

HYDROSUB

Version 5a, March 2002

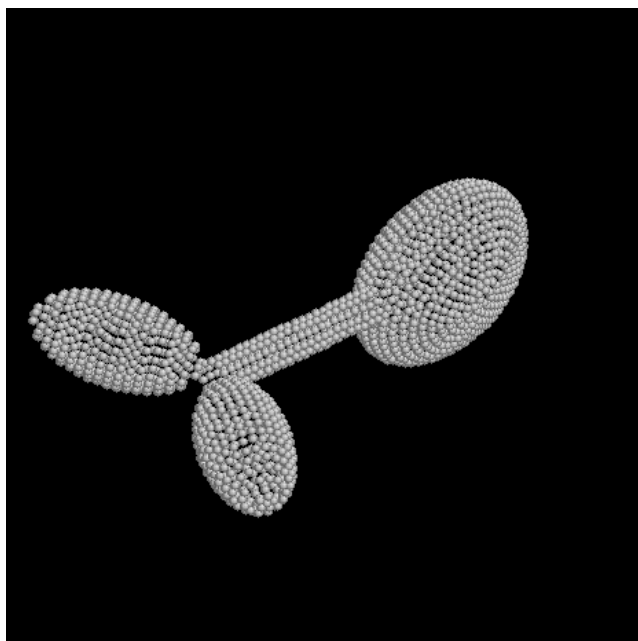
Index

1. Introduction to HYDROSUB
2. Literature
3. Running HYDROSUB. Input data files
4. Output files
5. Notes and hints
7. Release notes

1. Introduction to HYDROSUB

HYDROSUB is a computer program for the calculation of solution properties of a macromolecular or supramolecular structure modeled as an assembly of subunits having ellipsoidal (prolate, spherical or oblate) and/or cylindrical shapes.

For instance, the next figure shows the hydrodynamic model for an antibody molecule with two prolate Fab subunits, an oblate Fc subunit, and a long hinge



2. Literature

The primary reference 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).

If you wish to cite also the theoretical work on which the bead modeling procedure is based, a proper cite is our 1981 review in *Quarterly Reviews of Biophysics*. In our 1999 paper in *Biophysical Journal*, you can find an update of the theory, and a discussion on bead and shell modeling methodologies:

- J. Garcia de la Torre and V.A. Bloomfield, "Hydrodynamic properties of complex, rigid, biological macromolecules. Theory and applications". *Q. Rev. Biophy.*, 14, 81-139 (1981)
- B. Carrasco and J. Garcia de la Torre, "Hydrodynamic properties of rigid particles. Comparison of different modeling and computational strategies". *Biophys. J.* 76, 3044-3057 (1999).

3. Running HYDROSUB. Input data files

As in all the HYDRO family of programs, you will have to supply two input data files: (a) the main input data file, which will specify primary data such as temperature, solvent density, etc.; and (b) a structural data file, which will contain the information about the structure or geometry of the macromolecule or particle that you are considering.

In the case of HYDROSUB, the structural information will contain information on the size and shape of each subunit and its placement within the whole particle. This will be provided by the user in an ASCII file whose structure and contents are given in section 3.d.

The name of the main input data file for HYDROSUB will be `hydrosub.dat`, and it will contain the following lines:

3.a. First part of the input file.

Basically this part provides the information on the structure of the macromolecule. It contains the following lines (the FORTRAN types are specified):

- TITLE (CHARACTER*20) Title of the calculation
- FILENAME (CHARACTER*30) Name to be used for the various output files corresponding to each subcase in a many-cases execution. The various files produced will have names of the form `filename.xxx`, where xxx is an extension

depending on the file type (see section 4 below). This name would eventually include the path for the files.

- INPUT (CHARACTER*30) Name of the structural file, eventually including its path.

