density functional simulator for block copolymers
version 0.2.2
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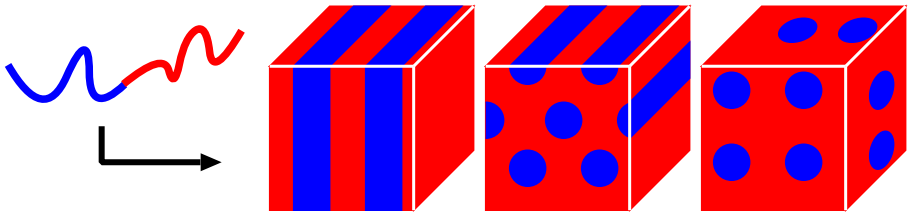
1 Introduction

It is widely known that most of the mixture of polymers causes phase separation at low temperature [Introduction to Polymer Physics, Scaling Concepts in Polymer Physics]. The block copolymers (polymers which consists on chemically connected subchains of different monomer species) causes phase separation at low temperature, too, but the its phase separation behavior is different from the case of homopolymers (polymers which consists on one monomer species) [Bates-Fredrickson-1999]. While the blends of homopolymers cause the phase separation macroscopically, the block copolymers cause the microscopic, chain-length scale phase separation. The former is called as the 'macro phase separation' and the latter is called as the 'micro phase separation'.

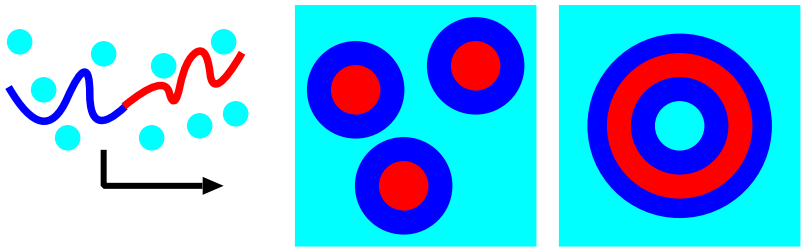


The micro phase separation takes various morphologies which depends on the structure of block copolymers or interaction of monomers. The scale of the micro phase separation structures is about the scale of polymer chains and is typically from $10nm$ - $1\mu m$.

To study the micro phase separation of block copolymers, various simulation method is proposed. The particle methods – the coarse-grained molecular dynamics (MD), the dissipative particle dynamics (DPD) [Groot-Warren-1997,Groot-Madden-1998,Groot-Madden-Tildesley-1999] – handle each polymer chains explicitly. These are good to study the dynamics of each chains, but takes too much memory and calculation time for studying the morphologies. The self consistent field (SCF) theory is widely used to study the morphologies of block copolymers [Helfand-Wasserman-1976,Helfand-Wasserman-1978,Helfand-Wasserman-1980, Matsen-Schick-1994,Matsen-Bates-1996,Fraaije-1993, Drolet-Fredrickson-1999,Fredrickson-Ganesan-Drolet-2002,Statistical Physics of Polymers: An Introduction]. It calculates the statistical weight of one polymer chain, based on the mean field theory. The SCF simulations are quite accurate and give very good results which is consistent with the experimental results quantitatively. While the SCF gives good results, it requires large memory and calculation time for large systems (for example, 3 dimensional systems or dynamics). The density functional (DF) theory is the theory which gives the free energy of the system as the functional of the subchain density fields [Joanny-Leibler-1978,de Gennes-1980,Leibler-1980,Ohta-Kawasaki-1986,Ohta-Kawasaki-1990, Kawasaki-Ohta-Kohrogui-1988,Nakazawa-Ohta-1993,Kawakatsu-1994,Ohta-Ito-1995, Bohbot-Raviv-Wang-2000,Uneyama-Doi-2005]. It requires small memory and calculation time compared with the SCF simulation while its accuracy is less than one of the SCF. The DF simulation is therefore suitable to survey the morphology of block copolymers qualitatively or to study the large systems which cannot be handled with the SCF simulation.

