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EXACT ARTIFICIAL BOUNDARY CONDITIONS FOR CONTINUUM AND DISCRETE ELASTICITY*

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Abstract. For the continuum and discrete elastic equations, we derive exact artificial boundary conditions (ABCs), often referred to as transparent boundary conditions, that can be applied at a planar interface below which there are no forces. Solution of the elasticity equations can then be performed using this interface as an artificial boundary, often with greatly reduced computational effort, but without loss of accuracy. A general solvability requirement is presented for the existence of an artificial boundary operator for discrete systems (such as discrete elasticity) on an unbounded (semi-infinite) domain. The solvability requirement is validated by introducing a sum-of-exponentials ansatz for the solution below the artificial boundary. We also derive a new expression for the total energy for the system, involving only the region above the artificial boundary. Numerical examples are provided to confirm and illustrate the accuracy and effectiveness of the results.

Key words. elasticity, discrete elasticity, artificial boundary conditions, transparent boundary conditions, atomistic strain

AMS subject classifications. Primary, 65N55; Secondary, 74B05, 70C20

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1. Introduction.

Many of the boundary value problems arising in applied mathematics are formulated on unbounded domains. It is in general a nontrivial task to solve such problems numerically [6], since the numerical solution naturally requires boundary conditions at a finite depth in the body.

The main motivation of the present work comes from the numerical simulation of strain fields in semi-infinite domains. For the strain equations, the use of a physical boundary condition, such as the zero displacement field at a certain depth, has been a common practice [21]. On the other hand, due to the long range of elastic interactions, the zero boundary condition must be imposed at considerable depth in order to accurately compute the strain field [4], which entails large computational cost.

The purpose of this paper is to derive exact *artificial boundary conditions* (ABCs) such that the solution on the (bounded) computational domain coincides with the exact solution on the unbounded domain. Such exact artificial boundary conditions are oftentimes referred to as *transparent boundary conditions* (TBCs) [6].

There have been various works on ABCs for a wide range of problems. For example, certain ABCs for the Poisson and Helmholtz equations on infinite domains are investigated in [1] using domain decomposition and Fourier techniques. For general elliptic problems, approximate ABCs and error estimates are performed within the finite element framework in [3]. Boundary element methods for homogeneous elasto-

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static and elastodynamic cases, linear elastostatic problems, time dependent heat and wave equations, and electromagnetic scattering problems are also treated in an exact manner using the Dirichlet to Neumann boundary condition in [2, 7, 8, 9].

For the elasticity problem, several local and nonlocal artificial boundary conditions are provided in terms of the finite element formulation in [12, 13, 14]. For a discrete elastic strain model for an epitaxial thin film, ABCs were derived recently by Russo and Smereka [20] using a formulation that is somewhat different from our model.

In the present work, we perform an analysis for the equations of both continuum and discrete elastic models. The discrete elastic equations correspond to an atomistic strain model introduced in the recent work by Schindler et al. [21]. Although full details are provided only for a discrete strain model, a general solvability requirement is formulated, which results in the well-posedness or the solvability of the system in an infinite domain. This work is a discrete analogue of the work by Hagstrom and Keller [11]. The solvability requirement is then validated by analyzing the solution on the exterior domain using a sum-of-exponentials ansatz. This framework, on the one hand, leads us to derive the abstract ABC operator in the form of a Schur complement operator and, on the other hand, guides the construction of the explicit ABC operator for actual implementations. Thanks to the ABC operator, the force balance equation that needs to be solved in the infinite domain can be posed as a reduced equation on the bounded domain, whose solution has been shown to coincide with the exact solution on the full (unbounded) domain. In addition, a new formula is derived for the total elastic energy of the system, involving only the solution above the artificial boundary. The latter is particularly important for practical applications such as thin epitaxial film growth simulations.

The rest of the paper is structured as follows. In section 2, we introduce some preliminaries and notation to ease the presentation. The ABCs, total energy formula, and variational principle for continuum elasticity are derived in section 3. In section 4, we briefly review the discrete elastic strain model and introduce the general solvability requirement, present an abstract form of the ABC operator, and derive explicit ABCs for a specific discrete strain model. The total energy formula and the variational principle for the discrete strain model are also presented. Several illustrative numerical results are provided in section 5. Conclusions are discussed in section 6. Some details are saved for the appendix.

2. Preliminaries. Suppose that the domain Ω is a half-infinite body, e.g., $\Omega = \{(x, y, z) \in \mathbb{R}^3 : z < h(x, y)\}$ for $h : \mathbb{R}^2 \mapsto \mathbb{R}$ being a bounded function. See Figure 2.1 for a schematic description. The interface Γ_2 on which the artificial boundary will be imposed is illustrated in Figure 2.1. For both the continuum and discrete problems, the domain Ω is divided into a finite part Ω_1 and a semi-infinite part (an exterior domain) $\Omega_2 = \Omega \backslash \Omega_1$. The requirement on the choice of Ω_2 is that its boundary Γ_2 is planar and normal to the depth variable and that there are no external forces in Ω_2. For the boundary condition for both continuum and discrete elasticity equations, we assume that the periodic conditions are imposed in x- and y-directions (lateral directions) and that the Neumann condition (i.e., the variational principle with no constraint at the boundary) is imposed on the top layer Γ_1 unless explicitly stated otherwise. Use of the Neumann condition is only for simplicity and to ensure that the problem is well-posed; it does not influence the resulting ABCs.

We use boldface lower case letters for vectors in $\mathbb{R}^d$ with $d = 2$ or 3 and boldface capital letters for symmetric tensors or square matrices. The differential operator ∂_k denotes the partial derivative with respect to the kth coordinate variable, i.e., $\partial/\partial x_k$,

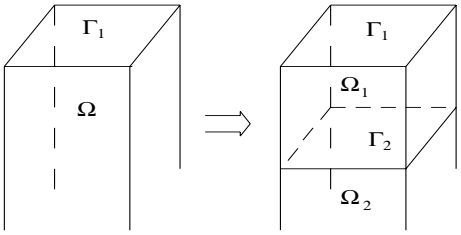

FIG. 2.1. *The domain decomposition: An artificial boundary* Γ_2 *(the horizontal plane) divides* Ω *into* Ω_1 *and* Ω_2. Γ_1 *is the top boundary (surface) of* Ω.

and the operator $\nabla\cdot$ is the standard *divergence* operator defined through

$$\nabla\cdot = (\partial/\partial x, \partial/\partial y)\cdot \qquad \text{for } d = 2,$$
$$\nabla\cdot = (\partial/\partial x, \partial/\partial y, \partial/\partial z)\cdot \qquad \text{for } d = 3.$$

The notation ∇ denotes the usual *gradient* operator for $d = 2$ and $d = 3$ given, respectively, as

$$\nabla = \begin{pmatrix} \partial/\partial x \\ \partial/\partial y \end{pmatrix}, \quad \nabla = \begin{pmatrix} \partial/\partial x \\ \partial/\partial y \\ \partial/\partial z \end{pmatrix},$$

and Δ is the *Laplace* operator $\nabla\cdot\nabla$.

For two vectors $\mathbf{u}$ and $\mathbf{v}$, $\mathbf{u}\cdot\mathbf{v}$ is the dot product; for a vector $\mathbf{v} = (v_k)_{k=1,\dots,d}$ and a tensor $\mathbf{N} = (N_{kl})_{k,l=1,\dots,d}$, $\mathbf{v}\cdot\mathbf{N} = \sum_{k=1}^{d} v_k N_{k\ell}$. The magnitude of a vector $\mathbf{u}$ will be denoted by $|\mathbf{u}| = (\mathbf{u}\cdot\mathbf{u})^{1/2}$.

Although the letters i, j, k are used for indices, we shall also use $\imath$ to denote the imaginary unit $\sqrt{-1}$, and the complex conjugate of a complex number v shall be denoted by $\overline{v}$. Also, for the matrix $\mathbf{N}$, $\mathbf{N}^H$ and $\mathbf{N}^T$ denote the complex conjugate transpose and the real transpose of $\mathbf{N}$, respectively. Finally, we shall use χ to denote the usual characteristic function that is defined as

$$\chi(x) = \begin{cases} 1 & \text{for } x \in \Omega_1, \\ 0 & \text{for } x \notin \Omega_1. \end{cases} \tag{2.1}$$

Some other notation will be introduced in each section as necessary.

3. The ABCs for continuum elasticity. In this section, we review the continuum elastic equations from an energetic viewpoint. We then derive the artificial boundary (or ABC) operator $\mathcal{A}$, as well as a new expression for the total energy and a formulation of the force balance equations depending on only the displacement on and above the interface Γ_2 on which the artificial boundary condition is given.

3.1. Continuum elasticity. Continuum elasticity is formulated in terms of a displacement field $\mathbf{u} = \mathbf{u}(\mathbf{x}) = \mathbf{y}(\mathbf{x}) - \mathbf{x}$ between the equilibrium position $\mathbf{x}$ of a material point and the elastically deformed position $\mathbf{y}(\mathbf{x})$ of that point. The strain tensor $\mathbf{S}$ has components defined as $S_{k\ell} = (\partial_k u_\ell + \partial_\ell u_k)/2$ in which u_k are the components of $\mathbf{u}$.

The derivation of the linear elasticity equations can be made via a variational principle for the total energy $\mathcal{E}$ in a domain Ω, namely,

$$\delta\mathcal{E} = 0. \tag{3.1}$$

The total elastic energy $\mathcal{E}$ for the linear elasticity is given as follows:

$$\mathcal{E} = \int_\Omega E d\mathbf{x}, \tag{3.2}$$

where the integrand is the energy density

$$E = \frac{1}{2}\sum_{k,\ell} S_{k\ell} T_{k\ell} - \mathbf{u}\cdot\mathbf{f}\,\chi, \tag{3.3}$$

$\mathbf{f} = (f_k)$ is a body force, and $\mathbf{T} = (T_{k\ell})$ is the stress tensor defined, for an isotropic material, as

$$T_{k\ell} = \lambda\delta_{k\ell}\sum_i S_{ii} + 2\tau S_{k\ell}. \tag{3.4}$$

The parameters λ and τ are the Lamé constants. In the absence of external force on the boundary Γ_1, (3.1) reduces to the classical Navier equations of linear elasticity, i.e.,

$$\begin{aligned} -\nabla\cdot\mathbf{T} &= \mathbf{f}\chi \quad \text{in } \Omega, \\ \mathbf{n}\cdot\mathbf{T} &= 0 \quad \text{on } \Gamma_1, \end{aligned} \tag{3.5}$$

where $\mathbf{n}$ is the outer unit normal vector.

For linear elasticity with cubic symmetry, the elastic energy density E is the following:

$$E = \frac{C_{11}}{2}\sum_i S_{ii}^2 + 2C_{44}\sum_{k\neq\ell} S_{k\ell}^2 + C_{12}\sum_{k\neq\ell} S_{kk}S_{\ell\ell}, \tag{3.6}$$

where C_{11}, C_{44}, and C_{12} are the cubic elastic moduli, i.e., the Voigt constants. The linear elasticity equations with cubic symmetry are

$$\begin{aligned} -C_{11}\partial_k\partial_k u_k - C_{44}\sum_{l\neq k}\partial_l\partial_l u_k \\ -(C_{12}+C_{44})\sum_{l\neq k}\partial_k\partial_l u_l = f_k\chi \quad \text{in } \Omega \end{aligned} \tag{3.7}$$

for $k = 1,\dots,d$. Note that the isotropic linear elasticity equations (3.5) can be recovered from (3.7) by choosing the following Voigt constants:

$$(C_{11}, C_{44}, C_{12}) = (\lambda+2\tau, \tau, \lambda). \tag{3.8}$$

For the study of the ABCs for continuum elasticity, we restrict our attention to the isotropic linear elasticity, namely, (3.7) with the Voigt constants given in (3.8), for simplicity. It is easily generalized to the anisotropic case.

