PIMD manual

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Description of the input file options

The input file is variable format and contains lines of the form *key value*, where 'key' is a case-sensitive name of a variable in the program, and *value* is a value. Boolean keys are specified as ".t." (true) or ".f" (false). The characters "!" or "#" may be used to comment lines, and blank lines are ignored.

Required options

fconfig	(string)	input filename - either a .xyz or .img (full bead simulation img)
fsave	(string)	label to be appended to all the output files
eq_timesteps	(int)	number of timesteps to equilibrate
run_timesteps	(int)	number of timesteps to run
delt	(real)	timestep in fs
pot_model	(int)	Model to be used: 2=ttm21f 3=ttm3f 4=qspcfw 5=spcf 6=SIESTA

Optional options

Output options

coord_out	(Bool, default .f.)	centroid coordinates output
momenta_out	(Bool, default .f.)	centroid velocities output
dip_out	(Bool, default .f.)	all dipoles output
Edip_out	(Bool, default .f.)	electronic (polarization) dipoles output
TD_out	(Bool, default .f.)	total dipole output
images_out	(Bool, default .f.)	coordinates for all images output
IMAGEDIPOLESOUT	(Bool, default .f.)	dipoles for all images output
TP_out	(Bool, default .f.)	Temp/Press (.t. to file, .f. to terminal)
ENERGYOUT	(Bool, default .f.)	total energy output (separate file)
HISTOUT	(Bool, default .t.)	OH histograms output (separate file)
BOXSIZEOUT	(Bool, default .f.)	box size running average output
CALCGEOMETRY	(Bool, default .t.)	compute average geometry of H2O molecules & output at end
CALCDIFFUSION	(Bool, default .t.)	computes diffusion constant of oxygen & output at end
read_method	(Bool, default 1)	.xyz file format (0 for OO....HHH and 1 for OHHOHH...)
CALCIRSPECTRA	(Bool, default .f.)	store dipole moments and calculate IR spectra at end of run
CALCDOS	(Bool, default .t.)	store H velocities and calculate DOS spectra at end of run
CALC_RADIUS_GYRATION	(Bool, default .t.)	output avg. radius of gyration (column in TempPress file)
DIELECTRICOUT	(Bool, default .t.)	output dielectric constant from running averages $\langle M^2\rangle - \langle M\rangle^2$(column in TempPress file)
CHARGESOUT	(Bool, default .f.)	charges on atoms output (to separate file)
WRITECHECKPOINTS	(Bool, default .t.)	configurations of all beads output (to separate file)
td_freq	(int, default 1)	Total dipole output frequency
tp_freq	(int, default 10)	Temp/Press output frequency
ti_freq	(int, default 2000)	all images output frequency
t_freq	(int, default 10)	Output frequency for everything else
checkpoint_freq	(int, default 2000)	checkpoint output frequency
RESTART	(Bool, default .f.)	restart? (this will append to previous output files)

MD options

Nbeads	(int, default 1)	Number of beads
setNMfreq	(real, default 0)	frequency (cm^{-1}) to scale normal modes to (0 for none/RPMD)
PIMD_type	(string, default 'full')	type of PIMD run ("full", "contracted", or "monomerPIMD")
intra_timesteps	(int, default 10)	ratio of slow timestep / fast timestep for contraction scheme
Rc	(real, default $L_{\min}/2$)	realspace cutoff (Å)
rc1	(real, default .8 *Rc*)	start of switched VdW cutoff (Å)
eps_ewald	(real, default 1.d-6)	eps for aewald
massO	(real, default 15.994)	mass of Oxygen (au)
massH	(real, default 1.008)	mass of Hyrdrogen (au)

Thermostat options

GENVEL	(Bool, default .t.)	generate velocities
THERMOSTAT	(Bool, default .f.)	Global Nose-Hoover thermostat?
BEADTHERMOSTAT	(Bool, default .f.)	Bead thermostat?
CENTROIDTHERMOSTAT	(Bool, default .f.)	thermostat bead centroid?
bead_thermostat_type	(string, default 'none')	type of bead thermostat - "Nose-Hoover", "Langevin"(PILE) or "none"
temp	(real, default 300)	Temperature (Kelvin)
tau	(real, default .1)	τ for global thermostat (ps)
tau_centroid	(real, default .1)	τ for centroid thermostat (ps)
global_chain_length	(int, default 4)	global Nose-Hoover chain length
bead_chain_length	(int, default 4)	bead Nose-Hoover chain length
BAROSTAT	(Bool, default .f.)	Berendson barostat (untested! probably not working)?
tau_P	(real, default 0.2)	τ for barostat (ps)
press	(real, default 1.0	reference pressure (bar)
PEQUIL	(Bool, default .f.)	pressure coupling during equilibration only?

TTM options

polar_maxiter	(int, default 15)	max polarization dipole iterations
polar_sor	(real, default 0.7)	TTM pol factor
polar_eps	(real, default 1.d-3)	accuracy to converge dipoles to (tweaked for speed)
guess_initdip	(Bool, default .t.)	guess initial, use predictor-corrector for dip iterations (increases speed)
print_dipiters	(Bool, default .f.)	print info about pol. dipole convergence

SIESTA related

sys_label	(string,required for SIESTA runs)	system label of .fdf file
mon_siesta_name	(string, required for SIESTA runs)	name of SIESTA executable for monomer calculation
siesta_name	(string, default "siesta")	name of siesta executable
num_SIESTA_nodes	(int, default 1)	# processors available for SIESTA calculations
SIESTA_MON_CALC	(Boolean, default .f.)	option to enable SIESTA monomer calculation

For backwards compatibility with the older type of input file, the keyword *old* may be placed at the top of an old-style input and it will be read accordingly.

0.1 Note on periodic boundary conditions

The current program only works for a cubic box, but it could be modified for arbitrary box. The box is automatically centered so that molecules span $[-L/2, L/2]$. The periodic boundary conditions follow the bead centroid - if the bead centroid crosses the edge of the box, then all the beads move with it. This means that at any time, some beads may lie outside the box. The potential() subroutine must be able to handle situations where beads are outside the box. All places in the code where PBCs are used are marked with *!PBC* in the code.