Brownian dynamics simulator for diblock copolymers and homopolymers
version 0.1.3
15 September 2020

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Table of Contents

1 Introduction

Block copolymer melts or polymer blends form various phase separation structures [Statistical Physics of Polymers: An Introduction]. Although static properties of phase separation structures are well understood by such as the Flory-Huggins theory or the self consistent field theory [Statistical Physics of Polymers: An Introduction], dynamic properties of these phase separated structures [The Structure and Rheology of Complex Fluids] are not so well understood.

Recently, a highly coarse-grained theory which models a polymer chain as an effective colloid particle is proposed [Louis-Bolhuis-Hansen-Meijer-2000]. The model is generalized to diblock copolymers [Addison-Hansen-Krakoviack-Louis-2005, Pierleoni-Addison-Hansen-Krakoviack-2006,Eurich-Karatchentsev-Baschnagel-Dieterich-Maass-2007] and thus it is possible to perform highly coarse-grained simulations for diblock copolymers or homopolymers. For example, by using the soft colloid model, micellar formation dynamics in diblock copolymer solutions [Cass-Heyes-English-2007,Cass-Heyes-Blanchard-English-2007] or rheology of lamellar structures [Uneyama-2009] can be simulated with small computational costs.

Dynamics simulations can be used to investigate the dynamic properties such as structure formation dynamics or rheology. `spreads` is a Brwonian dynamics simulator for diblock copolymers and homopolymers based on the soft particle model. It can handle blends of symmetric diblock copolymers and homopolymers. Because the soft particle model is a highly coarse-grained particle model, `spreads` enables numerically efficient simulations. Several interesting dynamics such as microphase separation under shear flow or viscoelastic properties can be studied with relatively small computational costs.

2 Installation of spreads

2.1 To Download the Latest Version of spreads

The latest version of spreads is available at the following URL. Access the web page and download the latest version via HTTP (FTP is not supported).

http://polymer-physics.jp/uneyama/spreads.html

2.2 Build and Install from the source

You can build and install spreads if the binary package of your system is not available, or if you want to customize the spreads. The source package of spreads is using GNU Automake and GNU Autoconf, therefore you can build and install spreads just like usual free software. Note that spreads requires zlib (http://www.zlib.net/) and Lua (http://www.lua.org/). You have to install them before building spreads.

The source package is distributed as the gzipped tar archive file, thus first extract it. To extract the archive, do

```
$ zcat spreads-0.1.3.tar.gz | tar xvf -
```

or if you are using GNU tar, do

```
$ tar zxvf spreads-0.1.3.tar.gz
```

Then the source directory will extracted. Move to the directory spreads-0.1.3.

```
$ cd spreads-0.1.3
```

To build spreads, do configure-make-make install just like other free software.

```
$ ./configure
$ make
$ su -
# make install
```

Now spreads will be installed under /usr/local of your system. If you have an error messages and the compilation is aborted, some commands or libraries may be missing. Install the required packages and retry.

If you want to customize or tune spreads,

```
$ ./configure --help
```

will help you.

2.3 Build and Install as the RPM package (for Linux)

The RPM package for your Linux system can be built from the source RPM (SRPM) package.Make sure that the headers and libraries and headers of zlib and lua is already installed to your system. If they are not installed, first you have to install them (zlib, zlib-devel,lua, and lua-devel). Of course you need standard development tools such as C compiler (gcc) or Make (make).

If you are using old system (rpm compatible with RedHat 7.3 or older), use the rpm command to build it.

```
# rpm --rebuild spreads-0.1.3-1.src.rpm
```

If you are using new system (`rpm` compatible with RedHat 8.0 or newer), use `rpmbuild` instead of `rpm`.

```
# rpmbuild --rebuild spreads-0.1.3-1.src.rpm
```

Now the binary RPM package for your system is stored in the directory which is shown in the output message of `rpm` or `rpmbuild`. Install it by `rpm`, for example, if you are using RedHat Linux or Fedora Core on a PC (or i386 compatible computer), like the following.

```
# rpm -Uvh /usr/src/redhat/RPMS/i386/spreads-0.1.3-1.i386.rpm
```

2.4 Compilation with Intel C++ Compiler (`icc`)

You may want to compile `spreads` Intel C++ Compiler (`icc`). `icc` is mostly compatible GNU C Compiler (`gcc`) and thus you can compiler `spreads` with `icc` easily. But the optimization flag `-ipo` will cause troubles when compiling `spreads`. Also note that the flag `-ipo` is automatically enabled if you set the optimization flag `-fast` or if you using `icc` version 9.0 or later.