3.2. Two dimensional case. In this section, we construct the artificial boundary operator $\mathcal{A}$ for the two dimensional case. The main idea is to analytically solve the force balance equation (3.7) on the exterior domain Ω_2 by introducing a sum-of-exponentials ansatz, which must be modified to include algebraic terms.

We assume that the solution is periodic in the x-direction with 2π periodicity and that the interface Γ_2 is a line, i.e., $\Gamma_2 = \{(x,y) \in \mathbb{R}^2 : y = 0\}$. We first look for a modal solution $\mathbf{u}(x,y)$ for $y < 0$ as

$$\begin{aligned}\mathbf{u}(x,y) &= \widehat{\mathbf{u}}(\mu,y)\,\mathrm{e}^{\imath\mu x} \\ &= \widehat{\mathbf{u}}(\mu)\,\mathrm{e}^{\beta y}\,\mathrm{e}^{\imath\mu x} = \begin{pmatrix} \hat{u}(\mu) \\ \hat{v}(\mu) \end{pmatrix}\mathrm{e}^{\beta y}\,\mathrm{e}^{\imath\mu x}.\end{aligned} \tag{3.9}$$

Since $\mathbf{u}$ in (3.9) is the solution to (3.7), for each μ, $\widehat{\mathbf{u}}(\mu)$ should satisfy the following linear system:

$$\mathbf{M}(\mu,\beta)\widehat{\mathbf{u}}(\mu) = 0,$$

where $\widehat{\mathbf{u}}(\mu) = (\widehat{u}(\mu), \widehat{v}(\mu))^T$ and

$$\mathbf{M}(\mu,\beta) = \begin{pmatrix} -(\lambda+2\tau)\mu^2 + \tau\beta^2 & \imath\mu(\lambda+\tau)\beta \\ \imath\mu(\lambda+\tau)\beta & -\tau\mu^2 + (\lambda+2\tau)\beta^2 \end{pmatrix}.$$

A nontrivial solution can be attained only if

$$\det \mathbf{M}(\mu,\beta) = \tau(\lambda+2\tau)(\beta^2-\mu^2)^2 = 0, \tag{3.10}$$

which implies that $\beta = \pm|\mu|$. Since the solution $\mathbf{u}$ should decay as $y \to -\infty$, then $\beta = |\mu|$ is the proper choice. Note that for $\mu = 0$, the only solution is $\beta = 0$, which corresponds to a trivial solution, the constant displacement field.

We now compute the zero eigenvector for $\mathbf{M}(\mu,|\mu|)$. It is easy to see that the matrix $\mathbf{M}(\mu,|\mu|)$ has a zero eigenvector given by $\mathbf{q}_1 = (\imath, \mu/|\mu|)^T$ and a generalized eigenvector $\mathbf{q}_2 = (0, -c/\mu)^T$ satisfying $\mathbf{M}(\mu)\mathbf{q}_1 = 0$ and $\mathbf{M}(\mu)\mathbf{q}_2 = -(\lambda+3\tau)|\mu|\mathbf{q}_1$ with $c = (\lambda+3\tau)/(\lambda+\tau)$, from which we obtain the general solution to the equation (3.7) as follows:

$$\widehat{\mathbf{u}}(\mu,y) = ((a_\mu + b_\mu y)\mathbf{q}_1 + b_\mu \mathbf{q}_2)\,\mathrm{e}^{\imath\mu x + |\mu| y}, \tag{3.11}$$

where

$$a_\mu = -\widehat{u}(\mu,0)\imath \quad \text{and} \quad b_\mu = -c^{-1}(\mu\widehat{v_0}(\mu,0) + \imath|\mu|\widehat{u}(\mu,0)). \tag{3.12}$$

From this, we obtain the following simple but important lemma.

LEMMA 3.1. *A solution to* (3.7) *on the domain* Ω_2 *with a given boundary value* $\mathbf{u}_0(x)$ *on* Γ_2 *is given by the following:*

$$\mathbf{u}(x,y) = \frac{1}{2\pi}\int_0^{2\pi} \mathbf{G}(x-x',y)\mathbf{u}_0(x')dx', \tag{3.13}$$

where $\mathbf{G}$ *is defined, using* $c = (\lambda+3\tau)/(\lambda+\tau)$, *as*

$$\begin{aligned}\mathbf{G}(x-x',y) &= \sum_{\mu=-\infty}^{\infty} \mathbf{G}_\mu(x-x',y), \\ \mathbf{G}_\mu(x-x',y) &= \begin{pmatrix} 1+\frac{|\mu|}{c}y & -\frac{\mu}{c}\imath y \\ -\frac{\mu}{c}\imath y & 1-\frac{|\mu|}{c}y \end{pmatrix}\mathrm{e}^{|\mu|y}\,\mathrm{e}^{\imath\mu(x-x')}.\end{aligned}$$

This analytic expression for the solution $\mathbf{u}$ on the domain Ω_2 is used to derive the ABC operator.

3.3. The ABC operator for the two dimensional case. In this section, using Lemma 3.1, we construct the ABC operator. First, consider the expression of the solution $\mathbf{u}$ in the exterior domain Ω_2 given in (3.13). By taking the derivative of $\mathbf{u}$ with respect to y, one finds that

$$\partial_y(\mathbf{u}(x,y)) = \frac{1}{2\pi}\int_0^{2\pi} \partial_y(\mathbf{G}_\mu(x-x',y))\mathbf{u}_0(x')\,dx'. \tag{3.14}$$

Note that the normal component of the stress tensor $\mathbf{n}\cdot\mathbf{T}$ is given by

$$\mathbf{n}\cdot\mathbf{T} = \begin{pmatrix} \tau(\partial_y u + \partial_x v) \\ (\lambda+2\tau)\partial_y v + \lambda\partial_x u \end{pmatrix}, \tag{3.15}$$

and observe that it can be written in terms of $\mathbf{u}$ on the interface Γ_2 as follows:

$$\mathbf{n}\cdot\mathbf{T} = \sum_{\mu=-\infty}^{\infty} \frac{1}{2\pi}\int_0^{2\pi} \mathbf{A}_\mu \mathbf{u}_0(x')\,dx', \tag{3.16}$$

where

$$\mathbf{A}_\mu = \frac{2}{\lambda+3\tau}\begin{pmatrix} \tau(\lambda+2\tau)|\mu| & \tau^2\imath\mu \\ -\tau^2\imath\mu & \tau(\lambda+2\tau)|\mu| \end{pmatrix} \mathrm{e}^{\imath\mu(x-x')}. \tag{3.17}$$

Define the artificial boundary operator $\mathcal{A}$ by the following:

$$\mathcal{A}\mathbf{u}_0(x) = \sum_{\mu=-\infty}^{\infty} \frac{1}{2\pi}\int_0^{2\pi} \mathbf{A}_\mu \mathbf{u}_0(x')\,dx'. \tag{3.18}$$

It is interesting to note that the operator $\mathcal{A}$ is real and symmetric since $\mathbf{A}_\mu(x-x') = \mathbf{A}_\mu^H(x'-x)$.

3.4. The ABC operator for the three dimensional case. We now extend the previous analysis to the three dimensional case by constructing the solution of the homogeneous linear elasticity problem in a semi-infinite domain, Ω_2. Assume that Γ_2 is the plane $z=0$. As in the two dimensional case, assume that in the lateral direction, the solution is periodic with 2π periodicity for both variables, x and y. The following result is the analogue to Lemma 3.1.

LEMMA 3.2. *A solution to* (3.7) *with given boundary data* $\mathbf{u}_0(x,y)$ *on the interface* Γ_2 *is given by the following:*

$$\mathbf{u}(x,y,z) = \frac{1}{4\pi^2}\int_0^{2\pi}\int_0^{2\pi} \mathbf{G}(x-x',y-y',z)\mathbf{u}_0(x',y')\,dx'dy', \tag{3.19}$$

where $\mathbf{G}$ *is defined, using* $c=(\lambda+3\tau)/(\lambda+\tau)$ *and* $d=|(\mu,\nu)|$, *as*

$$\begin{aligned}&\mathbf{G}(x-x',y-y',z)\\ &= \sum_{\mu,\nu=-\infty}^{\infty}\begin{pmatrix} 1+\frac{\mu^2}{cd}z & \frac{\mu\nu}{cd}z & -\frac{\mu}{c}\imath z \\ \frac{\mu\nu}{cd}z & 1+\frac{\nu^2}{cd}z & -\frac{\nu}{c}\imath z \\ -\frac{\mu}{c}\imath z & -\frac{\nu}{c}\imath z & 1-\frac{d}{c}z \end{pmatrix}\mathrm{e}^{dz}\mathrm{e}^{\imath(\mu,\nu)\cdot(x-x',y-y')}.\end{aligned}$$

For the definition of the artificial boundary operator $\mathcal{A}$, note that the normal component of the stress tensor $\mathbf{T}$ is

$$\mathbf{n}\cdot\mathbf{T}=\begin{pmatrix}\mu(\partial_z u+\partial_x w)\\ \mu(\partial_z v+\partial_y w)\\ (\lambda+2\tau)\partial_z w+\lambda(\partial_x u+\partial_y v)\end{pmatrix}, \tag{3.20}$$

where $\mathbf{n}$ is the outer unit normal vector to the interface Γ_2. It is easy to see that

$$\mathbf{n}\cdot\mathbf{T}=\sum_{\mu,\nu=-\infty}^{\infty}\frac{1}{4\pi^2}\int_0^{2\pi}\int_0^{2\pi}\mathbf{A}_{\mu,\nu}\mathbf{u}_0(x',y')\,dx'dy', \tag{3.21}$$

where

$$\mathbf{A}_{\mu,\nu}=\begin{pmatrix}\tau\left(\frac{\mu^2}{cd}+d\right) & \tau\frac{\mu\nu}{cd} & \frac{2\tau^2}{\lambda+3\tau}\imath\mu\\ \tau\frac{\mu\nu}{cd} & \tau\left(\frac{\nu^2}{cd}+d\right) & \frac{2\tau^2}{\lambda+3\tau}\imath\nu\\ -\frac{2\tau^2}{\lambda+3\tau}\imath\mu & -\frac{2\tau^2}{\lambda+3\tau}\imath\nu & (\lambda+2\tau)\left(-\frac{d}{c}+d\right)\end{pmatrix}\mathrm{e}^{\imath(\mu,\nu)\cdot(x-x',y-y')}.$$

Define the artificial boundary operator $\mathcal{A}$ as follows:

$$\mathcal{A}\mathbf{u}_0(x,y)=\sum_{\mu,\nu=-\infty}^{\infty}\frac{1}{4\pi^2}\int_0^{2\pi}\int_0^{2\pi}\mathbf{A}_{\mu,\nu}\mathbf{u}_0(x',y')\,dx'dy'. \tag{3.22}$$

Similarly to the two dimensional case, the operator $\mathcal{A}$ is symmetric.

3.5. The total energy and force balance equation. In this section, we find an alternative total energy formula for (3.2) and also a force balance equation for (3.5) that involve only the domain Ω_1 and Γ_2, using the ABC operator constructed in the previous sections. For convenience, denote $\mathbf{u}_0$ to be the displacement field of $\mathbf{u}$ at Γ_2.

