mathbf{A}$ is a symmetric matrix-valued function such that for two positive constants α and β,

$$\alpha|\xi|^2\le\xi\cdot\mathbf{A}(x)\xi\le\beta|\xi|^2,\ \forall x\in\mathbb{R}^2,\ \forall\xi\in\mathbb{R}^2. \tag{1.4}$$

We use the notation $C_{00}=(-0.5,0.5)^2$ and assume $D\subset C_{00}$ is a Lipschitz domain. We suppose $\mathbf{A}$ and c are bi-periodic with period of 1 except on the *defect cell* C_{00}. More

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precisely, for any $m,n\in\mathbb{Z}$ and $x=(x_1,x_2)\in\mathbb{R}^2$ with $x\notin C_{00}$ and $(x_1+m,x_2+n)\notin C_{00}$, we assume

$$\mathbf{A}(x_1+m,x_2+n)=\mathbf{A}(x_1,x_2),\ c(x_1+m,x_2+n)=c(x_1,x_2).$$

According to the analysis in [11], there exist a constant u_∞ and two positive constants C and δ such that for sufficiently large x, the solution of (1.1)-(1.3) satisfies

$$|u(x)-u_\infty|\le C|x|^{-\delta}. \tag{1.5}$$

This implies that the solution of (1.1) with a finite Dirichlet integral tends to a constant when the location point is far away from the coordinate origin. For instance, if $\mathbf{A}(x)=I_{2\times 2}$ and $c(x)=0$, then $\delta=1$, and if $c(x)\ge c_0>0$, then $u_\infty=0$ and δ can be made arbitrarily large since the solution decays exponentially fast at infinity.

Since the definition domain is an exterior region, the problem (1.1)-(1.3) is a so-called unbounded domain problem. If one is interested in the numerical behavior of such problems, a common practice is to introduce some suitable artificial boundary and confine the computation to a bounded domain. For the considered problem, a natural choice of this artificial boundary is the defect cell boundary ∂C_{00}. If the exact Dirichlet-to-Neumann (DtN) map on ∂C_{00}, denoted by $\mathcal{K}$, is derived for the governing Equation (1.1) on the residual unbounded domain $\mathbb{R}^2\backslash\bar{C}_{00}$, the solution of the problem

$$-\nabla\cdot(\mathbf{A}(x)\nabla u)+a_0(x)u=0,\ \forall x\in C_{00}\backslash\bar{D}, \tag{1.6}$$

$$u(x)=g(x),\ \forall x\in\partial D, \tag{1.7}$$

$$\mathbf{n}\cdot(\mathbf{A}(x)\nabla u(x))+\mathcal{K}[u|_{\partial C_{00}}](x)=0,\ \forall x\in\partial C_{00}, \tag{1.8}$$

will be the same as that of the original problem (1.1)-(1.3) restricted to the bounded domain $C_{00}\backslash\bar{D}$. Here $\mathbf{n}$ denotes the unit normal directed into $\mathbb{R}^2\backslash\bar{C}_{00}$. A suitable numerical method is then employed to compute the solution of the truncated domain problem (1.6)-(1.8).

The key ingredient of the above practice is the determination of the DtN map $\mathcal{K}$. This issue has been a research subject for nearly forty years under various problem settings. However, the closed form of this map is only available for some PDEs in special geometries. In general, a good approximation is the best one could expect. The readers are referred to [1, 7, 8, 9, 12] for some nice review papers. As far as the periodic structure problems are concerned, an analytical expression for the scattering operator in the form of a DtN map was presented in [13] for the one-dimensional Schrödinger equation with sinusoidal potential. Later this expression was extended to more general second-order ODE problems [5] in the case that the coefficient functions are symmetric. The DtN map for general one-dimensional periodic arrays was considered in [10, 3, 4]. Instead of seeking a closed form analytical expression, the authors of [10, 3, 4] proposed some viable algorithms for computing the DtN map in the discrete form. The underlying ideas had been further extended for bi-periodic structure problems in [6, 3].

In this paper, we propose a new approach of approximating the DtN map of bi-periodic elliptic problems by taking (1.1)-(1.3) as an example. Let us indicate G_n as the union of a $3^n\times 3^n$ bi-periodic array centered at the origin. It holds that $G_0=C_{00}$, $G_0\subset G_1\subset G_2\subset\cdots$, and $\lim_{n\to\infty}G_n=\mathbb{R}^2$. Put $D_n=G_{n+1}\backslash\bar{G}_n$. Then $\{D_n\}_{n=0}^{\infty}$ forms a non-overlapping decomposition of the residual domain $\mathbb{R}^2\backslash\bar{C}_{00}$; see Figure 1.1.

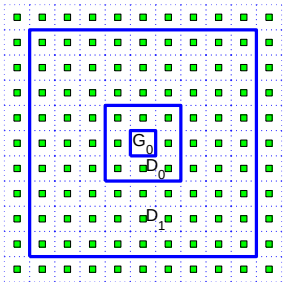

FIG. 1.1. *The residual unbounded domain* $\mathbb{R}^2\backslash\bar{C}_{00}=\mathbb{R}^2\backslash\bar{G}_0$ *is decomposed into a sequence of similar bounded domains* $\{D_n\}_{n=0}^{\infty}$. *Each* D_n *consists of eight identical cells or super-cells. Here* $G_0=C_{00}$ *denotes the defect cell.*

Confined to any D_n with $n\geq 0$, the governing Equation (1.1) is well-posed provided the Dirichlet boundary conditions are specified on the two disjointed boundaries ∂G_n and ∂G_{n+1}. A DtN map, denoted by $\mathcal{K}_{D_n}$, is thus uniquely determined. Setting the Dirichlet and Neumann data as

$$u_{n,D}=u|_{\partial G_n},\ u_{n,N}=\mathbf{n}\cdot\mathbf{A}(x)\nabla u(x)|_{\partial G_n},$$

with $\mathbf{n}$ being the unit normal directed to the exterior of G_n, we have

$$\begin{pmatrix}-u_{n,N}\\ u_{n+1,N}\end{pmatrix}=\mathcal{K}_{D_n}\begin{pmatrix}u_{n,D}\\ u_{n+1,D}\end{pmatrix},\ n=0,1,\cdots. \tag{1.9}$$

Note that $\mathcal{K}_{D_n}$ is non-negative in the sense that

$$\langle\mathcal{K}_{D_n}u|_{\partial D_n},u|_{\partial D_n}\rangle=\int_{\partial D_n}(\mathbf{n}\cdot\mathbf{A}(x)\nabla u(x))u(x)ds=\int_{D_n}\left[\nabla u\cdot\mathbf{A}(x)\nabla u+a_0(x)u^2\right]dx\geq 0.$$