`drops` is a simulator for block copolymer melts and blends based on the density functional theory [Uneyama-Doi-2005]. It can handle arbitrary block copolymer systems – block

copolymers with arbitrary structure and arbitrary blend of them. The required parameter sets which describes the block copolymers are the same parameter sets as ones required by the SCF simulation. Thus one can do the simulation by `drops` just like by using the simulator based on the SCF. `drops` enables fast and efficient simulation for the micro phase separation of the block copolymers. For example, 3D structure formed by block copolymers such as the onion structure [Koizumi-Hasegawa-Hashimoto-1994,Uneyama-Doi-2005] or micellar structures (spherical micelles, cylindrical micelles and vesicles) [Disher-Eisenberg-2002,Choucair-Eisenberg-2003,Uneyama-Doi-2005a] can be simulated by `drops`.



From version 0.2.0, the dynamic simulation scheme is implemented. Thus `drops` enables the dynamics simulations as well as statics simulations for polymer blends, block copolymers or micellar systems [Uneyama-2007].

2 Installation of drops

2.1 To Download the Latest Version of drops

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

http://www.ton.scphys.kyoto-u.ac.jp/~uneyama/drops.html

2.2 Install to Microsoft Windows by the Installer

The installer of drops for Microsoft Windows is now available. You can install drops just like other Windows applications, by executing the installer drops-0.2.2-win32-setup.exe. The installer is built by using Inno Setup (http://www.jrsoftware.org/isinfo.php) and works for most versions of Windows.

2.3 Build and Install from the source

You can build and install drops if the binary package of your system is not available, or if you want to customize the drops. The source package of drops is using GNU Automake and GNU Autoconf, therefore you can build and install drops just like usual free software. Note that drops requires zlib (http://www.zlib.net/), Lua (http://www.lua.org/) and FFTW3 (http://www.fftw.org/). You have to install them before build drops.

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

```
$ zcat drops-0.2.2.tar.gz | tar xvf -
```

or if you are using GNU tar, do

```
$ tar zxvf drops-0.2.2.tar.gz
```

Then the source directory will extracted. Move to the directory drops-0.2.2.

```
$ cd drops-0.2.2
```

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

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

Now drops 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 drops,

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

will help you.

2.4 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`, `lua` and `fftw3` is already installed to your system. If they are not installed, first you have to install them (`zlib`, `zlib-devel`,`lua`,`lua-devel`,`fftw3`, and `fftw3-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 drops-0.2.2-1.src.rpm
```

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

```
# rpmbuild --rebuild drops-0.2.2-1.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/drops-0.2.2-1.i386.rpm
```

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

You may want to compile `drops` Intel C++ Compiler (`icc`). `icc` is mostly compatible GNU C Compiler (`gcc`) and thus you can compiler `drops` with `icc` easily. But the optimization flag `-ipo` will cause troubles when compiling `drops`. 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 drops

The format for running the `drops` program is:

```
$ drops option ... input
```

input is the input file for `drops`. If no input file is specified, `drops` will read the default input file `dropsin.lua`.

`drops` supports the following options:

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

`--psi=`*psi*
`-p` *psi*
: Read the initial value of the psi-field (square root of the density) from the file *psi*. The psi-field input file *psi* must be the gzipped plain text. You can create one easily by using `gzip`. By default, drops set the density field to be homogeneous.

`--external=`*external*
`-e` *external*
: Read the external force field from the file *external*. The external force input file density must be the gzipped plain text. You can create one easily by using `gzip`. By default, drops does not apply any external force to the system.

`--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 `drops` (the input file and some scripts for plotting / visualization can be found in the directory `examples/`). But first of all, you have to install the `drops` to your system. If `drops` is not installed to your system, see the 'Install `drops`' section. We starts from the simplest block copolymer systems, the diblock copolymer melts. The input file is distributed with the source code or binary of `drops`. To run this example, move to the directory `examples/ab_melt_1d/` and just type `drops`

