Velocity Verlet algorithm for dissipative-particle-dynamics-based models of suspensions

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A velocity Verlet algorithm for velocity dependent forces is described for modeling a suspension of rigid body inclusions. The rigid body motion is determined from the quaternion-based scheme of Omelyan [Comput. Phys. **12**, 97 (1998)]. An iterative method to determine angular velocity in a self-consistent fashion for this quaternion-based algorithm is presented. This method is tested for the case of liquid water. We also describe a method for evaluating the stress tensor for a system of rigid bodies that is consistent with the velocity Verlet alogorithm. Results are compared to the constraint-based rattle algorithm of Anderson [J. Comput. Phys. **52**, 24 (1993)]. [S1063-651X(99)13203-3]

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I. INTRODUCTION

There has been recent interest in mesoscopic models of complex fluids called dissipative particle dynamics (DPD) that blend cellular automata ideas with molecular dynamics methods [1]. The original DPD algorithm utilized symmetry properties such as conservation of mass, momentum, and Galilean invariance to obtain hydrodynamic behavior for a system of ''mesoscopic'' particles which can be thought of as representing clusters of molecules or ''lumps'' of fluid. Later modifications of the DPD algorithm resulted in a more rigorous formulation which was consistent with the fluctuation dissipation theorem [2]. Improvements to the temperature behavior of the DPD algorithm were made by modification of a stocastic forcing term and incorporating a velocity Verlet algorithm which allowed a larger time step while still producing a satisfactory temperature control [3]. An algorithm for modeling the motion of arbitrarily shaped objects subject to hydrodynamic interactions by DPD was suggested by Koelman and Hoogerbrugge [4]. The rigid body is approximated by ''freezing'' a set of randomly placed particles where the solid inclusion is located and updating their position according to the Euler equations. The original DPD algorithm used an Euler algorithm for updating the positions of free particles, and a leap frog algorithm for updating the position of the rigid body. A motivation of this work was to develop an efficient algorithm to update both the free particles, and the rigid body position in a manner consistent with the velocity Verlet algorithm.

A commonly used velocity Verlet-based algorithm for updating the position of rigid bodies is the so called rattle algorithm [5]. The rattle routine solves a set of constraint equations that fix the relative positions of particles comprising the rigid body by a relaxation method. Further, the stress tensor (from an atomic view) can be directly obtained from the constraint forces calculated in the algorithm, and is completely symmetric. While the rattle routine is of order N^2 (where N is the number of particles in the inclusion) and, hence, can be prohibitively slow for the case of modeling the motion of solid inclusions composed of large numbers of particles, it serves as an accurate benchmark to test other algorithms.

In this Brief Report we show how the use of quaternions to represent the orientation of such objects [6,7] can greatly increase the computational efficiency of DPD simulations. Quaternions provide a convenient way to represent the orientation of rigid objects, since, in contrast to a representation in Euler angles, the transformations between body-fixed and laboratory coordinate reference frames contain no singularities when expressed as quaternions. First, we review the development of the equations of motion for the quaternions. Next we indicate how to efficiently apply the velocity Verlet algorithm [8,9] to the quaternion equations [10], and demonstrate its use in the simulation of water. We then discuss the modifications of the algorithm needed to include the velocity dependent dissipative forces in DPD simulations. A procedure for determining the rigid body's contribution to the stress tensor, consistent with the velocity Verlet algorithm, is given and compared to that derived from the rattle routine.

II. EQUATIONS OF MOTION

The equations of motion for the quaternions have been discussed by several authors [7,11–13] with varying degrees of completeness. Note that the explicit form for the matrix connecting the angular velocity of the object in the body-fixed frame and the time derivatives of the quaternions is not treated with a uniform notation, so care must be taken when comparing the elements of this matrix as presented by different authors. For this reason, we present the development of the equations of motion in detail.

