CANDELA User's Manual

This is the manual for CANDELA, which was developed in Mohan Chen's research group in Peking University.

Outline

In Section 1, we briefly introduce the functions of CANDELA. In Section 2, we introduce how to obtain and install CANDELA. In Section 3, a list of examples is provided. In Section 4, some key parameters are explained in detail. Finally, in section 5, the code structure is introduced.

1. Introduction

CANDELA is the office name of Mohan Chen when he was a postdoc at Princeton University, where the code was created. The code was designed in a way to read in data from either Quantum Espresso, VASP, PROFESS, ABACUS, LAMMPS etc., most of the data are molecular dynamics trajectories. Next, CANDELA is mainly designed for post processing and provides results like radial distribution functions, bond angle distribution functions, diffusion coefficients, and many others. It is convenience for users who use multiple packages and would like to analyze the data in a same manner.

2. Download:

The code is stored in the bitbucket website and can be downloaded from the website with the following address:
https://mohanchen@bitbucket.org/mohanchen/Candela.git

3. Structure of the CANDELA Code

Blue: commonly used.
Black: base modules.
Red: analysis for liquid water system.
Purple: analysis for mechanical properties.

atoms.cpp, atoms.h	Define the class of atoms
bdf.cpp, bdf.h	Calculate the bond angle distribution functions
bdf_rcut.cpp, bdf_rcut.h	Calculate the bond angle distribution functions within a radius cutoff
cell.cpp, cell.h	Cell Information
cellFile.cpp, cellFile.h	Cell Files from various kinds of software
cellABACUS.cpp	Read in cell information from ABACUS
cellLAMMPS.cpp	Read in cell information from LAMMPS
cellPROFESS.cpp	Read in cell information from PROFESS
cellPWmat.cpp	Read in cell information from PWmat
cellQE2.cpp	Read in cell information from Quantum Espresso
cellQE.cpp	Read in cell information from Quantum Espresso

cellRAW.cpp	Read in cell information from RAW format
cellVASP.cpp	Read in cell information from VASP
cellXYZ.cpp	Read in cell information from XYZ format
const.h	Define constants
density2D.cpp, density2D.h	For water, to plot two dimensional figures regarding the relation between density and length of covalent bonds.
dielectric.cpp, dielectric.h	Compute dielectric constants for liquid water.
distri2D.cpp, distri2D.h	Compute angle-distance relation for liquid water (2D).
distri3D_ions.cpp, distri3D_ions.h	Compute 3D distribution of atoms/MLWFs around ions(hydroxide,Cl), read by VESTA
Doc	Documents
dsf.cpp, dsf.h	Dynamic Structure Factors
ele_conductivity.cpp, ele_conductivity.h	Compute the electron conductivity.
examples	Include examples.
ext.cpp, ext.h	Extend the cells.
find_ion.cpp, find_ion.h	Find the ion positions in the interface of water-oil system.
gfun.cpp, gfun.h	Define globally used functions.
HBs.cpp, HBs.h	Define hydrogen bonds in liquid water.
Honeycutt.cpp Honeycutt.h	Honeycutt analysis (not used yet).
planarity.cpp, planarity.h	Compute the hyper structures of OH- ion via the order parameter named planarity.
ili_3D.cpp, ili_3D.h	Generate 3D data of Instantaneous Liquid Interface (ILI)
ili.cpp, ili.h	Compute Instantaneous Liquid Interface (ILI)
input.cpp, input.h	Input data.
insert.cpp, insert.h	Randomly insert atoms into existing structures.
iprof.cpp, iprof.h	Ionic density profile.
isf2.cpp, isf2.h	Compute intermediate scattering function, new by Qianrui.
isf.cpp, isf.h	Compute intermediate scattering function, old.
main.cpp	Main function of CANDELA package.
Makefile	Makfile of CANDELA package.
math.cpp, math.h	Math functions.
matrix3.cpp, matrix3.h	3-dimensional matrix format.
mdp2.cpp, mdp2.h	Compute mean density profile based on mean liquid interfaces.
mdp3.cpp, mdp3.h	Analysis based on Mean Density Profile and Instantaneous Liquid Interface
mdp.cpp, mdp.h	Compute mean density profile based on instantaneous liquid interface (ILI).
mj.cpp, mj.h	Provide proton transfer data.
movie_hexane.cpp, movie_hexane.h	Print movie data for hexane project.

