Two algorithms for numerical modeling of thermal decay of a metastable state

M V Chushnyakova\textsuperscript{1}, I I Gontchar\textsuperscript{2}, N A Khmyrova\textsuperscript{2}
\textsuperscript{1}Omsk State Technical University, 11 Mira ave., Omsk 644050, Russia
\textsuperscript{2}Physics and Chemistry Department, Omsk State Transport University, Omsk 644046, Russia

maria.chushnyakova@gmail.com

Abstract. We compare two numerical algorithms for the computer modeling of the thermal decay process (Kramers problem) solving the stochastic (Langevin) equations for the generalized coordinate and its conjugate momentum. These are known in the literature (i) the ALGO algorithm including in the fluctuation part the terms up to $\tau^{3/2}$ ($\tau$ is the time step of the numerical modeling) and (ii) the Euler-Maruyama algorithm including in the fluctuation part only the terms proportional to $\tau^{1/2}$. We concentrate on the quasistationary decay rate and transient time. The ALGO algorithm appears to be more efficient, however, the optimal size of the time step has a strong and non-trivial dependence upon the dissipation strength and governing parameter.

1. Introduction

The Brownian motion was first successfully interpreted theoretically more than 100 years ago [1,2]. The approach that was worked out in those two works later became a model applied in a variety of natural sciences. The case of the thermally activated decay of a metastable state was studied theoretically in [3,4] and formed a basis for describing many processes ranging from the nuclear fission (considered within the one-dimensional models [5–7] and multi-dimensional models [8–11]) with a typical spatial size 10 fm up to the single bio-molecule manipulating [12–14] with a typical size about 100 nm [13].

In all these studies, the decay rate plays a key role. Many works are devoted to the study of this rate (see, e.g., surveys [15–17]). The numerical modeling of the stochastic decay process serves here as a valuable tool [18–20]. In the present work, we consider a one-dimensional case when an imaginary Brownian particle initially is at rest at the metastable state separated from the global minimum of the potential $U(q)$ by a potential barrier whose height is $U_b$. The motion of this particle is described by the generalized coordinate $q$ and its conjugate momentum $p$. The corresponding Langevin Equations (LEs) read

\begin{align}
\frac{dp}{dt} &= -\frac{\eta}{m} p - \frac{dU}{dq} + g\Gamma, \quad (1) \\
\frac{dq}{dt} &= \frac{p}{m}. \quad (2)
\end{align}
Here \( m \) and \( \eta \) denote the inertia ("mass") and friction parameters, respectively; \( g = \sqrt{\eta \theta} \) is the amplitude of the random force (the thermal energy \( \theta \) is proportional to the temperature \( T \): \( \theta = k_B T \)); \( \langle \Gamma(t) \rangle = 0, \langle \Gamma(t_1) \Gamma(t_2) \rangle = 2 \delta(t_1 - t_2) \). All quantities \( m, \eta, \) and \( \theta \) are supposed to be \( g \)-independent.

In any explicit numerical scheme, the LEs are modeled as follows

\[
P^{(n+1)} = p^{(n)} + \Delta p, \tag{3}
\]

\[
q^{(n+1)} = q^{(n)} + \Delta q, \tag{4}
\]

The superscripts correspond to two moments of time separated by the time step \( \tau \). Different algorithms differ in a way they compute \( \Delta p \) and \( \Delta q \).

In the works related to the nuclear fission problem [6,21,22], the LEs are modeled usually using the Euler-Maruyama (EM) numerical scheme [23]. In our case it reads

\[
\Delta p = \left\{ -\beta p - \frac{dU}{dq} \right\} \tau + g b(t)^{1/2}, \tag{5}
\]

\[
\Delta q = \left( p^{(n)} + p^{(n+1)} \right)/(2m). \tag{6}
\]

Here we introduce the damping coefficient \( \beta = \eta / m \); the random number \( b \) entering the random force has a Gaussian distribution with zero average and variance 2. On the right-hand side of Eq. (5), all quantities are taken at the time moment \( t_n \).

