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BioVEC: A program for Biomolecule Visualization with Ellipsoidal Coarse-graining

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ABSTRACT

Biomolecule Visualization with Ellipsoidal Coarse-graining (BioVEC) is a tool for visualizing molecular dynamics simulation data while allowing coarse-grained residues to be rendered as ellipsoids. BioVEC reads in configuration files, which may be output from molecular dynamics simulations that include orientation output in either quaternion or ANISOU format, and can render frames of the trajectory in several common image formats for subsequent concatenation into a movie file. The BioVEC program is written in C++, uses the OpenGL API for rendering, and is open source. It is lightweight, allows for user-defined settings for and texture, and runs on either Windows or Linux platforms.

1. Introduction

The use of coarse-graining methods in biomolecular simulation is progressively increasing [1], mainly to circumvent the current time-scale problem that exists for all-atom molecular dynamics simulations, and to allow for the computational modeling of ever larger systems which address biologically relevant questions. However as the coarse-grained constituents encompass more atoms, the resulting residual objects become poorly approximated by spheres with corresponding isotropic potentials, while the steric character of the residues becomes more important. Such a scenario would exist for the coarse-graining of bases in DNA, or the coarse-graining of helices in a protein.

For these reasons, interest in ellipsoidal coarse-graining, perhaps the simplest non-spherical generalization, has recently increased [2–9]. Interest in industrial applications such as the manufacture of nanoparticle films has also motivated studies of ellipsoidal coarse-graining [10,11].

The molecular dynamics (MD) of rigid objects raises some new practical challenges, including a singularity-free representation of rigid body rotation [12–15] and corresponding energy conserving scheme for symplectic integration [16–18]. This is best done using quaternions [19,20], which MD simulation programs such as LAMMPS [7] currently allow one to employ.

Quite apart from the issues of coarse-graining and molecular dynamics, visualization tools for rendering thermal ellipsoids representing Debye–Waller factors have enjoyed a long and successful tradition [21]. However, in spite of widely used standards in crystallography, as well as the above-mentioned progress in coarse-graining and molecular dynamics of rigid bodies, to the authors' knowledge no currently available program allows for the straightforward visualization of the dynamical evolution of coarse-grained systems with ellipsoidal constituents. To facilitate our own analysis of such coarse-grained models, we have decided to develop our own program. The program is portable to either Windows or Linux systems, and could in principle be incorporated into many of the more versatile and widely used visualization programs such as VMD [22], Molmol [23], Molscript [24], PyMOL [25], Raster3D [26], Jmol [27], and Rasmol [28].

2. Methods

The program BioVEC presented in this paper, is a program to visualize the results of MD simulations of biomolecules that have been coarse-grained with ellipsoids. The functionality of BioVEC is simple and basic, as its purpose is not to compete with current molecular visualization packages but specifically to allow the scientist to visualize dynamical processes involving ellipsoidal coarse-graining. BioVEC automatically creates graphical images, which can be compiled to movie files in an external editor, such as Slide Show Movie Maker [29] (Windows) or MJPEG Tools [30] (*NIX). It is also possible for the user to manually step through the simulation, and to save the current view of the molecule to an image file in several formats, including png, bmp, and jpg. The representation used in BioVEC differs from techniques such as cartoon and ribbon representation, as these techniques aim to smooth out details, in, all-atom simulations for example. The aim

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of BioVEC is rather to show all the features of already coarse-grained simulation data.

BioVEC reads in molecular dynamics simulation data from a file containing the positions of the coarse-grained species and the orientations of the ellipsoids for all time steps in the molecular dynamics simulation. The input format for BioVEC is based on the output dump file format in LAMMPS [7], which is of the form:

```
species-no species-type position × 3 orientation × 4
```

for each time step. The program also reads in a file with information on the topology of the molecule, in order for the program to display bonds between the species. In the current version of the program, covalent bonds are not allowed to break or form between different time steps. The information in the topology file comes from the LAMMPS input file, and is of the form

```
bond-no bond-type 1st-species 2nd-species 1st-origin 2nd-orgin
```

where the bond goes from the `1st-origin` on the `1st-species` to the `2nd-origin` on the `2nd-species`, corresponding to the `species-no` in the simulation data file. Each ellipsoid can have an arbitrary number of bond origins, as specified in the input file. The `1st-origin` and `2nd-origin` entries in the topology file are optional if the species only have one bond origin each.

