Capacitance of the Unit Cube

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Computing the capacitance of the unit cube analytically is considered to be “one of the major unsolved problems of electrostatic theory.” However, due to improvements in computer performance and error analysis for “Walk on Spheres” (WOS) Monte Carlo algorithms, we can now calculate the capacitance of the unit cube to many more significant digits than previously possible by using a modified Brownian dynamics algorithm. In our algorithm, there are only two error sources: the error associated with the number of random walks \(N\) (sampling error) and the error associated with an \(\epsilon\)-absorption layer. The sampling error convergence is well-known as \(O(N^{-1/2})\), and error analysis for “Walk on Spheres” Monte Carlo algorithms enables us to control the error from the \(\epsilon\)-absorption layer and to get a more accurate capacitance value for the unit cube, \(0.666063 \pm 0.000005\). Our result supports the calculations by Given et al., by Greenspan et al. and by Read. However, the conjectured exact value proposed by Hubbard and Douglas is inconsistent with our calculations.

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Recently, Given et al. [11] numerically computed the capacitance of the unit cube by using their first-passage (FP) Monte Carlo algorithm. In the FP Monte Carlo algorithm, they refined the previous Brownian dynamics algorithm [7] to remove the \(\epsilon\)-absorption layer by using a set of Green’s functions to provide exact FP probability distributions to terminate the walks [see Fig. 1]. (“Walk on Spheres” (WOS) methods employ an \(\epsilon\)-shell to terminate the random walks [2,12–15]. The boundary, on which random walks terminate, is thickened by \(\epsilon\), and when a walker enters this \(\epsilon\)-shell, the walk is terminated by choosing the boundary point closest to this point on the \(\epsilon\)-shell, as shown in Fig. 2. As shown in the Table 1, there are significant differences between these calculations and the one by Given et al. [11]. Moreover, Given et al. claimed that their approach was exact in the sense that no systematic error was present.

To solve the inconsistencies in the unit cube capacitance, we need a simple error-controllable method. In this letter, using a modified Brownian dynamics algorithm and \(\epsilon\)-error control technique, we obtain an exact value of the cube capacitance up to five significant digits and thereby verify Given et al.’s claim. Due to ceaseless improvement in computer performance (compare 10 hours on a Convex C3830 computer at the time of Zhou et al. [2], with about 4 minutes on a 500-MHz Pentium III workstation) and error analysis for WOS [16].

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Monte Carlo algorithms, we can verify the calculation by Given et al. from recent numerical results obtained by using the modified Brownian dynamics algorithm [7] (Note that in the FP Monte Carlo algorithm, non-trivial Green’s functions were used).

The electrostatic capacitance of an arbitrarily shaped conducting object can be calculated by using the algorithm originally devised for calculating the diffusion-controlled reaction rate toward a target object [2]. The capacitance, \( C \), of an arbitrarily shaped conducting object can be obtained by computing the probability (relative capacitance with respect to the launching sphere), \( \beta \), of a random walk started on the “launching sphere,” a sphere of radius \( b \) completely enclosing the given object, and doing first-passage on the object in question [see Fig. 2]:

\[
C = b \beta. \quad (1)
\]

In addition, in this modified Brownian dynamics algorithm instead of using a fixed time step (Lamm and Schulten method [17]) we have no time variable whatsoever. Instead, we constantly endeavor to take as large a WOS step as is possible, repeating this until we either escape to infinity or terminate in the \( \epsilon \)-absorption boundary layer.

We calculate the quantity \( \beta \) by performing simulations as follows: A random walker is initially placed at a randomly determined position on the surface of the launching sphere. After that, each random walk is constructed as a series of first-passage propagation jumps, each from the present position of the random walker to a new position on a first-passage sphere drawn around the present position [see Fig. 2]. If the random walker is placed inside the launching sphere, another first-passage sphere large enough to touch the cube is drawn, and the first-passage propagation jumps are continued. When the walker enters the \( \epsilon \)-shell, the walk is terminated by choosing the boundary point closest to this point in the \( \epsilon \)-shell [see Fig. 2]. When the random walker is placed outside the launching sphere, to decide whether the random walker goes back to the launching sphere or to infinity we use the probability of going to infinity [18],

\[
P_{\text{inf}} = 1 - \frac{b}{r}. \quad (2)
\]

Here, \( b \) is the launching sphere radius and \( r \) the radial position of the random walker from the center of the launching sphere. When it is determined to go back to the launching sphere, we use the replacement distribution function [18]

\[
\omega(\theta, \phi) = \frac{1 - \alpha^2}{4\pi[1 - 2\alpha \cos \theta + \alpha^2]^{3/2}}. \quad (3)
\]

Here, \((\theta, \phi)\) are defined with respect to the polar axis that joins the position of the random walker to the launching sphere center and \( \alpha \) is \( b/r \) [see Fig. 3]. This distribution function has no \( \phi \) dependence due to symmetry. This procedure is repeated until the random walker ei-
Table 1. Capacitance of a unit cube.

