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ON LOCAL ALGORITHMS FOR ELECTROSTATICS

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Abstract. We study finite-difference approximations of the Poisson–Boltzmann (PB) electrostatic energy functional of ionic concentrations and electric displacements constrained by Gauss' law and the ionic mass conservation, and a class of local algorithms for minimizing the finite-difference discretized such energy functional. We prove that the discrete Boltzmann distributions characterize the finite-difference minimizer and obtain the uniform bounds and optimal error estimates in maximum norm for such a minimizer. The local algorithm is an iteration over all the grid boxes that locally minimizes the energy by updating the concentrations and displacement one grid box at a time, keeping Gauss' law and the mass conservation satisfied. A new local algorithm with a shift is constructed for minimizing the Poisson electrostatic energy (the part of the PB energy without ionic concentrations) with a variable dielectric coefficient. We prove the convergence of these local algorithms and present numerical tests to demonstrate the results of our analysis.

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1. Introduction

We study a class of local algorithms [3, 24, 25, 27, 35] for minimizing the non-dimensionalized Poisson–Boltzmann (PB) [2, 6, 10, 17, 43] electrostatic energy functional with constraints for periodic structures:

$$\text{Minimize} \qquad F[c, D] = \int_\Omega \left(\frac{1}{2\varepsilon}|D|^2 + \sum_{s=1}^{M} c_s \log c_s \right) \mathrm{d}x \qquad \text{(PB energy)}, \tag{1.1}$$

$$\text{subject to} \qquad \nabla \cdot D = \rho + \sum_{s=1}^{M} q_s c_s \quad \text{in } \Omega \qquad \text{(Gauss' law)}, \tag{1.2}$$

$$\int_\Omega c_s \, \mathrm{d}x = N_s, \quad s = 1, \ldots, M \qquad \text{(Conservation of mass)}. \tag{1.3}$$

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Here, $\Omega = (0, L)^3$ for some $L > 0$, $\varepsilon > 0$ and ρ are given variable dielectric coefficient and fixed charge density, respectively, $c = (c_1, \ldots, c_M)$ with each $c_s \geq 0$ the concentration of ions of the sth species (a total of M species assumed), and D is the vector field of electric displacement. For each s, $q_s \neq 0$ is the charge of an ion of species s and $N_s > 0$ is the total amount of concentrations of such ions, both known.

Let us cover $\overline{\Omega}$ with a finite-difference grid of size h. We approximate the displacement at half-grid points by $D_{i+1/2,j+1/2,k+1/2} = (u_{i+1/2,j,k}, v_{i,j+1/2,k}, w_{i,j,k+1/2})$ [21,26,40] and concentrations $c = (c_1, \ldots, c_M)$ at grid points by $c_{s,i,j,k} \geq 0$ for all s, i, j, k. The PB energy and Gauss' law are discretized by

$$F_h[c, D] := \frac{h^3}{2} \sum_{i,j,k} \left(\frac{u^2_{i+1/2,j,k}}{\varepsilon_{i+1/2,j,k}} + \frac{v^2_{i,j+1/2,k}}{\varepsilon_{i,j+1/2,k}} + \frac{w^2_{i,j,k+1/2}}{\varepsilon_{i,j,k+1/2}} \right) + h^3 \sum_s \sum_{i,j,k} c_{s,i,j,k} \log c_{s,i,j,k},$$

$$u_{i+1/2,j,k} - u_{i-1/2,j,k} + v_{i,j+1/2,k} - v_{i,j-1/2,k} + w_{i,j,k+1/2} - w_{i,j,k-1/2} = h \left(\rho^h_{i,j,k} + \sum_s q_s c_{s,i,j,k} \right),$$

respectively, where $\varepsilon_{i+1/2,j,k} = (\varepsilon(x_i, y_j, z_k) + \varepsilon(x_{i+1}, y_j, z_k))/2$ and $\varepsilon_{i,j+1/2,k}$ and $\varepsilon_{i,j,k+1/2}$ are similarly defined, and ρ^h is an approximation of ρ. The mass conservation can be discretized similarly. The local algorithm for minimizing the finite-difference PB energy functional with the constraints is to locally update the discretized ionic concentrations and displacement one grid box at a time to relax the energy while keeping the discretized Gauss' law and mass conservation satisfied. For instance, we update the concentration c_s and displacement D at neighboring grids, *e.g.*, (i, j, k) and $(i + 1, j, k)$, and at the edge connecting them, respectively, by

$$c_{s,i,j,k} \leftarrow c_{s,i,j,k} - \zeta, \quad c_{s,i+1,j,k} \leftarrow c_{s,i+1,j,k} + \zeta, \quad \text{and} \quad u_{i+1/2,j,k} \leftarrow u_{i+1/2,j,k} - hq_s\zeta,$$

with a single parameter ζ that can be computed readily to minimize the perturbed PB energy.

The PB model of electrostatics has many applications [2,7,13,36] and the periodic boundary conditions are commonly used for simulations of electrostatics [11,33,34]. The local algorithm was initially proposed for Monte Carlo simulations of the Poisson electrostatics and then extended to the PB electrostatics [3,24,25,27,35]. The discretization of displacement is a classical scheme for Maxwell's equation for isotropic media [21,26,40]. The constrained variational model that is the basis for the local algorithm has been extended to model ionic size effects [5,14,16,19,44]. Such a variational formulation, which seeks the minimizer of a convex functional rather than a saddle point of a nonconvex functional, preserves physical constraints and ensures stability at the discrete level [32,44]. Recently, the local algorithm has been incorporated into numerical methods for solving the Poisson–Nernst–Planck equations [30–32]. The locality of the algorithm makes it appealing for combining them with the fast binary level-set method for molecular simulations with a variational approach [23,41,42]. Potentially, the local algorithms are attractive for parallel implementations. The desirable properties and initial applications of local algorithms motivate a rigorous numerical analysis of such algorithms, which is the main contribution of this work.

We study the finite-difference approximations of the constrained electrostatic energy functional, the error estimates of such approximations, and the local algorithm for minimizing such energy. While we focus on the PB electrostatics, we also consider the Poisson electrostatics (*i.e.*, without ions) as it has a wide range of applications and the local algorithm was initially developed for such electrostatics. We present the analysis results for the Poisson case but omit most of their proofs as they are similar to (and often easier than) the PB case.

Let us now briefly describe and discuss our main results.

(1) *Characterization of finite-difference minimizers.* The unique minimizer $(c^h_{\min}, D^h_{\min})$ of the discrete constrained PB energy F_h is characterized by (i) the local equilibrium conditions that consist of the discrete Boltzmann distributions

$$\nabla_h \log c^h_{\min,s} = -q_s \nabla_h \phi^h_{\min} \quad (1 \leq s \leq M) \qquad \text{and} \qquad D^h_{\min} = -\varepsilon \nabla_h \phi^h_{\min},$$

where ∇_h is the discrete gradient and $\phi^h_{\min}$ is the discrete electrostatic potential which is the solution to the discrete charge-conserved PB equation (CCPBE), and (ii) the uniform bounds

$$0 < C_1 \le c^h_{\min,s} \le C_2 \qquad (s = 1, \ldots, M) \tag{1.4}$$

with C_1 and C_2 independent of h; cf. Theorems 2.1 and 2.2. A comparison argument [18] is used to obtain the bounds (1.4). We also characterize the minimizer of the Gauss' law constrained, discrete Poisson energy given by (1.1) and (1.2) without ions; cf. Theorem 2.3.

(2) *Error estimates.* Let $(c_{\min}, D_{\min})$ be the minimizer of the functional F with the constraints (cf. (1.1)–(1.3)). We prove the finite-difference error estimate

$$\|c_{\min} - c^h_{\min}\|_\infty + \|\mathscr{P}_h D_{\min} - D^h_{\min}\|_\infty \le Ch^2,$$

where $(\mathscr{P}_h D)_{i,j,k} = (u(x_{i+1/2,j,k}), v(y_{i,j+1/2,k}), w(z_{i,j,k+1/2}))$ and $C > 0$ is a constant independent of h; cf. Theorem 3.1. The proof relies on the uniform boundedness (1.4), a property of diagonally dominated matrix [38,39], and the known L^∞-stability for the discrete inverse Laplacian [4,28,29].

(3) *Convergence of the local algorithm.* The proof is based on the fact that $\delta^{(k)} \to 0$, where $\delta^{(k)}$ is the energy difference after the kth local update, and that the amount of perturbation of concentrations and displacement in each local update are controlled by the energy difference. Therefore, in the limit, the local equilibrium conditions are satisfied; cf. Theorem 4.1.

(4) *A new local algorithm with shift for minimizing the Poisson's energy with a variable dielectric coefficient* ε. Each local update in the original local algorithm for relaxing the discrete Poisson energy does not change $\sum_{i,j,k} D_{i+1/2,j+1/2,k+1/2}$ but will change $\sum_{i,j,k} (D/\varepsilon)_{i+1/2,j+1/2,k+1/2}$, not preserving the global constraint, if ε is not a constant. Therefore, the algorithm may not converge in general. To resolve this issue, we propose a new algorithm with a simple global shift to translate the displacement after many cycles of local updates to satisfy the required global constraint, with negligible computational cost. We prove the convergence of our new local algorithm; cf. Theorem 4.3.

(5) *Numerical tests.* We present numerical tests to demonstrate the results of our analysis on the error estimates and the convergence of local algorithms; cf. Section 5.

We end our introduction with a precise statement of the minimizer of the constrained variational problem for both PB and Poisson energy. We denote by $C_{\text{per}}(\overline{\Omega})$, $C^k_{\text{per}}(\overline{\Omega})$ $(k \in \mathbb{N})$, $L^p_{\text{per}}(\Omega)$ $(1 \le p \le \infty)$, and $W^{k,p}_{\text{per}}(\Omega)$, respectively, the subspaces of $\overline{\Omega}$-periodic C, C^k, L^p, and $W^{k,p}(\Omega)$ functions [1,9,12]. (Note that any $\phi \in L^p(\Omega)$ can be extended $\overline{\Omega}$-periodically to $\mathbb{R}^3$.) We define

$$\mathring{L}^p_{\text{per}}(\Omega) = \left\{ \phi \in L^p_{\text{per}}(\Omega) : \mathscr{A}_\Omega(\phi) = 0 \right\},$$
$$\mathring{W}^{k,p}_{\text{per}}(\Omega) = \left\{ \phi \in W^{k,p}_{\text{per}}(\Omega) : \mathscr{A}_\Omega(\phi) = 0 \right\},$$

where

$$\mathscr{A}_A(u) = \frac{1}{|A|} \int_A u \, \mathrm{d}x,$$

if $A \subset \mathbb{R}^d$ is a Lebesgue measurable set of finite Lebesgue measure $|A| > 0$ and u is Lebesgue integrable on A. We denote $H^k_{\text{per}}(\Omega) = W^{k,2}_{\text{per}}(\Omega)$, $\mathring{H}^k_{\text{per}}(\Omega) = \mathring{W}^{k,2}_{\text{per}}(\Omega)$, and

$$H(\text{div}, \Omega) = \{ D \in L^2(\Omega, \mathbb{R}^d) : \nabla \cdot D \in L^2(\Omega) \},$$

where $\nabla \cdot D$ is understood in the weak sense [37]. Note that $H(\text{div}, \Omega)$ is a Hilbert space with the norm $\|D\|_{H(\text{div},\Omega)} = \|D\|_{L^2(\Omega)} + \|\nabla \cdot D\|_{L^2(\Omega)}$ [37]. We denote by $H_{\text{per}}(\text{div}, \Omega)$ the $H(\text{div}, \Omega)$–closure of $C^1_{\text{per}}(\overline{\Omega}, \mathbb{R}^3)$–functions.

Let $\varepsilon \in L^\infty_{\rm per}(\Omega)$ and $\rho \in L^2_{\rm per}(\Omega)$. We assume

$$\text{Positive bounds:} \qquad 0 < \varepsilon_{\min} \le \varepsilon(x) \le \varepsilon_{\max} \qquad \forall x \in \Omega, \tag{1.5}$$

$$\text{Charge neutrality:} \qquad \sum_{s=1}^M q_s N_s + \int_\Omega \rho \, {\rm d}x = 0, \tag{1.6}$$

where $\varepsilon_{\min}$ and $\varepsilon_{\max}$ are two positive constants. We define $I : H^1_{\rm per}(\Omega) \to \mathbb{R} \cup \{+\infty\}$ by

$$I[\phi] = \int_\Omega \left(\frac{\varepsilon}{2} |\nabla \phi|^2 - \rho\phi \right) {\rm d}x + \sum_{s=1}^M N_s \log \left(\mathscr{A}_\Omega (e^{-q_s\phi}) \right) \qquad \forall \phi \in H^1_{\rm per}(\Omega). \tag{1.7}$$

The Euler–Lagrange equation for the functional I is the CCPBE [15]

$$\nabla \cdot \varepsilon \nabla \phi + \sum_{s=1}^M N_s q_s \left(\int_\Omega e^{-q_s\phi} \, {\rm d}x \right)^{-1} e^{-q_s \phi} = -\rho \qquad \text{in } \Omega. \tag{1.8}$$

We denote $c = (c_1, \ldots, c_M)$ and define

$$\begin{aligned} X_\rho = \big\{ &(c, D) \in L^2_{\rm per}(\Omega, \mathbb{R}^M) \times H_{\rm per}({\rm div}, \Omega) : c_s \ge 0 \text{ a.e. } \Omega \ (1 \le s \le M), \\ &(1.2) \text{ and } (1.3) \text{ hold true} \big\}, \\ \tilde{X}_0 = \Bigg\{ &(\tilde{c}, \tilde{D}) \in L^\infty_{\rm per}(\Omega, \mathbb{R}^M) \times H_{\rm per}({\rm div}, \Omega) : \int_\Omega \tilde{c}_s \, {\rm d}x = 0 \ (1 \le s \le M), \\ &\nabla \cdot \tilde{D} = \sum_{s=1}^M q_s \tilde{c}_s \Bigg\}. \end{aligned}$$

It can be verified readily that for any $\rho \in L^2_{\rm per}(\Omega)$ that $X_\rho \ne \emptyset$ if and only if (1.6) holds true. The following theorem summarizes the results on the PB equation and energy functional (cf. [15–18, 20] and the proof of Thm. 2.1 below):

Theorem 1.1. *Let $\varepsilon \in C^1_{\rm per}(\overline{\Omega})$ satisfy (1.5) and $\rho \in L^2_{\rm per}(\Omega)$ satisfy (1.6).*

(1) *There exists a unique $\phi_{\min} \in \mathring{H}^1_{\rm per}(\Omega)$ such that $I[\phi_{\min}] = \min_{\phi \in \mathring{H}^1_{\rm per}(\Omega)} I[\phi]$. Moreover, $\phi_{\min} \in L^\infty_{\rm per}(\Omega) \cap H^2_{\rm per}(\Omega)$ is the unique solution to the CCPBE (1.8).*

(2) *Let $(c_{\min}, D_{\min}) = (c_{\min,1}, \cdots, c_{\min,M}, D_{\min})$ be given by*

$$c_{\min,s} = N_s \left(\int_\Omega e^{-q_s \phi_{\min}} \, {\rm d}x \right)^{-1} e^{-q_s\phi_{\min}} \quad \text{and} \quad D_{\min} = -\varepsilon \nabla \phi_{\min} \quad \text{in } \mathbb{R}^3. \tag{1.9}$$

Then $(c_{\min}, D_{\min}) \in X_\rho$ is the unique minimizer of $F : X_\rho \to \mathbb{R} \cup \{+\infty\}$ defined in (1.1).

(3) *Let $(c, D) \in X_\rho$. Then $(c, D) = (c_{\min}, D_{\min})$ if and only if the following are satisfied:*
   (i) Positive bounds: *There exist $\theta_1, \theta_2 > 0$ such that $\theta_1 \le c_s \le \theta_2$ a.e. Ω and $s = 1, \ldots, M$;*
   (ii) Global equilibrium:

$$\int_\Omega \left(\frac{1}{\varepsilon} D \cdot \tilde{D} + \sum_{s=1}^M \tilde{c}_s \log c_s \right) {\rm d}x = 0 \qquad \forall (\tilde{c}, \tilde{D}) \in \tilde{X}_0.$$

Define now

$$\begin{aligned} S_\rho &= \{ D \in H_{\rm per}({\rm div}, \Omega) : \nabla \cdot D = \rho \text{ in } \Omega \}, \\ S_0 &= \{ D \in H_{\rm per}({\rm div}, \Omega) : \nabla \cdot D = 0 \text{ in } \Omega \}. \end{aligned}$$

The constraint $\nabla \cdot D = \rho$ here is the Gauss' law. It is verified that $S_\rho \neq \emptyset$ if and only if $\mathscr{A}_\Omega(\rho) = 0$. Clearly $S_0 \neq \emptyset$. We define

$$\hat{I}[\phi] = \int_\Omega \left(\frac{\varepsilon}{2} |\nabla \phi|^2 - \rho\phi \right) \mathrm{d}x \qquad \forall \phi \in H^1_{\mathrm{per}}(\Omega), \tag{1.10}$$

$$\hat{F}[D] = \int_\Omega \frac{1}{2\varepsilon} |D|^2 \, \mathrm{d}x \qquad \forall D \in S_\rho. \tag{1.11}$$

We call $\hat{F}[D]$ the Poisson electrostatic energy of the displacement D. The following theorem collects some properties of the Poisson energy minimization and its proof is omitted:

Theorem 1.2. *Let $\varepsilon \in L^\infty_{\mathrm{per}}(\Omega)$ satisfy (1.5) and $\rho \in L^2_{\mathrm{per}}(\Omega)$ satisfy $\mathscr{A}_\Omega(\rho) = 0$.*

(1) *There exists a unique $\hat{\phi}_{\min} \in \mathring{H}^1_{\mathrm{per}}(\Omega)$ such that $\hat{I}[\hat{\phi}_{\min}] = \min_{\phi \in \mathring{H}^1_{\mathrm{per}}(\Omega)} \hat{I}[\phi]$. Moreover, $\hat{\phi}_{\min}$ is the unique weak solution in $\mathring{H}_{\mathrm{per}}(\Omega)$ to Poisson's equation $\nabla \cdot \varepsilon \nabla \hat{\phi}_{\min} = -\rho$;*

(2) *There exists a unique $\hat{D}_{\min} \in S_\rho$ such that $\hat{F}[\hat{D}_{\min}] = \min_{D \in S_\rho} \hat{F}[D]$. Moreover, the minimizer $\hat{D}_{\min}$ is characterized by $\hat{D}_{\min} \in S_\rho$ and*

$$\int_\Omega \frac{1}{\varepsilon} \hat{D}_{\min} \cdot \tilde{D} \, \mathrm{d}x = 0 \qquad \forall \tilde{D} \in S_0.$$

(3) *We have $\hat{D}_{\min} = -\varepsilon \nabla \hat{\phi}_{\min}$.*

2. Finite-difference approximations

We first study the finite-difference approximation of the CCPBE. Let $N \geq 1$ be an integer. We cover $\overline{\Omega} = [0, L]^3$ with a uniform finite-difference grid of size $h = L/N$. Denote $h\mathbb{Z}^3 = \{(ih, jh, kh) : i, j, k \in \mathbb{Z}\}$. For $\phi : h\mathbb{Z}^3 \to \mathbb{R}$ and $i, j, k \in \mathbb{Z}$, we denote $\phi_{i,j,k} = \phi(ih, jh, kh)$, $\partial_1^h \phi_{i,j,k} = (\phi_{i+1,j,k} - \phi_{i,j,k})/h$, and $\partial_2^h \phi_{i,j,k}$ and $\partial_3^h \phi_{i,j,k}$ similarly. We define the discrete gradient $\nabla_h \phi = (\partial_1^h \phi, \partial_2^h \phi, \partial_3^h \phi)$ on $h\mathbb{Z}^3$, $\nabla_{-h} \phi_{i,j,k} = (\partial_1^h \phi_{i-1,j,k}, \partial_2^h \phi_{i,j-1,k}, \partial_3^h \phi_{i,j,k-1})$ $(i, j, k \in \mathbb{Z})$, and the discrete Laplacian $\Delta_h \phi = \nabla_{-h} \cdot \nabla_h \phi = \nabla_h \cdot \nabla_{-h} \phi$. A function $\phi : h\mathbb{Z}^3 \to \mathbb{R}$ is $\overline{\Omega}$-periodic, if $\phi_{i+N,j,k} = \phi_{i,j+N,k} = \phi_{i,j,k+N} = \phi_{i,j,k}$ $\forall i, j, k \in \mathbb{Z}$. We denote

$$V_h = \{\overline{\Omega}\text{-periodic grid functions } \phi : h\mathbb{Z}^3 \to \mathbb{R}\},$$
$$'\mathring{V}_h = \{\phi \in V_h : \mathscr{A}_h(\phi) = 0\},$$
$$\mathscr{A}_h(\phi) = \frac{1}{N^3} \sum_{i,j,k=0}^{N-1} \phi_{i,j,k} = \left(\frac{h}{L}\right)^3 \sum_{i,j,k=0}^{N-1} \phi_{i,j,k}.$$

Let $\varepsilon \in C_{\mathrm{per}}(\overline{\Omega})$ satisfy (1.5). We define a new function, still denoted ε, on half grid points by

$$\varepsilon_{i+1/2,j,k} = \frac{\varepsilon_{i,j,k} + \varepsilon_{i+1,j,k}}{2}, \quad \varepsilon_{i,j+1/2,k} = \frac{\varepsilon_{i,j,k} + \varepsilon_{i,j+1,k}}{2}, \quad \varepsilon_{i,j,k+1/2} = \frac{\varepsilon_{i,j,k} + \varepsilon_{i,j,k+1}}{2} \tag{2.1}$$

for all $i, j, k \in \mathbb{Z}$. For any $\phi \in V_h$, we define $A_h^\varepsilon[\phi] \in V_h$ by

$$A_h^\varepsilon[\phi]_{i,j,k} = \partial_1^h \left(\varepsilon_{i-1/2,j,k} \partial_1^h \phi_{i-1,j,k} \right) + \partial_2^h \left(\varepsilon_{i,j-1/2,k} \partial_2^h \phi_{i,j-1,k} \right) + \partial_3^h \left(\varepsilon_{i,j,k-1/2} \partial_3^h \phi_{i,j,k-1} \right) \tag{2.2}$$

for all $i, j, k \in \mathbb{Z}$. Clearly, $A_h^\varepsilon : V_h \to V_h$ is linear. If $\varepsilon = 1$ identically, then $A_h^\varepsilon = \Delta_h$. We denote for any $\phi, \psi \in V_h$

$$\langle \nabla_h \phi, \nabla_h \psi \rangle_{\varepsilon,h} = h^3 \sum_{i,j,k=0}^{N-1} \Big(\varepsilon_{i+1/2,j,k} \partial_1^h \phi_{i,j,k} \partial_1^h \psi_{i,j,k} + \varepsilon_{i,j+1/2,k} \partial_2^h \phi_{i,j,k} \partial_2^h \psi_{i,j,k}$$
$$+ \varepsilon_{i,j,k+1/2} \partial_3^h \phi_{i,j,k} \partial_3^h \psi_{i,j,k} \Big),$$
$$\|\nabla_h \phi\|_{\varepsilon,h} = \sqrt{\langle \nabla_h \phi, \nabla_h \phi \rangle_{\varepsilon,h}}.$$

If $\varepsilon = 1$ then we denote $\langle\cdot,\cdot\rangle_h = \langle\cdot,\cdot\rangle_{\varepsilon,h}$ and $\|\cdot\|_h = \|\cdot\|_{\varepsilon,h}$. We have the discrete Poincaré inequality

$$\|\phi\|_h \leq \frac{L}{4\sqrt{3}}\|\nabla_h\phi\|_h \qquad \forall \phi \in \mathring{V}_h.$$

This implies that $\langle\cdot,\cdot\rangle_{\varepsilon,h}$ is an inner product and $\|\cdot\|_{\varepsilon,h}$ the corresponding norm of $\mathring{V}_h$.

