

MD++ Reference Manual

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1 Class organizer (4 commands and 2 variables)

Commands

<code>quit</code>	Quit MD++. Print total CPU time.
<code>setnolog</code>	This command tells MD++ not to open the A.log file in the directory specified by <code>dirname</code> . Instead, the output is directed to the screen. Use this command before assigning variable <code>dirname</code> .
<code>setoverwrite</code>	By default, MD++ will abort if the directory specified by <code>dirname</code> already exists, to avoid overwriting previous simulation data. Use this command before assigning <code>dirname</code> if you want to remove this protection and allow overwriting the data in the existing directory.
<code>sleep</code>	Put MD++ to sleep for the number of seconds specified in <code>sleepseconds</code> .

Variables

dirname	Type: string. Default: none. MD++ immediately opens a directory specified by this variable and enters (i.e. <code>cd</code> into) this directory. This becomes the working directory for all future operations and the place for all output files. Output to screen is redirected to the <code>A.log</code> file in this directory if <code>setnolog</code> is not set beforehand.
sleepseconds	Type: integer. Default: 600. Number of seconds used by command <code>sleep</code> .

2 Class **md** (123 commands and 176 variables)

Commands

addtorque	no description file
allocchain	no description file
alloccolors	Allocate colors for the X-window display. Use after <code>openwin</code> and before <code>plot</code> . Variables <code>atomcolor</code> , <code>backgroundcolor</code> , <code>bondcolor</code> , <code>color00</code> , ..., <code>color10</code> may be set before calling this command.
alloccolorsX	no description file
annealpath	no description file
applystrain	no description file
atomeye	Call Atomeye to visualize atomic structure. Atomeye is an external visualization tool developed by Dr. Ju Li. Requires variables <code>atomeyepath</code> and <code>atomeyeexe</code> to be set before calling this command. MD++ saves the atomic configuration into file <code>atomeye.cfg</code> in the current directory before calling Atomeye.
calcentralsymmetry	Computes central symmetry deviation (CSD) parameter for each atom and store them in <code>TOPOL</code> array. Requires <code>NCS</code> to be set (number of nearest neighbors in CSD calculation). Also see <code>GnuPlotHistogram</code> .

<code>calHessian</code>	Compute Hessian matrix by numerical differentiation. The step size in (\AA) for numerical differentiation is specified by <code>timestep</code> . Result saved in <code>hessian.out</code> in the current directory. If <code>input[0]=0</code> , then the entire Hessian matrix is computed. If <code>input[0]≠0</code> , then <code>input[0]=n</code> specifies the number of atoms whose corresponding (3) columns in the Hessian matrix will be computed. The atom indices are specified in <code>input[1], ..., input[n]</code> .
<code>calmisfit</code>	no description file
<code>calphonondisp</code>	no description file
<code>changeH_keepR</code>	Requires <code>input = [i j α]</code> to be set beforehand. Change the supercell \mathbf{H} while keeping the real coordinates of the atoms \mathbf{r}^i constant. The scaled coordinates \mathbf{s}^i change because $\mathbf{r}^i = \mathbf{H} \cdot \mathbf{s}^i$. The matrix \mathbf{H} consists of three column vectors $[\mathbf{c}_1 \mathbf{c}_2 \mathbf{c}_3]$, and will be changed by $\mathbf{c}_i = \mathbf{c}_i + \alpha \mathbf{c}_j$. Same as <code>redefinepbc</code> .
<code>changeH_keepS</code>	Same as <code>changeH_keepR</code> except that the scaled coordinates of the atoms \mathbf{s}^i remain constant. The real coordinates \mathbf{r}^i change because $\mathbf{r}^i = \mathbf{H} \cdot \mathbf{s}^i$. Same as <code>shiftbox</code> .
<code>constrainedrelax</code>	no description file
<code>convertCNtoCFG</code>	no description file
<code>convertXDATCAR</code>	no description file
<code>cutpastecn</code>	no description file
<code>cutpath</code>	no description file
<code>cutslice</code>	no description file
<code>eval</code>	Call the potential function and compute total potential energy, force, kinetic energy, temperature and Virial stress for the current configuration. The total potential energy and stress are printed to the screen or to the A.log file (depending on whether or not <code>setnolog</code> is set).
<code>extendbox</code>	no description file
<code>findcore</code>	no description file
<code>fixallatoms</code>	Mark all atoms with <code>fixed[i] = 1, i = 0, ..., NP - 1</code> .