However, in Ref. [24], a different algorithm (ALGO) of a higher order with respect to \( \tau \) was proposed. That algorithm is expected allowing to use a larger time step thus winning the computer time. The algorithm reads

\[
\Delta p = \left\{ -\beta p - \frac{dU}{dq} \right\} \tau + g b_1 \tau^{1/2} - \beta g \left( \frac{b_1}{2} + \frac{b_2}{2\sqrt{3}} \right) \tau^{3/2}, \tag{7}
\]

\[
\Delta q = \frac{p}{m} + \frac{g}{m} \left( \frac{b_1}{2} + \frac{b_2}{2\sqrt{3}} \right) \tau^{3/2}. \tag{8}
\]

Here all the quantities on the right-hand side are taken at the time moment \( t_n \). A possible disadvantage of the ALGO is that it requires two random numbers \( b_1 \) and \( b_2 \) at each time step.

2. Results

The model used in the present work is described in detail in [20,25]. The numerical modeling results in a set of \( N_{tot} \) trajectories; each of them is terminated not later than at \( t = t_p \). We store a file with the information about each trajectory ("raw data") for the subsequent processing. Some of these trajectories cross the absorptive border \( q_a \) (sink) before \( t_p \). They contribute to the time-dependent decay rate \( R_n(t) \), calculated at the sink point according to the definition

\[
R_n(t) = \frac{1}{N_{tot} - N_e} \frac{\Delta N_e}{\Delta t}. \tag{9}
\]

Here \( N_e \) is the number of trajectories reaching \( q_a \) by the time moment \( t \); \( \Delta N_e \) denotes the number of trajectories arriving at the sink during the time lapse \( \Delta t \).

It was shown in [26] that the rate \( R_n(t) \) is basically defined by two dimensionless parameters: the governing parameter

\[
G = \frac{U_b}{\theta}, \tag{10}
\]

and damping parameter

\[
\varphi = \frac{\eta}{m\omega}, \tag{11}
\]
In Eq. (11), $\omega$ is the frequency of the oscillations near the bottom of the potential pocket. Note, that all the times below are measured in units of $\omega^{-1}$ unless the opposite is stated explicitly.

There are two most important values characterizing the time-dependent decay rate $R_n(t)$: its quasistationary value $R_D$ and transient time $T_n$ being the time moment at which $R_n(t)$ reaches a half of its quasistationary value.

Typical time-dependent rates divided by the corresponding values of $R_D$ are presented in Fig. 1 for different values of the damping parameter. In Fig. 1e the meaning of $T_n$ is illustrated by the dashed lines. These numerical rates are obtained using the EM algorithm with $\tau = 3 \cdot 10^{-5}$. This value has been proved to obey the plateau condition, i.e. the quantities we are interested in, $R_D$ and $T_n$, do not depend upon $\tau$ within the statistical errors. We call the maximum value of $\tau$, at which the plateau contains three points, the optimal value, $\tau_{opt}$. The latter is considered to be safe to be used for obtaining physical results through computer modeling. We present this plateau obtained using the EM algorithm for $R_D$ and $T_n$ in Fig. 2.

![Figure 1](image_url)

**Figure 1.** Normalized rates $R_n/R_D$ (red lines with symbols) versus the normalized time for several values of the damping parameter $\varphi$ (indicated in the panels). Horizontal blue lines are for convenience. The EM algorithm is used; $G = 3.5$; $\tau = 3 \cdot 10^{-5}$. 
Fig. 2. The quasistationary decay rate $R_D$ (a) and transient time $T_n$ (b) versus the time step $\tau$.

The EM algorithm is used; $\phi = 2.5 \cdot 10^{-3}; G = 3.5$.

In Fig. 2a one clearly sees the plateau: while $\tau$ is too large, the quasistationary rate appears to be big and depending upon $\tau$ significantly beyond the statistical errors. At $\tau \leq 10^{-4}$ this dependence disappears; we can choose $\tau_{opt} \approx 5 \cdot 10^{-5}$. Fig. 2b shows that in the whole interval of $\tau$ variation, the transient time changes within at most 5% around its average value.