Let $\rho^h \in V_h$ and assume (cf. (1.6))

$$\text{Discrete charge neutrality:} \qquad \sum_{s=1}^{M} q_s N_s + h^3 \sum_{i,j,k=0}^{N-1} \rho^h_{i,j,k} = 0. \tag{2.3}$$

We define

$$I_h[\phi] = \frac{1}{2}\|\nabla_h\phi\|^2_{\varepsilon,h} - \langle\rho^h,\phi\rangle_h + \sum_{s=1}^{M} N_s \log\left(\mathscr{A}_h\left(e^{-q_s\phi}\right)\right) \qquad \forall\phi\in V_h. \tag{2.4}$$

We verify that $I_h[\phi + a] = I_h[\phi]$ ($\phi \in V_h$ and $a \in \mathbb{R}$), $I_h : \mathring{V}_h \to \mathbb{R}$ is strictly convex, and there exist $K_1 > 0$ and $K_2 \in \mathbb{R}$, independent of h, such that $I_h[\phi] \geq K_1\|\nabla_h\phi\|^2_{\varepsilon,h} + K_2$ for all $\phi \in \mathring{V}_h$.

Theorem 2.1. *Let $\varepsilon \in C_{\rm per}(\overline{\Omega})$ satisfy (1.5) and $\rho^h \in V_h$ satisfy (2.3). There exists a unique $\phi^h_{\min} \in \mathring{V}_h$ such that $I_h[\phi^h_{\min}] = \min_{\phi\in\mathring{V}_h} I_h[\phi]$. Moreover, $\phi := \phi^h_{\min}$ is the unique solution in $\mathring{V}_h$ to the discrete charge-conserved PBE (CCPBE):*

$$A^\varepsilon_h[\phi] + \sum_{s=1}^{M}\frac{q_s N_s}{L^3\mathscr{A}_h(e^{-q_s\phi})}e^{-q_s\phi} = -\rho^h \quad \text{on} \quad h\mathbb{Z}^3. \tag{2.5}$$

If in addition $\sup_h\|\rho^h\|_\infty < \infty$, then $\sup_h\|\phi^h_{\min}\|_\infty < \infty$.

Proof. Since $\dim(\mathring{V}_h) < \infty$ and $I_h : \mathring{V}_h \to \mathbb{R}$ is strictly convex, there exists a unique minimizer $\phi^h_{\min} \in \mathring{V}_h$ of $I_h : \mathring{V}_h \to \mathbb{R}$. Thus, $\phi := \phi^h_{\min}$ satisfies

$$\langle\nabla_h\phi,\nabla_h\xi\rangle_{\varepsilon,h} - \sum_{s=1}^{M}\frac{N_s q_s}{L^3\mathscr{A}_h(e^{-q_s\phi})}\langle e^{-q_s\phi},\xi\rangle_h = \langle\rho^h,\xi\rangle_h \qquad \forall\xi\in\mathring{V}_h.$$

Since

$$\rho^h + \sum_{s=1}^{M}\frac{q_s N_s}{L^3\mathscr{A}_h(e^{-q_s\phi})}e^{-q_s\phi} \in \mathring{V}_h$$

by (2.3) and $\langle\nabla_h\phi,\nabla_h\xi\rangle_{\varepsilon,h} = \langle -A^\varepsilon_h[\phi],\xi\rangle_h$ for all $\xi\in\mathring{V}_h$ by summation by parts, we see that ϕ is the solution to the discrete CCPBE (2.5).

Now assume $\sup_h\|\rho^h\|_\infty < \infty$. Let $\phi^h_0 \in \mathring{V}_h$ be such that $\langle\nabla_h\phi^h_0,\nabla_h\xi\rangle_{\varepsilon,h} = \langle\rho^h,\xi\rangle_h$ for all $\xi\in\mathring{V}_h$. Note that $\phi^h_0 \in \mathring{V}_h$ is the unique solution to $A^\varepsilon_h[\phi^h_0] = -\rho^h$ on $h\mathbb{Z}^3$. By the uniform stability of the inverse of A^ε_h [4,28,29], there exists $C > 0$, independent of h, such that $|\phi^h_{0,i,j,k}| \leq C$ for all $i,j,k\in\mathbb{Z}$. Define

$$J_h[\psi] = \frac{1}{2}\|\nabla_h\psi\|^2_{\varepsilon,h} + \sum_{s=1}^{M} N_s\log\left(\mathscr{A}_h\left(e^{-q_s(\phi^h_0+\psi)}\right)\right) \qquad \forall\psi\in V_h.$$

Let $\psi\in V_h$ and $\bar\psi = \mathscr{A}_h(\psi)$. Since $\langle\nabla_h\phi^h_0,\nabla_h\psi\rangle_{\varepsilon,h} = \langle\rho^h,\psi-\bar\psi\rangle_h$ and $\|\nabla_h\phi^h_0\|^2_{\varepsilon,h} = \langle\rho^h,\phi^h_0\rangle_h$,

$$J_h[\psi] = J_h[\psi-\bar\psi] - \bar\psi\sum_{s=1}^{M}q_sN_s = I_h\left[\psi-\bar\psi+\phi^h_0\right] + \frac{1}{2}\left\|\nabla_h\phi^h_0\right\|^2_{\varepsilon,h} - \bar\psi\sum_{s=1}^{M}q_sN_s.$$

In particular, if $\psi \in \mathring{V}_h$ and $\phi = \psi + \phi_0^h \in \mathring{V}_h$, then

$$J_h[\psi] = I_h[\phi] + \frac{1}{2}\|\nabla_h \phi_0^h\|_{\varepsilon,h}^2.$$

Thus, $\psi_{\min}^h := \phi_{\min}^h - \phi_0^h \in \mathring{V}_h$ is the unique minimizer of $J_h : \mathring{V}_0 \to \mathbb{R}$. We show that $\psi_{\min}^h$ is bounded uniformly with respect to h. This will lead to the desired bound for $\phi_{\min}^h$.

For convenience, let us denote $\psi = \psi_{\min}^h$ and $\phi_0 = \phi_0^h$. We consider three cases.

Case 1: there exist $s', s'' \in \{1, \ldots, M\}$ such that $q_{s'} > 0$ and $q_{s''} < 0$. Let $\lambda > 0$ and

$$\hat{\psi}_\lambda = \begin{cases} \psi & \text{if } |\psi| \le \lambda, \\ \lambda & \text{if } \psi > \lambda, \\ -\lambda & \text{if } \psi < -\lambda, \end{cases} \qquad \text{and} \qquad \psi_\lambda = \hat{\psi}_\lambda - \mathscr{A}_h(\hat{\psi}_\lambda). \tag{2.6}$$

Clearly, $\hat{\psi}_\lambda \in V_h$ and $\psi_\lambda \in \mathring{V}_h$, hence $J_h[\psi] \le J_h[\psi_\lambda]$. Consider two neighboring grid points, *e.g.*, (i, j, k) and $(i + 1, j, k)$. Let $\alpha = \psi_{i,j,k}$ and $\beta = \psi_{i+1,j,k}$, and assume $\alpha \le \beta$. (The case that $\beta \ge \alpha$ is similar.) We can verify that $|\psi_{i+1,j,k} - \psi_{i,j,k}| \ge |\hat{\psi}_{\lambda,i+1,j,k} - \hat{\psi}_{\lambda,i,j,k}|$ by checking the following six cases: (1) $\alpha \le \beta \le -\lambda$; (2) $\alpha \le -\lambda \le \beta \le \lambda$; (3) $\alpha \le -\lambda < \lambda \le \beta$; (4) $-\lambda \le \alpha \le \beta \le \lambda$; (5) $-\lambda \le \alpha \le \lambda \le \beta$; and (6) $\lambda \le \alpha \le \beta$. Thus, $|\nabla_h \psi| \ge |\nabla_h \hat{\psi}_\lambda| = |\nabla_h \psi_\lambda|$ on $h\mathbb{Z}^3$. Applying Jensen's inequality to $u \mapsto -\log u$, we thus have

$$\begin{aligned}
0 &\ge \frac{1}{2}\|\nabla_h \hat{\psi}_\lambda\|_{\varepsilon,h}^2 - \frac{1}{2}\|\nabla_h \psi\|_{\varepsilon,h}^2 \\
&= J_h[\hat{\psi}_\lambda] - J_h[\psi] + \sum_{s=1}^M N_s \left[\log\left(\mathscr{A}_h(e^{-q_s(\phi_0+\psi)})\right) - \log\left(\mathscr{A}_h\left(e^{-q_s(\phi_0+\hat{\psi}_\lambda)}\right)\right)\right] \\
&= J_h[\psi_\lambda] - J_h[\psi] - \mathscr{A}_h\left(\hat{\psi}_\lambda\right)\sum_{s=1}^M q_s N_s \\
&\quad + \sum_{s=1}^M N_s \left[\log\left(\mathscr{A}_h\left(e^{-q_s(\phi_0+\psi)}\right)\right) - \log\left(\mathscr{A}_h\left(e^{-q_s(\phi_0+\hat{\psi}_\lambda)}\right)\right)\right] \\
&\ge \mathscr{A}_h\left(B_h(\phi_0+\psi) - B_h\left(\phi_0+\hat{\psi}_\lambda\right)\right) - \mathscr{A}_h(\hat{\psi}_\lambda)\sum_{s=1}^M q_s N_s,
\end{aligned} \tag{2.7}$$

where

$$B_h(u) = \sum_{s=1}^M \frac{N_s}{\alpha_{s,h}} e^{-q_s u} \qquad \text{and} \qquad \alpha_{s,h} = \mathscr{A}_h\left(e^{-q_s(\phi_0+\psi)}\right). \tag{2.8}$$

We claim that there are positive constants C_1 and C_2, independent of h, such that

$$0 < C_1 \le \alpha_{s,h} \le C_2 \qquad \forall s = 1, \ldots, M. \tag{2.9}$$

In fact, by applying Jensen's inequality to $u \mapsto -\log u$ and the fact that $\phi_0, \psi \in \mathring{V}_h$, we obtain that $\log \alpha_{s,h} \ge -q_s \mathscr{A}_h(\phi_0 + \psi) = 0$. Hence, $\alpha_{s,h} \ge 1 =: C_1$. Note by the uniform bound of $\phi_0 = \phi_0^h$ that $\sum_{s=1}^M N_s \log(\alpha_{s,h}) \le J_h[\psi] \le J_h[0] \le C$, where C is a constant independent of h. Since each $\alpha_{s,h} \ge C_1$, we have that each $\alpha_{s,h} \le C_2$ for some constant C_2 independent of h. Thus, (2.9) is true.

We show now there exists $\lambda > 0$ such that $|\psi_{i,j,k}| \le \lambda$ for all $i, j, k \in \mathbb{Z}$. Suppose this were not true. Then for any $\lambda > 0$ there is some h such that with $\psi = \psi_{\min}^h$ the set $\{(i, j, k) : \psi_{i,j,k} > \lambda\} \cup \{(i, j, k) : \psi_{i,j,k} < -\lambda\} \ne \emptyset$. We may assume both of these subsets of indices are nonempty as the case that one of them is empty is similar.

Set $b = \sum_{s=1}^M q_s N_s$. It is clear that B_h, defined in (2.8), is a convex function. Thus, by Jensen's inequality and the fact that $\mathscr{A}_h(\psi) = 0$, we can continue from (2.7) to get

$$\begin{aligned}0 &\geq \mathscr{A}_h\left(\left[B_h'\left(\phi_0 + \hat{\psi}_\lambda\right) + b\right]\left(\psi - \hat{\psi}_\lambda\right)\right)\\ &= h^3 \sum_{\psi_{i,j,k} > \lambda} \left[B_h'\left(\phi_{0,i,j,k} + \lambda\right) + b\right]\left(\psi_{i,j,k} - \lambda\right)\\ &\quad + h^3 \sum_{\psi_{i,j,k} < -\lambda} \left[B_h'\left(\phi_{0,i,j,k} - \lambda\right) + b\right]\left(\psi_{i,j,k} + \lambda\right). \end{aligned} \tag{2.10}$$

Since $q_{s'} > 0$ and $q_{s''} < 0$, it follows from (2.9) that for any $u \in \mathbb{R}$

$$B_h'(u) = \sum_{s=1}^M \frac{N_s}{\alpha_{s,h}}(-q_s)e^{-q_s u} \geq \sum_{s:\, q_s > 0} \frac{N_s}{C_1}(-q_s)e^{-q_s u} + \sum_{s:\, q_s < 0} \frac{N_s}{C_2}(-q_s)e^{-q_s u} =: b_h(u).$$

The h-dependent function $b_h(u)$ is an increasing function of $u \in \mathbb{R}$. Moreover, $b_h(+\infty) = +\infty$ and $b_h(-\infty) = -\infty$. By the uniform bound on $\phi_0 = \phi_0^h$, we can find $\lambda_+ > 0$ sufficiently large and independent of h such that

$$B_h'(\phi_{0,i,j,k} + \lambda) + b \geq b_h(\phi_{0,i,j,k} + \lambda) + b \geq 1 \qquad \forall \lambda \geq \lambda_+ \ \forall i, j, k \in \mathbb{Z}.$$

Similarly, there exists $\lambda_- > 0$ sufficiently large and independent of h such that

$$B_h'(\phi_{0,i,j,k} - \lambda) + b \leq -1 \qquad \forall \lambda \geq \lambda_- \ \forall i, j, k \in \mathbb{Z}.$$

Let $\lambda \geq \max\{\lambda_+, \lambda_-\}$. It thus follows from (2.10) that

$$0 \geq \sum_{i,j,k:\, \psi_{i,j,k} > \lambda} |\psi_{i,j,k} - \lambda| + \sum_{i,j,k:\, \psi_{i,j,k} < -\lambda} |\psi_{i,j,k} + \lambda|.$$

This is impossible.

Case 2: all $q_s < 0$ $(1 \leq s \leq M)$. Let $\lambda > 0$ and define $\hat{\psi}_\lambda = \psi$ if $\psi \leq \lambda$ and $\hat{\psi}_\lambda = \lambda$ if $\psi > \lambda$, and $\psi_\lambda = \hat{\psi}_\lambda - \mathscr{A}_h(\hat{\psi}_\lambda)$. In this case, the function $B_h(u)$ defined in (2.8) is convex and

$$B_h'(u) \geq \sum_{s=1}^M -\frac{q_s N_s}{C_2} e^{-q_s u} =: b_{+,h}(u) \qquad \forall u \in \mathbb{R},$$

where C_2 is the same as in (2.9). Thus, $b_{+,h}(u)$ is an increasing function of $u \in \mathbb{R}$ and $b_{+,h}(+\infty) = +\infty$. Hence, carrying out the same calculations as above with $\{\psi > \lambda\}$ replacing $\{|\psi| > \lambda\}$, we get $\psi \leq \lambda$ on $h\mathbb{Z}^3$ for any λ large enough and all h. Since $\psi = \psi_{\min}^h$ is the minimizer of $J_h : \mathring{V}_h \to \mathbb{R}$, it is a critical point of J_h, which implies

$$A_h^\varepsilon[\psi] + \sum_{s=1}^M \frac{q_s N_s}{L^3 \alpha_{s,h}} e^{-q_s(\phi_0 + \psi)} = 0 \qquad \text{on} \ \ h\mathbb{Z}^3,$$

where $\alpha_{s,h}$ is defined in (2.8). Since $q_s < 0$ for all s, $\phi_0 = \phi_0^h$ is uniformly bounded, and ψ is uniformly bounded above, we have by (2.9) and the uniform L^∞-stability of the inverse of $A_h^\varepsilon : \mathring{V}_h \to \mathring{V}_h$ [4, 28, 29] that ψ is also bounded below uniformly with respect to all $h > 0$.

Case 3: all $q_s > 0$ $(s = 1, \ldots, M)$. This is similar to Case 2. □

We now study the finite-difference approximation of the constrained PB energy functional. We define a discretized displacement $D = (u, v, w) : h(\mathbb{Z}+1/2)^3 \to \mathbb{R}^3$ by

$$D_{i+1/2,j+1/2,k+1/2} = (u_{i+1/2,j,k}, v_{i,j+1/2,k}, w_{i,j,k+1/2}) \qquad \forall i, j, k \in \mathbb{Z}. \tag{2.11}$$

Here, $u_{i+1/2,j,k}$, $v_{i,j+1/2,k}$, and $w_{i,j,k+1/2}$ are approximations of the first, second, and third components of a displacement at $((i+1/2)h, jh, kh)$, $(ih, (j+1/2)h, kh)$, and $(ih, jh, (k+1/2)h)$. We denote

$$Y_h = \{\overline{\Omega}\text{-periodic functions } D = (u, v, w) : h(\mathbb{Z}+1/2)^3 \to \mathbb{R}^3 \text{ in the form (2.11)}\}, \tag{2.12}$$

where D is $\overline{\Omega}$-periodic if

$$D(\xi + hNe) = D(\xi) \qquad \forall \xi \in h(\mathbb{Z}+1/2)^3 \ \forall e \in \{(1,0,0), (0,1,0), (0,0,1)\}.$$

Given $D = (u, v, w) \in Y_h$, we define the discrete divergence $\nabla_h \cdot D : h\mathbb{Z}^3 \to \mathbb{R}$ and the discrete curl $\nabla_h \times D : h(\mathbb{Z}+1/2)^3 \to \mathbb{R}^3$, respectively, by

$$(\nabla_h \cdot D)_{i,j,k} = \frac{1}{h}\left(u_{i+1/2,j,k} - u_{i-1/2,j,k} + v_{i,j+1/2,k} - v_{i,j-1/2,k} + w_{i,j,k+1/2} - w_{i,j,k-1/2}\right),$$
$$(\nabla_h \times D)_{i+1/2,j+1/2,k+1/2} = \frac{1}{h}\begin{pmatrix} w_{i,j+1,k+1/2} - w_{i,j,k+1/2} - v_{i,j+1/2,k+1} + v_{i,j+1/2,k} \\ u_{i+1/2,j,k+1} - u_{i+1/2,j,k} - w_{i+1,j,k+1/2} + w_{i,j,k+1/2} \\ v_{i+1,j+1/2,k} - v_{i,j+1/2,k} - u_{i+1/2,j+1,k} + u_{i+1/2,j,k} \end{pmatrix}.$$

Note that the discrete curl at $(i+1/2, j+1/2, k+1/2)$ is defined through the three grid faces of the grid box $(i,j,k) + [0,1]^3$ sharing the same grid (i,j,k).