The quaternion parameters, χ, η, ξ, and ζ for a individual body are related to the Euler angles, as described by Goldstein [14], by [7]

$$\chi = \cos(\theta/2)\cos((\psi+\phi)/2),$$

$$\eta = \sin(\theta/2)\cos((\psi-\phi)/2),$$

$$\xi = \sin(\theta/2)\sin((\psi-\phi)/2),$$

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$$\zeta = \cos(\theta/2)\sin((\psi+\phi)/2).$$

The quaternions satisfy the constraint

$$\chi^2+\eta^2+\xi^2+\zeta^2=1. \tag{1}$$

The connection of the quaternions with the description of the dynamics of the rigid object is through the matrix equation that connects the time derivatives of the quaternions with the principal angular velocity $\boldsymbol{\omega}_p$,

$$\begin{pmatrix} \dot{\xi} \\ \dot{\eta} \\ \dot{\zeta} \\ \dot{\chi} \end{pmatrix} = \begin{pmatrix} -\zeta, & -\chi, & \eta, & \xi \\ \chi, & -\zeta, & -\xi, & \eta \\ \xi, & \eta, & \chi, & \zeta \\ -\eta, & \xi, & -\zeta, & \chi \end{pmatrix} \begin{pmatrix} \omega_{px} \\ \omega_{py} \\ \omega_{pz} \\ 0 \end{pmatrix} \tag{2}$$

The 4×4 matrix in this equation is orthogonal, so that the transformation is singularity free.

Equations of motion for the quaternions are obtained by transforming the Euler equations for a rigid body that has the center of mass fixed, and is subject to torques **N**, in the principal frame,

$$\begin{aligned} \dot{\omega}_{px} &= N_x/I_x + \omega_{py}\omega_{pz}(I_y-I_z)/I_x, \\ \dot{\omega}_{py} &= N_y/I_y + \omega_{pz}\omega_{px}(I_z-I_x)/I_y, \\ \dot{\omega}_{pz} &= N_z/I_z + \omega_{px}\omega_{py}(I_x-I_z)/I_z, \end{aligned} \tag{3}$$

into a quaternion form using the following sequence of matrix operations. First, define matrices $Q=(\xi,\eta,\zeta,\chi)^T$ and $W=(\omega_{px},\omega_{py},\omega_{pz},0)^T$ so that Eq. (2) becomes

$$\dot{Q}_\alpha = \tfrac{1}{2} M_{\alpha\beta} W_\beta, \tag{4}$$

where repeated Greek indices are summed. Now

$$W_\gamma = 2M^T_{\gamma\alpha}\dot{Q}_\alpha \tag{5}$$

and

$$\dot{W}_\gamma = 2M^T_{\gamma\alpha}\ddot{Q}_\alpha + 2\dot{M}^T_{\gamma\alpha}\dot{Q}_\alpha = \mathcal{T}_\gamma, \tag{6}$$

where $\mathcal{T}$ is obtained from the right-hand side of Eq. (3) with $\mathcal{T}_4=0$. This reduces to

$$\ddot{Q}_\beta = \tfrac{1}{2} M_{\beta\gamma}\mathcal{T}_\gamma - M_{\beta\gamma}\dot{M}^T_{\gamma\alpha}\dot{Q}_\alpha, \tag{7}$$

which in turn simplifies to

$$\ddot{Q}_\beta = \tfrac{1}{2} M_{\beta\gamma}\mathcal{T}_\gamma - Q_\beta(\dot{Q}^T_\alpha\dot{Q}_\alpha), \tag{8}$$

when the conditions $Q_\alpha Q_\alpha=1$ and $Q_\alpha\dot{Q}_\alpha=0$ are applied.

Note that the explicit form of the matrix M depends on the order of the quaternion parameters in the matrix Q, and that different authors have made different choices. The general form for the equations of motion for Q_α is independent of this choice, but any given implementation must be internally consistent.

III. INTEGRATION OF THE EQUATIONS OF MOTION

The velocity Verlet algorithm [8] was initially introduced to improve the numerical stability of the leap frog scheme [15]. The velocity Verlet algorithm has subsequently been derived in a systematic way by means of a time-reversible partitioning of the Louville operator from Ref. [9], and is now widely used in simulations. It is an example of a second order symplectic integrator. It has the forms

$$\begin{aligned} x(\delta t) &= x(0) + \dot{x}(0)\,\delta t + \frac{(\delta t^2)}{2} a(0), \\ \dot{x}(\delta t) &= \dot{x}(0) + \frac{\delta t}{2}[a(0)+a(\delta t)], \end{aligned} \tag{9}$$

where $a(0)$ is the acceleration term evaluated using $x(0)$.

