Leapfrog discretization scheme for solid body tracking in Molecular Dynamics simulations

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I. MOVEMENT OF THE CENTER OF MASS

Input quantities at time t:

position	$\boldsymbol{x}(t)$
velocity	$\boldsymbol{v}\left(t-\frac{dt}{2}\right)$
acceleration	$\boldsymbol{a}(t)$

time	$t-dt/2$	t	$t+dt/2$	$t+dt$
$\boldsymbol{x}$		$\times$		
$\boldsymbol{v}$	$\times$			
$\boldsymbol{a}$		$\times$		

update velocity

$$\boldsymbol{v}\left(t+\frac{dt}{2}\right)=\boldsymbol{v}\left(t-\frac{dt}{2}\right)+\frac{\boldsymbol{a}\,(t)}{m}dt \tag{1}$$

update position

$$\boldsymbol{x}\,(t+dt)=\boldsymbol{x}\,(t)+\boldsymbol{v}\left(t+\frac{dt}{2}\right)dt \tag{2}$$

Output:

$\boldsymbol{x}\,(t+dt)\,,\boldsymbol{v}\left(t+\frac{dt}{2}\right)$

time	$t-dt/2$	t	$t+dt/2$	$t+dt$
$\boldsymbol{x}$				$\times$
$\boldsymbol{v}$			$\times$	
$\boldsymbol{a}$		$\times$		

II. PARTICLE ROTATION

Input quantities at time t:

quaternion	$\boldsymbol{q}(t)$
angular momentum	$\boldsymbol{l}\left(t-\frac{dt}{2}\right)$
torque	$\boldsymbol{\tau}(t)$

time	$t-dt/2$	t	$t+dt/2$	$t+dt$
$\boldsymbol{q}$		$\times$		
$\boldsymbol{l}$	$\times$			
$\boldsymbol{\tau}$		$\times$		

First part of the advancing scheme

Derive rotation matrices at integer time step

$$\boldsymbol{q}(t)\Rightarrow\mathcal{A}(t)\,,\ \mathcal{Q}(t) \tag{3}$$

where

$$\mathcal{A}=\begin{pmatrix} q_0^2+q_1^2-q_2^2-q_3^2 & 2(q_1q_2+q_0q_3) & 2(q_1q_3+q_0q_2) \\ 2(q_1q_2+q_0q_3) & q_0^2-q_1^2+q_2^2-q_3^2 & 2(q_2q_3+q_0q_1) \\ 2(q_1q_3+q_0q_2) & 2(q_2q_3+q_0q_1) & q_0^2-q_1^2-q_2^2+q_3^2 \end{pmatrix}\qquad \mathcal{Q}=\begin{pmatrix} q_0 & -q_1 & -q_2 & -q_3 \\ q_1 & q_0 & -q_3 & q_2 \\ q_2 & q_3 & q_0 & -q_1 \\ q_3 & -q_2 & q_1 & q_0 \end{pmatrix} \tag{4}$$

Estimate the angular momentum at time t

$$[\boldsymbol{l}\,(t)]_{estimate} = \boldsymbol{l}\left(t - \frac{dt}{2}\right) + \frac{dt}{2}\boldsymbol{\tau}(t) \tag{5}$$

Rotation to the body reference system

$$\left[\boldsymbol{l}^b\,(t)\right]_{estimate} = \mathcal{A}(t) \cdot [\boldsymbol{l}\,(t)]_{estimate}$$

Computation of angular velocity in the body frame

$$\left[\boldsymbol{\omega}^b\,(t)\right]_{estimate} = \frac{\left[\boldsymbol{l}^b\,(t)\right]_{estimate}}{\mathcal{I}_{ii}}, \qquad \mathcal{I} = \begin{pmatrix} I_{xx} & 0 & 0 \\ 0 & I_{yy} & 0 \\ 0 & 0 & I_{zz} \end{pmatrix}$$

Estimate the quaternions at time $t + dt/2$

$$[\dot{\boldsymbol{q}}(t)]_{estimate} = \frac{1}{2}\mathcal{Q}(t) \cdot \begin{pmatrix} 0 \\ \left[\boldsymbol{\omega}^b(t)\right]_{estimate} \end{pmatrix}$$

$$\left[\boldsymbol{q}\left(t + \frac{dt}{2}\right)\right]_{estimate} = \boldsymbol{q}\,(t) + \frac{dt}{2}\,[\dot{\boldsymbol{q}}(t)]_{estimate} \tag{6}$$

Enforce quaternion normalization $\boldsymbol{q} \cdot \boldsymbol{q} = 1$.

