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新的有偏扩散模型 LMC 仿真算法的精度

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摘要：已证实传统定时间步长 LMC 算法，能准确复现粒子分布的均值和方差。而存在漂移时，总产生非零的偏度。为进一步提高精度，设计了具有 5 个转移概率的新 LMC 有偏扩散模型算法，且新算法能准确地复现分布的前三阶矩。一旦给定漂移速度和扩散率，有效网格和时间步长的范围就能够数值计算出来。*引入了一种新的度量方法来研究新算法的精度特性。从而发现了一个特殊的网格步长，能让算法仿真的首步误差是最大误差。在该网格步长下，也能发现最优时间步长，使得最大误差达到最小。*

关键词：LMC 算法；扩散模型；精度度量；精度特性
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Introduction

It is an efficient and important method to use LMC simulation for biased diffusion models when difficult to get analytical solutions[1] or necessary to track the trajectory of particles[2]. Generally, the mathematical foundation of the LMC simulation algorithm is based on the theory of random walks on discrete lattices. The key of such algorithms is to find the appropriate transition probabilities[3] as well as the lattice step and the time step. Moreover, it is known that the numerical results of LMC simulation would be accord with the continuous systems[4] once

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the algorithm is designed rationally and the lattice step is small enough[5].

For the Fokker-Planck equation, the LMC algorithm with three transition probabilities has already been devised although it cannot be extended to the more general three dimensional case[6]. Moreover, it is already proved that the traditional fixed time step LMC algorithm can reproduce both the mean and the mean square displacement correctly in the long time limit[7]. However, it is also found that the algorithm always produces a significant non-zero skewness when there is a drift[8]. The error introduced in the skewness converges to zero very slowly in the long time limit[8].

The accuracy of such LMC simulations tops in the biased diffusion processes especially involving simultaneous reactions or interactions between particles[9]. However, the related work on accuracy of the traditional algorithms is totally based on three transition probabilities, which is not in accord with the nature of biased diffusion[10]. Thus, more transition probabilities are needed for the LMC algorithm of biased diffusion models. For the convenience of mathematical derivation and analysis, five transition probabilities are considered in this paper.

For the purpose of the accuracy characteristics of the new algorithm, this paper will only focus on the one-dimensional Fokker-Planck equation with constant drift and diffusivity. The paper is organized as follows. In Section 1, the fundamental background of the new fixed time step LMC algorithm, as well as the transition probabilities, is given. The valid scope of lattice step and time step is also discussed in this section. Then a new accuracy measurement is introduced to explore the potential accuracy characteristics of the new algorithm. In Section 2, some interesting and valuable features with the new accuracy measurement are found through emphatically studying several carefully-choosing diffusion models. In Section 3, some conclusions and the related work of the accuracy characteristics are briefly summarized.

1 The new LMC algorithm and its accuracy measurement

One-dimensional Fokker-Planck equation with constant drift q and diffusivity D can be formulated as

$$\frac{\partial}{\partial t}\rho(x,t) = -q\frac{\partial}{\partial x}\rho(x,t) + D\frac{\partial^2}{\partial x^2}\rho(x,t) \tag{1}$$

The analytical solution is

$$\rho(x,t) = \frac{1}{\sqrt{4\pi Dt}}\exp\left(-\frac{(x-qt)^2}{4Dt}\right) \tag{2}$$

with the initial condition $\rho(x,t=0)=\delta(x)$, where δ is the Dirac delta function. The mean μ, the variance σ^2 and the skewness η of the distribution are

$$\mu = qt, \sigma^2 = 2Dt, \eta = 0 \tag{3}$$

Consider a random walk that hops between its neighboring five sites on a one-dimensional lattice and suppose the lattice step is ℓ. Suppose each particle can stay put or jump to its nearby sites by one or two lattice steps with constant probabilities on discrete fixed time steps. Let p_0 be the probability to stay put and $p_i, i = \pm1, \pm2$ be the probability of jumping to its nearby sites by i lattice steps.