While the systematic derivation for translational degrees of freedom does not apply to rotation of a rigid body, one can still propose a velocity-Verlet-like algorithm for the quaternions. Here we adopt the scheme proposed by Omelyan [10]. The conditions on the quaternions, $Q_\alpha Q_\alpha=1$ and $Q_\alpha\dot{Q}_\alpha=0$, are incorporated into the coefficient Λ of a constraint force with the form $f_\alpha=-2\Lambda Q_\alpha$ so that the integrator for Q_α takes the form

$$Q_\alpha(\delta t) = Q_\alpha(0) + \dot{Q}_\alpha(0)\,\delta t + \frac{(\delta t)^2}{2}\ddot{Q}_\alpha(0) + f_\alpha(0)\frac{(\delta t)^2}{2}. \tag{10}$$

The condition $Q_\alpha(\delta t)Q_\alpha(\delta t)=1$ leads to an explicit expression for the coefficient Λ, namely,

$$(\delta t)^2\Lambda = 1 - s_1(\delta t)^2/2 - \sqrt{1 - s_1(\delta t)^2 - s_2(\delta t)^3 - (s_3 - s_1^2)(\delta t)^4/4}, \tag{11}$$

where the s_i terms are sums: $s_1=\dot{Q}_\alpha(0)\dot{Q}_\alpha(0)$, $s_2=\dot{Q}_\alpha(0)\ddot{Q}_\alpha(0)$, and $s_3=\ddot{Q}_\alpha(0)\ddot{Q}_\alpha(0)$. For small δt, $\Lambda \to s_2\delta t/2$.

The updated values for $\dot{Q}_\alpha(\delta t)$ and $\ddot{Q}_\alpha(\delta t)$ are obtained using Eqs. (4) and (8), with values for ω_{px}, ω_{py}, and ω_{pz} at δt obtained by solving the Euler equations [Eqs. (3)]. Since $\dot{\omega}_{p\alpha}$ is proportional to $\omega_{p\beta}\omega_{p\gamma}$, it is necessary to iterate the second member of Eq. (3) in order to obtain a self-consistent result. Here we suggest a scheme that converges rapidly.

First determine the ω-independent part of $\dot{\omega}_{p\alpha}(\delta t)$ which involves just the torques [Eq. (3)], and call it $T_\alpha(\delta t)$. A zeroth estimate for $\omega_{p\alpha}(\delta t)$ is then

$$\omega^{(0)}_{p\alpha}(\delta t) = \omega_{p\alpha}(0) + \frac{\delta t}{2}[\dot{\omega}_{p\alpha}(0) + T_\alpha(\delta t)]. \tag{12}$$

This estimate for $\omega_{p\alpha}(\delta t)$ is then used to estimate the ω-dependent part of the right-hand side of Eq. (3), say $g^{(0)}_\alpha[\omega^{(0)}(\delta t)]$. The first estimate for $\omega_{p\alpha}(\delta t)$ is then

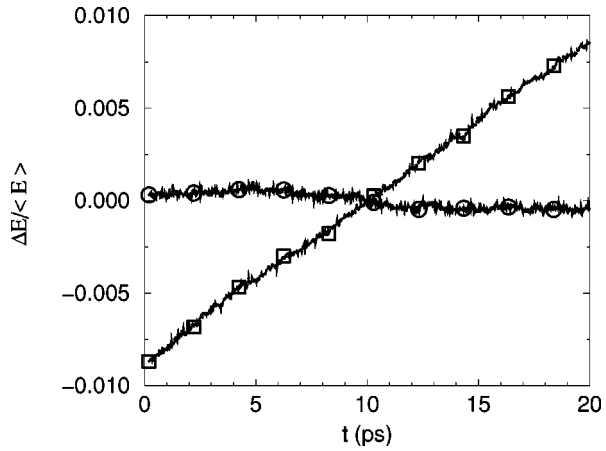

FIG. 1. The departures from the average energy for SPC/E water over a 20-ps time interval are shown for the algorithm discussed above as a line with circles, and for an algorithm where the constraints on the quaternions are imposed by scaling as a line with squares.