fixatoms_by_ID	Requires <code>input = [n i₁...i_n]</code> beforehand. Mark all atoms $i = i_1, \dots, i_n$ with <code>fixed[i] = 1</code> .
fixatoms_by_pos_topol	no description file
fixatoms_by_position	no description file
fortranrelax	no description file
freeallatoms	Mark all atoms with <code>fixed[i] = 0, i = 0, \dots, NP - 1</code> .
GnuPlotHistogram	Call gnuplot to plot the histogram of atom energy i.e. EPOT_IND. If <code>plot_color_axis = 2</code> then the histogram of TOPOL is plotted instead. TOPOL stores the computes the central symmetry deviation (CSD) parameters computed by <code>calcentralsymmetry</code> .
initRchain	no description file
initvelocity	no description file
makecn	Same as <code>makecrystal</code> .
makecrystal	no description file
makecut	no description file
makecylinder	no description file
makedipole	no description file
makedislcyllinder	no description file
makedislocation	no description file
makedisloop	no description file
makegb	no description file
makegrainboundary	no description file
maketorquehandle	no description file
makewave	no description file
markremovefixedatoms	no description file
moveatom	no description file
movefixedatoms	no description file
movegroup	no description file
multieval	no description file
multiplyvelocity	no description file
nebrelex	no description file
openintercnfile	no description file
openpropfile	no description file

openwin	Open X-window to display current atom position in 3D. Click and drag in the X-window to rotate. Press F1 for help. Usually used as <code>openwin alloccolors rotate saverot eval plot</code>
pbcsiftatom	no description file
plot	no description file
printatoms_in_sphere	no description file
randomposition	no description file
readcn	Requires <code>incnfile = file</code> to be set. Read atomic positions, velocities and other information from <i>file</i> to the current configuration.
readHessian	no description file
readLAMMPS	no description file
readMDCASK	no description file
readMDCASKJAIME	no description file
readPOSCAR	no description file
readRASMOLXYZ	no description file
readRchain	no description file
redefinepbc	Same as <code>changeH_keepR</code> .
refreshnnlist	no description file
relabelatom	no description file
relax	Conjugate gradient relaxation. Variables <code>conj_fevalmax</code> , <code>conj_fixbox</code> , <code>conj_fixboxvec</code> , <code>conj_ftol</code> should be set before calling this command.
removeellipsoid	no description file
removefixedatoms	no description file
removeoverlapatoms	no description file
removerectbox	no description file
reorientH	no description file
replacefreeatom	no description file
restoreH	no description file
reversefixedatoms	no description file
reversergb	no description file
reversespecies	no description file
rotate	no description file

<code>run</code>	Molecular dynamics simulation. Variables <code>totalsteps</code> , <code>integrator_type</code> , <code>saveprop</code> , <code>savecn</code> , etc. should be set before calling this command.
<code>runcommand</code>	no description file
<code>runMC</code>	no description file
<code>runMCSWITCH</code>	no description file
<code>runTAMC</code>	no description file
<code>saveH</code>	no description file
<code>saverot</code>	no description file
<code>scaleH</code>	no description file
<code>scaleVel</code>	no description file
<code>setconfig1</code>	no description file
<code>setconfig2</code>	no description file
<code>setfilecounter</code>	no description file
<code>setfixedatomsgroup</code>	no description file
<code>setfixedatomsspecies</code>	no description file
<code>setgroupcomvel</code>	no description file
<code>setH</code>	no description file
<code>shiftbox</code>	Same as <code>changeH.keepS</code> .
<code>splicecn</code>	no description file
<code>srand</code>	Randomize random number generator using <code>randseed</code> , which must be set before calling this command. This affects future calls to <code>drand48()</code> . Notice that by default MD++ uses <code>drand48()</code> (which is not affected by this command), and only if it is not available from the compiler does MD++ use <code>rand()</code> .
<code>srand48</code>	Randomize random number generator using <code>randseed</code> , which must be set before calling this command. This affects future calls to <code>drand48()</code> .
<code>srand48bytime</code>	Randomize random number generator using current CPU time as the seed. This affects future calls to <code>drand48()</code> .

srandbytime	Randomize random number generator using current CPU time as the seed. This affects future calls to <code>rand()</code> . Notice that by default MD++ uses <code>drand48()</code> (which is not affected by this command), and only if it is not available from the compiler does MD++ use <code>rand()</code> .
statedistance	no description file
step	no description file
switchconfig	no description file
testcolor	no description file
testpotential	no description file
wintogglepause	no description file
writeatomeyecfg	no description file
writeatomtv	no description file
writecn	Requires <code>finalcnfile = file</code> to be set before calling this command. Write atomic positions of the current configuration to <i>file</i> . If <code>write_all = 1</code> is also set, the atomic velocities and other information are written in <i>file</i> as well.
writeENERGY	no description file
writeFORCE	no description file
writeintercn	no description file
writeLAMMPS	no description file
writeMDCASK	no description file
writeMDCASKXYZ	no description file
writePINYMD	no description file
writePOSCAR	no description file
writePOSITION	no description file
writepovray	no description file
writeRASMOLXYZ	no description file
writeRchain	no description file

