Research Article

Continuous Finite Element Methods of Molecular Dynamics Simulations

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Molecular dynamics simulations are necessary to perform very long integration times. In this paper, we discuss continuous finite element methods for molecular dynamics simulation problems. Our numerical results about AB diatomic molecular system and A_2B triatomic molecules show that linear finite element and quadratic finite element methods can better preserve the motion characteristics of molecular dynamics, that is, properties of energy conservation and long-term stability. So finite element method is also a reliable method to simulate long-time classical trajectory of molecular systems.

1. Introduction

Molecular dynamics (MD) simulations can provide detailed information on molecular fluctuations and conformational changes and are used to investigate the thermodynamics and structure of chemical and biological molecules. Constructing efficient algorithms suitable for MD applications is an important task. Because of the very rapid oscillatory motions characteristic of MD, very small time steps of about a femtosecond (10^{-15}) are typically used in MD. This means that, in order to get estimates for parameters of interest from simulation, it is necessary to perform very long integration times for MD simulations. The total energy H , obtained by summing the kinetic and potential contributions, is a conserved quantity for the molecular system. Many numerical methods have been developed but the most effective for use in MD simulations should have superior long-term stability properties and energy conservation and permit a large integration time step [1–6]. It is important to construct discrete algorithms which preserve these basic properties.

Currently symplectic algorithm is the main choice in the long-time calculation to the MD. An important feature is that the molecular systems always remain Hamiltonian dynamical models. The Hamiltonian system has a symplectic

structure with strong geometric properties of a dynamical system and conserves the total energy $H(q, p)$ in which the phase-space points (q, p) are allowed on the constant energy hypersurface satisfying $H(q, p) = E$. Ruth, Feng, Sanz-Serna, and Marsden et al. constructed the symplectic algorithm to solve the Hamiltonian system, including the 4-stage, 4th-order explicit symplectic scheme (4SS) to the separable Hamiltonian system and 2-stage, 4th-order implicit symplectic Runge-Kutta scheme (4SRK) [4, 7–13]. It is a difference method that preserves the structure of the system. However, most numerical methods cannot maintain the two properties: Symplectic and energy conservation simultaneously in general according to Ge-Marsde theorem [14]. Symplectic algorithm can preserve symplectic properties, but it can only obtain approximate energy conservation for nonlinear Hamiltonian system. However, the energy conservation is very important to the MD system. If not, (p, q) do not stay near the energy surface very soon leading to unrealistic averages [4–6, 15].

Applying continuous finite element methods for Hamiltonian systems, there are two important advantages where finite element methods can preserve energy conservation and high accuracy approximation to symplectic structure. Zhong and Chen et al. [16–18] got good results. Based on the

importance of energy conservation and long time to the MD system, in this paper, we first use continuous finite element methods to solve MD simulation problems. In numerical experiments of AB diatomic molecular and A_2B triatomic molecules, the linear element and quadratic element methods can better preserve the motion characteristics of molecular system: conservation of energy and long-term stability properties, that reached the microscopic reaction need to be considered time. It is a reliable method for long-time classical trajectory simulations of MD.

2. Continuous Finite Element Methods for Hamiltonian Systems

Consider the first-order ordinary differential equation with initial value in the interval $J = [0, T]$:

$$\begin{aligned} \frac{du}{dt} &= u' = f(t, u), \\ u(0) &= u_0. \end{aligned} \quad (1)$$

Let $J^h : t_0 = 0 < t_1 < t_2 < \dots < t_N = T$ be a partition of J , with $I_j = (t_{j-1}, t_j)$, $h_j = t_j - t_{j-1}$. Consider $h = \max h_j$, $h_j \geq Ch$, $1 \leq j \leq N$. The constant C is independent of j and h . Define the m th degree continuous finite element space:

$$S^h = \{w \mid w \in C(J), w|_{I_j} \in P_m\}, \quad (2)$$

where P_m is a set of m th degree polynomials. In cell I_j , m th degree polynomial has $m + 1$ parameters. As it is an initial value problem, and we already knew the initial value $U(t_{j-1})$ in I_j , it has only m degrees of freedom. Defining m th degree continuous finite element $U \in S^h$ satisfies [19, 20]

$$\begin{aligned} \int_{I_j} (U' - f(t, U)) v dt &= 0, \quad v \in P_{m-1}, \\ U(0) &= u_0. \end{aligned} \quad (3)$$

That is, in cell I_j , it is orthogonal to arbitrary P_{m-1} . Taking $v \in S^h$, then its derivate $v' \in P_{m-1}$. In practical computation, take $v = (t - t_{j-1})^i$, $i = 0, 1, 2, \dots, m-1$.