Let $\varepsilon \in C_{\text{per}}(\overline{\Omega})$ satisfy (1.5) and $\rho^h \in V_h$ satisfy (2.3). We consider discrete concentrations $c_s \in V_h$ $(s = 1, \ldots, M)$ and electric displacement $D \in Y_h$ that satisfy the following conditions:

$$\text{Nonnegativity:} \qquad c_{s,i,j,k} \geq 0, \quad s = 1, \ldots, M; \ i, j, k = 1, \ldots, N; \tag{2.13}$$

$$\text{Discrete mass conservation:} \qquad h^3 \sum_{i,j,k=0}^{N-1} c_{s,i,j,k} = N_s, \quad s = 1, \ldots, M; \tag{2.14}$$

$$\text{Discrete Gauss' law:} \qquad \nabla_h \cdot D = \rho^h + \sum_{s=1}^{M} q_s c_s \quad \text{on} \ \ h\mathbb{Z}^3. \tag{2.15}$$

We define

$$X_{\rho,h} = \left\{(c, D) = (c_1, \ldots, c_M; D) \in V_h^M \times Y_h : \ \text{(2.13)–(2.15) hold true}\right\},$$
$$\tilde{X}_{0,h} = \left\{(\tilde{c}, \tilde{D}) = (\tilde{c}_1, \ldots, \tilde{c}_M; \tilde{D}) \in \mathring{V}_h^M \times Y_h : \nabla_h \cdot \tilde{D} = \sum_{s=1}^{M} q_s \tilde{c}_s \text{ on } h\mathbb{Z}^3\right\}.$$

Clearly, $X_{\rho,h} \neq \emptyset$ if $\rho^h \in V_h$ satisfies the condition (2.3), and $\tilde{X}_{0,h} \neq \emptyset$. Define for any $D = (u, v, w), \tilde{D} = (\tilde{u}, \tilde{v}, \tilde{w}) \in Y_h$

$$\langle D, \tilde{D}\rangle_{1/\varepsilon,h} = h^3 \sum_{i,j,k=0}^{N-1} \left(\frac{u_{i+1/2,j,k}\tilde{u}_{i+1/2,j,k}}{\varepsilon_{i+1/2,j,k}} + \frac{v_{i,j+1/2,k}\tilde{v}_{i,j+1/2,k}}{\varepsilon_{i,j+1/2,k}} + \frac{w_{i,j,k+1/2}\tilde{w}_{i,j,k+1/2}}{\varepsilon_{i,j,k+1/2}}\right),$$
$$\|D\|_{1/\varepsilon,h} = \sqrt{\langle D, D\rangle_{1/\varepsilon,h}}.$$

Note that $\langle \cdot, \cdot \rangle_{1/\varepsilon,h}$ and $\| \cdot \|_{1/\varepsilon,h}$ are an inner product and the corresponding norm of Y_h. If $\varepsilon = 1$, we simply write the subscript h. If $D = (u, v, w) \in Y_h$, we define $D/\varepsilon \in Y_h$ by

$$\left(\frac{D}{\varepsilon}\right)_{i+1/2,j+1/2,k+1/2} = \left(\frac{u_{i+1/2,j,k}}{\varepsilon_{i+1/2,j,k}}, \frac{v_{i,j+1/2,k}}{\varepsilon_{i,j+1/2,k}}, \frac{w_{i,j,k+1/2}}{\varepsilon_{i,j,k+1/2}}\right) \qquad \forall i, j, k \in \mathbb{Z}. \tag{2.16}$$

If $\phi \in V_h$, we define $D_h^\varepsilon[\phi] = (u, v, w) \in Y_h$ by

$$u_{i+1/2,j,k} = -\varepsilon_{i+1/2,j,k}\partial_1^h \phi_{i,j,k}, \quad v_{i,j+1/2,k} = -\varepsilon_{i,j+1/2,k}\partial_2^h \phi_{i,j,k}, \quad w_{i,j,k+1/2} = -\varepsilon_{i,j,k+1/2}\partial_3^h \phi_{i,j,k}. \tag{2.17}$$

It follows from the definition of A_h^ε (cf. (2.2)) that

$$A_h^\varepsilon[\phi] = -\nabla_h \cdot D_h^\varepsilon[\phi] \qquad \forall \phi \in V_h. \tag{2.18}$$

We define the discrete PB energy

$$F_h[c, D] = \frac{1}{2}\|D\|^2_{1/\varepsilon,h} + h^3 \sum_{s=1}^{M} \sum_{i,j,k=0}^{N-1} c_{s,i,j,k} \log c_{s,i,j,k} \qquad \forall (c, D) \in X_{\rho,h}. \tag{2.19}$$

Let $\phi^h_{\min}$ be the unique minimizer of the functional $I_h : \mathring{V}_h \to \mathbb{R}$ as in Theorem 2.1. Define

$$c^h_{\min,s} = \frac{N_s}{L^3 \mathscr{A}_h(e^{-q_s \phi^h_{\min}})} e^{-q_s \phi^h_{\min}} \quad (s = 1, \ldots, M) \quad \text{and} \quad D^h_{\min} = D^\varepsilon_h[\phi^h_{\min}]; \tag{2.20}$$

cf. (2.17) for the definition of D^ε_h. Denote $c^h_{\min} = (c^h_{\min,1}, \ldots, c^h_{\min,M})$. By direct calculations using (2.18) and applying Theorem 2.1, we obtain the following lemma:

Lemma 2.1. *Let* $(c, D) = (c^h_{\min}, D^h_{\min})$ *be defined by* (2.20). *Then* $(c, D) \in X_{\rho,h}$ *and* $\nabla_h \times (D/\varepsilon) = 0$ *on* $h(\mathbb{Z} + 1/2)^3$. *If in addition* $\sup_h \|\rho^h\|_\infty < \infty$, *then there exist positive constants* θ_1 *and* θ_2, *independent of* h, *such that* $0 < \theta_1 \le c_s \le \theta_2$ *on* $h\mathbb{Z}^3$ *for* $s = 1, \ldots, M$.

We remark that this lemma asserts the uniform (with respect to the grid size) positivity of finite-difference minimizers of ionic concentrations. At the continuum level, such positivity results from the entropic term (the integral of $c_s \log c_s$) [16, 17]. For finite-difference approximations, such positivity is also found in the numerical analysis of the Poisson–Nernst–Planck equations [8, 22].

Theorem 2.2. *That* $(c^h_{\min}, D^h_{\min})$ *defined in* (2.20) *is the unique minimizer of* $F_h : X_{\rho,h} \to \mathbb{R}$. *Moreover, if* $(c, D) = (c_1, \ldots, c_M; u, v, w) \in X_{\rho,h}$, *then the following are equivalent:*

(1) $(c, D) = (c^h_{\min}, D^h_{\min})$;
(2) (i) Positivity: $c_s > 0$ *on* $h\mathbb{Z}^3$ *for all* $s = 1, \ldots, M$; *and*
 (ii) Global equilibrium:

$$\langle D, \tilde{D} \rangle_{1/\varepsilon,h} + \sum_{s=1}^{M} \langle \tilde{c}_s, \log c_s \rangle_h = 0 \qquad \forall (\tilde{c}, \tilde{D}) = (\tilde{c}_1, \ldots, \tilde{c}_M; \tilde{D}) \in \tilde{X}_{0,h}; \tag{2.21}$$

(3) (i) Positivity: $c_s > 0$ *on* $h\mathbb{Z}^3$ *for all* $s = 1, \ldots, M$; *and*
 (ii) Local equilibrium—finite-difference Boltzmann distributions:

$$(\nabla_h \log c_s)_{i,j,k} = q_s \left(\frac{D}{\varepsilon}\right)_{i+1/2,j+1/2,k+1/2} \qquad \forall s \in \{1, \ldots, M\}\ \forall i, j, k \in \mathbb{Z}. \tag{2.22}$$

Proof. The functional $F_h : X_{\rho,h} \to \mathbb{R}$ is strictly convex and bounded below, and $F_h[c,D] \to \infty$ if $\|(c,D)\| \to +\infty$ (with any norm). Thus it has a unique minimizer.

We prove that Part (1) implies Part (2). Let $(\tilde{c}, \tilde{D}) = (\tilde{c}_1, \ldots, \tilde{c}_M; \tilde{D}) \in \tilde{X}_{0,h}$. Then, $\nabla \cdot \tilde{D} = \sum_{s=1}^M q_s \tilde{c}_s$. Since $(c,D) = (c^h_{\min}, D^h_{\min})$ by Part (1) and $D^h_{\min} = D^\varepsilon_h[\phi^h_{\min}]$ by (2.20), it follows from the definition of D^ε_h (cf. (2.17)) and summation by parts that

$$\langle D, \tilde{D} \rangle_{1/\varepsilon,h} = \langle \phi^h_{\min}, \nabla_h \cdot \tilde{D} \rangle_h = \sum_{s=1}^M q_s \langle \phi^h_{\min}, \tilde{c}_s \rangle_h. \tag{2.23}$$

Since $\mathscr{A}_h(\tilde{c}_s) = 0$ for all $s \in \{1, \ldots, M\}$, we get by (2.20) that

$$\sum_{s=1}^M \langle \tilde{c}_s, \log c_s \rangle_h = -\sum_{s=1}^M q_s \langle \tilde{c}_s, \phi^h_{\min} \rangle_h. \tag{2.24}$$

Now (2.23) and (2.24) imply Part (2)(ii), the global equilibrium property (2.21). Together with (2.20) which implies Part (2)(i), we see that Part (1) implies Part (2).

We now prove that Part (2) implies Part (1). Denoting by $(c_{\mathrm{m}}, D_{\mathrm{m}}) = (c^h_{\min}, D^h_{\min}) \in X_{\rho,h}$ the unique minimizer of F_h over $X_{\rho,h}$ and $(\tilde{c}, \tilde{D}) = (c_{\mathrm{m}} - c, D_{\mathrm{m}} - D) \in X_{0,h}$, we have by the convexity of $u \mapsto u \log u$, the fact that $\sum_{i,j,k=0}^{N-1} \tilde{c}_{s,i,j,k} = 0$ for all $s \in \{1, \ldots, M\}$, and the global equilibrium property (2.21) for (c,D) in Part (2) that

$$\begin{aligned}
&F_h[c_{\mathrm{m}}, D_{\mathrm{m}}] - F_h[c,D] \\
&\quad \ge \langle D, \tilde{D} \rangle_{1/\varepsilon,h} + h^3 \sum_{s=1}^M \sum_{i,j,k=0}^{N-1} \left[(c_{s,i,j,k} + \tilde{c}_{s,i,j,k}) \log(c_{s,i,j,k} + \tilde{c}_{s,i,j,k}) - c_{s,i,j,k} \log c_{s,i,j,k} \right] \\
&\quad \ge \langle D, \tilde{D} \rangle_{1/\varepsilon,h} + h^3 \sum_{s=1}^M \sum_{i,j,k=0}^{N-1} \tilde{c}_{s,i,j,k} (1 + \log c_{s,i,j,k}) \\
&\quad = 0.
\end{aligned}$$

Thus, $F_h[c,D] \le F_h[c_{\mathrm{m}}, D_{\mathrm{m}}]$, and (c,D) is the minimizer of $F_h : X_{\rho,h} \to \mathbb{R}$. Hence, Part (2) implies Part (1).

We now prove that Part (1) implies Part (3). Let $(c,D) = (c^h_{\min}, D^h_{\min}) \in X_{\rho,h}$ be the minimizer of $F_h : X_{\rho,h} \to \mathbb{R}$. We need only to prove the local equilibrium property (2.22), as (2.20) implies Part (3)(i). Let us fix $s \in \{1, \ldots, M\}$ and a grid point (i,j,k) with $0 \le i,j,k \le N-1$. Define $\hat{c}_s = c_s$ at all (p,q,r) with $0 \le p,q,r \le N-1$ except $\hat{c}_{s,i,j,k} = c_{s,i,j,k} + \delta$ and $\hat{c}_{s,i+1,j,k} = c_{s,i+1,j,k} - \delta$, where $\delta \in \mathbb{R}$ is such that $-c_{s,i,j,k} < \delta < c_{s,i+1,j,k}$. Extend $\hat{c}_s$ periodically. For $s' \ne s$, we set $\hat{c}_{s'} = c_{s'}$. Let us also define $\hat{D} = (\hat{u}, \hat{v}, \hat{w}) \in Y_h$ by setting $\hat{v} = v$ and $\hat{w} = w$ everywhere, and $\hat{u} = u$ everywhere except $\hat{u}_{i+1/2,j,k} = u_{i+1/2,j,k} + hq_s\delta$ (extended periodically). We verify that $(\hat{c}, \hat{D}) = (\hat{c}_1, \ldots, \hat{c}_M; \hat{D}) \in X_{\rho,h}$. Let

$$\begin{aligned}
g(\delta) &:= \hat{F}_h[\hat{c}, \hat{D}] - \hat{F}_h[c,D] \\
&= \frac{1}{2} h^3 \frac{\left(u_{i+1/2,j,k} + hq_s\delta\right)^2 - u^2_{i+1/2,j,k}}{\varepsilon_{i+1/2,j,k}} + h^3 \left[(c_{s,i,j,k} + \delta) \log(c_{s,i,j,k} + \delta) - c_{s,i,j,k} \log c_{s,i,j,k} \right. \\
&\quad \left. + (c_{s,i+1,j,k} - \delta) \log (c_{s,i+1,j,k} - \delta) - c_{s,i+1,j,k} \log c_{s,i+1,j,k} \right].
\end{aligned}$$

If $\delta = 0$ then $(\hat{c}, \hat{D}) = (c,D)$, which is the minimizer of $F_h : X_{\rho,h} \to \mathbb{R}$. Thus, g is minimized at $\delta = 0$ and $g'(\delta) = 0$. This leads to $\partial^h_1 \log c_{s,i,j,k} = q_s u_{i+1/2,j,k} / \varepsilon_{i+1/2,j,k}$. Same is true for the other components of (2.22). Hence, (2.22), and Part (3), is true.

Finally, we prove that Part (3) implies Part (2). We need only to prove the global equilibrium property (2.21). Let $(c,D) \in X_{\rho,h}$ and assume it satisfies (i) and (ii) of Part (3). We need only to prove the global equilibrium property (2.21). Let $(\tilde{c}, \tilde{D}) = (\tilde{c}_1, \ldots, \tilde{c}_M; \tilde{u}, \tilde{v}, \tilde{w}) \in \tilde{X}_{0,h}$. Fix $\sigma \in \{1, \ldots, M\}$ and fix $j, k \in \{0, \ldots, N-1\}$. By (2.22) and summation by parts,

$$\sum_{i=0}^{N-1} \frac{u_{i+1/2,j,k}\tilde{u}_{i+1/2,j,k}}{\varepsilon_{i+1/2,j,k}} = \frac{1}{hq_\sigma} \sum_{i=0}^{N-1} (\log c_{\sigma,i+1,j,k} - \log c_{\sigma,i,j,k})\, \tilde{u}_{i+1/2,j,k}$$
$$= -\frac{1}{hq_\sigma} \sum_{i=0}^{N-1} \left(\tilde{u}_{i+1/2,j,k} - \tilde{u}_{i-1/2,j,k}\right) \log c_{\sigma,i,j,k}.$$

Similar identities for $\tilde{v}$ and $\tilde{w}$ hold true. Thus, it follows from the definition of $\nabla_h \cdot \tilde{D}$ and $\nabla_h \cdot \tilde{D} = \sum_{s=1}^{M} q_s \tilde{c}_s$ as $(\tilde{c}, \tilde{D}) \in X_{0,h}$ that

$$\langle D, \tilde{D}\rangle_{1/\varepsilon,h} = -\frac{1}{q_\sigma}\langle \nabla_h \cdot \tilde{D}, \log c_\sigma\rangle_h = -\sum_{s=1}^{M} \frac{q_s}{q_\sigma}\langle \tilde{c}_s, \log c_\sigma\rangle_h.$$

Hence,

$$\langle D, \tilde{D}\rangle_{1/\varepsilon,h} + \sum_{s=1}^{M}\langle \tilde{c}_s, \log c_s\rangle_h = \sum_{s=1}^{M} q_s \left\langle \tilde{c}_s, \frac{1}{q_s}\log c_s - \frac{1}{q_\sigma}\log c_\sigma \right\rangle_h. \tag{2.25}$$

For each s, we define $\phi_s \in V_h$ by

$$\phi_{s,i,j,k} = -\frac{1}{q_s}\log c_{s,i,j,k} + \xi_s \qquad \forall i, j, k \in \mathbb{Z},$$

where $\xi_s = N^{-3} q_s^{-1} \sum_{p,q,r=0}^{N-1} \log c_{s,p,q,r}$. Clearly, $\phi_s \in \mathring{V}_h$. It follows from (2.22) that

$$(\nabla_h \phi_s)_{i,j,k} = -\frac{1}{q_s}(\nabla_h \log c_s)_{i,j,k} = -h\left(\frac{u_{i+1/2,j,k}}{\varepsilon_{i+1/2,j,k}}, \frac{v_{i,j+1/2,k}}{\varepsilon_{i,j+1/2,k}}, \frac{w_{i,j,k+1/2}}{\varepsilon_{i,j,k+1/2}}\right) \quad \forall i, j, k \in \mathbb{Z}.$$

The right-hand side is independent of s. So, if $s, s' \in \{1, \ldots, M\}$, then $\nabla_h(\phi_s - \phi_{s'}) = 0$ on $h\mathbb{Z}^3$, which implies $\phi_s = \phi_{s'}$, since $\mathscr{A}_h(\phi_s - \phi_{s'}) = 0$. Thus,

$$\frac{1}{q_s}\log c_{s,i,j,k} - \frac{1}{q_\sigma}\log c_{\sigma,i,j,k} = \xi_s - \xi_\sigma \qquad \forall i, j, k \in \mathbb{Z}.$$

Since $\mathscr{A}_h(\tilde{c}_s) = 0$ for each s, this and (2.25) imply the global equilibrium property (2.21). $\square$

We finally consider the discrete Poisson electrostatic energy. Let $\rho^h \in V_h$. We define

$$S_{\rho,h} = \{D \in Y_h : \nabla_h \cdot D = \rho^h \text{ on } h\mathbb{Z}^3\},$$
$$S_{0,h} = \{D \in Y_h : \nabla_h \cdot D = 0 \text{ on } h\mathbb{Z}^3\}.$$

We verify that $S_{\rho,h} \neq \emptyset$ if and only if $\rho^h \in \mathring{V}_h$.

Let $\rho^h \in \mathring{V}_h$ and define

$$\hat{I}_h[\phi] = \frac{1}{2}\|\nabla_h \phi\|_{\varepsilon,h}^2 - \langle \rho^h, \phi\rangle_h \qquad \forall \phi \in \mathring{V}_h, \tag{2.26}$$

$$\hat{F}_h[D] = \frac{1}{2}\|D\|_{1/\varepsilon,h}^2 \qquad \forall D \in S_{\rho,h}. \tag{2.27}$$

Lemma 2.2. (1) *There exists a unique minimizer* $\hat{\phi}_{\min}^h$ *of* $\hat{I}_h : \mathring{V}_h \to \mathbb{R}$, *characterized by* $\hat{\phi}_{\min}^h \in \mathring{V}_h$ *and* $\langle \nabla_h \hat{\phi}_h, \nabla_h \xi\rangle_{\varepsilon,h} = \langle \rho^h, \xi\rangle_h$ *for all* $\xi \in \mathring{V}_h$. *Equivalently, it is the unique solution in* $\mathring{V}_h$ *of the discrete Poisson equation* $A_h^\varepsilon[\hat{\phi}_h] = -\rho^h$ *on* $h\mathbb{Z}^3$.

(2) *If* $\sup_h \|\rho^h\|_\infty < \infty$*, then there exists a constant* $C > 0$*, independent of* h*, such that* $\|\hat{\phi}^h_{\min}\|_\infty + \|\nabla_h \hat{\phi}^h_{\min}\|_\infty \le C$.

Proof. Part (1) is standard. Part (2) is proved in [28, 29] (cf. also [4]). $\square$

Theorem 2.3. *Let* $\varepsilon \in C(\overline{\Omega})$ *satisfy* (1.5) *and* $\rho^h \in \mathring{V}_h$*. There exists a unique* $\hat{D}^h_{\min} \in S_{\rho,h}$ *such that* $\hat{F}_h[\hat{D}^h_{\min}] = \min_{D \in S_{\rho,h}} \hat{F}_h[D]$*. Moreover, if* $D \in S_{\rho,h}$*, then the following are equivalent:*

(1) Minimizer: $D = \hat{D}^h_{\min}$ *is the minimizer of* $\hat{F}_h : Y_h \to \mathbb{R}$*;*
(2) Global equilibrium: $\langle D, \tilde{D}\rangle_{1/\varepsilon,h} = 0$ *for all* $\tilde{D} \in S_{0,h}$*;*
(3) $D = D^\varepsilon_h[\hat{\phi}^h_{\min}]$ *with* $\hat{\phi}^h_{\min} \in \mathring{V}_h$ *the unique solution to* $A^\varepsilon_h[\hat{\phi}^h_{\min}] = -\rho^h$ *on* $h\mathbb{Z}^3$ *as in Lemma* 2.2*;*
(4) (i) Local equilibrium: D/ε *is curl free, i.e.,* $\nabla_h \times (D/\varepsilon) = 0$ *on* $h(\mathbb{Z} + 1/2)^3$*; and*
(ii) Zero total field: $\mathscr{A}_h(D/\varepsilon) = 0$ *in* $\mathbb{R}^3$.

Proof. The existence and uniqueness of the minimizer and the equivalence between Part (1) and Part (2) follow from usual arguments.

We prove that Part (1) and Part (3) are equivalent, *i.e.*, $\hat{D}^h_{\min} = D^h_\varepsilon[\hat{\phi}^h_{\min}]$; cf. (2.17) for the definition of D^h_ε. We first note by (2.18) that $\nabla_h \cdot D^\varepsilon_h[\hat{\phi}^h_{\min}] = -A^\varepsilon_h[\hat{\phi}^h_{\min}] = \rho^h$ on $h\mathbb{Z}^3$. Thus, $D^\varepsilon_h[\hat{\phi}^h] \in S_{\rho,h}$. We now denote $\phi = \hat{\phi}^h_{\min} \in \mathring{V}_h$ and $D = D^\varepsilon_h[\hat{\phi}^h_{\min}] = (u, v, w)$. Let $\tilde{D} = (\tilde{u}, \tilde{v}, \tilde{w}) \in S_{0,h}$. For fixed j and k, we have by (2.17) and summation by parts that

$$\sum_{i=0}^{N-1} \frac{u_{i+1/2,j,k}\tilde{u}_{i+1/2,j,k}}{\varepsilon_{i+1/2,j,k}} = \frac{1}{h}\sum_{i=0}^{N-1} \phi_{i,j,k}(\tilde{u}_{i+1/2,j,k} - \tilde{u}_{i-1/2,j,k}). \tag{2.28}$$

Similar identities hold for the v and w components. Summing both sides of all these identities, we obtain by the fact that $\nabla_h \cdot \tilde{D} = 0$ that $\langle D, \tilde{D}\rangle_{1/\varepsilon,h} = \langle \phi, \nabla_h \cdot \tilde{D}\rangle_h = 0$. This is Part (2), which is equivalent to Part (1). Hence, $D \in S_{\rho,h}$ is the unique minimizer. Consequently, Part (1) and Part (3) are equivalent.

