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# Modified RATTLE Method for Rigid Body Dynamics in Cartesian Coordinates

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**Abstract.** In this paper, we describe a modified RATTLE (M-RATTLE) method for rigid body dynamics directly in Cartesian coordinates. The M-RATTLE method introduces a new way of resetting the coordinates to satisfy the constraints at each step, which is designed for the rigid body dynamics calculations in the Cartesian coordinates. M-RATTLE is algebraically equivalent to the RATTLE method and the cost of performing rigid body dynamics by M-RATTLE is independent of the number of constraints. The interaction forces between atoms belonging to the same rigid molecule do not need to be computed and explicit expressions of the constraints of internal degrees of freedom are unnecessary. The performance and sampling results of the proposed method are compared with those of the symplectic splitting method for an isolated rigid benz molecule and for a cluster of twenty-seven benz molecules.

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**Key words**: Rigid body dynamics, RATTLE method, symplectic splitting method, Cartesian formulation.

## 1 Introduction

There has been great interest in developing stable and efficient algorithms for rigid body dynamics, see, e.g., [1–3]. There are three formulations for rigid body dynamics: the rotation matrix formulation, the formulation based on the Euler equations, and the Cartesian formulation [19]. During the past three decades, a number of algorithms have been developed under these formulations, which include the Gear predictor-corrector algorithm [8],

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the linear constraints method [5], the symplectic splitting methods [6,26,29], the symplectic quaternion scheme [22], the leapfrog scheme [25], the symplectic constrained rotation matrix integration [15,21] and the algorithm proposed by Neto et al. [24].

For rigid molecules whose potentials are expressed in terms of interactions between atomic sites, it is natural to consider calculating the rigid body dynamics directly in Cartesian coordinates. The Cartesian formulation is believed to have good stability property, which can also avoid many complications of Euler equations and quaternions. In the Cartesian formulation, the dynamics are determined by integrating the equations of motion of each atom, subject to the constraints that make the molecules rigid (constraining all internal degrees of freedom). The equations of motion of constrained dynamics are

$$\begin{cases} M\ddot{X}(t) = -\dfrac{\partial U(X(t))}{\partial X} - \dfrac{\partial g(X(t))}{\partial X}^T \lambda, \\ g(X(t)) = 0, \end{cases} \tag{1.1}$$

where $M = \text{diag}\{m_1, m_1, m_1, \cdots, m_N, m_N, m_N\}$ is the $3N \times 3N$ mass matrix, $N$ is the number of atoms, $m_i$ is the mass of atom $i$, $X$ is the coordinate of all atoms, $U(X)$ is the potential, $g$ is the $m$-dimensional vector of constraints, $\lambda$ is the $m$ vector of Lagrange multipliers, and $m$ is the number of constraints. The underlying system of ordinary differential equations,

$$\ddot{X} = (I - M^{-1}B^T(BM^{-1}B^T)^{-1}B)M^{-1}F - M^{-1}B^T(BM^{-1}B^T)^{-1}\frac{dB}{dt}\dot{X}, \tag{1.2}$$

is equivalent to (1.1) provided that the matrix $BM^{-1}B^T$ is invertible, where $B = \partial g(X)/\partial X$ and $F = -\partial U(X)/\partial X$. If the initial values $X(0)$ and $\dot{X}(0)$ satisfy the constraints, then solutions of (1.2) will continue to satisfy the constraints. In practice, we can discretize (1.2) directly, but the numerical error leads to drifts of the constraints. This is why we prefer SHAKE or RATTLE which are direct discretizations of the equations (1.1).

In [27], Rychaert et al. proposed SHAKE discretization for (1.1) based on the leap-frog Verlet scheme,

$$\begin{cases} MV_{n+1/2} = MV_{n-1/2} + hF_n - hB_n^T\lambda_n, \\ X_{n+1} = X_n + hV_{n+1/2}, \\ g(X_{n+1}) = 0, \end{cases} \tag{1.3}$$

where $F_n = -\partial U(X_n)/\partial X$ and $B_n = \partial g(X_n)/\partial X$, $h$ is the size of the time-step, and $\{X_n, V_n\}$ are the coordinates and velocities of all atoms at step $n$. An alternative velocity-level formulation, RATTLE, was proposed by Andersen [1]:

$$\begin{cases} MV_{n+1/2} = MV_n + hF_n/2 - hB_n{}^T\lambda_n/2, \\ X_{n+1} = X_n + hV_{n+1/2}, \\ g(X_{n+1}) = 0, \\ MV_{n+1} = MV_{n+1/2} + hF_{n+1}/2 - hB_{n+1}{}^T\lambda^v_{n+1}/2, \\ B_{n+1}V_{n+1} = 0. \end{cases} \tag{1.4}$$