Molecular Dynamics FF, Manual , version 0.2.2

30 novembre 2011

1 But

Le but de ce document est de repertorier les differents algorithmes utilisés par MDFF. Notamment, definir les commandes (TAG) et leurs valeurs par défaut. Mais également, les réferences aux codes, articles originaux, livres dont sont extraits les différents algorithmes, ou preciser dans le cas contraire (i.e FMV!) ce que fait la routine point par point. Ce travail de documentation permettra de faciliter la découverte de bug qui independamment de ma volonté sont (et seront) forcément présents.

2 Usage

MDFFonly needs one input file usually called control.F [1]

2.1 Minimum settings : the input file

The input file is composed of different sections. Each section is defined by &SECTIONNAME and &END. Everything outside the sections is ignored.

In MDFF, five sections are always required :
- &controltag ... &end → General control parameters for calculation
- &mdtag ... &end → General Molecular dynamics parameters.
- &configtag ... &end → Information on the configuration
- &fieldtag ... &end → Set the Force-Field.
- &proptag ... &end → Calculation of properties

Using this minimum settings (5 empty sections) the code runs with default values. It correspond to a molecular dynamics trajectory of 10 unit of times of a fcc lennard-jones crystal (256 atoms) at ρ =1.0 at T =1.0. In the next sextion we show the standard output of this minimum setting.

1. the .F extension permits to get nice colors with vim

2.2 Minimum setting : standart output

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============================================================

MOLECULAR DYNAMICS ...for fun
mdff.0.2.0
parallel version
filipe.manuel.vasconcelos@gmail.com
Running on   1 nodes
time     : 2011/11/05    15:50:14
calc     : md

============================================================

periodic boundary conditions in cubic cell
verlet list used
units reduced by the number of atom
dynamic calculation
NVE ensemble --- velocity verlet integrator
with equilibration:
berendsen scaling ( is not canonical ...and so NVE)
number of steps                      =         10
timestep                             = .10000E-02
time range                           = .10000E-01
temperature                          =    1.00000
number of equilibration steps        =         10
equilibration period                 =          1
Berendsen thermo time scale          = .10000E-02
tauberendsen = dt -> simple rescale
print thermo  periodicity            =          1

============================================================

structure generated from the code
Face-centered cubic structure :  4x  4x  4
system                               : fcc
natm                                 =        256
cell parameter                       =     6.3496
volume                               =   256.0000
```

```
density                                =     1.0000
distance check subroutine
smallest distance =   1.12

============================================================

force field information :
no masses are implemented
LENNARD-JONES

       eps    /    / sigma* \ q       / sigma*  \ p \
 V = ------- |  p | ------- |    - q | -------- |   |
      q - p   \    \   r    /         \    r    /   /

USER DEFINED MODEL
cutoff  =    2.50000

A-A interactions:
sigmaAA =    1.00000
epsAA   =    1.00000
qAA     =   12.00000
pAA     =    6.00000
long range correction :         -0.535433102

paralelisation - atom decomposition
rank    0 atom    1 to  256
============================================================
...
============================================================

