AnalysisTools user manual

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Contents

1. Introduction

AnalysisTools is a set of utilities to (mainly) analyse trajectories of particle-based simulations. The 34 utilities (including one from the DL_MESO simulation package) can be roughly divided into four types:

- utilities to calculate system-wide properties; e.g., pair correlation functions or particle densities along a simulation box axis
- utilities to calculate per-molecule or per-aggregate properties (where aggregate stands for any supramolecular structure); e.g., shape descriptors for individual molecules or whole micelles
- utilities to manipulate a configuration; e.g., create initial configuration for a simulation from scratch or by adding molecules to an existing one
- helper utilities to analyse text files; e.g., calculate averages and standard deviations of a data series

The `Examples` directory contains examples showcasing capabilities of individual utilities as well as possible workflows chaining several utilities.

1.1 Installation

AnalysisTools requires `C` and `Fortran` compilers and `cmake`. The utilities should be compiled in a separate directory, typically `<root>/build` (where `<root>` is the AnalysisTools root directory). The following generates a `Makefile` within `<root>/build`:

```
mkdir <root>/build; cd <root>/build; cmake ../
```

To then compile the utilities, simply run `make` (to compile all utilities) or `make <utility name>` (to compile a single utility) in `<root>/build`. The binaries are located in the `<root>/build/bin` directory.

2. Format of input/output files

This section describes several file types used by many of the AnalysisTools utilities. Output files for the utilities themselves are described in their respective sections in chapter 3.

Input files are divided into two categories: structure and coordinate files. The structure files contain information about the system composition, that is, number of beads and molecules, bead properties (mass, charge, etc.), molecule properties (number and types of beads, connectivity, etc.). The coordinate files contain individual timesteps with beads' coordinates (and, possibly, velocities, forces, etc.). Some files can be used as both a structure and a coordinate file, but using a different structure file may be essential. For example, an `xyz` file (see below) may be used as both, but because it only provides bead names, using a separate structure file would provide additional information (bead and/or molecule properties).

For working with aggregates, AnalysisTools' `agg` file format (see below) describes their compositions in terms of molecule numbers from a structure file used to generate it. Any of the `Aggregates` (section 3.2) utilities can create the `agg` file.

2.1 Structure files

As structure files, any of the following formats can be used; example files for a simple 'sandbox' system are provided in the `Examples/InputFiles` directory. Utilities load a specific structure using the `-i <file>` option; if the option is missing, it is usually assumed the structure file is the same as the coordinate file.

`Info` utility (section 3.6) can convert these formats between each other via the `-o <file>` option.

2.1.1 VTF format

See here for complete description and `in.vtf` and `in.vsf` for example files (a `vtf` file contains a structure part followed by a coordinate part, but a `vsf` file contains only the structure part). In this format, every bead is defined on its own line and all bonds all listed.

Not all keywords listed on the web page for the 'Atom lines' are recognized; keyword `n[ame]` is mandatory and optional keywords are `m[ass]`, `charge|q`, `r[adius]`, `resid`, and `res[name]`. For the `<aid-specifier>`, only a single bead index number or the `default` keyword can be used. Other keywords are ignored.

AnalysisTools groups beads (and molecules) into bead (and molecule) types. Generally, only name defines types of beads, i.e., should two beads share the name, they will be of the same type; their mass, charge, and radius will each equal to that for the bead type's topmost atom line containing the corresponding keyword.

If the keyword is missing from all atom lines, that characteristic is undefined. The `--detailed` command line option triggers detailed recognition, where beads that share the name but differ in mass, charge, and/or radius will be of different type.

Different molecule types, on the other hand, are always distinguished based on all their characteristics, i.e., name, connectivity, and order of beads (order of its `vsf` indices). However, molecule types can also be affected by the `--detailed` option because of the bead type definition

For the effect of the `--detailed` option, see the `Examples/Info` directory.

For bond lines, only single bonds are recognized (i.e., `bond <index1>:<index2>` format).

Periodic boundary condition can be included as `pbc <x> <y> <z>` for a cuboid box or `pbc <a> <b> <c> <alpha> <beta> <gamma>` for a general rhomboid box.

2.1.2 FIELD format

A format similar to the `FIELD` input file for DL_MESO_DPD simulation package; see `in.FIELD` for an example. This concise format defines species of beads and molecules, providing number of beads/molecules of given species as well as their properties.

The `species` section is the same as in the `DL_MESO FIELD` file, but the `molecules` section differs slightly. Besides the `beads` part, every molecule can have `bonds`, `angles`, `dihedrals`, but even though up to three parameters for potential parameters are read, AnalysisTools does not recognize the potential keywords (`harm`, `cos`, etc.). Moreover, these potential parameters are only used for generating new LAMMPS data files via the `Info` utility (section 3.6). The `molecules` section can also contain one extra part: `impropers` for improper angles which has the same format as the `dihedrals` section (this was added because the LAMMPS molecular dynamics simulator distinguishes between the two).

Note that the `FIELD` file does not have to contain `Interactions` section; this part is ignored.

However, using this file in conjunction with coordinate files is not recommended. Because `FIELD` contains only numbers of beads of given types, it is not possible to ensure that bead indices in the coordinate file will line up with the correct bead types in the `FIELD` file. The indices are assigned to the beads from `FIELD` on the 'first read, first labelled' basis, that is, the unbonded bonds are first (in the order of the lines in the `species` section) followed by beads from the molecules. Should one want to check the bead index assignments, the `Info` utility can be used to generate, e.g., a `vsf` file from the `FIELD` file.

Nevertheless, the file can be used to supply extra information for bead and molecule types for the `Info` utility's `-i[!]` option as these do not depend on individual beads but rather on bead and molecule type names (see section 3.6 for details). Moreover, `FIELD` is used as an input file to add extra species into an existing system or to create a new system from scratch via, e.g., AddRandomToSystem (section 3.1) or ref GenSystem, GenLayers, or some such.

To be recognized by AnalysisTools utilities, the file must either be called `FIELD` or have a `.FIELD` extension.

2.1.3 XYZ format

This is the simplest and probably best known format, see, e.g., here for the description and `in.xyz` for an example. An `xyz` file is essentially a file with timesteps (bead coordinates), and the only structure information are bead names.

The comment line at the beginning of each timestep can contain periodic boundary conditions as `<x> <y> <z>` (cuboid box) or `<a> <b> <c> <alpha> <beta> <gamma>` (general rhomboid box); it is similar to the `pbc` keyword in `vtf` file. To use this box definition, use `-pbc <n>` option where `<n>` is the position of the first number on the comment line (e.g., `1` if the comment line starts with the box size).

