File:multihydro3.doc

MULTIHYDRO

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1. Introduction to MULTIHYDRO

MULTIHYDRO is a computer program that generates possible conformations of a particle, providing a convenient interface with the HYDRO computer program, so that the files for the calculations for all the conformations are automatically generated.

Essentially, there are two general uses for MULTIHYDRO

(1) Structural search of a rigid particle, generating multiple possible conformations and facilitating the HYDRO calculation for each of them. The user would later decide the ones that best fit some experimental data

(2) Simulation of solution properties of a flexible particle. As in the first case, the user would provide the generation of the possible conformations, and would also be in charge of doing the *a posteriori* averaging proper of the rigid particle

In both cases, the program has a friendly interface with HYDRO, whose output `summary.txt` file is a convenient for either search or averaging.

As described below, MULTIHYDRO is supplied as a set of pieces of source code, written in FORTRAN, and it is intended to be a sample, or template, of the program that the user has to write for his/her particular model

2. Literature

The primary reference for MULTIHYDRO is:

- J.Garcia de la Torre, A. Ortega, H.E. Pérez Sánchez and J.G. Hernandez Cifre, "MULTIHYDRO and MONTEHYDRO: Conformational search and Monte Carlo

calculation of the solution properties of rigid and flexible bead models", *Biophys. Chem.* 116, 121-128 (2005).

The general, primary reference for HYDRO is:

- J. Garcia de la Torre, S. Navarro, M.C. Lopez Martinez, F.G. Diaz, J. Lopez Cascales. HYDRO. A computer software for the prediction of hydrodynamic properties of macromolecules. *Biophys. J.* 67, 530-531 (1994).

3. Writing your own MULTIHYDRO program

As mentioned above, the source code that we supplied for MULTIHYDRO is intended to be a template that you will employ to write the MULTIHYDRO program for your own case. With this purpose in mind, we have written the supplied MULHYDRO 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 and insert in the proper places within the 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 (compulsory data) contains values that the user has to supply for the following variables

- **`icase`** `(INTEGER)` Type of hydrodynamic calculation in the HYDRO++ calculation. Please consult the HYDRO++ manual for a description of the several types.
- **`temp`** `(REAL)` Temperature, Centigrade
- **`eta0`** `(REAL)` Solvent viscosity, poise
- **`rm`** `(REAL)` Molecular weight
- **`vbar`** `(REAL)` Partial specific volume of solute, g/cm3
- **`solden`** `(REAL)` Solution density, cm3/g
- **`title`** `(CHARACTER*20)` Title for the calculation; up to 20 characters
- **`filename`** `(CHARACTER*5)` Generic file name to be user for output files, with 5 characters (not more or less).
- **`nconf`** `(INTEGER)` Number of conformations to be generated

This section will have necessarily the format:

```
icase= ……
temp= ……
eta0= ……
rm= ……
vbar= ……
solden= ……
```

```
title='……'
filename='……'
nconf=……
```

where …… means the user data

NOTE: **rm** is needed only for the calculation of the sedimentation coefficient and the intrinsic viscosity. **vbar** and **solden** are needed only for the sedimentation coefficient. Please, see the HYDRO User's Manual, as it is HYDRO the program that will do the hydrodynamic calculations.

3) Specific, user-written section no. 3 will contain data specific of the structure whose multiple conformations have to be generated. Lengths, sizes, dimensions, etc., will be given in Angstrom units.

4) General section no. 4 initiates a Fortran DO loop over the conformations to be generated.

5) Specific, user-written section no. 5 will contain the specific instructions to construct each conformation, with the information provided in Section 3. At the end of this section, the number n , of beads, and the coordinates , **x(i,k)**, k=1,2,3, i=1,…,n , and radius, **e(i)**, of each bead must be defined. Some generated structures could be perhaps rejected, for reasons such as bead overlapping. The criterion for rejection has to be programmed by the user. Note that within section 6 we provide some utility subroutines for that purpose.

6) General section no. 6 is the last section in the program. First, it records the generated (and eventually accepted) conformation in the files required for the HYDRO calculation. It also contains some utility subroutines that may be used (not necessarily) in the construction of the conformations of the user's model, for purposes like checking bead overlap, random number generator.

The code supply for MultiHydro will contain also general purpose subprograms. Presently, there is one to detect overlapping in an array of beads, and another that generates conformations of a freely jointed chain.

4. Ouput files. Running HYDRO

MULTHYDRO will produce the following files:

- One file named `hydro.dat`, which will be the main input data file for the subsequent HYDRO calculation

- **nconf** files, named `xxxxx001.txt, xxxxx002.txt,` etc, where `xxxxx` is **filename**, which will be structural files for the subsequent HYDRO calculation

After running MULTIHYDRO, you will run HYDRO to compute the hydrodynamic

properties. The procedure is very simple, because you already have the input files `hydro.dat` and `xxxxx001.txt, xxxxx002.txt,` etc. Just launch the HYDRO executable and you will obtain the final results. As this is a "multi-case" HYDRO 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 have to analyze the set of values obtained for each individual conformation. For this purpose, you can open `summary.txt` with an spreadsheet like EXCEL. Similarly, it can be easily read by a any user written programThe handling of this set of results. The handling of the individual data will be according to your purpose when using MULTIHYDRO. Some examples could be:

a) In the structural search of a rigid particle, you would plan to find the conformation whose properties are closest to available experimental data

b) If you are doing a Monte Carlo type calculation, you will have to obtain the averages (with the proper weights) of the values of each property over all the generated conformations.