                 TOTAL :  cpu time     0.15
                    MD :  cpu time     0.01

main subroutines:
MD:
    engforce_bmlj      :  cpu time     0.01
    engforce_coul_DS   :  cpu time     0.00
    vnlistcheck        :  cpu time     0.00
============================================================
```

2.3 Miniumim setting : Output files

For this minimum setting, the code generates 4 files :
- OUTFF : close to the standard output
- OSZIFF : thermodynamic parameters
- TRAJFF : trajectory file (empty in this case)
- CONTFF : final configuration

theses files and other output files are described in a following section.

2.4 Input file : Description

2.4.1 &controltag

Where : `SUBROUTINE control_init` in `control.f90`

`lbmlj`	(LOGICAL)
`lcoulomb`	(LOGICAL)
`lvnlist`	(LOGICAL)
`lstatic`	(LOGICAL)
`calc`	(CHARACTER)
`dgauss`	(CHARACTER)
`lpbc`	(LOGICAL)
`longrange`	(CHARACTER)
`cutoff`	(DOUBLE PRECISION)
`skindiff`	(DOUBLE PRECISION)
`restart`	()
`lreduced`	(LOGICAL)
`lshiftpot`	(LOGICAL)
`ltest`	(LOGICAL)

2.4.2 &mdtag

Where : `SUBROUTINE md_init` in `md.f90`

`npas`	(INTEGER)
`integrator`	(CHARACTER)
`dt`	(DOUBLE PRECISION)
`temp`	(DOUBLE PRECISION)
`nequil`	(INTEGER)
`nequil_period`	(INTEGER)
`nprint`	(INTEGER)
`fprint`	(INTEGER)
`ltraj`	(LOGICAL)
`itraj_start`	(INTEGER)
`itraj_period`	(INTEGER)
`spas`	(INTEGER)
`setvel`	(CHARACTER)
`nuandersen`	(DOUBLE PRECISION)
`tauberendsen`	(DOUBLE PRECISION)
`Qnosehoover`	(DOUBLE PRECISION)

2.4.3 &configtag

Where : `SUBROUTINE config_init` in `config.f90`

`system` (CHARACTER)

`rho` (DOUBLE PRECISION)

`box` (DOUBLE PRECISION)

`ntype` (INTEGER)

`natm` (INTEGER)

`struct` (CHARACTER)

`lfcc` (LOGICAL)

`lsc` (LOGICAL)

`lbcc` (LOGICAL)

`ncell` (INTEGER)

`xna` (DOUBLE PRECISION)

`xnb` (DOUBLE PRECISION)

`lgenconf` (LOGICAL)

2.4.4 &fieldtag

Where : `SUBROUTINE field_init` in `field.f90`

epsAA (DOUBLE PRECISION)

epsAB (DOUBLE PRECISION)

epsBB (DOUBLE PRECISION)

sigmaAA (DOUBLE PRECISION)

sigmaAB (DOUBLE PRECISION)

sigmaBB (DOUBLE PRECISION)

qljAA (DOUBLE PRECISION)

pljAA (DOUBLE PRECISION)

qljAB (DOUBLE PRECISION)

pljAB (DOUBLE PRECISION)

qljBB (DOUBLE PRECISION)

pljBB (DOUBLE PRECISION)

mA (DOUBLE PRECISION)

mB (DOUBLE PRECISION)

qa (DOUBLE PRECISION)

qb (DOUBLE PRECISION)

ncelldirect (INTEGER)

ncellewald (INTEGER)

lKA (LOGICAL)

alphaES (DOUBLE PRECISION)

2.4.5 &proptag

Where : SUBROUTINE prop_init in prop.f90

`nprop_start` (INTEGER)

`nprop` (INTEGER)

`nprop_print` (INTEGER)

`lefg` (LOGICAL)

`lgr` (LOGICAL)

`lstrfac` (LOGICAL)

`lmsd` (LOGICAL)

`lvacf` (LOGICAL)

2.4.6 &opttag

Where : `SUBROUTINE opt_init` in `opt.f90`

`ncopt` (INTEGER)

`nskipopt` (INTEGER)

`nmaxopt` (INTEGER)

`optalgo` (CHARACTER)

2.4.7 &vibtag

Where : `SUBROUTINE vib_init` in `vib.f90`

`ncvib` (INTEGER)

`ngconf` (INTEGER)

`lwrite_vectff` (LOGICAL)

`imod` (INTEGER)

`nkphon`

`resdos` (DOUBLE PRECISION)

`omegamax` (DOUBLE PRECISION)

`ksx,ksy,ksz`

`kfx,kfy,kfz`

2.4.8 &efgtag

Where : `SUBROUTINE efg_init` in `efg.f90`

`lefgprintall` (LOGICAL)

`ncelldirect` (INTEGER)

`ncefg` (INTEGER)

`ncellewald` (INTEGER)

`cutefg` (DOUBLE PRECISION)

`alphaES` (DOUBLE PRECISION)

`resvzz` (DOUBLE PRECISION)

`reseta` (DOUBLE PRECISION)

`resu` (DOUBLE PRECISION)

`vzzmin` (DOUBLE PRECISION)

`umin` (DOUBLE PRECISION)

`ntcor`

2.4.9 &msdtag

Where : `SUBROUTINE msd_init` in `msd.f90`

`tdifmax` (DOUBLE PRECISION)

`nblock` (DOUBLE PRECISION)

`ibmax` (DOUBLE PRECISION)

2.4.10 &grtag

Where : `SUBROUTINE control_init` in `radial_distribution.f90`

`resg` (DOUBLE PRECISION) resolution in the radial distribution function

2.4.11 &vacftag

Where : `SUBROUTINE vacf_init` in `vacf.f90`

`tdifmax` (DOUBLE PRECISION)

`it0` (DOUBLE PRECISION)

2.5 Output files : description

3 Commands

4 Theory

[1]

Références

[1] M. P. Allen and D. J. Tildesley, *Computer simulation of liquids*, Oxford University Press, Oxford UK, 1987.