2.1.4 LAMMPS data format

This rather complicated format comes from the LAMMPS molecular dynamics simulator and lists the numbers of beads, bonds, angles, etc., as well as individual beads, bonds, angles, etc., and information about potentials for bonds, angles, etc. See here for description of the format and `in.data` for an example.

AnalysisTools reads the header information as well as `Masses`, `Atoms`, `Velocities`, `Bonds`, `Angles`, `Dihedrals`, `Impropers`. It also reads `Bond Coeffs`, `Angle Coeffs`, `Dihedral Coeffs`, and `Improper Coeffs` sections.

The `Atoms` section must have `atom_style full` format, that is every bead line must have the format `<id> <mol id> <bead type> <q> <x> <y> <z>`, where `<id>` is a bead index, `<mol id>` is a molecule index (-1 means the bead is in no molecule), `<bead type>` is the bead type index corresponding to a line in the `Masses` section, `<q>` is charge, and `<x> <y> <z>` are coordinates.

For the `Bond Coeffs` and `Angle Coeffs` sections, harmonic potential is assumed, and the first value of each bond/angle type is multiplied by 2 because LAMMPS uses harmonic spring strength of $k/2$ (as opposed to, e.g., DL_MESO which uses k).

For the `Dihedral Coeffs` and `Improper Coeffs` sections, AnalysisTools reads at most three numbers without assuming any specific potential.

All the `Coeffs` sections are used only for generating new structure files via the utility Info (section 3.6), (specifically, only to generate `FIELD` and LAMMPS `data` files because no other supported file contains this information).

To be recognized by AnalysisTools utilities, the file must have an extension `.data`.

2.1.5 LAMMPS lammpstrj format

This mainly coordinate file format comes from the LAMMPS dump style custom command. See `in.lammpstrj` for an example.

Of the possible LAMMPS attributes, AnalysisTools recognizes only `id` (bead index – mandatory), `element` (bead name), `x y z` (bead coordinates), `vx vy vz` (bead velocities), and `fx fy fz` (bead forces). Any other attribute is ignored. Note that if `element` is missing, all beads are considered of the same type called `bt`.

To be recognized by AnalysisTools utilities, the file must have an extension `.lammpstrj`.

2.2 Coordinate files

As coordinate files, any of the following formats can be used; example files for a simple 'sandbox' system are provided in the `Examples/InputFiles` directory. These files can be combined with any of the above-described structure files (via the `-i <file>` option), but some may be used as both the structure and coordinate file.

Utility Selected (section 3.8) can generate any of these file types, converting between the formats; all utilities that require coordinate file can use any of these formats.

2.2.1 VTF format

See here for the description of a coordinate part of the `vtf` format and `in.vtf` and `in.vcf` for example files (a `vtf` file contains the coordinate part after a structure part, while a `vcf` file contains only the coordinate part).

AnalysisTools recognizes both ordered and indexed timesteps as well as a `pbc` line defining box dimensions.

If an AnalysisTools utility is not provided with an extra structure file (`-i <file>` option), the same filename is assumed but with the `.vsf` extension instead of the `.vcf` extension.

2.2.2 XYZ format

This is the simplest and probably best known format, see, e.g., here for the description and `in.xyz` for an example.

The comment line at the beginning of each timestep can contain periodic boundary conditions as `<x> <y> <z>` (cuboid box) or `<a> <b> <c> <alpha> <beta> <gamma>` (general rhomboid box); it is similar to the `pbc` keyword in `vtf` file. To use this box definition, use `-pbc <n>` option where `<n>` is the position of the first number on the comment line (e.g., `1` if the comment line starts with the box size).

The `xyz` coordinate file will be used as a structure file as well unless an extra structure file is provided via the `-i <file>` option.

2.2.3 LAMMPS lammpstrj format

This coordinate file format comes from the LAMMPS dump style custom command. See `in.lammpstrj` for an example.

Of the possible LAMMPS attributes, AnalysisTools recognizes only `id` (bead index – mandatory), `element` (bead name), `x y z` (bead coordinates), `vx vy vz` (bead velocities), and `fx fy fz` (bead forces). Any other attribute is ignored. Note that if `element` is missing, all beads are considered of the same type called `bt`.

To be recognized by AnalysisTools utilities, the file must have an extension `.lammpstrj`.

This coordinate file will be used as a structure file as well unless an extra structure file is provided via the `-i <file>` option.

2.3 Aggregate file

A `file.agg` is generated using `Aggregates` (or `Aggregates-NotSameBeads`) utility. The file contains information about the number of aggregates in each timestep and which molecules and monomeric (i.e., unbonded) beads belong to which aggregate. It serves as an additional input file for utilities that calculate aggregate properties; `agg` file is, therefore, linked to the `vcf` file that was used to generate it.

The `agg` file is a simple text file. The first two lines are just comments (the second one should contain the command used to generate the file as parts of the command may be used by subsequent aggregate analysis). From third line, the data for individual timesteps are shown. It follows these rules:

- each timestep starts with `Step: <int>`
- the second line is the number of aggregates in the given timestep
- for each aggregate, there is a single line in the format `<size> : <id1> <id2> ... <idsize>`; the `<id#>` are molecular indices from the input structure file
- no blank or comment lines are allowed
- not all molecules present in the `vcf` file used to generate this file must be present in every timestep

Note that the term aggregate also refers to free chains (i.e., fully dissolved chains).

When keywords `Last Step: <int>` are encountered in place of `Step:` line, it signalizes the end of the `agg` file; no utility will read anything beyond this line.

If `vtf` format is used for the coordinates, the indices from `agg` file can be used in vmd to visualize, e.g., only a specific aggregate by using `resid <id1> ... <id#>` in the `Selected Atoms` box inside the vmd. A bash script `scripts/VisualizeAgg.sh` (and the accompanied picture VisualizeAgg.jpg) is a rough example of visualizing aggregates by different colours (it takes `vtf` and `agg` files as command line arguments).

An example of an `agg` file can be found in the `Examples/DistrAgg` directory.

3. Utilities

All utilities have command line options affecting their behaviour. The following options are common for many utilities, so they are described here rather than at the individual utilities where only list of the possible options is provided.

