Molecular Dynamics FF, Manual , version 0.2.2

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Avant-Propos

Actually there is three general reason, why I start this code :

– for research :

EFG + MD = nowhere could be useful in futur

– for education :

Try to teach Computational Physics with a real connection to codes. Interactive figures and animation

– for fun :

Molecular Dynamics (and Statistical Physics) is really fun ... (beautiful and intuitive theoretical physic)

the actual version is 0.2.0 ... but I never wrote any documentation for the intermediate versions. I'm not following the code name convention quite well. Basically since 0.2.0 Ewald sum where introduced. The first digit is for humility

The document will be partlty in french ;)

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.

En ce qui concerne l'historique de ce code : il, complétement réecrit depuis, est basé sur le code de dynamique moléculaire de F. Affouard et S. Sastry, utilisée au cours de mon Master á Lille. Il en a gardé certaines particularités. Il est orientée dans le but d'étudier un systemes de particules en interactions avec des potentiels simples (Lennard-Jones , Coulomb). Cependant dans le but de la recherche, il ne devrait être utiliser en production que pour l'étude du gradient de champ électrique (EFG).

2 Usage

MDFFne necessite qu'un seul fichier d'entrée, géneralement appelé control.F [1], mais peut porter n'importe quel autre nom. Ce fichier gère toutes les parties du code et toutes les actions.

2.1 Minimum settings : the input file

The input file is composed of different sections. Each section is started by &SECTIONNAME and ended by &END (We are closely following italian codes ;)). All input 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 Field-Force.
- &proptag ... &end → Calculation of properties

Using this minimum settings (empty section) 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. l'extension .F permet d'avoir de jolie couleur avec vim

2.2 Minimum setting : standart output

```
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                         -(o o)-
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          ____    ____  ______   ________  ________
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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`
`it0`

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.