File: montehydro-4b.doc

MONTEHYDRO

Version 4b, January 2014

Index

1. Introduction to MONTEHYDRO

MONTEHYDRO is a computer program that generates possible conformations of a "beads-and-connectors" model particle, employing the Monte Carlo importance sampling procedure. In addition, the program may calculate directly some solution properties, particularly mean dimensions and hydrodynamic properties in the so-called "Monte Carlo rigid-body" (MCRB) treatment.

The model consists of beads – like in typical bead models for rigid particles – joined by connectors. More properly and generally speaking, there are intramolecular interaction potentials between the beads that account not only for bead connectivity, but also may describe partial flexibility, excluded volume interactions, etc. Presently, these interactions are of the following types:

- "Bonds": Pairs of beads (I, J) that are joined by a connector.
- "Angles": Trios of beads (I, J, K) such that I and J are connected, and J and K are connected. The angle, of which J is the vertex, is restricted by some potential.
- "Torsion": Quartet of beads (I, J, K, L) such that I and J are connected, J and K are connected, and K and L are connected, being J and K the central ones. The dihedral angle formed by the two planes defined by the beads IJK and the beads JKL is restricted by some potential.
- "Non-bonded beads" ("excluded volume", "electrostatic"…): Pairs of beads (I, J) that are not joined by a connector, nor involved in an angle interaction, which interact by means of some (usually repulsive) potential.

2. Literature

The primary reference for MONTEHYDRO is:

- J.García de la Torre, A. Ortega, H.E. Pérez Sánchez and J.G. Hernández 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, used in the calculation of solution properties:

- J. García de la Torre, S. Navarro, M.C. López Martínez, F.G. Díaz, J. López Cascales. "HYDRO. A computer software for the prediction of hydrodynamic properties of macromolecules", *Biophys. J.* 67, 530-531 (1994).

If you consider the intrinsic viscosity or the rotational coefficients or relaxation times, then be aware that this version of MONTEHYDRO includes our last improvements in the calculation of these properties, which has been reported in:

- J. García de la Torre, G. Del Río Echenique and A. Ortega "Improved calculation of rotational diffusion and intrinsic viscosity of bead models for macromolecules and nanoparticles", *Journal of Physical Chemistry B* 111, 955-961 (2007).

Some early publications on the MCRB treatment for fully flexible macromolecules and semiflexible particles, respectively, are:

- J. García de la Torre, A. Jiménez and J.J. Freire, "Monte Carlo calculation of hydrodynamic properties of freely jointed, freely rotating and real polymethylene chains, *Macromolecules* 15, 148-154 (1982).

- A. Iniesta, F.G. Díaz and J. García de la Torre, "Transport properties of rigid bent-rod macromolecules and semiflexible broken rods in the rigid-body approximation", *Biophys. J.* 54, 269-275 (1988).

3. Input files. Running MONTEHYDRO

You may launch **`MONTEHYDRO`** by clicking the corresponding icon in MS/Windows or – what is better recommended – at the system prompt in a MS/DOS console. You can do it similarly at the system prompt in a Linux console. Alternatively, you can write script files to launch the program automatically containing the instruction to execute the program and the name of the main input file.

There is a **main input data file** whose name is given by the user. The program asks for entering its name after launching it.

Moving and non-moving beads: if all of the beads in the chain model move, the previously mentioned main input data file will be the only input file. If some beads of the model does not move (i.e. they keep their possitions during the simulation), then there must be a second input file which is compulsory termed `nomove.txt` that contains the parameters of the non-moving beads as specified below.

Possibility of several cases in a run: a series of cases can be processed in the same run (one after other, i.e. one at a time) **if every bead in every case moves** (a series of cases including non-moving beads is incompatible with this version because of fix name of the file `nomove.txt`). The end-of-file (no more cases) will be an asterisk (*). NOTE: this is not the same as a multiexecution using a batch queue.