Lemma 1 (see [20]). *The m th degree continuous finite element of ordinary differential equation has superconvergence in cell node t_j :*

$$(u - U)(t_j) = O(h^{2m}) \|u\|_{m+1, \infty}. \quad (4)$$

We take finite dimension autonomous Hamiltonian $H(p, q)$ canonical systems as

$$\begin{aligned} \frac{dp}{dt} &= -\frac{\partial H}{\partial q}, \\ \frac{dq}{dt} &= \frac{\partial H}{\partial p}, \end{aligned} \quad (5)$$

where $p = (p_1, p_2, \dots, p_n)^T$, $q = (q_1, q_2, \dots, q_n)^T$, and matrix transpose is defined by “ T .” In applications to MD, q , p , and H represent the n particles positions, the canonical momentum, and the total energy of the systems, respectively.

Let $z = [p, q]^T$; (5) can be written as

$$\frac{dz}{dt} = z' = J^{-1} H_z = f(z), \quad (6)$$

where $J = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}$, I_n is the n order identity matrix, and $H_z = \begin{bmatrix} H_p \\ H_q \end{bmatrix}$.

Define (6)’s m th degree continuous finite element $Z = [P, Q]^T$ of z ; it satisfies orthogonal relation:

$$\begin{aligned} \int_{I_j} (Z' + JH_z) v' dt &= 0, \\ Z(0) &= z_0. \end{aligned} \quad (7)$$

Taking $v = [Q, P]^T$, we obtain

$$\begin{aligned} \int_{I_j} (P' + H_q(P, Q)) Q' dt &= 0, \\ P(0) &= p_0, \end{aligned} \quad (8)$$

$$\begin{aligned} \int_{I_j} (Q' - H_p(P, Q)) P' dt &= 0, \\ Q(0) &= q_0. \end{aligned} \quad (9)$$

By subtracting (9) from (8),

$$\int_{I_j} (H_p P' + H_q Q') dt = \int_{I_j} \frac{d}{dt} H(P, Q) dt = 0. \quad (10)$$

Hence, in each node t_j , we prove that

$$\begin{aligned} H(P(t_j), Q(t_j)) &= H(P(t_{j-1}), Q(t_{j-1})) = \dots \\ &= H(P(0), Q(0)) = H(p_0, q_0). \end{aligned} \quad (11)$$

Then we can prove the following.

Lemma 2 (see [16]). *Applying arbitrary degree continuous finite element to solve Hamilton equation, it preserves energy conservation; that is, $H(P(t_j), Q(t_j)) = H(p_0, q_0)$.*

Using continuous finite element methods to solve nonautonomous Hamiltonian $H(p, q, t)$ systems, from (7), we can obtain

$$\int_{I_j} (P' + H_q(P, Q, t)) Q' dt = 0, \quad (12)$$

$$P(0) = p_0,$$

$$\int_{I_j} (Q' - H_p(P, Q, t)) P' dt = 0, \quad (13)$$

$$Q(0) = q_0.$$

By subtracting (13) from (12),

$$\begin{aligned} & \int_{I_j} (H_p(P, Q, t) P' + H_q(P, Q, t) Q') dt \\ &= \int_{I_j} \left(\frac{d}{dt} H(P, Q, t) - H_t(P, Q, t) \right) dt = 0. \end{aligned} \quad (14)$$

It is a nonautonomous Hamiltonian system; in general $\int_{I_j} H_t(p, q, t) dt \neq 0$ for every cell I_j . Hence, in node t_j ,

$$H(P(t_j), Q(t_j), t_j) \neq H(p_0, q_0, t_0). \quad (15)$$

Theorem 3. The continuous finite element methods cannot preserve the energy to nonautonomous Hamiltonian systems.

Theorem 3 verifies that the nonautonomous Hamiltonian systems $H(p, q, t)$ do not have the energy conservation, which coincides with the actual case.

Definition 4 (see [21]). A transformation $z \rightarrow \hat{z}$ of R^{2n} is called canonical, or symplectic, if it is a local diffeomorphism whose Jacobian $\partial \hat{z} / \partial z$ is everywhere symplectic; that is,

$$\left(\frac{\partial \hat{z}}{\partial z} \right)^T J \frac{\partial \hat{z}}{\partial z} = J. \quad (16)$$

Utilizing Legendre orthogonal polynomial and Lemmas 1 and 2, we can prove the following.