Write the total elastic energy in Ω in terms of the total energy $\mathcal{E}_1$ in Ω_1 and the total energy $\mathcal{E}_2$ in Ω_2 as follows:

$$\begin{aligned}\mathcal{E}_{total}&=\frac{1}{2}\int_\Omega\mathbf{S}:\mathbf{T}\,d\mathbf{x}-\int_\Omega\mathbf{u}\cdot\mathbf{f}\chi\,d\mathbf{x}\\ &=\frac{1}{2}\left\{\int_{\Omega_1}\mathbf{S}:\mathbf{T}\,d\mathbf{x}-\int_{\Omega_1}\mathbf{u}\cdot\mathbf{f}\,d\mathbf{x}\right\}+\frac{1}{2}\int_{\Omega_2}\mathbf{S}:\mathbf{T}\,d\mathbf{x}\\ &=\mathcal{E}_1+\mathcal{E}_2.\end{aligned}$$

Let $\mathcal{L}$ denote the linear elasticity operator:

$$\mathcal{L}\mathbf{u}=\tau\Delta\mathbf{u}+(\lambda+\tau)\nabla(\nabla\cdot\mathbf{u}).$$

Note that $\mathcal{E}_2$ can be written in terms of the boundary data $\mathbf{u}_0(\mathbf{x})$ on the interface Γ_2 as follows:

$$\begin{aligned}\mathcal{E}_2&=\frac{1}{2}\int_{\Omega_2}\mathbf{S}:\mathbf{T}\,d\mathbf{x}\\ &=-\frac{1}{2}\int_{\Omega_2}\mathbf{u}\cdot\mathcal{L}\mathbf{u}\,d\mathbf{x}+\frac{1}{2}\int_{\Gamma_2}\mathbf{u}_0\cdot(\mathbf{n}\cdot\mathbf{T})\,d\Gamma\\ &=\frac{1}{2}\int_{\Gamma_2}\mathbf{u}_0\cdot\mathcal{A}\mathbf{u}_0\,d\Gamma,\end{aligned}$$

where we use the fact that $\mathcal{L}\mathbf{u} = 0$ in the domain Ω_2 and the definition (3.22) of the artificial boundary operator $\mathcal{A}$.

Consequently, the total energy $\mathcal{E}_{total}$ in the domain Ω is

$$\begin{aligned}\mathcal{E}_{total} &= \mathcal{E}_1 + \mathcal{E}_2 \\ &= \frac{1}{2}\int_{\Omega_1} \mathbf{S} : \mathbf{T}\, d\mathbf{x} - \int_{\Omega_1} \mathbf{u}\cdot\mathbf{f} + \frac{1}{2}\int_{\Gamma_2} \mathbf{u}_0 \cdot \mathcal{A}\mathbf{u}_0\, d\Gamma.\end{aligned} \tag{3.23}$$

This is the new formula for the total energy (3.2) that involves only the domain Ω_1 and Γ_2. Now apply integration by parts to the first term in (3.23) and obtain

$$\begin{aligned}\mathcal{E}_{total} = &-\frac{1}{2}\int_{\Omega_1} \mathbf{u}\cdot\mathcal{L}\mathbf{u}\, d\mathbf{x} - \int_{\Omega_1} \mathbf{u}\cdot\mathbf{f}\, d\mathbf{x} \\ &+\frac{1}{2}\int_{\Gamma_2} \mathbf{u}_0\cdot\mathcal{A}\mathbf{u}_0 - \mathbf{u}_0\cdot(\mathbf{n}\cdot\mathbf{T})\, d\Gamma.\end{aligned} \tag{3.24}$$

Application of the variational principle for the new expression of the total energy (3.24) results in the following force balance equations, which use the ABC operator $\mathcal{A}$ in the ABC on Γ_2:

$$\begin{aligned}-\mathcal{L}\mathbf{u} &= \mathbf{f} \qquad \text{in } \Omega_1, \\ \mathbf{n}\cdot\mathbf{T} &= \mathcal{A}\mathbf{u}_0 \quad \text{on } \Gamma_2.\end{aligned}$$

4. The ABCs for discrete elasticity. In this section, we study the analogue of the ABCs for discrete elasticity. In particular, we discuss the solvability (well-posedness) of the discrete strain model in an unbounded or semi-infinite domain.

It is not trivial to show directly the well-posedness of the discrete strain model in an infinite domain. As discussed in Hagstrom and Keller [11], the well-posedness can be derived from a so-called solvability requirement, which is a solvability condition for the exterior domain problem for which the force term is zero. Generally, the validation of this solvability requirement is done by introducing a sum-of-exponentials ansatz for the solution below the artificial boundary. It is difficult, however, to validate this condition fully in an analytic manner [11] except for simple problems such as the Laplace equation. Numerical validation is partially used, since an analytic validation could not be made fully for the current problem of interest.

The importance of the framework developed in this section is that it identifies how the solvability requirement can be used to show well-posedness of the discrete equations posed on the unbounded domain, and also clarifies why an appropriate use of the ABC operator leads to the exact boundary condition. To the best of our knowledge, it is the first attempt to formulate a general discussion on the solvability of discrete systems in an infinite domain in terms of solvability requirements. Furthermore, this formal discussion leads to an understanding of the ABC operator as a Schur complement operator and reveals various properties of the resulting reduced system on the finite domain. These properties of the reduced system are important when one attempts to develop an appropriate solver for the reduced system (see the concluding remark in section 6).

Throughout this section, we assume that the lattice of the discrete strain model is connected [19]. We begin this section by briefly reviewing the discrete elastic model introduced in [21].

4.1. Discrete elasticity. To describe the strain energy at each atom, $\mathbf{i} = (i, j, k)$, introduce the translation operators, $T_k^{\pm}$, and the discrete difference operators, $D_k^{\pm}$, D_k^0, defined as follows:

$$\begin{aligned} T_k^{\pm} f(\mathbf{i}) &= f(\mathbf{i} \pm \mathbf{e_k}), \\ D_k^{+} f(\mathbf{i}) &= \frac{(T_k^{+} - 1) f(\mathbf{i})}{h}, \\ D_k^{-} f(\mathbf{i}) &= \frac{(1 - T_k^{-}) f(\mathbf{i})}{h}, \\ D_k^{0} f(\mathbf{i}) &= \frac{(T_k^{+} - T_k^{-}) f(\mathbf{i})}{2h}, \end{aligned}$$

where h is the lattice constant and $\mathbf{e}_k$ is the vector in the kth direction for $k = 1, 2, 3$ with $\|\mathbf{e}_k\| = h$. Throughout this paper, we assume the lattice constant $h = 1$ for simplicity. We use i for the depth-like index, with $-\infty < i \leq n$. Here n is the maximum height of the material. An ABC is sought at $i = 0$, assuming that there is no force for $i < 0$.

Let $\mathbf{u}(\mathbf{i}) = (u_k(\mathbf{i}))_{k=1,\dots,d}$ be the displacement at the discrete point $\mathbf{i}$ relative to an equilibrium lattice. The discrete strain components defined below ((4.1) and (4.2)) can be used to describe the discrete elastic energy. For $k, \ell = 1, 2, 3$ and $p, q = \pm$,

$$S_{k\ell}^{\pm}(\mathbf{u}(\mathbf{i})) = D_{\ell}^{\pm} u_k(\mathbf{i}), \tag{4.1}$$

$$S_{k\ell}^{pq}(\mathbf{u}(\mathbf{i})) = \frac{1}{2}(D_{\ell}^{q} u_k(\mathbf{i}) + D_k^{p} u_{\ell}(\mathbf{i})). \tag{4.2}$$

The discrete energy density at a point $\mathbf{i}$ is then given by

$$E(\mathbf{i})(\mathbf{u}, \mathbf{u}) = \sum_{k,p} \alpha_k^p (S_{kk}^p(\mathbf{u}))^2 + \sum_{k \neq \ell, p, q} \left\{ 2\beta_{k\ell}^{pq} (S_{k\ell}^{pq}(\mathbf{u}))^2 + \gamma_{k\ell}^{pq} S_{kk}^p(\mathbf{u}) S_{\ell\ell}^q(\mathbf{u}) \right\}.$$

The subsequent discussion uses three constant displacement fields, denoted by $\mathbf{1}_k$ for $k = 1, 2, 3$, for a constant displacement in the kth component. For convenience, denote $\mathbf{1}$ for any constant vector. With some abuse of notation, it is used to denote a constant vector formed by taking the linear combinations of $\mathbf{1}_k$ and $\mathbf{1}_\ell$ with $k \neq \ell$.

The elastic constants should be chosen to ensure positivity of the (total) energy density, as discussed, for example, in [17]. A sufficient condition for the positivity is

$$\min_{k,p} \alpha_k^p \geq \max_{pq} \gamma^{pq} + c \tag{4.3}$$

for some positive constant $c > 0$. One consequence of positivity is that rigid body motions are the only local displacements that entail no internal energy.

A discrete version of the elastic energy density E at a lattice point $\mathbf{i} = (i, j, k)$ is then given as follows:

$$\mathcal{E}_{total} = \mathcal{E}_{total}(\mathsf{U}, \mathsf{U}) = \widetilde{\mathcal{E}}(\mathsf{U}, \mathsf{U}) - (\mathsf{F}, \mathsf{U}), \tag{4.4}$$

where

$$\widetilde{\mathcal{E}}(\mathsf{U}, \mathsf{U}) = \sum_{\mathbf{i}} E(\mathbf{i})(\mathbf{u}, \mathbf{u}), \tag{4.5}$$

$$\begin{aligned} \mathsf{U} &= (U_n, \dots, U_1, U_0, U_{-1}, \dots)^T, \\ \mathsf{F} &= (F_n, \dots, F_1, F_0, F_{-1}, \dots)^T, \end{aligned} \tag{4.6}$$

where U_i and F_i are the vectors of size N consisting of displacement components $\mathbf{u}$ and force components $\mathbf{f}$ at depth i. The total energy formula (4.4) is modified in section 5.3 to include effects of lattice mismatch. Under traction-free (i.e., Neumann) boundary conditions on the surface Γ_1, the external force vector F must be orthogonal to any constant vector field. As shown in (5.6) in section 5.3, this is also true for the effective force due to lattice mismatch in a thin film. Now, due to the boundary condition, the periodic condition in the lateral direction, and Neumann condition on the surface Γ_1, and from the assumption that the lattice is connected, it follows that

$$\widetilde{\mathcal{E}}(\mathsf{U},\mathsf{U}) = 0 \quad \Longleftrightarrow \quad \mathsf{U} = \mathbf{1}; \tag{4.7}$$

see also Martinsson and Babuska [19] for further discussion on connectivity.

As described in detail in section 4.5, the total energy $\mathcal{E}_{total}$ has the following alternative form:

$$\mathcal{E}_{total} = \mathcal{E}_{total}(\mathsf{U},\mathsf{U}) = \frac{1}{2}(\mathbf{H}\mathsf{U},\mathsf{U}) - (\mathsf{F},\mathsf{U}), \tag{4.8}$$

where

$$\mathbf{H} = \begin{pmatrix} \cdots & \cdots & 0 & 0 & 0 & 0 & \cdots \\ \cdots & A_{i+1i+1} & A_{i+1i} & 0 & \ddots & 0 & \vdots \\ \vdots & A_{ii+1} & A_{ii} & A_{ii-1} & 0 & \ddots & \vdots \\ \vdots & 0 & A_{i-1i} & A_{i-1i-1} & A_{i-1i-2} & 0 & \vdots \\ \vdots & \cdots & 0 & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & \cdots & \cdots & \ddots & \ddots & \vdots \end{pmatrix}. \tag{4.9}$$

The discrete strain equations are derived from the following optimization problem:

$$\min \mathcal{E}_{total} = \min \left(\frac{1}{2}(\mathbf{H}\mathsf{U},\mathsf{U}) - (\mathsf{F},\mathsf{U}) \right). \tag{4.10}$$

Note that the off-diagonal block matrices satisfy $A_{i+1i} = A_{ii+1}^T$ for all $i \le n$. Furthermore, since the material is homogeneous below the artificial boundary, $A_{ii+1} = A_{-10}$ and $A_{ii} = A_{00}$ are independent of i for all $i < 0$. Both A_{00} and A_{-10} are invertible. In particular, the proof that A_{-10} is invertible is included in the appendix.