We show that Part (1) implies Part (4). Assume $D = \hat{D}^h_{\min}$. Since Parts (1)–(3) are equivalent, $D = D^h_\varepsilon[\hat{\phi}^h_{\min}]$, and hence $D := (u, v, w)$ is given by (2.17) with $\hat{\phi}^h_{\min}$ replacing ϕ. By the definition of D/ε (cf. (2.16)) and that of the discrete curl operator, we can directly verify that D/ε is curl free. Hence, Part (1) implies Part (4)(i). For any $(a, b, c) \in \mathbb{R}^3$, $D + (a, b, c) \in S_{\rho,h}$. Since $g(a, b, c) := \hat{F}_h[D + (a, b, c)]$ $(a, b, c \in \mathbb{R})$ reaches its minimum at $a = b = c = 0$, we have $\partial_a g(0, 0, 0) = \partial_b g(0, 0, 0) = \partial_c g(0, 0, 0) = 0$, implying Part (4)(ii). Thus, Part (1) implies Part (4).

Finally, we prove that Part (4) implies Part (2). Suppose Part (4) is true. It follows from Lemma 2.3 below, applied to D/ε, that $D/\varepsilon = -\nabla_h \phi$ for a unique $\phi \in \mathring{V}_h$, and thus $(D/\varepsilon)_{i+1/2,j+1/2,k+1/2} = -\nabla_h \phi_{i,j,k}$ for all $i, j, k \in \mathbb{Z}$. Consequently, setting $D = (u, v, w)$, we have by the same argument used above (cf. (2.28)) that $\langle D, \tilde{D}\rangle_{1/\varepsilon,h} = 0$ for any $\tilde{D} = (\tilde{u}, \tilde{v}, \tilde{w}) \in S_{0,h}$. Thus, Part (4) implies Part (2). $\square$

Lemma 2.3. *If* $D = (u, v, w) \in Y_h$ *satisfies* $\nabla_h \times D = 0$ *on* $h(\mathbb{Z} + 1/2)^3$ *and* $\mathscr{A}_h(D) = 0$ *in* $\mathbb{R}^3$*, then there exists a unique* $\phi \in \mathring{V}_h$ *such that* $D = D^\varepsilon_h[\phi]$ *with* $\varepsilon = 1$ *identically.*

Proof. If $\phi_1, \phi_2 \in \mathring{V}_h$ and $\nabla_h \phi_1 = \nabla_h \phi_2$, then $\nabla_h(\phi_1 - \phi_2) = 0$. Thus $\phi_1 - \phi_2$ is a constant on $h\mathbb{Z}^3$. Since $\phi_1 - \phi_2 \in \mathring{V}_h$, this constant must be 0 and hence $\phi_1 = \phi_2$. This is the uniqueness.

Let $\rho^h = \nabla_h \cdot D \in V_h$. The periodicity of D implies that $\rho^h \in \mathring{V}_h$. By Lemma 2.2, there exists a unique $\phi \in \mathring{V}_h$ such that $A^\varepsilon_h[\phi] = -\rho^h$ on $h\mathbb{Z}^3$ with $\varepsilon = 1$. We define $\hat{D} = (\hat{u}, \hat{v}, \hat{w}) \in Y_h$ by $\hat{D} = D^\varepsilon_h[\phi]$ with $\varepsilon = 1$, *i.e.*, by (2.17) with $\hat{u}$, $\hat{v}$, and $\hat{w}$ replacing u, v, and w, respectively, and with $\varepsilon = 1$ identically. Since $\varepsilon = 1$, $\mathscr{A}_h(\hat{D}) = 0$. By (2.18),

$$\nabla_h \cdot \hat{D} = -\nabla_h \cdot D^\varepsilon_h[\phi] = -A^\varepsilon_h[\phi] = \rho^h \qquad \text{on } h\mathbb{Z}^3.$$

By the definition of discrete curl operator and direct calculations using (2.17) with $\hat{u}$, $\hat{v}$, and $\hat{w}$ replacing u, v, and w, respectively, we have $\nabla_h \times \hat{D} = 0$ on $h(\mathbb{Z} + 1/2)^3$. Denoting $\tilde{D} = (\tilde{u}, \tilde{v}, \tilde{w}) := D - \hat{D} \in Y_h$, we have

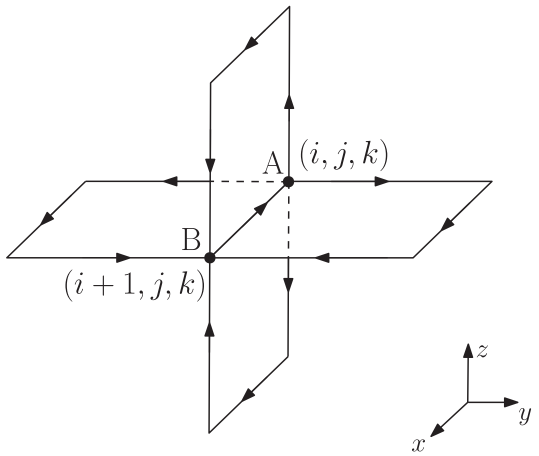

FIGURE 1. The divergence-free of the displacement $\tilde{D}$ at the two vertices A and B (cf. (2.29) and (2.30)) and the zero circulation along the four edges of each of the four faces sharing the edge AB that results from the curl-free of $\tilde{D}$ (cf. (2.31)–(2.34)) lead to the mean-value property of the $\tilde{u}$-component of $\tilde{D}$ at the midpoint of the edge AB (cf. the last equation above). An arrow indicates the sign of a component of $\tilde{D}$, positive (negative) if the arrow points in the positive (negative) coordinate direction. Note that the current from B to A is counted six times.

$\nabla_h \cdot \tilde{D} = 0$ on $h\mathbb{Z}^3$, $\nabla_h \times \tilde{D} = 0$ on $h(\mathbb{Z}+1/2)^3$, and $\mathscr{A}_h(\tilde{D}) = 0$ in $\mathbb{R}^3$. We shall show that $\tilde{D} = 0$ identically which will imply that $D = \hat{D} = D_h^\varepsilon[\phi] = -\nabla_h \phi$, the desired existence.

We claim that each component of $\tilde{D} = (\tilde{u}, \tilde{v}, \tilde{w})$ is a discrete harmonic function. Fix $i, j, k \in \mathbb{Z}$. We consider the two adjacent grid points labeled by $A = (i, j, k)$ and $B = (i+1, j, k)$, and also the four faces of grid boxes that share the common edge AB connecting these two grid points; cf. Figure 1. Since $-(\nabla_h \cdot \tilde{D})_{i,j,k} = 0$ and $(\nabla_h \cdot \tilde{D})_{i+1,j,k} = 0$, we have

$$\tilde{u}_{i-1/2,j,k} - \tilde{u}_{i+1/2,j,k} + \tilde{v}_{i,j-1/2,k} - \tilde{v}_{i,j+1/2,k} + \tilde{w}_{i,j,k-1/2} - \tilde{w}_{i,j,k+1/2} = 0, \tag{2.29}$$

$$\tilde{u}_{i+3/2,j,k} - \tilde{u}_{i+1/2,j,k} + \tilde{v}_{i+1,j+1/2,k} - \tilde{v}_{i+1,j-1/2,k} + \tilde{w}_{i+1,j,k+1/2} - \tilde{w}_{i+1,j,k-1/2} = 0. \tag{2.30}$$

Two of the four faces sharing the edge AB are on the plane $y = jh$, one with the vertices A, B, $(i, j, k-1)$, and $(i+1, j, k-1)$, and the other A, B, $(i, j, k+1)$, and $(i+1, j, k+1)$, respectively. The other two faces are on the coordinate plane $z = kh$, with vertices A, B, $(i, j-1, k)$, and $(i+1, j-1, k)$, and A, B, $(i, j+1, k)$, and $(i+1, j+1, k)$, respectively. Since $\nabla_h \times \tilde{D} = 0$, we have, by keeping the term $u_{i+1/2,j,k}$ with a negative sign, the four circulation-free equations on these four faces (cf. Fig. 1)

$$\tilde{u}_{i+1/2,j,k-1} - \tilde{u}_{i+1/2,j,k} + \tilde{w}_{i+1,j,k+1/2} - \tilde{w}_{i,j,k+1/2} = 0, \tag{2.31}$$

$$\tilde{u}_{i+1/2,j,k+1} - \tilde{u}_{i+1/2,j,k} + \tilde{w}_{i,j,k+1/2} - \tilde{w}_{i+1,j,k+1/2} = 0, \tag{2.32}$$

$$\tilde{u}_{i+1/2,j-1,k} - \tilde{u}_{i+1/2,j,k} + \tilde{v}_{i+1,j-1/2,k} - \tilde{v}_{i,j-1/2,k} = 0, \tag{2.33}$$

$$\tilde{u}_{i+1/2,j+1,k} - \tilde{u}_{i+1/2,j,k} + \tilde{v}_{i,j+1/2,k} - \tilde{v}_{i+1,j+1/2,k} = 0. \tag{2.34}$$

Adding the same sides of all (2.29)–(2.34) leads to

$$\tilde{u}_{i+3/2,j,k} + \tilde{u}_{i-1/2,j,k} + \tilde{u}_{i+1/2,j,k-1} + \tilde{u}_{i+1/2,j+1,k} + \tilde{u}_{i+1/2,j,k-1} + \tilde{u}_{i+1/2,j+1,k} - 6\tilde{u}_{i+1/2,j,k} = 0.$$

Since $i, j, k \in \mathbb{Z}$ are arbitrary, this means that $\tilde{u}$ satisfies the discrete mean-value property, *i.e.*, $\tilde{u}$ is a discrete harmonic function. Similarly, $\tilde{v}$ and $\tilde{w}$ are discrete harmonic functions.

Let $p, q, r \in \mathbb{Z}$ be such that $\tilde{u}_{p+1/2,q,r} = \max_{i,j,k\in\mathbb{Z}} \tilde{u}_{i+1/2,j,k}$. Then, it follows from the mean-value property (cf. the last equation above) with $(i,j,k) = (p,q,r)$ that $\tilde{u}$ also achieves its maximum value at the 6 neighboring points. Applying this argument to these 6 neighboring points, and to the 6 points neighboring each of these 6 points, and so on, we see that all $\tilde{u}_{i+1/2,j,k}$ equal the maximum value. Hence $\tilde{u}$ is a constant. But, $\sum_{i,j,k=0}^{N-1} \tilde{u}_{i+1/2,j,k} = 0$. Hence, $\tilde{u} = 0$ identically. Similarly, $\tilde{v} = 0$ and $\tilde{w} = 0$. Hence $\tilde{D} = 0$. □

3. Error estimates

Let $f \in C_{\text{per}}(\overline{\Omega})$ and $D = (u, v, w) \in C_{\text{per}}(\overline{\Omega}, \mathbb{R}^3)$. We define $\mathscr{Q}_h f \in V_h$ by

$$\mathscr{Q}_h f = f + \mathscr{A}_\Omega(f) - \mathscr{A}_h(f) \qquad \text{on} \quad h\mathbb{Z}^3$$

and also define $\mathscr{P}_h D \in Y_h$ (cf. (2.12) for the notation Y_h) by

$$(\mathscr{P}_h D)_{i+1/2,j+1/2,k+1/2} = (u((i+1/2)h, jh, kh), v(ih, (j+1/2)h, kh), w(ih, jh, (k+1/2)h))$$

for all $i, j, k \in \mathbb{Z}$. We denote by $C > 0$ a generic constant, independent of h. We omit the proof of the following elementary lemma:

Lemma 3.1. (1) *If $f \in C^2_{\text{per}}(\overline{\Omega})$, then*

$$|\mathscr{Q}_h f - f| = |\mathscr{A}_\Omega(f) - \mathscr{A}_h(f)| \le Ch^2 \qquad \text{on} \quad h\mathbb{Z}^3.$$

(2) *If $D \in C^3_{\text{per}}(\overline{\Omega}, \mathbb{R}^3)$, then*

$$\nabla_h \cdot \mathscr{P}_h D = \nabla \cdot D + h^2 \sigma^h \quad \text{with } \sigma^h \in V_h \text{ and } |\sigma^h| \le C \quad \text{on } h\mathbb{Z}^3.$$

(3) *If $\varepsilon \in C^2_{\text{per}}(\overline{\Omega})$ satisfies (1.5), $\phi \in C^3_{\text{per}}(\overline{\Omega})$, and $D = -\varepsilon\nabla\phi \in C^3_{\text{per}}(\overline{\Omega}, \mathbb{R}^3)$, then*

$$\mathscr{P}_h D = D_h^\varepsilon[\phi] + h^2 T^h \quad \text{with } T^h \in Y_h \text{ and } |T^h| \le C \qquad \text{on} \quad h(\mathbb{Z}+1/2)^3.$$

(4) *If $\varepsilon \in C^2_{\text{per}}(\overline{\Omega})$ satisfies (1.5), $\phi \in C^4_{\text{per}}(\overline{\Omega})$, and $D = -\varepsilon\nabla\phi \in C^3_{\text{per}}(\overline{\Omega}, \mathbb{R}^3)$, then*

$$\nabla \cdot \varepsilon \nabla \phi = A_h^\varepsilon[\phi] + h^2 \tau^h \quad \text{with } \tau^h \in V_h \text{ and } |\tau^h| \le C \qquad \text{on} \quad h\mathbb{Z}^3.$$

For any $D = (u, v, w) \in Y_h$ (cf. (2.12)), we define $m_h[D] : h\mathbb{Z}^3 \to \mathbb{R}^3$ by

$$(m_h[D])_{i,j,k} = \left(\frac{u_{i+1/2,j,k} + u_{i-1/2,j,k}}{2}, \frac{v_{i,j+1/2,k} + v_{i,j-1/2,k}}{2}, \frac{w_{i,j,k+1/2} + w_{i,j,k-1/2}}{2} \right) \ \forall i,j,k \in \mathbb{Z}.$$

Theorem 3.1. *Let $\varepsilon \in C^2_{\text{per}}(\overline{\Omega})$ satisfy (1.5), $\rho \in C^2_{\text{per}}(\overline{\Omega})$ satisfy (1.6), and $\rho^h := \mathscr{Q}_h \rho$ with*

$$\mathscr{Q}_h \rho = \rho + \mathscr{A}_\Omega(\rho) - \mathscr{A}_h(\rho) = \rho - \frac{1}{L^3} \sum_{s=1}^{M} q_s N_s - \frac{1}{N^3} \sum_{l,m,n=0}^{N-1} \rho(lh, mh, nh). \tag{3.1}$$

Let $\phi_{\min} \in \mathring{H}^1_{\text{per}}(\Omega)$, $\phi^h_{\min} \in \mathring{V}_h$, $(c_{\min}, D_{\min}) \in X_\rho$, and $(c^h_{\min}, D^h_{\min}) \in X_{\rho,h}$ be the unique minimizer of $I : \mathring{H}^1_{\text{per}}(\Omega) \to \mathbb{R} \cup \{+\infty\}$, $I_h : \mathring{V}_h \to \mathbb{R}$, $F : X_\rho \to \mathbb{R}$, and $F_h : X_{\rho,h} \to \mathbb{R}$, respectively. Assume $\phi_{\min} \in C^3_{\text{per}}(\overline{\Omega})$ and $D_{\min} \in C^3_{\text{per}}(\overline{\Omega}, \mathbb{R}^3)$. Then, we have

$$\|c_{\min} - c^h_{\min}\|_h + \|\mathscr{P}_h D_{\min} - D^h_{\min}\|_h + \|\phi_{\min} - \phi^h_{\min}\|_h \le Ch^2. \tag{3.2}$$

If $\phi_{\min} \in C^4_{\text{per}}(\overline{\Omega})$, then we also have

$$\|c_{\min} - c^h_{\min}\|_\infty + \|\mathscr{P}_h D_{\min} - D^h_{\min}\|_\infty + \left\| \frac{m_h[-D^h_{\min}]}{\varepsilon} - \nabla\phi_{\min} \right\|_\infty \le Ch^2. \tag{3.3}$$

Proof. Let us denote

$$\phi = \phi_{\min}, \quad \phi^h = \phi^h_{\min}, \quad c = c_{\min}, \quad D = D_{\min}, \quad c^h = c^h_{\min}, \quad D^h = D^h_{\min}.$$

By Theorem 1.1, $D = -\varepsilon \nabla \phi$. Thus, it follows from Lemma 3.1 that

$$\mathscr{P}_h D = D_h^\varepsilon[\phi] + h^2 T^h \quad \text{with } |T^h| \le C \text{ on } h(\mathbb{Z}+1/2)^3.$$

Let $(\tilde{c}, \tilde{D}) \in \tilde{X}_{0,h}$. Summation by parts leads to

$$\langle \mathscr{P}_h D, \tilde{D}\rangle_{1/\varepsilon,h} \le \langle D_h^\varepsilon[\phi^e], \tilde{D}\rangle_{1/\varepsilon,h} + C\langle 1, \tilde{D}\rangle h^2 \le \langle \phi, \nabla_h \cdot \tilde{D}\rangle_h + Ch^2 \|\tilde{D}\|_h. \tag{3.4}$$

It follows from (1.9) in Theorem 1.1 that for each $s \in \{1, \ldots, M\}$

$$\log c_s = \xi_s - q_s \phi \quad \text{with } \xi_s = -\log\left(N_s^{-1} L^3 \mathscr{A}_h(e^{-q_s\phi})\right).$$

Since each $\tilde{c}_s \in \mathring{V}_h$, which implies $\langle c_s, \xi_s\rangle_h = 0$, and $\nabla_h \cdot \tilde{D} = \sum_{s=1}^M q_s \tilde{c}_s$, we have

$$\sum_{s=1}^M \langle \tilde{c}_s, \log c_s\rangle_h = \sum_{s=1}^M \langle \tilde{c}_s, \xi_s - q_s\phi\rangle_h = -\langle \phi, \nabla_h \cdot \tilde{D}\rangle_h.$$

This and (3.4) lead to

$$\langle \mathscr{P}_h D, \tilde{D}\rangle_{1/\varepsilon,h} + \sum_{s=1}^M \langle \tilde{c}_s, \log c_s\rangle_h \le Ch^2\|\tilde{D}\|_h \qquad \forall (\tilde{c}, \tilde{D}) \in \tilde{X}_{0,h}. \tag{3.5}$$

Let $e_h^D = \mathscr{P}_h D - D^h$. By Theorem 2.2, $(c^h, D^h) \in X_{\rho,h}$ satisfies the global equilibrium condition (2.21), which together with (3.5) imply

$$\langle e_h^D, \tilde{D}\rangle_{1/\varepsilon,h} + \sum_{s=1}^M \langle \tilde{c}_s, \log c_s - \log c_s^h\rangle_h \le Ch^2\|\tilde{D}\|_h \qquad \forall (\tilde{c}, \tilde{D}) \in \tilde{X}_{0,h}. \tag{3.6}$$

Since $(c, D) \in X_\rho$ and $(c^h, D^h) \in X_{\rho,h}$, we have

$$\nabla \cdot D = \rho + \sum_{s=1}^M q_s c_s \qquad \text{in } \mathbb{R}^3,$$

$$\nabla_h \cdot D^h = \rho^h + \sum_{s=1}^M q_s c_s^h \qquad \text{on } h\mathbb{Z}^3.$$

Moreover, by Lemma 3.1,

$$\nabla_h \cdot \mathscr{P}_h D = \nabla \cdot D + \sigma^h h^2 \qquad \text{on } h\mathbb{Z}^3$$

for some $\sigma^h \in V_h$ such that $|\sigma^h| \le C$ on $h\mathbb{Z}^3$. Thus,

$$\nabla_h \cdot e_h^D = \nabla_h \cdot \left(\mathscr{P}_h D - D^h\right) = \sum_{s=1}^M q_s(c_s - c_s^h) + \rho - \rho^h + \sigma^h h^2 \qquad \text{on } h\mathbb{Z}^3. \tag{3.7}$$

Define

$$\tilde{c}_s = c_s - c_s^h + \mathscr{A}_\Omega(c_s) - \mathscr{A}_h(c_s) \qquad (s = 1, \ldots, M).$$

Since $c \in X_\rho$ and $c^h \in X_{\rho,h}$, $\mathscr{A}_\Omega(c_s) = \mathscr{A}_h(c_s^h) = N_s L^{-3}$. Hence, $\tilde{c}_s \in \mathring{V}_h$. It then follows from (3.7) that

$$\nabla_h \cdot e_h^D = \sum_{s=1}^M q_s \tilde{c}_s + h^2 \gamma^h, \tag{3.8}$$

where

$$h^2\gamma^h = -\sum_{s=1}^M q_s \left[\mathscr{A}_\Omega(c_s) - \mathscr{A}_h(c_s)\right] + \rho - \rho^h + \sigma^h h^2.$$

By Lemma 3.1, $|\gamma^h| \le C$ on $h\mathbb{Z}^3$. Moreover, $\gamma^h \in \mathring{V}_h$, since e_h^D is periodic and each $\tilde{c}_s \in \mathring{V}_h$. Let $\psi^h \in \mathring{V}_h$ be such that $\Delta_h \psi^h = -\gamma^h$. We thus have $|\psi^h| \le C$ on $h\mathbb{Z}^3$ by Lemma 2.2. Denoting $G^h = -\nabla_h \psi^h \in Y_h$ and $\tilde{D} = e_h^D - h^2 G^h \in Y_h$, we then have by (3.8) that $\nabla_h \cdot \tilde{D} = \sum_{s=1}^M q_s \tilde{c}_s$. Hence, setting $\tilde{c} = (\tilde{c}_s, \ldots, \tilde{c}_M)$, we have $(\tilde{c}, \tilde{D}) \in \tilde{X}_{0,h}$.