```
$ drops
```

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

4.2 Plot or Visualize Output Data

The output file of `drops` 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. For example, here we plot the output data of the previous simulation by using Gnuplot (http://www.gnuplot.info/). For Gnuplot 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 phi.dat.gz
$ gnuplot
gnuplot> plot "phi.dat" using 1:2 with lines
```

This will show the density profile of the 'A' subchain. The second way is to use `zcat`.

```
$ gnuplot
gnuplot> plot "< zcat phi.dat.gz" using 1:2 with lines
```

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 =
{
    optimize_lattice = false,

    use_multigrid_solver = false,

    dynamics_simulation = false,

    save_psi_sequential = false,
    save_density_sequential = false,
    save_chemical_potential_sequential = false,
```

```
    save_free_energy_sequential = false,
    save_geometry_sequential = false,
    save_dx_sequential = false,

    error_tolerance = 1.0e-12,
    seed = 19876,
    noise = 0.0e-2,
    initial_noise = 1.0e-3,

    phi_min = -1.0,

    iteration_max = 5000,
    interval = 500,
    omega = 0.1,
}

file =
{
    wisdom = "fftw.wisdom",

    psi_output = "psi.dat.gz",
    density_output = "phi.dat.gz",
    chemical_potential_output = "mu.dat.gz",
    free_energy_output = "fe.dat",
    geometry_output = "geometry.dat",
    dx_output = "dropsout.dx",

    psi_template = "psi.%d.dat.gz",
    density_template = "phi.%d.dat.gz",
    chemical_potential_template = "mu.%d.dat.gz",
    free_energy_template = "fe.%d.dat",
    geometry_template = "geometry.%d.dat",
    dx_template = "ppoutput.%d.dx"
}

multigrid =
{
    n_cycle = 10,
    n_pre = 5,
    n_post = 5,
    error_tolerance = 1.0e-4
}

geometry =
{
    dimension = 1,
```

```
    nx = 256,
    ny = 1,
    nz = 1,

    lx = 32,
    ly = 1,
    lz = 1
}

blend =
{
    polymer = {"AB_diblock"},
    volume_fraction = {1}
}

monomer =
{
    name = {"A", "B"},
    b = {1, 1},
    chi = {{0, 3.0},
           {0, 0  }}
}

AB_diblock =
{
    N = 40,
    f = {0.5, 0.5},
    a = {{false, true },
         {false, false}},
    monomer = {"A", "B"},
    lambda = 20
}
```

There are many parameters required by `drops`. 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,

    nx = 32,
    ny = 32,
    nz = 1,

    lx = 16,
```

```
    ly = 16,
    lz = 1
}
```

`dimension` means the dimension(s) of the system. `nx,ny,nz` and `lx,ly,lz` mean the number of division and edge length for x, y, z axis. Thus the parameters shown above mean the 2 dimensional system with each edge length is 16 and divided into 32.

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"},
    volume_fraction = {0.5, 0.5}
}

A_homo =
{
    N = 10,
    f = {1},
    a = {{false}},
    monomer = {"A"},
    lambda = 0
}

