File:multisub1b.doc

MULTISUB
(formerly MONTESUB)

Version 1-b, May 2005

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1. Introduction to MULTISUB

MULTISUB is a computer program that generates possible conformations a multisubunit model, in the sense employed in program HYDROSUB. The particle will consist of:

- *"Subunits"* of ellipsoidal or cylindrical shape
- *"Linkers", or "chains"*, which will be modeled as arrays of spheres

MULTISUB produces the files needed for the calculation the properties of each individual conformation using HYDROSUB Version 5b-2 or higher

The supplied source code of MULTISUB, written in FORTRAN, is intended to be a sample, or template, of the program that the user has to write for his/her particular model.

MULTISUB can be used for either of the following purposes

- A conformational search for a rigid particle, generating multiple possible conformations whose properties, computed by HYDROSUB, would be compared to experimental data in order to find the best fitting one.
- Monte Carlo calculation of properties for a flexible particle, of which many possible conformations have to be generated, and their properties evaluated afterwards using HYDROSUB in order to evaluate the Monte Carlo averages

In either case, MULTISUB facilitates the task of creating the files that will be needed in the subsequent HYDROSUB calculation.

2. Literature

The primary reference for MULTISUB (its first versions was named MONTESUB) is:

- J.Garcia de la Torre, H.E. Perez Sanchez, A. Ortega, J.G. Hernandez, F.G.Diaz and M.C. Lopez Martinez, "Calculation of the solution properties of flexible macromolecules: methods and applications", *Eur. Biophys. J.* 32, 477-486 (2003)

The general, primary refereence for HYDROSUB is:

- J. García de la Torre and B. Carrasco, "Hydrodynamic properties of rigid macromolecules composed of ellipsoidal and cylindrical subunits", *Biopolymers* 63, 163-167 (2002).

3. Writing your own MULTISUB program

As mentioned above, the source code that we supplied for MULTISUB is intended to be a template that you will employ to write the MULTISUB program for your own case. With this purpose in mind, we have written the supplied MULTISUB code in such a way that it contains:

- *General* sections, that you must keep in your program without any modification and in the same place
- *Specific* sections, that the user will write, replacing the specific sections of the sample code

The purpose and placement of the sections (look at the sample code) are as follows:

1) General section no. 1 contains comments, declaration of variables used in other general sections.
2) Specific, user-written section no. 2 will contain the declaration of variables used in your own specific sections.
3) General section no. 3 reads a general data file, **`multisub-dat.txt`** , and writes a general data file, **`hydrosub.dat`** .
4) Specific, user-written section no. 4 will be where the program reads the data needed for the model under study.
5) General section no. 5 contains a DO loop over the number of conformations to be produced. For each conformation, generates the name of the structural file and opens this file. See the HYDROSUB User Guide.
6) Specific, user-written section no. 6 will contain the calculations that generate the data for each conformation, to be written in the structural file. The variables to which values will be assigned here are as follows (for more details, see HYDROSUB Users' Guide) :

- NSUB: Number of subunits
- ITYPE: (dimensioned to NSUB) type of each subunit (1, 2, 3, 4 see HYDROSUB Users's Guide)
- SEMILONG, SEMISHORT (dimensioned to NSUB) long and short semiaxes of subunits (in Ansgstroms)
- XC, YC, ZC, T, F (dimensioned to NSUB), the three Cartesian coordinates (in Angstroms) of the center of the subunit, and the polar angles theta and phi (in degrees) defining its orientation
- NESF: number of spheres in the linkers or chains (may be zero)
- X , Y, Z, E (dimensioned to NESF), Cartesian coordinates and radii of the spheres

7) General section no. 7 writes the information for each conformation to the individual structural files. Main program ends here
8) Specific, section no. 8 (if needed) may contain user-written subroutines for the construction of the conformations

4. Utilities in MONTESUB

The provided source code contains some FORTRAN subroutines that may be useful for building your models. Presently, this are:

- Testing overlap between spheres and/or ellipsoids
- Generation of a freely jointed chain, with side groups, with excluded volume restrictions
- Generation of random numbers
- …. More utilities will be added in future releases

5. Input data files

The name of the main (general) input data file for HYDROSUB will be `multisub-dat.txt,` and it will contain the following lines:

- TITLE`(CHARACTER*20)` Title for the model

- FILENAME5 `(CHARACTER*5)` Name to be used for the various output files corresponding to each generated conformation. The various files produced will have names of the form `xxxxxnnn.txt`, where xxxxx is the name that you give for FILENAME5, and nnn will be a number assigned by the program: 001, 002, etc

- NSIG `(INTEGER)` Number of values of the radius of the minibead.

- SIGMIN `(REAL)` Lowest value of sigma, the minibead radius

- SIGMAX `(REAL)` Highest value of sigma, the minibead radius

- TEMP `(REAL)` Temperature, Kelvin

- ETA (REAL) Solvent viscosity, poises
- RM (REAL) Molecular weight .
- VBAR (REAL) Partial specific volume, cm^3/g
- RHO (REAL) Solution (approx. Solvent) density, g/cm^3
- IDIF is a flag that indicates (if IDIF is 1) that you wish a detailed report of the diffusivity of the particle.
- NCONF (INTEGER) Number of conformations to be generated

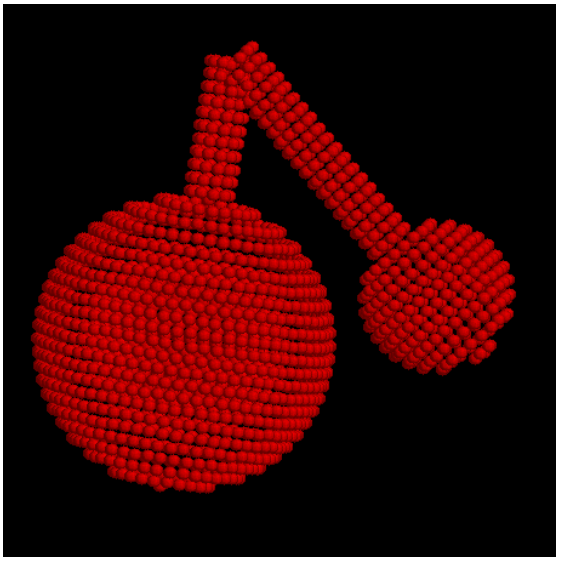
More details about TITLE, NSIG, SIGMIN, SIGMAX, TEMP, ETA, RM, VBAR, RHO and IDIF can be found in the HYDROSUB User's Guide.

6. Ouput files. Running HYDROSUB

MULTISUB will produce the following files:

- A log file, named **multisub-log.txt** , which reports messages during program execution
- One file named **hydrosub.dat**, which will be main input data file for the subsequent HYDROSUB calculation
- NCONF files, named **xxxxx001.txt, xxxxx002.txt,** etc, where **xxxxx** is FILANEME5, which will be structural files for the subsequent HYDROSUB calculation

After running MULTISUB, you will run HYDROSUB to compute the hydrodynamic properties. The procedure is very simple, because you already have the input files **hydrosub.dat** and **xxxxx001.txt, xxxxx002.t**xt, etc. Just launch the HYDROSUB executable and you will obtain the final results. As this is a "multi-case" HYDROSUB run, the output file named **summary.txt** will be particularly helpful. This is a numeric archive containing NCONF lines, one for each conformation. It has 13 columns containing (1) first 10 characters of title; (2) translational diffusion coefficient; (3) radius of gyration; (4) volume; (5-9) the five relaxation times; (10) intrinsic viscosity; (11) sedimentation coefficient; (12) longest distance; (13) covolume.



Afterwards, you will obtain the final results for properties of the flexible particle by averaging, for each property, all the individual values over the NCONF conformations. For this purpose, you can open `summary.txt` with an spreadsheet like EXCEL or anyother, to easily obtain the average for property (i.e. for each column).

