

# HYDRO

Version 5a, March 2002

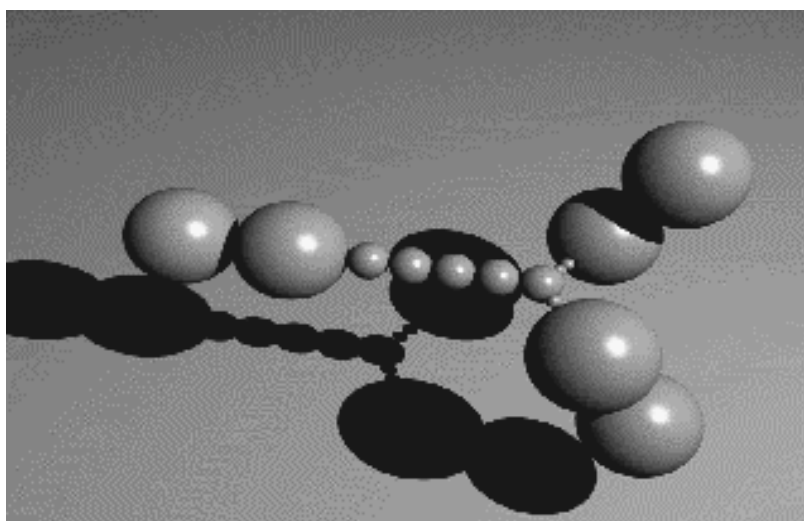
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## 1. Introduction to HYDRO

HYDRO is a program for the calculation of hydrodynamic coefficients and other solution properties of rigid macromolecules, colloidal particles, etc, employing bead models. In strict sense, bead models are those in which the shape and volume of the particle are modeled as an array of spheres (beads) of arbitrary – equal or unequal – size. It is the classical program that has been available from us for many years. Note that there is another, different, modeling strategy based on bead-shell models. This alternative methodology is implemented in other programs of our suite (HYDROPRO, HYDRONMR, HYDROMIC, HYDROPIX, HYDROSUB, etc). The user of HYDRO has to build previously the bead model, which will be specified as a list of Cartesian coordinates and radii of the beads.

The following figure illustrates a bead model, for the HYDRO, calculation of the IgG3 human antibody, made up of only 15 beads.



## 2. Literature

The 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).

If you employ scattering related properties (distribution of distances, longest distance, scattering function), or the covolume – which is related to the second virial coefficient – then the you may also cite the reference where these calculations are described:

- J. Garcia de la Torre, B. Carrasco and S. E. Harding, “Calculation of NMR relaxation, covolume and scattering-related properties of bead models using the SOLPRO computer program”, *Eur. Biophys. J.*, 28, 119-132" (1999).

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. Biophys.*, 14, 81-139 (1981)
- B. Carrasco and J. Garcia de la Torre, “Hydrodynamic properties of rigid particles. Comparison of different modeling and computational strategies”. *Biophysical Journal* 76, 3044-3057 (2000). (XXX-REVISAR-CITA. CREO QUE ES 1999)

## 3. Running HYDRO. Input data files

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. The name of the structural file will be one of the data in the main input data file. The name of the main input data file for HYDRO will be `hydro.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 (separate) file containing the information on the bead model, eventually including its path. It will have the following lines: (1) (REAL) `U`, unit of length (in cm) in which coordinates and radii are given (2) (INTEGER) Number of beads, and (following `N` lines), in each line, four comma-or space-separated values: three Cartesian coordinates and radii of beads

### 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,  $\text{cm}^3/\text{g}$
- `RHO` (REAL) Solution (approx. Solvent) density,  $\text{g}/\text{cm}^3$

### 3.C. Third part of the input file.

This part is intended for the calculation of some non-hydrodynamic properties that, in previous versions of our software, were considered separately in the computer program SOLPRO. These properties are the scattering form factor (Debye expression), the distribution of intramolecular distances, and the covolume, and are calculated from the coordinates of the spheres.

For bead models, this calculation is made from the bead coordinates and sizes.

The data that you have to supply are:

- `NH` (INTEGER), the number of values of the scattering (angular) variable, `h`. If you wish to omit the scattering calculation, the value given here should be 0, and the following line (`HMAX`) is omitted.
- `HMAX` (REAL), the largest value of `h` ( $\text{cm}^{-1}$ ), so that the scattering variable will range from 0 to `HMAX`

- `NS (INTEGER)`, the number of intervals for the distribution of distances. The values of the intramolecular distances will be varied between 0 and the longest distance, which is determined by the program. If you wish to omit the calculation of the distribution of distances, the value given here should be 0.
- `NTRIALS (INTEGER)` is the number of trials or MonteCarlo moves in the calculation of the covolume. Set this value to 0 if you wish to omit the covolume calculation. Recall that this calculation is very time-consuming, and must be restricted to models with not too many beads.

The most important quantities related to translational and rotational diffusion are the translational and rotational diffusion coefficients and the rotational relaxation times. The program will give you these quantities. For some special purposes you may also want the full 6x6 diffusion tensor, which contains the 3x3 translational diffusion tensor, rotational diffusion tensor, and the translation-rotation coupling tensor, as well as the center of diffusion.

- `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.D. 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.

## 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 main results, with the name specified in the input file
- `.bea` is a pdb-formatted file containing the coordinates of the original bead model (mode HYDRO), to be viewed with RASMOL, that is produced when the model contains identical beads. No provision of unequal beads is considered so far.
- `.sol` is a binary 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 RasWin 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 and 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. HYDROMIC 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

The main changes in this new version are:

- The unit of length, number of beads, and bead coordinates are no longer part of `hydro.dat`. This data are now given apart, in the structural file.
- A file for visualization is given in the case of beads of the same size
- Optional calculation of scattering related properties (distribution of distances, scattering function) and covolume
- Optional report on the full translational/rotational tensors and hydrodynamic (diffusion) center.
- File for subsequent SOLPRO calculation

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.