According to our derivation, the five probabilities are

$$p_1 = \frac{-q^3T^3 + (-q^2\ell - 6qD)T^2 + (4q\ell^2 - 2D\ell)T}{6\ell^3} + \frac{2}{3}(1-p_0) \tag{4}$$

$$p_{-1} = \frac{q^3T^3 + (-q^2\ell + 6qD)T^2 - (4q\ell^2 + 2D\ell)T}{6\ell^3} + \frac{2}{3}(1-p_0) \tag{5}$$

$$p_2 = \frac{q^3T^3 + (2q^2\ell + 6qD)T^2 + (-q\ell^2 + 4D\ell)T}{12\ell^3} - \frac{1}{6}(1-p_0) \tag{6}$$

$$p_{-2} = \frac{-q^3T^3 + (2q^2\ell - 6qD)T^2 + (q\ell^2 + 4D\ell)T}{12\ell^3} - \frac{1}{6}(1-p_0) \tag{7}$$

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$$p_0 = 1 - 4\pi D^2 \cosh\left(\frac{\ell q}{2D}\right)\sum_{n=1}^{\infty}\frac{n\sin(n\pi/2)}{\pi^2 D^2 n^2 + q^2\ell^2}\times \left[1-\exp\left(\frac{-\pi^2 D^2 n^2 - q^2\ell^2}{4D\ell^2}T\right)\right]. \quad (8)$$

Clearly, to make the probabilities meaningful, there must be

$$0 \leqslant p_i < 1, i = 0, \pm 1, \pm 2 \quad (9)$$

Consequently, the lattice step and the time step are constrained by Eq. (9), which guarantees that the algorithm is valid. Further, it is known that p_0 is always meaningful for any lattice step and time step.

It is also found that there exist maximums for both lattice step and time step, namely $\ell_{\max}$ and $T_{\max}$, which are determined by the special case

$$p_{-1} = p_{-2} = 0 \quad (10)$$

Then, we can obtain

$$T_{\max} = \frac{\ell_{\max}}{q} = \frac{2D\xi}{q^2} \quad (11)$$

$$\sum_{n=1}^{\infty}\frac{n\sin\left(\frac{n\pi}{2}\right)}{4\xi^2+\pi^2 n^2}\left[1-\exp\left(\frac{-\xi}{2}-\frac{\pi^2 n^2}{8\xi}\right)\right] = \frac{2\xi - 1}{8\pi\xi\cosh(\xi)} \quad (12)$$

where $\xi = \ell_{\max} q/(2D)$.

Eq. (12) can be solved numerically and a valid algorithm can always be derived for this special case. Then, another three transition probabilities are

$$p_0 = p_2 = 1/2\xi \quad (13)$$

$$p_1 = 1 - 1/\xi \quad (14)$$

For more general cases, the scope of valid lattice step and time step can be calculated numerically. The plot of the scope is shown in Fig. 1 for some typical biased diffusion models. Note the log-log scale is used. q and D are marked in the parenthesis. The typical models are selected carefully on the ratio of D/q. The values of the ratio can take 0.1, 1 and 10. The value, 0.1 (10), means that the drift (the diffusivity) is dominant, while 1 indicates that the drift and the diffusivity occupy the same weight in the diffusion models. Then, the values of q and D are all chosen from 0.1, 1 and 10, which would be easier to investigate the effect of q or D on the scope of lattice step and time step, according to the principle of controlling variable method.

It indicates that both the maximum lattice step and the maximum time step are just determined by Eq. (10). The maximum lattice step only depends on D/q. For any valid lattice step, valid time step can always be found. Although its lower bound is always determined by p_{-1}, its upper bound is determined by either p_1 or p_{-2}.

