BioVEC - README

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Abstract

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1 Copyright

2 Installation

2.1 Downloads

The BioVEC program can be downloaded from

http://www.phas.ubc.ca/~steve/BioVEC/

The download consists of a few separate packages: Precompiled Windows executable; the source code for compiling on either Windows or Linux; and a package containing a few examples of the needed input files. BioVEC also comes with a helper program for creating smoother animations from LAMMPS simulation data.

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2.2 Windows

2.2.1 Precompiled executable

The precompiled Windows version of BioVEC is installed by placing the executable and the dll-files in the same directory. In order to run, BioVEC requires dll:s from the DevIL library (`DevIL.dll`, `ILU.dll`, and `ILUT.dll`), and the GNU Scientific Library (`libgsl.dll` and `libgslcblas.dll`).

The Microsoft Visual C++ Runtime Files are also needed in order to run the program. On some computers only the `msvcr80.dll` file is needed. It can be downloaded from

http://www.phas.ubc.ca/~steve/BioVEC/Files/msvcr80.zip

Just unzip the msvcr80.dll file into the BioVEC directory with a zip tool of your choice.

If errors such as "The application failed to initialize properly (0xc0150002)", or "This application has failed to start because MSVC***.dll was not found", please install either the .NET framework, or the Microsoft Visual C++ 2008 Redistributable Package. Hopefully all these problems will be solved in future releases of BioVEC.

2.2.2 Compiling from source

In order to compile from source, the SDK versions of DevIL, GLS, and OpenGLUT needs to be installed. The precompiled DevIL SKD, or the DevIL source code, can be downloaded from

http://openil.sourceforge.net.

A precompiled Windows version, or the source code, of OpenGLUT can be downloaded from

http://openglut.sourceforge.net

The GNU Scientific Library can be downloaded from

http://www.gnu.org/software/gsl/.

The BioVEC source comes with Visual C++ 2008 and Dev-C++ project files for easy setup and compilation on Windows. BioVEC needs to be linked to the OpenGL32, GLU32, OpenGLUT, GLS, GSLCBLAS, IL, ILU, and ILUT libraries. It is recommended that the OpenGLUT library is used, even though most features of BioVEC will work with the FreeGLUT or GLUT libraries.

2.3 Linux

2.3.1 Compiling from source

In order to compile from source, the DevIL, GSL, and OpenGLUT libraries needs to be installed on the system. These libraries can either be downloaded and compiled from source, or downloaded from the system package manager of the Linux system. Make sure that both the runtime support and the development files are installed for all packages. It is recommended that the OpenGLUT

library is used, even though most features of BioVEC will work with the FreeGLUT or GLUT libraries.

The DevIL library can be downloaded from

http://openil.sourceforge.net

and the OpenGLUT library can be downloaded from

http://openglut.sourceforge.net.

The GNU Scientific Library can be downloaded from

http://www.gnu.org/software/gsl.

Please refer to their respective manuals for instructions on compilation and installation.

After the libraries are installed, it might be a good idea to do

```
sudo ldconfig
```

to make sure that all libraries are properly linked. It might also be necessary to edit the

```
/usr/local/include/IL/ilut.h
```

file. Insert a new line before line 128:

```
#define ILUT_USE_OPENGL.
```

After the needed packages are installed, the BioVEC program is compiled with, for example, GCC:

```
gcc -Wall -o BioVEC.exe
   -lglut -lGL -lGLU  -lIL -lILU -lILUT -lgsl -gslcblas -lm
   BioVEC.cpp
```

3 BioVEC Manual

3.1 Running the program

The operation and usage of BioVEC is very simple and intuitive. The program can be run from a command prompt or an Explorer window. BioVEC is started by typing (Windows)

```
BioVEC <inputfile.in>
```

or (Linux)

```
./BioVEC <inputfile.in>
```

in the command prompt. If no input file is specified, or the program is started from an Explorer window, BioVEC will ask the user supply one in the command prompt. The input files should be given with a path relative to the executable, or with an absolute path.

3.2 Input files

BioVEC needs three files to visualize the molecular data: A file containing simulation data, an optional file containing information about the topology of the molecule, and an input file created by the user, containing information about the coarse-graining of the system, as well as information about colors and similar visual information.

Currently there are few checks of the consistency of the input files. If the files are not correctly formatted, the program might crash without explanation. Care should be taken when creating the input files.

