JBFM 1.4

Documentation

applet written by Ron Dockhorn[1] (**dockhorn@ipfdd.de**)
documentation written by Max Hoffmann[1] (**hoffmann-max@ipfdd.de**)

[1] **Leibniz-Institut für Polymerforschung Dresden e.V.**

Model

The bond fluctuation model (BFM) used in this applet was first introduced by Carmesin and Kremer in 1988 in order to simulate conformations and dynamics of polymer systems.

In this model the monomers are represented by cubes on a regular cubic lattice with each cube occupying eight lattice positions. Each lattice position can only be occupied by one monomer in order to model excluded volume. The monomers are connected by a bond vector, which is taken from a set of typically 108 bond vectors. There are different definitions for this vector set. As example we provide the one used in the applet: The allowed bond vectors are made up from six base vectors, using permutation and sign variation of the three vector components in each direction:

$$\boldsymbol{B} = P_{\pm}\begin{pmatrix} 2 \\ 0 \\ 0 \end{pmatrix} \cup P_{\pm}\begin{pmatrix} 2 \\ 1 \\ 0 \end{pmatrix} \cup P_{\pm}\begin{pmatrix} 2 \\ 1 \\ 1 \end{pmatrix} \cup P_{\pm}\begin{pmatrix} 2 \\ 2 \\ 1 \end{pmatrix} \cup P_{\pm}\begin{pmatrix} 3 \\ 0 \\ 0 \end{pmatrix} \cup P_{\pm}\begin{pmatrix} 3 \\ 1 \\ 0 \end{pmatrix}$$

The combination of bond vector set and monomer shape in this model ensures cut avoidance of strands (polymer strands cannot cross each other) without explicit test of the local topology.

A single attempt to move one monomer consists of the following steps which are standard for Monte Carlo methods:

1. Select a monomer m and a direction d ($P_{\pm}(1,0,0)$) randomly
2. Check list of conditions (see below)
3. If all conditions are fulfilled, perform move

The conditions to perform a move can be subdivided into mandatory and optional ones.

Mandatory conditions:

1. Four lattice sites next monomer m in the direction d are empty
2. The move does not lead to bonds that are not contained in the bond vector set.

Optional conditions: If the move leads to an energetic difference ΔU for example due to an electric field or an adsorbing force on the walls. In this case a Metropolis algorithm is applied: The Metroplis rate p_m which is defined as

$$p_M = e^{-\frac{\Delta U}{k_B T}}$$

is compared to a random number r from the interval [0,1). If the Metropolis rate is smaller than r the move is rejected, otherwise it is accepted.

The number of Monte Carlo steps of the total system is defined as:

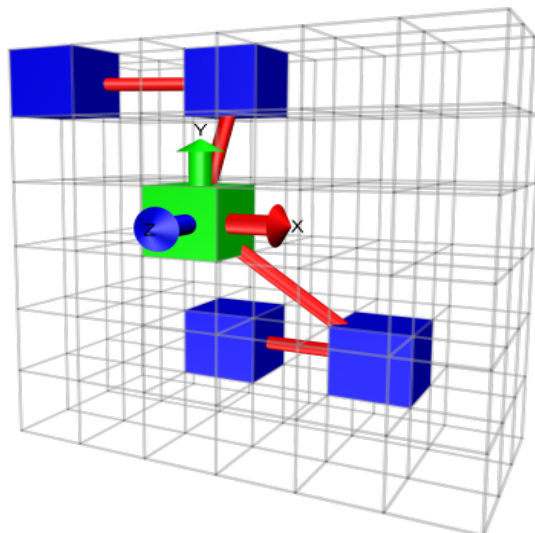$$\#MCS = \frac{\#\,attempts}{\#\,monomers}$$

Figure 1: Bond Fluctuation Model

Applet

Window "BFM-Model" (standard graphics engine)
or "BFM3D" (Java3D graphics engine)

The *simulation cube* can be *rotated* by moving the mouse while clicking the left mouse button. Moving the mouse while clicking the right mouse button *moves the cube*. *Zooming in or out* is possible by either using the scrollwheel or the "+" and "−" keys on your keyboard (if you are using Java3D the "+" and "−" keys only set the zoom speed; to actually zoom in or out one has to use the arrow-keys). Pressing the "r" key will *reset the viewpoint* (feature not available when using Java3D).

