Lattice Evolution Solution for the Nonlinear Poisson- Boltzmann Equation in Confined Domains

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Abstract: The lattice evolution method for solving the nonlinear Poisson-Boltzmann equation in confined domain is developed by introducing the second-order accurate Dirichlet and Neumann boundary implements, which are consistent with the non-slip model in lattice Boltzmann method for fluid flows. The lattice evolution method is validated by comparing with various analytical solutions and shows superior to the classical numerical solvers of the nonlinear Poisson equations with Neumann boundary conditions. The accuracy and stability of the method are discussed. This lattice evolution nonlinear Poisson-Boltzmann solver is suitable for efficient parallel computing, complex geometry conditions, and easy extension to three dimensional cases.

Keywords: Lattice evolution method; Poisson-Boltzmann Equation; numerical solution; electrical double layer; Neumann boundary condition

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I. INTRODUCTION

Electrostatic potentials play a fundamental role in many biochemical and biophysical processes, such as bio-macromolecules interactions in electrolyte solutions [1,2], transport phenomena in ion channels in cells [3-7]. Similar applications can also be found in MEMS/NEMS devices [8-10] and fuel cells [11]. A complete understanding of these physical and chemical processes needs correct mathematical descriptions and accurate solutions of the electrostatic potential distributions. One of the most widespread models for the electrostatic interactions is the Poisson-Boltzmann equation (PBE) [2]

$$-\nabla\cdot\varepsilon(r)\nabla\psi(r)+\bar{\kappa}^2(r)\sinh\psi(r)=f(r). \qquad (1)$$

This second-order nonlinear elliptic partial differential equation relates the electrostatic potential (ψ) to the dielectric properties of the solute and solvent (ε), the ionic strength of the solution and the accessibility of ions to the solute interior ($\bar{\kappa}^2$), and the distribution of solute atomic partial charges (f). To expedite solution of the equation, this nonlinear PBE is often approximated by the linearized PBE by assuming $\sinh\psi(r)\approx\psi(r)$. Several numerical techniques have been used to solve the nonlinear PBE and linearized PBE, including boundary element [12,13], finite element [14,15], finite difference algorithms [16-18], and multigrid method [19-23]. Efficient computer codes have also been developed for the PBE numerical solutions with applications in chemical and biological analyses, such as APBS [20], DELPHI [22], ITPCT [14], and Mainfold code [15]. However, due to the complexity of the nonlinear PBE, there is hardly a completely universal approach for the solution. Lots of efforts have always been put on the development of efficient methods to solve the PBE. Up to now, hundreds of relative research papers per year appear on various scientific journals [24].

This work will present an alternative solution for the nonlinear PBE in non-periodic domains by a lattice evolution method (LEM), based on the spirit of the lattice Boltzmann method solving Navier-Stokes equation [25, 26]. Chen *et al*. [27] were the first ones to solve Poisson equation by a lattice evolution method. They introduced the multicolor cellular automaton (CA) model into the lattice gas algorithm. The method was validated numerically for simple Poisson equations; however, as well known, the lattice gas method was in low efficiency [25]. Along Chen's way, Hirabayashi *et al.* [28] solved the Poisson equation by a lattice BGK model as the upgrade of lattice gas model. This lattice BGK solver was also used to solve the time independent Kardar-Parisi-Zhang (KPZ) equation for porous media flows [29]. Hirahayashi's solver increased the efficiency greatly except for it can be only suitable for linear or weak nonlinear Poisson equations. Warren [30] first introduced the "moment propagation" method [31] into the Lattice Boltzmann method to solve the electrical potential distribution. He and Li [32] proposed a different scheme for analyzing the electrochemical processes in an electrolyte by using an independent lattice Boltzmann method to solve the Poisson equation for the ion diffusion. However, this method was based on a locally electrically neutral assumption so it was not suitable for analyzing the dynamics of charged suspensions [33]. Guo *et al.* [34] developed a finite-difference-based lattice Boltzmann (FDLB) algorithm to investigate the Joule heating effect of electro-osmotic flow in microfluidic devices. Wang *et al.* [35,36] proposed a lattice Poisson-Boltzmann method (LPBM) to simulate the electroosmotic flow and its mixing enhancement applications recently.

