6.2 Minimization

IMIN: Flag to run minimization

= 0 No minimization (only do molecular dynamics; default)

= 1 Perform minimization (and no molecular dynamics)

MAXCYC: Maximum number of cycles of minimization. Default 1.

NCYC: After NCYC cycles the method of minimization is switched from steepest descent to the conjugate gradient method. Default 10.

NTMIN: Flag for the method of minimization.

= 0 Full conjugate gradient minimization. The first 10 cycles are steepest descent at the start of the run and after every nonbonded pairlist update

= 1 For NCYC cycles the steepest descent method is used then conjugate gradient is switched on (default).

= 2 Only steepest descent method is used.

= 3 Only Limited Memory BFGS method is used. This method usually performs faster than conjugate gradient minimization (see Liu and Nocedal, Mathematical Programming 45 (1989) 503-528).

DX0: The initial step length. (Note: it is DX zero not DX letter O)

If the initial step length is big then the minimizer will try to leap across the energy surface and sometimes the first few cycles will give a huge energy, however the minimizer is generally smart enough to adjust itself. Default 0.01.

DXM: The maximum step length allowed. Default 0.5.

DRMS: Convergence criterion for the energy gradient: minimization will halt when the root-mean-square of the Cartesian elements of the gradient is less than DRMS. Default 1.0E-4 kcal/mole Å

6.3 Molecular Dynamics

NRUN: Number of MD-runs of NSTLIM steps to be performed.

Since the restart coordinates are written only at the end of each ”run”, it is sometimes advisable to break a long MD calculations into several ”runs”. The number of picoseconds of molecular dynamics is equal to the product of NRUN x NSTLIM x DT. Default 1

NSTLIM: Number of MD-steps per NRUN to be performed. Default 1.

NDFMIN: Number of degrees of freedom that will be subtracted from the total number of degrees of freedom.

If either NTCM or NSCM. NE. 0 then this option should be set equal to 6. Otherwise, NDFMIN should be 0. NDFMIN, NTCM, and NSCM are ignored for belly dynamics. Default 0.

NTCM: Flag for the removal of translational and rotational motion at the beginning of the simulation.

= 0 The translational and rotational motion about the center of mass is not removed (default)

= 1 The above motion is removed one time at the beginning of the simulation.

NSCM: Flag for the removal of translational and rotational motion at regular intervals.

After every NSCM steps, translational and rotational motion will be removed. This flag is ignored for both belly and periodic simulations. Default 0.

INIT: Flag for different starting procedures.

If option NTX is less than 4, INIT should be equal to 3. If option NTX is greater than or equal to 4, this option should be equal to 4.

= 3 Starting velocities are assigned from a Maxwellian distribution at TEMPI K. If input TEMPI = 0, TEMPI is set to 10 K. Net momentum of the entire system will be removed.

= 4 Input velocities (NTX = 4) are read from the ”inpcrd” file.

Note: The Nosé-Hoover chain/reversible algorithm used in ROAR conserves the linear momentum of the system. When restarting a run with velocities and if the net momentum is not zero, it will be conserved. If one wants to have zero net momentum during the simulation, one should restart a run using ROAR without velocities, then ROAR will choose the initial velocities and remove the net momentum.

T: The time at the start (ps). This is for your own reference and is not critical. Start time is taken from the coordinate input file. Default 0.0.

DT: The time step (ps).

Recommended MAXIMUM is .002 if SHAKE is used, or .001 if it isn’t. Note that for temperatures above 300K, the step size should be reduced since greater temperatures mean increased velocities and longer distances traveled between each force evaluation, which can lead to anomalously high energies and temperatures. Default 0.001.

NTB: Flag indicates if periodic boundary condition is used.

Required input parameters

If NTB = 0 then a boundary is NOT applied regardless of any boundary condition information in the topology file. The value of NTB specifies whether constant volume or constant pressure dynamics will be used. Options for constant pressure are described in the NHC section.

= 0 no periodicity is applied

= 1 constant volume simulation

= 2 constant pressure simulation

Note: If NTB .NE. 0, there must be a periodic boundary in the topology file. Constant pressure is not used in minimization (IMIN=1, above).

For a periodic system, constant pressure is the only way to equilibrate the density of the system if the starting state is not correct. For example, the solvent packing scheme used in EDIT can result in voids being generated when solvent molecules are subtracted from the system. Another consideration is the shrinkage of the box during a constant pressure MD simulation which can result in solvent molecules ‘seeing’ parts of the solute in opposite directions if the initial box size was chosen too small. The remedy for this is to build a large enough box when beginning a constant pressure MD simulation.