B_homo =
{
    N = 10,
    f = {1},
    a = {{false}},
    monomer = {"B"},
    lambda = 0
}
```

The `blend` is changed to simulate the blend of A homopolymer / B homopolymer. The polymer species which the blend is consists on is listed in `polymer`. The volume fractions of each polymer species are specified by `volume_fraction`. 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). `N` is the degree of polymerization, `f` is the block ratio, `a` is the adjacency matrix for subchains and `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 `drops`. 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`. `drops` 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

Adjacency matrices and Flory-Huggins chi parameter matrices are symmteric. Thus we don't need to set all the elements in these matrices. In the input file for `drops`, adjacency matrices are required to set their upper triangular part and chi parameter matrices are required to set their diagonal and uppser triangular part. `drops` automatically fill the lower critical part by copying the values of upper triangular elements. (See examples in previous sections.)

5 Reporting Bugs

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

If you find a bug in `drops`, please send electronic mail to uneyama@ton.scphys.kyoto-u.ac.jp. Include the version number, which you can find by running `drops --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 `drops`, contact the author via electronic mail to uneyama@ton.scphys.kyoto-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 `drops` 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 will be set as the table `condition`. The following elements are required.

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

Whether to perform the lattice optimization or not. If `condition.optimize_lattice` is set to `true`, `drops` automatically modify the size of the system `lx,ly,lz` to minimize the free energy.

`condition.use_multigrid_solver`
(*bollean* or *number*)

Whether to use the multigrid solver for Poisson equation or not. If `condition.use_multigrid_solver` is set to `true`, `drops` uses the multigrid Poisson equation. If it is set to `false`, the fast solver using FFT is used.

`condition.dynamics_simulation`
(*bollean* or *number*)

Whether to perform the dynamics simulation or not. If `condition.dynamics_simulation` is set to `true`, `drops` performs the dynamics simulation. If it is set to `false`, it performs the statics (equilibrium) simulation.

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

Whether to save the psi-field sequentially or not. If `condition.save_psi_sequential` is set to `true`, `drops` saves the psi-field every `condition.interval` steps. The output file name is generated from `file.psi_template`. If it is set to `false`, `drops` saves psi-field to the output file named `file.psi_output` every `condition.interval` steps (in other words, the output file is overwritten). This behavior is the same for other output files (the chemical potential field, the density field, the free energy, the geometry and the DX output).

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

Whether to save the chemical potential field sequentially or not. See `condition.save_psi_sequential` for detail.

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

Whether to save the density field sequentially or not. See `condition.save_psi_sequential` for detail.

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

Whether to save the free energy sequentially or not. See `condition.save_psi_sequential` for detail.

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

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

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

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

`condition.error_tolerance`
(*number*)

Allowed error for the free energy. `drops` stops the simulation if the absolute value of the difference of the free energy is smaller than `condition.error_tolerance`.

`condition.seed`
(*number*)

Seed for the Mersenne twister random number generator.

`condition.noise`
(*number*)

Magnification of the random noise added to the chemical potential field. Set to `0` if you do not want to apply any random force.

`condition.initial_noise`
(*number*)

Magnification of the random noise added to the density field at the beginning of the simulations. Set to `0` if you do not want to add any random noise to the field.

`condition.phi_min`
(*number*)

Allower minimum value of the density field for dynamics simulations. If the value of the density, `phi`, is lower than `condition.phi_min`, `drops` automatically correct the density field. If `condition.phi_min` is positive value, the density correction is not performed. This parameter is only for dynamics simulations, and not used in the statics simulations.

`condition.iteration_max`
(*number*)

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

`condition.interval`
(*number*)

Interval for the lattice optimization, file output or calculating the difference of the free energy.

`condition.omega`
(*number*)

Acceleration factor for the density evolution. Too large `condition.omega` causes numerical instability associated with the employed numerical scheme.

6.2 Input / Output Files