3.1. Contents of the `main input file`

For each case (of a "one-at-a-time multicase run") contained in the main input file, there will be a block of lines with the following information:

- **`GENERICFILENAME`** (C*22) Common part (first part) of all the output files generated by the program, used to construct the full names of those files.

- **`TITLE`** (C*30) Title of case.

- **`NSUB`** (I) Number of subsamples into which the simulation is subdivided; this is convenient to get estimates or errors. For instance (recommended): 5.

- **`NSTEPS`** (I) Number of Monte Carlo steps per subsample in the simulation. Every "moving bead" in the model is moved at each step. The total number of steps in the simulation will be **`NSTEPS*NSUB.`**

- **`NCONF`** (I) Number of conformations in each subsample of the Monte Carlo trajectory. A new conformation is generated at each step; however, the resulting conformation may be quite similar to that before the step, and it is convenient not to register all of them (the output file could be exceedingly large) but a number, **`NCONF*NSUB`**, that will be a fraction, i.e. an integer divisor, of the total number of steps, **`NSTEPS*NSUB.`**

- **`ISEED`** (I) Integer random number (recommended five or six digits, more than six is not allowed).

- **`ULENGTH`** (R) Unit or "token" of length, u_L, expressed in cm, used internally to avoid large powers of 10 in data and calculations. For instance (recommended) u_L =1 nm = 10^{-7} cm.

- **`UENER`** (R) Unit or "token" of energy, u_E, expressed in erg, used internally for the same purpose. For instance (recommended) $u_E = k_BT$ = 1.3805e-16 x 293 = 4.04 x 10^{-14} erg, the thermal energy at 20ºC.

- **DELTA** (R) "Typical" amplitude (length) of Monte Carlo bead moves. From this general **DELTA**, the program will find an individual δ for each bead, according to its size. **DELTA** is a crucial parameter in MC simulation. It must be quite smaller than the average bead size. The value given to **DELTA** will determine the probability of accepting the new step as valid in the importance sampling procedure. The percentage of rejected new conformations should be small, and this is achieved with small **DELTA**. However, a too small **DELTA** values would result in a slow sampling of conformational space. A compromise is to use values of **DELTA** such that the percentage of rejections is 10-30%. The percentage, which is reported by the program, is reliable even with small **NSTEPS.** Thus, **DELTA** can be adjusted in trials with short simulations. The value must be in units of **ULENGTH**.

- **NMOV** (I) Number of "moving beads" (less or equal than total number of beads, N). The indices of these beads go from 1 to NMOV.

- Following **NMOV** lines: **X, Y, Z, SIG** (R): x_i, y_i, z_i, σ_i, Cartesian coordinates and radius of moving bead *i* in units of u_L.

- **NBOND** (I) Number of bonds or connectors between beads.

- Following **NBOND** lines: **I** (I), **J** (I), **ITYPEBOND** (I), **PARAM(1)** (R), **PARAM(2)** (R),…, corresponding to pair of beads *i, j,* type of connector and parameters for this connector. In the present version, the allowed types of bonds and the corresponding parameters are:

  ITYPEBOND =1, Hookean spring with equilibrium length d_{ij} and Hookean constant *H*. The potential is $V_{ij}(r_{ij}) = (1/2)\, H\, (r_{ij} - d_{ij})^2$. **PARAM(1)** is *H* in units of u_E / u_L^2, **PARAM(2)** is d_{ij} in units of u_L. This potential may be employed to simulate quasirigid bonds (bonds with exactly fixed length are not allowed in this methodology). To do so, give *H* a value much larger than k_BT/ d_{ij}^2. For instance, for $H = 100\, k_BT/ d_{ij}^2$, the root-mean-squared fluctuation in r_{ij} is only 2% of d_{ij}.

  ITYPEBOND =2, Hookean spring with zero equilibrium length and Hookean constant *H*. The potential is $V_{ij}(r_{ij}) = (1/2)\, H\, r_{ij}^2$ (Gaussian springs). **PARAM(1)** is *H* in units of u_E / u_L^2. This potential is usually employed to simulate Gaussian subchains in fully flexible chain polymers. The value of *H* will be parameterized taking into account that the mean square connector length is $\langle r_{ij}^2 \rangle = 3\, k_BT/H$.