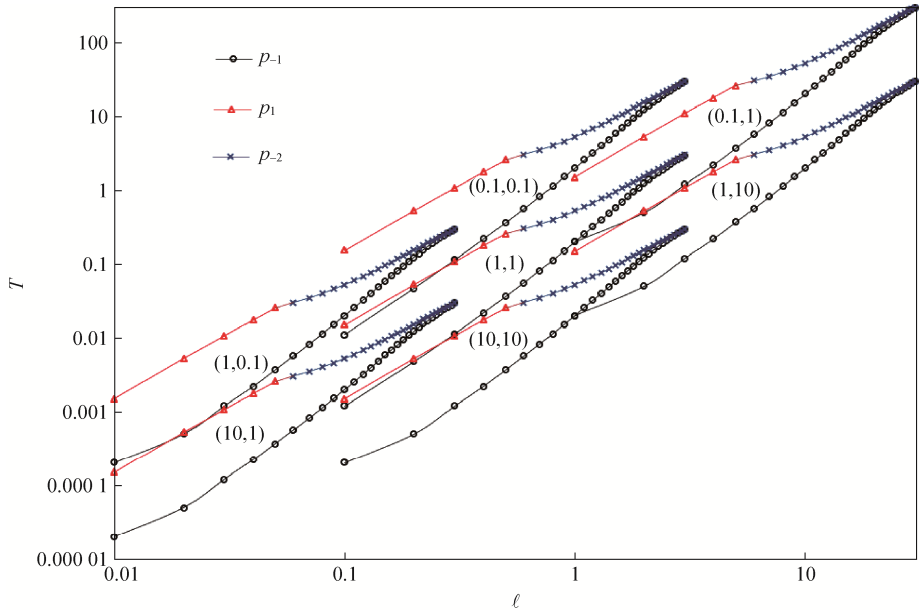

Fig. 1 Scope of valid lattice step and time step

For the accuracy of the one-dimensional fixed time step LMC simulation, three main quantitative estimates are discussed concretely in Ref.[8]. It indicates that the first one is always nonzero in principle for any positive lattice step, no matter how accurate the algorithm is. While the error of the second one can actually be zero, if the number of particles in each site is correct. The third one is proposed through the second one divided by the lattice step. However, the lattice step cannot be given the specific mathematical formula for more general cases. Then it is less meaningful to use the third one than the second. Thus, to discover the accuracy characteristics of the new algorithm, it is more advisable[8] to employ the second one

$$\Delta(t=NT+)=\left\{\sum_{i=-\infty}^{+\infty}\left[\Phi\left(\frac{i\ell+\frac{\ell}{2}-NqT}{\sqrt{2NDT}}\right)-\Phi\left(\frac{i\ell-\frac{\ell}{2}-NqT}{\sqrt{2NDT}}\right)-P(i,t)\right]^2\right\}^{\frac{1}{2}} \quad (15)$$

where $P(i, t)$ is the ratio between particle number at site i and the total particle number of all sites; Φ is the cumulative distribution function of the standard normal distribution and the "+" sign in $t=NT+$ indicates that all the quantities are measured after the jump, rather than before.

For the special case $p_{-1}=p_{-2}=0$, according to Eqs. (11) and (12), the error defined by Eq. (15) can be formulated as

$$\Delta(t=NT+)=\left\{\sum_{i=-\infty}^{+\infty}\left[\Phi\left(\frac{(i+\frac{1}{2}-N)\sqrt{\xi}}{\sqrt{N}}\right)-\Phi\left(\frac{(i-\frac{1}{2}-N)\sqrt{\xi}}{\sqrt{N}}\right)-n_i(NT)\right]^2\right\}^{\frac{1}{2}} \quad (16)$$

Upon using the combined generating function and Fourier transform on the master equation, we obtain

$$n_i(t=NT+)=\sum_{m=\max\{N-i,0\}}^{N-\frac{i}{2}}\frac{N!{p_0}^m{p_1}^{2N-2m-i}{p_2}^{i-N+m}}{m!(2N-2m-i)!(i-N+m)!}=\sum_{m=\max\{N-i,0\}}^{N-\frac{i}{2}}\frac{(\xi-1)^{2N-2m-i}N!}{2^{i-N+2m}\xi^N m!(2N-2m-i)!(i-N+m)!} \quad (17)$$

where $n_i(t)$ is the mean particle number at site i.

2 Numerical results

According to Eqs. (4)~(14), it is not difficult to implement the LMC simulation algorithm of the one-dimensional biased diffusion model with Wolfram Mathematica 8 and Visual Studio 2012. The simulation algorithm is based on the master equation

$$n_i(t+T)=p_0n_i(t)+p_{-1}n_{i+1}(t)+p_{-2}n_{i+2}(t)+p_1n_{i-1}(t)+p_2n_{i-2}(t). \quad (18)$$

According to Eq. (15), the plot of the errors, calculated by Δ as a function of the number of simulation steps with q=1 $\mu m/s$ and D=1 $\mu m^2/s$, is in Fig. 2. ℓ and T are marked in the parenthesis. Note the special case is marked by $\ell_{\max}$ and $T_{\max}$. The subplot reveals the details of Δ with large number of simulation steps. The logarithmic scale is only used for number of steps in the plot, while the log-log scale is used in the subplot.