After $\mathcal{K}_{D_n}$ has been determined, the DtN map on $\cup_{n=0}^{L}D_n=G_{L+1}\backslash\bar{C}_{00}$ for any $L\geq 1$ can be derived by the following *gluing procedure*. Take the case $L=1$ as an example. Rewriting $\mathcal{K}_{D_0}$ and $\mathcal{K}_{D_1}$ into the block form $(\mathcal{A}_{ij})$ and $(\mathcal{B}_{ij})$, we have

$$\begin{pmatrix}-u_{0,N}\\ u_{1,N}\end{pmatrix}=\begin{pmatrix}\mathcal{A}_{11}&\mathcal{A}_{12}\\ \mathcal{A}_{21}&\mathcal{A}_{22}\end{pmatrix}\begin{pmatrix}u_{0,D}\\ u_{1,D}\end{pmatrix},\ \begin{pmatrix}-u_{1,N}\\ u_{2,N}\end{pmatrix}=\begin{pmatrix}\mathcal{B}_{11}&\mathcal{B}_{12}\\ \mathcal{B}_{21}&\mathcal{B}_{22}\end{pmatrix}\begin{pmatrix}u_{1,D}\\ u_{2,D}\end{pmatrix}$$

or, equivalently,

$$-u_{0,N}=\mathcal{A}_{11}u_{0,D}+\mathcal{A}_{12}u_{1,D}, \tag{1.10}$$
$$u_{1,N}=\mathcal{A}_{21}u_{0,D}+\mathcal{A}_{22}u_{1,D}, \tag{1.11}$$
$$-u_{1,N}=\mathcal{B}_{11}u_{1,D}+\mathcal{B}_{12}u_{2,D}, \tag{1.12}$$
$$u_{2,N}=\mathcal{B}_{21}u_{1,D}+\mathcal{B}_{22}u_{2,D}. \tag{1.13}$$

Adding (1.11) and (1.12) together yields

$$u_{1,D}=-(\mathcal{A}_{22}+\mathcal{B}_{11})^{-1}(\mathcal{A}_{21}u_{0,D}+\mathcal{B}_{12}u_{2,D}). \tag{1.14}$$

The invertibility of $\mathcal{A}_{22}+\mathcal{B}_{11}$ is ensured by the well-posedness of governing Equation (1.1) in conjunction with the Dirichlet boundary conditions on ∂G_0 and ∂G_2.

Substituting (1.14) into (1.10) and (1.13) gives

$$-u_{0,N} = \left[\mathcal{A}_{11} - \mathcal{A}_{12}(\mathcal{A}_{22}+\mathcal{B}_{11})^{-1}\mathcal{A}_{21}\right] u_{0,D} - \mathcal{A}_{12}(\mathcal{A}_{22}+\mathcal{B}_{11})^{-1}\mathcal{B}_{12}u_{2,D}, \quad (1.15)$$

$$u_{2,N} = -\mathcal{B}_{21}(\mathcal{A}_{22}+\mathcal{B}_{11})^{-1}\mathcal{A}_{21}u_{0,D} + \left[\mathcal{B}_{22} - \mathcal{B}_{21}(\mathcal{A}_{22}+\mathcal{B}_{11})^{-1}\mathcal{B}_{12}\right] u_{2,D}, \quad (1.16)$$

which implies

$$\mathcal{K}_{D_0\cup D_1} = \begin{pmatrix} \mathcal{A}_{11} - \mathcal{A}_{12}(\mathcal{A}_{22}+\mathcal{B}_{11})^{-1}\mathcal{A}_{21} & -\mathcal{A}_{12}(\mathcal{A}_{22}+\mathcal{B}_{11})^{-1}\mathcal{B}_{12} \\ -\mathcal{B}_{21}(\mathcal{A}_{22}+\mathcal{B}_{11})^{-1}\mathcal{A}_{21} & \mathcal{B}_{22} - \mathcal{B}_{21}(\mathcal{A}_{22}+\mathcal{B}_{11})^{-1}\mathcal{B}_{12} \end{pmatrix}.$$

For $L \geq 2$, the DtN map $\mathcal{K}_{D_0\cup\cdots\cup D_L}$ is derived by repeating the above gluing procedure L times.

Since the size of domain G_L grows exponentially fast with respect to L, in terms of (1.5), we can terminate the gluing procedure for a moderately large L and impose the homogeneous Neumann boundary condition at ∂G_{L+1}. Rewriting $\mathcal{K}_{D_0\cup\cdots\cup D_L}$ into a block form $(\mathcal{C}_{ij,L})$ we have

$$\begin{pmatrix} -u_{0,N} \\ u_{L+1,N} \end{pmatrix} = \begin{pmatrix} \mathcal{C}_{11,L} & \mathcal{C}_{12,L} \\ \mathcal{C}_{21,L} & \mathcal{C}_{22,L} \end{pmatrix} \begin{pmatrix} u_{0,D} \\ u_{L+1,D} \end{pmatrix}, \; u_{L+1,N} = 0.$$

From these equations we derive

$$-u_{0,N} = \mathcal{K}_L u_{0,D}, \; \mathcal{K}_L = \mathcal{C}_{11,L} - \mathcal{C}_{12,L}\mathcal{C}_{22,L}^{-1}\mathcal{C}_{21,L}.$$

The operator $\mathcal{K}_L$ gives an approximation of the exact DtN map $\mathcal{K}$ on ∂G_0, and $\lim_{L\to\infty}\mathcal{K}_L = \mathcal{K}$ in a suitable sense.

Intuitively, the above idea of deriving an approximate DtN map is not limited to the considered periodic structure problems, and is seemingly applicable in a much more general case. Practically, however, unless some symmetry is prescribed in the problem setting, this idea is of no use since the computational cost of the DtN map in a large domain is very expensive for a general variable coefficient problem. Fortunately, the problem considered in this paper fulfills the symmetry requirement perfectly; the whole domain consists of identical periodic cells except only one defect cell. In this special case, the DtN map on the large domain can be derived very efficiently. For example, after the DtN map on a single periodic cell has been derived, the DtN map $\mathcal{K}_{D_0}$ can be computed by gluing together 8 single cell DtN maps. The domain D_1 consists of $9\times 8 = 72$ periodic cells, much more than D_0 does. However, if the DtN map on a super-cell, a 3×3 bi-periodic array, has been derived successfully, one can compute $\mathcal{K}_{D_1}$ by merely gluing 8 super-cell DtN maps. The computation of other $\mathcal{K}_{D_n}$ is analogous. We will study these technical issues in detail in the next section.