msd.cpp, msd.h	Compute the mean square displacements.
msd_multiple.cpp, msd_multiple.h	Compute the mean square displacements through multiple trajectories.
pdf2d.cpp, pdf2d.h	PDF for 2d materials.
pdf5.cpp, pdf5.h	Compute PDF for each shell of neighboring atoms.
pdf_added.cpp, pdf_added.h	The extra functions used in computing the PDF of systems.
pdf.cpp, pdf.h	Compute the radial distribution functions.
powers.cpp, powers.h	Compute the power spectra of system (FFT of VAF).
presolvation.cpp, presolvation.h	Compute the presolvation structure (yes/no).
local_pseudopotential.cpp, local_pseudopotential.h	Change the form of the readin pseudopotential.
random.h	Compute the random numbers.
README.md	Change log, important.
reorganize.cpp, reorganize.h	Reorganize the input trajectories through nbin,
binftream.cpp, binfstream.h	Read in binary data.
ssf.cpp, ssf.h	Compute static structure factors
ssf_selected.cpp, ssf_selected.h	Compute static structure factors for selected q points.
tetra_order.cpp, tetra_order.h	Tetrahedral order parameter computed for each water molecule.
vacuum.cpp, vacuum.h	Add vacuum for a structure.
vec3.h	Vector3 format.
velcor.cpp, velcor.h	Velocity autocorrelation functions.
vel.cpp, vel.h	Compute the distribution of velocities.
void.cpp, void.h	Create a void in a material.
wannier1.cpp, wannier1.h	Compute distributions of Wannier functions, including 1D, 2D, and 3D.
wannier.cpp, wannier.h	Compute Infrared Spectra from Wannier functions, plot distribution of dipoles.
water.cpp, water.h	Construct a water class for each read-in water.
waterwire2.cpp, waterwire2.h	Compute the free energy map of waterwire involving single and double proton transfer.
waterwire.cpp, waterwire.h	Compute the free energy map of waterwire involving single and double proton transfer.
wavefunc.cpp, wavefunc.h	Wave functions, added by Qianrui
wfFile.cpp, wfFile.h	Wave functions, added by Qianrui.
wfPWmat.cpp, wfPWmat.h	Wave functions, added by Qianrui.
wfqe.cpp, wfqe.h	Wave functions, added by Qianrui
wfRead.cpp, wfRead.h	Wave functions, added by Qianrui.
write.cpp, write.h	Wave functions, added by Qianrui.
ww_compress.cpp, ww_compress.h	Compute the compression of water wires.
xsf.cpp, xsf.h	Compute the properties from 3D data in XSF format.

4. List of Examples:

1) Radial distribution functions for O-O with varying cells
2) Bond angle distribution function for O triplets with varying cells
3) Bond angle distribution function for O triplets with cutoff in varying cells
4) Hydrogen bond analysis
5) Mean square displacement
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4.1）Radial distribution functions for O-O with varying cells

```
calculation  pdf # Pair Distribution Function.
system water
geo_in_type  QE
geo_directory  ../SCAN_volume/water.pos
cell_file ../SCAN_volume/water.cel
geo_1        1
geo_2        122517
geo_interval 1
geo_ignore   20836 ! first 5 ps

geo_out      pdf.txt # output pdf name.

ntype        2        # number of different types of atoms.
natom        192      # total number of atoms.
natom1       64
natom2       128
dr           0.01     # delta r in real space
rcut         6.22     # real space cutoff

id1 O
id2 H
ele1 O
ele2 O

struf_dgx   0.05
struf_ng    480
```

4.2）Bond Angle distribution function for O triplets with varying cells

```
calculation  bdf_rcut
system water
geo_in_type  QE  #PROFESS/VASP/QE/ABINIT/MESIA/XYZ/PIMD
geo_directory  ../SCAN_volume/water.pos
cell_file ../SCAN_volume/water.cel
geo_1        1
geo_2        122517
geo_interval 1
geo_ignore   20836 ! ignore first 5 ps

ntype        2         # number of different types of atoms.
natom        192      # total number of atoms.
natom1       64
natom2       128

dr           0.01      # delta r in real space

id1 O
id2 H

rcut1        4.0
bdf_rcut     3.154
bdf_dtheta   0.5     # d(theta) for degree between (0,180]

ele1 O
ele2 O

func 1

factor 0.9834679045
x0 2.25
y0 40
nx 50
ny 70
dx 0.025
dy 2.0
```