In this work, we developed the lattice evolution solution based on the previous work [35] for any kinds of nonlinear Poisson equations, particularly the non-linearized Poisson-Boltzmann equation (PBE), emphasizing implements for different type boundary conditions. The current method is validated by comparing with the theoretical and numerical data. Especially, this method is also proved useable for some cases where the classical PDE solvers are hardly suitable. Finally, the stability and accuracy will be discussed.

II. THE ALGORITHM

A. Evolution equation

As well known, the lattice Boltzmann method (LBM) simulates transport phenomena by tracking the movements of molecule ensembles through the evolution of the distribution function [25]. It actually solves the continuous Boltzmann-BGK equation

$$\frac{Df}{Dt} \equiv \partial_t f + (\boldsymbol{\xi} \cdot \nabla) f = -\frac{f - f^{eq}}{\tau_v} + F , \tag{2}$$

where $f \equiv f(x, \boldsymbol{\xi}, t)$ is the single particle distribution function in the phase space $(x, \boldsymbol{\xi})$, $\boldsymbol{\xi}$ is the microscopic velocity, τ_v is the relaxation time, f^{eq} is the Maxwell-Boltzmann equilibrium distribution, and F is an external force term. Through the Chapman-Enskog expansion, it was proved that LBM could provide the correct solution for the continuum Navier-Stokes equations [26],

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla P + \mu \nabla^2 \mathbf{u} + \mathbf{F} , \tag{3}$$

where ρ is the solution density, P is the pressure, μ is the dynamic fluid viscosity and $\mathbf{F}$ is the external force vector.

From this point of view, we adapt Eq. (1) into

$$\nabla^2 \psi(r) - G(\psi, r) = 0 \tag{4}$$

for an uniform dielectric property ε, where $G(\psi, r) = \frac{1}{\varepsilon}\left(\bar{\kappa}^2(r) \sinh \psi(r) - f(r)\right)$.

The Eq. (4) can be regarded as the steady solution of the equation:

$$\frac{\partial \psi(\mathbf{r}, t)}{\partial t} = \nabla^2 \psi(\mathbf{r}, t) + \bar{g}_s(\mathbf{r}, \psi, t) , \tag{5}$$

where $\bar{g}_s = -G$. Based on the thermal lattice evolution schemes [37,38], here we propose the evolution equation for the electrical potential on the two-dimensional nine-direction discrete lattices:

$$g_\alpha(\mathbf{r} + e_\alpha \delta_t, t + \delta_t) - g_\alpha(\mathbf{r}, t) = -\frac{1}{\tau_g}\left[g_\alpha(\mathbf{r}, t) - g_\alpha^{eq}(\mathbf{r}, t) \right] + (1 - \frac{0.5}{\tau_g}) \delta_t \omega_\alpha \bar{g}_s , \tag{6}$$

where

$$\omega_\alpha = \begin{cases} 4/9 & \alpha = 0 \\ 1/9 & \alpha = 1,2,3,4 \\ 1/36 & \alpha = 5,6,7,8 \end{cases} , \tag{7}$$

and the equilibrium distribution of g

$$g_\alpha^{eq} = \varpi_\alpha \psi \text{ , with } \varpi_\alpha = \begin{cases} 0 & \alpha = 0 \\ 1/6 & \alpha = 1,2,3,4 \\ 1/12 & \alpha = 5,6,7,8 \end{cases} . \tag{8}$$

The time step in Eq. (6) is $\delta_t = \delta_x / c$, where c is a *pseudo* sound speed. In fact it can be artificial to vary the time step to influence the accuracy at the boundaries, which will be stated latter. The dimensionless relaxation time for Eq. (6) is

$$\tau_g = \frac{3\chi\delta_t}{2\delta_x^2} + 0.5 , \tag{9}$$

where χ, which is equal to unity in the simulations, is defined as the potential diffusivity.