2. Discrete approximation of the DtN map

Given a bounded Lipschitz domain $\Omega \subset \mathbb{R}^2 \backslash \bar{C}_{00}$, set

$$a_\Omega(u,v) \stackrel{def}{=} (\mathbf{A}(x)\nabla u, \nabla v)_\Omega + (a_0(x)u, v)_\Omega, \; \forall u, v \in H^1(\Omega). \quad (2.1)$$

According to the Assumption (1.4), $a_\Omega(\cdot,\cdot)$ defines a bounded symmetric bilinear form on $H^1(\Omega)$. For any $f \in H^{\frac{1}{2}}(\partial\Omega)$, let us consider the minimization problem

$$J_{\partial\Omega}(f) \stackrel{def}{=} \inf_{v|_{\partial\Omega}=f, v\in H^1(\Omega)} \frac{a_\Omega(v,v)}{2}. \quad (2.2)$$

By Dirichlet's principle, the infimum is attained by $\mathcal{S}(f)\in H^1(\Omega)$ which uniquely solves the following variational problem:
Find $u\in H^1(\Omega)$ with $u|_{\partial\Omega}=f\in H^{\frac{1}{2}}(\partial\Omega)$ such that

$$a_\Omega(u,v)=0,\ \forall v\in H_0^1(\Omega). \tag{2.3}$$

Therefore, it holds that

$$J_{\partial\Omega}(f)=\frac{a_\Omega(\mathcal{S}(f),\mathcal{S}(f))}{2}.$$

The variation of $J_{\partial\Omega}$ is

$$<\delta J_{\partial\Omega}(f),g>_{\partial\Omega}=a_\Omega(\mathcal{S}(f),\mathcal{S}(g)),\ \forall g\in H^{\frac{1}{2}}(\partial\Omega),$$

which implies that $\delta J_{\partial\Omega}$ is simply the DtN map $\mathcal{K}_\Omega$ on the domain Ω.

Let $\mathcal{B}_{\partial\Omega}^h$ be a boundary triangulation of $\partial\Omega$ with the characteristic mesh size h, and $\mathcal{T}_\Omega^h$ a triangulation of Ω by triangles and/or rectangles compatible with $\mathcal{B}_{\partial\Omega}^h$. Let P_k denote the polynomials of total degree k, and Q_k the polynomials of maximum degree k for each spatial variable. If $T\in\mathcal{T}_\Omega^h$ is a triangle, put $V(T)=P^k(T)$, and if T is a rectangle, put $V(T)=Q^k(T)$. Set

$$\begin{aligned} V_\Omega^h&=\left\{v\in\mathcal{C}(\bar{\Omega}):v|_T\in V(T),\forall T\in\mathcal{T}_\Omega^h\right\},\\ B_{\partial\Omega}^h&=\left\{w\in\mathcal{C}(\partial\Omega):w|_e\in P_k(e),\forall e\in\mathcal{B}_{\partial\Omega}^h\right\}. \end{aligned} \tag{2.4}$$

For any $f^h\in B_{\partial\Omega}^h$, let us consider the discrete counterpart of the minimization problem (2.2):

$$J_{\partial\Omega}^h(f^h)=\inf_{v|_{\partial\Omega}=f^h,\,v\in V_\Omega^h}\frac{a_\Omega(v,v)}{2}. \tag{2.5}$$

The infimum is attained by $\mathcal{S}^h(f^h)\in V_\Omega^h$, which uniquely solves the following discrete variational problem:
Find $u^h\in V_\Omega^h$ with $u^h|_{\partial\Omega}=f^h$ such that

$$a_\Omega(u^h,v)=0,\ \forall v\in V_\Omega^h \text{ with } v|_{\partial\Omega}=0. \tag{2.6}$$

Similar to the continuous case, it holds that

$$J_{\partial\Omega}^h(f^h)=\frac{a_\Omega(\mathcal{S}^h(f^h),\mathcal{S}^h(f^h))}{2}. \tag{2.7}$$

The variation of $J_{\partial\Omega}^h$ is

$$(\delta J_{\partial\Omega}^h(f^h),g^h)_{\partial\Omega}=a_\Omega(\mathcal{S}^h(f^h),\mathcal{S}^h(g^h)),\ \forall g^h\in B_{\partial\Omega}^h. \tag{2.8}$$

Therefore, $\delta J_{\partial\Omega}^h$ gives a discrete approximation of the exact DtN map $\delta J_{\partial\Omega}=\mathcal{K}_\Omega$. Note that by setting $\mathcal{K}_\Omega^h=\delta J_{\partial\Omega}^h$, we have

$$J_{\partial\Omega}^h(f^h)=\frac{(\mathcal{K}_\Omega^h f^h,f^h)_{\partial\Omega}}{2}. \tag{2.9}$$

2.1. Single cell DtN map. In this part we compute the discrete DtN map $\mathcal{K}_C^h$ for a single periodic cell C. More precisely, we will compute the matrix representation of $\mathcal{K}_C^h$ under a suitable set of basis functions. Here and hereafter, by matrix representation of an operator $\mathcal{L}$ in some Hilbert space V, we mean a matrix $B=(b_{ij})$ such that

$$b_{ij}=(\mathcal{L}\varphi_i,\varphi_j)_V,$$

where $(\cdot,\cdot)_V$ stands for the inner product and $\{\varphi_i\}$ consists of a complete set of basis functions in V.

Let $\mathcal{B}_{\partial C}^h$ be a boundary triangulation of ∂C obtained by decomposing each of four edges into $M=1/h$ equivalent segments, and let $\mathcal{T}_C^h$ be a triangulation of C by triangles and/or rectangles compatible with $\mathcal{B}_{\partial C}^h$. The finite element spaces V_C^h and $B_{\partial C}^h$ are defined as (2.4).