  ITYPEBOND =3, Finitely extensible, non-linear (FENE) springs. At low elongation they tend to the Gaussian behaviour, but elongation is limited by a maximum value $d_{ij,max}$. The potential is $V_{ij}(r_{ij}) = -(1/2)\, H\, d_{ij,max}^2 \ln [1 - (r_{ij}/d_{ij,max})^2]$. **PARAM(1)** is *H* in units of u_E / u_L^2 and **PARAM(2)** is $d_{ij,max}$ in units of u_L.

ITYPEBOND =6, Finitely extensible, non-linear (FENE) springs with equilibrium length d_{ij} and Hookean constant H (hard-FENE). Elongation is limited by a maximum value $d_{ij,max.}$ The potential is $V_{ij}(r_{ij}) = -(1/2)\ H\ d_{ij,max}^2\ \ln\ [1 - (r_{ij}/d_{ij,max})^2] + (1/2)\ H\ d_{ij,max}\ d_{ij}\ \ln[(d_{ij,max} + r_{ij})\ /\ (d_{ij,max} - r_{ij})]$. **PARAM(1)** is H in units of $u_E\ /u_L^2$, **PARAM(2)** is d_{ij} in units of u_L, and **PARAM(3)** is $d_{ij,max}$ in units of u_L.

- **NANGLES** (I) Number of angular, bending interactions. Give zero if there are no angles.

- Following **NANGLES** lines: **I** (I), **J** (I), **K** (I), **ITYPEANG** (I), **PARAM(1)** (R), **PARAM(2)** (R),…, corresponding to the three involved beads *i, j, k* (*j* is the central one), type of angle and parameters for this angle. In the present version, the allowed types of angle and the corresponding parameters are:

  ITYPEANG =1, Hookean angular spring with potential $V_{ijk}(\alpha_{ijk}) = (1/2)\ Q\ (\alpha_{ijk} - \alpha_{0,ijk})^2$ where α_{ijk} is the instantaneous angle subtended by the prolongation of bond *i-j* and bond *j-k* (note that the angle is zero for a straight, colinear conformation) and $\alpha_{0,ijk}$ is the equilibrium value of this angle, in radians. **PARAM(1)** is $\alpha_{0,ijk}$ and **PARAM(2)** is Q in units of u_E. Exactly fixed values of the angles are not possible; a quasi-rigid angle can be simulated with a large value of Q, for instance $Q = 100\ k_BT$.

  ITYPEANG =3, Anharmonic angular potential $V_{ijk}(\alpha_{ijk}) = (1/2)\ K(\alpha_{ijk} - \alpha_{0,ijk})^2 + (1/3)\ K'(\alpha_{ijk} - \alpha_{0,ijk})^3 + (1/4)\ K''(\alpha_{ijk} - \alpha_{0,ijk})^4$ where α_{ijk} is the instantaneous angle subtended by the prolongation of bond *i-j* and bond *j-k* (note that the angle is zero for a straight, colinear conformation) and $\alpha_{0,ijk}$ is the equilibrium value of this angle, in radians. **PARAM(1)** is $\alpha_{0,ijk}$ and **PARAM(2), PARAM(3), PARAM(4)** are K, K', K'' in units of u_E.

- **NTORS** (I) Number of torsion interactions. Give zero if there are no dihedral angles.