It can be proved that the evolution equations (6-9) are consistent with the macroscopic Poisson-Boltzmann equation (4). After evolving on the discrete lattices, the macroscopic electrical potential can be calculated using

$$\psi = \sum_\alpha g_\alpha + \frac{1}{2}\delta_t \bar{g}_s . \tag{10}$$

Though the evolution equations of the electrical potential are in an un-steady form, they are limited in the steady

application right now, because the electromagneticsusceptibility has not been considered in the present form. Clearly, the current method inherits most advantages of the Lattice Boltzmann method. It is suitable for complex flows and parallel computing. Though 2D cases are mainly used in this paper, the algorithm is easily to extend to 3D case.

B. Boundary conditions

Boundary condition implements are very important for any numerical method. For the current lattice evolution method, the classical bounce-back model in the standard LBM can be used on the charged surfaces. However, the bounce-back model was reported only in first order accuracy [39-41]. Therefore we introduce here the adapted "counter-slip" approach into the boundary condition implements for electric potential calculations [42,43], which could be consistent with the non-slip boundary in fluid flow simulations [44]. In the so called "counter-slip" approach here, the incoming unknown potential populations are assumed to be equilibrium distributed with a counter-slip potential ψ_0. The value of ψ_0 is determined by suitable constraints, such as given zeta potential (ζ) or surface charge density (σ). Physically, zeta potential accords to the Dirichlet boundary condition and surface charge density accords to the Neumann boundary condition on the wall surface. For clear indication of the boundary condition implements, Fig. 1 shows the simple flat plan channel domain with two charged walls.

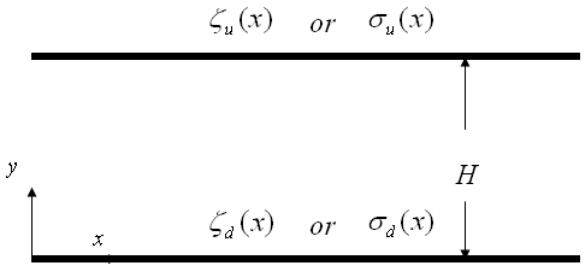

Fig. 1 Boundary conditions for the electric potential in a channel

Dirichlet boundary condition

For the Dirichlet boundary, the unknown distribution functions were calculated from the local equilibrium distribution with the source, $\overline{g}_s$. For example, for the upper wall, g_4, g_7, and g_8, which are unknown, can be obtained from the equilibrium distribution of the local ψ_0:

$$\psi_0 = 3\psi_s - 3S_p - 1.5\delta_t \overline{g}_s, \tag{11}$$

where ψ_s is the potential on the surface (here equals to the zeta potential), S_p is the sum of known populations coming from the internal nodes and nearest wall nodes

$$S_p = g_0 + g_1 + g_2 + g_3 + g_5 + g_6. \tag{12}$$

Thus the unknown distributions are

$$g_\alpha = \varpi_\alpha \psi_0. \tag{13}$$

The corner can be treated in a similar way, with five unknowns at the corner. The upper-right corner, for example, has the unknown populations g_3, g_4, g_6, g_7, and g_8. They also follow from Eq. (23) with

$$\psi_0 = \frac{12\psi_s - 6\delta_t \overline{g}_s - 12S_p}{7}, \tag{14}$$

where

$$S_p = g_0 + g_1 + g_2 + g_5. \tag{15}$$

Neumann boundary condition

For the Neumann boundary, the unknown distribution functions were also calculated by Eq. (13). For the upper wall as an example, introducing the relationship

$$\left.\frac{d\psi}{dy}\right|_s = \frac{1}{\chi}\left[\sum_i (\mathbf{e}_\alpha)_y g_i\right]\left(\frac{\tau_c - 0.5}{\tau_c}\right) \tag{16}$$

leads to

$$\psi_0 = 3S_p - 3\chi\frac{1}{c}\left(\frac{\tau_c}{\tau_c - 0.5}\right)\left.\frac{d\psi}{dy}\right|_s, \tag{17}$$

with

$$S_p = g_2 + g_5 + g_6, \tag{18}$$

and $\left.\frac{d\psi}{dy}\right|_s$ is the potential gradient on the surface, which is determined by the surface charge density

$$\left.\frac{d\psi}{dy}\right|_{y=0} = -\left.\frac{d\psi}{dy}\right|_{y=H} = -\frac{\sigma}{\varepsilon}. \tag{19}$$

Eqs (17) and (13) can be used to determine the unknown populations g_4, g_7 and g_8 for the Neumann boundary condition.