General options	
`--verbose`	print information about all bead and molecule types to the screen
`--silent`	run silently, i.e., without any output at all (overrides `--verbose` option)
`--help`	print short description of the utility and usage
`--version`	print version of the utilities and exit
Options for structure and coordinate input files	
`-i <name>`	use specified structure file, see section 2.1 for possible formats
`--detailed`	only `vtf` structure file: detailed recognition for bead (and, consequently, molecule) types based on the bead names as well as charges, masses, and radii
`-st <n>`	any coordinate file: start calculations at `n`-th timestep
`-e <n>`	any coordinate file: end calculations at `n`-th timestep
`-sk <n>`	any coordinate file: skip every `n` timesteps during calculations

For `vtf` structure files, the bead types are defined solely based on their name by default; the other properties (mass, charge, and radius) are taken from the first `a[tom]` line with the bead of that name that contains the appropriate keyword. For example, lines

```
atom default name A m 1
atom 1 name B
atom 2 name B m 2
atom 3 name A m 2
atom 4 name A
```

would define two bead type called `A` and `B` with masses equal to 1 and 2, respectively. Using the `--detailed` option would split the `A` beads into three types: `A` and `A_1` with masses equal to 1 and 2, respectively, and `A_2` with undefined mass (it remains undefined because there is an ambiguity—should the last bead have mass 1 or 2?). On the other hand, the `B` beads would be assigned the same bead type with mass equal to 2 (there is no ambiguity because only one mass is specified for the `B` beads). See `Examples/Info` directory for other examples.

Which timesteps are used by the utility can be controlled via the `-st`, `-e`, and `-sk` options. For example, specifying `-st 2 -e 10 -sk 2` would use timesteps 2, 5, and 8.

3.1 AddRandomToSystem

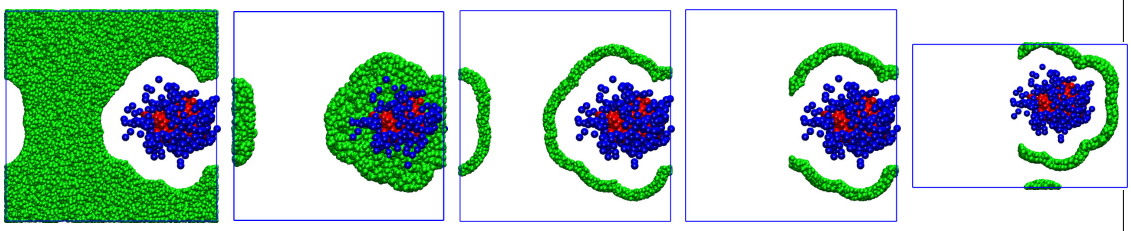
This utility takes an existing system (or an empty system, i.e., creates new sytem from scratch) and adds new beads (read from a `FIELD` file) into it, placing them either completely randomly or according to supplied constraints.

There are two types of constraints which can be combined: place new beads (i) specified distance from other beads or (ii) in a specified interval in x-, y-, and/or z-axis directions. In (i), options `-ld` and/or `-hd` specify the distance; if present, these must be accompanied by `-bt` or `--bonded` option. The new beads are then placed at least `-ld <float>` and at most `-hd <float>` distance from beads specified by the `-bt` option or from any bonded bead (`--bonded` option).

In (ii), options `-cx`, `-cy`, and `-cz` basically change the box size for the added beads. By default, this constraint is specified in units relative to the box dimensions (i.e., allowed values go from 0 to 1); use the `--real` option for absolute units. For example, `-cx 0.5 1` would generate x coordinates between 50% and 100% of the box's x sidelength. All these options can be combined, but note that `AddRandomToSystem` does not perform any sanity checks; that is, if any combination of the provided options is impossible to achieve, the utility will run forever. See figure 3.1 for schematic examples.

For added molecules, either the molecule's geometric centre (default behaviour) or its first bead (`--head` option) obey these constraints. The coordinates of the remaining beads in the molecule are governed by the coordinates in the `FIELD` file. Therefore, not all the molecular beads necessarily obey the constraining rules. Molecules are added with a random orientation unless the `--no-rotate` switch is used.

By default, the new beads are exchanged for beads in the original system; what bead type to exchange is either the most numerous one (default behaviour) or provided via the `-xb` option. Note that the utility doesn't check whether exchanged beads are in a molecule, so a bonded bead may be exchanged, leaving only part of



(a) (b) (c) (d) (e)

Figure 3.1: Examples of distance checks: (a) `-ld 3 -bt A B` specifies that any added bead (green) is at least at a distance of three from any `A` or `B` bead (red and blue, respectively); (b) `-hd 4 -bt A B` specifies added beads are at most four units away from any `A` or `B` bead; (c) combines (a) and (b) into `-ld 3 -hd 4 -bt A B`, that is, new beads are added at a distance between three and for from any `A` or `B` bead; (d) combines (c) with axis constraint into `-ld 3 -hd 4 -cx 0.5 1 -bt A B` which constrains the x-coordinate of new beads between 50% and 100% of the box's x sidelength; (e) adds `-b 30 20 25` to the options in (d), changing the box size.

the molecule in the new system. If beads are to be added into the system rather than switched, use the `--add` option.

The size of the new simulation box can be changed using the `-b` option. Any constraints for placing beads are applied to this box rather than the one in the original system. The new system is placed so the centres of the original box and the new one coincide. Note that in the end, all coordinates are wrapped into the output box (i.e., periodic boundary conditions are applied).

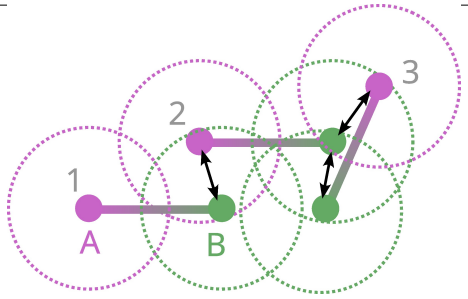
To create a new system instead of adding to an existing one, use `-` instead of an `<input>` file. An extra structure file can be generated via the `-o` option; this can be useful to, e.g., generate both `vtf` file for visualization and `data` file for use by LAMMPS.

Examples of using the utility are provided in the `Examples/AddRandomToSystem` folder (including those in figure 3.1).

Usage: `AddToSystem <input.vcf> <out.vsf> <out.vcf> [options]`

Mandatory arguments	
`<input>/-`	input coordinate file (or create a system from scratch)
`<in.field>`	input `FIELD` structure file for the new system
`<output>`	output coordinate file for the new system

options	
`-o <file>`	extra output structure file
`-s <int>`	seed for random number generator
`--add`	replace original beads instead of increasing the total number of beads
`-b <x> <y> <z>`	side lengths of the new simulation box
`--centre`	place the original simulation box in the middle of the new one re-implement probably
`--no-rotate`	do not randomly rotate added molecules
`-ld <float>`	lowest distance from beads specified by `-bt` option
`-hd <float>`	highest distance from beads specified by `-bt` option
`-bt <bead name(s)>`	bead types to use in conjunction with `-ld` and/or `-hd` options
`--bonded`	use bonded beads for the distance condition (overwrites `-bt` option)
`--head`	use molecule's first bead for distance check (default: molecule's geometric centre)
`-cx 2<float>`	constrain x coordinate to interval $\langle num, num2)$ (units relative to box size)
`-cy 2<float>`	constrain y coordinate to interval $\langle num, num2)$ (units relative to box size)
`-cz 2<float>`	constrain z coordinate to interval $\langle num, num2)$ (units relative to box size)
`--real`	use 'real' units instead of relative ones for `-cx`/`-cy`/`-cz` options



`Aggregates ... A B`
⇒ 3 contact pairs
`Aggregates-NotSameBeads ... A B`
⇒ 2 contact pairs

Figure 3.2: Simple example of distance checks—three two-bead molecules, where dotted lines represent maximum pair distance (`-d` option) and black arrows show contact pairs.