Menu bar[1]

Select *"file" menu* to take a screenshot or (if you have POV-Ray[2] installed) create a rendered picture of the current configuration. The screenshot and the rendered picture (named screen.png and rendered.png) will be saved in your home directory (on Linux and Mac) or in C:/Documents and Settings/*user* (on Windows). In addition a PovRay Script will be created.

The simulation speed can be changed using the *"simulation speed" menu*.

The size, shape, and colour of the monomers as well as the background colour are modified using the *"view" menu*. Depending on the polymer architecture the colours of the monomers represent different features for example the center monomer. One can also enable smoothing (which means averaging the visualisation over multiple configurations). The smoothing rate can be set in the appropriate submenu.

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1 Please note that most of the following features are only available when using Java3D, also note that if running Mac OS X the menus are positoned in the main system menu bar.

2 POV-Ray – The Persistence of Vision Raytracer: http://www.povray.org

Window "JBFM"

A click on the *"start simulation"-button* will start and stop the simulation.

The *"BFM"-button* will reopen the window "BFM-Model" or "BFM3D" (depending on the graphics engine used).

Clicking the *"radius of gyration"-button* will open a new window, in which the components of the radius of gyration you want to look at can be chosen. Clicking the buttons will open the appropriate graphs. The radius of gyration is calculated by

$$R_g^2 = \frac{1}{N} \sum_{i=1}^{N} (\vec{r}_i - \vec{r}_{CM})^2 = \frac{1}{N} \sum_{i=1}^{N} (\Delta x^2 + \Delta y^2 + \Delta z^2)$$

whereby $\vec{r}_{CM}$ is the position of the center of mass and $\vec{r}_i$ the position of monomer i.

The *"end-to-end distance"-button* opens a graph displaying the distance from the first to the last monomer. The end-to-end-distance is calculated by

$$R_{E2E} = |\vec{r}_N - \vec{r}_1|$$

The *"adsorption parameter"-button* will open a window in which it can be toggled whether the walls should adsorb monomers or not and if yes to what degree by setting the parameter a belonging to the Metropolis rate p_m for adsorbing one monomer (see optional conditions in the model section):

$$p_M = e^{-a}$$

A click on the "order parameter"-button will open a graph displaying the total degree of adsorption (which is calculated as the number of monomers touching a wall divided by the total number of monomers) and the degree of adsorption for the particular directions.

Using the *"electric field"-button* an electric field can be applied. The strength and direction can be chosen in the newly opened window by modifying the Metropolis rate:

$$\Delta U = -q\, \vec{E}\, \Delta \vec{r}$$

$$p_M = \mathrm{e}^{-\frac{\Delta U}{k_B T}} = \mathrm{e}^{-\frac{f}{k_B T}}$$

whereby f is the parameter that can be changed in the applet.

To notice an influence of the electric field, the charge of some monomers has to be non-zero; charge of monomers is adjusted via the "change charges"-button.

With the *"boundary condition"-button* periodic boundary conditions can be set (for each direction separately).

A click on the *"single monomer move"-checkbox* (only possible while simulation is stopped) will open a new window which gives a detailed view of each attempted monomer movement and whether it is accepted or not (and if not for what reason). The speed of this single monomer movement simulation can be changed by using the scrollbar below the checkbox.

The *"statistics of Rg²"*, the *"statistics of R_end"* and the *"statistics of adsorption"-buttons* open new windows with the statistical evaluation of the respective values (which can be started and stopped with the "start" and "stop"-buttons at the bottom). The graph of the running average can also be viewed.

The *"new init"-button* resets the simulation.

Saving your current simulation can be done by clicking on the *"save coordinates"-button*. Please use the "Save"-button in the new window (due to an Java-AWT issue the use of the "Enter"-key will cause problems). Previously saved coordinates can be loaded with the *"load coordinates"-button*.

The *"setup"-button* opens a new window in which one can change the lattice size and also choose between polymers of different architecture and environment, for example star and ring polymers and polymer brushes. Please note that some of

the above mentioned options and graphs may not be available for all polymer types.

The *"Info"-button* will open the credits and the *"Quit"-button* terminates the applet.

If you have questions or comments about the applet or this documentation please send an e-mail to the respective author.