III. RESULTS AND DISCUSSION

To test the present lattice evolution method for solving nonlinear Poisson-Boltzmann equation, we have carried out numerical simulations for electric potential distributions in dilute electrolyte solution in microchannels with charged walls under Dirichlet or Neumann boundary conditions. For simplicity, we only carried out two-dimensional simulation although the extension to three dimensions is straightforward. For the Poisson equation with a Neumann boundary, the current lattice evolution method shows superior to any other numerical methods due to its self-accommodation characteristic.

Consider a 1:1 electrolyte solution in a simple microchannel, as shown in Fig. 1, with periodic inlet/outlet boundaries and homogeneous walls. The Poisson-Boltzmann equation Eq. (1) can therefore be simplified into the one-dimensional form:

$$\frac{d^2\psi}{dy^2} = \frac{2n_\infty ze}{\varepsilon}\sinh\left(\frac{ze}{kT}\psi\right). \tag{20}$$

Based on the Debye-Huckel theory, if $ze\psi/kT$ is small, $\sinh(ze\psi/kT) \approx ze\psi/kT$. Eq. (20) can then be linearized as:

$$\frac{d^2\psi}{dy^2} = \frac{2n_\infty z^2e^2}{\varepsilon kT}\psi = \kappa^2\psi, \tag{21}$$

where $\kappa = \sqrt{\frac{2n_\infty z^2e^2}{\varepsilon kT}}$ is defined as the reciprocal of the Debye length. The linear one-dimensional ordinary differential equation Eq. (21) has a simple analytical solution for a specified set of boundary conditions.

Figure 2 compares the present LEM results for the nonlinear Poisson-Boltzmann equation Eq. (20) and the analytical solutions of the linearized equation Eq. (21), together with numerical solution using the standard multi-grid method. The parameters are the ionic molar concentration $c_\infty = 10^{-4}M$, $n_\infty = c_\infty N_A$ where N_A is the Avogadro's number, $z = 1$, the dielectric constant of the solution $\varepsilon = 6.95\times10^{-10}C^2/J\cdot m$, the temperature $T = 273K$, and $\zeta_u = \zeta_d = \zeta_0$ with ζ_0 as a constant.

In general, the linearization is accurate when ζ_0 is small. Figure 2 shows that the LEM results agree perfectly with multigrid solutions at all zeta potentials and with the analytical solution of the linearized equation when the absolute value of the surface zeta potential ζ is small, less than about 30 mV. This validates the accuracy of the present LEM. When

the absolute value of zeta potential is large (> 30 mV), the linearized analytical solutions deviate from the LEM numerical results as expected [18,45,46].

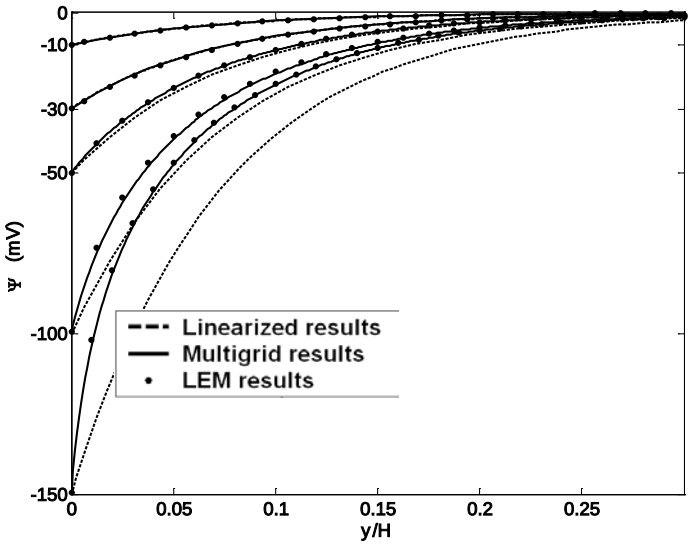

Fig. 2 LEM results (line) compared with the 1D linearization results (cycles) for various surface zeta potentials (-10 mV, -30 mV, -50 mV, -100 mV and -150 mV).