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

`file.wisdom`
(*string*)

FFTW wisdom file used by the FFTW library. If the file named `file.wisdom` exists already, FFTW reads the wisdom from it. If the file does not exist FFTW saves its wisdom to the file which can be used for latter simulations.

`file.psi_output`
(*string*)

Output file name for the psi-field. This is used when `condition.save_psi_sequential` is set to `false`. If the `file.psi_output` is set to the null string (`""`), no output file will be created. It is the same for for other output files (the chemical potential field, the density field, the free energy, the geometry and the DX output).

`file.density_output`
(*string*)

Output file name for the density field.

`file.chemical_potential_output`
(*string*)

Output file name for the chemical potential field.

`file.free_energy_output`
(*string*)

Output file name for the free energy.

`file.geometry_output`
(*string*)

Output file name for the geometry.

`file.dx_output`
(*string*)

Output file name for the DX output file.

`file.psi_template`
(*string*)

Template for the output file of the psi-field. `file.psi_template` must contains `%d` once. `%d` will be replaced by the sequential number `1,2,3,...` If `file.psi_template` is set to the null string (`""`), no output file is created.

`file.density_template`
(*string*)

Template for the output file of the density field.

`file.chemical_potential_template`
(*string*)

Template for the output file of the chemical potential field.

`file.free_energy_template`
(*string*)

Template for the output file of the free energy.

`file.geometry_template`
(*string*)

Template for the output file of the geometry.

`file.dx_template`
(*string*)

Template for the output file of the DX output file.

6.3 Multigrid Solver

The input / output file names are set as the `multigrid` table. The multigrid solver is not used if `condition.use_multigird_solver` is set to `false`.

`multigrid.n_cycle`
(*number*)

Number of iteration for multigrid V-cycle.

`multigrid.n_pre`
(*number*)

Number of iteration for pre-smoothing Gauss-Seidel method.

`multigrid.n_post`
(*number*)

Number of iteration for post-smoothing Gauss-Seidel method.

`multigrid.error_tolerance`
(*number*)

Allowed error for the Poisson equation. The multigrid solver stops relaxation if the mean square residual is less than `multigrid.error_tolerance`.

6.4 Geometry of Simulation Box

6.5 geometry

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

`geometry.dimension`
(*number*)

Number of dimension(s). This must be set to `1`,`2` or `3`.

`geometry.nx`
(*number*)

Number of division in x-direction.

`geometry.ny`
(*number*)

Number of division in y-direction (not used for 1 dimensional systems).

`geometry.nz`
(*number*)

Number of division in z-direction (not used for 1, 2 dimensional systems).

`geometry.lx`
(*number*)

Length of the edge of the simulation box in x-direction.

`geometry.ly`
(*number*)

Length of the edge of the simulation box in x-direction (not used for 1 dimensional systems).

`geometry.lz`
(*number*)

Length of the edge of the simulation box in x-direction (not used for 1,2 dimensional systems).

6.6 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.volume_fraction`
(*array of numbers*)

Volume fraction of each polymers (`drops` automatically normalize `blend.volume_fraction`).

6.7 Monomer Species

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

`monomer.name`
(*array of strings*)

Names for each monomers.

`monomer.b`
(*array of numbers*)

Kuhn length (effective segment size) for each monomers.

`monomer.chi`
(*array of array of numbers*)

Flory-Huggins chi parameters for monomers. Only the diagonal and upper triangular part are used.

6.8 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`.N`
: (*number*)
Polymerization index of the polymer.

polymer`.f`
: (*array of numbers*)
Block ratio for each subchains (`drops` automatically normalize *polymer*`.f`).

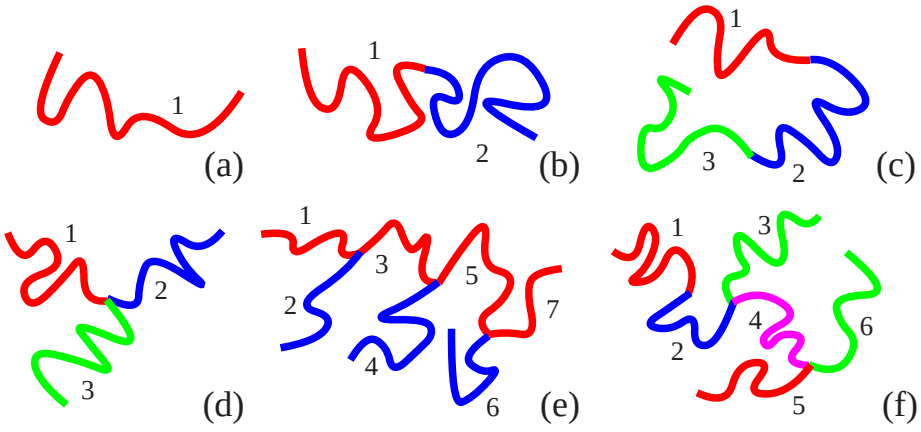
polymer`.a`
: (*array of array of booleans or numbers*)
Adjacency matrix. *polymer*`.a` specifies the topology of the polymer (connectivity of subchains). Only the upper triangular part is used.

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

polymer`.lambda`
: Tang-Freed type cutoff length for the long range interaction. If *polymer*.lambda is negative or 0, cutoff length is set to infinity (no cutoff length).

6.9 How to Determine the Adjacency Matricies

Most of the input parameters are easy to understand. The most confusing parameters are the adjacency matrix `polymer.a` which represents the connectivity of subchains. Here we show how to determine the adjacency matricies for block copolymers.



The above figure shows some polymer species; (a) homopolymer, (b) diblock copolymer, (c) triblock linear copolymer, (d) triblock star copolymer, (e) comb copolymer, (f) copolymer with complicated structure. The numbers (`1,2,...`) shown in figure corresponds to the index of the subchains.

The adjacency matricies for these polymer species are determined as follows.

(a) homopolymer

The homopolymer has only one subchain. Since there are no non-diagonal elements, the adjacency matrix has no meaning (but it must be specified, or `drops` won't work).