- Following **NTORS** lines: **I** (I), **J** (I), **K** (I), **L** (I), **ITYPETOR** (I), **PARAM(1)** (R), **PARAM(2)** (R),…, corresponding to the four involved beads *i, j, k, l* (*j, k* are the central ones), type of torsion and parameters for this torsion. In the following, ϕ_{ijkl} is the instantaneous dihedral angle (in radians) subtended by the two planes defined by beads *i,j,k* and beads *j,k,l* (ϕ_{ijkl}=0 if beads *i* and *l* are in "trans", ϕ_{ijkl}=2.094 if beads *i* and *l* are in "gauche+", ϕ_{ijkl}=4.189 if beads *i* and *l* are in "gauche-" conformations). In the present version, the allowed types of torsion and the corresponding parameters are:

  ITYPETOR =1, $V_{ijkl}(\phi_{ijkl}) = c_0 + c_1\cos(\phi_{ijkl}) + c_2\cos^2(\phi_{ijkl}) + c_3\cos^3(\phi_{ijkl}) + c_4\cos^4(\phi_{ijkl}) + c_5\cos^5(\phi_{ijkl})$; used when the torsion is performed around a bond between carbon atoms sp^3-sp^3. **PARAM(n)** (n=1,2,3,4,5,6) is c_{n-1} in units of u_E. Typical values of c_{n-1} (in Kcal/mol) are

Author	c_0	c_1	c_2	c_3	c_4	c_5
Ryckaert and Bellemans *Chem. Phys. Lett.* 30, 123-125, 1975	2.217	2.905	-3.135	-0.731	6.271	-7.527
Rey et al. *J. Chem. Phys.* 97, 1240-1249, 1992	1.941	3.73	-1.071	-3.703	2.141	-3.034

ITYPETOR =2, $V_{ijkl}(\phi_{ijkl})$ =K_ϕ[1+cos(3ϕ_{ijkl})]; used when the torsion is performed around a bond between carbon atoms sp^3-sp^3. **PARAM(1)** is K_ϕ in units of u_E. See Lamm and Szabo *J. Chem. Phys.* 85, 7334-7348, 1986 that set K_ϕ=1.0 Kcal/mol.

ITYPETOR =3, $V_{ijkl}(\phi_{ijkl})$=(K_ϕ/2)[x(1-cos(ϕ_{ijkl}))+(1-x)(1-cos(3ϕ_{ijkl}))]; used when the torsion is performed around a bond between carbon atoms sp^3-sp^3. **PARAM(1)** is K_ϕ in units of u_E and **PARAM(2)** is x (dimensionless). See Winkler et al. *J. Chem. Phys.* 98, 729-736, 1992 that set K_ϕ=4.1 Kcal/mol and x=0.163.

ITYPETOR=4, $V_{ijkl}(\phi_{ijkl})$=c_1[1-cos(ϕ_{ijkl})]+c_2[1-cos(2ϕ_{ijkl})]+c_3[1-cos(3ϕ_{ijkl})]; used when the torsion is performed around a bond between carbon atoms sp^3-sp^2. **PARAM(n)** (n=1,2,3) is c_n in units of u_E. See Wiberg et al. *J. Am. Chem. Soc.* 107, 5035-5041, 1985 (note: constants c_n here are constants V_n/2 in that paper).

ITYPETOR =5, $V_{ijkl}(\phi_{ijkl})$=c_1[cos(ϕ_{ijkl})- cos($\phi_{0,ijkl}$)]^2 where $\phi_{0,ijkl}$ is the equilibrium value of the dihedral angle subtended by the two planes defined by beads *i,j,k* and beads *j,k,l*, in radians; used when the torsion is performed around a bond between carbon atoms sp^2-sp^2. **PARAM(1)** is $\phi_{0,ijkl}$ and **PARAM(2)** is c_1 in units of u_E. See Rey et al. *J. Chem. Phys.* 97, 1240-1249, 1992 (note: constant c_1 here is constant k_ϕ/2 in that paper).

ITYPETOR =6, $V_{ijkl}(\phi_{ijkl})$=k_1[1+cos(ϕ_{ijkl}-$\phi_{0,ijkl}$)]+k_3[1+cos3(ϕ_{ijkl}-$\phi_{0,ijkl}$)] where $\phi_{0,ijkl}$ is the equilibrium value of the dihedral angle subtended by the two planes defined by beads *i,j,k* and beads *j,k,l*, in radians. **PARAM(1)** is $\phi_{0,ijkl}$, **PARAM(2)** is k_1 in units of u_E, and **PARAM(2)** is k_3 in units of u_E. See Elcock *PloS Comput. Biology* 2, 2006.