$$\omega_{p\alpha}^{(1)}(\delta t)=\omega_{p\alpha}^{(0)}(\delta t)+\frac{\delta t}{2}g_{\alpha}^{(0)}. \tag{13}$$

Now use $\omega_{p\alpha}^{(1)}(\delta t)$ to construct $g_{\alpha}^{(1)}[\omega^{(1)}(\delta t)]$, and then to generate the second estimate for $\omega_{p\alpha}(\delta t)$:

$$\omega_{p\alpha}^{(2)}(\delta t)=\omega_{p\alpha}^{(0)}(\delta t)+\frac{\delta t}{2}g_{\alpha}^{(1)}. \tag{14}$$

This process can be continued until the desired level of convergence has been reached. We find that three iterations are sufficient for the examples discussed in Sec. IV. Equations (10)–(14) constitute the ''constraint force algorithm.''

A related algorithm for integrating the equations of motion for quaternions, that is patterned after the original Verlet algorithm, was described by Svanberg [16]. His ''mid-step implicit algorithm'' is similar to a velocity Verlet algorithm that iterates $\dot{Q}_{\alpha}$ and imposes the $Q_{\alpha}Q_{\alpha}=1$ and $Q_{\alpha}\dot{Q}_{\alpha}=0$ conditions by scaling. Omelyan [10] showed that a velocity Verlet algorithm with scaling for quaternions is inferior to the version described above. This is illustrated by the example discussed next.

IV. ENERGY CONSERVATION FOR WATER

The constraint force algorithm has been used to integrate the equations of motion of 216 SPC/E [17] water molecules at ambient conditions with a time step $\delta t=2$ fs. Results for a 20-ps interval are displayed in Fig. 1 as a ragged line with circles. The quantity $\langle E\rangle$ is the average energy for the 20-ps interval, and $\Delta E=E(t)-\langle E\rangle$. The sloping line with squares is for the same system using a ''scaling algorithm,'' where a velocity Verlet algorithm is used to integrate Q_{α} and $\dot{Q}_{\alpha}$ with scaling to impose the constraints. Clearly this demonstrates the superiority of the constraint force algorithm over the scaling algorithm. Note that a similar figure was given by Omelyan [10]. However, in this case the running average $\langle E(t)\rangle$ instead of $\langle E\rangle$ is used in the denominator. Use of the running average can be misleading because it can mask a systematic drift in energy.

V. DPD MOTION OF LARGE RIGID BODIES

Forces in DPD depend both on the relative positions and velocities of particles. Hence a predictor velocity must be estimated to input into the force calculations. A reasonable approach to determine a predictor velocity could be based on an estimate of angular velocity at $t=\delta t/2$ derived from the quaternion equations of motion. However, to match more closely the trajectories obtained from the rattle routine that strictly follow the velocity Verlet algorithm, the predictor velocity was simply based on the average velocity obtained in moving from position $x(0)$ to $x(\delta t)$ in Eq. (9). Otherwise, the quaternion and rattle routines may not be consistent except in the limit of infinitesimally small time step.

The following modifications were then made to velocity equation in Eq. (9):

$$\tilde{\dot{x}}\left(\frac{\delta t}{2}\right)=\dot{x}(0)+\lambda\,\delta t\,a(0)\approx\frac{x(\delta t)-x(0)}{\delta t} \tag{15}$$

and

$$\dot{x}(\delta t)=\dot{x}(0)+\frac{\delta t}{2}\left[a(0)+a\left(\delta t,\tilde{\dot{x}}\left(\frac{\delta t}{2}\right)\right)\right] \tag{16}$$

for the rattle routine and for the center of mass motion of the rigid body when using the quaternion-based algorithm. In addition Eq. (15) is used to determine the DPD forces between particles for both the rattle and quaternion algorithm. The final position and velocity of the solid body's constituent particles is derived from the quaternion equations. We used $\lambda=\frac{1}{2}$ for our simulations. For further discussion of the effect of varying λ, see Ref. [3].