Lemma 5 (see [17]). The linear finite element for nonlinear Hamiltonian systems is an approximately symplectic algorithm which has the accuracy of third order to Hamiltonian systems symplectic structure; that is, $(\partial Z_{j+1} / \partial Z_j)^T J (\partial Z_{j+1} / \partial Z_j) = J + O(h^3)$. It also possesses second-order accuracy and preserves the energy.

Lemma 6 (see [17]). The quadratic finite element for nonlinear Hamiltonian systems is an approximately symplectic algorithm which has the accuracy of fifth order to Hamiltonian systems symplectic structure; that is, $(\partial Z_{j+1} / \partial Z_j)^T J (\partial Z_{j+1} / \partial Z_j) = J + O(h^5)$. It also possesses fourth-order accuracy and preserves the energy.

The specific calculation format of the linear continuous finite element (1FE) $Z = ((1-x)/2)Z_{j-1} + ((1+x)/2)Z_j$, $x \in [-1, 1]$, is as follows:

$$Z_j - Z_{j-1} = \frac{h_j}{2} J \int_{-1}^1 H_z(Z) dx, \quad j = 0, 1, \dots, N-1. \quad (17)$$

The specific calculation format of the quadratic continuous finite element (2FE) $Z = ((x^2-x)/2)Z_{j-1} + (1-x^2)Z_{j-1/2} + ((x^2+x)/2)Z_j$, $Z_{j-1/2} = Z((t_{j-1} + t_j)/2)$, $x \in [-1, 1]$, is as follows:

$$\begin{aligned} Z_j - Z_{j-1} &= \frac{h_j}{2} J \int_{-1}^1 H_z(Z) dx, \\ \frac{5}{6}Z_j - \frac{2}{3}Z_{j-1/2} - \frac{1}{6}Z_{j-1} &= \frac{h_j}{4} J \int_{-1}^1 H_z(Z) (x+1) dx. \end{aligned} \quad (18)$$

We utilize high accuracy numerical integration such as at least $m+1$ points of the Gaussian quadrature formula to the m th degree continuous finite element at the right of (17) or (18). From above equation set, we can solve Z_j on cell $I_j = (t_{j-1}, t_j)$, and then we can get the value Z_j , $j = 1, \dots, N$.

3. Numerical Experiments

3.1. Diatomic Molecular System. Consider the classical motion of AB diatomic molecule in the electronic potential, where the mass of atom A is m_1 and that of atom B is m_2 . The coordinates of A and B are x_1 and x_2 , respectively. $q = R = x_1 + x_2$ is the canonical coordinate; $m = (m_1 + m_2)/(m_1 m_2)$ is the canonical mass. Then $p = mq_t$ and $U = p^2/(2m)$ are the momentum and canonical kinetics, respectively. Morse potentials have been used to describe vibrational levels of diatomic molecules. We take the Morse potential as $V(q) = D(e^{-2\alpha(q-q_0)} - e^{-\alpha(q-q_0)})$ [6]. In each case, the parameters D , α , and q_0 of the corresponding Morse potential are specified. The total energy of the AB diatomic molecule system is

$$H(p, q) = U(p) + V(q) = \frac{1}{2m} p^2 + V(q). \quad (19)$$

And the Hamiltonian equation is

$$\begin{aligned} \frac{dp}{dt} &= -\frac{\partial H}{\partial q} = -\frac{\partial V(q)}{\partial q}, \\ \frac{dq}{dt} &= \frac{\partial H}{\partial p} = \frac{\partial U(p)}{\partial p}. \end{aligned} \quad (20)$$

Since it is a separated Hamiltonian system, symplectic scheme can be used to solve this system [6]. We consider 2-stage, 4th-order implicit symplectic Runge-Kutta scheme (4SRK):

$$\begin{aligned} Y_1 &= z^n + h \left(\frac{1}{4} f(Y_1) + \left(\frac{1}{4} - \frac{\sqrt{3}}{6} \right) f(Y_2) \right), \\ Y_2 &= z^n + h \left(\left(\frac{1}{4} + \frac{\sqrt{3}}{6} \right) f(Y_1) + \frac{1}{4} f(Y_2) \right), \\ z^{n+1} &= z^n + \frac{h}{2} (f(Y_1) + f(Y_2)). \end{aligned} \quad (21)$$