4.3）Bond Angle distribution function for O triplets with cutoff in varying cells

Notes: if func_b==1, do nothing; func_b==2, both bonded; func_b==3, both are not boned; func_b==4, one bonded, the other not bonded.

```
calculation  bdf_rcut       #
system water
geo_in_type  QE   #PROFESS/VASP/QE/ABINIT/MESIA/XYZ/PIMD
geo_directory  ../../SCAN_volume/water.pos
cell_file ../../SCAN_volume/water.cel
geo_1        1
geo_2        122517
geo_interval 1
geo_ignore   20836 ! first 5 ps

ntype        2         # number of different types of atoms.
natom        192      # total number of atoms.
natom1       64
natom2       128

dr           0.01      # delta r in real space

id1 O
id2 H

rcut1        4.0
bdf_rcut     3.154     # cutoff for O triplets
bdf_out      3.154.dat  # output file name
bdf_dtheta   0.5     # d(theta) for degree between (0,180]

ele1 O
ele2 O
func_b  2

factor 1.1542012927
x0 2.25
y0 40
nx 50
ny 70
dx 0.02
dy 2.0
```

4.4）Hydrogen bond analysis

```
calculation  hbs  # hydrogen bond analysis
system water
geo_in_type  QE   #PROFESS/VASP/QE/ABINIT/ABACUS
geo_directory  ../SCAN_volume/water.pos
cell_file ../SCAN_volume/water.cel
geo_out      PBE0_OH_HBs.dat
geo_1        1
geo_2        122517
geo_interval 1   # geometry selected with this interval
geo_ignore   20836

ntype        2         # number of different types of atoms.
natom        192       # total number of atoms.

natom1 64 # O
natom2 128 # H
id1 O
id2 H

rcut_oo 3.5
rcut_oh 1.24
acut_hoo 30
```

---------- FOR LAMMPS ----------

```
calculation    hbs    # hydrogen bond analysis
system water
geo_in_type    LAMMPS
geo_directory    ../dump.lammpstrj
geo_1            1
geo_2            100 40001
geo_interval 1
geo_ignore     0 ! first 5 ps

ntype            2             # number of different types of atoms.
natom            96           # total number of atoms.

natom1 32 # O
natom2 64 # H
id1 O
id2 H

rcut_oo 3.5
```

rcut_oh 1.24
acut_hoo 30

cartesian 1

4.5）Mean square displacement

```
calculation  msd     # pair Distribution Function.
system water
geo_in_type  QE   #PROFESS/VASP/QE/ABINIT/MESIA
geo_directory  ../SCAN_volume/water.pos
cell_file ../SCAN_volume/water.cel
geo_1       1
geo_2      122517
geo_interval 1
geo_ignore   0

geo_out     pdf.txt # output pdf name.

ntype       2        # number of different types of atoms.
natom       192     # total number of atoms.
natom1      64
natom2      128
dr          0.01     # delta r in real space
rcut        6.22    # real space cutoff

id1 O
id2 H
ele1 O
ele2 O

struf_dgx   0.05
struf_ng    480

func 2

cartesian 1
msd_dt 0.005
```