Second part of the advancing scheme

Derive rotation matrices at half time step

$$\left[\boldsymbol{q}\left(t + \frac{dt}{2}\right)\right]_{estimate} \Rightarrow \mathcal{A}\left(t + \frac{dt}{2}\right),\, \mathcal{Q}\left(t + \frac{dt}{2}\right) \tag{6}$$

update angular momentum

$$\boldsymbol{l}\left(t + \frac{dt}{2}\right) = \boldsymbol{l}\left(t - \frac{dt}{2}\right) + dt\boldsymbol{\tau}(t) \tag{6}$$

Rotation to the body reference system

$$\boldsymbol{l}^b\left(t + \frac{dt}{2}\right) = \mathcal{A}\left(t + \frac{dt}{2}\right) \cdot \boldsymbol{l}\left(t + \frac{dt}{2}\right)$$

Computation of angular velocity in the body frame

$$\boldsymbol{\omega}^b\left(t + \frac{dt}{2}\right) = \frac{\boldsymbol{l}^b\left(t + \frac{dt}{2}\right)}{\mathcal{I}}$$

Computation of angular velocity in the fixed frame

$$\boldsymbol{\omega}\left(t + \frac{dt}{2}\right) = \mathcal{A}^T(t + \frac{dt}{2}) \cdot \boldsymbol{\omega}^b\,(t)$$

update quaternions

$$\dot{\boldsymbol{q}}\left(t + \frac{dt}{2}\right) = \frac{1}{2}\mathcal{Q}\left(t + \frac{dt}{2}\right) \cdot \begin{pmatrix} 0 \\ \boldsymbol{\omega}^b(t + \frac{dt}{2}) \end{pmatrix}$$

$$\boldsymbol{q}\,(t + dt) = \boldsymbol{q}\,(t) + dt\dot{\boldsymbol{q}}\left(t + \frac{dt}{2}\right) \tag{6}$$

Enforce quaternion normalization $\boldsymbol{q} \cdot \boldsymbol{q} = 1$.

Output:

$\boldsymbol{x}\left(t+dt\right), \boldsymbol{v}\left(t+\frac{dt}{2}\right)$

time	$t-dt/2$	t	$t+dt/2$	$t+dt$
$\boldsymbol{q}$				$\times$
$\boldsymbol{l}$			$\times$	
$\boldsymbol{\tau}$		$\times$		

III. COMPUTING THE NEW FORCE AND TORQUE

In order to estimate $\boldsymbol{a}(t+dt)$ and $\boldsymbol{\tau}(t+dt)$ one needs the values of the linear $\boldsymbol{v}$ and angular velocity $\boldsymbol{\omega}$ at an integer time step. These values will be use to compute the velocity of the particle-fluid interface .
One has two options, either using the mean values $\boldsymbol{v}\left(t\right)$ and $\boldsymbol{\omega}\left(t\right)$

$$\boldsymbol{v}\left(t\right)=\frac{1}{2}\left(\boldsymbol{v}\left(t+\frac{dt}{2}\right)+\boldsymbol{v}\left(t-\frac{dt}{2}\right)\right) \tag{7}$$

$$\boldsymbol{\omega}\left(t\right)=\frac{1}{2}\left(\boldsymbol{\omega}\left(t+\frac{dt}{2}\right)+\boldsymbol{\omega}\left(t-\frac{dt}{2}\right)\right) \tag{8}$$

or the linear extrapolations $[\boldsymbol{v}(t+dt)]_{estimate}$ and $[\boldsymbol{\omega}(t+dt)]_{estimate}$

$$[\boldsymbol{v}(t+dt)]_{estimate}=\frac{1}{2}\left(3\boldsymbol{v}\left(t+\frac{dt}{2}\right)+\boldsymbol{v}\left(t-\frac{dt}{2}\right)\right) \tag{9}$$

$$[\boldsymbol{\omega}(t+dt)]_{estimate}=\frac{1}{2}\left(3\boldsymbol{\omega}\left(t+\frac{dt}{2}\right)+\boldsymbol{\omega}\left(t-\frac{dt}{2}\right)\right) \tag{10}$$

IV. APPENDIX

Note that the following relations holds:

$$\boldsymbol{l}^b=\mathcal{I}\cdot\boldsymbol{\omega}^b \tag{10}$$