Denote

$$\mathsf{U} = \begin{pmatrix} \mathsf{U}^+ \\ U_0 \\ \mathsf{U}^- \end{pmatrix} \quad \text{and} \quad \mathsf{F} = \begin{pmatrix} \mathsf{F}^+ \\ F_0 \\ 0 \end{pmatrix}, \tag{4.11}$$

in which U^- and U^+ are vectors consisting of all U_i for $i < 0$ and $i > 0$, respectively. The vector F^+ of forces is defined similarly. Correspondingly, write $\mathbf{H}$ as follows:

$$\mathbf{H} = \begin{pmatrix} \mathsf{A}_{II} & \mathsf{A}_{I0}^T & 0 \\ \mathsf{A}_{I0} & A_{00} & \mathsf{B}^T \\ 0 & \mathsf{B} & \mathsf{M} \end{pmatrix}, \tag{4.12}$$

where A_{II} acts on U^+, A_{00} acts on U_0, and M acts on U^-.

An analysis in section 4.2 shows that under an appropriate solvability condition, the optimization problem (4.10) leads to the force balance equation

$$\mathbf{H}\mathsf{U} = \mathsf{F}. \tag{4.13}$$

Moreover, the analysis shows that (4.13) and the optimization problem (4.10) are well-posed.

Since the displacement $\mathbf{u}$ decays as $i \to -\infty$, one might expect that the space ℓ^2 would be the appropriate admissible solution space for the optimization problem (4.10). Coercivity of the operator $\mathbf{H}$ fails, however, for the space ℓ^2, so that it is difficult to show the solvability of the problem (4.10) directly. The solvability requirement of the next section remedies this lack of coercivity.

4.2. The solvability requirement and the general form of the ABC operator. In the region $i < 0$, i.e., below the artificial boundary, the solution of the problem (4.10) satisfies

$$\begin{aligned} A_{-10}U_0 + A_{00}U_{-1} + A_{-10}^T U_{-2} &= 0, \\ A_{-10}U_{-1} + A_{00}U_{-2} + A_{-10}^T U_{-3} &= 0, \\ A_{-10}U_{-2} + A_{00}U_{-3} + A_{-10}^T U_{-4} &= 0, \\ &\vdots\ . \end{aligned} \tag{4.14}$$

The solvability condition is phrased in terms of solutions for (4.14) that are decaying or constant.

Condition 4.1. *There exists an invertible matrix* C *such that for any* $U_0 \in \mathbb{R}^{\mathrm{N}}$, *the vector* $(U_0, U_{-1}, U_{-2}, \dots)$ *with*

$$U_i = \mathsf{C}^i U_0 \quad \forall i \le 0 \tag{4.15}$$

(where C^0 *is the identity matrix) satisfies* (4.14). *In addition,*

$$\mathsf{C}^i U_0 = U_0 \quad \forall i \le 0, \quad \forall\, U_0 \in \operatorname{span}\{\mathbf{1}_k : k = 1, 2, 3\} \quad \textit{and} \tag{4.16}$$

$$\mathsf{C}^i U_0 \to 0 \quad \textit{as} \quad i \to -\infty \quad \forall\, U_0 \in \operatorname{span}\{\mathbf{1}_k : k = 1, 2, 3\}^{\perp}. \tag{4.17}$$

Note that the constant displacement field is a trivial solution to (4.14) since it is the discretization of the differential operator $\mathcal{L}$, which is reflected in the statement (4.16). The second statement (4.17) says that if U_0 is orthogonal to all constant fields, then the solution decays to 0 at infinity.

Condition 4.1, which is validated in section 4.3, has a number of important consequences, as described in the following subsections.

4.2.1. On the general ABC operator $\mathcal{A}$. The general form of the ABC operator, under Condition 4.1, is described in this subsection.

Define the following two special vector spaces:

$$\Theta = \left\{ \mathsf{V} = (V_{-1}, V_{-2}, \dots) : \inf_{\xi \in \mathbb{R}} \|\mathsf{V} + \xi \mathbf{1}\|_{\ell^2} < \infty \quad \Psi(V_i) = 0 \quad \forall i < -1 \right\},$$

where

$$\Psi(V_i) = A_{-10}V_{i+1} + A_{00}V_i + A_{-10}^T V_{i-1}, \tag{4.18}$$

and

$$\Theta^* = \{\mathsf{G} = (G_{-1}, 0, \dots, 0, \dots) : G_{-1} \in \mathbb{R}^{\mathrm{N}}\}. \tag{4.19}$$

It is clear that both spaces Θ and Θ^* are finite dimensional. In particular, due to the constraints (4.18), the space Θ is completely determined by the first two vectors V_{-1} and V_{-2}. Due to Condition 4.1, the dimension of the space Θ is at least N; in fact, as shown below, its dimension is exactly N. By defining $\|\mathsf{V}\|_\Theta = \sum_{k=-1,-2} \|V_k\|_{\ell^2}$ as a norm on Θ, the space Θ is a Banach space, as is Θ^*. The following lemma is simple but important for the subsequent discussion (the proof can be found in the appendix).

LEMMA 4.1. *Under Condition* 4.1*, the matrix* M*, given as*

$$\mathsf{M} = \begin{pmatrix} A_{00} & A_{-10}^T & 0 & 0 & 0 & \cdots \\ A_{-10} & A_{00} & A_{-10}^T & 0 & 0 & \vdots \\ 0 & A_{-10} & A_{00} & A_{-10}^T & 0 & \vdots \\ \vdots & 0 & A_{-10} & A_{00} & \cdots & \vdots \\ \vdots & 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \cdots & \cdots & \ddots & \ddots & \vdots \end{pmatrix}, \tag{4.20}$$

is an isomorphic mapping from Θ *to* Θ^**.*

Since M is isomorphic, the following equation is solvable:

$$\mathsf{M}\mathsf{U}^- = \mathsf{G}, \tag{4.21}$$

where

$$\mathsf{U}^- = (U_{-1}, U_{-2}, U_{-3}, \dots)^T$$
$$\text{and} \quad \mathsf{G} = (-A_{-10}U_0, 0, 0, \dots)^T.$$

In particular, $\mathsf{U}^- = \mathsf{M}^{-1}\mathsf{G}$. Multiplying both sides of this equation by $\mathsf{B} = (A_{-10}^T, 0, \dots, 0)$ yields the relation

$$A_{-10}^T U_{-1} = -\mathsf{B}\mathsf{M}^{-1}\mathsf{B}^T U_0. \tag{4.22}$$

The general form of the ABC operator $\mathcal{A}$ is defined by

$$\mathcal{A} = \mathsf{B}\mathsf{M}^{-1}\mathsf{B}^T. \tag{4.23}$$

Note that the operator $\mathcal{A}$ relates U_{i-1} and U_i for $i \le 0$. Since U^- belongs to the space Θ, U_i should decay as $i \to -\infty$, unless U_0 has a nonzero component that is a constant vector.

4.2.2. The total energy formula for the system above the artificial boundary. This section introduces the new energy formula that is a by-product of the ABC operator.

Since $A_{-10}U_{i+1} + A_{00}U_i + A_{-10}^T U_{i-1} = 0$ and $F_i = 0$ for $i < 0$, the total energy

$\mathcal{E}_{total}$ from (4.8) can be written as follows:

$$\begin{aligned}\mathcal{E}_{total} &= \sum_{i\geq 0} \frac{1}{2}\left(U_i, (A_{ii+1}U_{i+1} + A_{ii}U_i + A_{ii-1}U_{i-1})\right) - (U_i, F_i)\\ &= \frac{1}{2}\left(U_0, \left(A_{01}U_1 + A_{00}U_0 + A_{-10}^T U_{-1}\right)\right) - (U_0, F_0)\\ &\quad + \sum_{i>0} \frac{1}{2}\left(U_i, (A_{ii+1}U_{i+1} + A_{ii}U_i + A_{ii-1}U_{i-1})\right) - (U_i, F_i)\,.\end{aligned}$$

This formula, however, depends on the displacement field U_{-1} below the artificial boundary. To remove this dependence and obtain an energy formula (and a reduced force balance equation) that involves displacement fields only above the artificial boundary, use the operator $\mathcal{A}$ to obtain the following alternative formula:

$$\begin{aligned}\mathcal{E}_{total} &= \frac{1}{2}\left(U_0, (A_{01}U_1 + (A_{00} - \mathcal{A})U_0)\right) - (U_0, F_0)\\ &\quad + \sum_{i>0} \frac{1}{2}\left(U_i, (A_{ii-1}U_{i-1} + A_{ii}U_i + A_{ii+1}U_{i+1})\right) - (U_i, F_i)\,.\end{aligned} \tag{4.24}$$

Note that the energy formula given in (4.24) depends only on the displacement fields U_0 and U^+ above the artificial boundary, but it includes the energy in the strain field below the artificial boundary. In addition, optimization of this formula for the energy yields the reduced equation on the upper domain with the ABC using the operator $\mathcal{A}$, as shown in the next subsection.

4.2.3. The force balance equation. Define the following admissible solution space for the optimization problem (4.10):

$$\mathbf{V} = \left\{\mathsf{V} = (V_n, \dots, V_0, V_{-1}, \dots) : \inf_{\xi\in\mathbb{R}} \|\mathsf{V} + \xi\mathbf{1}\|_{\ell^2} < \infty, \quad \Psi(V_i) = 0 \quad \forall i < 0\right\}.$$

Thanks to Condition 4.1, the force balance equation that results from minimizing the total energy in its reduced form (4.24) is

$$\widehat{\mathbf{H}}\begin{pmatrix}\mathsf{U}^+\\ U_0\end{pmatrix} = \begin{pmatrix}\mathsf{A}_{II} & \mathsf{A}_{I0}^T\\ \mathsf{A}_{I0} & A_{00} - \mathcal{A}\end{pmatrix}\begin{pmatrix}\mathsf{U}^+\\ U_0\end{pmatrix} = \begin{pmatrix}\mathsf{F}^+\\ F_0\end{pmatrix}. \tag{4.25}$$

The reduced form (4.25) of the force balance equation, as well as its properties, is the main result of this work. Note that (4.25) involves the *Schur complement* of the matrix A_{00} in the original force balance equation (4.13).

The properties of the matrices $\mathcal{A}$ and $\widehat{\mathbf{H}}$ are summarized in the following lemma, whose proof is provided in the appendix.

LEMMA 4.2. *The matrix $\mathcal{A}$ is symmetric and positive definite, the matrix $\widehat{\mathbf{H}}$ is symmetric and nonnegative definite, and the null space of $\widehat{\mathbf{H}}$ consists of the constant displacement fields* $\operatorname{span}\{\mathbf{1}_k : k = 1, 2, 3\}$.

The analysis in this section is performed for the Neumann boundary condition at the top boundary Γ_1, by which we mean that the variational principle (4.10) involves no constraint on the solution at Γ_1. In this case, it is most important to note that (4.25) is solvable since (F^+, F_0) belongs to the range of $\widehat{\mathbf{H}}$; namely, (F^+, F_0) is orthogonal to the constant vector fields, which is exactly the null space of $\widehat{\mathbf{H}}$ as noted in Lemma 4.2. In addition, the solution to (4.25) is determined up to a constant

vector. However, the additional contribution of the constant vector does not affect the total energy evaluation since the total energy is invariant with respect to the constant displacement. Furthermore, use of the Neumann condition is only to simplify the analysis. It does not affect the ABC operator $\mathcal{A}$, which can be used for any choice of boundary conditions on the top.

In passing to the next section, we summarize the most important properties of the ABC operator $\mathcal{A}$, which guide its construction.

P1 The operator $\mathcal{A}$ is a symmetric and positive definite matrix mapping $\mathbb{R}^N$ to $\mathbb{R}^N$.

P2 The relation between U_{-1} and U_0 is that $U_{-1} = -(A_{-10}^T)^{-1}\mathcal{A}U_0 = \mathsf{C}U_0$.