4.6）Mean square displacement computed by multiple sections

Example 1 for QE and Example 2 for LAMMPS

```
calculation  msd_multiple  # mean square displacements
system hydroxide
geo_in_type  QE   #PROFESS/VASP/QE/ABINIT/MESIA
geo_directory  ../SCAN_volume/water.pos
cell_file ../SCAN_volume/water.cel
geo_1       1
geo_2       122517
geo_interval 1

ntype       2        # number of different types of atoms.
natom       192      # total number of atoms.

natom1 64 # O
natom2 128 # H
id1 O
id2 H

rcut_oo 3.5
rcut_oh 1.24
acut_hoo 30

msd_n  5  # number of msd needed
msd_t0 5 # starting point of msd
msd_t 12.20 # length of msd (in ps)
msd_dt0 3 # difference between different different MSD
msd_dt .00084661 # delta t between 2 snapshots
msd_natom 192
msd_stokes 0
system water
```

```
calculation msd_multiple # mean square displacements
system water
geo_in_type LAMMPS
geo_directory  ../lmp.nve.64/dump.lammpstrj
geo_1       1
geo_2       200001
geo_interval 1
geo_ignore   1000 ! first 5 ps

ntype 2 # number of different types of atoms.
```

```
natom 192 # total number of atoms.
natom1 64 # O
natom2 128 # H
id1 O
id2 H
rcut_oo 3.5
rcut_oh 1.24
acut_hoo 30
msd_n 10 # number of msd needed
msd_t0 0 # starting point of msd
msd_t 100 # length of msd (in ps)
msd_dt0 100 # difference between different different MSD
msd_dt 0.005 # delta t between 2 snapshots (ps)
msd_natom 192
 msd_stokes 0
```

```
calculation  msd_multiple
geo_in_type PROFESS
geo_directory  ../out/
geo_1 4000
geo_2 400000
geo_interval 4
geo_ignore 0

ntype 2
natom 128
natom1 118
natom2 10
id1 L7
id2 L6
msd_single 1 #1: open msd for only one type 0: close(by default)
msd_type 0   # type id (starts from 0)
msd_natom 10

msd_n 10
msd_t0 1
msd_t 10
msd_dt0 10
msd_dt 0.01
msd_stokes 0
dt_snapshots 0.00025
```

4.7）Wannier centers and dipoles

```
  calculation  wannier      # pair Distribution Function.
  system water
  geo_in_type  QE   # input type of geometry file:
PROFESS/VASP/QE/ABINIT/MESIA
  geo_directory  ../SCAN_volume/water.pos
  cell_file ../SCAN_volume/water.cel
  wannier_file ../SCAN_volume/water.wfc
  geo_1       1
  geo_2       122517
  geo_interval 1
  geo_ignore   20836

  ntype       2        # number of different types of atoms.
  natom       192     # total number of atoms.
  natom1      64
  natom2      128

  id1 O
  id2 H
  ele1 O

  nbands 256

  dr 0.001
  rcut 1.00

  dz 0.02  # for dipole moment
  rcut1 10.0 # for dipole moment

  nx 70
  ny 70
  x0 0.95
  y0 0.25
  dx 0.0025
  dy 0.005
```

4.8）Tetrahedrality

```
  calculation  top  # hydrogen bond analysis
  system hydroxide
  geo_in_type  QE   # input type of geometry file:
PROFESS/VASP/QE/ABINIT/MESIA
  geo_directory  ../SCAN_volume/water.pos
  cell_file ../SCAN_volume/water.cel
  geo_1       1
  geo_2       122517
  geo_interval 1
  geo_ignore   20836 ! first 5 ps

  ntype       2        # number of different types of atoms.
  natom       192     # total number of atoms.
  natom1      64
  natom2      128
  id1 O
  id2 H

  rcut_oo 3.5
  rcut_oh 1.24
  acut_hoo 30

  bdf_rcut 3.15
```

4.9）Reorganize

```
calculation  reorganize
system water         # system is water
geo_in_type  QE      # PROFESS/VASP/QE/ABINIT/MESIA
geo_directory  ../SCAN_volume/water.pos
wannier_file ../SCAN_volume/water.wfc
cell_file ../SCAN_volume/water.cel

geo_1       1
geo_2       122517
geo_interval 1
geo_ignore   20836 ! first 5 ps


ntype       2       # number of different types of atoms.
natom       192     # total number of atoms.
natom1      64
natom2      128
id1 O
id2 H

nbands 256 # number of bands for the system

nbin 10
```