There are two way to avoid troubles with the flag `-ipo`. One way is to add the flag `-ipo_obj`. This means, to run `configure` like

```
$ ./configure CC=icc CFLAGS='-O3 -ipo -ipo_obj'
```

(Here note that, this method can be used only for `icc` version 8. If you are using `icc` version 9, you should use the following method.) Another way is to use `xiar`,`xild` instead of `ar`,`ld`. In this case, the additional flag `-ipo_obj` is not needed.

```
$ ./configure CC=icc CFLAGS='-O3 -ipo'
$ make AR=xiar LD=xild
```

See the manual of Intel C++ Compiler for more information.

3 Invoking spreads

The format for running the `spreads` program is:

```
$ spreads option ... input
```

input is the input file for `spreads`. If no input file is specified, `spreads` will read the default input file `spreadsin.lua`.

`spreads` supports the following options:

`--input=`*input*
`-i` *input*
: Read the parameters for simulation from the input file *input*. If no input file is specified, spreads will read the input file named `spreadsin.lua`.

`--position=`*position*
`-p` *position*
: Read the initial positions of the particles from the file *position*. The position input file *position* must be the gzipped plain text. You can create one easily by using `gzip`. By default, spreads set the positions randomly.

`--help`
`-h`
: Show summary of options.

`--version`
`-v`
: Show version of program.

4 Tutorial

4.1 Simple Example

Here are a simple examples how to use `spreads` (the input file and some scripts for visualization can be found in the directory `examples/`). But first you have to install the `spreads` to your system. If `spreads` is not installed to your system, see the 'Install `spreads`' section. We starts from the microphase separation dynamics of a diblock copolymer melt. The input file is distributed with the source code or binary of `spreads`. To run this example, move to the directory `examples/ab_melt_3d/` and just type `spreads`

```
$ spreads
```

`spreads` will output some information about the simulation, and starts the simulation. The simulation will end in several hours. You can find output files.

4.2 Visualize Output Data

The output file of `spreads` is gzipped plain text and the OpenDX (http://www.opendx.org/) data format. If you have OpenDX, you can visualize it directly. The gzipped plain text is more portable and can be handled by most of the plotting / visualizing applications. Most of applications cannot handle the gzipped text directly, we have to decompress it. There are two way to do it. The first way is to use `gunzip` and then plot the decompressed data.

```
$ gunzip position.dat.gz
```

The second way is to use `zcat` and pipe.

```
$ zcat position.dat.gz | program
```

where `program` reads the input data from `stdin`. The result is just the same as the first way.

4.3 Changing Input File

The input file is the Lua script which sets the parameters needed for the DF simulation. The following is the input file used in the previous section.

```
condition =
{
    save_position_sequential = true,
    save_stress_sequential = true,
    save_energy_sequential = false,
    save_geometry_sequential = false,
    save_dx_sequential = true,
    seed = 11583192,

    apply_shear = false,

    iteration_max = 5000,
    interval = 50,
    dt = 0.02,
    omega = 0.0,
```

```
    kappa = 0.0
}

file =
{
    position_output = "position.dat.gz",
    stress_output = "stress.dat",
    energy_output = "energy.dat",
    geometry_output = "geometry.dat",
    dx_output = "spreadsout.dx",

    position_template = "position.%d.dat.gz",
    dx_template = "spreadsout.%d.dx"
}

geometry =
{
    dimension = 3,

    l = {16, 16, 16}
}

blend =
{
    polymer = {"AB_diblock"},
    number = {2048}
}

monomer =
{
    name = {"A", "B"},
    epsilon = {{30, 40},
               {0,  30}}
}

AB_diblock =
{
    monomer = {"A", "B"}
}
```

There are many parameters required by `spreads`. The detail of the input file will be expressed in the section 'Input File Format'.

Here we modify this input file simply. The first example is to change the size and dimension(s) of the simulations box. This can be done by changing the `geometry` in the input file. Change the `geometry` in the input file as follows.

```
geometry =
{
```

```
    dimension = 2,

    l = {64, 64}
}
```

`dimension` means the dimension(s) of the system. `l` means the size of the simulation box. Thus the parameters shown above mean the 2 dimensional with the size 16 times 16.

The second example is to change the polymers used in the simulation. This needs more complicated changes. The change will be as follows.

```
blend =
{
    polymer = {"A_homo", "B_homo"},
    number = {2048, 2048}
}

A_homo =
{
    monomer = {"A"}
}

B_homo =
{
    monomer = {"B"}
}
```

`blend` is changed to simulate the blend of A homopolymer / B homopolymer. The polymer species which the blend is consists on are listed in `polymer`. The numbers of each polymer species are specified by `number`. The A homopolymer `A_homo` and the B homopolymer `B_homo` is defined as well (the `AB_diblock` is no longer needed and can be deleted because now it is not used). `monomer` is the monomer species.