`-i`, `-st`, `--detailed`, `--verbose`, `--silent`, `--help`, `--version`

3.2 Aggregates and Aggregates-NotSameBeads

These utilities determine which molecules belong to which aggregates (note that 'aggregate' is used for any supramolecular structure) according to a simple criterion: two molecules belong to the same aggregate if they share at least a specified number of contact pairs. A contact pair is a pair of two beads belonging to different molecules which are closer than a specified distance. The information is written into an `.agg` text file described in Section 2.3.

Periodic boundary conditions can be removed from whole aggregates via the `-j` option; the aggregate's centre of mass is always inside the simulation box. This is useful for visualization (an aggregate will no longer be split by the walls of the simulation box, but it may stretch far outside the boundaries of the box) as well as for further analysis (the other utilities do not have to join the aggregates, possibly speeding up the analysis).

While the `Aggregates` utility uses all possible pairs of given bead types, `Aggregates-NotSameBeads` does not use same-type pairs. For example, if bead types `A` and `B` are given, `Aggregates` will use all three possible bead type pairs (i.e., `A-A`, `A-B`, and `B-B`), but `Aggregates-NotSameBeads` will use only `A-B` bead type pairs. Fig 3.2 illustrates the behaviour: using `Aggregates ... A B` would find one contact pair between molecules 1 and 2 and two contacts between molecules 2 and 3, whereas `Aggregates-NotSameBeads ... A B` would ignore A-A and B-B pairs, finding no contact pair between molecules 1 and 2 and only one between molecules 2 and 3.

Note that when `-st`, `-e`, or `-sk` options are used, the resulting `agg` file is no longer coupled to the original coordinate file (i.e., they cannot be used together for further analysis), but it is coupled to the optional output file with joined coordinates (`-j` option).

Usage: `Aggregates <input> <out.agg> <bead type(s)> [options]`

Mandatory arguments

`<input>`	input coordinate file
`<out.agg>`	output `agg` file
Options	
`-d <num>`	maximum distance for contact (default: 1)
`-c <num>`	minimum number of contacts (default: 1)
`-j <file>`	save coordinates of joined aggregate to a coordinate file
Other options (see the beginning of Chapter 3)	
`-st`, `-e`, `-sk`, `-i`, `--detailed`, `--verbose`, `--silent`, `--help`, `--version`	

3.3 Average

This utility calculates one of three types of averages based on a used option from specified column(s) of data in the input text file (all `#`-starting lines and blank lines are ignored). It either produces an overall average with statistical error and an autocorrelation time estimate (`-tau` option), block averages (`-b` option), or moving averages (`-m` option). While the `-tau` option appends a single line to the output file, either of the `-b` or `-m` options creates a new output file with somewhat smoother data.

The first and last lines used for the average calculation can be controlled using the standard `-st` and `-e` options.

3.3.1 Estimate autocorrelation time via -tau option

The average value of an observable $\mathcal{O}$ is a simple arithmetic mean,

$$\langle \mathcal{O} \rangle = \frac{1}{N} \sum_{i=1}^{N} \mathcal{O}_i, \tag{3.1}$$

where N is the number of measurements and the subscript i denotes individual measurements. If the measurements are independent (i.e., uncorrelated), the statistical error, ϵ, is given by:

$$\epsilon^2 = \frac{\sigma^2_{\mathcal{O}_i}}{N}, \tag{3.2}$$

where $\sigma^2_{\mathcal{O}_i}$ is the variance of the individual measurements,

$$\sigma^2_{\mathcal{O}_i} = \frac{1}{N-1} \sum_{i=1}^{N} (\mathcal{O}_i - \langle \mathcal{O} \rangle)^2. \tag{3.3}$$

For correlated data, the autocorrelation time, τ, representing the number of steps between two uncorrelated measurements must be determined. Every τ-th measurement is uncorrelated, so the equation (3.2) can then be used to estimate the error.

A commonly used method to estimate τ is the binning (or block) method. In this method, the correlated data are divided into N_B non-overlapping blocks of size k ($N = kN_\mathrm{B}$) with per-block averages, $\mathcal{O}_{\mathrm{B},n}$, defined as:

$$\mathcal{O}_{\mathrm{B},n} = \frac{1}{k} \sum_{\substack{i=1+ \\ (n-1)k}}^{kn} \mathcal{O}_i. \tag{3.4}$$

If $k \gg \tau$, the blocks are assumed to be uncorrelated and equation (3.2) can be used:

$$\epsilon^2 = \frac{\sigma_\mathrm{B}^2}{N_\mathrm{B}} = \frac{1}{N_\mathrm{B}(N_\mathrm{B}-1)} \sum_{n=1}^{N_\mathrm{B}} (\mathcal{O}_{\mathrm{B},n} - \overline{\mathcal{O}})^2. \tag{3.5}$$

An estimate of the autocorrelation time can be obtained using the following formula:

$$\tau_\mathcal{O} = \frac{k\sigma_\mathrm{B}^2}{2\sigma_{\mathcal{O}_i}^2}. \tag{3.6}$$

The number of blocks, N_B, is supplied as an argument of the `-tau` option and Average then appends a single line to the `<output>` file; the line starts with N_B and continues with three values ($\langle\mathcal{O}\rangle$, ϵ, and $\tau_\mathcal{O}$) per every data column specified in the Average command.

A way to quickly get a τ estimate is to use a wide range of N_B values and plot $\tau_\mathcal{O}$ from equation (3.6) as a function of N_B. Because the number of data points in one block should be significantly larger than the autocorrelation time (e.g., ten times larger), plotting $f(x) = N/(10x)$ will produce a monotonously decreasing curve that intersects the $\tau_\mathcal{O}$ vs. N_B curve. A value of $\tau_\mathcal{O}$ near the intersection (but to the left, where the decreasing curve is above $\tau_\mathcal{O}$ vs. N_B curve) can be considered a safe estimate of τ.

3.3.2 Block averages via -b option

Besides estimating the autocorrelation time, the per-block averages can be themselves plotted to get (probably) smoother dataset. Using the `-b` option, the number of datapoints per block to average, k, is supplied, and the utility prints the per-block averages from equation (3.4) to the output file.