Let $\{\Phi_{b,k}(x)\}_{k=1}^{\dim B_{\partial C}^h}$ be the boundary element basis functions of $B_{\partial C}^h$. We use the same notation $\Phi_{b,k}(x)$ to indicate its natural extension into V_C^h. Besides, let $\{\Phi_{i,k}(x)\}_{k=1}^{\dim V_C^h-\dim B_{\partial C}^h}$ be the finite element basis functions of V_C^h associated with the interior degrees of freedom of $\mathcal{T}_C^h$. We denote the stiffness matrix associated with the bilinear form $a_C(\cdot,\cdot)$ (see (2.1)) by

$$A=\begin{pmatrix}A_{11} & A_{12}\\ A_{21} & A_{22}\end{pmatrix},\ A_{mn}=(a_{mn;kl}),$$

where

$$a_{11;kl}=a_C(\Phi_{b,l},\Phi_{b,k}),\ a_{12;kl}=a_{21;lk}=a_C(\Phi_{i,l},\Phi_{b,k}),\ a_{22;kl}=a_C(\Phi_{i,l},\Phi_{i,k}).$$

Set

$$B=A_{11}-A_{12}A_{22}^{-1}A_{21},\ B=(b_{kl}).$$

According to (2.8) and (2.6) we have

$$b_{kl}=\left(\mathcal{K}_C^h\Phi_{b,l},\Phi_{b,k}\right)_{\partial C},$$

which implies that B is the matrix representation of $\mathcal{K}_C^h$ under the boundary element basis functions $\{\Phi_{b,k}(x)\}_{k=1}^{\dim B_{\partial C}^h}$ of $B_{\partial C}^h$.

PROPOSITION 2.1. *$\mathcal{K}_C^h$ is a symmetric non-negative definite operator from $B_{\partial C}^h$ to $B_{\partial C}^h$. Besides, the only possible null functions of $\mathcal{K}_C^h$ are constant. Any operator with these properties is regarded* almost symmetric positive definite (SPD).

Proof. By (2.8), $\mathcal{K}_C^h$ is symmetric and non-negative definite. If there exists $f^h\in B_{\partial C}^h$ satisfying $\mathcal{K}_C^h f^h=0$, then $J_{\partial C}^h(f^h)=0$ by (2.9). In terms of (2.7), it holds that

$$a_C(\mathcal{S}^h(f^h),\mathcal{S}^h(f^h))=0.$$

Since (see (1.4))

$$a_C(\mathcal{S}^h(f^h),\mathcal{S}^h(f^h))\geq\alpha|\mathcal{S}^h(f^h)|_{1,C}^2,$$

$\mathcal{S}^h(f^h)$ is constant. Therefore, f^h should be constant. This ends the proof. ∎

2.2. DtN gluing. Suppose $\{\Omega_i\}_{i=1}^N$ are N non-overlapping bounded domains such that $\Omega=\cup_{i=1}^N\bar{\Omega}_i$ has a connected interior part. See Figure 2.1 for two typical examples. Let $B^h_{\partial\Omega_i}$ be the boundary function space on $\partial\Omega_i$. Suppose $\{B^h_{\partial\Omega_i}\}_{i=1}^N$ is consistent in the sense that their restricted spaces are the same on any shared part of boundary. With this assumption, $\{B^h_{\partial\Omega_i}\}_{i=1}^N$ induces an interface function space, denoted by $B^h_{\cup_{i=1}^N\partial\Omega_i}$, which is defined on the union of all $\partial\Omega_i$. $\{B^h_{\partial\Omega_i}\}_{i=1}^N$ also induces the boundary function space $B^h_{\partial\Omega}$ on $\partial\Omega$. We should point out that the consistency requirement is automatically satisfied if all Ω_i consist of identical periodic cells and all periodic cells are meshed in the same manner as in the last subsection.

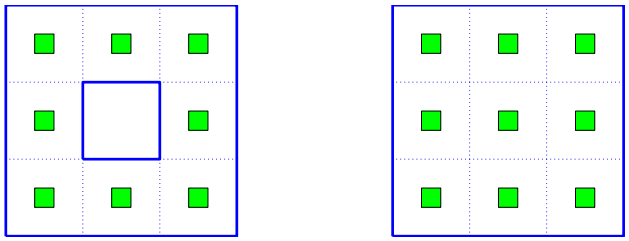

FIG. 2.1. *Left: Gluing 8 cell DtN maps for the ring-shaped domain. Right: Gluing 9 cell DtN maps for the super-cell.*

The approximate DtN map $\mathcal{K}^h_\Omega$ can surely be determined with the method in the last subsection. However, if the approximate DtN maps $\mathcal{K}^h_{\Omega_i}$ on the sub-domains Ω_i have been derived, then $\mathcal{K}^h_\Omega$ can be computed more efficiently, as shown in the following.

For any $f^h\in B^h_{\partial\Omega}$, according to (2.5) and (2.9) we have

$$\begin{aligned}
J^h_{\partial\Omega}(f^h)&=\inf_{v|_{\partial\Omega}=f^h,\,v\in V^h_\Omega}\frac{a_\Omega(v,v)}{2}=\inf_{v|_{\partial\Omega}=f^h,\,v\in V^h_\Omega}\sum_{i=1}^N\frac{a_{\Omega_i}(v,v)}{2}\\
&=\inf_{w|_{\partial\Omega}=f^h,\,w\in B^h_{\cup_{i=1}^N\partial\Omega_i}}\ \inf_{v_i|_{\partial\Omega_i}=w|_{\partial\Omega_i},\,v_i\in V^h_{\Omega_i}}\sum_{i=1}^N\frac{a_{\Omega_i}(v_i,v_i)}{2}\\
&=\inf_{w|_{\partial\Omega}=f^h,\,w\in B^h_{\cup_{i=1}^N\partial\Omega_i}}\sum_{i=1}^N J^h_{\partial\Omega_i}(w|_{\partial\Omega_i})\\
&=\inf_{w|_{\partial\Omega}=f^h,\,w\in B^h_{\cup_{i=1}^N\partial\Omega_i}}\sum_{i=1}^N\frac{(\mathcal{K}^h_{\Omega_i}w|_{\partial\Omega_i},w|_{\partial\Omega_i})_{\partial\Omega_i}}{2}.
\end{aligned}$$

Set

$$b_\Omega(v,w)\overset{def}{=}\sum_{i=1}^N(\mathcal{K}^h_{\Omega_i}v|_{\partial\Omega_i},w|_{\partial\Omega_i})_{\partial\Omega_i},\ \forall v,w\in B^h_{\cup_{i=1}^N\partial\Omega_i},\tag{2.10}$$

then we have

$$J^h_{\partial\Omega}(f^h)=\inf_{w|_{\partial\Omega}=f^h,\,w\in B^h_{\cup_{i=1}^N\partial\Omega_i}}\frac{b_\Omega(w,w)}{2}.$$

The infimum of the above minimization problem is attained by $\mathcal{S}^*(f^h) \in B^h_{\cup_{i=1}^N \partial\Omega_i}$ which solves the following interface variational problem:
Find $v \in B^h_{\cup_{i=1}^N \partial\Omega_i}$ with $v|_{\partial\Omega} = f^h$ such that

$$b_\Omega(v,w) = 0,\ \forall w \in B^h_{\cup_{i=1}^N \partial\Omega_i} \text{with } w|_{\partial\Omega} = 0. \tag{2.11}$$