ITYPETOR =7, $V_{ijkl}(\phi_{ijkl})$=k_1[1-cos(ϕ_{ijkl}-$\phi_{0,ijkl}$)]+k_3[1-cos3(ϕ_{ijkl}-$\phi_{0,ijkl}$)] where $\phi_{0,ijkl}$ is the equilibrium value of the dihedral angle subtended by the two planes defined by beads *i,j,k* and beads *j,k,l*, in radians. **PARAM(1)** is $\phi_{0,ijkl}$, **PARAM(2)** is k_1 in units of u_E, and **PARAM(2)** is k_3 in units of u_E. See Elcock *J. Chem. Theory Comput.* 5, 242, 2009.

NOTE: conformations generated with potential 6 are mirror images of conformations generated with potential 7. Potential 6 reproduces the crystalline protein structure as given in the PDB file.

- **NNONBOND** (I) Number of non-bonded interactions, between pairs of beads not involved in a bond or an angle. Give zero if there are no such interactions.

- Following **NNONBOND** lines: **I** (I), **J** (I), **ITYPENONB** (I), **PARAM(1)** (R), **PARAM(2)** (R),…, corresponding to pair of beads *i, j,* type of interaction and parameters for this interaction. In the present version, the allowed types of bonds and the corresponding parameters are:

  ITYPENONB =1, Lennard-Jones C12-C6 potential, $V_{ij}(r_{ij})=C12/r^{12}-C6/r^{6}$, with $V_{ij}(r_{ij})=0$ for $r_{ij}>r_{cutoff}$. **PARAM(1)** is *C12* in units of u_E x u_L^{12} ; **PARAM(2)** is *C6* in units of u_E x u_L^{6}; **PARAM(3)** is r_{cutoff} in units of u_L.

  ITYPENONB =2, Purely repulsive, Gaussianly decaying potential, $V_{ij}(r_{ij})=A\exp(-Br_{ij}^{2})$, with $V_{ij}(r_{ij})=0$ for $r_{ij}>r_{cutoff}$. **PARAM(1)** is *A* in units of u_E ; **PARAM(2)** is *B* in units of u_L^{-2}; **PARAM(3)** is r_{cutoff} in units of u_L.

  ITYPENONB =3, Purely repulsive, exponentially decaying potential, $V_{ij}(r_{ij})=A\exp(-Br_{ij})$, with $V_{ij}(r_{ij})=0$ for $r_{ij}>r_{cutoff}$. **PARAM(1)** is *A* in units of u_E ; **PARAM(2)** is *B* in units of u_L^{-1}; **PARAM(3)** is r_{cutoff} in units of u_L.

  ITYPENONB =4, Electrostatic pure (Coulomb) or screened (Debye-Hückel) potential, $V_{ij}(r_{ij})=A\exp(-Kr_{ij})/r_{ij}$, with $V_{ij}(r_{ij})=0$ for $r_{ij}>r_{cutoff}$. **PARAM(1)** is *A* in units of u_E x u_L ; **PARAM(2)** is *K* in units of u_L^{-1}; **PARAM(3)** is r_{cutoff} in units of u_L. For screened Debye-Hückel, *K* must be positive. For non-screened, pure Coulomb, give any negative number (e.g. –9.) for *K*.

  ITYPENONB =5, Lennard-Jones interaction, whose potential is $V_{ij}(r_{ij}) = 4\varepsilon[(\sigma/ r_{ij})^{12}- (\sigma/ r_{ij})^{6}]$, with $V_{ij}(r_{ij})=0$ for $r_{ij}>r_{cutoff}$. **PARAM(1)** is ε in units of u_E, **PARAM(2)** is σ in units of u_L, and **PARAM(3)** is r_{cutoff} in units of u_L.

