QUICK-SHEET for molsim

Action	Specifier	Input values	Output values
load	**xyz**	**File name (string)**	
	top	**File name (string)**	
save		**1 Types (string)** **2 File name (string)**	
set	**timestep**	**Time step (scalar – default 0.005)**	
	temperature	**Temperature (scalar – default 1.0)**	
	cutoff	**Max. cutoff (scalar – default 2.5)**	
	omp	**No. threads (int scalar – default 1)**	
	exclusion	**'bonded' or 'molecule'** **(string – default 'all')**	
	temperaturerelax	**Temp. relaxation time** **(scalar – default 0.01)**	
	compressionfactor	**Compression factor** **(scalar – default 0.99995)**	
	types	**Particle types (string)**	
	skin	**Buffer-skin for neighbourlist** **(scalar – default 0.25)**	
	charges	**Atom charges (vector)**	
get	**numbpart**		**Scalar**
	box		**Vector**
	energies		**Vector (E_{kin}, E_{pot})**
	velocities		**Matrix**
	positions		**Matrix**
	forces		**Matrix**
	types		**String**
	molpositions		**Matrix**
	pressure		**Scalar**
calcforce	**lj**	**1 Types (string)** **2 Cutoff (scalar)** **3 σ (scalar)** **4 ε (scalar)** **5 aw (scalar)**	

	bond	**1 Bond type (int scalar)** **2 Bond length (scalar)** **3 Spring constant(scalar)**
	angle	**1 Angle type (int scalar)** **2 Eq. angle (scalar)** **3 Spring constant (scalar)**
	torsion	**1 Torsion type (int scalar)** **2 Potential parameters (vector)**
	coulomb	**1 Algorithm (“sf” or “wolf”)** **2 Cutoff (scalar)** **3 <OPT for “wolf”:> Screening (Scalar)**
	lattice	**1 Particle type (string)** **2 Spring constant (scalar)**
	dpd	**1 Types (string)** **2 Cutoff (scalar)** **3 Repulsion parameter (scalar)** **4 σ (scalar)**

integrate	**leapfrog**	
	dpd	**λ (scalar)**

thermostate	**relax**	**1 Particle type (string)** **2 Temperature (scalar)** **3 Thermostat relax time (scalar)**
	nosehoover	**1 Particle type (string)** **2 Temperature (scalar)** **3 Thermostat mass (scalar)**

sample	**vacf/mcvacf**	**1 Length vector (int scalar)** **2 Time span (scalar)**
	sacf/msacf	**1 Length vector (int scalar)** **2 Time span (scalar)**
	hydrocorrelations/ **mhydrocorrelations**	**1 Length vector (int scalar)** **2 Time span (scalar)** **3 No. wavevectors (int scalar)**
	profiles	**1 Particle type (string)** **2 Length vector (int scalar)** **3 Sample freq. (int scalar)**
	msd	**1 Length vector (int scalar)** **2 Time span (scalar)** **3 No. wavevectors (int scalar)** **4 Particle type (string)**
	do	
task	**lj**	**1 Types (string)** **2 Cutoff (scalar)** **3 σ (scalar)**

		4 ε (scalar) 5 Block no.
	bond	1 Bond type (int scalar) 2 Bond length (scalar) 3 Spring constant(scalar) 4 Block no.
	angle	1 Angle type (int scalar) 2 Eq. angle (scalar) 3 Spring constant (scalar) 4 Block no.
	torsion	1 Torsion type (int scalar) 2 Potential parameters (vector) 3 Block no.
	coulomb	1 Cutoff (scalar) 2 Block no.
	do	1 Total no. blocks

compress		Target density

add	force	1 Forces (vector) 2 Direction (int scalar)

clear