Now, plugging the newly constructed $(\tilde{c}, \tilde{D}) \in \tilde{X}_{0,h}$ in (3.6), we obtain

$$\langle e_h^D, e_h^D - h^2 G^h\rangle_{1/\varepsilon,h} + \sum_{s=1}^M \langle c_s - c_s^h + \mathscr{A}_\Omega(c_s) - \mathscr{A}_h(c_s), \log c_s - \log c_s^h\rangle_h \le Ch^2 \|e_h^D - h^2 G^h\|_h.$$

Consequently, since $|\mathscr{A}_\Omega(c_s) - \mathscr{A}_h(c_s)| \le Ch^2$ for all s by Lemma 3.1, we have

$$\begin{aligned}\langle e_h^D, e_h^D - h^2 G^h\rangle_{1/\varepsilon,h} &+ \sum_{s=1}^M \langle c_s - c_s^h, \log c_s - \log c_s^h\rangle_h \\ &\le Ch^2\|e_h^D\|_h + Ch^4\|G^h\|_h + Ch^2\|\log c_s - \log c_s^h\|_h.\end{aligned} \tag{3.9}$$

Since $0 < C_1 \le c_s, c_s^h \le C_2$ on $h\mathbb{Z}^3$ for all h and s (cf. Thms. 1.1 and 2.2), we have by the Mean-Value Theorem that

$$\langle c_s - c_s^h, \log c_s - \log c_s^h\rangle_h \ge \frac{1}{C_2}\|c_s - c_s^h\|_h^2 \quad \text{and} \quad \|\log c_s - \log c_s^h\|_h \le \frac{1}{C_1}\|c_s - c_s^h\|_h. \tag{3.10}$$

Moreover, since $G^h = -\nabla_h \psi^h \in Y_h$, by summation by parts and the Cauchy–Schwarz inequality, we get

$$\|G^h\|_h^2 = \langle G^h, -\nabla_h \psi^h\rangle_h = \langle \nabla_h \cdot G^h, \psi^h\rangle_h = \langle \gamma^h, \psi^h\rangle_h \le \|\gamma^h\|_h \, \|\psi^h\|_h \le C. \tag{3.11}$$

It now follows from (3.9)–(3.11) and the equivalence of the norms $\|\cdot\|_{1/\varepsilon,h}$ and $\|\cdot\|_h$ that

$$\begin{aligned}&\|e_h^D\|_{1/\varepsilon,h}^2 + \frac{1}{C_2}\|c - c^h\|_h^2 \\ &\quad \le \langle e_h^D, e_h^D - h^2 G^h\rangle_{1/\varepsilon,h} + \langle e_h^D, h^2 G^h\rangle_{1/\varepsilon,h} + \sum_{s=1}^M \langle c_s - c_s^h, \log c_s - \log c_s^h\rangle_h \\ &\quad \le Ch^2\|e_h^D\|_h + Ch^4 + Ch^2\|c_s - c_s^h\|_h \\ &\quad \le \frac{1}{2}\|e_h^D\|_h^2 + \frac{1}{2C_2}\|c_s - c_s^h\|_h^2 + Ch^4.\end{aligned} \tag{3.12}$$

By Lemma 3.1 and the fact that $D^h = D_h^\varepsilon[\phi^h]$, we have

$$\|\nabla_h \phi - \nabla_h \phi^h\|_h \le C_3\|D_h^\varepsilon[\phi] - D_h^\varepsilon[\phi^h]\| \le C_3\|\mathscr{P}_h D - D^h\|_h + C_3 h^2 \le Ch^2.$$

Since ϕ^h and $\mathscr{Q}_h\phi$ are in $\mathring{V}_h$ and $\phi^h - \mathscr{Q}_h\phi$ is constant on $h\mathbb{Z}^3$, the discrete Poincaré inequality then implies that

$$\|\mathscr{Q}_h\phi - \phi^h\|_h \le C\|\nabla_h \mathscr{Q}_h \phi - \nabla_h \phi^h\|_h = C\|\nabla_h\phi - \nabla_h\phi^h\|_h \le Ch^2.$$

This and Lemma 3.1, together with (3.12), then imply the estimates (3.2).

Assume now $\phi \in C^4_{\rm per}(\overline{\Omega})$. Since ϕ and ϕ^h are solutions to the CCPBE (1.8) and the discrete CCPBE (2.5), respectively, it follows that

$$\nabla \cdot \varepsilon \nabla \phi - A_h^\varepsilon[\phi^h] + \sum_{s=1}^M \frac{q_s N_s}{L^3} \left[\frac{e^{-q_s\phi}}{\mathscr{A}_\Omega(e^{-q_s\phi})} - \frac{e^{-q_s\phi^h}}{\mathscr{A}_h(e^{-q_s\phi^h})} \right] = \rho^h - \rho \quad \text{on} \quad h\mathbb{Z}^3. \tag{3.13}$$

By Lemma 3.1, the definition $\rho^h = \mathscr{Q}_h \rho$, and (3.1), we have

$$|\nabla \cdot \varepsilon \nabla \phi - A_h^\varepsilon[\phi]| \le Ch^2 \quad \text{and} \quad |\rho - \rho^h| \le Ch^2 \qquad \text{on} \quad h\mathbb{Z}^3. \tag{3.14}$$

Clearly, $\|\rho^h\|_\infty \le C$. Thus, it follows from Theorem 2.1 that $\|\phi^h\|_\infty \le C$ and that all $\|e^{-q_s\phi^h}\|_\infty$, $\mathscr{A}_\Omega(e^{-q_s\phi^h})$, and $\mathscr{A}_h(e^{-q_s\phi^h})$ are bounded below and above by positive constants independent of h. Consequently, the Mean-Value Theorem, the Cauchy–Schwarz inequality, and (3.2) together imply that

$$\begin{aligned} \left| \mathscr{A}_h(e^{-q_s\phi}) - \mathscr{A}_h(e^{-q_s\phi^h}) \right| &\le \frac{1}{N^3} \sum_{i,j,k=0}^{N-1} \left| e^{-q_s\phi_{i,j,k}} - e^{-q_s\phi^h_{i,j,k}} \right| \\ &\le \frac{C}{N^3} \sum_{i,j,k=0}^{N-1} \left| \phi_{i,j,k} - \phi^h_{i,j,k} \right| \\ &\le C\|\phi - \phi^h\|_h \\ &\le Ch^2, \qquad s = 1, \ldots, M. \end{aligned}$$

This and Lemma 3.1 imply

$$\begin{aligned} |\mathscr{A}_\Omega(e^{-q_s\phi}) - \mathscr{A}_h(e^{-q_s\phi^h})| &\le |\mathscr{A}_\Omega(e^{-q_s\phi}) - \mathscr{A}_h(e^{-q_s\phi})| + |\mathscr{A}_h(e^{-q_s\phi}) - \mathscr{A}_h(e^{-q_s\phi^h})| \\ &\le Ch^2. \end{aligned} \tag{3.15}$$

Moreover, by the fact again that $\mathscr{A}_h(e^{-q_s\phi^h})$ is bounded below by a positive constant independent of h (cf. the argument below (3.14)), we obtain by (3.15) that

$$\left| \left[\frac{e^{-q_s\phi}}{\mathscr{A}_\Omega(e^{-q_s\phi})} - \frac{e^{-q_s\phi^h}}{\mathscr{A}_h(e^{-q_s\phi^h})} \right] - \frac{1}{\mathscr{A}_\Omega\left(e^{-q_s\phi}\right)} \left(e^{-q_s\phi} - e^{-q_s\phi^h} \right) \right| \le Ch^2, \qquad 1 \le s \le M.$$

Denoting the error $r_h^\phi := \phi - \phi^h$, this and (3.14) allow us to rewrite (3.13) into

$$A_h^\varepsilon[r_h^\phi] + \sum_{s=1}^M \frac{q_s N_s}{L^3 \mathscr{A}_\Omega(e^{-q_s\phi})} \left(e^{-q_s\phi} - e^{-q_s\phi^h} \right) = h^2 \alpha^h \qquad \text{on} \quad h\mathbb{Z}^3, \tag{3.16}$$

where $\alpha^h \in V_h$ satisfies $|\alpha^h| \le C$ on $h\mathbb{Z}^3$. Since $e^{-q_s\phi} - e^{-q_s\phi^h} = -q_s e^{-q_s\psi_s^h} r_h^\phi$ for some $\psi_s^h \in V_h$ which lies in between ϕ and ϕ^h at each (i, j, k), the error equation (3.16) for r_h^ϕ becomes

$$-A_h^\varepsilon[r_h^\phi] + b^h r_h^\phi = -h^2 \alpha^h, \tag{3.17}$$

where

$$b^h = \sum_{s=1}^M \frac{q_s^2 N_s e^{-q_s\psi_s^h}}{L^3 \mathscr{A}_\Omega(e^{-q_s\phi})} \in V_h \quad \text{and} \quad C_4 \le b^h \le C_5$$

for some constants $C_4 > 0$ and $C_5 > 0$ independent of h.

The linear operator $M_h : V_h \to V_h$ defined by

$$M_h \xi_h = -A_h^\varepsilon[\xi_h] + b^h \xi_h \qquad (\xi_h \in V_h)$$

can be represented by a matrix $\mathbf{M}_h := \mathbf{B}_h - \mathbf{A}_h^\varepsilon$, where $\mathbf{B}_h$ is the diagonal matrix with diagonal entries $b^h_{i,j,k}$ $(0 \le i, j, k \le N-1)$ and $\mathbf{A}_h^\varepsilon$ is the matrix representing the difference operator A_h^ε. By (2.2) and (2.1), $\mathbf{B}_h - \mathbf{A}_h^\varepsilon$ is strictly diagonally dominant. In fact, if $M_{h,(i,j,k),(l,m,n)}$ is the entry of $\mathbf{M}_h$ in the row and column corresponding to (i, j, k) and (l, m, n), respectively, then we can verify that

$$\min_{(i,j,k)} \left(|M_{h,(i,j,k),(i,j,k)}| - \sum_{(l,m,n)\neq(i,j,k)} |M_{h,(i,j,k),(l,m,n)}| \right) = \min_{(i,j,k)} b^h_{i,j,k} \ge C_4 > 0.$$

Therefore, the matrix $\mathbf{M}_h$ is invertible and $\|\mathbf{M}_h^{-1}\|_\infty \le 1/C_4$; cf. [38,39]. Hence, $M_h : V_h \to V_h$ is invertible and $\|M_h^{-1}\|_\infty \le 1/C_4$. Since $|\alpha^h| \le C$ on $h\mathbb{Z}^3$, we have by (3.17) that

$$\|r_h^\phi\|_\infty = h^2 \|M_h^{-1}\alpha^h\|_\infty \le h^2 \|M_h^{-1}\|_\infty \|\alpha^h\|_\infty \le Ch^2. \tag{3.18}$$

By Theorems 1.1, 2.2, (3.15), (3.18), and the bound $\|\phi^h\|_\infty \le C$, we have

$$\|c_s - c_s^h\|_\infty = \frac{N_s}{L^3} \left\| \frac{e^{-q_s\phi}}{\mathscr{A}_\Omega(e^{-q_s\phi})} - \frac{e^{-q_s\phi^h}}{\mathscr{A}_h(e^{-q_s\phi^h})} \right\|_\infty \le Ch^2, \qquad s = 1, \dots, M. \tag{3.19}$$

Let

$$\bar{r}_h^\phi = r_h^\phi - \mathscr{A}_h(r_h^\phi) \in \mathring{V}_h \qquad \text{and} \qquad \beta^h = h^2\alpha^h + b^h r_h^\phi \in V_h.$$

Then (3.17) becomes $A_h^\varepsilon[\bar{r}_h^\phi] = \beta^h$ on $h\mathbb{Z}^3$. This implies $\beta^h \in \mathring{V}_h$. Moreover, $\|\beta^h\|_\infty \le Ch^2$ by (3.18). Since $A_h^\varepsilon : \mathring{V}_h \to \mathring{V}_h$ is invertible, we have $\bar{r}_h^\phi = (A_h^\varepsilon)^{-1}\beta^h$. It follows now from the stability of $(A_h^\varepsilon)^{-1}$ [4,28,29] that

$$\|\partial_m^h r_h^\phi\|_\infty = \|\partial_m^h \bar{r}_h^\phi\|_\infty \le \|\partial_m^h (A_h^\varepsilon)^{-1}\|_\infty \|\beta^h\|_\infty \le Ch^2 \qquad (m = 1, 2, 3).$$

This and Part (3) of Lemma 3.1 imply

$$\|\mathscr{P}_h D - D^h\|_\infty \le \|\mathscr{P}_h D - D_h^\varepsilon[\phi]\|_\infty + \|D_h^\varepsilon[r_h^\phi]\|_\infty \le Ch^2, \tag{3.20}$$

Finally, Taylor expanding $(\varepsilon\partial_1\phi)((i+1/2)h, jh, kh)$ and $(\varepsilon\partial_1\phi((i-1/2)h, jh, kh)$ at (i, j, k) leads to

$$\left| \frac{1}{2}(u_{i+1/2,j,k} + u_{i-1/2,j,k}) + (\varepsilon\partial_1\phi)(i, j, k) \right| \le Ch^2 \qquad \forall i, j, k \in \mathbb{Z}.$$

Similar inequalities hold with respect to ∂_2 and ∂_3. Hence, by the definition of m_h, $|m_h[\mathscr{P}_h D] + \varepsilon\nabla\phi| \le Ch^2$ on $h\mathbb{Z}^3$. But (3.20) implies that $|m_h[D^h] - m_h[\mathscr{P}_h D]| \le Ch^2$ on $h\mathbb{Z}^3$. Therefore,

$$\left| m_h[-D^h] - \varepsilon\nabla\phi \right| \le Ch^2 \qquad \text{on} \quad h\mathbb{Z}^3.$$

This, together with (3.19) and (3.20), implies (3.3). □

We now present the error estimate for the finite-difference approximation of the Poisson energy but omit its proof.

Theorem 3.2. *Assume* $\varepsilon \in C^2_{\rm per}(\overline{\Omega})$ *satisfies* (1.5), $\rho \in C^2_{\rm per}(\overline{\Omega})$ *satisfies* $\mathscr{A}_\Omega(\rho) = 0$, *and* $\rho^h := \mathscr{Q}_h\rho \in \mathring{V}_h$. *Let* $\hat{\phi}_{\min} \in \mathring{H}^1_{\rm per}(\Omega)$, $\hat{\phi}^h_{\min} \in \mathring{V}_h$, $\hat{D}_{\min} \in S_\rho$, *and* $\hat{D}^h_{\min} \in S_{\rho,h}$ *be the unique minimizers of the functionals* $\hat{I} : \mathring{H}^1_{\rm per}(\Omega) \to \mathbb{R}$, $\hat{I}_h : \mathring{V}_h \to \mathbb{R}$, $\hat{F} : S_\rho \to \mathbb{R}$, *and* $\hat{F}_h : S_{\rho,h} \to \mathbb{R}$, *respectively. Assume that* $\hat{\phi}_{\min} \in C^3_{\rm per}(\overline{\Omega})$ *and* $\hat{D}_{\min} \in C^3_{\rm per}(\overline{\Omega}, \mathbb{R}^3)$, *then there exists a constant* $C = C(\varepsilon, \rho, \Omega) > 0$, *independent of* h, *such that*

$$\|\mathscr{P}_h \hat{D}_{\min} - \hat{D}^h_{\min}\|_h + \left\| \frac{m_h[-\hat{D}^h_{\min}]}{\varepsilon} - \nabla \hat{\phi}_{\min} \right\|_h \le Ch^2.$$

If in addition $\hat{\phi}_{\min} \in C^4_{\rm per}(\overline{\Omega})$, *then*

$$\|\mathscr{P}_h \hat{D}_{\min} - \hat{D}^h_{\min}\|_\infty + \left\| \frac{m_h[-\hat{D}^h_{\min}]}{\varepsilon} - \nabla \hat{\phi}_{\min} \right\|_\infty \le Ch^2.$$

4. Local algorithms and their convergence

We first describe the local algorithm for minimizing the discrete PB energy $F_h : X_{\rho,h} \to \mathbb{R}$ defined in (2.19) with $\varepsilon \in V_h$ such that $\varepsilon > 0$ on $h\mathbb{Z}^3$ and $\rho^h \in V_h$ satisfying (2.3). We define $c^{(0)} = (c_1^{(0)}, \ldots, c_M^{(0)})$ with $c^{(0)}_{s,i,j,k} = L^{-3}N_s$ for all $i, j, k \in \mathbb{Z}$ and $s = 1, \ldots, M$. Let $\tau^h = \rho^h + \sum_{s=1}^M q_s c_s^{(0)}$. We define [3]

$$\forall i, j \in \{0, \ldots, N-1\}: \ w^{(0)}_{i,j,1/2} = 0,\ w^{(0)}_{i,j,k+1/2} = w^{(0)}_{i,j,k-1/2} + hp_k, \quad k = 1, \ldots, N-1, \tag{4.1}$$

$$\forall i, k \in \{0, \ldots, N-1\}: \ v^{(0)}_{i,1/2,k} = 0,\ v^{(0)}_{i,j+1/2,k} = v^{(0)}_{i,j-1/2,k} + hq_{j,k}, \quad j = 1, \ldots, N-1, \tag{4.2}$$

$$\forall j, k \in \{0, \ldots, N-1\}: \ u^{(0)}_{1/2,j,k} = 0,\ u^{(0)}_{i+1/2,j,k} = u^{(0)}_{i-1/2,j,k} + h(\tau^h_{i,j,k} - p_k - q_{j,k}), \tag{4.3}$$

$$i = 1, \ldots, N-1, \tag{4.4}$$

where

$$p_k = \frac{1}{N^2}\sum_{l,m=0}^{N-1} \tau^h_{l,m,k} \quad \text{and} \quad q_{j,k} = \frac{1}{N}\sum_{l=0}^{N-1} \tau^h_{l,j,k} - p_k \qquad (j, k = 0, \ldots, N-1). \tag{4.5}$$

We verify that our initialization $(c^{(0)}, D^{(0)}) \in X_{\rho,h}$.

To describe the local updates, let $(c, D) = (c_1, \ldots, c_M; u, v, w) \in X_{\rho,h}$ with $c_{s,i,j,k} > 0$ for all s and i, j, k. Fix s and (i, j, k). Define $(\check{c}, \check{D})$ to be the same as (c, D) except

$$\check{c}_{s,i,j,k} := c_{s,i,j,k} - \zeta_s, \quad \check{c}_{s,i+1,j,k} := c_{s,i+1,j,k} + \zeta_s, \quad \check{u}_{i+1/2,j,k} := u_{i+1/2,j,k} - hq_s\zeta_s,$$

where $\zeta_s \in (-c_{s,i+1,j,k}, c_{s,i,j,k})$ is to be determined. One verifies that $(\check{c}, \check{D}) \in X_{\rho,h}$ and all the components of $\check{c}$ are still strictly positive. We choose ζ_s to minimize the perturbed energy $F_h[\check{c}, \check{D}]$, equivalently, the energy change

$$\begin{aligned}\Delta F_h(\zeta_s) &:= F_h[\check{c}, \check{D}] - F_h[c, D] \\ &= h^3\left[(c_{s,i,j,k} - \zeta_s)\log(c_{s,i,j,k} - \zeta_s) + (c_{s,i+1,j,k} + \zeta_s)\log(c_{s,i+1,j,k} + \zeta_s)\right. \\ &\quad \left. - c_{s,i,j,k}\log c_{s,i,j,k} - c_{s,i+1,j,k}\log c_{s,i+1,j,k}\right] \\ &\quad + \frac{h^3}{2}\left[\frac{\left(u_{i+1/2,j,k} - hq_s\zeta_s\right)^2 - u^2_{i+1/2,j,k}}{\varepsilon_{i+1/2,j,k}}\right]\end{aligned} \tag{4.6}$$

for all $\zeta_s \in (-c_{s,i+1,j,k}, c_{s,i,j,k})$. We verify that $(\Delta F_h)'' > 0$ and ΔF_h attains its unique minimum at some $\zeta_{s,i+1/2,j,k} \in (-c_{s,i+1,j,k}, c_{s,i,j,k})$, which is determined by $(\Delta F_h)'(\zeta_{s,i+1/2,j,k}) = 0$, *i.e.*,

$$\log\left(c_{s,i+1,j,k} + \zeta_{s,i+1/2,j,k}\right) - \log\left(c_{s,i,j,k} - \zeta_{s,i+1/2,j,k}\right) - \frac{hq_s\left(u_{i+1/2,j,k} - hq_s\zeta_{s,i+1/2,j,k}\right)}{\varepsilon_{i+1/2,j,k}} = 0. \tag{4.7}$$