4.4 Notes on Input File

4.4.1 Boolean Variables

There are many boolean variables (of which value is `true` or `false`) in the input file for `spreads`. However it may seem verbous to write many boolean values (especially for large adjacency matrices). In such situations one can use `1` and `0` instead of `true` and `false`. `spreads` automatically converts `1` and `0` into boolean values, `true` and `false`, for the boolean variables. (Strictly speaking, number value `0` corresponds to `false` and non-zero numbers, including `1`, correspond to `true`. This is just the same as the standard C mannar.)

4.4.2 Symmetric Matrices

The effective interaction parameter matrix, `monomer.epsilon` are symmteric. Thus we don't need to set all the elements in these matrices. In the input file for `spreads`, the interaction parameter matrice is required to set their upper triangular part. `spreads` automatically fill the lower triangular part by copying the values of upper triangular elements. (See examples in previous sections.)

5 Reporting Bugs

Currently, the error handling routines in `spreads` is not complete and therefore `spreads` may suddenly stops if some input error or calculation error is caused.

If you find a bug in `spreads`, please send electronic mail to uneyama@mp.pse.nagoya-u.ac.jp. Include the version number, which you can find by running `spreads --version`. Also include in your message the output that the program produced and the output you expected.

If you have other questions, comments or suggestions about `spreads`, contact the author via electronic mail to uneyama@mp.pse.nagoya-u.ac.jp. The author will try to help you out, although he may not have time to fix your problems.

6 Input File Format

In this section, the input file format for `spreads` is expressed. The input file is the Lua script which sets the parameters. The parameters are set as the table variables.

6.1 Simulation Condition

The simulation condition is set as the table `condition`. The following elements are required.

`condition.save_position_sequential`
(*boolean* or *number*)

Whether to save the particle positions or not. If `condition.save_position_sequential` is set to `true`, `spreads` saves the positions every `condition.interval` steps. The output file name is generated from `file.positions_template`. If it is set to `false`, `spreads` saves positions to the output file named `file.positions_output` every `condition.interval` steps (in other words, the output file is overwritten). The behavior is the same for following items.

`condition.save_stress_sequential`
(*boolean* or *number*)

Whether to save the stress tensor sequentially or not. See `condition.save_position_sequential` for detail.

`condition.save_energy_sequential`
(*boolean* or *number*)

Whether to save the energy sequentially or not. The energy output routime is not implemented yet and currently this item has no meaning. See `condition.save_position_sequential` for detail.

`condition.save_geometry_sequential`
(*boolean* or *number*)

Whether to save the geometry field sequentially or not. See `condition.save_position_sequential` for detail.

`condition.save_dx_sequential`
(*boolean* or *number*)

Whether to save the DX output sequentially or not. See `condition.save_position_sequential` for detail.

`condition.seed`
(*number*)

Seed for the Mersenne twister random number generator.

`condition.apply_shear`
(*boolean* or *number*)

Whether to apply the external shear flow field or not. The shear flow condition can be set by `condition.kappa` and `condition.omega`.

`condition.iteration_max`
(*number*)

Maximum number of iterations for the simulation. `spreads` ends the simulation if the number of iterations reaches `condition.iteration_max`.

`condition.interval`
(*number*)

Interval for the data output into files.

`condition.dt`
(*number*)

The size of the time step. Too large `condition.dt` will lead unstable simulations or incorrect data.

`condition.omega`
(*number*)

The frequency of the external shear flow field. If this is set to `0`, steady shear is applied.

`condition.kappa`
(*number*)

The maximum shear strain rate.

6.2 Input / Output Files

The input / output file names are set as the `file` table.

`file.position_output`
(*string*)

Output file name for the positions of particles. This is used when `condition.save_position_sequential` is set to `false`. If the `file.position_output` is set to the null string (`""`), no output file will be created and the data will be discarded. The behaviour is the same for the other output files.

`file.stress_output`
(*string*)

Output file name for the stress tensor.

`file.energy_output`
(*string*)

Output file name for the free energy.

`file.geometry_output`
(*string*)

Output file name for the box geometry.

`file.dx_output`
(*string*)

Output file name for the DX output file.

`file.position_template`
(*string*)
Template for the output file of the positions of particles. `file.position_template` must contains `%d` once. `%d` will be replaced by the sequential numbers `1,2,3,...` If `file.positions_template` is set to the null string (`""`), no output file will be created.

`file.dx_template`
(*string*)
Template for the output file of the DX output file.