This way of averaging could be useful for example with density data produced by DensityBox or related utilities; if the bin width supplied to the DensityBox was too small, it is (possibly much) faster to block-average the densities rather than rerun DensityBox. For this case, specify the first column (distance) along with any density columns from the density file.

3.3.3 Moving averages via -m option

More common way to smoothing noisy data is to use the moving (or rolling or running) average (or moving mean or rolling mean); this common method does have many names.

Similarly to the block-average, the first element of the moving average is a simple mean of k values. Unlike with block-average, however, the k values for the next element are obtained by ignoring only one value and taking the next k values; i.e., $k-1$ values from the previous element of the moving average are always reused as opposed to the block-average where the blocks of data are not overlapping.

The moving average elements, $\mathcal{O}_{\mathrm{M},n}$, are defined as

$$\mathcal{O}_{\mathrm{M},n} = \frac{1}{k}\sum_{n}^{n+k-1}\mathcal{O}_i. \tag{3.7}$$

Usage: `Average <input> <output> <column(s)> [options]`

Mandatory arguments	
`<input>`	input text file
`<output>`	output text file
`<column(s)>`	at least one column number from `<input>`

Options	
`-tau <int>`	τ estimation where `<int>` represents the number of blocks N_{B}
`-b <int>`	block-average printing mode where `<int>` represents the number of datapoints per one block, k (equation (3.4))
`-m <int>`	moving average mode where `<int>` represents the number of datapoints per one moving block, k (equation (3.7))

Other options (see the beginning of Chapter 3)
`-st`, `-e`, `--verbose`, `--silent`, `--help`, `--version`

3.4 DensityBox

This utility calculates number density for all bead types along all three axes directions of the simulation box, generating one file per axis. The density is calculated from 0 to box length in the given direction, that is, the box is 'sliced' into blocks with width `<width>`, and numbers of different bead types are counted in each 'slice'. Or to put it in other words, a density profile for a bead type i along an axis α, $\rho(\alpha)$, is calculated as

$$\rho_i(\alpha) = \frac{\sum_j \delta(\alpha-\alpha_j^i)}{\Delta\alpha L_\beta L_\gamma}, \tag{3.8}$$

where $\delta(\alpha-\alpha_i^j)$ gives the number of i beads inside a slice of the simulation box of the thickness $\Delta\alpha$ (i.e., `<width>`) along the α-axis; L_β and L_γ represent box side lengths along the two remaining axes.

The utility does not distinguish between beads with the same name in different molecules, so if one bead type is in more than one molecule type, its density will be averaged over all molecule types it appears in. If one requires densities specific to certain molecules containing the same bead types, the `-x` option can be used

to first run the utility without one molecule type and then rerun it, excluding the other molecule type. Thus, two output files (per axis) are generated, each missing densities from the specified molecule types.

Note that this utility assumes orthogonal box with constant side lengths; in case of triclinic box and/or varying box size, undefined behaviour may occur i.e., the utility may crash or freeze, and any results will not be reliable.

Usage: `DensityBox <input> <width> <output> [options]`

Mandatory arguments	
`<input>`	input coordinate file (either `vcf` or `vtf` format)
`<width>`	width of each bin of the distribution
`<output>`	three output files with automatic `-x.rho`, `-y.rho`, and `-x.rho` endings
Options	
`-x <mol name(s)>`	exclude specified molecule type(s) (i.e., do not calculate density for beads in molecules `<mol name(s)>`)
Other options (see the beginning of Chapter 3)	
`-st`, `-e`, `-sk`, `-i`, `--help`, `--detailed`, `--verbose`, `--silent`, `--version`	

Format of output files:
1) `<output>` – bead densities; one file per x-, y-, and z-axis
- first line: AnalysisTools version
- second line: command used to generate the file
- third line: column headers
  - first is the centre of each bin (governed by `<width>`); i.e., if `<width>` is 0.1, then the centre of bin 0 to 0.1 is 0.05, centre of bin 0.1 to 0.2 is 0.15, etc.
  - the rest are for the calculated data: each column corresponds to the number density of the specified bead type
- the rest of the file are data lines

3.5 DistrAgg

This utility calculates average aggregate mass and aggregation number for each timestep (i.e., time evolution) and the averages over all timesteps from a supplied `agg` file (see Section 2.3 for its format). It calculates number, weight, and z averages. It also calculates distribution functions of aggregation sizes.

Generally, for a quantity $\mathcal{O}$, the number, weight, and z averages, $\langle\mathcal{O}\rangle_{\mathrm{n}}$, $\langle\mathcal{O}\rangle_{\mathrm{w}}$, and $\langle\mathcal{O}\rangle_{\mathrm{z}}$, respectively, are defined as

$$\langle\mathcal{O}\rangle_{\mathrm{n}} = \frac{\sum_i N_i\mathcal{O}_i}{N}, \quad \langle\mathcal{O}\rangle_{\mathrm{w}} = \frac{\sum_i N_i m_i\mathcal{O}_i}{\sum_i N_i m_i}, \text{ and } \quad \langle\mathcal{O}\rangle_{\mathrm{z}} = \frac{\sum_i N_i m_i^2\mathcal{O}_i}{\sum_i N_i m_i^2}, \tag{3.9}$$

where N is the total number of measurements, i.e., the total number of aggregates for per-aggregate averages (or molecules for per-molecule averages); N_i is the number

of measurements with the value $\mathcal{O}_i$, and m_i is mass of an aggregate i (or a molecule i).

Number, weight, and z distribution functions of aggregate sizes, $F_{\mathrm{n}}(A_{\mathrm{S}})$, $F_{\mathrm{w}}(A_{\mathrm{S}})$, and $F_{\mathrm{z}}(A_{\mathrm{S}})$, respectively, are defined as

$$\begin{aligned} F_{\mathrm{n}}(A_{\mathrm{S}}) &= \frac{N_{A_{\mathrm{S}}}}{\sum_{A_{\mathrm{S}}} N_i} = \frac{N_{A_{\mathrm{S}}}}{N}, \\ F_{\mathrm{w}}(A_{\mathrm{S}}) &= \frac{N_{A_{\mathrm{S}}} m_{A_{\mathrm{S}}}}{\sum_{A_{\mathrm{S}}} N_i m_i} = \frac{N_{A_{\mathrm{S}}} m_{A_{\mathrm{S}}}}{\sum_{i=1}^{N} m_i} = \frac{N_{A_{\mathrm{S}}} m_{A_{\mathrm{S}}}}{M}, \text{ and} \\ F_{\mathrm{z}}(A_{\mathrm{S}}) &= \frac{N_{A_{\mathrm{S}}} m_{A_{\mathrm{S}}}^2}{\sum_{A_{\mathrm{S}}} N_i m_i^2} = \frac{N_{A_{\mathrm{S}}} m_{A_{\mathrm{S}}}^2}{\sum_{i=1}^{N} m_i^2}, \end{aligned} \tag{3.10}$$

where $N_{A_{\mathrm{S}}}$ and $m_{A_{\mathrm{S}}}$ stand for the number and mass, respectively, of aggregates with aggregate size A_{S}; M is the total mass of all aggregates. The equations are normalised so that $\sum F_x(A_{\mathrm{S}}) = 1$.