To facilitate the accuracy analysis, the values of the lattice step can take 0.1, 0.2, 0.4 and $\ell_{\max}$. According to the former theoretical analysis, if the lattice step is less than its maximum, a valid scope of time step can always be found and calculated numerically. Given the lattice step, the values of the time step are always selected starting from its scope's lower bound. Then, the results of ten representative models are shown in the plot. Although the errors exhibit rather complicated behavior regarding number of simulation steps, some underlying information about Δ can still be discovered.

Through the subplot, it indicates that the errors fit well to the power law in the $N\to\infty$ limit. In addition, it is found that the differences of power exponents between different models are pretty small, so the curves seem parallel to each other.

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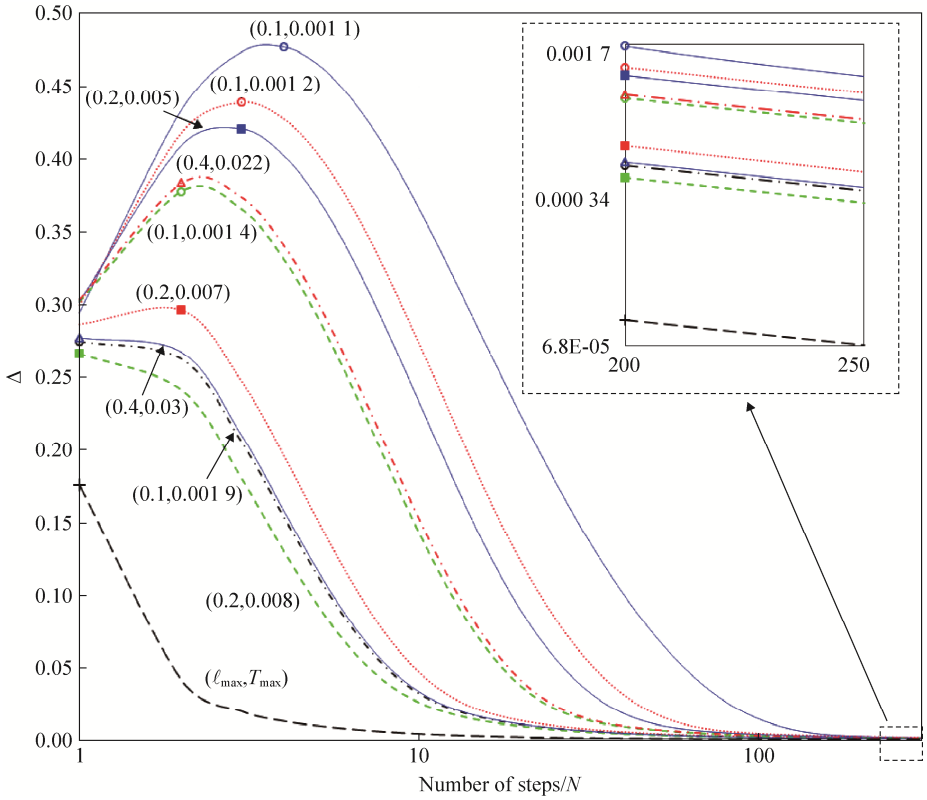

Fig. 2 Errors calculated by Δ versus number of simulation steps with q=1 $\mu m/s$, D=1 $\mu m^2/s$

For the special case, it is found that no matter what the drift and the diffusivity are, errors calculated by Δ always behave in the same way as shown in Fig. 2. It clearly shows that the errors decrease monotonically, so the first step error (Δ_F) is just the maximum error (Δ_m), which is about 0.175 55. For more general cases, several representative models have been studied deeply. According to Fig. 2, given the lattice step, it is observed that some a valid time step can be searched out to make Δ_F be Δ_m. Furthermore, it can be seen that Δ_m, with the time step taking its lower bound, gradually becomes the fourth, third, second, first step error with the lattice step taking 0.1, 0.2, 0.4, $\ell_{\max}$ in turn. Consequently, it naturally leads to the fact that a particular lattice step, namely ℓ^*, can be found out so that Δ_F is just Δ_m. Moreover, it is inspiring to search out the particular lattice steps regarding several typical cases, which greatly validates the fact.