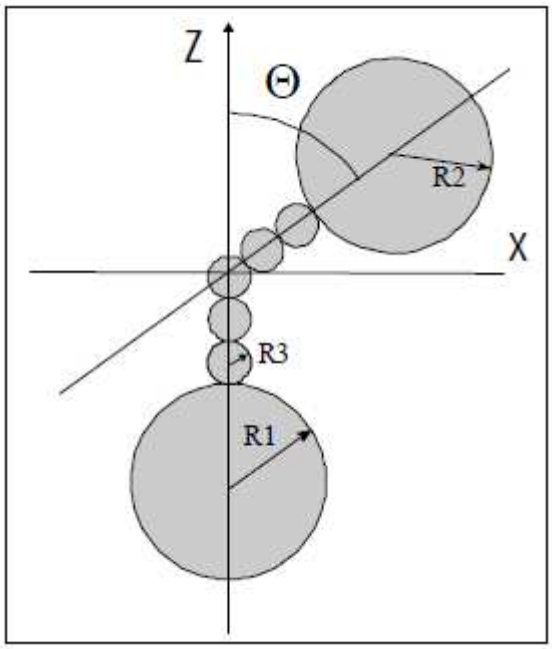
In both cases the tabular format of `summary.txt` will be helpful.

For more details, see the HYDRO Users's Guide

5. Example.

As an example of the use of MULTIHYDRO, we present a case in which the structure being modeled has two globular domains connected by a rodlike connector, with either a rigid bent or a flexible hinge; we call this structure the "bent" or "broken dumbbell". The globules are represented by spheres of radii r_1 and r_2. The connector is represented by a string of n_C beads of radius r_3 (its total length is $L = 2n_C r_3$). There are n_1–1 beads in one of the arms, 1 bead at the bent or hinge, and n_2 beads at the second arm, so that $n_C = n_1+n_2$ beads and the total number of beads in the model is $n=n_1+ n_2+2$.

The conformation is determined by angle θ, subtended second arm and the prolongation of the first one, as indicated in the Figure. The beads are placed in the (x,z) plane, with the first arm along the negative part of the z axis. Thus the coordinates of beads i=1,…,n_1 are (0, 0, $2(i$-1$)\ r_3$) and those of the first globule are (0, 0, $2(n_1$-1$)\ r_3+r_1$). The coordinates of the second arm and second globule are of the form (ρu_x, 0 , ρu_z) where $u_x=\sin\theta$ and $u_z=\cos\theta$ are the components of a unitary vector along the arm, and $\rho=2ir_3$ for the beads i=1,…,n_2 in the connector and , $\rho=2\ n_2 r_3+r_2$ for the second globule.



A number of conformations **nconf**=36 is generated, with values of the angle (in radians) $\theta=(i_C\text{-}1)\pi/$**nconf**, with i_C=1,…**nconf,** or $\theta = 5(i_C\text{-}1)$ in degrees for the 36 conformations. Subroutine **CHECK_OVERLAP** is used to detect, and reject, conformations with overlapping beads. MULTIHYDRO produces the input files for the HYDRO calculation on the accepted conformations, that is done straightforwardly. File `summary.txt` from the HYDRO calculation can be readily inspected or inserted in an Excel spreadsheet.

If the problem were a conformational search of the rigidly bent dumbbell , in this case the determination of the bent angle could be done comparing the results with experimental data.

Another possibility is that of the flexibly hinged dumbbell. For any property, say p, the final value is a conformational average, over the values for the successive θ's, of the form $p = (\Sigma w_k p_k) / (\Sigma w_k)$ where w_k is some statistical weight, which would eventually contain an energetic and/or a geometric contribution.

6. Hints and notes.

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This version of the program does not consider the calculation of scattering intensities, distribution of distances and covolume, and assumes that the full diffusion tensor is to be calculated. Therefore it fills the file named `hydro.dat` file with the required lines for the variables NH, NS,NTRIALS and IDIF with the values 0, 0, 0 and 1. This is done in the lines of code:

```
WRITE(1,250) 0
WRITE(1,250) 0
WRITE(1,250) 0
WRITE(1,250) 1
```

These lines could be changed if these calculations are required. In order to introduce your changes, please consult the HYDRO++ User Guide for instructions on how this information must be provided

7. Release notes

- This FORTRAN has been tested in two platforms: (a) PC/Windows with Visual Fortran 6.5 compiler and (b) Linux Red Hat 7.2 with g77 compiler. The FORTRAN code is fully standard and therefore should compiled succesfully in any other platform.

- The previous released version was 2, October 2010. The change in this version is that temperature is expressed in centrigrades, and some aspects of compatibility with version 10 of HYDRO++ . The change in version 2 with respect to the previous one, 1c of May 2005, was the inclusion of variable icase for type of hydrodynamic calculation, as required by HYDRO++ program (versions 8 and successive ones).