NAMD Version 1.5 Configuration File Parameters

Keyword	Allowable Values	Default Value	Description

Input Files

Keyword	Allowable Values	Default Value	Description
`coordinates`	filename	–	PDB file with initial coordinates
`structure`	filename	–	X-PLOR compatable psf file name
`parameters`	filename	–	Multiple occurances used for multiple files
`velocities`	filename	–	PDB with initial velocities
`binvelocities`	filename	–	Binary file containing initial velocities
`bincoordinates`	filename	–	Binary restart file with initial coordinates
`cwd`	directory	–	Default working directory. All filenames not starting with / will assumed to be here.

Output Files

Keyword	Allowable Values	Default Value	Description
`outputname`	filename	–	Prefix for final coordinate and velocity output
`restartname`	filename	–	Prefix for restart output
`restartfreq`	int > 0	–	Frequency of restart file generation
`binaryrestart`	`yes` or `no`	`yes`	Should the restart files be in binary format?
`DCDfile`	filename	–	DCD trajectory file name
`DCDfreq`	int > 0	–	Frequency of trajectory output in timesteps
`velDCDfile`	filename	–	Velocity DCD file name
`velDCDfreq`	int > 0	–	Frequency of velocity DCD output
`electForceDCDfile`	filename	–	Electrostatic force DCD file prefix. Short range will have `.s` and long range will have `.l` appended.
`electForceDCDfreq`	int > 0	–	Frequency of electrostatic force DCD output
`allForceDCDfile`	filename	–	Total force DCD file name
`allForceDCDfreq`	int > 0	–	Frequency of total force DCD output
`outputEnergies`	int > 0	1	Specify how often to print energies

Timestep Parameters

Keyword	Allowable Values	Default Value	Description
`numsteps`	int > 0	req	Number of timesteps to perform
`timestep`	dec > 0	1.0	Timestep size (fs)
`firsttimestep`	int ≥ 0	0	Timestep to start with. Must be a multiple of `stepspercycle`. Should be 0 unless restarting.
`stepspercycle`	int > 0	15	Steps between pairlist generation and FMA

Simulation Space Partitioning

Keyword	Allowable Values	Default Value	Description
`eleccutoff`	dec > 0	–	Local electrostatic cutoff distance (Å)
`vdwcutoff`	dec > 0	–	Local van der Waals cutoff distance (Å)
`cutoff`	dec > 0	–	Common electrostatic and van der Waals cutoff distance (Å)
`switching`	`on` or `off`	`off`	Use switching functions?
`elecswitchdist`	$0 <$ dec $<$ `eleccutoff`	–	Distance for electrostatic switching function activation (Å)
`vdwswitchdist`	$0 <$ dec $<$ `vdwcutoff`	–	Distance for van der Waals switching function activation (Å)
`switchdist`	$0 <$ dec $<$ `cutoff`	–	Common distance for switching function activation (Å)
`pairlistdist`	dec $\geq$ `cutoff`	`cutoff`+1.0	Pairlist inclusion distance (Å)
`margin`	dec > 0	1.0	Patch width margin
`plMarginCheck`	`on` or `off`	`on`	Should pairlist margin checking be performed?

Basic Dynamics

Keyword	Allowable Values	Default Value	Description
`exclude`	`none`, `1-2`, `1-3`, `1-4`, `scaled1-4`	req	Electrostatic exclusion policy
`temperature`	dec > 0	–	Temperature for random velocity assignment
`COMmotion`	`yes` or `no`	`no`	Should center of mass move?
`dielectric`	dec ≥ 1	1.0	Dielectric constant
`1-4scaling`	dec > 0	1.0	1-4 electrostatic scaling factor
`seed`	int > 0	random	Specify a random number seed
`rigidBonds`	`none` or `water` or `all`	none	Select which bonds with hydrogen to constrain
`rigidTolerance`	dec > 0	0.000001	Convergence parameter for bond lengths with ShakeH
`rigidIterations`	int > 0	100	Convergence fails after this many ShakeH iterations

NAMD Version 1.5 Configuration File Parameters (cont.)