Also, as described in the HYDROSUB User's Guide, you obtain a graphics file to be visualized with our displaying program, VISUALBEADS.

7. Examples

We provide two examples that illustrate the use of MULTISUB, implemented in full, working versions of the code

Example 1 (**`multisub_1b-brodum.for`**) is a model composed of two spherical globules joined by a connector that resembles a bent or broken rod, consisting of two rodlike arms, which make some angle , θ, (between the prolongation of the first arm and the second one), which is varied from 0 to 140^o, because for higher angles the two speheres overlap

The specific sections have the following purpose:

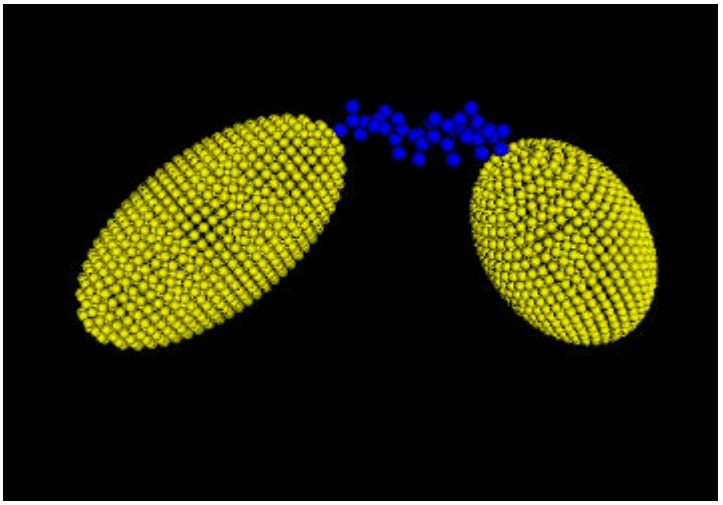
- Specific section 2 declares the variables used in the other specific sections
- Specific section 4 gives the dimensions of the globules and arms
- Specific section 6 determines, for each value of the angle θ, the position and orientation of the four subunits:.

Example 2 (**`multisub_1b-dimer.for`**) is for a model with two globular, ellipsoidal domains, linked by a flexible chain consisting of a skeleton and side groups. The symmetry axes of the first and second ellipsoid are directed along the line of centers of the two first and two last, respectively, skeletal beads. The chain is a freely jointed flexible chain with random bond angles greater than 60^o . All the skeletal beads except the two terminal ones have a side bead (representing a side group) of the same size as the skeletal ones, and directed along the other diagonal of the bond angle. Any

overlap, between beads, between the two ellipsoids or between beads and ellipsoids are forbidden.

The specific sections have the following purpose:

- Specific section 2 declares the variables used in the other specific sections
- Specific section 4 reads a file, **`dimerdata.tx`**t, containing the structural information. See the commented lines in the code for the meaning of the structural variables
- Specific section 6 constructs one possible conformation of the model. First, a conformation of the chain, including the side beads, free of excluded volume (overlapping) effects is generated. Then, ellipsoids are attached to the ends. Finally, the conformation is tested for overlapping between ellipsoids and between ellipsoids and the beads
- Specific section 8 contains some subroutines for the above specific purposes



8. Hints and notes.

- Recall that HYDROSUB Version 5-a (March, 2002) considered only subunits, represented as shell of minibeads, but not spheres. Now you must use HYDROSUB Version 5-b2 (May 2005) or a later version. For a proper understanding of MULTISUB, you should understand first how HYDROSUB works

9. Release notes

This is the first released version of MULTISUB. In future releases this section will contain a description of the main changes.

This FORTRAN has been tested in two platforms: (a) PC/Windows with Visual Fortran 5.0 and (b) Linux RedHat with g77. The FORTRAN code is fully standard and therefore should compiled succesfully in any other platform.