3.2.1 Simulation data file

The simulation data file is taken from the output format of the LAMMPS molecular dynamics package. The orientation of the ellipsoids are given as quaternions in the vector format. No editing of the LAMMPS dump files is (or should be) needed. The format of the simulation data in the dump file is

```
atomno atomtype posX posY posZ q0 q1 q2 q3
```

where `atomno` is the number of the species, `atomtype` defines the type of coarse-graining of the species as specified in the simulation, `posX posY posZ` are the Cartesian coordinates of the species, and `q0 q1 q2 q3` is the orientation of the species, given in quaternions. A short example of a simulation data file is given below:

```
ITEM: TIMESTEP
0
ITEM: NUMBER OF ATOMS
6
ITEM: BOX BOUNDS
-1500 1500
-1500 1500
-1500 1500
ITEM: ATOMS
1 1 2.056 5.582 -0.099 1 0 0 0
2 2 -0.500 9.684 1.828 1 0 0 0
3 3 0.571 2.204 0.185 0.4946 0 0 0.8691
4 1 -1.335 5.706 3.687 1 0 0 0
5 2 -6.103 7.464 5.078 1 0 0 0
6 3 -1.818 2.658 3.754 0.9243 8.80e-11 1.29e-10 0.3817
ITEM: TIMESTEP
1
ITEM: NUMBER OF ATOMS
6
ITEM: BOX BOUNDS
-1500 1500
-1500 1500
-1500 1500
ITEM: ATOMS
1 1  1.917 5.621 -0.011 1 0 0 0
2 2 -0.686 9.819  1.830 1 0 0 0
3 3  0.562 2.181  0.156 0.477 0.0037 -0.0153 0.8783
4 1 -1.350 5.752  3.622 1 0 0 0
5 2 -6.393 7.420  4.959 1 0 0 0
6 3 -1.772 2.696  3.699 0.919 -0.0202 -0.0306 0.3913
```

Not all the information is used by BioVEC, such as the box bounds. This is to simplify usage of the LAMMPS output files, without the need to edit them.

3.2.2 ANISOU data file

The BioVEC program can also read and visualize ANISOU anisotropic temperature factor records in PDB standard form The format of the ANISOU data is described at http://www.wwpdb.org/documentation/format23/sect9.html#ANISOU . The keyword `CRYS` (from the PDB entry `CRYST1`) is used to separate different time steps. The PDB file must always contain the keyword `CRYS`, even if the file contains only one time step.

3.2.3 Topology file

The topology file contains information about which species is bonded to which. If a topology file is supplied by the user, BioVEC utilizes this information to draw bonds between species. The information in the topology file is given by the input file to the LAMMPS molecular dynamics simulation, after the keyword `bonds`. This information can be used in the topology file. The format of the topology file is

`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. If no bond origins are specified, BioVEC assumes the bond goes from the first origin on both species. The information in `bondno` and `bondtype` is not used by BioVEC. An example of a topology file with multiple bond origins is given below:

```
bonds

1 2 1 3 1 2
2 5 1 2 1 1
3 6 2 4
4 1 4 6 2 1
5 5 4 5
```

3.2.4 Input file

The input file is created by the user. This file should contain the names of the simulation data file, and the topology file. It also contains information on the number of different coarse-grained species, the ellipsoid-radii, and the bond vectors of the different coarse-grained species. Furthermore it should contain information about the colors of the different coarse-grained species, background color of the screen, and the name of any texture file used when

rendering. Comments in the input file are indicated with a number sign (#) at the beginning of the line. Blank lines are ignored. The filenames of the data, topology, and other files should be given with a path relative to the executable, or with an absolute path. No path is needed if the files are in the same directory as the executable.

Commands The BioVEC input consists of commands with corresponding arguments. Some keywords are optional, and generally the order of the commands is not important, with a few exceptions, as outlined below.

- `dumpfile` — The file containing the LAMMPS simulation data.
- `anisoufile` — The file containing ANISOU data. The `dumpfile` and the `anisoufile` commands are mutually exclusive. The `anisoufile` command will create half radii, bond vectors, and colours for each ellipsoid. The number of species will be equal to the number of atoms in the file. Thus, the commands `species`, `bond_vector`, `half_radii`, and `color` are ignored when `anisoufile` is specified.
- `bondfile` — The file containing information about the bonds. Optional, if no bonds are to be drawn.
- `solid_bonds` — Specify if bonds should be drawn as solid cylinders. Followed by the thickness of the bond. Optional, if the bonds should be drawn as lines, for faster rendering.
- `species` — The number of different species in the simulation. Ignored if `anisoufile` is used.
- `bond_vector` — Specifies the vectors from which the bonds should be drawn. The `bond_vector` command must come after the `species` command. Each ellipsoid can have any number of bond vectors. The command is followed (on the same line) by the species number, the bond origin number, and the x, y, z components of the bond vector, relative to the principal axis of the ellipsoid. The bond vectors are given by the same vectors as were used in the molecular simulation. Ignored if `anisoufile` is used.
- `half_radii` — The half-radii of the ellipsoids. The command is followed by the species number and the three half-radii. The `half_radii` command must come after the `species` command. Ignored if `anisoufile` is used.
- `color` — The colours of the ellipsoids. The command is followed by the species number and the colour in RGB format. The `color` command must come after the `species` command. Ignored if `anisoufile` is used.
- `background` — The background color. The command is followed by color in RGB format.

