

HYDROPIX

(Including MAKEPIXB)

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1. Introduction to HYDROPIX

HYDROPIX is a computer program for the calculation of solution properties of macromolecular or supramolecular structures having an arbitrary shape, using bead-shell models. The task of building and specifying the hydrodynamic model is left to the user, but for this purpose we provide an ancillary FORTRAN program, MAKEPIXB, which just requires some extra lines of code that specify the dimensions and shape of the structure.

2. Literature

The primary reference for HYDROPIX and MAKEPIXB is:

- J. García de la Torre, "Building hydrodynamic bead-shell models for rigid bioparticles of arbitrary shape" *Biophys. Chem.*, 94, 265-274 (2001).

If you employ scattering related properties (distribution of distances, longest distance, scattering function), or the covolume, 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”. *Biophys. J.* 76, 3044-3057 (1999).

3. Running HYDROPIX. 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 HYDROPIX, the structural information is in the *pixbit* file, usually named `xxxxxxx.pxb`, with the `.pxb` extension. The name of the structural file will be one of the data in the main input data file. This file is previously produced by the user with the help of the ancillary program MAKEPIXB. Instructions of this previous step are given in section 3.e.

The name of the main input data file for HYDROMIC will be `hydropix.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 *pixbit* file, eventually including its path.

HYDROPIX 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 sigma; 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 sigma, the minibead radius
- SIGMAX (REAL) Highest value of sigma, 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, cm³/g
- RHO (REAL) Solution (approx. Solvent) density, g/cm³

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 *pixbit* structures, the coordinates are taken from the last filling model

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 (HMAX) line is omitted.

- `HMAX` (`REAL`), the largest value of h (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.

In `HYDROPIX`, the calculation of scattering and distances is a bit lengthy, but still feasible. However, the calculation of the volume can be extremely long. It may be advisable to avoid these calculations in the way indicated above.

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.

3.e. `MAKEPIXB`: An ancillary program for `HYDROPIX` calculations

Prior to the `HYDROPIX` calculation, you have to build a structural file that specifies the size and shape of the particle that you are considering. For this purpose, I supply the source code of the FORTRAN program `MAKEPIXB`, and the user has to write two additional pieces of FORTRAN code, namely the files `maxdims.for` and `conditions.for`. You have to imagine the particle placed in the (+,+,+) octant of a system of Cartesian coordinates. The particle will be as close as possible to the origin of the system of axes, but none of its points will have a negative coordinate. Imagine a box (parallelepiped) of dimensions `XMAX`, `YMAX`, `ZMAX`, whose two diagonally opposite corners are (0,0,0) – i.e., the origin – and (`XMAX`,`YMAX`,`ZMAX`). The particle must be fully enclosed within this box. The coordinates of points within the box will be discretized as intervals with some `SPACING` (note that the number of points is inversely proportional to the third power of the spacing).

Your first FORTRAN file, `maxdims.for`, will contain just the values of `XMAX`, `YMAX`, `ZMAX` and `SPACING`. In addition to this, you have to specify the shape of the

particle. This is done by means of the condition that a point in the box must satisfy if it belongs to the particle. This is done in your second FORTRAN file, `conditions.for`. This file contain as many FORTRAN statements as needed, the last of which will be of the form `CONDITION =` where `CONDITION` is a FORTRAN LOGICAL variable, and `.` is a valid LOGICAL expression that is `.TRUE.` if the point belongs to the particle.

For instance, the following two files specify a particle whose shape is a disk with a central hole, with inner radius 15 Angstroms, outer radius 40 Angstroms and thickness (height) 20 Angstroms:

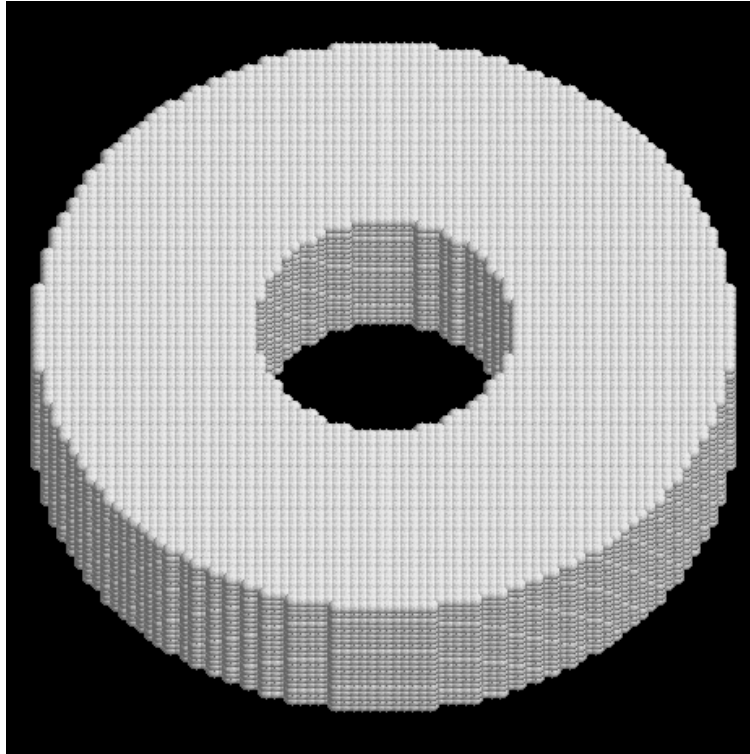
```
C-----
C File: maxdims.for
C This is for a disk-shape particle, with height 20 and outer radius
C 40, having a central hole of radius 15
C Spacing is 1.0=20/20, so that along the shortest dimension of
C the box there are NX=20 pixels
      XMAX=80.
      YMAX=80.
      ZMAX=20.
      SPACING=1.0
C-----

C-----
C File: conditions.for
C This is for a disk-shape particle, with height 20 and outer radius
C 40, having a central hole of radius 15
      R=SQRT((X-40.)**2+(Y-40.)**2)
      CONDITION = R.GE.15.AND.R.LE.40.
C-----
```

In our above mentioned paper describing this programs you can find further examples.

When you run `MAKEPIXB`, you will be informed on the number of pixels that represent the particle. The maximum value that `HYDROPIX` will accept is 300000. If you see that this values is exceeded, increase the `SPACING`. There is also another condition: the number of cells or cubelets within the box will be, obviously, equal to $(XMAX*YMAX*ZMAX)/SPACING**3$. This must be an integer number multiple of 8. If this does not happen, you will get an error message from `MAKEPIXB`. The remedy is to increase slightly one of the dimensions `XMAX`, `YMAX` and `ZMAX` of the box (the box dimensions can be larger than the maximum dimensions of the particle), or vary `SPACING`. An advisable trick is that `XMAX/SPACING`, `YMAX/SPACING`, and `ZMAX/SPACING`, be all integer, even numbers.

The next figure displays the hydrodynamic model a the hollow disk generated with `MAKEPIXB`, used in the `HYDROPIX` calculation



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
- `.ext` contains details of the shell-model extrapolations of the various properties.
- `.pri` is a pdb-formatted file representing the primary hydrodynamic 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 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. HYDROPIX 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 HYDROPIX. 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.