HYDROSUB employs the shell-model methodology. The primary hydrodynamic model is not used in the hydrodynamic calculations. Instead, a shell model, composed of ‘minibeads’ of radius σ is derived from it, and extrapolation to the shell model limit of $\sigma=0$ is carried out. For this purpose, the following information has to be supplied next in the main input data file

- NSIG (INTEGER) Number of values of the radius of the minibead. This radius will range from SIGMIN to SIGMAX. It must be greater than 2 (typically 5 to 8). There is also the possibility of letting to the program the task of estimating the two extreme values of σ ; this will be indicated giving the value -1 for NSIG, and in this case you will omit the two following lines with the values of SIGMIN and SIGMAX.
- SIGMIN (REAL) Lowest value of σ , the minibead radius
- SIGMAX (REAL) Highest value of σ , the minibead radius

The smaller the size of the minibeads, the larger the number of them needed to cover the surface of the particle. The present version of the program works with a maximum of 2000 minibeads. If SIGMIN is too small, an error message will be obtained and the program will stop. The value of SIGMAX should be taken such that the number of minibeads is not too small, say in the range 200-400.

3.b. Second part of the input file.

This part provides information on some basic properties of macromolecule and solvent. It contains the following lines:

- T (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, including the full (anisotropic) translational, rotational and coupling tensor, and the position of the hydrodynamic (diffusion) center.

3.c. End of calculation or next case

- Next or final line: If this case is the only or the final one, in the next line you will put an asterisk followed by 19 spaces.

3.d. The structural file for HYDROSUB.

Prior to the HYDROSUB calculation, you have to build a structural file that specifies the size and shape of the particle that you are considering. Positions and orientations of the subunits are referred to an arbitrarily chosen system of Cartesian axis. You have to specify, for each subunit:

- The type of the subunit, given by `ITYPE` (`INTEGER`) which can take the following values: 1(prolate), 2(uncapped cylinder), 3(oblate), 4 (capped cylinder or disk)
- The subunit sizes, in Angstroms, given by `SEMILONG` and `SEMISHORT` (`both REAL`). For ellipsoids, `SEMILONG` and `SEMISHORT` are, respectively, the longest and shortest semiaxes. For cylinders, `SEMILONG` and `SEMISHORT` are, respectively, **half** of the length and the radius. A disk is a cylinder for which `SEMILONG` is half of the height or thickness.
- The Cartesian coordinates, in Angstroms, `XCEN`, `YCEN`, `ZCEN` (`all REAL`) of the geometric center of each subunit
- The spherico-polar angles `THETA` and `PHI` in degrees (`both REAL`), that specify the orientation of the main (revolution symmetry) axis of the ellipsoid or cylinder. `THETA` is the angle subtended by the main particle axis and the Z Cartesian axis. `PHI` is the angle subtended by the projection of the main particle axis on the (X,Y) plane and the X Cartesian axis.

The structural file can have any name, and its contents will be:

- A first line with the value of `NSUB` (`INTEGER`), the number of subunits
- A number of lines equal to `NSUB`, containing (separated by spaces) the values of `ITYPE`, `XCEN`, `YCEN`, `ZCEN`, `THETA`, `PHI`, `SEMILONG` and `SEMISHORT`

4. Output files

Several files are produced at execution time. There will be a set of files for each case included in a single run. All these files will have a common name, given by the filename specified for each case in the input file, and a different extension. The extensions correspond to:

- `.res` Output file containing the mains results, with the name specified in the input file
- `.she` is a pdb-formatted file containing the coordinates of the last shell model, that can be viewed with RASMOL.
- `.sol` is an ASCII file containing data needed if you wish to run the separate program SOLPRO

Other files are:

- `summary.txt` is a numeric archive containing a line for each case in the calculation. 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.

NOTE: Do not forget to specify: Display / SpaceFill in the RasMol menu to see the the visualization files.

5. Hints and notes.

- The molecular weight is used in the calculation of the intrinsic viscosity and the sedimentation coefficient, and the specific volume of the solute and the solution density are only used for the sedimentation coefficient. If you do not know these quantities, you may give then some approximate or estimated values in the data files. HYDROSUB will still be useful, because all the other solution properties (diffusion coefficients, relaxation times, radius of gyration, scattering properties, covolume, etc) will be correct.

6. Release notes

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

This program has been developed in a Windows PC. The MS DOS/Windows executable can be started from Windows, but we advise to open a MS DOS session in a window for program execution, while doing the other tasks (editing, visualization, etc) as usually in Windows. Executables of this program are also available for other platforms: Linux, Silicon Graphics and Compaq-DEC Alpha.