```
homopolymer.a = {0}
```

(b) diblock copolymer

This is the simplest block copolymer except for the homopolymer. Subchain `1` and subchain `2` are connected, so `a[1][2] = 1`.

```
diblock.a = {{0, 1},
             {1, 0}}
```

Note that we can use `true` and `false` instead of `1` and `0`. Also note that the diagonal term and lower triangular part of the matrix are actually not used.

(c) triblock linear copolymer

The triblock linear copolymer and the triblock star copolymer (d) are good example for determining adjecency matrices. For linear copolymer, Subhain `1` is connected to subchain `2`, but not connected to subchain `3`. Subchain `2` is connected to subchain `3`. Thus `a[1][2] = 1, a[1][3] = 0, a[2][3] = 1`.

```
triblock_linear.a = {{0, 1, 0},
                     {1, 0, 0},
                     {0, 1, 0}}
```

(d) triblock star copolymer

The triblock star copolymer contains three subchains, but the connectivity is different from the triblock linear copolymer (c). In this case, all subchains are connected each other. `a[1][2] = a[1][3] = a[2][3] = 1`.

```
triblock_star.a = {{0, 1, 1},
                   {1, 0, 1},
                   {1, 1, 0}}
```

(e) comb copolymer

Here we consider the comb copolymer which contains seven subchains. Although it may look complicated, but determining the adjecency matrix is not so complicated. First, the backbone subchains `1,3,5,7` is connected just like the linear copolymer. Thus `a[1][3] = a[3][5] = a[5][7] = 1`. Next, each side subchains `2,4,6` is connected to two backbone subchains. `a[1][2] = a[3][2] = 1, a[3][4] = a[5][4] = 1, a[5][6] = a[5][7] = 1`. Any other elements are equal to 0. Finally `a` is expressed as