With $\zeta := \zeta_{s,i+1/2,j,k}$, $\alpha := c_{s,i,j,k}$, $\beta := c_{s,i+1,j,k}$, $\gamma := u_{i+1/2,j,k}$, $a = h^2q_s^2/\varepsilon_{i+1/2,j,k} > 0$, and $b = hq_s/\varepsilon_{i+1/2,j,k} \in \mathbb{R}$, (4.7) becomes $f(\alpha,\beta,\gamma,\zeta) = 0$, where

$$f(\alpha,\beta,\gamma,\zeta) = \log(\beta+\zeta) - \log(\alpha-\zeta) - b\gamma + a\zeta,$$

and it is defined for $\alpha > 0$, $\beta > 0$, $-\infty < \gamma < \infty$, and $-\beta < \zeta < \alpha$. Clearly, f is a continuously differentiable function. Moreover, $\partial_\zeta f(\alpha,\beta,\gamma,\zeta) = 1/(\beta+\zeta) + 1/(\alpha-\zeta) + a > 0$. Since $f(\alpha,\beta,\gamma,\zeta) = 0$ has a unique solution $\zeta = \zeta(\alpha,\beta,\gamma)$ for $\alpha > 0$, $\beta > 0$, and $-\infty < \gamma < \infty$, it follows from the Implicit Function Theorem that $\zeta = \zeta(\alpha,\beta,\gamma)$ is a continuously differentiable function of (α,β,γ). Taking the partial derivative on both sides of $f(\alpha,\beta,\gamma,\zeta) = 0$, we obtain

$$\partial_\alpha\zeta = \frac{\beta+\zeta}{q(\zeta)}, \quad \partial_\beta\zeta = \frac{\zeta-\alpha}{q(\zeta)}, \quad \partial_\gamma\zeta = \frac{b(\alpha-\zeta)(\beta+\zeta)}{q(\zeta)},$$

where $q(\zeta) = a(\alpha-\zeta)(\beta+\zeta) + \beta + \alpha$. Therefore, $0 < \partial_\alpha\zeta < 1$, $-1 < \partial_\beta\zeta < 0$, and $|\partial_\gamma\zeta| \le |b|/a$, and hence $\zeta = \zeta(\alpha,\beta,\gamma)$ is Lipschitz-continuous for $\alpha > 0$, $\beta > 0$, $-\infty < \gamma < \infty$, and $-\beta < \zeta < \alpha$. By (4.6), (4.7), and the fact that $\log(1+a) \le a$ if $a \in (-1,1)$, we have

$$\begin{aligned}\Delta F_h(\zeta_{s,i+1/2,j,k}) &= h^3\left[c_{s,i,j,k}\log\left(1 - \frac{\zeta_{s,i+1/2,j,k}}{c_{s,i,j,k}}\right) + c_{s,i+1,j,k}\log\left(1 + \frac{\zeta_{s,i+1/2,j,k}}{c_{s,i+1,j,k}}\right)\right] \\ &\quad - \frac{h^5q_s^2\zeta_{s,i+1/2,j,k}^2}{2\varepsilon_{i+1/2,j,k}} \\ &\le -\frac{h^5q_s^2\zeta_{s,i+1/2,j,k}^2}{2\varepsilon_{i+1/2,j,k}}.\end{aligned}$$

To summarize, we update $c_{s,i,j,k}$, $c_{s,i+1,j,k}$, and $u_{i+1/2,j,k}$ to

$$\check{c}_{s,i,j,k} = c_{s,i,j,k} - \zeta_{s,i+1/2,j,k} \quad \text{and} \quad \check{c}_{s,i+1,j,k} = c_{s,i+1,j,k} + \zeta_{s,i+1/2,j,k}, \tag{4.8}$$

$$\check{u}_{i+1/2,j,k} = u_{i+1/2,j,k} - hq_s\zeta_{s,i+1/2,j,k}, \tag{4.9}$$

where $\zeta_{s,i+1/2,j,k} \in (-c_{s,i+1,j,k}, c_{s,i,j,k})$ is determined by (4.7). Similarly, we update $c_{s,i,j,k}$, $c_{s,i,j+1,k}$, $v_{i,j+1/2,k}$, and $c_{s,i,j,k}$, $c_{s,i,j,k+1}$, $w_{i,j,k+1/2}$, respectively, by

$$\check{c}_{s,i,j,k} = c_{s,i,j,k} - \zeta_{s,i,j+1/2,k} \quad \text{and} \quad \check{c}_{s,i,j+1,k} = c_{s,i,j+1,k} + \zeta_{s,i,j+1/2,k}, \tag{4.10}$$

$$\check{v}_{i,j+1/2,k} = v_{i,j+1/2,k} - hq_s\zeta_{s,i,j+1/2,k}, \tag{4.11}$$

$$\check{c}_{s,i,j,k} = c_{s,i,j,k} - \zeta_{s,i,j,k+1/2} \quad \text{and} \quad \check{c}_{s,i,j,k+1} = c_{s,i,j,k+1} + \zeta_{s,i,j,k+1/2}, \tag{4.12}$$

$$\check{w}_{i,j,k+1/2} = w_{i,j,k+1/2} - hq_s\zeta_{s,i,j,k+1/2}, \tag{4.13}$$

where $\zeta_{s,i,j+1/2,k} \in (-c_{s,i,j+1,k}, c_{s,i,j,k})$ and $\zeta_{s,i,j,k+1/2} \in (-c_{s,i,j,k+1}, c_{s,i,j,k})$ are uniquely determined by

$$\log\left(c_{s,i,j+1,k} + \zeta_{s,i,j+1/2,,k}\right) - \log\left(c_{s,i,j,k} - \zeta_{s,i,j+1/2,k}\right) - \frac{hq_s\left(v_{i,j+1/2,k} - hq_s\zeta_{s,i,j+1/2,k}\right)}{\varepsilon_{i,j+1/2,k}} = 0, \tag{4.14}$$

$$\log\left(c_{s,i,j,k+1} + \zeta_{s,i,j,k+1/2}\right) - \log\left(c_{s,i,j,k} - \zeta_{s,i,j,k+1/2}\right) - \frac{hq_s\left(w_{i,j,k+1/2} - hq_s\zeta_{s,i,j,k+1/2}\right)}{\varepsilon_{i,j,k+1/2}} = 0, \tag{4.15}$$

respectively. We solve (4.7), (4.14), and (4.15) using Newton's iteration.

We summarize some of the properties of these local updates in the following:

Lemma 4.1. *Let* $(c, D) = (c_1, \ldots, c_M, u, v, w) \in X_{\rho,h}$ *satisfy* $c_s > 0$ *on* $h\mathbb{Z}^3$ *for all* $s = 1, \ldots, M$. *Let* $0 \le i, j, k \le N - 1$ *and* $1 \le s \le M$. *Update* (c, D) *to* $(\check{c}, \check{D}) \in X_{\rho,h}$ *by* (4.8)–(4.13) *with* $\zeta_{s,i+1/2,j,k}$, $\zeta_{s,i,j+1/2,k}$, *and* $\zeta_{s,i,j,k+1/2}$ *given in* (4.7), (4.14), *and* (4.15), *respectively.*

(1) *Each update keeps the components of* c *to be still positive at all the grid points.*
(2) *All* $\zeta_{s,i+1/2,j,k} \in (-c_{s,i+1,j,k}, c_{s,i,j,k})$, $\zeta_{s,i,j+1/2,k} \in (-c_{s,i,j+1,k}, c_{s,i,j,k})$, *and* $\zeta_{s,i,j,k+1/2} \in (-c_{s,i,j,k+1}, c_{s,i,j,k})$ *are Lipschitz-continuous functions of* $(c_{s,i,j,k}, c_{s,i+1,j,k}, u_{i+1/2,j,k})$, $(c_{s,i,j,k}, c_{s,i,j+1,k}, v_{i,j+1/2,k})$; *and* $(c_{s,i,j,k},\ c_{s,i,j,k+1}, w_{i,j,k+1/2})$, *respectively.*
(3) *The energy change* $\Delta F_h(\zeta) = F_h[\check{c}, \check{D}] - F_h[c, D]$ *from the three updates from* (c, D) *to* $(\check{c}, \check{D})$ *for given* s, i, j, k *satisfy*

$$|\Delta F_h(\zeta_{s,\sigma})| \ge h^5 q_s^2 \zeta_{s,\sigma}^2/(2\varepsilon_\sigma) \qquad \text{for } \sigma \in \{(i + 1/2, j, k), (i, j + 1/2, k), (i, j, k + 1/2)\}.$$

(4) *The updates of* (c, D) *at all grid points do not decrease the energy, i.e.,*

$$\zeta_{s,i+1/2,j,k} = \zeta_{s,i,j+1/2,k} = \zeta_{s,i,j,k+1/2} = 0 \qquad \forall s, i, j, k,$$

if and only if the local equilibrium conditions (2.22) *are satisfied.*

Local algorithm for minimizing the discrete PB energy $F_h : X_{\rho,h} \to \mathbb{R}$

Step 1. Initialize $(c^{(0)}, D^{(0)}) \in X_{\rho,h}$ and set $m = 0$.
Step 2. Update $(c, D) := (c^{(m)}, D^{(m)})$ at all the grid boxes one by one in a fixed order. Set $(c^{(m+1)}, D^{(m+1)}) = (c, D)$.
Step 3. If the updates of (c, D) at all the grid points do not further decrease the energy, then stop. Otherwise, set $m := m + 1$ and go to Step 2.

We denote by $(c^{(t)}, D^{(t)})$ $(t = 0, 1, \ldots)$ the sequence of updates produced by the local algorithm. For each $t \ge 1$, $(c^{(t+1)}, D^{(t+1)})$ is obtained from $(c^{(t)}, D^{(t)})$ by one of the $3M$ updates associated with the M components of $c^{(t)}$ and the three edges connected to one of the N^3 grid points. Since there are a total of N^3 grid points with three edges for each grid point and there are M ionic species, for any $t \ge 0$, $(c^{(t+3MN^3)}, D^{(t+3MN^3)})$ and $(c^{(t)}, D^{(t)})$ are updates on the same component of the concentration and displacement on the same edge of a grid point.

Theorem 4.1. *Let* $(c^{(t)}, D^{(t)}) \in X_{\rho,h}$ $(t = 0, 1, \ldots)$ *be the sequence generated by the local algorithm and* $(c^h_{\min}, D^h_{\min}) \in X_{\rho,h}$ *be the unique minimizer of* $F_h : X_{\rho,h} \to \mathbb{R}$. *We have*

$$\lim_{t\to\infty} \left(c^{(t)}, D^{(t)}\right) = \left(c^h_{\min}, D^h_{\min}\right) \text{ on } V_h^M \times Y_h \quad \text{and} \quad \lim_{t\to\infty} F_h\left[c^{(t)}, D^{(t)}\right] = F_h\left[c^h_{\min}, D^h_{\min}\right].$$

Proof. We may assume the sequence is infinite for otherwise the conclusions follow from Lemma 4.1 and Theorem 2.2. Since $\sigma \mapsto \sigma \log \sigma$ ($\sigma \geq 0$) is bounded below, the discrete energy functional $F_h : X_{\rho,h} \to \mathbb{R}$ is bounded below. Since each update in the local algorithm decreases the energy, the sequence $F_h[c^{(t)}, D^{(t)}]$ ($t = 0, 1, \dots$) decreases monotonically and is bounded below. Thus, $F_{h,\infty} := \lim_{t\to\infty} F_h[c^{(t)}, D^{(t)}] \in \mathbb{R}$ exists. Denoting

$$\delta_t = F_h\left[c^{(t)}, D^{(t)}\right] - F_h\left[c^{(t+1)}, D^{(t+1)}\right] \qquad (t = 0, 1, \dots),$$

we have all $\delta_t \geq 0$ and $0 \leq \sum_{t=0}^{\infty} \delta_t \leq F_h[c^{(0)}, D^{(0)}] - F_{h,\infty} < \infty$. Hence, $\lim_{t\to\infty} \delta_t = 0$.

Let us denote $(c^{(t)}, D^{(t)}) = (c_1^{(t)}, \dots, c_M^{(t)}; u^{(t)}, v^{(t)}, w^{(t)})$ ($t = 0, 1, \dots$). For any $s, i, j, k \in \mathbb{Z}$ ($1 \leq s \leq M$ and $0 \leq i, j, k \leq N-1$) and any $t \geq 0$, we define $\zeta^{(t)}_{s,i+1/2,j,k}$ to be the unique solution to (4.7) with $c^{(t)}_{s,i,j,k}$, $c^{(t)}_{s,i+1,j,k}$, and $u^{(t)}_{s,i+1/2,j,k}$ replacing those without the superscript (t). Similarly, we define $\zeta^{(t)}_{s,i,j+1/2,k}$ and $\zeta^{(t)}_{s,i,j,k+1/2}$; cf. (4.14) and (4.15). We claim that

$$\zeta^{(t)}_{s,i+1/2,j,k} \to 0, \quad \zeta^{(t)}_{s,i,j+1/2,k} \to 0, \quad \text{and} \quad \zeta^{(t)}_{s,i,j,k+1/2} \to 0 \quad \text{as } t \to \infty. \tag{4.16}$$

We shall prove the first convergence as the other two are similar.

Fix t, s, i, j, and k. The values of $c^{(t)}_{s,i,j,k}$, $c^{(t)}_{s,i+1,j,k}$, and $u^{(t)}_{s,i+1/2,j,k}$, which are the only components of $c^{(t)}$ and $D^{(t)}$ used to define $\zeta^{(t)}_{s,i+1/2,j,k}$ are possibly obtained by several local updates (instead of just one single update) at grid points nearby and including (i, j, k). Assume that the last local update that determines all $c^{(t)}_{s,i,j,k}$, $c^{(t)}_{s,i+1,j,k}$, and $u^{(t)}_{i+1/2,j,k}$ is from $(c^{(t'-1)}, D^{(t'-1)})$ to $(c^{(t')}, D^{(t')})$, where $t' \leq t < t' + 3MN^3$. This means that $c^{(t)}_{s,i,j,k} = c^{(t')}_{s,i,j,k}$, $c^{(t)}_{s,i+1,j,k} = c^{(t')}_{s,i+1,j,k}$, and $u^{(t)}_{i+1/2,j,k} = u^{(t')}_{i+1/2,j,k}$, and hence $\zeta^{(t')}_{s,i+1/2,j,k} = \zeta^{(t)}_{s,i+1/2,j,k}$. The update is given by

$$c^{(t')}_{s,i,j,k} = c^{(t'-1)}_{s,i,j,k} + \delta_i^{(t'-1)}, \quad c^{(t')}_{s,i+1,j,k} = c^{(t'-1)}_{s,i+1,j,k} + \delta_{i+1}^{(t'-1)}, \quad u^{(t')}_{s,i+1/2,j,k} = u^{(t'-1)}_{s,i+1/2,j,k} + \delta_{i+1/2}^{(t'-1)}.$$

Some of these perturbations $\delta_i^{(t'-1)}$, $\delta_{i+1}^{(t'-1)}$, and $\delta_{i+1/2}^{(t'-1)}$ maybe 0 but at least one of them is nonzero. Assume that this last local update is associated with an edge connecting some grid points (l, m, n) and $(l+1, m, n)$ or $(l, m+1, n)$ or $(l, m, n+1)$ and with the species s' that may be different from s. If we denote the corresponding optimal perturbation by $\zeta^{(t'-1)}_{s',l,m,n}$ (cf. (4.7), (4.14), and (4.15)), then we can write

$$\delta_i^{(t'-1)} = \sigma_i \zeta^{(t'-1)}_{s',l,m,n}, \quad \delta_{i+1}^{(t'-1)} = \sigma_{i+1} \zeta^{(t'-1)}_{s',l,m,n}, \quad \delta_{i+1/2}^{(t'-1)} = -\sigma_{i+1/2} h q_{s'} \zeta^{(t'-1)}_{s',l,m,n},$$

where $\sigma_i, \sigma_{i+1}, \sigma_{i+1/2} \in \{0, 1, -1\}$ and at least one of them is nonzero. By Part (3) of Lemma 4.1, $(\zeta^{(t'-1)}_{s',l,m,n})^2$ is bounded by the energy change resulting from this local update. Consequently, it follows from the definition of δ_t, the fact that $\delta_t \to 0$, and the fact that $t' \to \infty$ if $t \to \infty$ that

$$\lim_{t\to\infty} \zeta^{(t'-1)}_{s',l,m,n} = 0. \tag{4.17}$$

Therefore, by the formula of local update (cf. (4.8)),

$$\lim_{t\to\infty} \left[\left(c^{(t')}, D^{(t')}\right) - \left(c^{(t'-1)}, D^{(t'-1)}\right)\right] = 0. \tag{4.18}$$

By Part (2) of Lemma 4.1, $\zeta^{(t'-1)}_{s',l,m,n}$ and $\zeta^{(t')}_{s,i+1/2,j,k}$ depend respectively on $(c^{(t'-1)}, D^{(t'-1)})$ and $(c^{(t')}, D^{(t')})$ Lipschitz-continuously. Therefore, it follows from (4.18) that $\zeta^{(t')}_{s,i+1/2,j,k} - \zeta^{(t'-1)}_{s',l,m,n} \to 0$ as $t \to \infty$. Consequently, by (4.17) again, $\zeta^{(t)}_{s,i+1/2,j,k} = \zeta^{(t')}_{s,i+1/2,j,k} \to 0$ as $t \to \infty$.

We now prove $(c^{(t)}, D^{(t)}) \to (c^h_{\min}, D^h_{\min})$ which implies $F_h[c^{(t)}, D^{(t)}] \to F_h[c^h_{\min}, D^h_{\min}]$. Assume that

$$\lim_{r\to\infty} \left(c^{(t_r)}, D^{(t_r)}\right) = \left(c^{(\infty)}, D^{(\infty)}\right) \tag{4.19}$$

for a convergent subsequence $\{(c^{(t_r)}, D^{(t_r)})\}_{r=1}^{\infty}$ of $\{(c^{(t)}, D^{(t)})\}_{t=1}^{\infty}$ and some discrete and vector-valued functions $c^{(\infty)}$ and $D^{(\infty)}$. We show that $(c^{(\infty)}, D^{(\infty)}) = (c^h_{\min}, D^h_{\min})$. This will complete the proof. Since clearly $(c^{(\infty)}, D^{(\infty)}) \in X_{\rho,h}$, by Theorem 2.2, we need only to show that $c^{(\infty)}_{s,i,j,k} > 0$ for all s, i, j, k and that $(c^{(\infty)}, D^{(\infty)})$ satisfies (2.22).

If there exists $s \in \{1, \ldots, M\}$ such that $c^{(\infty)}_s = 0$ at some grid point, then by (2.14) and the nonnegativity of $c^{(\infty)}_s$, we may assume without loss of generality that $\alpha_\infty := c^{(\infty)}_{s,l,m,n} > 0$ but $c^{(\infty)}_{s,l+1,m,n} = 0$ for some (l, m, n). Let $c^{(\infty)} = (c^{(\infty)}_1, \ldots, c^{(\infty)}_M)$ and $D^{(\infty)} = (u^{(\infty)}, v^{(\infty)}, w^{(\infty)})$. Since $c^{(t_r)} \to c^{(\infty)}$ and $D^{(t_r)} \to D^{(\infty)}$, we have

$$\alpha_r := c^{(t_r)}_{s,l,m,n} \to \alpha_\infty > 0, \quad \beta_r := c^{(t_r)}_{s,l+1,m,n} \to 0, \quad \gamma_r := u^{(t_r)}_{s,l+1/2,m,n} \to \gamma_\infty := u^{(\infty)}_{s,l+1/2,m,n},$$

as $r \to \infty$. By (4.16), $\zeta_r := \zeta^{(t_r)}_{s,l+1/2,m,n} \to 0$. On the other hand, by (4.7), ζ_r is uniquely determined by

$$\log(\beta_r + \zeta_r) - \log(\alpha_r - \zeta_r) + a\zeta_r - b\gamma_r = 0, \tag{4.20}$$

where $a = h^2 q_s^2/\varepsilon_{l+1/2,m,n}$ and $b = hq_s/\varepsilon_{l+1/2,m,n}$ are independent of r. As $r \to \infty$, the left-hand side of (4.20) diverges to $-\infty$, while the right-hand side remains 0. This is a contradiction. Thus $c^{(\infty)}_{s,i,j,k} > 0$ for all s, i, j, k.

Fix any s, i, j, k and set $\zeta^{(\infty)}_{s,i+1/2,j,k}$ by (4.7) with $c^{(\infty)}_{s,i,j,k}$, $c^{(\infty)}_{s,i+1,j,k}$, and $u^{(\infty)}_{i+1/2,j,k}$ replacing $c_{s,i,j,k}$, $c_{s,i+1,j,k}$, and $u_{i+1/2,j,k}$, respectively. Then, by Part (1)(ii) of Lemma 4.1 and the fact $(c^{(t_r)}, D^{(t_r)}) \to (c^{\infty}, D^{(\infty)})$, $\zeta^{(t_r)}_{s,i+1/2,j,k} \to \zeta^{(\infty)}_{s,i+1/2,j,k}$ as $r \to \infty$. But $\zeta^{(t_r)}_{s,i+1/2,j,k} \to 0$ by (4.16). Hence $\zeta^{(\infty)}_{s,i+1/2,j,k} = 0$. Similarly, $\zeta^{(\infty)}_{s,i,j+1/2,k} = \zeta^{(\infty)}_{s,i,j,k+1/2} = 0$. Part (4) of Lemma 4.1 implies that $(c^{(\infty)}, D^{(\infty)})$ satisfies (2.22). □

We now describe the local algorithm [24,25] for minimizing the discrete Poisson energy $\hat{F}_h : S_{\rho,h} \to \mathbb{R}$ defined in (2.27), given $\varepsilon \in V_h$ with $\varepsilon > 0$ and $\rho^h \in \mathring{V}_h$. The update of the displacement in this algorithm can be added to the local algorithm for minimizing the PB energy as described above. The initialization of $D^{(0)} \in S_{\rho,h}$ can be defined by (4.1)–(4.5) with ρ^h replacing τ^h. Note in this case we have $\mathscr{A}_h(D^{(0)}) = 0$ if $\varepsilon \in V_h$ is a constant.

To describe the local update, we set $D = (u, v, w) \in S_{\rho,h}$. Fix (i, j, k) with $0 \le i, j, k \le N-1$ and consider the grid box $B_{i,j,k} = (i, j, k) + [0, 1]^3$; cf. Figure 2 (Left). We update D on the edges of the three faces of $B_{i,j,k}$ (on the plane $x = ih$, $y = jh$, and $z = kh$) that share the vertex (i, j, k).