Variables

allocmultiple	Type: integer. If <code>allocmultiple = n</code> is set before <code>readcn</code> or <code>makecrystal</code> , then the memory for $NP \times n$ atoms is allocated, where NP is the actual number of atoms. Useful for <code>extendbox</code> .
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annealspec	no description file
applieshear	no description file
atomcolor	no description file
atomeyeexe	no description file
atomeyepath	no description file
atomeyerepeat	no description file
atommass	no description file
atomradius	no description file
atomTcpl	no description file
autowritegiffreq	no description file
backgroundcolor	no description file
bondcolor	no description file
bondlength	no description file
bondradius	no description file
boxdamp	no description file
boxTcpl	no description file
chainlength	no description file
command	no description file
conj_dfpred	no description file
conj_fevalmax	no description file
conj_fixatoms	no description file
conj_fixbox	no description file
conj_fixboxvec	no description file
conj_fixdir	no description file
conj_fixshape	no description file
conj_ftol	no description file
conj_g2res	no description file
conj_itmax	no description file
constrainatoms	no description file
constrainS	no description file
crystalstructure	no description file
curstep	no description file
dEdlambda	no description file
dH	no description file
DOUBLE_T	no description file
Ecoh	no description file
ecspring	no description file
energycolorbar	no description file
EPBOX	no description file
EPOT	no description file
EPOTO	no description file
EPOT_IND	no description file

equilsteps	no description file
ESTRAIN	no description file
extforce	no description file
F	no description file
F0	no description file
Fext	no description file
filecounter	no description file
finalcnfile	no description file
fixatomcolor	no description file
fixbox	no description file
fixboxvec	no description file
fixed	no description file
fixedatomenergypartition	no description file
forcemul	no description file
fortranexe	no description file
fortranpath	no description file
GH	no description file
group	no description file
H	no description file
H0	no description file
H_11	no description file
H_12	no description file
H_13	no description file
H_21	no description file
H_22	no description file
H_23	no description file
H_31	no description file
H_32	no description file
H_33	no description file
HELM	no description file
HELMP	no description file
highlightcolor	no description file
hprecond	no description file
image	no description file
incnfile	no description file
input	no description file
integrator_type	no description file
intercnfile	no description file
KATOM	no description file
KBOX	no description file
lambda0	no description file
lambda1	no description file

latticeconst	no description file
latticesize	no description file
latticestructure	no description file
makecnspec	no description file
MC_accept_ratio	no description file
MC_dr	no description file
mcatom	no description file
MDCASKpot	no description file
mkcylinderspec	no description file
mkdipole	no description file
mkdislspec	no description file
myname	no description file
NCS	no description file
nebspec	no description file
NIC	no description file
NNM	no description file
NP	no description file
nspecies	no description file
OMEGA	no description file
outpropfile	no description file
output	no description file
output_fmt	no description file
plot_atom_info	no description file
plot_color_axis	no description file
plot_color_bar	no description file
plot_color_windows	no description file
plot_limits	no description file
plot_map_pbc	no description file
plotfreq	no description file
potfile	no description file
PRESSURE	no description file
pressureadd	no description file
printfreq	no description file
PSTRESS	no description file
R	no description file
R0	no description file
randseed	no description file
refpotential	no description file
RLIST	no description file
rotateangles	no description file
savecn	no description file
savecnfreq	no description file

SAVEMEMORY	no description file
saveprop	no description file
savepropfreq	no description file
shearrate	no description file
SIGMA	no description file
species	no description file
SR	no description file
storedr	no description file
stress	no description file
stressmul	no description file
switchfreq	no description file
switchfunc	no description file
switchoffatoms	no description file
T_OBJ	no description file
timestep	no description file
Tinst	no description file
TOPOL	no description file
torquespec	no description file
totalsteps	no description file
TSTRESS	no description file
TSTRESS_xx	no description file
TSTRESS_xy	no description file
TSTRESS_xz	no description file
TSTRESS_yx	no description file
TSTRESS_yy	no description file
TSTRESS_yz	no description file
TSTRESS_zx	no description file
TSTRESS_zy	no description file
TSTRESS_zz	no description file
usenosehoover	no description file
usescalevelocity	no description file
vacuumratio	no description file
VH	no description file
VIRIAL	no description file
VIRIAL_IND	no description file
VR	no description file
VSR	no description file
vt2	no description file
wallmass	no description file
win_height	no description file
win_width	no description file
writeall	no description file