The statistical error for $R_D$ is estimated as the doubled root mean square deviation. For $T_n$ finding the statistical errors is challenging. We adopt the following algorithm: after the value of $R_D$ has been found, we process our raw data several times with different values of the upper limit $t_{up} \leq t_D$. The resulting values of $T_n$ are presented in Fig. 3 for two parameter sets (left for $\phi = 0.50$ and $G = 1.0$; right for $\phi = 5.0$ and $G = 5.7$). These calculations have been performed using the ALGO algorithm. We estimate the relative error of $T_n$ as $\varepsilon_{T_n} = 0.5(T_{n,\text{max}} - T_{n,\text{min}})/(T_n)$ where $\langle T_n \rangle$ is the average value of $T_n$ in the interval of $t_{up}$-variation. This procedure results in $\varepsilon_{T_n} = 2\%$.

Let us now go over to the main question of our work: to what extent the ALGO algorithm is advanced in comparison to the EM algorithm. To answer this question, one needs to consider Fig. 4. Here we present the quantities $R_D$ and $T_n$, evaluated with the different values of $\tau$ using the ALGO algorithm and divided by the corresponding value resulting from the EM algorithm at $\tau = 3 \cdot 10^{-5}$. The relative value of $R_D$, changing most drastically, is shown in each column of this figure twice in different scales for the convenience.
Figure 3. The relative values of the transient time $T_n$ versus the value of $t_{up}$. The values obtained at different $t_{up}$ are divided by the average value in the given domain of $t_{up}$. (a) $\tau = 10^{-3}$, $\varphi = 0.50$, $G = 1.0$; (b) $\tau = 2 \cdot 10^{-3}$, $\varphi = 5.0$, $G = 5.7$. The ALGO algorithm is used.

In general, one learns from Fig. 4 that, within the framework of the ALGO algorithm, the value of $\tau$ at which the plateau condition is obeyed strongly depends upon $G$ and $\varphi$. At $G = 1.0$, in the overdamping regime ($\varphi \gg 1$) the optimal value of the time step is extremely large ($\tau \approx 10^{-2}$) giving enormous profit for the computer modeling. However, as the damping parameter becomes smaller, the optimal value of the time step becomes significantly smaller too (see Figs. 4a and 4b) and at $\varphi = 10^{-3}$ the advantage of the ALGO algorithm disappears.

At the larger value of the governing parameter, $G = 5.7$, the situation becomes even worse (see Figs. 4d-4f). In the overdamping regime, the ALGO algorithm again demonstrates a significant advantage, but this advantage disappears already at $\varphi = 10^{-2}$.

3. Conclusions

Despite many works devoted to the Kramers problem, its universal analytical solution (i.e. the one which is valid at any values of the governing and damping parameters, $G$ and $\varphi$) has not been found yet. Therefore, numerical modeling proves to be extremely useful for finding the quasistationary decay rate $R_D$. In the present work, we compare two numerical algorithms, Euler-Maruyama (EM) and ALGO used in the literature for this purpose.

The decay process is modeled numerically by solving the stochastic (Langevin) equations for the generalized coordinate and its conjugate momentum. We determine the main characteristics of the process: the quasistationary decay rate $R_D$ and transient time $T_n$ as functions of the time step $\tau$. The value of this step at which the plateau condition is obeyed, $\tau_{opt}$ (optimal time step) has been found to depend significantly upon the values of $G$ and $\varphi$; whereas at small $G$ and large $\varphi$ the ALGO algorithm makes computer modeling faster by a factor of 200, at $G = 5.7$ and $\varphi = 10^{-2}$ the advantage of the ALGO algorithm totally disappears. Thus, one should be extremely careful using the ALGO algorithm for modeling the decay process of the metastable state.
Figure 4. The relative values of two quantities characterizing the time-dependent decay rate are shown versus the time step \( \tau \): (a), (b), (d), and (e) the quasistationary rate \( R_D \) in the different scales (c) and (f) the transient time \( T_n \). Both \( R_D \) and \( T_n \) are calculated within the framework of the ALGO algorithm and are normalized to the value obtained using the EM algorithm at \( \tau = 3 \cdot 10^{-5} \). Different symbols correspond to the different values of \( \varphi \) as shown in panel (a). Left column: \( G = 1.0 \); right column: \( G = 5.7 \).

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