4.3. Validation of the solvability requirement, Condition 4.1. In this section, Condition 4.1 is derived by introducing a sum-of-exponentials ansatz. Much of the derivation, including the most crucial steps, is analytic, but some steps are based on numerical evidence. In related work on the Laplace equation, Hagstrom and Keller [11] performed a completely analytic validation of the analogue of Condition 4.1.

The following presentation is mostly based on the thesis of Lee [18] and is similar to the work by Russo and Smereka [20], which used the palindromic eigenvalue problem [15, 16]. Although these works did not state a general solvability condition like Condition 4.1, their analysis is equivalent to a validation of this condition. Throughout this section, denote $\mathcal{F}$ and $\mathcal{F}^{-1}$ to be the discrete forward and backward Fourier transforms, respectively.

4.3.1. Two dimensional case. The force balance equations at a point $(x_m, y_i) = (m, i)$ are

$$\begin{aligned} -(\mathcal{L}\mathbf{u})_1 &= -C_{11}D_x^+D_x^-u - C_{44}D_y^+D_y^-u - (C_{12}+C_{44})D_y^0D_x^0v = 0, \\ -(\mathcal{L}\mathbf{u})_2 &= -C_{44}D_x^+D_x^-v - C_{11}D_y^+D_y^-v - (C_{12}+C_{44})D_x^0D_y^0u = 0. \end{aligned} \tag{4.26}$$

Since the solution is periodic in the x-direction, we introduce the following ansatz:

$$\begin{aligned} \mathbf{u}(m,i) &= \frac{1}{N_x}\sum_{\mu=0}^{N_x-1}\widehat{\mathbf{u}}(\mu,i)\,\mathrm{e}^{2\pi\imath\mu m/N_x} \\ &= \frac{1}{N_x}\sum_{\mu=0}^{N_x-1}\widehat{\mathbf{u}}(\mu)\gamma^i\,\mathrm{e}^{2\pi\imath\mu m/N_x}, \end{aligned} \tag{4.27}$$

where N_x is such that $\mathbf{u}(m,i) = \mathbf{u}(N_x+m,i)$ for all m.

From (4.27), the force balance equations (4.26) become

$$P(\mu,\gamma)\widehat{\mathbf{u}}(\mu,i) = \left(\gamma^2\widehat{A}_{-10}(\mu) + \gamma\widehat{A}_{00}(\mu) + \widehat{A}_{-10}^H(\mu)\right)\widehat{\mathbf{u}}(\mu,i) = 0 \tag{4.28}$$

for $\mu = 0, 1, \ldots, N_x - 1$, where

$$\widehat{A}_{-10}(\mu) = \begin{pmatrix} -C_{44} & -\imath\frac{C_{12}+C_{44}}{2}\sin(2\pi\mu/N_x) \\ -\imath\frac{C_{12}+C_{44}}{2}\sin(2\pi\mu/N_x) & -C_{11} \end{pmatrix},$$

$$\widehat{A}_{00}(\mu) = \begin{pmatrix} 2C_{44}+2C_{11}(1-\cos(2\pi\mu/N_x)) & 0 \\ 0 & 2C_{11}+2C_{44}(1-\cos(2\pi\mu/N_x)) \end{pmatrix},$$

and $\widehat{A}_{-10}^H$ is the complex transpose of the matrix $\widehat{A}_{-10}$.

Nontrivial solutions for this system require that

$$\det P(\mu,\gamma)=0. \tag{4.29}$$

This is the well-known palindromic eigenvalue problem [15, 16, 20]. Note that for $\mu=0$, which corresponds to the constant vector in the Fourier expansion of the solution ansatz (4.27), the only solution to (4.29) is $\gamma=1$, which corresponds to the constant solution to (4.14).

For $\mu\neq 0$, (4.29) has four solutions that occur in pairs $(\gamma_k,\overline{\gamma}_k{}^{-1})$ for $k=1,2$, since

$$\det(P(\mu,\gamma))=0 \quad\Longleftrightarrow\quad \overline{\det(P(\mu,\gamma))}=0 \tag{4.30}$$

and

$$\overline{P(\mu,\gamma)}=\overline{\gamma}^2 P(\mu,\overline{\gamma}^{\,-1}).$$

We then pick a pair of solutions (γ_1,γ_2) with $|\gamma_k|>1$ for $k=1,2$, which are the relevant choices since the corresponding solution is decaying as $i\to-\infty$ for $\mu\neq 0$, and we also pick two linearly independent eigenvectors $\mathbf{q}_1(\mu)$ and $\mathbf{q}_2(\mu)$ that correspond to γ_1 and γ_2, respectively [10, 20]; i.e.,

$$P(\mu,\gamma_1)\mathbf{q}_1(\mu)=P(\mu,\gamma_2)\mathbf{q}_2(\mu)=0. \tag{4.31}$$

It is possible that $|\gamma_k|=1$ or that $\gamma_1=\gamma_2$ and there is a generalized eigenvector, but these possibilities have not been seen numerically. Indeed, the occurrence of a generalized eigenvector in the continuous case (cf. section 3.2) does not seem to have consequences for the discrete case.

We then arrive at the general solution for $\widehat{\mathbf{u}}(\mu,i)$ given as follows:

$$\widehat{\mathbf{u}}(\mu,i)=\mathbf{q}_1(\mu)\gamma_1^i+\mathbf{q}_2(\mu)\gamma_2^i. \tag{4.32}$$

For the zero mode $\mu=0$, two linearly independent vectors $\mathbf{q}_k(0)$ are $\mathbf{q}_1=(1,0)^T$ and $\mathbf{q}_2=(0,1)^T$. Note that omitting this mode would make 0 an eigenvalue for the operator $\mathcal{A}$, but that $\mathcal{A}$ should be positive definite as indicated in property **P1** in subsection 4.2.3.

4.3.2. Three dimensional case. As in the two dimensional case, consider the force balance equations at a point $(x_m,y_n,z_i)=(m,n,i)$:

$$\begin{aligned}
-(\mathcal{L}\mathbf{u})_1 &= -C_{11}D_x^+D_x^-u-C_{44}(D_y^+D_y^-u+D_z^+D_z^-u)\\
&\quad -(C_{12}+C_{44})(D_y^0D_x^0v+D_z^0D_x^0w)\\
&= 0,\\
-(\mathcal{L}\mathbf{u})_2 &= -C_{11}D_y^+D_y^-v-C_{44}(D_x^+D_x^-v+D_z^+D_z^-v)\\
&\quad -(C_{12}+C_{44})(D_y^0D_x^0u+D_z^0D_y^0w)\\
&= 0,\\
-(\mathcal{L}\mathbf{u})_3 &= -C_{11}D_z^+D_z^-w-C_{44}(D_x^+D_x^-w+D_y^+D_y^-w)\\
&\quad -(C_{12}+C_{44})(D_z^0D_x^0u+D_z^0D_y^0v)\\
&= 0.
\end{aligned} \tag{4.33}$$

Introduce the solution ansatz as follows:

$$\mathbf{u}(m,n,i) = \frac{1}{N_x N_y}\sum_{\mu=0}^{N_x-1}\sum_{\nu=0}^{N_y-1}\widehat{\mathbf{u}}(\mu,\nu,i)\,\mathrm{e}^{(2\pi\imath\mu m)/N_x+(2\pi\imath\nu n)/N_y} = \frac{1}{N_x N_y}\sum_{\mu=0}^{N_x-1}\sum_{\nu=0}^{N_y-1}\widehat{\mathbf{u}}(\mu,\nu)\gamma^i\,\mathrm{e}^{(2\pi\imath\mu m)/N_x+(2\pi\imath\nu n)/N_y}, \tag{4.34}$$

where N_x and N_y are the periods in x and y for $\mathbf{u}$. From ansatz (4.34), the force balance equations become

$$P(\mu,\nu,\gamma)\widehat{\mathbf{u}}(\mu,\nu,i) = \left(\gamma^2\widehat{A}_{-10}(\mu,\nu)+\gamma\widehat{A}_{00}(\mu,\nu)+\widehat{A}^H_{-10}(\mu,\nu)\right)\widehat{\mathbf{u}}(\mu,\nu,i) = 0 \tag{4.35}$$

for each $\mu = 0,1,\ldots,N_x$ and $\nu = 0,1,\ldots,N_y$, where $\widehat{A}_{-10} = \widehat{A}_{-10}(\mu,\nu)$ and $\widehat{A}_{00} = \widehat{A}_{00}(\mu,\nu)$ are given by

$$\widehat{A}_{-10} = \begin{pmatrix} -C_{44} & 0 & -s_1 \\ 0 & -C_{44} & -s_2 \\ -s_1 & -s_2 & -C_{11} \end{pmatrix},$$

$$\widehat{A}_{00} = \begin{pmatrix} a_{11} & a_{12} & 0 \\ a_{21} & a_{22} & 0 \\ 0 & 0 & a_{33} \end{pmatrix},$$

in which

$$s_1 = \imath\frac{C_{12}+C_{44}}{2}\sin(2\pi\mu/N_x),$$
$$s_2 = \imath\frac{C_{12}+C_{44}}{2}\sin(2\pi\nu/N_y)$$

and

$$\begin{aligned} a_{11} &= 2C_{11}(1-\cos(2\pi\mu/N_x)) + 2C_{44}(1-\cos(2\pi\nu/N_y)) + 2C_{44},\\ a_{12} &= -(C_{12}+C_{44})\sin(2\pi\mu/N_x)\sin(2\pi\nu/N_y),\\ a_{21} &= a_{12},\\ a_{22} &= 2C_{44}(1-\cos(2\pi\mu/N_x)) + 2C_{11}(1-\cos(2\pi\nu/N_y)) + 2C_{44},\\ a_{33} &= 2C_{44}(1-\cos(2\pi\mu/N_x)) + 2C_{44}(1-\cos(2\pi\nu/N_y)) + 2C_{11}. \end{aligned}$$

A nontrivial solution can be found only if

$$\det P(\mu,\nu,\gamma) = 0. \tag{4.36}$$

As in the two dimensional case, for $\mu = \nu = 0$, the only solution is $\gamma = 1$, and for $(\mu,\nu) \neq (0,0)$, there are three pairs of eigenvalues, namely $(\gamma_k, \overline{\gamma}_k{}^{-1})$ with $|\gamma_k| > 1$ for $k = 1,2,3$, and corresponding eigenvectors $\mathbf{q}_k(\mu,\nu)$ that are mutually linearly independent, from which the general solution can be given as follows:

$$\widehat{\mathbf{u}}(\mu,\nu,i) = \mathbf{q}_1(\mu,\nu)\gamma_1^i + \mathbf{q}_2(\mu,\nu)\gamma_2^i + \mathbf{q}_3(\mu,\nu)\gamma_3^i. \tag{4.37}$$

Note that if the three values γ_k are distinct, then it can be seen directly that there exist three linearly independent eigenvectors $\mathbf{q}_k(\mu,\nu)$ corresponding to the three eigenvalues γ_k (see the appendix). Often in our computation, as seen in the work by Russo and Smereka [20], it happens that $\gamma_k = \gamma_\ell$ with $k \neq \ell$. When this happens, it is difficult to establish analytically the existence of linearly independent eigenvectors; this is always found to be the case, however, in the numerical computations.

4.4. On the discrete ABC operator $\mathcal{A}$ and Condition 4.1. In this section, the ABC operator $\mathcal{A}$ is constructed for the three dimensional case only, since the two dimensional construction is similar but simpler. We first construct the operator C that relates U_{i-1} and U_i by $U_{i-1} = \mathsf{C}U_i$, as indicated in **P2**. We then construct $\mathcal{A} = -(A_{-10}^T)\mathsf{C}$. Finally, we discuss the validation of Condition 4.1.