- `texture` — The name of the image file for adding texture to the ellipsoids. All ellipsoids are given the same texture, blended with the unique color of the species. Optional, if no texture is to be used.
- `texture_bonds` —The name of the image file for adding texture to the bonds. Optional, if no texture is to be used.

An example of an input file is given below:

```
# This is an example of BioVEC input

# The file with simulation data
dumpfile  ex.dump

# A file with ANISOU data. Not used in this example
#anisoufile ex.anisou.pdb

# The file with the topology
bondfile  ex.bonds

# This example have three species
species 3
half_radii 1 0.7    0.7    0.7             P
half_radii 2 0.5    0.5    0.5             S
half_radii 3 2.3127 1.7950 0.39028         C

# One bond origin per ellipsoid in this example
bond_vector 1 1  0.0      0.0      0.0      P
bond_vector 2 1  0.0      0.0      0.0      S
bond_vector 3 1 -2.04544  0.72828  0.00648  C
# If the third ellipsoid would have a second bond origin
# it would look like
# bond_vector 3 2 1.50411 -0.85552 -0.54021   C

# Solid bonds with a thickness of 0.15
solid_bonds 0.15
color 1 0.25   0.95   0.25                 C
color 2 0.1    0.6    1.0                  P
color 3 0.05   0.05   1.0                  S
background 1.0 1.0 1.0
texture CoarseGrid.bmp
#No textures on the bonds in this example
#texture_bonds CoarseGrid.bmp
```

More examples of input files can be downloaded from the BioVEC website http://www.phas.ubc.ca/∼steve/BioVEC/.

3.3 Using the program

BioVEC has two main parts – the main rendering window; and the command prompt. The user will mainly interact with the main window, occasionally entering information in the command prompt. The interaction with the program is done through mouse movement (left-click or mouse wheel), a mouse menu (right-click) and keyboard commands.

3.3.1 Mouse menu

BioVEC gives the option to perform some basic tasks through a right-click mouse menu. The most crucial item in this menu is the `Print` selection. By choosing the option `Print Images`, the animation will print the view to file as the molecular simulation data is displayed. The file name of the created image files will be

`<infile>_<frame no>.<format>`.

The format of the file is chosen in the `File format` submenu. The default format is JPEG.

If the item `Print This Screen` is chosen in the `Print` selection, or the Enter key is pressed, the current view is saved to file. The name of this file will be

`Screen_<screen no>_<frame no>.<format>`,

where `<screen no>` is a count of the number of images that has been saved, and `<frame no>` is the current time step of the simulation.

The `Light` item in the menu lets the user choose between `Stationary Light`, where the light sources are stationary with respect to the screen, or `Moving Light`, where the light sources are fixed with respect to the molecule, and follow its rotations and movements.

The `Timestep` item in the menu hides or shows the time step in the simulation, shown in the .

3.3.2 Mouse movement

The view can be rotated in the x and y axis by left-click and moving the mouse. By holding the `Shift` key the view is rotated around the z-axis. The view is zoomed by holding the `Ctrl` key.

3.3.3 Keyboard commands

- Movement

  Rotation: a, s, d, q, w, e

  Translation: $\leftarrow$, $\rightarrow$, $\uparrow$, $\downarrow$

  Zoom: + (or =), - (or _), mouse wheel

- Animation

  Start / pause animation: Space

Previous frame: p

Next frame: n

Go back a tenth of the simulation: P

Go forward a tenth of the simulation: N

Go to frame: G (enter frame number in command prompt)

Go to first frame: r

Go to last frame: f

- File handling

  Load new input file: L (enter file name in command prompt)

- Graphics

  Print current view to file: Enter

  Hide / show timestep text: t

- Quit

  Quit: Esc, Q

4 Helper programs

4.1 Smooth

BioVEC comes with a program called Smooth. This program calculates a weighted average of the ellipsoidal coordinates over consecutive time steps. These averaged coordinates are output to a new data file for BioVEC. This is useful for creating smoother movements of the ellipsoids during the animation.

5 Movie Software

BioVEC does not come with the ability to compile images to movies. Do to this, external programs are needed. There are probably several options for most systems, but here are two recommendations for Windows and Linux.

5.1 Slide Show Movie Maker

Slide Show Movie Maker (http://homepage.mac.com/joernthiemann/tools/SSMM/index.html) is a is a free Windows program that can create an AVI-file from a series of .bmp or .jpg images. The program has not been updated in quite a while, but still works well, and it's easy to work with.

5.2 MJPEG Tools

The package MJPEG Tools (http://mjpeg.sourceforge.net) can create movie files from a series of .jpg images. As always with Linux, it has a steep learning curve, but the very comprehensive *MJPEG HOWTO - An introduction to the MJPEG-tools* (http://sourceforge.net/docman/display_doc.php?docid=3456&group_id=5776) should get you started in no time.

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