  ITYPENONB =6, Shifted, purely repulsive Lennard-Jones interaction, whose potential is $V_{ij}(r_{ij}) = \varepsilon +4\varepsilon [(\sigma/ r_{ij})^{12}-(\sigma/ r_{ij})^{6}]$, with $V_{ij}(r_{ij})=0$ for $r_{ij}>2^{1/6}\sigma$. **PARAM(1)** is ε in units of u_E ; **PARAM(2)** is σ in units of u_L .

  ITYPENONB =7, Hard-spheres potential, $V_{ij}(r_{ij}) = V_0$ for $r_{ij}< r_{cutoff}$ and $V_{ij}(r_{ij}) = 0$ if $r_{ij}> r_{cutoff}$. It is suggested that $r_{cutoff.} = \sigma_1+\sigma_2$, i.e. the sum of the radii of the two beads. The two beads would be prevented to overlap, in the spirit of the hard-spheres potential, if $V_0 >>> k_BT$, for instance $V_0 = 200\ k_BT$. **PARAM(1)** is V_0 in units of u_E, and **PARAM(2)** is r_{cutoff} in units of u_L.

  ITYPENONB =8, 12-10 Lennard-Jones interaction, whose potential is $V_{ij}(r_{ij}) = \varepsilon[5(\sigma/ r_{ij})^{12}- 6(\sigma/ r_{ij})^{10}]$, with $V_{ij}(r_{ij})=0$ for $r_{ij}>r_{cutoff}$. **PARAM(1)** is ε in units of u_E, **PARAM(2)** is σ in units of u_L, **PARAM(3)** is r_{cutoff} in units of u_L. (Before Generic Lennard-Jones interaction, whose potential is $V_{ij}(r_{ij}) = A\varepsilon[B(\sigma/ r_{ij})^{e1}- C(\sigma/ r_{ij})^{e2}]$).

ITYPENONB =9, Repulsive exponent-12 Lennard-Jones interaction, whose potential is $V_{ij}(r_{ij}) = \varepsilon(\sigma/ r_{ij})^{12}$, with $V_{ij}(r_{ij})$=0 for r_{ij}>r_{cutoff}. **PARAM(1)** is ε in units of u_E, **PARAM(2)** is σ in units of u_L, **PARAM(3)** is r_{cutoff} in units of u_L.

- **TEMP** (R), temperature (kelvin). This value is always needed for the calculation of the Boltzmann factor, k_BT, in the Monte Carlo method. Eventually, it would be also needed for the translational and rotational diffusion coefficient. If you do not have a specific value, give 293 K to obtain standard results at 20ºC.

- **PROPSMODE** (I), flag to indicate which properties will be calculated "on line" (see following section). Presently allowed values for any working mode are only: **PROPSMODE=3** and **PROPSMODE=4.** Values of **PROPSMODE** that are not allowed will result in an error message. Value of **PROPSMODE** should match with that in **modefile.txt**

If **PROPSMODE=4** there will be two additional lines:

- **ETA** (R), solvent viscosity, η_0 (poise). This value is only needed for the calculation of the translational coefficient (which is proportional to the value that you supply for this quantity). If you ignore this value, give 0.010 poise to obtain standard results in water at 20ºC.

- **RM** (R), molecular weight, M. This value is only needed for the calculation of the intrinsic viscosity (which is proportional to the value that you supply for this quantity). If you ignore this value, give just an estimate and ignore the result for the intrinsic viscosity.

(I), (R) and (C*n) mean the FORTRAN variable types integer, real, and character*n, respectively.

After the successive blocks (in case of a one-at-a-time multicase run), the end of this file will be indicated with a line whose first character will be one asterisk (*).

3.2. Contents of the `nomove.txt` file (only valid if running a single case)

For the simulation of just one case containing non-moving beads, there must exists the input file `nomove.txt` with the following lines:

- **NNMOV** (I) Number of non-moving beads (less than total number of beads, N). The indices of these beads go from NMOV+1 to NMOV+NNMOV.
- Following **NNMOV** lines: **X, Y, Z, SIG** (R): x_i, y_i, z_i, σ_i, Cartesian coordinates and radius of non-moving bead i in units of u_L.