For the accuracy of the new fixed time step LMC algorithm simulation, it would be more interesting to investigate into Δ_m. Thus, it is worthy of plotting Δ_m versus time step in Fig. 4 to study some potential properties, based on several representative models with $q=\{0.1,1,10\}\mu m/s$, $D=\{0.1,1,10\}\mu m^2/s$ and the particular lattice steps. Note the time step of each model is calculated numerically.

According to Fig. 3, it seems that the trend of Δ_m has nothing to do with the drift and the diffusivity, and is always presented in the shape of "V", when the particular lattice steps are used in the biased diffusion models. As a result, an optimal time step, namely T_{op}, can always be found to make Δ_m reach its minimum (approximately 0.04). Since it is hard to get more information about ℓ^* and T_{op} by mathematical analysis, two empirical formulas are obtained, which are $\ell^* = 0.8D/q$ and $T_{op} = 0.29D/q^2$ based on the data from a large number of simulation tests.

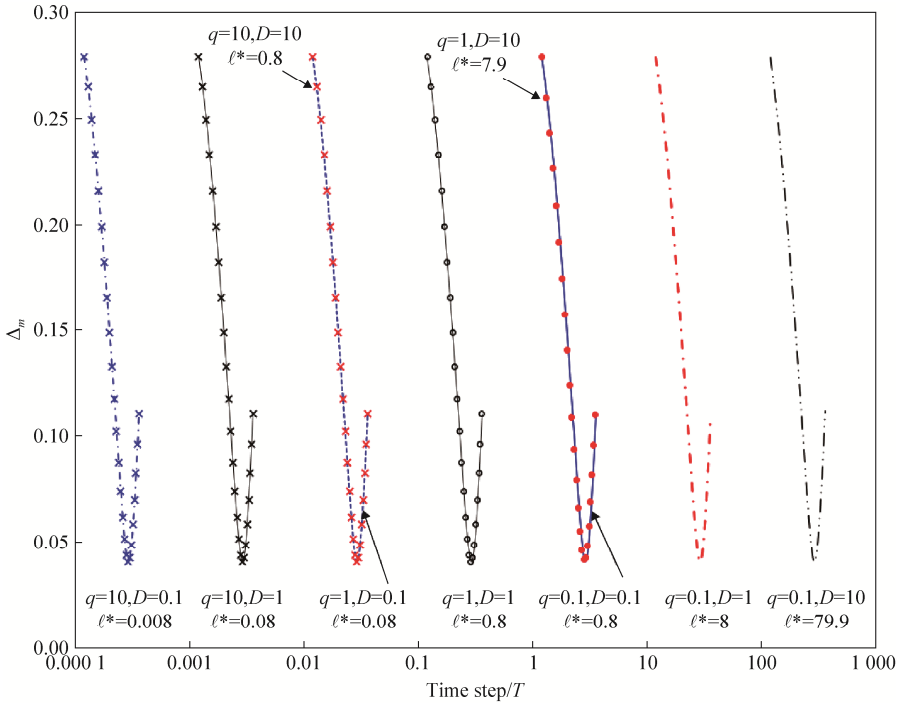

Fig. 3 Maximum errors calculated by Δ versus time step.

If considering the parameter $\ell q/(2D)$, i.e., the Péclet number, it can be found that the maximum error at optimal time step and the error at any simulation step are less than those (the maximum error is about 0.05) in traditional algorithm.

Given that Δ_m concerns us a lot and may lead to some unexpected properties, then the plot of Δ_m versus time step with q=1 μm/s, D=1 μm^2/s and $\ell=\{\ell_{\max},2\ell^*,\ell^*,\ell^*/2,\ell^*/4,\ell^*/8,\ell^*/16,\ell^*/32,\ell^*/64\}$μm is drawn in Fig. 4. The lattice steps are shown beside each curve. Note that all the minimums of Δ_m are marked particularly with circle or square.