4.10）Radial distribution function of O*H in hydroxide solution

```
calculation  pdf      # pair Distribution Function.
system hydroxide
geo_in_type  QE   # PROFESS/VASP/QE/ABINIT/MESIA
geo_directory OH_PBE0_vdW.pos
geo_1       1
geo_2       95306
geo_interval 1

geo_out     pdf.txt # output pdf name.

ntype       2        # number of different types of atoms.
natom       191      # total number of atoms.
natom1      64
natom2      127
dr          0.002     # delta r in real space
rcut        6.2    # real space cutoff

id1 O
id2 H
ele1 O
ele2 H

celldm1 12.444655509
celldm2 12.444655509
celldm3 12.444655509
```

4.11）Hydrogen bonds for hydroxide

```
calculation  hbs  # hydrogen bond analysis
system hydroxide
geo_in_type  QE   # PROFESS/VASP/QE/ABINIT/MESIA
geo_directory OH_PBE0_vdW.pos
geo_out     PBE0_OH_HBs.dat
geo_1       1
geo_2       95306
geo_interval 1   # pick up geometry with this interval
ntype       2        # number of different types of atoms.
natom       191      # total number of atoms.

natom1 64 # O
natom2 127 # H
id1 O
id2 H

celldm1 12.444655509
celldm2 12.444655509
celldm3 12.444655509

rcut_oo 3.5
rcut_oh 1.24
acut_hoo 30
```

4.12）Multiple jumps

```
calculation  mj  # multiple jump
system hydroxide
geo_in_type  QE   #PROFESS/VASP/QE/ABINIT/ABACUS
geo_2        87

ntype       2        # number of different types of atoms.
natom       191      # total number of atoms.

natom1 64 # O
natom2 127 # H
id1 O
id2 H

celldm1 12.444655509
celldm2 12.444655509
celldm3 12.444655509

func 2
```

4.13）Planarity of hydroxide ion and its neighbors

Note: If delta is not set, then the criterion is not used.

Nacc set to 4 suggests that the hyper coordinated structures are selected,

Ndon set to 1 suggests that only those water molecules who donate 1 HB are selected.

```
calculation  hyper  # instantaneous liquid interfaces
system hydroxide
geo_in_type  QE   # PROFESS/VASP/QE/ABINIT/MESIA
geo_directory OH-_PBE0_vdW.pos
geo_out     hyper.dat
geo_1       1    #
geo_2       95306 #
geo_interval 1   # pick up geometry with this interval
ntype       2        # number of different types of atoms.
natom       191      # total number of atoms.

natom1 64 # O
natom2 127 # H
id1 O
id2 H

celldm1 12.444655509
celldm2 12.444655509
celldm3 12.444655509

rcut_oo 3.5
rcut_oh 1.24
acut_hoo 30

rcut  6.0
dr 0.1
nacc 4
delta -0.1
```

4. 14）Movie

```
calculation  movie  # instantaneous liquid interfaces
geo_in_type  QE   #PROFESS/VASP/QE/ABINIT/ABACUS
geo_directory OH-_PBE0_vdW.pos
geo_out     movie.xyz
geo_1       1
geo_2       62338
geo_interval 62338
ntype       2       # number of different types of atoms.
natom       191      # total number of atoms.

natom1 64 # O
natom2 127 # H
id1 O
id2 H

snatom 5 49 15 16 58 62

celldm1 12.444655509
celldm2 12.444655509
celldm3 12.444655509 # celldm3 in Angstrom

func 2
```

4.15) Distance 2D

```
 calculation  dist
 system hydroxide
 geo_in_type  QE
 geo_directory OH-_PBE0_vdW.pos
 geo_1       1
 geo_2        95306
 geo_interval 1

 ntype       2        # number of different types of atoms.
 natom       191      # total number of atoms.

 natom1 64 # O
 natom2 127 # H
 id1 O
 id2 H

 celldm1 12.444655509
 celldm2 12.444655509
 celldm3 12.444655509

 rcut_oo 3.5
 rcut_oh 1.24
 acut_hoo 30

 rcut  12.0
 rcut1  4.0
 dr 0.1

 nx 61
 ny 21

 u1 41
 u2 41
 u3 61

 func 1
ele1 O
```