```
comb.a = {{0, 1, 1, 0, 0, 0, 0},
          {1, 0, 1, 0, 0, 0, 0},
          {1, 1, 0, 1, 1, 0, 0},
          {0, 0, 1, 0, 1, 0, 0},
          {0, 0, 1, 1, 0, 1, 1},
          {0, 0, 0, 0, 1, 0, 1},
          {0, 0, 0, 0, 1, 1, 0}}
```

(f) general block copolymer (with complicated structure)

As a final example, here we show the general block copolymer with complicated structure. This block copolymer has 6 subchians. We start from the subchain `1`. It is connected to subchain `2`, so `a[1][2] = 1`. Subchain `2` is connected subchains `3` and `4` (of course it is connected to `1`, but we already know it). `a[2][3] = a[2][4] = 1`. Subchain `3` is connected to subchain `4`. `a[3][4] = 1`. Subchain `4` is connected to subchains `5` and `6`. `a[4][5] = a[5][6] = 1`. Subchain `5` is connected to subchain `6`. Thus we scanned all the connectivity. Now the adjacency matrix is

```
general.a = {{0, 1, 0, 0, 0, 0},
             {1, 0, 1, 1, 0, 0},
             {0, 1, 0, 1, 0, 0},
             {0, 1, 1, 0, 1, 1},
             {0, 0, 0, 1, 0, 1},
             {0, 0, 0, 1, 1, 0}}
```

7 Output File Format

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

7.1 Psi-Field

The output file for the psi-field is gzipped text. Each low corresponds to the one lattice point and each column corresponds to the subchain. For example, if `blend.polymer` is set to `{AB_diblock, C_homo}` and `AB_diblock.monomer` is set to `{"A","B"}`, The output data is like the following data (the output file itself is gzipped).

```
0.0241512 0.29688  0.954609
0.0240064 0.291801 0.956178
0.0238619 0.286763 0.957704
0.0237176 0.281766 0.95919
0.0235735 0.276813 0.960634
0.0234294 0.271903 0.962039
0.0232853 0.267038 0.963404
0.0231412 0.262219 0.964731
    :         :        :
```

The first and second column correspond to the psi-field of A subchain and B subchain of AB diblock copolymer, The third column corresponds to one of C homopolymer. You can deflate the output file by using `gunzip` or `zcat`.

7.2 Density Field

The output file for the density field is gzipped text. The format is like the psi-field output file, but contains position data. The first column (and the second, third column(s) if the dimensions of the system is greater than 1) is the position.

```
0       0.000583278 0.0881376 0.911279
0.03125 0.000576307 0.0851477 0.914276
0.0625  0.000569391 0.0822328 0.917197
0.09375 0.000562526 0.0793923 0.920045
0.125   0.000555708 0.0766254 0.922819
0.15625 0.000548935 0.0739314 0.925519
0.1875  0.000542204 0.0713094 0.928148
0.21875 0.000535514 0.0687586 0.930705
   :         :          :         :
```

It is convenient to use `gnuplot` to plot the 1D or 2D density data. For example, to plot 1D data, `gnuplot` command will be

```
gnuplot> plot "< zcat phi.dat.gz" using 1:2 title "A" with lines, \
                                  using 1:3 title "B" with lines, \
                                  using 1:4 title "C" with lines
```

and to plot 2D data, the command will be

```
gnuplot> splot "< zcat phi.dat.gz" using 1:2:3 title "A" with lines, \
                                    using 1:2:4 title "B" with lines, \
                                    using 1:2:5 title "C" with lines
```

7.3 Chemical Potential Field

The output file for the chemical potential field is gzipped text. The data format is same as the density output file.

7.4 Free Energy

The output file for the free energy is text file. The total free energy, the long range term, the local term, the gradient term are stored in this order. The sample output file is as follows.

```
-0.0925369 0.00859006 -0.13708 0.0359527
```

7.5 Geometry

The output file for the geometry is text file. The first row describes dimension(s) of the system, the second row describes number(s) of division and the third row describes length(es) of the edge of the simulation box. The sample output file is as follows.

```
1
1024
32
```

7.6 DX Output File

The DX output file is the data format for OpenDX (visualization software). It contains the density field (`phi0,phi1,...`) and the chemical potential field (`mu0,mu1,...`). You can visualize it by using OpenDX. The sample OpenDX program to visualize the OpenDX format `drops` output data will be found in the `example/` directory.

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