The variational problem (2.11) is uniquely solvable since all $\mathcal{K}^h_{\Omega_i}$ are almost SPD. Therefore, we have

$$J^h_{\partial\Omega}(f^h) = \frac{b_\Omega(\mathcal{S}^*(f^h), \mathcal{S}^*(f^h))}{2},$$

and

$$(\mathcal{K}^h_\Omega f^h, g^h)_{\partial\Omega} = (\delta J^h_{\partial\Omega}(f^h), g^h)_{\partial\Omega} = b_\Omega(\mathcal{S}^*(f^h), \mathcal{S}^*(g^h)),\ \forall f^h, g^h \in B^h_{\partial\Omega}. \tag{2.12}$$

The determination of $\mathcal{K}^h_\Omega$ is much similar to that of the cell DtN map explained in the last subsection. Let $\{\Phi_{b,k}(x)\}_{k=1}^{\dim B^h_{\partial\Omega}}$ be the boundary element basis functions of $B^h_{\partial\Omega}$. We use the same notation $\Phi_{b,k}(x)$ to indicate its natural extension into the interface function space $B^h_{\cup_{i=1}^N \partial\Omega_i}$. Besides, let $\{\Phi_{i,k}(x)\}_{k=1}^{\dim B^h_{\cup_{i=1}^N \partial\Omega_i} - \dim B^h_{\partial\Omega}}$ be the interface element basis functions of $B^h_{\cup_{i=1}^N \partial\Omega_i}$ associated with the interior degrees of freedom. The stiffness matrix associated with the bilinear form $b_\Omega(\cdot,\cdot)$ (see (2.10)) is denoted by

$$B = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix},\ B_{mn} = (b_{mn;kl}),$$

where

$$\begin{aligned} b_{11;kl} &= \sum_{i=1}^N (\mathcal{K}^h_{\Omega_i} \Phi_{b,l}, \Phi_{b,k})_{\partial\Omega_i}, \\ b_{12;kl} = b_{21;lk} &= \sum_{i=1}^N (\mathcal{K}^h_{\Omega_i} \Phi_{i,l}, \Phi_{b,k})_{\partial\Omega_i}, \\ b_{22;kl} &= \sum_{i=1}^N (\mathcal{K}^h_{\Omega_i} \Phi_{i,l}, \Phi_{i,k})_{\partial\Omega_i}. \end{aligned}$$

B can be easily written out if the matrix representations of $\mathcal{K}^h_{\Omega_i}$ are available. Set

$$C \overset{def}{=} B_{11} - B_{12} B_{22}^{-1} B_{21},\ C = (c_{kl}).$$

According to (2.12) and (2.11) we then have

$$c_{kl} = \left(\mathcal{K}^h_\Omega \Phi_{b,l}, \Phi_{b,k}\right)_{\partial\Omega}.$$

This implies that C is the matrix representation of $\mathcal{K}^h_\Omega$ under the boundary element basis functions $\{\Phi_{b,k}(x)\}_{k=1}^{\dim B^h_{\partial\Omega}}$ of $B^h_{\partial\Omega}$.

PROPOSITION 2.2. *If all $\mathcal{K}^h_{\Omega_i}$ are almost SPD, then so is $\mathcal{K}^h_\Omega$.* The proof is analogous

to that of Proposition 2.1, and we omit it here.

The benefit of the proposed gluing method is obvious: the approximate DtN map in a large domain can be determined merely through the DtN maps on individual components, without consulting the details of the interior mesh structure. The computational cost is nearly cubic to the dimension of the interface function space. This is a remarkable reduction of complexity compared with the direct method in the last subsection, since the latter involves the invertibility of a matrix whose rank is the total number of degrees of freedom in the solid domain.

2.3. DtN homogenization. After the single cell DtN map $\mathcal{K}_C^h$ has been derived as in the Subsection 2.1, one glues eight such cell DtN maps to derive $\mathcal{K}_{D_0}^h$, the approximation of the DtN map $\mathcal{K}_{D_0}$ on D_0. To approximate $\mathcal{K}_{D_1}$, one can first glue nine cells' DtN maps to derive the DtN map $\mathcal{K}_{1,C}^h$ for a super-cell consisting of a 3×3 bi-periodic array, and then glue eight $\mathcal{K}_{1,C}^h$ to obtain $\mathcal{K}_{D_1}^h$. The approximation of $\mathcal{K}_{D_n}$ with $n\geq 2$ is derived recursively. With the above treatment, however, one immediately realizes that since the number of operations needed for $\mathcal{K}_{D_n}^h$ is of $\mathcal{O}((\dim B_{\partial G_n}^h)^3)$, and $\dim B_{\partial G_n}^h$ is tripled each time as n increases, the computational cost tends to a heavy burden quickly. In this part, we propose a novel technique called *DtN homogenization* to avoid this complexity disaster.

The basic idea of this technique is to control the dimension of the representative space of the DtN map. It is known that $\mathcal{K}_{D_0}^h$ is an almost SPD operator defined on $B_{\partial G_0}^h \oplus B_{\partial G_1}^h$. Let $\mathcal{P}_h$ be the L^2 projection from $B_{\partial G_1}^h$ to $B_{\partial G_1}^{3h} \subset B_{\partial G_1}^h$, where $B_{\partial G_1}^{3h}$ denotes the boundary function space with a characteristic mesh size $3h$. Set

$$\tilde{\mathcal{K}}_{D_0}^h = (I\otimes \mathcal{P}_h)\mathcal{K}_{D_0}^h (I\otimes \mathcal{P}_h^\top).$$

Here $\mathcal{P}_h^\top$ denotes the adjoint operator of $\mathcal{P}_h$, which identically embeds $B_{\partial G_1}^{3h}$ into $B_{\partial G_1}^h$. Then $\tilde{\mathcal{K}}_{D_0}^h$, acting on $B_{\partial G_0}^h \oplus B_{\partial G_1}^{3h}$, gives a simplified version of the discrete DtN map $\mathcal{K}_{D_0}^h$ by coarsening the representations of both Dirichlet and Neumann data at ∂G_1. Note that since $\dim B_{\partial G_1}^{3h} = \dim B_{\partial G_0}^h$, we have used the same number of degrees of freedom on ∂G_0 and ∂G_1, the two disjointed boundaries of D_0.