The user supplies the names of the simulation data and topology files in an input file with information about the coarse-graining of the system. This file should contain the number of coarse-grained species, the radii of the different ellipsoids and spheres, as well as the vector from the centre of mass of the ellipsoid to the location of the bond connecting the ellipsoidal residue to its covalently bonded partner. Spheres are treated as ellipsoids with all three radii equal. Information about the colouring and texture of the species is also entered into the input file.

The BioVEC program can also read and visualize ANISOU anisotropic temperature factor records in PDB standard form [31].

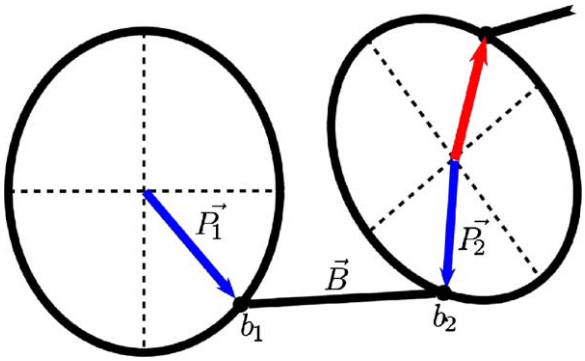

Fig. 1. Representation of the bond vectors. The bond $\vec{B}$ is formed between the points b_1 and b_2, given by the bond vectors $\vec{P}_1$ and $\vec{P}_2$. A second bond vector for the right ellipsoid is indicated by a red arrow. The bond vectors are given relative to the principal axis (dotted lines) of the ellipsoids.

2.1. Quaternions

Quaternions [19] are frequently used in computer graphics to represent rotations and orientation in 3-dimensional space. One of the main advantages of quaternions over other representations, such as Euler angles, is the absence of singularities in the quaternion representation.

A quaternion is a four-dimensional extension to the complex numbers,

$$\mathbf{q} = q_0\mathbf{u} + q_1\mathbf{i} + q_2\mathbf{j} + q_3\mathbf{k}, \tag{1}$$

where q_0, q_1, q_2, and q_3 are real numbers, and $\mathbf{u}$, $\mathbf{i}$, $\mathbf{j}$, and $\mathbf{k}$ are such that $\mathbf{i}^2 = \mathbf{j}^2 = \mathbf{k}^2 = \mathbf{ij}\,\mathbf{k} = -\mathbf{u}^2 = -1$, and $\mathbf{ij} = -\mathbf{ji} = \mathbf{k}$. Quaternions are often written in a more compact vector form,

$$\mathbf{q} = [q_0, q_1, q_2, q_3], \tag{2}$$

where the quantities q_0, q_1, q_2, and q_3 again are real numbers.

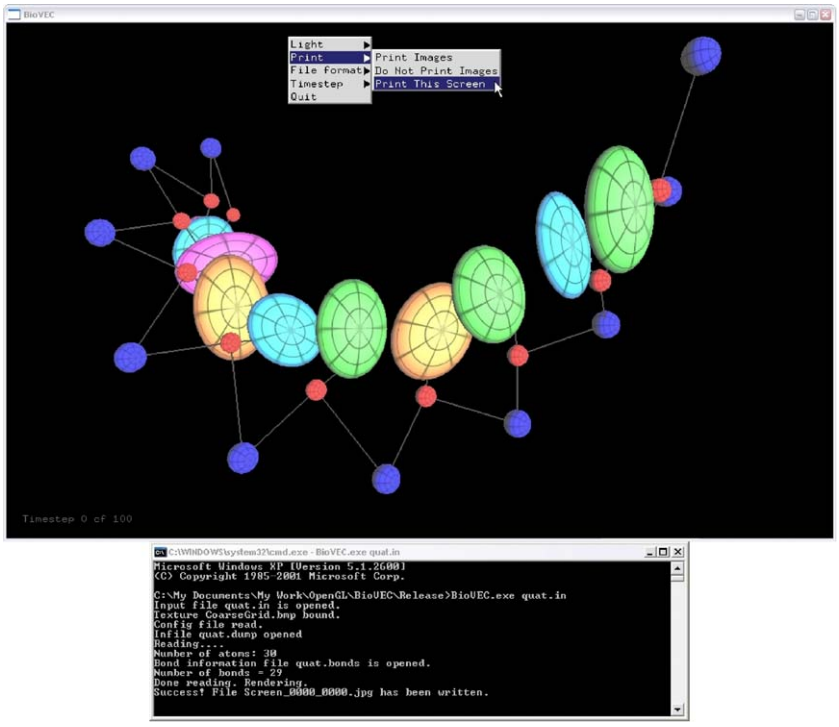

Fig. 2. View of the BioVEC interface, running on Windows XP.