Consider the face on the plane $z = kh$, the square of vertices $P = (i, j, k)$, $Q = (i+1, j, k)$, $R = (i+1, j+1, k)$, and $S = (i, j+1, k)$; cf. Figure 2 (Right). To update the 4 values $u_{i+1/2,j,k}$, $u_{i+1/2,j+1,k}$, $v_{i,j+1/2,k}$, and $v_{i+1,j+1/2,k}$ of D on the 4 edges of the face $PQRS$, we define a locally perturbed displacement $\check{D} = (\check{u}, \check{v}, \check{w}) \in S_{\rho,h}$ by $\check{D} = D$ everywhere except

$$\begin{aligned} \check{u}_{i+1/2,j,k} &= u_{i+1/2,j,k} + \alpha, \quad \check{v}_{i+1,j+1/2,k} = v_{i+1,j+1/2,k} + \beta, \\ \check{u}_{i+1/2,j+1,k} &= u_{i+1/2,j+1,k} + \gamma, \quad \check{v}_{i,j+1/2,k} = v_{i,j+1/2,k} + \delta, \end{aligned}$$

where $\alpha, \beta, \gamma, \delta \in \mathbb{R}$ are to be determined. In order for $\check{D} \in S_{\rho,h}$, the discrete Gauss' law $\nabla_h \cdot D = \rho^h$ at the 4 vertices P, Q, R, S should be satisfied. Consequently,

$$\alpha + \delta = 0, \quad -\alpha + \beta = 0, \quad -\beta - \gamma = 0, \quad \gamma - \delta = 0.$$

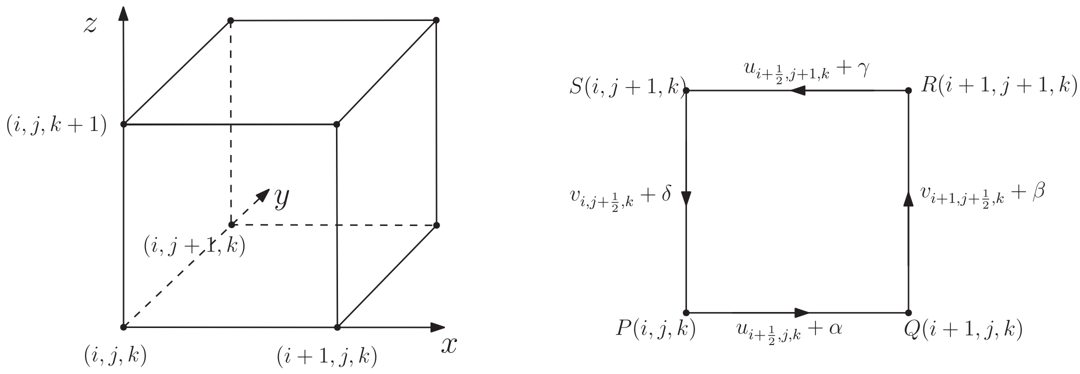

FIGURE 2. *Left*: grid box $B_{i,j,k} = (i,j,k) + [0,1]^3$. *Right*: grid face of box $B_{i,j,k}$ with vertices P, Q, R, and S. The perturbations α, β, γ and δ of u and v with subscript, the corresponding components of the displacement D, are to be determined.

Thus, $\alpha = \beta = -\gamma = -\delta =: \eta \in \mathbb{R}$. The optimal value of η is set to minimize the perturbed energy $\hat{F}_h[\check{D}]$, or equivalently, the energy change

$$\begin{aligned}\Delta\hat{F}_h(\eta) &:= \hat{F}_h[\check{D}] - \hat{F}_h[D] \\ &= \frac{\varepsilon_{z,i,j,k}h^3}{2}\eta^2 + 2\eta\left(\frac{u_{i+1/2,j,k}}{\varepsilon_{i+1/2,j,k}} + \frac{v_{i+1,j+1/2,k}}{\varepsilon_{i+1,j+1/2,k}} - \frac{u_{i+1/2,j+1,k}}{\varepsilon_{i+1/2,j+1,k}} - \frac{v_{i,j+1/2,k}}{\varepsilon_{i,j+1/2,k}}\right),\end{aligned}$$

$$\text{with} \quad \varepsilon_{z,i,j,k} = \frac{1}{\varepsilon_{i+1/2,j,k}} + \frac{1}{\varepsilon_{i+1,j+1/2,k}} + \frac{1}{\varepsilon_{i+1/2,j+1,k}} + \frac{1}{\varepsilon_{i,j+1/2,k}}.$$

This is minimized uniquely at $\eta = \eta_{z,i,j,k}$ with the minimum $\Delta\hat{F}_{z,i,j,k} := \min_{\eta\in\mathbb{R}} \Delta\hat{F}_h(\eta)$ given by

$$\eta_{z,i,j,k} = -\frac{1}{\varepsilon_{z,i,j,k}}\left(\frac{u_{i+1/2,j,k}}{\varepsilon_{i+1/2,j,k}} + \frac{v_{i+1,j+1/2,k}}{\varepsilon_{i+1,j+1/2,k}} - \frac{u_{i+1/2,j+1,k}}{\varepsilon_{i+1/2,j+1,k}} - \frac{v_{i,j+1/2,k}}{\varepsilon_{i,j+1/2,k}}\right), \tag{4.21}$$

$$\Delta\hat{F}_{z,i,j,k} = -\frac{1}{2}\varepsilon_{z,i,j,k}h^3\eta_{z,i,j,k}^2. \tag{4.22}$$

Therefore, we update D by

$$u_{i+1/2,j,k} \leftarrow u_{i+1/2,j,k} + \eta_{z,i,j,k}, \qquad v_{i+1,j+1/2,k} \leftarrow v_{i+1,j+1/2,k} + \eta_{z,i,j,k}, \tag{4.23}$$

$$u_{i+1/2,j+1,k} \leftarrow u_{i+1/2,j+1,k} - \eta_{z,i,j,k}, \qquad v_{i,j+1/2,k} \leftarrow v_{i,j+1/2,k} - \eta_{z,i,j,k}. \tag{4.24}$$

We denote by $D^z \in S_{\rho,h}$ this updated displacement.

Similarly, we update D on the 4 edges of the face of the grid box $B_{i,j,k}$ on the plane $y = jh$ and $x = ih$ to get the updated displacement $D^y \in S_{\rho,h}$ and $D^x \in S_{\rho,h}$, respectively, by

$$w_{i,j,k+1/2} \leftarrow w_{i,j,k+1/2} + \eta_{y,i,j,k}, \qquad u_{i+1/2,j,k+1} \leftarrow u_{i+1/2,j,k+1} + \eta_{y,i,j,k}, \tag{4.25}$$

$$w_{i+1,j,k+1/2} \leftarrow w_{i+1,j,k+1/2} - \eta_{y,i,j,k}, \qquad u_{i+1/2,j,k} \leftarrow u_{i+1/2,j,k} - \eta_{y,i,j,k}, \tag{4.26}$$

$$v_{i,j+1/2,k} \leftarrow v_{i,j+1/2,k} + \eta_{x,i,j,k}, \qquad w_{i,j+1,k+1/2} \leftarrow w_{i,j+1,k+1/2} + \eta_{x,i,j,k}, \tag{4.27}$$

$$v_{i,j+1/2,k+1} \leftarrow v_{i,j+1/2,k+1} - \eta_{x,i,j,k}, \qquad w_{i,j,k+1/2} \leftarrow w_{i,j,k+1/2} - \eta_{x,i,j,k}. \tag{4.28}$$

Note that the sign of each of the perturbations $\eta_{x,i,j,k}$, $\eta_{y,i,j,k}$, and $\eta_{z,i,j,k}$ follows from the right-hand rule for orientations; cf. Figure 2 (Right). The optimal perturbations $\eta_{y,i,j,k}$ and $\eta_{x,i,j,k}$ and the corresponding energy differences $\Delta \hat{F}_{y,i,j,k}$ and $\Delta \hat{F}_{x,i,j,k}$ are given by

$$\eta_{y,i,j,k} = -\frac{1}{\varepsilon_{y,i,j,k}} \left(\frac{w_{i,j,k+1/2}}{\varepsilon_{i,j,k+1/2}} + \frac{u_{i+1/2,j,k+1}}{\varepsilon_{i+1/2,j,k+1}} - \frac{w_{i+1,j,k+1/2}}{\varepsilon_{i+1,j,k+1/2}} - \frac{u_{i+1/2,j,k}}{\varepsilon_{i+1/2,j,k}} \right), \tag{4.29}$$

$$\eta_{x,i,j,k} = -\frac{1}{\varepsilon_{x,i,j,k}} \left(\frac{v_{i,j+1/2,k}}{\varepsilon_{i,j+1/2,k}} + \frac{w_{i,j+1,k+1/2}}{\varepsilon_{i,j+1,k+1/2}} - \frac{v_{i,j+1/2,k+1}}{\varepsilon_{i,j+1/2,k+1}} - \frac{w_{i,j,k+1/2}}{\varepsilon_{i,j,k+1/2}} \right), \tag{4.30}$$

$$\Delta \hat{F}_{y,i,j,k} = -\frac{1}{2}\varepsilon_{y,i,j,k} h^3 \eta^2_{y,i,j,k}, \quad \text{and} \quad \Delta \hat{F}_{x,i,j,k} = -\frac{1}{2}\varepsilon_{x,i,j,k} h^3 \eta^2_{x,i,j,k}, \tag{4.31}$$

$$\text{where} \quad \varepsilon_{y,i,j,k} = \frac{1}{\varepsilon_{i,j,k+1/2}} + \frac{1}{\varepsilon_{i+1/2,j,k+1}} + \frac{1}{\varepsilon_{i+1,j,k+1/2}} + \frac{1}{\varepsilon_{i+1/2,j,k}},$$

$$\varepsilon_{x,i,j,k} = \frac{1}{\varepsilon_{i,j+1/2,k}} + \frac{1}{\varepsilon_{i,j+1,k+1/2}} + \frac{1}{\varepsilon_{i,j+1/2,k+1}} + \frac{1}{\varepsilon_{i,j,k+1/2}}.$$

Note that, by (4.30), (4.29), (4.21), and the definition of the discrete curl, we have

$$h(\varepsilon_{x,i,j,k}\eta_{x,i,j,k}, \varepsilon_{y,i,j,k}\eta_{y,i,j,k}, \varepsilon_{z,i,j,k}\eta_{z,i,j,k}) = -\left(\nabla_h \times (D/\varepsilon)\right)_{i+1/2,j+1/2,k+1/2} \qquad \forall i,j,k \in \mathbb{Z}.$$

We summarize these calculations in the following lemma:

Lemma 4.2. *Let $D = (u, v, w) \in S_{\rho,h}$.*

(1) *Given $i, j, k \in \{0, \dots, N-1\}$. Let D^x, D^y, and D^z be updated from D by (4.23)–(4.28) with $\eta_{x,i,j,k}$, $\eta_{y,i,j,k}$, $\eta_{z,i,j,k}$, $\Delta \hat{F}_{x,i,j,k}$, $\Delta \hat{F}_{y,i,j,k}$, and $\Delta \hat{F}_{z,i,j,k}$ given in (4.21), (4.22), and (4.29)–(4.31), respectively. Then $D^x, D^y, D^z \in S_{\rho,h}$, $\mathscr{A}_h(D^x) = \mathscr{A}_h(D^y) = \mathscr{A}_h(D^z) = \mathscr{A}_h(D)$, and*

$$\eta^2_{\sigma,i,j,k} = \frac{1}{4}\|D^\sigma - D\|_h^2 = -\frac{2}{\varepsilon_{\sigma,i,j,k} h^3} \Delta \hat{F}_{\sigma,i,j,k}, \qquad \sigma \in \{x, y, z\}.$$

(2) *That $\nabla_h \times (D/\varepsilon) = 0$ on $h(\mathbb{Z} + 1/2)^3$ if and only if $\eta_{z,i,j,k} = \eta_{y,i,j,k} = \eta_{x,i,j,k} = 0$ for all i, j, k.*

Here is the local algorithm for a constant coefficient ε. In this case, the expressions of all those subscripted η and $\Delta \hat{F}$ can be simplified.

Local algorithm for minimizing the discrete Poisson energy $\hat{F}_h : S_{\rho,h} \to \mathbb{R}$ with a constant dielectric coefficient ε

Step 1. Initialize a displacement $D^{(0)} \in S_{\rho,h}$ with $\mathscr{A}_h(D^{(0)}) = 0$. Set $m = 0$.
Step 2. Update $D := D^{(m)}$.
For $i, j, k = 0, \dots, N-1$
  Update $D \to D^x$ and $D \leftarrow D^x$;
  Update $D \to D^y$ and $D \leftarrow D^y$;
  Update $D \to D^z$ and $D \leftarrow D^z$.
End for
Step 3. If $\eta_{x,i,j,k} = \eta_{y,i,j,k} = \eta_{z,i,j,k} = 0$ for all $i, j, k = 0, \dots, N-1$, then stop.
Otherwise, set $D^{(m+1)} = D$ and $m := m + 1$ and go to Step 2.

We denote by $D^{(t)}$ $(t = 0, 1, \dots)$ the sequence of updates produced by the local algorithm. For each $t \geq 1$, $D^{(t+1)}$ is obtained from $D^{(t)}$ by an update on one of the three grid faces of a grid box associated with a grid point. Since there are a total of N^3 grid points, for any $t \geq 0$, $D^{(t+3N^3)}$ and $D^{(t)}$ are updates on the same displacement on the same grid face.

Theorem 4.2. *Let $\varepsilon > 0$ be a constant, $\rho^h \in \mathring{V}_h$, and $\hat{D}^h_{\min} \in S_{\rho,h}$ be the unique minimizer of $\hat{F}_h : S_{\rho,h} \to \mathbb{R}$. Let $D^{(t)} \in S_{\rho,h}$ $(t = 0, 1, \dots)$ be the sequence of displacements generated by the local algorithm with $\mathscr{A}_h(D^{(0)}) = 0$. Then*

$$\lim_{t\to\infty} D^{(t)} = \hat{D}^h_{\min} \quad \text{on} \quad h(\mathbb{Z} + 1/2)^3 \qquad \textit{and} \qquad \lim_{t\to\infty} \hat{F}_h[D^{(t)}] = \hat{F}[\hat{D}^h_{\min}].$$

Proof. We may assume the sequence is infinite for otherwise the conclusions follow from Lemma 4.2 and Theorem 2.3. Note that for each $t \in \mathbb{N}$, the iteration from $D^{(t)}$ to $D^{(t+1)}$ consists of a cycle of $3N^3$ local updates (with 1 on each of the 3 faces of the grid box associated with each grid point and a total of N^3 grid points). Let us redefine the sequence of updates, still denoted $D^{(t)}$ $(t = 1, 2, \dots)$, by a single-step local update, *i.e.*, $D^{(t+1)}$ is obtained by updating $D^{(t)}$ on one of the $3N^3$ grid faces. The new $D^{(t+3N^3)}$ and $D^{(t)}$ are updates on the same grid face for each $t \geq 1$. Clearly, the original sequence is a subsequence of the new one. We prove that this new sequence converges to $D^h_{\min}$, which will imply that the original sequence converges to $D^h_{\min}$.

By Lemma 4.2, $\hat{F}_h[D^{(t)}]$ decreases as t increases. Since $0 \leq \hat{F}_h[D^{(t)}] \leq \hat{F}_h[D^{(0)}]$ for all $t \geq 1$, the limit $\hat{F}_{h,\infty} := \lim_{t\to\infty} \hat{F}_h[D^{(t)}]$ exists and $\hat{F}_{h,\infty} \geq 0$. Denoting

$$\delta_t = \hat{F}_h[D^{(t)}] - \hat{F}_h[D^{(t+1)}] \geq 0 \qquad (t = 0, 1, \dots),$$

we have as before $0 \leq \sum_{t=0}^{\infty} \delta_t \leq \hat{F}_h[D^{(0)}] - \hat{F}_{h,\infty} \leq \hat{F}_h[D^{(0)}]$. Hence, $\lim_{t\to\infty} \delta_t = 0$.

To show $D^{(t)} \to \hat{D}^h_{\min}$, which implies immediately $\hat{F}_h[D^{(t)}] \to \hat{F}_h[\hat{D}^h_{\min}]$, it suffices to show that the limit of any convergent subsequence of $\{D^{(t)}\}_{t=1}^{\infty}$ is $\hat{D}^h_{\min}$. Let $\{D^{(t_r)}\}_{r=1}^{\infty}$ be such a subsequence and assume $D^{(\infty)} = \lim_{r\to\infty} D^{(t_r)}$. Since $D^{(t)} \in S_{\rho,h}$ and $\mathscr{A}_h(D^{(t)}) = 0$ for all $t \geq 1$ by Lemma 4.2, $D^{(\infty)} \in S_{\rho,h}$ and $\mathscr{A}_h(D^{(\infty)}) = 0$. By Theorem 2.3, it suffices to show that $D^{(\infty)}$ is locally in equilibrium, *i.e.*, $\nabla_h \times (D^{(\infty)}/\varepsilon) = 0$ which is the same as $\nabla_h \times D^{(\infty)} = 0$ since ε is a constant.

Since $\{D^{(t_r)}\}_{r=1}^{\infty}$ is an infinite sequence and there are only finitely many grid faces, there exists a grid face with vertices, say, $(i + \hat{\delta}_1, j + \hat{\delta}_2, k)$ with $\hat{\delta}_1, \hat{\delta}_2 \in \{0, 1\}$, on which $D^{(t_r)}$ is updated for infinitely many r's. Therefore, there exists a subsequence of $\{D^{(t_r)}\}_{r=1}^{\infty}$, not relabeled, such that for each $r \geq 1$, $D^{(t_r)}$ is updated on that same grid face. Since $D^{(t_r)} \to D^{(\infty)}$, $\eta^{(t_r)}_{z,i,j,k} \to \eta^{(\infty)}_{z,i,j,k}$, where $\eta^{(t_r)}_{z,i,j,k}$ and $\eta^{(\infty)}_{z,i,j,k}$ are the η_z values as defined in (4.21) with $D^{(t_r)}$ and $D^{(\infty)}$ replacing D, respectively. On the other hand, since $\delta_t \to 0$, Lemma 4.2 implies that $[\eta^{(t_r)}_{z,i,j,k}]^2 \to 0$. Hence, $\eta^{(\infty)}_{z,i,j,k} = 0$.

Finally, fix any grid point (l, m, n). We show $\eta^{(\infty)}_{z,l,m,n} = \eta^{(\infty)}_{y,l,m,n} = \eta^{(\infty)}_{x,l,m,n} = 0$, where these η-values are defined as in (4.21), (4.29), and (4.30) with $D^{(\infty)}$ and (l, m, n) replacing D and (i, j, k), respectively. This will imply that $D^{(\infty)}$ is in local equilibrium, and complete the proof.

Note that in the local algorithm a cycle of $3N^3$ local updates are done for all the grid faces before next cycle starts. Thus, for each $r \geq 1$, there exists an integer τ_r such that $1 \leq \tau_r \leq 3N^3$ and $D^{(t_r+\tau_r)}$ is updated, with the perturbation $\eta^{(t_r+\tau_r)}_{z,l,m,n}$, on the grid face parallel to the z-plane of the grid box $B_{l,m,n} = (l, m, n) + [0, 1]^3$; cf. Figure 2 (Left). (Since the order of grid points is fixed for local updates, τ_r is independent of r.) Since $\delta_t \to 0$, Lemma 4.2 implies $\|D^{(t+1)} - D^{(t)}\|_h \to 0$ as $t \to \infty$. Thus,

$$\|D^{(t_r+\tau_r)} - D^{(t_r)}\|_h \leq \sum_{s=1}^{3N^3} \|D^{(t_r+s)} - D^{(t_r+s-1)}\|_h \to 0 \qquad \text{as } r \to \infty.$$

But $D^{(t_r)} \to D^{(\infty)}$. Hence, $D^{(t_r+\tau_r)} \to D^{(\infty)}$. Thus, by Lemma 4.2, $\eta^{(\infty)}_{z,l,m,n} = \lim_{r\to\infty} \eta^{(t_r+\tau_r)}_{z,l,m,n} = 0$. Similarly, $\eta^{(\infty)}_{x,l,m,n} = 0$ and $\eta^{(\infty)}_{y,l,m,n} = 0$. ∎

To treat the case of a variable coefficient ε, we propose a new local algorithm based on the following lemma whose proof is omitted:

Lemma 4.3. *Let $\varepsilon \in V_h$ be such that $\varepsilon > 0$, $\rho^h \in \mathring{V}_h$, $D = (u, v, w) \in S_{\rho,h}$, and*

$$(\hat{a}, \hat{b}, \hat{c}) = -\sum_{i,j,k=0}^{N-1} \left(\frac{u_{i+1/2,j,k}/\varepsilon_{i+1/2,j,k}}{\sum_{l,m,n=0}^{N-1} 1/\varepsilon_{l+1/2,m,n}}, \frac{v_{i,j+1/2,k}/\varepsilon_{i,j+1/2,k}}{\sum_{l,m,n=0}^{N-1} 1/\varepsilon_{l,m+1/2,n}}, \frac{w_{i,j,k+1/2}/\varepsilon_{i,j,k+1/2}}{\sum_{l,m,n=0}^{N-1} 1/\varepsilon_{l,m,n+1/2}} \right).$$

Then $D + (a, b, c) \in S_{\rho,h}$ for any $a, b, c \in \mathbb{R}$, $(\hat{a}, \hat{b}, \hat{c})$ is the unique minimizer of $g(a, b, c) := \hat{F}_h[D + (a, b, c)] - \hat{F}_h[D]$ $(a, b, c \in \mathbb{R})$, and the minimum of $g : \mathbb{R}^3 \to \mathbb{R}$ is

$$g(\hat{a}, \hat{b}, \hat{c}) = -\frac{h^3}{2} \left[\left(\sum_{i,j,k=0}^{N-1} \frac{1}{\varepsilon_{i+1/2,j,k}} \right) \hat{a}^2 + \left(\sum_{i,j,k=0}^{N-1} \frac{1}{\varepsilon_{i,j+1/2,k}} \right) \hat{b}^2 + \left(\sum_{i,j,k=0}^{N-1} \frac{1}{\varepsilon_{i,j,k+1/2}} \right) \hat{c}^2 \right].$$

Moreover, $\mathscr{A}_h((D + (\hat{a}, \hat{b}, \hat{c}))/\varepsilon) = 0$.

