

Brownmove-Read-Me

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Overview

Brownmove is a simulation package for Brownian Dynamics (BD) and Langevin Dynamics (LD) simulations of many-particle systems, which handles variable numbers of rigid and bead-spring particles with electrostatic, van-der-Waals, hydrodynamic, and external interactions plus elastic and hydrogen bonds. The particles, called proteins, are assembled hierarchically from one or more spherical shapes representing the different types of interactions. In addition to these moving proteins, the simulation box can be bounded with fixed walls of various types (reflecting, periodic, interfaces to reservoirs, or walls with physical interactions), which may also contain fixed structures. Protein and wall definitions can be set up at runtime from configuration files.

The brownmove package was designed and started in 2003 by Tihamér Geyer, Jörg Niggemann, and Christian Gorba with the aim to set up a general purpose simulation library which would be easily extensible for new interactions, physical objects, or propagation schemes. To achieve this modularity, an object-oriented approach was taken using C++ for the general structure and plain C for the more time-critical computation parts. Most of the code filling up this concept (and later changes to it) was written 2003-2010 by Tihamér Geyer. Contributions to the hydrodynamic interactions are from 2008 by Uwe Winter.

The underlying concept is that a physical particle, which is called a "Protein" in brownmove and can be, e.g., a polymer or a biological protein, is constructed from rigid subunits, the "Gestalt" objects. Each of these Gestalt objects may contain an EStatShape, a vdWShape, a BondShape, and an HiShape. These shape objects are responsible for their respective type of interaction.

Getting Help

Contact Information

To obtain the brownmove-code, for bug reports, open questions, or feature requests, please contact the main author Tihamér Geyer, preferred via email at tihamer.geyer@bioinformatik.uni-saarland.de. Further contact information can be obtained at <http://gepard.bioinformatik.uni-saarland.de/people/geyer>.

Documentation

Beyond this ReadMe file there is an explanation of the structure of the setup files in the "BrownDef-Doku". An introduction with some example scenarios can be found in the Tutorials folder. From the code itself, a

comprehensive documentation can be created via doxygen ("make doc"). Start reading by opening the file "doc/html/index.html" in your favourite web browser.

Obtaining and Installation

Licensing

The brownmove package is free for private or academic use. This means that the author retains the copyright, but you are free to use and modify the code for yourself or your non-commercial research projects. However, modifications must be clearly marked and documented and the reference to the original authors may not be deleted, when you redistribute the code or parts thereof. The brownmove code comes with absolutely no warranty, you are using it on your own risk.

If you want to use the code in a commercial product, please contact the author directly.

Building and using "brownmove"

To build and run the brownmove package you need an Ansi C++ compiler with the standard template library (STL) and the Gnu Scientific Library (GSL) available at <http://www.gnu.org/software/gsl/>. The code was developed and tested on Linux (RedHat 7.3 and OpenSUSE 10.0) and Mac OSX (10.3 to 10.5) systems and compiles with g++ versions 2.95 to 4.2.

From the GSL only the random number generation is used — which means that you can easily replace the GSL random numbers by any other RNG. On current Linux systems, the GSL is usually installed by default, while on MacOSX the GSL from the fink package was used (but any other variant should work, too).

Building the basic brownmove application is straightforward. The code is distributed as a gzip-compressed tar-archive. Thus, unpack:

```
$> tar xvzf brownmove.tgz,  
$> cd brownmove
```

Depending on your system you should check for the library paths in the file config.mk (defaults are for building on MacOSX with the fink-GSL). Then

```
$> make  
$> make doc
```

will build you the executable and the doxygen-documentation (start from doc/html/index.html).

If you are using brownmove for the first time, you can get an overview through the Tutorials.