After opening this file, NNMOV and the total number of beads N (=NMOV+NNMOV) are shown on screen and a pause is made waiting for confirmation to proceed.

4. Output files.

For each case there will be a set of output files, with the names constructed by using the **GENERICFILENAME** given in input file with a different end according to the content of the file. All of them will have upto 30 characters (C*30).

4.a. Results file

Its name is ended in "**-RES.TXT**": **GENERICFILENAME-RES.TXT**
A file that contains the results of the Monte Carlo basic calculations:

(1) A summary of the main data.

(2) The program also reports the percent of rejected (in the importance-sampling sense) Monte Carlo moves. According to experience an acceptable result is 10 – 30 %. Increase Delta if this is too low, or decrease it if it is too high.

(3) Depending on **PROPSMODE** following properties will be calculated "on line":
If **PROPSMODE=3**

- 1, Mean square end-to-end (1-N, center-to-center) distance
- 2, Mean square radius of gyration, including the effect of finite bead size.

If **PROPSMODE=4**

- 1, Mean square end-to-end (1-N, center-to-center) distance
- 2, Mean square radius of gyration, including the effect of finite bead size
- 3, Translational diffusion coefficient
- 3, Intrinsic viscosity (NOTE: in public released version, with the adjusted finite-bead size effect as described in *J. Phys. Chem. B* 111, 955-961 (2007) by default)

4.b. Monte Carlo sample (trajectory) file

Its name is ended in "**-TMC.TXT**": **GENERICFILENAME-TMC.TXT**
It contains:

(1) A reproduction of all the data in the main data file, pertaining to this case.

(2) **nsub** blocks of **nconf+1** records with the 3N coordinates, written by the statement:

```
WRITE(nunittrajmc,*) isub,icon,(r(ii),ii=1,n3)
```

where **isub=1,…nsub, icon=0,…nconf** and the **n3=3*n** coordinates are placed in: **r(1)=x(1), r(2)=y(1), r(3)=z(1), r(4)=x(2),…, r(n3)=z(n)**

4.c. Average values file

Its name is ended in "**-VAL.TXT**": **GENERICFILENAME-VAL.TXT**
It contains in a column a collection of the average values and errors of the properties calculated "on line" according to **PROPSMODE**. It is useful in a multiexecution (batch queue) run, which is ready for future versions. In this version you can ignore it.

4.d. Final coordinates file

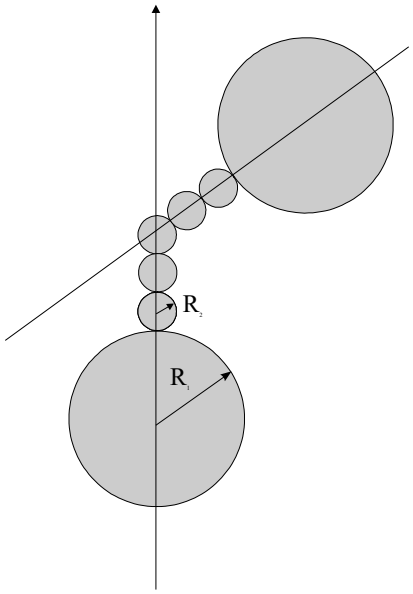
When program ends, a file with composed name is generated. The name is made of two pieces, the first (fixed) is **finalcoor** and the second (variable) is the name of the main input file (useful when a multiexecution –batch queue– is run): **finalcoor + main-input-file-name.txt**. Every one of those files consists of N (number of beads) lines and three columns (Cartesian coordinates); for each execution, they contain the Cartesian coordinates of the last conformation in the unit of length specified in the main input file (usually cm). Thus, simulations can be continued starting from the last conformation.

4.e. Scratch files

For each case in a one-at-a-time multicase run or in a multiexecution (batch queue) run, the program will produce three small files, named **brownxxx.txt, initxxx.txt** and **molecxxx.txt** (**xxx** composed of a serial number and the name of the input file). They are just scratch files internally employed by the program. Please, delete them.