According to Fig. 4, it clearly indicates that an optimal time step can always be found to minimize Δ_m for any valid lattice step. Looking into the relation between the minimum error and the lattice step, we can get such a judgment that the minimum error does not approach zero, but closes to some a specific positive in the $\ell \to 0$ limit.

Likewise, it is worth considering the performance of error defined by Δ in the $q\to 0$ limit. It is easy to get

$$p_1 = p_{-1} = -\frac{x}{3} + \frac{2}{3}(1 - p_0) \tag{19}$$

$$p_2 = p_{-2} = \frac{x}{3} - \frac{1}{6}(1 - p_0) \tag{20}$$

$$p_0 = 1 - \frac{4}{\pi}\sum_{n=1}^{\infty}\frac{\sin(n\pi/2)}{n}\left[1 - \exp\left(-\frac{\pi^2 n^2}{4}x\right)\right] \tag{21}$$

where $x = DT/\ell^2$.

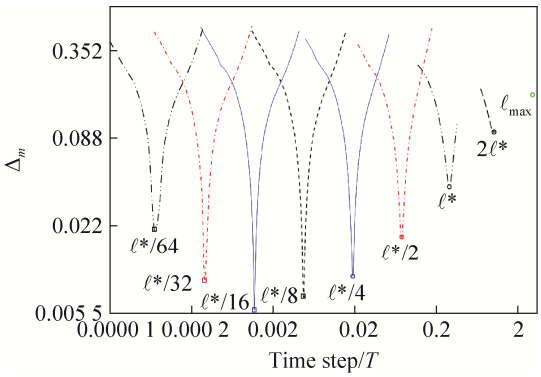

Fig. 4 Maximum errors calculated by Δ versus the time step with q=1 μm/s, D=1 μm^2/s

It agrees with our common sense that the particles jump to right and left with same probabilities when the velocity is zero. It is surprising to see the diffusivity, the time step and the lattice step

are coupled together. But judging from the dimension, x is just a scalar, containing no specific physical meaning at present.

To make $p_i, i = 0, \pm 1, \pm 2$ meaningful, the scope of x can be calculated numerically. Then the plot of Δ versus x is shown in Fig. 5.

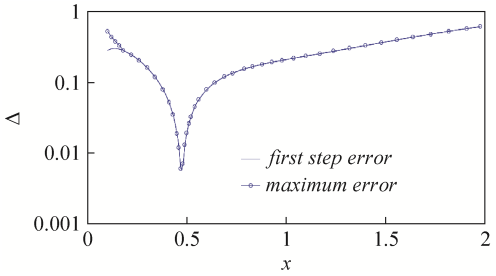

Fig. 5 First step error and maximum error calculated by Δ versus x in the $q \to 0$ limit

According to Fig. 5, the trends of first step error and maximum error are similar to the cases of non-zero velocity and the lattice step which is smaller than the particular lattice step. Clearly, it can be found that the two curves overlap at $x \approx 0.18$. This means that Δ only decreases monotonically when $x > 0.18$. Otherwise, Δ is nonmonotonic. Moreover, it is observed that the optimal x (approximately 0.47), leads to the minimum of Δ_m, which is about 0.005 973.

3 Conclusions

In summary, although we have devised the new algorithm with five transition probability and have proved that the first three moments of the distribution can all be reproduced exactly, the accuracy of the new fixed time step LMC simulation can never be a trivial matter. Instead, it is significant to probe into the characteristic of the accuracy measured by different criterions, since the different criterions will be appropriate for different purposes or make sense in different contexts[8], such as the accuracy measurement defined by Δ.

On the one hand, according to our numerical results, it clearly shows that a particular lattice step can be found in which case the first step error equals the maximum error. More importantly, we sum up two empirical formulas of the particular lattice step and the optimal time step, which fit well in many different models. The formulas are valuable to us as they provide a more simple and feasible way to select the lattice step and the time step for more general cases instead of calculating numerically. Besides, they themselves represent considerably specific meanings.

On the other hand, the new fixed time step LMC algorithm with more transition probabilities indeed improves the accuracy compared with traditional algorithm. But the improvement does not seem significant on the numerical results as we expected, which is more likely caused by the round-off errors introduced in the iterative calculations.

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