The 4-stage, 4th-order explicit symplectic difference scheme (4SS) is

$$\begin{aligned} H(p, q) &= T(p) + V(q), \\ \alpha &= (2 - 2^{1/3})^{-1}, \\ \beta &= 1 - 2\alpha, \\ p_1 &= p^n - c_1 h \left(\frac{\partial V(q)}{\partial q} \right)_{q^n}, \end{aligned}$$

$$\begin{aligned}
q_1 &= q^n + d_1 h \left(\frac{\partial T(p)}{\partial p} \right)_{p_1}, \\
p_2 &= p^n - c_2 h \left(\frac{\partial V(q)}{\partial q} \right)_{q_1}, \\
q_2 &= q^n + d_2 h \left(\frac{\partial T(p)}{\partial p} \right)_{p_2}, \\
p_3 &= p^n - c_3 h \left(\frac{\partial V(q)}{\partial q} \right)_{q_2}, \\
q_3 &= q^n + d_3 h \left(\frac{\partial T(p)}{\partial p} \right)_{p_3}, \\
p^{n+1} &= p^n - c_4 h \left(\frac{\partial V(q)}{\partial q} \right)_{q_3}, \\
q_{n+1} &= q^n + d_4 h \left(\frac{\partial T(p)}{\partial p} \right)_{p^{n+1}},
\end{aligned} \tag{22}$$

where $c_1 = c_4 = \alpha/2$, $c_2 = c_3 = (\alpha + \beta)/2$, $d_1 = d_2 = \alpha$, $d_3 = \beta$, and $d_4 = 0$.

Take the potential parameters $D = 88575.905 \text{ cm}^{-1}$, $\alpha = 2.3425473 \text{ \AA}^{-1}$, $m_1 = 22036 \text{ a.u.}$, $m_2 = 29376 \text{ a.u.}$, $m = (m_1 * m_2)/(m_1 + m_2)$, and $q_0 = 1.128323 \text{ \AA}$ to the CO molecule [5]. Initial condition $q(0) = q_0$, $p(0) = \sqrt{2MD} - 0.01$, stepsize $h = 3$, computing $K = 10^8$ step, and integral interval $T = [0, 3 * 10^8]$. Respectively, we utilize 2FE, 4SRK, and 4SS to compute the energy error; two atoms oscillate versus time and (q, p) classical trajectories of the CO diatomic systems as follows (Figures 1–6).

Take the potential parameters $D = 51443.117 \text{ cm}^{-1}$, $\alpha = 24.251821 \text{ nm}^{-1}$, $m_1 = 25704 \text{ a.u.}$, $m_2 = m_1$, $m = m_1/2$, and $q_0 = 0.12203 \text{ nm}$ to the N_2 molecule [5]. Initial condition $q(0) = q_0$, $p(0) = \sqrt{2MD} - 0.01$, stepsize $h = 3$, computing $K = 10^8$ step, and integral interval $T = [0, 3 * 10^8]$. Respectively, we utilize 2FE, 4SRK, and 4SS to compute the energy error and (q, p) classical trajectories of the N_2 diatomic systems as follows (Figures 7–9).

Figures 1, 3, 5, 7, 8, and 9 show the evolution of the energy and the phase trajectories of CO, N_2 molecule versus time. Figures 2, 4, and 6 indicate that two atoms oscillate in the evolution process, respectively, utilizing 2FE, 4SRK, and 4SS. It is observed from Figures 1–9 that the numerical results computed by 2FE are in agreement with the theoretical analysis, the phase trajectories in phase space are steady, and two atoms oscillate periodically in the evolution process (Figures 1, 2, and 7) which indicates that 2FE can keep approximate high accuracy of symplectic structure just as the symplectic difference method (Figures 3, 4, 5, 6, 8, and 9) which preserves the structure of phase space in a long time ($T = [0, 3 * 10^8]$). The energy error computed by 2FE is only 10^{-15} (Figures 1 and 7) which indicates conservation of energy over long time intervals $T = 3 * 10^8$ under a large stepsize

FIGURE 1: 2FE, computing $K = 10^8$ step, the final 100000 points' corresponding energy error curve and phase trajectories of CO molecule in the phase space (q, p) .

FIGURE 2: 2FE, computing $K = 10^8$ step, the evolution of the final 100000 points $p(t), q(t)$.

$h = 3$, but the energy deviation is comparatively larger by symplectic difference scheme, energy error up to 10^{-9} (4SRK, Figures 3 and 8) and 10^{-7} (4SS, Figures 5 and 9), which is only approximately conservative.

3.2. A_2B Triatomic Molecules. Basing Banerjee and Adams constructed a transformation method; we consider the motion of A_2B triatomic molecule such as water (H_2O) within the C_{2v} symmetry; take the Cartesian coordinate system yOz , with origin at the center of mass O , and the z -axis is the C_2 axis; the coordinates of the two A atoms and B atom are $A(y_1, z_1)$, $A(y_2, z_2)$, and $B(y_3, z_3)$. The generalized

FIGURE 3: 4SRK, computing $K = 10^8$ step, the final 100000 points' corresponding energy error curve and phase trajectories of CO molecule in the phase space (q, p) .