Let $\{\Phi_{\partial G_0,k}^h(x)\}_{k=1}^{\dim B_{\partial G_0}^h}$, $\{\Phi_{\partial G_1,k}^h(x)\}_{k=1}^{\dim B_{\partial G_1}^h}$, and $\{\Phi_{\partial G_1,k}^{3h}(x)\}_{k=1}^{\dim B_{\partial G_1}^{3h}}$ be the boundary element basis functions of $B_{\partial G_0}^h$, $B_{\partial G_1}^h$, and $B_{\partial G_1}^{3h}$ respectively. Suppose $P=(p_{kl})$ satisfies

$$\Phi_{\partial G_1,k}^{3h}(x) = \sum_l p_{kl}\Phi_{\partial G_1,l}^h(x),$$

and $C=(c_{kl})$ is the matrix representation of $\mathcal{K}_{D_0}^h$ under the basis functions $\{\Phi_{\partial G_0,k}^h(x)\}_{k=1}^{\dim B_{\partial G_0}^h}$ and $\{\Phi_{\partial G_1,k}^h(x)\}_{k=1}^{\dim B_{\partial G_1}^h}$, then under the basis functions $\{\Phi_{\partial G_0,k}^h(x)\}_{k=1}^{\dim B_{\partial G_0}^h}$ and $\{\Phi_{\partial G_1,k}^{3h}(x)\}_{k=1}^{\dim B_{\partial G_1}^{3h}}$, the matrix representation of $\tilde{\mathcal{K}}_{D_0}^h$ is simply

$$\tilde{C} = \begin{pmatrix} I & 0 \\ 0 & P \end{pmatrix} C \begin{pmatrix} I & 0 \\ 0 & P^T \end{pmatrix}.$$

The matrix elements of P are easily determined if the order of finite elements is specified.

To derive an approximation of $\mathcal{K}_{D_1}$, we first compute the super-cell DtN map $\mathcal{K}^h_{1,C}$ with the gluing procedure. Note that $\mathcal{K}^h_{1,C}$ is defined on $B^h_{\partial G_1}$. A homogenized version of $\mathcal{K}^h_{1,C}$ is then derived as

$$\mathcal{K}^{3h}_{1,C} = \mathcal{P}_h \mathcal{K}^h_{1,C} \mathcal{P}_h^\top.$$

This operator is defined on $B^{3h}_{\partial G_1}$. The approximate DtN map of $\mathcal{K}_{D_1}$, denoted by $\tilde{\mathcal{K}}^{3h}_{D_1}$, is derived by first gluing eight super-cell DtN maps $\mathcal{K}^{3h}_{1,C}$, and then applying the DtN homogenization on the exterior boundary ∂G_2. Therefore, $\tilde{\mathcal{K}}^{3h}_{D_1}$ is defined on the space $B^{3h}_{\partial G_1} \oplus B^{9h}_{\partial G_2}$. The approximations of $\mathcal{K}_{D_n}$ with $n \geq 2$, denoted by $\tilde{\mathcal{K}}^{3^n h}_{D_n}$, are computed recursively.

For the ease of reference, we write the entire algorithm.

Step 1 Given h, generate the boundary mesh $\mathcal{B}^h_{\partial C}$ and the interior mesh $\mathcal{T}^h_C$ for a single periodic cell.

Step 2 Specify the order of finite elements. Form the boundary element space $B^h_{\partial C}$ and the interior finite element space T^h_C. Compute the single cell DtN map $\mathcal{K}^h_C$.

Step 3 Set the zeroth level super-cell DtN map $\mathcal{K}^h_{0,C} = \mathcal{K}^h_C$. For $n = 0, 1, \cdots$, we perform

- Derive $\mathcal{K}^{3^n h}_{D_n}$ by gluing together eight n-th level super-cell DtN maps $\mathcal{K}^{3^n h}_{n,C}$. Set

$$\tilde{\mathcal{K}}^{3^n h}_{D_n} = (I \otimes \mathcal{P}) \mathcal{K}^{3^n h}_{D_n} (I \otimes \mathcal{P}^\top),$$

  where $\mathcal{P}$ is the L^2 projection from $B^{3^n h}_{\partial G_{n+1}}$ to $B^{3^{n+1} h}_{\partial G_{n+1}}$.

- Derive $n+1$-st level super-cell DtN map $\mathcal{K}^{3^n h}_{n+1,C}$ by gluing together nine n-th level super-cell DtN maps $\mathcal{K}^{3^n h}_{n,C}$. Set the homogenized $n+1$-st level super-cell DtN map as

$$\mathcal{K}^{3^{n+1} h}_{n+1,C} = \mathcal{P} \mathcal{K}^{3^n h}_{n+1,C} \mathcal{P}^\top.$$

It should be pointed out that what we really derive from the above algorithm are the matrix representations of $\tilde{\mathcal{K}}^{3^n h}_{D_n}$ under the natural boundary element basis functions $\{\Phi^h_{\partial G_n, k}(x)\}_{k=1}^{\dim B^{3^n h}_{\partial G_n}}$ of $B^{3^n h}_{\partial G_n}$ and $\{\Phi^{3^{n+1} h}_{\partial G_{n+1}, k}(x)\}_{k=1}^{\dim B^{3^{n+1} h}_{\partial G_{n+1}}}$ of $B^{3^{n+1} h}_{\partial G_{n+1}}$.

PROPOSITION 2.1. *If $\mathcal{K}^h_C$ is almost SPD, so are $\mathcal{K}^{3^n h}_{n,C}$ and $\tilde{\mathcal{K}}^{3^n h}_{D_n}$.*

Proof. It suffices to prove that $\mathcal{K}^{3h}_{1,C}$ and $\tilde{\mathcal{K}}^h_{D_0}$ are almost SPD. By Proposition 2.2, $\mathcal{K}^h_{1,C}$ and $\mathcal{K}^h_{D_0}$ are almost SPD. Thus both $\mathcal{K}^{3h}_{1,C}$ and $\tilde{\mathcal{K}}^h_{D_0}$ are non-negative definite. If there exists a function $v \in B^{3h}_{\partial G_1}$ such that $\mathcal{K}^{3h}_{1,C} v = 0$, then $\mathcal{P}^\top v$ should be constant, since $\mathcal{K}^h_{1,C}$ is almost SPD. This implies that v is constant, considering $\mathcal{P}^\top$ is the embedding operator from $B^{3h}_{\partial G_1}$ to $B^h_{\partial G_1}$. This indicates that $\mathcal{K}^{3h}_{1,C}$ is almost SPD. The proof for $\tilde{\mathcal{K}}^h_{D_0}$ is analogous. ∎

2.4. Truncated domain problem. With the gluing and homogenization techniques, we have derived a sequence of approximate DtN maps $\tilde{\mathcal{K}}^{3^n h}_{D_n}$ of $\mathcal{K}_{D_n}$ on the domain D_n, which acts on $B^{3^n h}_{\partial G_n} \oplus B^{3^{n+1} h}_{\partial G_{n+1}}$. By Proposition 2.1, all $\tilde{\mathcal{K}}^{3^n h}_{D_n}$ are almost SPD. For any $L \geq 0$, we can employ the gluing procedure again to derive an

approximate DtN map on $\cup_{n=0}^{L} D_n = G_{L+1}\backslash \bar{G}_0$. We denote this map by $\tilde{\mathcal{K}}_L^h$, which is also an almost SPD operator. Recall that the size of domain $\cup_{n=0}^{L} D_n$ increases exponentially fast with respect to L. In terms of (1.5), we can terminate the above gluing process at a moderately large L, and apply the homogeneous Neumann boundary condition at ∂G_{L+1}.