In our local algorithm with shift for minimizing the discrete Poisson energy with a variable coefficient ε, the initial $D^{(0)}$ is not necessary to satisfy $\mathscr{A}_h(D^{(0)}) = 0$. Moreover, we introduce $N_{\text{local}} \in \mathbb{N}$ to control the number of cycles of local updates followed by one shift of displacement.

Local algorithm with shift for minimizing the discrete Poisson energy $\hat{F}_h : S_{\rho,h} \to \mathbb{R}$ with a variable dielectric coefficient ε

Step 1. Initialize a displacement $D^{(0)} \in S_{\rho,h}$. Set $m = 0$.
Step 2. Update locally $D := D^{(m)}$.
  For $n = 1, \ldots N_{\text{local}}$
    For $i, j, k = 0, \ldots, N - 1$
      Update $D \to D^x$ and $D \leftarrow D^x$;
      Update $D \to D^y$ and $D \leftarrow D^y$;
      Update $D \to D^z$ and $D \leftarrow D^z$.
    End for
  End for
Step 3. Shift D : Compute $\hat{a}$, $\hat{b}$, $\hat{c}$ and $D \leftarrow D + (\hat{a}, \hat{b}, \hat{c})$.
Step 4. If $\eta_{x,i,j,k} = \eta_{y,i,j,k} = \eta_{z,i,j,k} = 0$ for all $i, j, k = 0, \ldots, N - 1$ and $\hat{a} = \hat{b} = \hat{c} = 0$, then stop.
  Otherwise, set $D^{(m+1)} = D$ and $m := m + 1$. Go to Step 2.

Theorem 4.3. *Let $\varepsilon \in V_h$ with $\varepsilon > 0$, $\rho_h \in \mathring{V}_h$, and $\hat{D}^h_{\min} \in S_{\rho,h}$ be the unique minimizer of $\hat{F}_h : S_{\rho,h} \to \mathbb{R}$. Let $D^{(0)} \in S_{\rho,h}$ and $D^{(t)} \in S_{\rho,h}$ $(t = 0, 1, \ldots)$ be the sequence generated by the local algorithm with shift. Then*

$$\lim_{t\to\infty} D^{(t)} = \hat{D}^h_{\min} \quad \text{on} \quad h(\mathbb{Z} + 1/2)^3 \qquad \textit{and} \qquad \lim_{t\to\infty} \hat{F}_h[D^{(t)}] = \hat{F}[\hat{D}^h_{\min}].$$

Proof. We again assume the sequence of updates is infinite. For any $D = (u, v, w) \in S_{\rho,h}$, we define $\eta = \eta(D) = (\eta_x, \eta_y, \eta_z)$ by (4.30), (4.29), and (4.21) at any (i, j, k). We also define $G = G(D) = (\hat{a}, \hat{b}, \hat{c}) \in \mathbb{R}^3$ with $\hat{a}$, $\hat{b}$, and $\hat{c}$ given in Lemma 4.3. Clearly, both $\eta(D)$ and $G(D)$ depend on D linearly and hence continuously. We claim that

$$\lim_{t\to\infty} \eta(D^{(t)}) = (0, 0, 0) \quad \text{(at all the grid points)} \quad \text{and} \quad \lim_{t\to\infty} G(D^{(t)}) = (0, 0, 0). \tag{4.32}$$

Suppose (4.32) is true. We prove that $D^{(t)} \to D^h_{\min}$, which implies $\hat{F}_h[D^{(t)}] \to \hat{F}_h[D^h_{\min}]$. It suffices to show the following: assume that $D^{(t_r)}$ $(r = 1, 2, \ldots)$ is a convergent subsequence of $D^{(t)}$ $(t = 1, 2, \ldots)$ and $D^{(t_r)} \to D^{(\infty)}$, then $D^{(\infty)} = D^h_{\min}$. In fact, with such an assumption, $D^{(\infty)} \in S_{\rho,h}$, and $\eta(D^{(\infty)}) = (0, 0, 0)$ and $G(D^{(\infty)}) = (0, 0, 0)$ by (4.32). Hence, $\nabla_h \times (D^{(\infty)}/\varepsilon) = 0$ by Lemma 4.2 and $\mathscr{A}_h(D^{(\infty)}/\varepsilon) = 0$ by Lemma 4.3. Consequently, $D^{(\infty)} = \hat{D}^h_{\min}$ by Theorem 2.3.

We now proceed to prove (4.32). By Lemmas 4.2 and 4.3, $\hat{F}_h[D^{(t)}] \geq 0$ decreases as t increases. Thus, the limit $\hat{F}_{h,\infty} := \lim_{t\to\infty} \hat{F}_h[D^{(t)}] \geq 0$ exits. Denoting

$$\delta_t = \hat{F}_h[D^{(t)}] - \hat{F}_h[D^{(t+1)}] \geq 0 \qquad (t = 0, 1, \dots),$$

we have as before that $0 \leq \sum_{t=1}^{\infty} \delta_t \leq \hat{F}_h[D^{(0)}]$ and hence $\lim_{t\to\infty} \delta_t = 0$.

Denote $\eta^{(t)} = (\eta_x^{(t)}, \eta_y^{(t)}, \eta_z^{(t)}) = \eta(D^{(t)})$ and $G^{(t)} = G(D^{(t)}) = (\hat{a}^{(t)}, \hat{b}^{(t)}, \hat{c}^{(t)})$ $(t = 1, 2, \dots)$. We show that $\eta_z^{(t)} \to 0$ at all i, j, k as $t \to \infty$. Let us fix $t \geq 1$ and also i, j, k. By (4.21), $\eta_{z,i,j,k}^{(t)}$ is a linear combination of $u_{i+1/2,j,k}^{(t)}$, $u_{i+1/2,j+1,k}^{(t)}$, $v_{i,j+1/2,k}^{(t)}$, and $v_{i+1,j+1/2,k}^{(t)}$. Each of these values is obtained from some previous local updates or a global update. There are two cases: one is that the last update that determines all these values is local, and the other global.

Consider the first case. Assume the last update that determines all $u_{i+1/2,j,k}^{(t)}$, $u_{i+1/2,j+1,k}^{(t)}$, $v_{i,j+1/2,k}^{(t)}$, and $v_{i+1,j+1/2,k}^{(t)}$ is a local update from $D^{(t'-1)}$ to $D^{(t')}$ with some t' such that $t' \leq t < t' + 3N^3 + 1$. (This 1 accounts for a possible global update.) Note that some of the four $u^{(t)}$ and $v^{(t)}$-values might have been possibly updated before this last update. Assume also the perturbation associated with this last local update is $\eta_{\theta,l,m,n}^{(t'-1)}$ for some l, m, n with $\theta = x$ or y or z. All l, m, n, and θ depend on t' and hence t, and (l, m, n) may not be the same as (i, j, k). By Lemma 4.2, that fact that $\delta_t \to 0$, and $t' \to \infty$ as $t \to \infty$,

$$\lim_{t\to\infty} \eta_{\theta,l,m,n}^{(t'-1)} = 0. \tag{4.33}$$

This, together with Lemma 4.2 again, implies

$$\|D^{(t')} - D^{(t'-1)}\|_h^2 = 4[\eta_{\theta,l,m,n}^{(t'-1)}]^2 \to 0 \quad \text{as } t \to \infty. \tag{4.34}$$

Note that, after that last local update from $(t'-1)$ to (t'), all the values of $u_{i+1/2,j,k}^{(t)}$, $u_{i+1/2,j+1,k}^{(t)}$, $v_{i,j+1/2,k}^{(t)}$, and $v_{i+1,j+1/2,k}^{(t)}$ are not changed before the next update from $D^{(t)}$ to $D^{(t+1)}$. Thus, $u_{i+1/2,j,k}^{(t)} = u_{i+1/2,j,k}^{(t')}$, $u_{i+1/2,j+1,k}^{(t)} = u_{i+1/2,j+1,k}^{(t')}$, $v_{i,j+1/2,k}^{(t)} = v_{i,j+1/2,k}^{(t')}$, and $v_{i+1,j+1/2,k}^{(t)} = v_{i+1,j+1/2,k}^{(t')}$. Consequently, $\eta_{z,i,j,k}^{(t)} = \eta_{z,i,j,k}^{(t')}$. By (4.21), $\eta_{z,i,j,k}^{(t')}$ and $\eta_{\theta,l,m,n}^{(t'-1)}$ depend linearly and hence continuously on $D^{(t')}$ and $D^{(t'-1)}$, respectively. Hence, it follows from (4.34) that $\eta_{z,i,j,k}^{(t')} - \eta_{\theta,l,m,n}^{(t'-1)} \to 0$ as $t \to \infty$. This and (4.33) imply $\eta_{z,i,j,k}^{(t)} = \eta_{z,i,j,k}^{(t')} \to 0$ as $t \to \infty$. Similarly, $\eta_{x,i,j,k}^{(t)} \to 0$ and $\eta_{y,i,j,k}^{(t)} \to 0$.

Now the second case: the update from $D^{(t-1)}$ to $D^{(t)}$ is global, *i.e.*, $D^{(t)} = D^{(t-1)} + (\hat{a}^{(t-1)}, \hat{b}^{(t-1)}, \hat{c}^{(t-1)})$. By Lemma 4.3 and the fact that $\delta_t \to 0$, all $\hat{a}^{(t)}$, $\hat{b}^{(t)}$, $\hat{c}^{(t)}$ converge to 0. Therefore, since $\eta_{z,i,j,k} = \eta_{z,i,j,k}(D)$ depends on D linearly, $\eta_{z,i,j,k}^{(t)} - \eta_{z,i,j,k}^{(t-1)} \to 0$. Note that $\eta_{z,i,j,k}^{(t-1)}$ is a linear combination of $u_{i+1/2,j,k}^{(t-1)}$, $u_{i+1/2,j,k}^{(t-1)}$, $v_{i,j+1/2,k}^{(t-1)}$, and $v_{i+1,j+1/2,k}^{(t-1)}$. Since the update from $D^{(t-1)}$ to $D^{(t)}$ is global, the last update that determines those four values of $D^{(t-1)}$ must be a local update. By case 1 above, we have $\eta_{z,i,j,k}^{(t-1)} \to 0$, and hence $\eta_{z,i,j,k}^{(t)} \to 0$. Similarly, $\eta_{x,i,j,k}^{(t)} \to 0$ and $\eta_{y,i,j,k}^{(t)} \to 0$. The first limit in (4.32) is proved.

We now prove the second limit in (4.32). Let $t \geq 0$. If the update from $D^{(t)}$ to $D^{(t+1)}$ is global, then $G(D^{(t)}) \to (0, 0, 0)$ as $t \to \infty$ by Lemma 4.3 and the fact that $\delta_t \to 0$. Suppose the update is local. Then, there exists an integer $m = m(t)$ such that $1 \leq m \leq 3N_{\text{local}}N^3$, and with the notation $t_0 = t - m$, the update from $D^{(t_0)}$ to $D^{(t_0+1)}$ is global but all the updates from $D^{(t_0+n)}$ to $D^{(t_0+n+1)}$ $(n = 1, \dots, m-1)$ are local. It follows from Lemma 4.3, the fact that $\delta_t \to 0$, and the fact that $t_0 \to \infty$ as $t \to \infty$ that

$$\|G(D^{(t_0)})\|^2 \leq C(\varepsilon) h^{-3} \delta_{t_0} \to 0 \quad \text{as } t \to \infty, \tag{4.35}$$

where $C(\varepsilon) > 0$ is a constant independent of h and t_0. By Lemma 4.2, Lemma 4.3, and the fact that $\delta_t \to 0$, $\|D^{(t')} - D^{(t'-1)}\|_h \to 0$ as $t' \to \infty$. Thus,

$$\|D^{(t)} - D^{(t_0)}\|_h \leq \sum_{n=1}^{m} \|D^{(t_0+n)} - D^{(t_0+n-1)}\|_h \to 0.$$

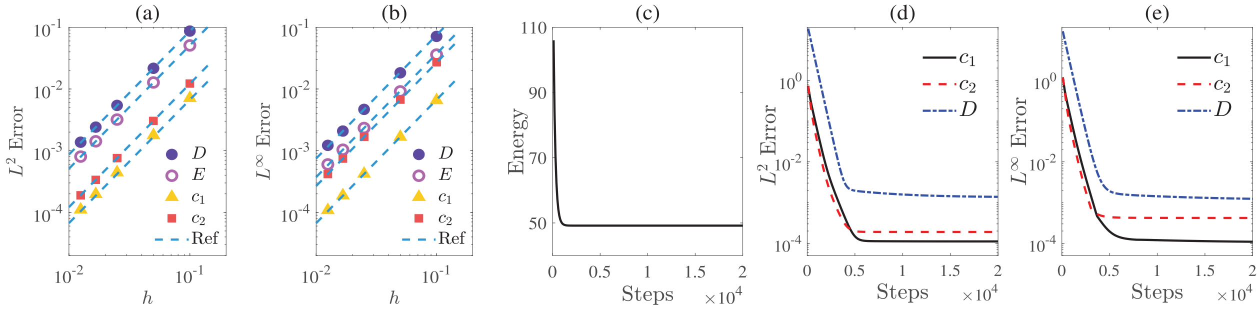

FIGURE 3. (a) and (b): Log–log plots of the L^2-error (a) and the L^∞-error (b) for the approximation of $(c_h, D_h) = (c_{1,h}, c_{2,h}; D_h)$ of $(c, D) = (c_1, c_2, D)$ (marked c_1, c_2, and D), respectively, and for the approximation $E_h := m_h[D_h]/\varepsilon$ of the electric field $E := -\nabla\phi$ (marked E). The blue dashed lines (marked Ref) are reference lines indicating the $O(h^2)$ convergence rate. (c)–(e): The discrete energy (c), the L^2-error (d), and the L^∞-error (e) for the approximations $(c_h^{(k)}, D_h^{(k)})$ *vs.* the iteration step k in the local algorithm.

This and (4.35), together with the continuity of $G(D)$ on D by Lemma 4.3, imply that $G(D^{(t)}) \to (0, 0, 0)$. □

5. NUMERICAL TESTS

We present two tests: one for the PB energy and the other for the Poisson energy with a variable dielectric coefficient ε.

Test 1. The PB energy. We set $\Omega = (0, 2)^3$ (*i.e.*, $L = 2$), $M = 2$, $q_1 = -q_2 = 1$, $c_s = e^{-q_s\phi}$ $(s = 1, 2)$, $D = -\varepsilon\nabla\phi$, and

$$\varepsilon(x_1, x_2, x_3) = 3 - \cos(\pi x_1)\cos(\pi x_2)\cos(\pi x_3),$$
$$\phi(x_1, x_2, x_3) = -\cos(\pi x_1)\cos(\pi x_2)\cos(\pi x_3),$$
$$\rho(x) = -\nabla\cdot\varepsilon\nabla\phi(x) - \sum_{s=1}^{2} q_s e^{-q_s\phi(x)},$$
$$N_s = \int_\Omega e^{-q_s\phi}\,\mathrm{d}x \quad (s = 1, 2).$$

Note that we do not need to compute the integral that defines N_s. It can be verified that ϕ is the unique periodic solution to the CCPBE (1.8) and $(c, D) = (c_1, c_2; D) \in X_\rho$ is the unique minimizer of $F : X_\rho \to \mathbb{R} \cup \{+\infty\}$. For a given finite-difference grid of size h, we denote by $(c_h, D_h) = (c_{1,h}, c_{2,h}; D_h) \in X_{\rho,h}$ the unique minimizer of the discrete PB energy functional $F_h : X_{\rho,h} \to \mathbb{R}$, same as $(c^h_{\min}, D^h_{\min})$ in Theorem 2.2, where ρ^h in the definition of $X_{\rho,h}$ is constructed in Theorem 3.1. We also denote by $(c_h^{(k)}, D_h^{(k)}) = (c_{1,h}^{(k)}, c_{2,h}^{(k)}; D_h^{(k)})$ $(k = 0, 1, \dots)$ the iterates produced by the local algorithm. Figures 3a and 3b show in the log–log scale the L^2 and L^∞ errors for the approximation $c_{s,h}$ of c_s $(s = 1, 2)$ and D_h of D, and also the approximation $E_h := m_h[D_h]/\varepsilon$ of the electric field $-\nabla\phi$, respectively, against the finite-difference grid size h. Figures 3c–3e show the discrete energy $F_h[c_h^{(k)}, D_h^{(k)}]$, L^2-errors $\|c_s - c_{s,h}\|_h$ $(s = 1, 2)$ and $\|\mathscr{P}_h D - D_h^{(k)}\|_h$, and L^∞-errors $\|c_s - c_{s,h}\|_\infty$ $(s = 1, 2)$ and $\|\mathscr{P}_h D - D_h^{(k)}\|_\infty$, respectively, *vs.* the iteration step k of local update with $h = L/N = 2/160 = 0.0125$. We observe from Figures 3c–3e the monotonic decrease of all the energy and errors during iteration. In fact, the errors converge to some values that are set by the grid size h. We observe from Figures 3a and 3b the $O(h^2)$ convergence rate as predicted by Theorem 3.1.

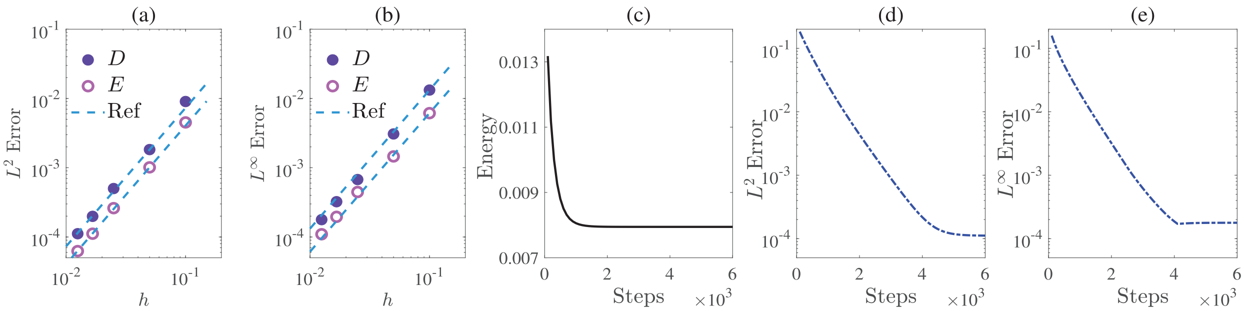

FIGURE 4. (a) and (b): Log–log plots of the L^2-error (a) and the L^∞-error (b) for the approximation $\hat{D}_h$ of the displacement D (marked D) and the reconstructed approximation $\hat{E}_h := m_h[\hat{D}_h]/\varepsilon$ of the electric field $E := -\nabla\phi$ (marked E) for Test 2. The blue dashed lines (marked Ref) are reference lines indicating the $O(h^2)$ convergence rate. (c)–(e): The discrete energy (c), L^2-error (d), and L^∞-error (e) for the displacement $\hat{D}_h^{(k)}$ *vs.* the iteration step k in the local algorithm with shift for Test 2.

Test 2. The Poisson energy with a variable permittivity. We set $\Omega = (0,2)^3$ and define

$$\begin{aligned} \varepsilon(x_1,x_2,x_3) &= 3 - \cos(\pi x_1), \\ \phi(x_1,x_2,x_3) &= f(x_1)\cos(\pi x_2)\cos(\pi x_3), \\ f(x_1) &= \begin{cases} e^{\frac{1}{(x_1-1)^2-0.5^2}} & \text{if } |x_1 - 1| < 0.5, \\ 0 & \text{if } 0 \le x_1 \le 0.5 \text{ or } 1.5 \le x_1 \le 2, \end{cases} \end{aligned}$$

first for $(x_1,x_2,x_3) \in [0,2]^3$ and then extend them $[0,2]^3$-periodically to $\mathbb{R}^3$, Note that f is a C^∞-function. We define $\rho = -\nabla\cdot\varepsilon\nabla\phi$ and $D = -\varepsilon\nabla\phi$. So, ϕ is the periodic solution to Poisson's equation $\nabla\cdot\varepsilon\nabla\phi = -\rho$ and $D \in S_\rho$ is the minimizer of $\hat{F} : S_\rho \to \mathbb{R}$ defined in (1.11). For a finite-difference grid with grid size $h = L/N$ for some $N \in \mathbb{N}$, we denote by $\hat{D}_h \in S_{\rho,h}$ the finite-difference displacement that minimizes the discrete energy $\hat{F}_h : S_{\rho,h} \to \mathbb{R}$ defined in (2.27). Note that $\hat{D}_h$ is the same as $\hat{D}^h_{\min}$ in Theorem 2.3, where ρ^h is constructed as in Theorem 3.2. We also denote by $\hat{D}_h^{(k)}$ $(k = 0,1,\dots)$ the iterates produced by the local algorithm with shift. Figures 4a and 4b show in the log–log scale the L^2 and L^∞ errors for the approximation $\hat{D}_h$ of the exact minimizer D and also for the approximation $\hat{E}_h := m_h[\hat{D}_h]/\varepsilon$ of the electric field $-\nabla\phi$, respectively, against the finite-difference grid size h. We observe the $O(h^2)$ convergence rate as predicted by Theorem 3.2. Figures 4c and 4d show the discrete energy $\hat{F}_h[\hat{D}_h^{(k)}]$, L^2-error $\|\mathscr{P}_h D - \hat{D}_h^{(k)}\|_h$, and L^∞-error $\|\mathscr{P}_h D - \hat{D}_h^{(k)}\|_\infty$ *vs.* the iteration step k of local update with the grid size $h = L/N = 2/160 = 0.0125$. We again observe a fast decrease of the energy at the beginning of iteration and then slow decrease of the energy afterwards. The errors converge to some values that are set by the grid size h.

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