Per-timestep averages are written to the `<output avg>` and distributions into the `<output distr>` file. Overall averages are appended as comments (with commented legend) to both `<output avg>` and `<output distr>` files.

Lastly, `DistrAgg` can calculate distribution of composition for aggregates with specified size(s) (`-c` option). Two versions of a 'composition distribution' are generated. The first is the distribution of numbers of each molecule type in the aggregates of that size. The second is a distribution of ratios of all possible molecular pairs in those aggregates The distribution of numbers of each molecule type is written into `<file>-<size>.txt` file, and the distribution of all ratios of all possible bead pairs is written into `<file>-ratio_<size>.txt` file; that is, two files are created for each aggregate size. In both cases, the number distribution for aggregates with aggregation number A_{S}, $F_{A_{\mathrm{S}}}(i)$, is defined as

$$F_{A_{\mathrm{S}}}(i) = \frac{N_{A_{\mathrm{S}},i}}{N_{A_{\mathrm{S}}}}, \tag{3.11}$$

where $N_{A_{\mathrm{S}}}$ is the total number of aggregates with aggregation number A_{S}. The $N_{A_{\mathrm{S}},i}$ is the number of aggregates with size A_{S} that either contain i molecules of given type (the first distribution type) or has the ratio of molecules `mol1` and `mol2`; i.e., $i =$ `mol1`/`mol2` (the second distribution type).

The `<avg file>` contains averages for all timesteps regardless of `-st`, `-e`, and `-sk` options. The starting and ending timesteps as well as the number of skipped timesteps are taken into account for all the distributions and overall averages.

The definition of aggregate size is flexible. If none of `-m`, `-x`, or `--only` options is used, aggregate size is the 'true' aggregation number, i.e., the number of all molecules in the aggregate; if `-m` is used, aggregate size is the sum of only specified molecule type(s); if `-x` is used, aggregates containing only specified molecule type(s) are disregarded; if `--only` is used, only aggregates composed of the specified molecule type(s) are taken into account. These options can be mixed. For example, consider a system containing three aggregates composed of various numbers of three different molecule types:

Molecule types	Aggregate composition
Mol_A	Agg_1: 1 Mol_A +2 Mol_B +3 Mol_C = 6 molecules
Mol_B	Agg_2: 1 Mol_A +2 Mol_B = 3 molecules
Mol_C	Agg_3: 1 Mol_A = 1 molecule

Here is a list of some of the possibilities depending on the option(s) used:
1) if none of -m, -x, --only is used, all three aggregates are counted and their sizes are their 'true' aggregation numbers, i.e., $A_S = 6$, 3, and 1
2) if -m Mol_A Mol_B is used, all three aggregates are counted, but their size is the sum of only Mol_A and Mol_B molecules: Agg_1 – 3; Agg_2 – 3; Agg_3 – 1
3) if -m Mol_B Mol_C is used, Agg_3 is not counted, because its size would be zero; DistrAgg would detect only two aggregates with sizes: Agg_1 – 5; Agg_2 – 2
4) if -x Mol_A Mol_B is used, Agg_2 and Agg_3 are not counted, because neither contains anything else than Mol_A and/or Mol_B; DistrAgg would detect only one aggregate with size: Agg_1 – 6
5) if -x Mol_A Mol_B is combined with -m Mol_A Mol_B, DistrAgg would again detect only Agg_1, but its size would be 3
6) if --only Mol_A Mol_B is used, Agg_1 is not counted, because it contains a molecule not specified by --only; DistrAgg would detect two aggregates with sizes: Agg_2 – 3; Agg_3 – 1
7) if --only Mol_A Mol_B is combined with -m Mol_A, the two detected aggregates have sizes: Agg_2 – 1; Agg_3 – 1
8) if --only Mol_A Mol_B is combined with -x Mol_A, only Agg_2 is detected as it is the only one composed of only Mol_A and Mol_B molecules and its size would be 3
9) if --only Mol_A Mol_B and -x Mol_A are combined with -m Mol_A, the size of the one detected aggregate would be 1

Note that aggregate mass is always taken as the total mass, e.g., in the above points 8) and 9), the mass of the one detected aggregate would be the sum of masses of all the molecules in the aggregate even though the size is defined differently.

Should the -c option be used (without any of the -x, -m, or -only options), the output <file>-<size>.txt file would contain three data columns, one for each molecule type; the output <file>-ratio_<size>.txt file would contain three columns for the three ratios, that is Mol_A/Mol_B, Mol_A/Mol_C, and Mol_B/Mol_C.

Moreover, only a specified range of aggregate sizes can be taken into account (-n <int> <int> option). These sizes are defined by the -m, -x, and --only options as well.

Usage:

```
DistrAgg <input.agg> <distr file> <avg file> <options>
```

Mandatory arguments	
<input>	input structure file
<input.agg>	input agg file

`<distr file>`	output file with distribution of aggregate sizes
`<avg file>`	output file with per-timestep averages
Non-standard options	
`-n <int> <int>`	use aggregate sizes in a given range
`-m <mol name(s)>`	use number of specified molecule(s) as aggregate size
`-x <mol name(s)>`	exclude aggregates containing only specified molecule(s)
`--only <mol name(s)>`	use only aggregates composed of specified molecule(s)
`-c <file> <int(s)>`	save composition distribution for specified aggregate size(s) to `<output>` file
Other options (see the beginning of Chapter 3)	
`-st`, `-e`, `-sk`, `--help`, `--detailed`, `--verbose`, `--silent`, `--version`	

Format of output files:

1) `<output distr>` – distributions of aggregate sizes
   - first line: AnalysisTools version
   - second line: command used to generate the file
   - third line: column headers
     - first is the aggregate size, `As` – either true aggregation number or the size specified by options
     - `F_n(As)`, `F_w(As)`, and `F_z(As)` are number, weight, and z distribution of aggregate sizes (Equation (3.10))
     - next is the total number of aggregates with specified size (sum from all timesteps)
     - the remaining columns (`<mol name>_n`) show average numbers of every molecule type in an aggregate with the specified size
   - data lines follow
   - second to last line: column headers for overall averages
     - `<As>_n`, `<As>_w`, and `<As>_z` are number, weight, and z averages, respectively, of aggregate numbers (see Equation (3.9) for definitions)
     - `<M>_n`, `<M>_w`, and `<M>_z` are number, weight, and z averages, respectively, of aggregate masses (see Equation (3.9) for definitions)
     - next are average numbers of every molecule type in an aggregate with the specified size (`<mol name>_n`)
     - average number of aggregates per timestep, `<n_agg>`
   - last line: the overall averages

2) `<output avg>` – per-timestep averages
   - first line: AnalysisTools version
   - second line: command used to generate the file
   - third line: column headers
     - first is simulation timestep
     - the calculated data follow: number, weight, and z average aggregate size (`<As>_n`, `<As>_w`, and `<As>_z`, respectively) and mass (`<M>_n`, `<M>_w`, and `<M>_z`, respectively)
     - the last column is the number of aggregates in the given step

- data lines follow
- the last two lines are the same as in `<output distr>`

3) `<file>-<size>.txt` from `-c` option – composition distribution of numbers of molecules
- first line: AnalysisTools version
- second line: command used to generate the file
- third line: number of aggregates of given size (sum from all timesteps)
- fourth line: column headers
  - first is the number of molecules in the aggregate
  - the rest are the number distributions of for each molecule type in the given aggregate size
- data lines follow

4) `<file>-ratio_<size>.txt` from `-c` option – composition distribution of ratios of molecular pairs
- first line: AnalysisTools version
- second line: command used to generate the file
- third line: number of aggregates of given size (sum from all timesteps)
- fourth line: column headers
  - first is the ratio of the two molecules (going from 0 to aggregate size with the interval of 0.1)
  - the rest are the ratios of all molecular pairs
- data lines follow

3.6 Info

This utility prints the system information read from an input structure file, possibly augmenting it with information from another structure file (`-i[!] <file>` option) and/or pruning the system to contain only beads from a provided coordinate file (`-c` option). For the effects of these options, see the `Examples/Info` folder.

Note that using LAMMPS `data` , `lammpstrj` or `xyz` input structure file automatically reads coordinates in those files, but using `vtf` does not. This is because a `vtf` timestep does not necessarily contain all beads defined in the `vtf` file, in which case `Info` would automatically prune the system. If coordinates should be read from the input `vtf` structure file (and the system potentially pruned), just use the `-c` option with that filename.

Using the `-i` option with an extra structure file asigns bead mass, charge, and/or radius from the extra file if the bead types in the original file have unspecified values; this is done only for bead types that share names. Also, if the two structure files share molecules that have the same bead type order (which can be initially checked via individual `Info` runs on the two files), bond types, angles and angle type can be added to the molecule types in the original file. Using `-i!` first exchanges beads in the original molecules with those from the extra file (if the molecules have the same number of beads) before adding the extra information. See `Examples/Info` folder for examples; note that this functionality can give unexpected results.

`Info` can also write this information into a new structure file of the given format (`-o` option). Allowed output files are `vtf/vsf` file, LAMMPS `data` file (either with

the extension `.data` or a filename without any recognizable extension), and DL_MESO FIELD file (called `FIELD` or with the extension `.FIELD`).

Coordinates are printed to output files that support them, i.e., LAMMPS `data` or `vtf` file. These coordinates are 0 if no coordinate file is specified or the input structure file does not contain them.

There are a few options for the output structure file. For LAMMPS `data` file, `--mass` can be used to specify LAMMPS atom types by their mass, but print different charges in the `Atoms` section (i.e., `Info`-recognized bead types which differ only in charge are aggregated into the same LAMMPS atom types in the `Mass` section). Furthermore, extra atom types (with mass 1) can be added via the `-ebt` option; these atoms do not appear in the `Atoms` section of the `data` file and can be used as, e.g., extra atom type when srp potential (i.e., non-crossing bonds created by adding ghost particles between bonded beads) is used. For `vtf/vsf` file, `atom default` bead type can be specified via the `-def` option; by default, the bead type with the most unbonded beads is used as the `atom default` type.

Usage: `Info <input> [options]`

Mandatory argument	
`<input>`	input structure file
Options for input files	
`-i[!] <file>`	extra input structure file; see `Examples/Info` directory for the effect of `-i` and `-i!` options (default: None)
`-c <file>`	input coordinate file (default: None)
Options for output file	
`-o <file>`	output coordinate file (default: None)
`-def <bead>`	only `vtf` structure file: use bead type `<bead>` for the 'atom default' line (default:bead type with the most unbonded beads)
`--mass`	only `data` structure file: define LAMMPS atom types by mass but print per-atom charges in the `Atoms` section (default: atom types are the same as `Info`-recognized bead types)
`-ebt <int>`	only `data` structure file: number of extra atom types (for, e.g., srp)
Other options (see the beginning of Chapter 3)	
`-st`, `--detailed`, `--verbose`, `--silent`, `--help`, `--version`	

3.7 JoinSystems

This utility takes two existing systems and joins them into a single system that contains all beads from the two coordinate files.

The second system can be offset against the first one (`-off` option). In each direction, all beads in the second system can be moved by specified distance (only positive numbers are allowed) or moved so that the centre of that box side is in the

centre of the first box's side (use `c` instead of a number as an argument). The final box size is defined as the smallest box that encompasses the two original boxes after the second one is moved. However, the final box size can be redefined via the `-b` option; the centre of the new box is aligned with the centre of the original 'smallest encompassing box'. Note that no check is done whether the bead coordinates are within the new box.

Figure 3.3 illustrates the above-described behaviour (the red and blue lines and balls represent the two original systems while the green lines and transparent balls represent the new system). Figure 3.3b shows the simplest case when two systems are put into one larger system. In figure 3.3c, the final box size is also redefined; the positions of the beads is unchanged, only the box size changes. Note that the absolute bead coordinates remain unchanged only when the output coordinate file supports defining the bounds of the simulation box; e.g., in `lammpstrj` file, the lower and upper bounds of the box are defined while for `vtf` file, only the sidelengths of the box are specified. Should `vtf` be used as the output file, the saved coordinates