In fact the zeta potential is not a pure physical characteristic though it provides great convenience to the Poisson-Boltzmann equation solutions, and may be measured experimentally [47]. The wall surface charge density actually plays the physical characteristic role instead, and becomes more and more important in micro scale simulations [48,49]. However it meets troubles to solve the Poisson equations with Neumann boundary conditions, because a second-order Poisson equation with a first-order boundary condition has a series of uncertain solutions. This violates the exclusiveness of physics. The charge conservation condition was suggested as one restriction, which is however hard to implement. Here we tried to simulate the PBE in the Fig. 1 domain with only a Neumann boundary condition. It is surprising to find the LEM gave one and only solution for such a case. When $\sigma/\varepsilon = -0.5\times10^{6}$ V/m and other properties were same as the above example, an electric potential distribution and therefore the zeta potential were calculated by LEM. The LEM results are compared with the linearized PBE Eq.(21) solutions in Fig. 3. The resulted zeta potential is low ($|\zeta|<15$ mV) so that the linearization of PBE has good accuracy. The excellent agreement between LEM numerical results and the linearized PBE semi-analytical solutions validates the Neumann boundary implement of LEM.

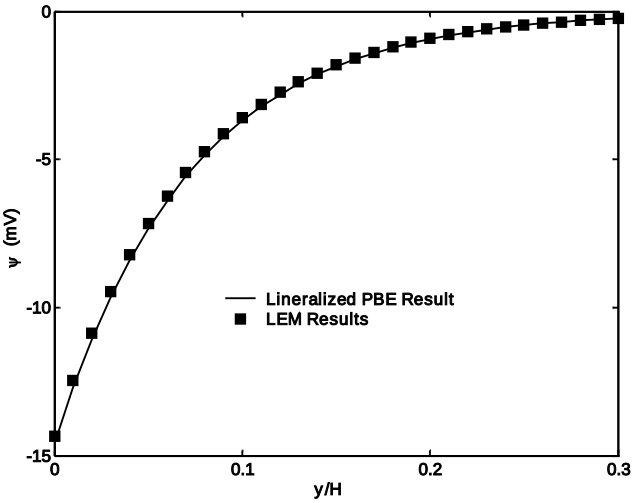

Fig. 3 Implement of Neumann boundary condition of LEM

However the result from Fig. 3 does not prove the only solution of LEM is the exact solution of the original PBE.

Based on the electrical dynamics theory, Ohshima and Furusawa [50] gave a linear relationship between the surface zeta potential and the wall surface charge density at low charge density values. In the book of surface science [51], a more complex one was presented for general dilute electrolytes for the present PBE form Eq. (20),

$$\sigma = \frac{2\varepsilon kT\kappa}{ze}\sinh\left(\frac{ze\zeta}{2kT}\right). \tag{22}$$

Here we carried out LEM simulations for various wall surface charge densities. For each case, we got one value of the electric potential on the wall surface which was treated same as the zeta potential. Fig. 4 compares of numerical results with the analytical results of Eq. (22). Both results agree quite well for a wide charge density region. Thus, we can therefore believe that the LEM for the nonlinear PBE is able to provide the exact only solution for a Neumann boundary condition, which is hard for classical numerical methods. The reason lies on the conversation restriction is automatically kept during the potential evolution process on the lattices.