Note that the Fourier transforms $\widehat{A}_{-10}$ and $\widehat{A}_{00}$ of A_{-10} and A_{00} consist of 3×3 block matrices $\widehat{A}_{-10}(\mu,\nu)$ and $\widehat{A}_{00}(\mu,\nu)$. Since the vectors $\mathbf{q}_i(\mu,\nu)$ from (4.37) are mutually independent, define the following mutually orthonormal vectors:

$$\widetilde{\mathbf{q}}_i = c_i(\mathbf{q}_{i'} \times \mathbf{q}_{i''}),$$

in which each triple (i,i',i'') is a rearrangement of $(1,2,3)$ and the constants c_i's are chosen so that

$$\widetilde{\mathbf{q}}_i \cdot \mathbf{q}_j = \delta_{ij} \quad \text{for } i,j = 1,2,3. \tag{4.38}$$

It follows that

$$\widehat{\mathbf{u}}(\mu,\nu,k-1) = \mathbf{C}(\mu,\nu)\widehat{\mathbf{u}}(\mu,\nu,k), \tag{4.39}$$

in which

$$\mathbf{C}(\mu,\nu) = \begin{pmatrix} \widetilde{\mathbf{q}}_1^T \\ \widetilde{\mathbf{q}}_2^T \\ \widetilde{\mathbf{q}}_3^T \end{pmatrix}^{-1} \begin{pmatrix} \gamma_1^{-1}\widetilde{\mathbf{q}}_1^T \\ \gamma_2^{-1}\widetilde{\mathbf{q}}_2^T \\ \gamma_3^{-1}\widetilde{\mathbf{q}}_3^T \end{pmatrix}. \tag{4.40}$$

The matrix C is

$$\mathsf{C} = \mathcal{F}^{-1}\mathbf{C}\mathcal{F}, \tag{4.41}$$

in which

$$\mathbf{C} = \operatorname{diag}(\mathbf{C}(\mu,\nu))_{\mu=0,\ldots,N_x-1,\nu=0,\ldots,N_y-1}. \tag{4.42}$$

To construct the ABC operator $\mathcal{A}$, multiply $-\widehat{A}_{-10}^H(\mu,\nu)$ by $\mathbf{C}(\mu,\nu)$. Note that $\mathcal{A} = \mathcal{F}^{-1}\mathbf{A}\mathcal{F}$, where $\mathbf{A}$ is a diagonal block matrix consisting of the submatrices $\mathbf{A}(\mu,\nu) = -\widehat{A}_{-10}^H(\mu,\nu)\mathbf{C}(\mu,\nu)$ for $\mu = 0,\ldots,N_x-1$ and $\nu = 0,\ldots,N_y-1$, namely,

$$\mathbf{A} = \operatorname{diag}(\mathbf{A}(\mu,\nu))_{\mu=0,\ldots,N_x-1,\,\nu=0,\ldots,N_y-1}, \tag{4.43}$$

and also for both two and three dimensional cases, the operator $\mathcal{A} = \mathcal{F}^{-1}\mathbf{A}\mathcal{F}$ is symmetric and positive definite. It is quite difficult to see this directly from the Fourier analysis discussed in this section, but it follows from the variational principle based on the general form of the ABC operator as discussed in section 4.2.

Finally, Condition 4.1 can be validated from the construction of the matrix C. For any data $U_0 \in \mathbb{R}^{\mathrm{N}}$ which consists of displacement $\mathbf{u}$ on the interface $i = 0$, the vectors U_i for all $i < 0$ can be written as follows:

$$U_i = \mathcal{F}^{-1}\mathbf{C}^i\mathcal{F}U_0 = \mathsf{C}^i U_0. \tag{4.44}$$

The matrix C is invertible. It satisfies (4.17), because $|\gamma| > 1$ for $(\mu, \nu) \neq 0$, while for $(\mu, \nu) = 0$, $\gamma = 1$ and the corresponding term in (4.34) has no dependence on m and n, so that (4.16) is also satisfied. This completes the validation of Condition 4.1.

4.5. Total energy. In this section we derive alternative general energy formulas that involve a product of stress and strain. Note that in the section 4.2, the energy and the variational principle are written in terms of displacement times force. For some applications, such as a heteroepitaxial thin film, as described in section 5.3, it is much more convenient to write the energy in the form of stress times strain, as in (4.3).

The analysis of this section relies on the following "summation by parts" formulas:

$$\sum_{j\le 0}(D^+f)_j g_j = f_1 g_0 - \sum_{j\le 0} f_j (D^- g)_j, \tag{4.45}$$

$$\sum_{j\le 0}(D^-f)_j g_j = f_0 g_1 - \sum_{j\le 0} f_j (D^+ g)_j, \tag{4.46}$$

$$\sum_{j\le 0}(D^0f)_j g_j = \frac{1}{2}\left(f_1 g_0 + f_0 g_1\right) - \sum_{j\le 0} f_j (D^0 g)_j, \tag{4.47}$$

where D^+, D^-, and D^0 are the forward, backward, and centered finite difference operators, respectively. The total energy can be decomposed into two parts:

$$\mathcal{E}_{total} = \mathcal{E}_{i\ge 0} + \mathcal{E}_{i\le -1}, \tag{4.48}$$

where $\mathcal{E}_{i\ge 0} = \sum_{i\ge 0} E_i$ and $\mathcal{E}_{i\le -1} = \sum_{i\le -1} E_i$, and $i = 0$ is the layer in which the ABCs are imposed. Use (4.45)–(4.47) to derive the following relations, in two and three space dimensions, respectively:

$$\begin{aligned}\mathcal{E}_{i\le -1} = &\sum_{i_1} \alpha v_0 (D_y^+ v)_{-1} + \beta u_0 (D_y^+ u)_{-1} \\ &+ \sum_{i_1} \alpha v_{-1} (D_y^- v)_0 + \beta u_{-1} (D_y^- u)_0 \\ &+ \sum_{i_1} \big[\beta (u_0 (D_x^0 v)_{-1} + u_{-1} (D_x^0 v)_0) \\ &\qquad + \gamma \left(v_0 (D_x^0 u)_{-1} + v_{-1} (D_x^0 u)_0\right)\big] \\ &- \sum_{i_1, i\le -1} \frac{1}{2}\mathbf{u}_i \cdot (\mathcal{L}\mathbf{u}_i) - \mathbf{u}_i \cdot \mathbf{f}_i\end{aligned} \tag{4.49}$$

and

$$
\begin{aligned}
(4.50)\quad \mathcal{E}_{i\le -1} = &\sum_{i_1,i_2} \alpha w_0 (D_z^+ w)_{-1} + \beta (u_0 (D_z^+ u)_{-1} + v_0 (D_z^+ v)_{-1}) \\
&+ \sum_{i_1,i_2} \alpha w_{-1} (D_z^- w)_0 + \beta (u_{-1} (D_z^- u)_0 + v_{-1} (D_z^- v)_0) \\
&+ \sum_{i_1,i_2} \big[\beta \left(v_0 (D_y^0 w)_{-1} + v_{-1} (D_y^0 w)_0 + u_0 (D_x^0 w)_{-1} + u_{-1} (D_x^0 w)_0\right) \\
&\qquad + \gamma \left(w_0 (D_y^0 v)_{-1} + w_{-1} (D_y^0 v)_0 + w_{-1} (D_x^0 u)_0 + w_0 (D_x^0 u)_{-1}\right)\big] \\
&- \sum_{i_1,i_2,i\le -1} \frac{1}{2} \mathbf{u}_i \cdot (\mathcal{L} \mathbf{u}_i) - \mathbf{u}_i \cdot \mathbf{f}_i,
\end{aligned}
$$

in which $\mathcal{L}$ is the operator introduced in (4.26) and (4.33) and $\mathbf{f}_i$ is the force. In these formulas, the subscript refers to the depth-like index i.

Due to the assumption that $\mathbf{f}_i = 0$ for $i \le -1$, the last terms are zero in both the two and three dimensional cases. This leads to the following formulas:

$$
\begin{aligned}
(4.51)\qquad \mathcal{E}_{total} = &\mathcal{E}_{i\ge 0} + \sum_{i_1} \alpha v_0 (D_y^+ v)_{-1} + \beta u_0 (D_y^+ u)_{-1} \\
&+ \sum_{i_1} \alpha v_{-1} (D_y^- v)_0 + \beta u_{-1} (D_y^- u)_0 \\
&+ \sum_{i_1} \big[\beta (u_0 (D_x^0 v)_{-1} + u_{-1} (D_x^0 v)_0) \\
&\qquad + \gamma \left(v_0 (D_x^0 u)_{-1} + v_{-1} (D_x^0 u)_0\right)\big]
\end{aligned}
$$

in two dimensions and

$$
\begin{aligned}
(4.52)\quad \mathcal{E}_{total} = &\mathcal{E}_{i\ge 0} + \sum_{i_1,i_2} \alpha w_0 (D_z^+ w)_{-1} + \beta (u_0 (D_z^+ u)_{-1} + v_0 (D_z^+ v)_{-1}) \\
&+ \sum_{i_1,i_2} \alpha w_{-1} (D_z^- w)_0 + \beta (u_{-1} (D_z^- u)_0 + v_{-1} (D_z^- v)_0) \\
&+ \sum_{i_1,i_2} \big[\beta \left(v_0 (D_y^0 w)_{-1} + v_{-1} (D_y^0 w)_0 + u_0 (D_x^0 w)_{-1} + u_{-1} (D_x^0 w)_0\right) \\
&\qquad + \gamma \left(w_0 (D_y^0 v)_{-1} + w_{-1} (D_y^0 v)_0 + w_{-1} (D_x^0 u)_0 + w_0 (D_x^0 u)_{-1}\right)\big]
\end{aligned}
$$

in three dimensions. In both (4.51) and (4.52), we replace U_{-1} by $\mathsf{C}U_0$ whenever $\mathbf{u}_{-1}$ appears.

If the ABCs are imposed on the layer $i = 0$ where there is no force, then the total energy could be computed by the following new energy formulas that do not involve U_{-1} or the operator C:

$$
\begin{aligned}
(4.53)\qquad \mathcal{E}_{total} = &\mathcal{E}_{i>0} + \sum_{i_1} \alpha v_1 (D_y^+ v)_0 + \beta u_1 (D_y^+ u)_0 \\
&+ \sum_{i_1} \alpha v_0 (D_y^- v)_1 + \beta u_0 (D_y^- u)_1 \\
&+ \sum_{i_1} \big[\beta (u_1 (D_x^0 v)_0 + u_0 (D_x^0 v)_1) \\
&\qquad + \gamma \left(v_1 (D_x^0 u)_0 + v_0 (D_x^0 u)_1\right)\big]
\end{aligned}
$$

in two space dimensions and

$$\begin{aligned}(4.54)\quad \mathcal{E}_{total} = \mathcal{E}_{i>0} &+ \sum_{i_1,i_2} \alpha w_1(D_z^+ w)_0 + \beta(u_1(D_z^+ u)_0 + v_1(D_z^+ v)_0) \\ &+ \sum_{i_1,i_2} \alpha w_0(D_z^- w)_1 + \beta(u_0(D_z^- u)_1 + v_0(D_z^- v)_1) \\ &+ \sum_{i_1,i_2} \big[\beta\left(v_1(D_y^0 w)_0 + v_0(D_y^0 w)_1 + u_1(D_x^0 w)_0 + u_0(D_x^0 w)_1\right) \\ &\qquad + \gamma\left(w_1(D_y^0 v)_0 + w_0(D_y^0 v)_1 + w_0(D_x^0 u)_1 + w_1(D_x^0 u)_0\right)\big]\end{aligned}$$

in three space dimensions, respectively. In both (4.53) and (4.54), we replace U_{-1} by $-(A_{-10}^T)^{-1}\mathcal{A}U_0$ whenever $\mathbf{u}_{-1}$ appears.