<code>writevelocity</code>	no description file
<code>xprecond</code>	no description file
<code>yprecond</code>	no description file
<code>zeta</code>	no description file
<code>zetaa</code>	no description file
<code>zetav</code>	no description file
<code>zprecond</code>	no description file

3 Class `mdparallel` (9 commands and 15 variables)

Commands

<code>alloc_all</code>	Every processor (master and slave) allocate memory (such as <code>SR</code> , <code>F</code> arrays) according to the number of atoms <code>NP</code> . Needed before <code>eval_parallel</code> . Effective only when MD++ is compiled for parallel runs, e.g. with <code>SYS = mpicc</code> or <code>SYS = mpigpp</code> .
<code>Broadcast_Atoms</code>	CPU 0 (master) broadcast all atom positions to other CPUs (slaves). Needed before <code>eval_parallel</code> . Effective only when MD++ is compiled for parallel runs, e.g. with <code>SYS = mpicc</code> or <code>SYS = mpigpp</code> .
<code>eval_parallel</code>	CPU 0 (Master) calls <code>eval</code> with the help of all other CPUs (slaves). Requires <code>Broadcast_Atoms</code> to be called beforehand.
<code>Mark_Local_Atoms</code>	no description file
<code>Master_to_Slave</code>	Requires <code>command = cmd</code> to be set beforehand. CPU 0 (master) request other CPUs (slaves) to execute <code>cmd</code> , which can be any MD++ command or variable assignment.
<code>Partition_Domains</code>	no description file
<code>quit_all</code>	Equivalent of <code>quit</code> in parallel.
<code>run_parallel</code>	no description file
<code>Slave_to_Master_Atoms</code>	no description file

Variables

domainID	no description file
myDomain	no description file
myIX	no description file
myIY	no description file
myIZ	no description file
myXmax	no description file
myXmin	no description file
myYmax	no description file
myYmin	no description file
myZmax	no description file
myZmin	no description file
numDomains	no description file
nXdoms	no description file
nYdoms	no description file
nZdoms	no description file

4 Class fs (1 commands and 10 variables)

Commands

readpot	no description file
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Variables

A	no description file
alpha	no description file
B	no description file
b0	no description file
beta	no description file
c	no description file
c0	no description file
c1	no description file
c2	no description file
d	no description file

5 Class **lj2** (1 commands and 6 variables)

Commands

initLJ	no description file
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Variables

C6_00	no description file
C6_01	no description file
C6_11	no description file
C12_00	no description file
C12_01	no description file
C12_11	no description file

6 Class **eam** (2 commands and 3 variables)

Commands

readeam	no description file
readMEAM	no description file

Variables

eamfiletype	no description file
eamgrid	no description file
pottype	no description file

7 Class **meam** (3 commands and 18 variables)

Commands

Broadcast_MEAM_Param	no description file
printpairpot	no description file
readMEAM	no description file

Variables

a8b	no description file
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ag	no description file
atpe2b	no description file
atpe3b	no description file
b8c	no description file
c8a	no description file
cg8c	no description file
d8d	no description file
dang1	no description file
dang2	no description file
embf	no description file
enable_square_rscrn	no description file
enable_zbl_fdimer	no description file
rhotot	no description file
rhsq	no description file
tav	no description file
xzbl	no description file
xzbl0	no description file

8 Class meam-baskes (2 commands and 11 variables)

Commands

printpairpot	no description file
readMEAM	no description file

Variables

cmin0	no description file
ename0	no description file
ename1	no description file
ename2	no description file
kode0	no description file
kode1	no description file
kode2	no description file
meafile	no description file
meamfile	no description file
ntypes	no description file
rcut	no description file

9 Class meam-lammps (3 commands and 19 variables)

Commands

Broadcast_MEAM_Param	no description file
printpairpot	no description file
readMEAM	no description file

Variables

arho1	no description file
arho2	no description file
arho2b	no description file
arho3	no description file
arho3b	no description file
dgamma1	no description file
dgamma2	no description file
dgamma3	no description file
frhop	no description file
gamma	no description file
meafile	no description file
meamfile	no description file
rcut	no description file
rho	no description file
rho0	no description file
rho1	no description file
rho2	no description file
rho3	no description file
t_ave	no description file