Let $u_{n,D/N}^{3^n h} \in B_{\partial G_n}^{3^n h}$ be the approximate Dirichlet/Neumann data. Rewriting $\tilde{\mathcal{K}}_L^h$ into a block form gives

$$\begin{pmatrix} -u_{0,N}^h \\ u_{L+1,N}^{3^{L+1}h} \end{pmatrix} = \tilde{\mathcal{K}}_L^h \begin{pmatrix} u_{0,D}^h \\ u_{L+1,D}^{3^{L+1}h} \end{pmatrix} = \begin{pmatrix} \mathcal{C}_{11,L} & \mathcal{C}_{12,L} \\ \mathcal{C}_{21,L} & \mathcal{C}_{22,L} \end{pmatrix} \begin{pmatrix} u_{0,D}^h \\ u_{L+1,D}^{3^{L+1}h} \end{pmatrix}, \tag{2.13}$$

where $(\mathcal{C}_{ij,L})$ is the block representation of $\tilde{\mathcal{K}}_L^h$. Let $u_{L+1,N}^{3^{L+1}h} = 0$. We have

$$\mathcal{C}_{21,L} u_{0,D}^h + \mathcal{C}_{22,L} u_{L+1,D}^{3^{L+1}h} = 0. \tag{2.14}$$

$\mathcal{C}_{22,L}$ is an SPD operator since $\tilde{\mathcal{K}}_L^h$ is almost SPD. From (2.14) we have

$$u_{L+1,D}^{3^{L+1}h} = -\mathcal{C}_{22,L}^{-1} \mathcal{C}_{21,L} u_{0,D}^h.$$

Substituting the above into the first equation of (2.13) gives

$$-u_{0,N}^h = \left[\mathcal{C}_{11,L} - \mathcal{C}_{12,L}\mathcal{C}_{22,L}^{-1}\mathcal{C}_{21,L}\right] u_{0,D}^h \equiv \mathcal{K}_L^h u_{0,D}^h.$$

PROPOSITION 2.2. *$\mathcal{K}_L^h$ is an almost SPD operator.*

Proof. Obviously $\mathcal{K}_L^h$ is symmetric. Note that

$$\begin{aligned} &(u_{0,D}^h, \mathcal{K}_L^h u_{0,D}^h)_{\partial G_0} = (u_{0,D}^h, -u_{0,N}^h)_{\partial G_0} \\ &= \left(\begin{pmatrix} u_{0,D}^h \\ u_{L+1,D}^{3^{L+1}h} \end{pmatrix}, \begin{pmatrix} -u_{0,N}^h \\ u_{L+1,N}^{3^{L+1}h} \end{pmatrix} \right)_{\partial G_0 \cup \partial G_{L+1}} = \left(\begin{pmatrix} u_{0,D}^h \\ u_{L+1,D}^{3^{L+1}h} \end{pmatrix}, \tilde{\mathcal{K}}_L^h \begin{pmatrix} u_{0,D}^h \\ u_{L+1,D}^{3^{L+1}h} \end{pmatrix} \right)_{\partial G_0 \cup \partial G_{L+1}}. \end{aligned}$$

If $(u_{0,D}^h, \mathcal{K}_L^h u_{0,D}^h)_{\partial G_0}$ equals zero, then $u_{0,D}^h$ should be constant since $\tilde{\mathcal{K}}_L^h$ is almost SPD. This implies $\mathcal{K}_L^h$ is almost SPD. ∎

Let $\{\Phi_{\partial G_0,k}^h(x)\}_{k=1}^{\dim B_{\partial G_0}^h}$ and $\{\Phi_{\partial G_{L+1},k}^{3^{L+1}h}(x)\}_{k=1}^{\dim B_{\partial G_{L+1}}^{3^{L+1}h}}$ be the boundary element basis functions of $B_{\partial G_0}^h$ and $B_{\partial G_{L+1}}^{3^{L+1}h}$, and let C_L be the matrix representation of $\tilde{\mathcal{K}}_L^h$ under this set of basis functions. Suppose

$$C_L = \begin{pmatrix} C_{11,L} & C_{12,L} \\ C_{21,L} & C_{22,L} \end{pmatrix}$$

is in block form. Then

$$C_{11,L} - C_{12,L} C_{22,L}^{-1} C_{21,L}$$

gives the matrix representation of $\mathcal{K}_L^h$ under the boundary element basis functions $\{\Phi_{\partial G_0,k}^h(x)\}_{k=1}^{\dim B_{\partial G_0}^h}$ of $B_{\partial G_0}^h$.

Now we are ready to consider the numerical solution of (1.1)-(1.3) restricted to the defect cell. Set $\Omega = G_0 \backslash \bar{D} = C_{00} \backslash \bar{D}$. Let $\mathcal{T}_\Omega^h$ be a triangulation of Ω, with

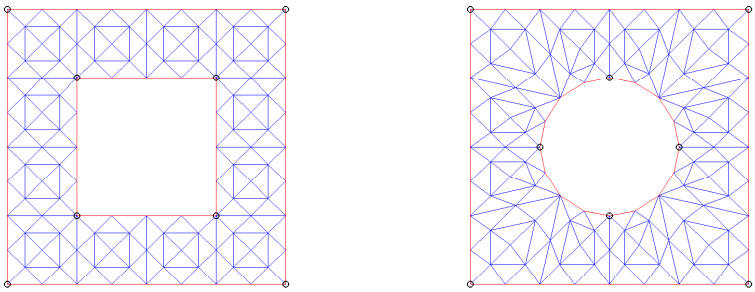

FIG. 3.1. *Meshes used in the computation.* $M=8$. *Left: Example A. Right: Example B.*

rectangles and/or triangles, which is compatible with $\mathcal{B}^h_{\partial G_0}$. Let V^h_Ω be the k-th degree conforming Lagrangian finite element space. With the DtN map $\mathcal{K}^h_L$ imposed at $B^h_{\partial G_0}$, the approximate variational problem with truncated domain Ω reads:
Find $u^h \in V^h_\Omega$ with $u^h|_{\partial D} = I_h g$, such that

$$(\mathbf{A}(x)\nabla u^h, \nabla v)_\Omega + (a_0(x)u^h, v)_\Omega + (\mathcal{K}^h_L u^h, v)_{\partial G_0} = 0, \ \forall v \in V^h_\Omega \text{ with } v|_{\partial D} = 0. \quad (2.15)$$

Here I_h is the standard Lagrangian interpolating operator. Since $\mathcal{K}^h_L$ is non-negative, the following proposition is obvious.