5. Numerical results. In this section, sample computations are performed to validate and illustrate the ABCs developed in previous sections. Throughout this section, the elastic constants C_{11}, C_{12}, C_{44} are assumed to be $C_{11} = 8$, $C_{12} = 4$, and $C_{44} = 4$ unless explicitly stated otherwise.

5.1. The ABCs for continuum elasticity. This section shows the effectiveness of the ABCs for continuum elasticity equations (3.7). The Lamé constants are chosen to be $\lambda = 1$ and $\tau = 1$.

The test problem is (3.7) on $\Omega = [0, 2\pi)\times(-\infty, 0)$ with data on $\Gamma_1 = [0, 2\pi)\times\{y = 0\}$. Periodicity is assumed in the lateral direction, and there is no body force; i.e., $\mathbf{f} = 0$. The interface Γ_2 at which the artificial boundary condition is imposed is the line $[0, 2\pi) \times \{y = -1\}$.

The Dirichlet data given on Γ_1 is as follows:

$$\mathbf{u} = (u, v) = (\cos x + \sin 2x, 0),$$

for which the exact solution to (3.7) is

$$(5.1)\qquad \mathbf{u} = \left(\left(1 + \frac{y}{2}\right)\cos x\, \mathrm{e}^y + (1 + y)\sin 2x\, \mathrm{e}^{2y}, \frac{7}{2}\sin x\, \mathrm{e}^y - y\cos 2x\, \mathrm{e}^{2y}\right).$$

This exact solution is compared to the solution of (3.7) with the exact artificial boundary condition (3.16) on the interface Γ_2 and also to the solutions with the following two alternative boundary conditions:

- The zero Dirichlet boundary condition $\mathbf{u}(x, -1) = 0$.
- The Neumann boundary condition $\mathbf{n}\cdot\mathbf{T} = 0$ on $y = -1$.

Figure 5.1 shows the u-displacement field at the line $y = -0.75$ for the exact solution, the solution using ABCs, and the two alternative solutions. Although there is still error, due to discretization of the continuum equation, it is clear that the solution obtained with the exact ABCs (3.16) is in good agreement with the analytic solution (5.1). On the other hand, the solutions obtained with the other two boundary conditions are in error by about 20%–30% at the peaks.

5.2. The ABCs for discrete elasticity. In this section, we investigate the ABCs for the discrete elastic equations for both two and three space dimensions with the Dirichlet data given on the boundary Γ_1. As in the continuum case, there are no external forces, and periodic boundary conditions are imposed in the lateral directions.

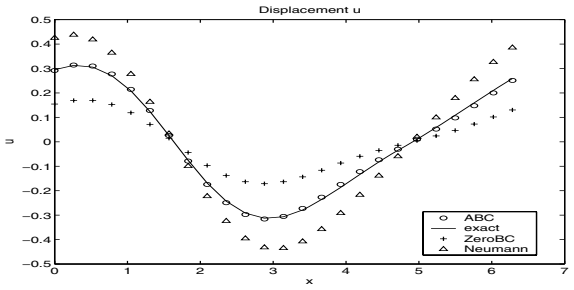

FIG. 5.1. *Test of the ABCs for the continuum solution in two space dimensions. Comparison of the u-displacement field of* $\mathbf{u} = (u, v)$ *given at* $y = -0.75$ *for the exact solution (line) and for the following boundary conditions: ABC (circle), zero-displacement (plus), and Neumann (triangle).*

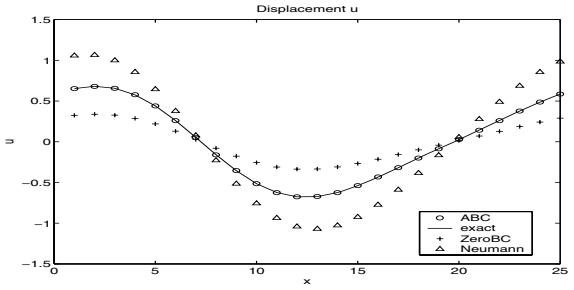

FIG. 5.2. *Test of the exact discrete ABCs in two dimensions: a comparison of the u-displacement field of* $\mathbf{u} = (u, v)$ *at* $(x, y) = (x, 3)$. *The boundary* Γ_1 *is at* $y = 1$, *and the interface* Γ_2 *is at* $y = 5$ *for the exact solution (line) and for the following boundary conditions: ABC (circle), zero-displacement (plus), and Neumann (triangle).*

More precisely, for the two dimensional case, the lattice Ω consists of $N_x = 25$ layers in the x-direction and $N_y = 5$ in the y-direction, and the prescribed Dirichlet boundary condition for $\mathbf{u}$ on $\Gamma_1 = \{y = 1\}$ is

$$\mathbf{u} = (\cos x + \sin 2x, \sin x). \tag{5.2}$$

For the three dimensional case, the lattice Ω consists of $N_x = N_y = 25$ layers in the x- and y-directions and $N_z = 4$ layers in the z-direction, and the Dirichlet data on $\Gamma_1 = \{z = 1\}$ is

$$\mathbf{u} = (\cos x + \sin 2x, \sin y, \sin x). \tag{5.3}$$

Numerical results are plotted in Figures 5.2 and 5.3. For numerical experiments, the exact ABCs and other approximate boundary conditions are imposed on $\Gamma_2 = \{y = 5\}$ for the two dimensional case and $\Gamma_2 = \{z = 4\}$ for the three dimensional case, respectively. The results show that the solution with the ABCs is much more accurate than those from the Dirichlet and Neumann boundary conditions. Indeed, the accuracy obtained with the ABCs operator is within the round-off error, i.e., $O(10^{-14})$.

5.3. Numerical simulations for thin films. In heteroepitaxial growth, a thin film of one material (e.g., Ge) is grown on top of a substrate of a second material (e.g., Si), with perfect, single crystalline structure in both materials and with the lattice

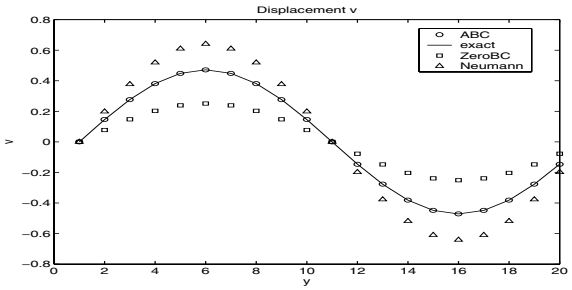

FIG. 5.3. *Test of the exact discrete ABCs in three dimensions: a comparison of the v-displacement field of* $\mathbf{u} = (u, v, w)$ *at* $(x, y, z) = (10, y, 3)$. *The boundary* Γ_1 *is at* $z = 1$, *and the interface* Γ_2 *is at* $z = 4$ *for the exact solution (line) and for the following boundary conditions: ABC (circle), zero-displacement (square), and Neumann (triangle).*

structure of the film determined by the substrate. If the lattice constants a_f and a_s for the film and substrate are different (e.g., $a_{Ge} = 1.04 \times a_{Si}$), then strain is generated in the film. This strain has important effects on the material structure, as well as on its electronic properties.

For this system, it is most convenient to define the atomic displacement relative to a single reference lattice, for example, the equilibrium lattice of the substrate, so that the displacement $\mathbf{u}$ in the film is defined relative to a nonequilibrium reference lattice. The bond displacement $\mathbf{d}^{\mathbf{k}\pm}$ is then

$$\mathbf{d}^{\mathbf{k}\pm}(\mathbf{i}) = (d_1^{k\pm}, d_2^{k\pm}, d_3^{k\pm}) = D_k^{\pm}\mathbf{u}(\mathbf{i}) - \epsilon \mathbf{e}_{\mathbf{k}}\chi, \tag{5.4}$$

in which $\epsilon = \frac{a_f - a_s}{a_s}$ is the relative lattice displacement, and χ is 0 in the substrate and 1 in the film. The resulting discrete strain equations have a force of size ϵ along the film/substrate interface, and the energy has the form

$$\mathcal{E}_{total} = \frac{1}{2}(\mathbf{H}\mathsf{U}, \mathsf{U}) - (\mathsf{F}, \mathsf{U}) + \mathcal{G}(\epsilon), \tag{5.5}$$

where

$$(\mathsf{F}, \mathsf{U}) = \sum_i \sum_{p=\pm, k=1,2,3} \epsilon\, D_k^p u_k \chi. \tag{5.6}$$

Further details are given, for example, in [5].

In this section, we compare the displacement fields $\mathbf{u}$ that are computed with the ABCs and with zero boundary conditions for a heteroepitaxial thin film. Since the forces lie on the film/substrate boundary, the artificial boundary can be taken to be any plane below this interface. Our computational domain is three dimensional with Γ_2 being of size 10×10. As in the last section, we denote NC to be the thickness of the substrate, including Γ_2. Note that on the top boundary Γ_1, the homogeneous Neumann boundary condition (no external force) is imposed.

To demonstrate the effectiveness of the ABCs, we first compute the displacement field $\mathbf{u}$ by imposing the ABCs on Γ_2 with substrate thickness NC = 1 and take it as the reference solution. We then compute two displacement fields that are generated by imposing zero boundary conditions on the bottom boundary with NC = 2 and NC = 8. For these three solutions, Figure 5.4 shows a comparison of the u component

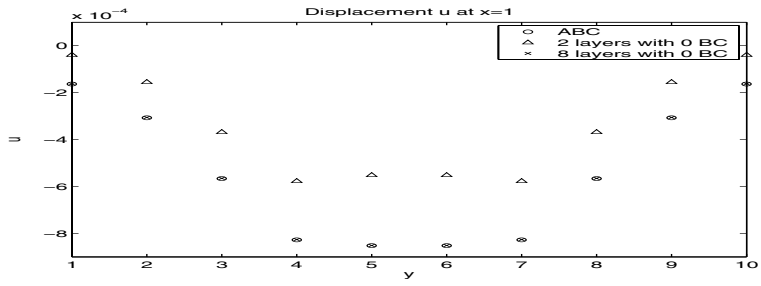

FIG. 5.4. *The comparison of u-displacement on the second layer from the top boundary* Γ_1 *with* $x = 1$. *The u-displacement computed with the ABC (circle) imposed on the first substrate layer and u-displacement computed with zero boundary condition with* NC $= 2$ *(triangle) and* NC $= 8$ *(cross).*

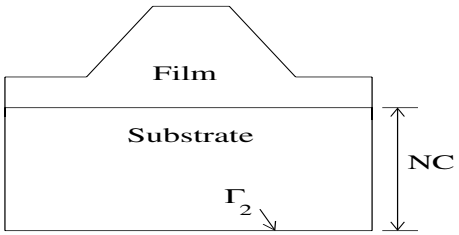

FIG. 5.5. *Schematic drawing of quantum dot geometry.*

of the displacement vector $\mathbf{u} = (u, v, w)$ on the line $x = 1$ in the second layer from the top. It is clear that the displacement field computed with the zero boundary conditions approaches the reference displacement field as the number of substrate layers increases. In addition (not shown in Figure 5.4), the results from the ABC are found to be independent (i.e., within round-off error) of the depth at which the ABC is applied.

5.4. Energy computation. This section presents results to validate the total energy formulas (4.51) and (4.52) derived in section 4.5. As in the previous section, NC denotes the number of substrate layers, including Γ_2 itself. In addition, E_A denotes the total energy computed by imposing the ABC on Γ_2, and E_Z denotes the total energy computed with the zero boundary condition on Γ_2.

For computational purposes, we take a geometry corresponding to a periodic array of quantum dots. A typical geometry is illustrated in Figure 5.5. For two space dimensions, Γ_2 is one dimensional with the material system of size $N_x = 128$ and the quantum dot of base size 64. For three space dimensions, Γ_2 is two dimensional with the material system of size $N_x = N_y = 10$ and the quantum dot of base size 8×8.