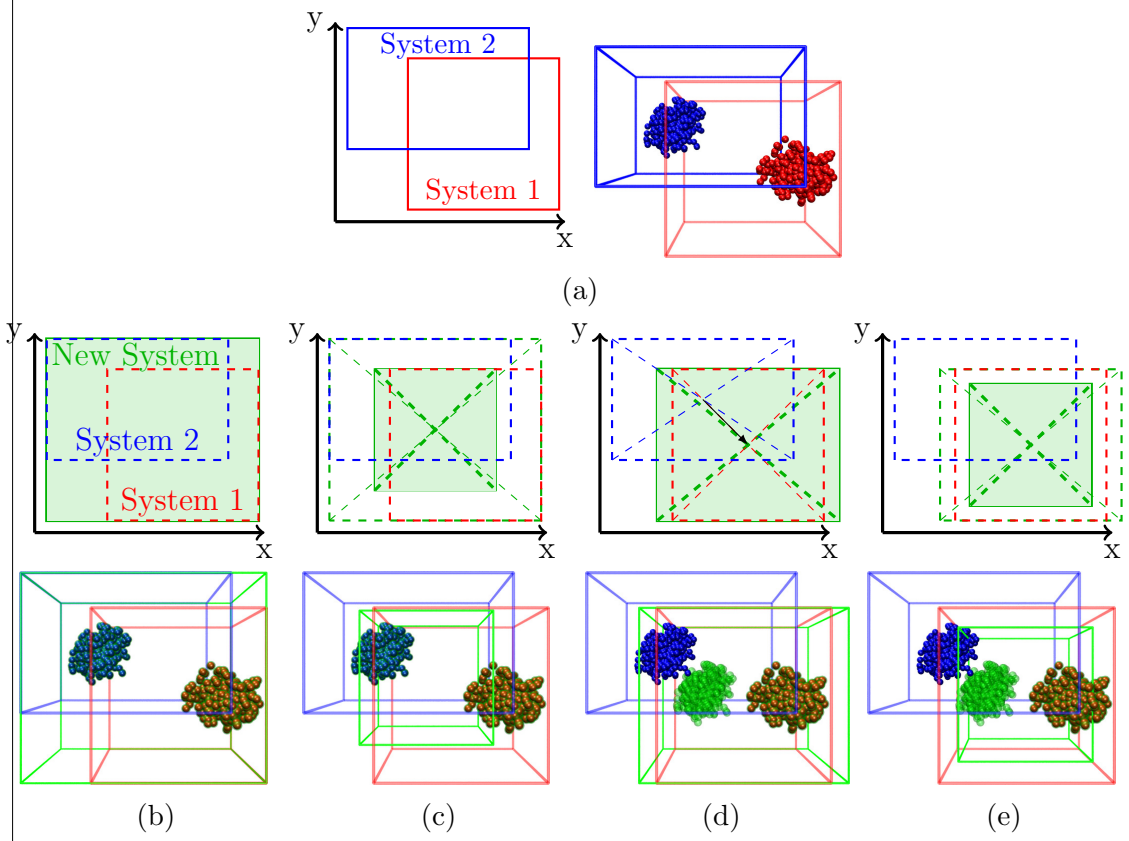


Figure 3.3: Schematic representation and corresponding snapshots illustrating `JoinSystems` behaviour. (a) The original systems: `System1.lammpstrj` (red) and `System2.lammpstrj` (blue) in the `Examples/JoinSystems` folder. The rest show examples of possible options (green rectangles and transparent balls represent the new systems): (b) no options; (c) `-b 20 20 20` option; (d) `-off c c c`; (e) `-b 20 20 20 -off c c c`, i.e., combining (c) and (d). These new systems are in the `Examples/JoinSystems` folder as `NewSystem_#.lammpstrj`, where `#` is `b`, `c`, `d`, or `e`.

would therefore move so the box's origin is in the coordinate beginning.

Using the `-off c c c` option in figure 3.3d moves the second system (the blue one), so that the centre of its box (in all three dimensions) lies on top of the centre of the first system's box (see the arrow in the schematic in figure 3.3d); coordinates of only the second system are adjusted, changing the relative coordinates of beads from the two original systems. If the `-off` and `-b` options are combined (as in figure 3.3e), the system created via the `-off` option is then assigned a new box size.

These examples are also provided in the `Examples/JoinSystems` directory.

The output file can be any file that supports coordinates, and an extra structure file can be created via the `-o` option. Note that if an output `vcf` coordinate file is used, a `vsf` structure file (with the same name except for the extension) is also created.

Usage: `JoinSystems <input1> <input2> <output> [options]`

Mandatory arguments	
`<input1>`	first input coordinate file
`<input2>`	second input coordinate file
`<output>`	output file with the new system
Options	
`-off <x>|c <y>|c <z>|c`	offset of the second system against the first (`c` to place it in the middle of the first system)
`-b <x> <y> <z>`	side lengths of the new simulation box
`-o <file>`	optional output structure file
Other options (see the beginning of chapter 3) As two input coordinate/structure files are needed, some options have 1 or 2 appended to specify which file they correspond to	
`-i1/-i2`, `-st1/-st2`, `--detailed1/--detailed2`, `--verbose`, `--silent`, `--help`, `--version`	

3.8 Selected

This utility creates a new coordinate file of the `xyz` , `vtf/vcf` , or `lammpstrj` format. By default, the utility saves all bead and molecules types (basically transforming one coordinate file format into another), but using `-bt` and/or `-mt` options specifies which bead and/or molecule types to exclude from the output file. If `--reverse` option is used, the specified bead and/or molecule types are instead the only ones that are written into the output file. Should both `-bt` and `-mt` (as well as `--reverse`) be omitted, the utility effectively transforms between the supported coordinate file types.

Besides the standard `-st`, `-e`, and `-sk` options, which timesteps to save can be explicitly specified via the `-n` option that can take a maximum of 100 arguments (the `-st`, `-e`, and `-sk` are then ignored). Also, using `--last` option saves only the last valid step from the input coordinate file (all the previous options are ignored

if `--last` is used). If lammps `data` file is used as a coordinate file, all the above options are ignored as the `data` file contains by definition only a single timestep.

There is also an option to remove periodic boundary conditions for molecules (i.e., to join them) via the `--join` switch. Conversely, the simulation box can be wrapped (i.e., the periodic boundary conditions applied, putting all beads inside the box) via the `--wrap` switch. If both `--wrap` and `--join` options are used, the simulation box is first wrapped and then the molecules are joined.

Usage: `Selected <input> <output> <bead type(s)> [options]`

Mandatory arguments	
`<input>`	input coordinate file
`<output>`	output coordinate file
Options	
`-bt <bead type>`	bead types to exclude
`-mt <mol type>`	molecule types to exclude
`--reverse`	save only specified types instead of excluding them
`--join`	join molecules by removing periodic boundary conditions
`--wrap`	wrap simulation box (i.e., apply periodic boundary conditions)
`-n <int(s)>`	save only specified timesteps
`--last`	save only the last step
Other options (see the beginning of Chapter 3)	
`-st`, `-e`, `-sk`, `-i`, `--detailed`, `--verbose`, `--silent`, `--help`, `--version`	