uniformly charged spheres instead of point charges, thus removing the numerical difficulties associated with a singular δ function. Moreover, to compute the dielectric boundary force, it is only necessary to compute with good accuracy the derivative at the center of the sphere and there is no need to perform the volume integral (4). For the case of a Langevin simulation of many charged particles, in which the force on each of the simulated particles is recomputed at every time step of the simulation, our analysis shows that by modeling the mobile particles as charged spheres, one needs to compute only the total electrostatic potential (the solution of Poisson's equation) and then compute the total force on each particle by computing the gradient of the total electrostatic potential at the center of a particle's sphere. Since these forces are independent of the size of the particles, one can solve Poisson's equation with spheres of larger radius than of the physical particles, for better stability and convergence of the numerical scheme.

We note that recently Allen *et al.* have proposed a different approach for the numerical computation of both the induced polarization charges and their effective forces, based on a variational approach [9]. In their method, a numerical computation of the DBC is performed on a two-dimensional grid at different dielectric boundaries, which should be more computationally efficient than solving a three-dimensional Poisson equation.

III. THE DIELECTRIC BOUNDARY FORCE IN TWO SIMPLE GEOMETRIES

We now present explicit computations of the dielectric boundary force for two simple generic geometries. The first is the standard and well-known problem of a charge near an infinite planar dielectric wall, where a closed analytical expression is known, and the other is the dielectric boundary force on the axis of a narrow gramicidin-like channel geometry. In general, closed form analytical solutions are possible only for very few cases, see, e.g., Refs. [7,9–11], so for most practical problems it is necessary to resort to numerical computations.

A. A point charge near a planar dielectric wall

Consider an infinite planar wall located on the (yz) plane, separating two regions with dielectric coefficients ε_1 for $x>0$ and ε_2 for $x<0$. Consider a point charge located at a point $(d,0,0)$ $(d>0)$ in cartesian coordinates. In this case, by the method of images, we can solve explicitly for the electric potential Φ. In Cartesian coordinates, $\boldsymbol{x}=(x,y,z)$, it is given by

$$\Phi(\boldsymbol{x})=\begin{cases}\dfrac{1}{4\pi\varepsilon_0\varepsilon_1}\left(\dfrac{q}{|\boldsymbol{x}-(d,0,0)|}+\dfrac{q'}{|\boldsymbol{x}-(-d,0,0)|}\right), & x>0\\[2ex] \dfrac{1}{4\pi\varepsilon_0\varepsilon_2}\dfrac{q''}{|\boldsymbol{x}-(d,0,0)|}, & x<0,\end{cases} \tag{18}$$

where the image charges q' and q'' are given by

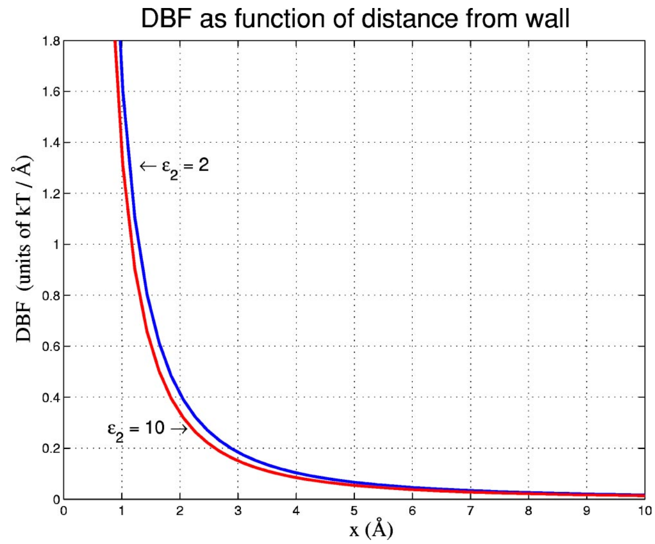

FIG. 1. (Color online) The dielectric boundary force on a single point charge of strength e inside an aqueous solution with $\varepsilon_1=80$ near a dielectric wall with $\varepsilon_2=2$ (upper curve) and with $\varepsilon_2=10$ (lower curve).

$$q'=\frac{\varepsilon_1-\varepsilon_2}{\varepsilon_1+\varepsilon_2}q,\quad q''=\frac{2\varepsilon_2}{\varepsilon_1+\varepsilon_2}q. \tag{19}$$

Therefore, according to Eq. (11), the force on the charge is only in the x direction and is given by

$$F_{ind,x}=\frac{1}{16\pi\varepsilon_0\varepsilon_1}\frac{\varepsilon_1-\varepsilon_2}{\varepsilon_1+\varepsilon_2}\frac{q^2}{d^2}. \tag{20}$$

The top curve in Fig. 1 shows a plot of this force near a dielectric wall with values $\varepsilon_1=80$ and $\varepsilon_2=2$. As seen from the figure, the dielectric boundary force is not exceedingly large even at microscopic distances from the wall. It also does not change much as long as $\varepsilon_1 \gg \varepsilon_2$, as can be seen both from the graph and from formula (20).

However, as pointed out in Ref. [12], the fact that a point charge induces surface charges on the wall has additional consequences apart from the DBF on the particle that induced them. For example, in the study of a multiparticle system, the presence of induced surface charges leads to additional interaction forces between any two charged particles near the dielectric wall, other than their standard Coulombic force. For example, consider two equal point charges of strength q located at $\boldsymbol{r}_1=(d,0,0)$ and at $\boldsymbol{r}_2=(3d,0,0)$. In this case the force on particle 2 due to particle 1 is only in the x direction and is given by

$$F_{2,1}=\frac{q^2}{4\pi\varepsilon_0\varepsilon_1}\left[-\frac{1}{(2d)^2}+\frac{\varepsilon_1-\varepsilon_2}{\varepsilon_1+\varepsilon_2}\frac{1}{(4d)^2}\right].$$

This force should be compared to the standard Coulombic interaction between the two charges. For $\varepsilon_1 \gg \varepsilon_2$, this force is only about 75% of the original Coulombic force between the two particles. Similarly, the force on particle 1 is increased by 25% relative to the free space Coulomb interac-