In order to validate the total energy formulas (4.51) and (4.52), by numerical computation we show first that the total energy E_A does not depend on the thickness of the substrate NC and second that the total energy E_Z obtained by imposing zero boundary conditions on Γ_2 approaches the total energy E_A as the thickness of substrates NC increases. These computational results are demonstrated in Figure 5.6, in which the thickness of the substrate NC varies from NC $= 2$ to NC $= 120$ for two space dimensions and from NC $= 2$ to NC $= 14$ for three space dimensions. The units of the total energy are 10^{12}dyne/cm^2.

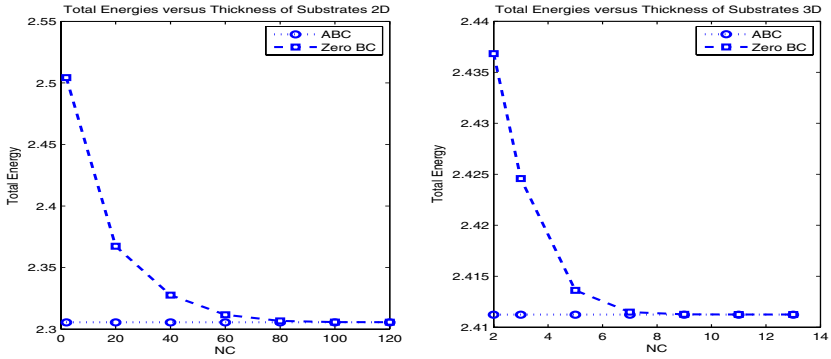

FIG. 5.6. *Total energies obtained by applying the ABC (circle) and zero boundary condition (square) as a function of the thickness of substrates for two dimensions (left) ($N_x = 128$) and three dimensions (right) ($N_x = N_y = 10$).*

6. Conclusions. In this paper, we have derived the ABCs for continuum and discrete elasticity equations. A solvability condition has been formulated and validated, under which the discrete equations in an unbounded domain can be shown to be well-posed and the reduced force balance equation can be derived. Its solution coincides with the exact solution when restricted to the bounded domain. Furthermore, a new total energy formula has been derived so that it can be computed by using only the displacement field in the region above the artificial boundary.

These results are currently being used for modeling and simulation of the growth of thin epitaxial films. By exploiting the symmetry of the resulting force balance equations in further work, we shall combine the ABCs with a multigrid method to get an accelerated simulation method for various applications.

Appendix. Several technical lemmas.

LEMMA A.1. *The matrix A_{-10} is invertible.*

Proof. Observe that

$$A_{-10}U_i = \mathcal{F}^{-1}\widehat{A}_{-10}\mathcal{F}(U_i), \tag{A.1}$$

where $\mathcal{F}$ and $\mathcal{F}^{-1}$ are Fourier and inverse Fourier transformations and $\widehat{A}_{-10}$ is a 3×3 (2×2 in two space dimensions) block matrix, such that for any given Fourier mode (μ,ν),

$$\widehat{A}_{-10}(\mu,\nu) = \begin{pmatrix} -C_{44} & 0 & -s_1 \\ 0 & -C_{44} & -s_2 \\ -s_1 & -s_2 & -C_{11} \end{pmatrix}, \tag{A.2}$$

where

$$s_1 = \imath\frac{(C_{12}+C_{44})}{2}\sin\left(\frac{2\pi\mu}{N_x}\right),$$
$$s_2 = \imath\frac{(C_{12}+C_{44})}{2}\sin\left(\frac{2\pi\nu}{N_y}\right).$$

The eigenvalues for $\widehat{A}_{-10}(\mu,\nu)$ can be obtained by solving the following equation:

$$\begin{aligned}\det(\widehat{A}_{-10}(\mu,\nu)-\lambda \mathrm{I}) &= -(C_{44}+\lambda)\left[(C_{44}+\lambda)(C_{11}+\lambda)-s_1^2-s_2^2\right]\\ &= -(C_{44}+\lambda)\left[\lambda^2+(C_{11}+C_{44})\lambda+C_{11}C_{44}\right.\\ &\qquad +\sin^2(2\pi\mu/N_x)(C_{12}+C_{44})^2/4\\ &\qquad \left.+\sin^2(2\pi\nu/N_y)(C_{12}+C_{44})^2/4\right].\end{aligned} \tag{A.3}$$

Hence, three eigenvalues λ_1,λ_2, and λ_3 are given as follows:

$$\begin{aligned}\lambda_1 &= -C_{44},\\ 2\lambda_2 &= -(C_{11}+C_{44})\\ &\quad +\sqrt{(C_{11}-C_{44})^2-(\sin^2(2\pi\mu/N_x)+\sin^2(2\pi\nu/N_y))(C_{12}+C_{44})^2},\\ 2\lambda_3 &= -(C_{11}+C_{44})\\ &\quad -\sqrt{(C_{11}-C_{44})^2-(\sin^2(2\pi\mu/N_x)+\sin^2(2\pi\nu/N_y))(C_{12}+C_{44})^2}.\end{aligned}$$

The eigenvalue with the smallest magnitude is λ_2 with $\sin(2\pi\nu/N_x)=\sin(2\pi\mu/N_y)=0$, in which case

$$2\lambda_2 = (-(C_{11}+C_{44})+|C_{11}-C_{44}|) = -2\min(C_{11},C_{44}). \tag{A.4}$$

It follows that no eigenvalues can be zero; hence A_{-10} is invertible. This completes the proof. ∎

LEMMA A.2. *For $\gamma_i \neq \gamma_j$, the corresponding eigenvectors $\mathbf{q}_i$ and $\mathbf{q}_j$ are linearly independent.*

Proof. Consider the linear reformulation of the palindromic eigenvalue problem (4.30) by introducing $x=\gamma y$ as follows: With $P(\mu,\nu,\gamma)=\gamma^2\widehat{A}_{-10}+\gamma\widehat{A}_{00}+\widehat{A}_{-10}^H$,

$$\begin{pmatrix} 0 & I \\ -\widehat{A}_{-10}^H & -\widehat{A}_{00}\end{pmatrix}\begin{pmatrix} y\\ x\end{pmatrix} = \gamma\begin{pmatrix} I & 0\\ 0 & \widehat{A}_{-10}\end{pmatrix}\begin{pmatrix} y\\ x\end{pmatrix}. \tag{A.5}$$

From the fact that $\widehat{A}_{-10}$ is invertible, it is obvious that the eigenvectors $\mathbf{q}_i$ and $\mathbf{q}_j$ that correspond to different eigenvalues γ_i and γ_j must be linearly independent. ∎

LEMMA A.3. *Under Condition* 4.1, *the matrix* M *given in* (4.20) *is an isomorphic mapping from* Θ *to* Θ^*.

Proof. For $\mathsf{V}^- = (V_{-1},V_{-2},\dots)^T \in \Theta$ with $V_i = \mathsf{C}^i V_0$ for $i\le 0$, as in Condition 4.1,

$$\begin{aligned}\mathsf{M}\mathsf{V}^- &= (-A_{-10}V_0,0,\dots,0,\dots)^T\\ &= \mathsf{G} = (G_{-1},0,\dots,0,\dots)^T\end{aligned} \tag{A.6}$$

if $G_{-1}=-A_{-10}V_0$. Since A_{-10} is invertible, this shows that the matrix M is onto.

To show that M is one to one, it is enough to show that $\mathsf{M}\mathsf{V}^-=0$ implies $\mathsf{V}^-=0$. Consider the energy

$$\mathcal{E}^- = \sum_{i<0} E_i \tag{A.7}$$

over the space Θ and observe that

$$(\mathsf{M}\mathsf{V}^-,\mathsf{V}^-) = \widehat{\mathcal{E}}^-, \tag{A.8}$$

in which $\widehat{\mathcal{E}}^-$ is $\mathcal{E}^-$ for $V_0 = 0$. Therefore, $\mathsf{MV}^- = 0$ implies that $\widehat{\mathcal{E}}^- = 0$. Connectivity of the lattice and $U_0 = 0$ then imply that $U_i = 0$ for all $i < 0$. This shows that the matrix M is one to one. Therefore, $\mathsf{M} : \Theta \mapsto \Theta^*$ is isomorphic. ∎

Proof of Lemma 4.2.

First, we show that $\mathcal{A}$ is symmetric. For any $\mathsf{U} = (0, 0, \dots, 0, U_0, U_{-1}, \dots, \dots)^T$ and $\mathsf{V} = (0, 0, \dots, 0, V_0, V_{-1}, \dots, \dots)^T$ that belong to the space $\mathbf{V}$, Condition 4.1 implies that

$$A_{-10}^T V_{-1} = -\mathcal{A} V_0 \quad \text{and} \quad A_{-10}^T U_{-1} = -\mathcal{A} U_0. \tag{A.9}$$

Note also that $\widetilde{\mathcal{E}}(\mathsf{U}, \mathsf{V}) = \widetilde{\mathcal{E}}(\mathsf{V}, \mathsf{U})$; i.e.,

$$\begin{aligned} \widetilde{\mathcal{E}}(\mathsf{U}, \mathsf{V}) &= \frac{1}{2}\left(U_0, \left(A_{00} V_0 + A_{-10}^T V_{-1}\right)\right) \\ &= \frac{1}{2}\left(V_0, \left(A_{00} U_0 + A_{-10}^T U_{-1}\right)\right) = \widetilde{\mathcal{E}}(\mathsf{V}, \mathsf{U}). \end{aligned} \tag{A.10}$$

Use (A.9) in (A.11) to obtain

$$(U_0, (A_{00} V_0 - \mathcal{A} V_0)) = (V_0, (A_{00} U_0 - \mathcal{A} U_0)).$$

Since A_{00} is symmetric, this implies that $(U_0, \mathcal{A} V_0) = (V_0, \mathcal{A} U_0)$ for all $U_0, V_0 \in \mathbb{R}^N$ and therefore, that $\mathcal{A}$ is symmetric. The symmetry of the operator $\mathcal{A}$ implies that the matrix $\widehat{\mathbf{H}}$ is symmetric.

Next, we show that $\mathcal{A}$ is positive definite since for $U_0 \neq 0 \in \mathbb{R}^N$,

$$\begin{aligned} (U_0, \mathcal{A} U_0) &= (U_0, \mathsf{B}\mathsf{M}^{-1}\mathsf{B}^T U_0) = (\mathsf{B}^T U_0, \mathsf{M}^{-1}\mathsf{B}^T U_0) \\ &= (\mathsf{M}\mathsf{U}^-, \mathsf{M}^{-1}\mathsf{M}\mathsf{U}^-) = (\mathsf{M}\mathsf{U}^-, \mathsf{U}^-) = \widehat{\mathcal{E}}^- > 0, \end{aligned}$$

where U^- is the unique solution of $\mathsf{M}\mathsf{U}^- = \mathsf{B}^T U_0$. Finally, we show that the matrix $\widehat{\mathbf{H}}$ is nonnegative definite. First note that $\widehat{\mathbf{H}}\mathbf{1} = 0$. Furthermore, there is no other null space for $\widehat{\mathbf{H}}$, since

$$\begin{aligned} \widehat{\mathbf{H}} \begin{pmatrix} \mathsf{U}^+ \\ U_0 \end{pmatrix} = 0 &\Longleftrightarrow (U_0, (A_{01} U_1 + (A_{00} - \mathcal{A}) U_0)) \\ &\quad + \sum_{i>0} (U_i, (A_{ii-1} U_{i-1} + A_{ii} U_i + A_{ii+1} U_{i+1})) = 0 \\ &\Longleftrightarrow \widetilde{\mathcal{E}}(\mathsf{U}, \mathsf{U}) = 0 \quad \text{with} \quad \mathsf{U} \in \mathbf{V} \\ &\Longleftrightarrow \mathsf{U} = \mathbf{1} \quad \text{by connectivity of the lattice.} \end{aligned}$$

This completes the proof of Lemma 4.2. ∎

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