5. Example

The example is the "symmetric broken dumbbell" (see our Biophys. Chem. paper). It has two beads of radius 2.5 nm joined by a rodlike connector consisting of five beads of 0.5 nm. The connector behaves as a "broken rod": it has two arms, and the central bead acts as a fully flexible joint.



The data file is as follows:

```
BroDumb                                    !generic file name
A symmetric broken dumb-bell                  !Title
  5         !Number of subsamples
  5000000   !nstepts
    20000   !nconf
   654321   !iseed
 1.E-7      !Unit of length (cm)  (1 nm)
 4.04e-14   !Unit of energy (erg) (1 kT)
    0.005   !delta
  7         !number of beads: x,y,z,sigma
   0.0  0.0 -5.0  2.5
   0.0  0.0 -2.0  0.5
   0.0  0.0 -1.0  0.5
   0.0  0.0  0.0  0.5
   1.0  0.0  0.0  0.5
   2.0  0.0  0.0  0.5
   5.0  0.0  0.0  2.5
  6        !number of bonds: i,j,type,param1,param2,...
  1   2   1   10.  3.0
   2   3   1  100.  1.0
   3   4   1  100.  1.0
   4   5   1  100.  1.0
   5   6   1  100.  1.0
   6   7   1   10.  3.0
  4  !number of angles: i,j,k,type,param1,param2,...
   1   2   3  1  0.0   100.0
   2   3   4  1  0.0   100.0
   4   5   6  1  0.0   100.0
   5   6   7  1  0.0   100.0
  0  !number of dihedral angles: i,j,k,l,type,param1,...
 10  !number of pairs: i,j,type,param1,param2,param3
 1 4 5 0.3 3.  9.
 1 5 5 0.3 3.  9.
 1 6 5 0.3 3.  9.
 1 7 5 0.6 5. 15.
 2 5 5 0.1 1.  3.
 2 6 5 0.1 1.  3.
 2 7 5 0.3 3.  9.
 3 6 5 0.1 1.  3.
 3 7 5 0.3 3.  9.
 4 7 5 0.3 3.  9.
   293.0        !Kelvin temperature
4   !propsmode
   0.010    !Solvent viscosity
115000.        !molecular weight
*
```

Among other things, you may note that:

- The coordinates given to the initial conformation are those for a bending angle of 90º. Recall that the choice of the initial conformation is irrelevant.
- The equilibrium connector lengths, d_{ij}, are the sums of the radii of the connected beads.
- The Hookean constant, H, for the connectors is approximately 100 k_BT/ d_{ij}^2.
- The small beads with numbers 2, 3, 5 and 6 are the central beads of angles with $\alpha_{0,ijk}$ =0 and a large Q; thus the two arms are kept stiff and straigth. However, there is no angle centered at bead 4, because this is the central hinge, which is fully flexible in this model.
- For all the pairs of beads not involved in connectors or angles, we assume a Lennard-Jones excluded volume potential with the indicated choices for the parameters. Alternatively, a simpler hard-spheres interaction could be used, with r_{cutoff} equal to the sum of radii and a large V_0. You may confirm that the results are practically identical.
- The calculated properties are the hydrodynamic ones, and this requires providing values of M and η_0.

6. Notes and hints.

- The user may write his/her own program to analyze the Monte Carlo sample of conformations, evaluating other averages, distributions,…. Note that the importance sampling Monte Carlo procedure takes into account potentials, statistical weights, probabilities, etc, in the simulation itself. Thus the sample averages will be simple arithmetic (unweighted) means over the values for each conformation.

7. Release notes

- This is the fourth release of the MONTEHYDRO User Guide.
- Some modifications in the text of this user guide have been performed in order to clarify program features and correct some mistakes. The program features are the same as the latest version. We remind that the main novelties introduced in the most recent versions are:
    a. Inclusion of new torsion and non-bonded potentials.
    b. Possibility of non-moving beads.
    c. Use of optimized mathematic libraries (MKL) to perform some vector and matrix operations.