PROPOSITION 2.3. *The discrete variational problem* (2.15) *is uniquely solvable.*

Since the matrix elements of $\mathcal{K}^h_L$ have been computed with the gluing and homogenization techniques, the discrete variational problem (2.15) is now solvable with the standard choice of finite element basis functions.

3. Numerical examples

In this section, we present two numerical tests to demonstrate the performance of the proposed algorithm.

3.1. Example A. As a first example, we consider an exterior problem of Laplace's equation. Let D be a square of width 0.5 centered at the origin, and let $g(x) = \frac{x_1}{x_1^2+x_2^2}$ be the Dirichlet boundary data at ∂D. The exact solution of this exterior problem is simply

$$u(x) = \frac{x_1}{x_1^2 + x_2^2}.$$

We consider the underlying homogeneous medium as a special instance of bi-periodic structures with the period of 1. In the left of Figure 3.1 we show the coarsest mesh with $M=8$ for the defect cell used in the computation. The mesh for periodic cells is generated with identical square elements. We plot the relative L^2 errors of the numerical solution u_h in Figure 3.2, where L is the parameter in the approximate DtN map $\mathcal{K}^h_L$; see Subsection 2.4. Remember that we derive $\mathcal{K}^h_L$ by truncating the residual unbounded domain $\mathbb{R}^2 \backslash \bar{C}_{00}$ and applying the homogeneous Neumann data at ∂G_{L+1}. For $L=10$, the errors degenerate almost with a rate of second order for the linear finite elements, and a rate of fourth order for the quadratic finite elements. This implies that in the mesh regime considered in this numerical test, the error from

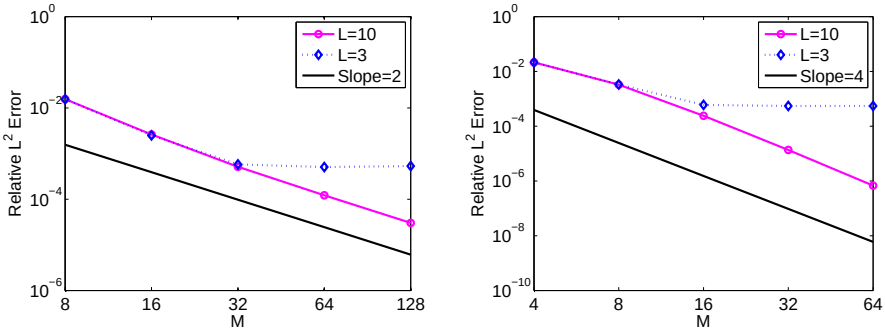

FIG. 3.2. *Example A. Left: linear finite elements. Right: quadratic finite elements.*

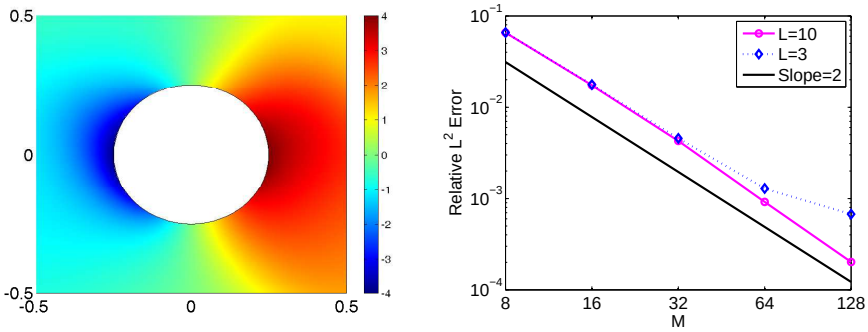

FIG. 3.3. *Example B. Error plot for the computed displacement field* u_h.

the approximate DtN map on the artificial boundary is negligible. An interesting thing that we cannot explain is the super-convergence behavior of the quadratic finite elements. For $L=3$, the errors first decrease and then saturate when the mesh is successively refined. This typically indicates that the artificial boundary condition for $L=3$ is not accurate enough.

3.2. Example B. In this numerical test, we consider a non-trivial bi-periodic structure problem of period 1 by setting

$$a(x)=\exp(\sin(2\pi(x_1+x_2))),\ c(x)=0.$$

The domain D is a circle of radius 0.25, and the Dirichlet data g is the same as in Example A. For this problem, the exact solution with closed form is not available. To evaluate the quality of numerical solutions, we compute a reference solution with the fourth order finite elements by setting $M=32$ and $L=10$. The mesh for $M=8$ is illustrated in the right of Figure 3.1, and the reference solution restricted to the defect cell is shown in the left of Figure 3.3. The relative L^2 errors with linear finite elements are plotted in the right of Figure 3.3, from which an analogous observation can be made as for Example A.

4. Conclusion

We proposed a new approach of designing approximate DtN map in a discrete form for a specific bi-periodic elliptic problem. The basic idea consists of several steps.

First, the residual unbounded domain is partitioned into a sequence of bounded domains $\{D_n\}_{n=0}^{\infty}$ with similar shape. Second, after the single cell DtN map is determined, the DtN map $\mathcal{K}_n$ for each D_n is computed by gluing eight cell (or super-cell) DtN maps. The gluing technique is also used to derive the DtN map for $\cup_{n=0}^{L} D_n$, which approaches the whole residual domain as L goes to infinity. Third, an approximate DtN map for the residual domain is derived by truncating the residual domain and imposing homogeneous Neumann boundary condition at a suitable place. This approximate DtN map is finally combined with the governing elliptic equation to determine the solution only in the local defect region.

At the discrete level, to control the growth of degrees of freedom involved in $\mathcal{K}_n$ we introduced a new concept — DtN homogenization. The underlying idea is to coarsen the representations of both Dirichlet and Neumann data while maintaining the energy of the smooth part of the data as much as possible. We proved the unique solvability for the discrete variational problem. Though the error analysis is beyond our capability at the moment, the numerical tests showed that the proposed techniques are promising.

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