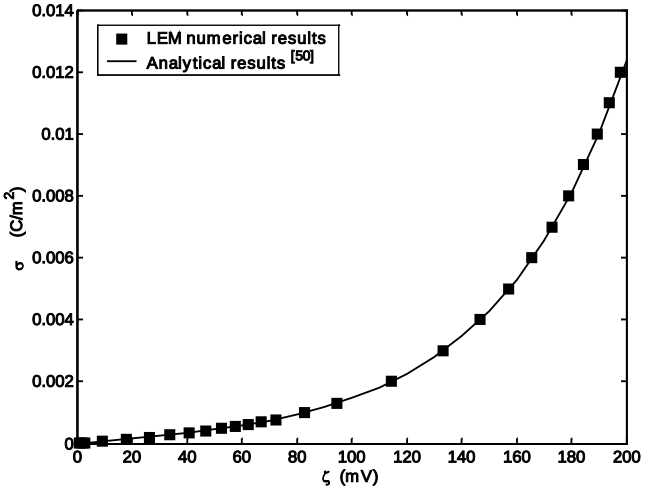

Fig. 4 LEM results (solid squares) compared with the analytical results (line) for the relationship between wall charge density and surface zeta potential.

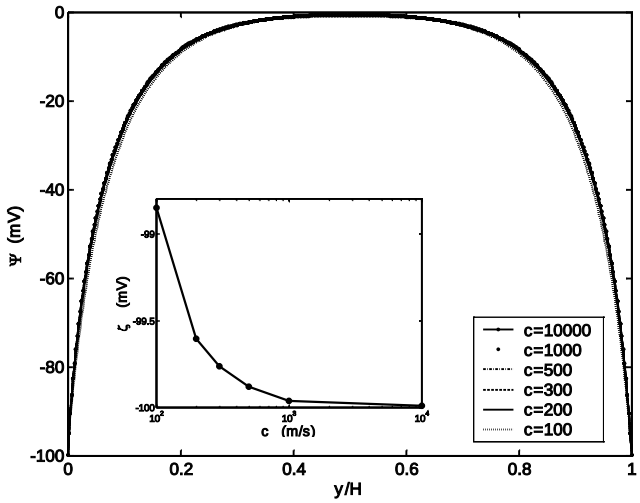

Fig. 5 The effects of the *pseudo* sound speed values on the potential distribution (big figure) and the zeta potential (sub figure) for the Dirichlet boundary condition calculations at $\zeta_0 = -100$ mV.

As a numerical method, the accuracy and stability of the lattice evolution method are also concerned. Inheriting from the standard LBM, the accuracy of current method is mainly influenced by the lattice size and the time step. Especially, for the strong boundary-layer structure distribution of electric potential, the lattice size affects the accuracy greatly. A finer lattice leads to more accurate results and wider potential regions, but costs more computational efforts. In fact, the local refinement [52-54] is very suitable for such cases. The lattices are only refined near the wall boundaries, while coarse lattices are used far from the boundaries. As mentioned above, the *pseudo* sound speed c can be artificially

changed due to its non-physical significance in electric potential evolution. Fig. 5 shows the c value effects on the results. The Dirichlet boundary is pre-specified as $\zeta_0 = -100$ mV. The results show that the electric potential distribution is little influenced by c. The sub plot in Fig. 5 shows the c values affect the calculated zeta potential on the surface. A larger c value leads to a closer zeta potential to the pre-specified value. However, when the c value is larger than 300, the deviation may be below 0.3%. Calculations at a larger value of c need more computational time to reach stable results. One can get a balance between efficiency and accuracy according to the detail requirements.

The present lattice evolution method for the nonlinear Poisson-Boltzmann equation has the advantages of suitability for parallel computations and straightness for three-dimensional extension. Although the efficiency is not high due to the long wavelength limit, it can deal well with complex ion charge structures, not limiting to N : N solutions like many PDE solvers, and complex geometry boundaries with little additional computational costs. The conversation is automatically kept in the electrostatic interactions with boundaries without additional restricts.

IV. CONCLUSIONS

This paper developed the lattice evolution solver for the nonlinear Poisson-Boltzmann equation in confined domains. The Dirichlet and Neumann boundary implement methods are given with second-order accuracy, which are consistent with the non-slip model in LBM for fluid flows. The method is validated by comparing with various analytical solutions and shows superior to the classical numerical solvers for nonlinear Poisson equations with Neumann boundary conditions. The local refinement technique and suitable parameters lead to a stable accurate solution of the nonlinear Poisson-Boltzmann equation with various boundary conditions by the current lattice evolution method. The present lattice evolution method is suitable for parallel computing and it three dimensional extension is easily straightforward.

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