FIGURE 5: 4SS, computing $K = 10^8$ step, the final 100000 points' corresponding energy error curve and phase trajectories of CO molecule in the phase space (q, p) .

FIGURE 4: 4SRK, computing $K = 10^8$ step, the evolution of the final 100000 points $p(t), q(t)$.

FIGURE 6: 4SS, computing $K = 10^8$ step, the evolution of the final 100000 points $p(t), q(t)$.

coordinates $q_1 = y_1 - y_2, q_2 = z_1 - 2z_3 + z_2$, and the generalized momenta $p_1 = 0.25(dq_1/dt), p_2 = 0.5(dq_2/dt)$. Hamiltonian function of A_2B type molecule is $H(q, p) = K(p) + V(q)$, where $K(p) = 2p_1^2 + p_2^2$ is the kinetic energy and $V(q)$ is the potential energy:

$$\begin{aligned}
 V(q) &= 5\pi^2 (D^2 - 5D + 6.5) + 4D^{-1} \\
 &\quad + 0.5\pi^2 (|q_2| - 1.5)^2 + |q_2|^{-1}, \\
 D &= (q_1^2 + q_2^2)^{1/2}.
 \end{aligned} \tag{23}$$

The canonical differential equations are

$$\begin{aligned}
 \frac{dq_1}{dt} &= \frac{\partial H}{\partial p_1}, \\
 \frac{dq_2}{dt} &= \frac{\partial H}{\partial p_2}, \\
 \frac{dp_1}{dt} &= -\frac{\partial H}{\partial q_1}, \\
 \frac{dp_2}{dt} &= -\frac{\partial H}{\partial q_2}.
 \end{aligned} \tag{24}$$

FIGURE 7: 2FE, computing $K = 10^8$ step, the final 100000 points' corresponding energy error curve and phase trajectories of N_2 molecule in the phase space (q, p) .

FIGURE 9: 4SS, computing $K = 10^8$ step, the final 100000 points' corresponding energy error curve and phase trajectories of N_2 molecule in the phase space (q, p) .

FIGURE 8: 4SRK, computing $K = 10^8$ step, the final 100000 points' corresponding energy error curve and phase trajectories of N_2 molecule in the phase space (q, p) .

Initial condition: $q_1(0) = 3, q_2(0) = 3/2, p_1(0) = 0, p_2(0) = 0$, and $H(0) = 50.1951$. Taking stepsize $h = 0.01$, computing $K = 10^8$ step, integral interval $T = [0, 10^6]$.

The second-order symplectic difference scheme (2SS) is

$$z_{k+1} = z_k + hJ^{-1}H_z\left(\frac{z_{k+1} + z_k}{2}\right). \quad (25)$$

We use the linear element method (1FE), general Leapfrog method [1], 2SS, and 4SS to compute the classical trajectories of A_2B type molecule in phase spaces and energy error $H_h - H$ as follows (Figures 10–13).

It is observed from Figures 10–13 that the numerical results computed by the linear element methods are in agreement with the theoretical analysis; atom B and two A atoms in A_2B type molecule vibrate quasi-periodically

FIGURE 10: 1FE, computing $K = 10^8$ step, the final 1000 nodes classical trajectories in phase space and corresponding energy error curve.

and the phase spaces are not squeezed together (Figure 10) which indicates that 1FE can for a long time preserve the characteristic of the oscillatory motions when $T = 1000000$, just as the symplectic difference method (Figures 11 and 12). The energy error computed by the linear element methods is only 10^{-10} when $T = 1000000$, it reached the microscopic reaction needed to be considered time $T = h * K = 10^6$, but the energy deviation is comparatively larger by symplectic difference scheme, energy error up to 10^{-1} (Leapfrog method, Figure 11), 10^{-2} (2SS, Figure 12), and 10^{-3} (4SS, Figure 13), which is only approximately conservative.

FIGURE 11: General Leapfrog method, computing $K = 10^8$ step, the final 1000 nodes classical trajectories in phase space and corresponding energy error curve.

FIGURE 12: 2SS, computing $K = 10^8$ step, the final 1000 nodes classical trajectories in phase space and corresponding energy error curve.

4. Conclusion

The above computations indicate that the finite element methods can preserve less energy drift and are extremely stable over long runs to MD, which leads to an excellent long-time behaviour. These just meet the requirements of MD simulations which have superior long-term stability properties, conservation of energy, and a large integration time step.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

FIGURE 13: 4SS, computing $K = 10^8$ step, the final 1000 nodes classical trajectories in phase space and corresponding energy error curve.

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