6.3 Geometry of Simulation Box

6.4 geometry

The simulation box geometry are set as the `geometry` table.

`geometry.dimension`
(*number*)
Number of dimension(s). This must be set to `2` or `3`.

`geometry.l`
(*array of numbers*)
Lengthes of the the simulation box.

6.5 Polymer Blend

The information about the polymer blend is set as the `blend` table. The polymers which is contained in the system is set as the individual tables.

`blend.polymer`
(*array of strings*)
Polymers which is contained in the blend. The polymers used here must be defined as individual tables.

`blend.number`
(*array of numbers*)
Numbers of each polymers

6.6 Monomer Species

The information about monomers is set as the `monomer` table.

`monomer.name`
(*array of strings*)
Names for each monomers.

`monomer.epsilon`
(*array of array of numbers*)
The effective interaction parameters between monomers. Only the diagonal and upper triangular parts are used.

6.7 Polymer Species

The polymers which is used in `blend.polymer` is defined as individual tables of which name is same as the element of `blend.polymer`. For example, if `blend.polymer` is set to `{AB_diblock, C_homo}` the tables `AB_diblock` and `C_homo` must be defined.

polymer`.monomer`
(*array of strings*)
Monomers for each subchains.

7 Output File Format

In this section, the output file format for `spreads` is described.

7.1 Positions of Particles

An output file of the positions of particles is a gzipped text file. The first line shows the dimensions and number of particle species, and the second line shows the number of particles. After that the position data are stored. Each low corresponds to one particle position and each column corresponds to the x,y, and z component. The output data is like the following data (the output file itself is gzipped).

```
# 3 2
# 2048 2048

1.482591 2.522368 8.503859
14.678206 9.115228 14.011614
6.584831 1.590900 14.042807
10.338461 5.101233 2.578110
3.443631 15.092652 4.027328
8.133353 0.291188 5.869824
14.790443 7.885689 13.788454
6.382475 11.639057 8.738407
    :         :        :
```

You can deflate the output file by using `gunzip` or `zcat`.

7.2 Stress Tensor

An output file of the stress tensor is a text file. It contains 6 stress tensor components (`xx`,`yy`,`zz`, `xy`,`yz`,and `zx`) as follows.

```
-31.587779 -31.638428 -31.601666 0.011065 0.010575 -0.020566
```

7.3 Energy

The energy output routine is not implemented yet.

7.4 Box Geometry

An output file of the box geometry is a text file. The first line shows dimension(s) of the system, the second line shows the box size, and the third line shows the gap size between periodic boxes caused by the shear strain. For example, an output file for a three dimensional system becomes as follows.

```
3
16.000000 16.000000 16.000000
0.000000
```

7.5 DX Output File

The DX output file is the data format for OpenDX (visualization software). It contains the particle positions (`position0,position1,...`), the box geometry (`box`), and the gap size (`delta_l`). You can visualize it by using OpenDX. The sample OpenDX program to visualize the OpenDX format `spreads` output data will be found in the `example/` directory.

8 Utility Programs

8.1 Converter for DX Output Files

The utility programs `spreads-dx2position` and `spreads-dx2geometry` convert an OpenDX format output file generated by `spreads` into gzipped text files. `spreads-dx2position` or `spreads-dx2geometry` convert the positions of particles or the box geometry in the DX file into text files.

To convert particle positions in a DX output file `spreadsout.dx` into a gzipped text file `position.dat.gz`, execute `spreads-dx2position` as follows.

```
$ spreads-dx2position spreadsout.dx position.dat.gz
```

`spreads-dx2geometry` can be used in the same way.

```
$ spreads-dx2geometry spreadsout.dx geometry.dat
```

8.2 Converter for Gzipped Text Files

The utility program `spreads-position2bond` converts a gzipped text file of particle positions into another gzipped text file of bond vectors. This program is experimental one and thus you may encounter errors if you specify incorrect input files. Please use the only the position files of diblock copolymer melts.

To convert position file `position.dat.gz` into a bond vector file `bond.dat.gz`, execute `spreads-position2bond` as

```
$ spreads-dx2phi position.dat.gz geometry.dat bond.dat.gz
```

Notice that a box geometry file is needed for this program.

8.3 Utility to Calculate Shear Relaxation Modulus

The utility program `spreads-stress2relaxation` calculates shear relaxation modulus from sequentially saved output stress tensor files.

To calculate shear relaxation modulus from stress tensor files, execute `spreads-stress2relaxation` as follows.

```
$ spreads-stress2relaxation spreadsin.lua modulus.dat
```

All the parameters will be read from `spreadsin.lua` automatically.

9 References

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END OF TERMS AND CONDITIONS

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```
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```
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```
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Concept Index