<table>
<thead>
<tr>
<th>Method</th>
<th>Method</th>
<th>Capacitance</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reitan-Higgins [1]</td>
<td>surface charge method</td>
<td>0.6555</td>
</tr>
<tr>
<td>Greenspan-Silverman [4,9]</td>
<td>finite difference method</td>
<td>0.661</td>
</tr>
<tr>
<td>Cochran [7]</td>
<td>boundary element method</td>
<td>0.6596</td>
</tr>
<tr>
<td>Goto-Shi-Yoshida [5]</td>
<td>surface charge method</td>
<td>0.6606747 ± 5 × 10^{-7}</td>
</tr>
<tr>
<td>Conjectured Hubbard-Douglas [3]</td>
<td>analytic conjecture</td>
<td>0.65946...</td>
</tr>
<tr>
<td>Douglas-Zhou-Hubbard [7]</td>
<td>Brownian dynamics algorithm</td>
<td>0.6632 ± 0.0003</td>
</tr>
<tr>
<td>Given-Hubbard-Douglas [11]</td>
<td>refined Brownian dynamics algorithm</td>
<td>0.660675 ± 0.00001</td>
</tr>
<tr>
<td>Read [6]</td>
<td>refined boundary element method</td>
<td>0.660683 ± 6 × 10^{-7}</td>
</tr>
<tr>
<td>our result</td>
<td>modified Brownian dynamics algorithm</td>
<td>0.660683 ± 0.000005</td>
</tr>
</tbody>
</table>

Further reaches the target cube or goes to infinity. After doing the procedure $N$ times, we get the probability, $\beta$, 

$$\beta = \frac{N_{fp}}{N},$$

where $N_{fp}$ is the number of times of doing first-passage on the cube.

In this modified algorithm, there are only two error sources: the error associated with the number of random walks (sampling error) and the error associated with the $\epsilon$-absorption layer. The sampling fractional error corresponding to one standard deviation is given by [11]

$$\sqrt{1-p} \frac{1}{p \sqrt{N}},$$

where $p$ is the probability of contacting the target object of a single random walker, and $N$ is the number of random walks. The error from the $\epsilon$-absorption layer can be investigated empirically if we have enough random walks so that the statistical sampling error is much smaller than the error from the $\epsilon$-absorption layer [16]. Using this technique, we show here that the $\epsilon$-layer error grows linearly in $\epsilon$ for small $\epsilon$. Also, this error analysis enables us to choose the $\epsilon$-absorption layer thickness so that the error associated with the $\epsilon$-absorption is sufficiently smaller than the sampling error.

In Fig. 4, we show that the $\epsilon$-layer error is linear in $\epsilon$ for small $\epsilon$. After simulating 120 runs of $10^9$ [19] random walks with $\epsilon = 10^{-9}$, our result is 0.660683 ± 0.000005. From the linear regression of Fig. 4, it should be noted that the error from the $\epsilon$-absorption layer is much less than the statistical one, 0.000005, which is approximately $10^{-9}$. The calculations by Given et al. [11], by Greenspan et al. [9], and by Read [6] fall within our error bounds; however, the exact value conjectured by Hubbard and Douglas [3] falls outside these bounds. Also, note that the calculations by Goto et al. [5] fall outside these bounds even though their claimed error is much less.

Fig. 3. This illustration shows the usage of the replacement distribution density function $\omega(\theta, \phi)$ when the first-passage jump from the launching sphere is outside the launching sphere, and the probability $P_{\alpha,f}$ decides that the diffusing particle goes back to the launching sphere.

Fig. 4. Solid line shows the linear regression result when the error due to the $\epsilon$-layer with $10^8$ random walks is linear in $\epsilon$ for small $\epsilon$. 
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REFERENCES