While the rigid body contribution to the stress tensor is readily calculated from the rattle routine, the constraint forces contributions are not immediately obtained from our quaternion algorithm. However, because the motion of the rigid body closely follows the trajectory obtained by the rattle routine, we can approximate the constraint forces contributions by considering the velocity Verlet algorithm. Let $a_i(0)$ be the acceleration of particle i on the rigid body which results from the sum of nonconstraint forces due to all particles (including those in the rigid body) and the constraint forces from particles in the rigid body. That is, $m\vec{a}_i=\vec{F}_i=\vec{F}^{\rm nc}{}_i+\vec{F}^{c}{}_i$, where the superscripts nc and c correspond to nonconstraint forces and the constraint forces, respectively. Since all the nonconstraint forces are known, as well as the velocity and positions of the particle at $t=0$ and $t=\delta t$, the sum of the constraint forces on particle i can be derived by assuming that particles follow the same time evolution as that derived from the rattle routine using Eqs. (9) and (16).

We now show that the sum of the constraint forces on each particle is all that is needed to determine correctly the constraint force contribution to the stress tensor. First, the contribution to the stress tensor from constraint forces is

$$\sigma_{\alpha\beta}^{c}=\tfrac{1}{2}\sum_{i,j}F_{ij\alpha}^{c}(\vec{r}_i-\vec{r}_j)_{\beta} \tag{17}$$

where i and j correspond to all particles in the rigid body. Note that $\vec{F}^c_{ij} = -\vec{F}^c_{ji}$, and that the sum of constraint forces on particle i due to particles j is $\vec{F}^c_i = \Sigma_j \vec{F}^c_{ij}$. We can then write

$$\begin{aligned}\sigma^c_{\alpha\beta} &= \tfrac{1}{2}\sum_{i,j} F^c_{ij\alpha}(\vec{r}_i - \vec{r}_j)_\beta \\ &= \tfrac{1}{2}\sum_{i,j} F^c_{ij\alpha}\vec{r}_{i_\beta} - \tfrac{1}{2}\sum_{i,j} F^c_{ij\alpha}\vec{r}_{j_\beta} \\ &= \tfrac{1}{2}\sum_{i} F^c_{i\alpha}\vec{r}_{i_\beta} + \tfrac{1}{2}\sum_{j} F^c_{j\alpha}\vec{r}_{j_\beta} \\ &= \sum_{i} F^c_{i\alpha}\vec{r}_{i_\beta}.\end{aligned}$$

Since $\vec{F}^{nc}$ is known and $\vec{a}_i$ can be estimated from Eqs. (9) and (16), we can determine $\vec{F}^c$ to the accuracy of the algorithm, and determine contributions to the stress tensor from the two parts of the velocity Verlet algorithm. Comparing stress tensor values between the rattle and our quaternion algorithm, we found agreement to six significant figures and, further, that the stress tensor was symmetric to the same order. Indeed, for the time step used here, $\delta t = 0.01$, out results are consistent with $\mathcal{O}(\delta t^3)$, the accuracy of the velocity Verlet algorithm.

VI. CONCLUSION

We have developed and tested a velocity Verlet algorithm for a dissipative-particle-dynamics-based model describing the motion of rigid body inclusions. A simple procedure for calculating the stress tensor contribution from the rigid body which is consistent with the velocity Verlet algorithm was given. The velocity Verlet algorithm for DPD is less sensitive to variation in time step size than the Euler algorithm presented in the original DPD papers, thus significantly improving numerical accuracy at little computational cost. Although the original motivation of the paper was to improve upon the original DPD algorithm such that the DPD particles which represent a solvent and the rigid body motion are treated in a self-consistent fashion, the numerical techniques presented in this paper should not be limited to DPD.

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