Keyword	Allowable Values	Default Value	Description

DPMTA Parameters

Keyword	Allowable Values	Default Value	Description
`FMA`	`on` or `off`	`off`	Use FMA?
`FMALevels`	int > 0	5	Tree levels to use in FMA
`FMAMp`	int > 0	8	Number of multipole terms to use in FMA
`FMAFFT`	`on` or `off`	`on`	Use FFT enhancement?
`FMAfrequency`	int > 0	–	Number of timesteps between FMA calculations
`FMAtheta`	dec	0.715	DPMTA θ parameter (radians)
`FMAFFTBlock`	int > 0	4	FFT blocking factor
`FullDirect`	`yes` or `no`	`no`	Compute full electrostatics directly. For testing purposes only.

MTS Parameters

Keyword	Allowable Values	Default Value	Description
`MTSAlgorithm`	`naive`, `verletI`, or `verletX`	`naive`	Specify a multiple timestep scheme to use
`longSplitting`	`sharp`, `xplor`, or `c1`	`sharp`	Specify a long/short range splitting scheme

Harmonic Constraints

Keyword	Allowable Values	Default Value	Description
`constraints`	`on` or `off`	`off`	Use harmonic constraints?
`consexp`	even int > 0	2	Exponent for harmonic potential
`consref`	filename	`coordinates`	PDB file containing reference positions
`conskfile`	filename	`coordinates`	PDB file containing force constants
`conskcol`	`X`, `Y`, `Z`, `O`, `B`	`O`	Column of PDB containing force constant
`movingConstraints`	`on` or `off`	`off`	Use moving constraints?
`movingConsVel`	vector `vx vy vz`	–	Velocity of reference point movement (Å/timestep)
`movingConsAtom`	int ≥ 0	–	Index of the restrained atom to move

Energy Minimization

Keyword	Allowable Values	Default Value	Description
`minimization`	`on` or `off`	`off`	Perform minimization?
`maximumMove`	dec > 0	$\frac{0.75 \times \texttt{cutoff}}{\texttt{stepsPerCycle}}$	Maximum atom movement per step (Å)

Langevin Dynamics

Keyword	Allowable Values	Default Value	Description
`langevin`	`on` or `off`	`off`	Use Langevin dynamics?
`langevinTemp`	dec > 0	–	T_0 for Langevin forces (K)
`langevinFile`	filename	`coordinates`	PDB file for b_i
`langevinCol`	`X`, `Y`, `Z`, `O`, `B`	`O`	Column to use in PDB file for b_i

Temperature Coupling

Keyword	Allowable Values	Default Value	Description
`tCouple`	`on` or `off`	`off`	Should temperature coupling be active?
`tCoupleTemp`	dec > 0	–	Temperature of heat bath (K)
`tCoupleFile`	filename	`coordinates`	PDB file for b_i
`tCoupleCol`	`X`, `Y`, `Z`, `O`, `B`	`O`	Column to use in PDB file for b_i

Temperature Rescaling

Keyword	Allowable Values	Default Value	Description
`rescaleFreq`	int > 0	–	Number of steps between velocity rescaling. Omit `rescaleFreq` to disable rescaling.
`rescaleTemp`	dec > 0	–	Equilibration temperature (K)

Spherical Boundary Conditions

Keyword	Allowable Values	Default Value	Description
`sphericalBC`	`on` or `off`	`off`	Use spherical boundary conditions?
`sphericalBCr1`	dec > 0	–	Radius for first sphere potential (Å)
`sphericalBCk1`	dec	–	Force constant for first sphere potential + value inward force, – value outward force
`sphericalBCexp1`	even int > 0	2	Exponent for first sphere potential
`sphericalBCr2`	dec > 0	–	Radius for second sphere potential (Å)
`sphericalBCk2`	dec	–	Force constant for second sphere potential + value inward force, – value outward force
`sphericalBCexp2`	even int > 0	2	Exponent for second sphere potential

Applied Electric Field

Keyword	Allowable Values	Default Value	Description
`eFieldOn`	`yes` or `no`	`no`	Apply a constant electric field?
`eField`	filename	–	file containing vector defining electric field