4.16) XSF 3D

Nacc40-plot the *.xsf file (3D pot)

```
 calculation  dist
system hydroxide
geo_in_type  QE
geo_directory OH-_PBE0_vdW.pos
geo_1       1
geo_2       95306
geo_interval 1
ntype       2        # number of different types of atoms.
natom       191      # total number of atoms.

natom1 64 # O
natom2 127 # H
id1 O
id2 H

celldm1 12.444655509
celldm2 12.444655509
celldm3 12.444655509

rcut_oo 3.5
rcut_oh 1.24
acut_hoo 30

rcut  12.0
rcut1  4.0
dr 0.1

nx 61
ny 41

nacc 40
func 2

u1 41
u2 41
u3 61

ele1 O
```

Add the following header in the front part of dist3D.dat file, change the name to 3d.xsf

```
CRYSTAL
PRIMVEC
    8.0 0 0
    0 8.0 0
    0  0 12.0
PRIMCOORD
        2 1
O    4.0 4.0 6.0
H    4.0 4.0 7.0
 BEGIN_BLOCK_DATAGRID_3D
 3D_PWSCF
 DATAGRID_3D_UNKNOWN
       41 41 61
 0.000  0.000 0.000
8 0 0
0 8 0
0 0 12
```

4.17) Distance 2D wannier

```
calculation  dist  # instantaneous liquid interfaces
system hydroxide
geo_in_type  QE   #PROFESS/VASP/QE/ABINIT/ABACUS
geo_directory OH_PBE0_vdW.pos
wannier_file  OH_PBE0_vdW.wfc
nbands 256
geo_1       1
geo_2       95306
geo_interval 1
ntype       2        # number of different types of atoms.
natom       191      # total number of atoms.

natom1 64 # O
natom2 127 # H
id1 O
id2 H

celldm1 12.444655509
celldm2 12.444655509
celldm3 12.444655509

rcut_oo 3.5
rcut_oh 1.24
acut_hoo 30

rcut  3.0
rcut1  1.0
dr 0.1

nx 60
ny 20

#nacc 30
func 4
```

4.18) PDF O(donate)-O(accept)

```
calculation  pdf
system hydroxide
geo_in_type  QE
geo_directory OH-_PBE0_vdW.pos
geo_1       1
geo_2      10000 95306

geo_interval 1

geo_out     pdf.txt # output pdf name.

ntype       2        # number of different types of atoms.
natom       191      # total number of atoms.
natom1      64
natom2      127
dr          0.02     # delta r in real space
rcut        6.22

id1 O
id2 H
ele1 O
ele2 O

celldm1 12.444655509
celldm2 12.444655509
celldm3 12.444655509

nacc 4
func 2 # g(O_donate, O_accept)
```

4.19) Presolvation

```
calculation  pre  # hydrogen bond analysis
system hydroxide
geo_in_type  QE
geo_directory OH_PBE0_vdW.pos
geo_1       1
geo_2      95306
geo_interval 1

ntype       2        # number of different types of atoms.
natom       191      # total number of atoms.

natom1 64 # O
natom2 127 # H
id1 O
id2 H

celldm1 12.444655509
celldm2 12.444655509
celldm3 12.444655509

rcut_oo 3.5
rcut_oh 1.24
acut_hoo 30

rcut 5
dr 0.01
```

4.20) Hydroxide Wannier

Note: add “nacc 5” can select those hydroxide ions with 5 accepted HBs

```
calculation  wannier
system hydroxide
geo_in_type  QE
geo_directory  OH-_PBE0_vdW.pos
wannier_file  OH_PBE0_vdW.wfc
geo_1       1
geo_2       95306
geo_interval 1
ntype       2        # number of different types of atoms.
natom       191      # total number of atoms.
nbands      256

natom1 64 # O
natom2 127 # H
id1 O
id2 H

celldm1 12.444655509
celldm2 12.444655509
celldm3 12.444655509

dr 0.005
rcut 1.00
ele1 O
```

4.21) Waterwire 2

```
 calculation  waterwire2  # hydrogen bond analysis
 system hydroxide
 geo_in_type  QE
 geo_directory OH_PBE0_vdW.pos
 geo_1       1
 geo_2       95306
 geo_interval 1
 ntype       2        # number of different types of atoms.
 natom       191      # total number of atoms.

 natom1 64 # O
 natom2 127 # H

 id1 O
 id2 H

 celldm1 12.444655509
 celldm2 12.444655509
 celldm3 12.444655509

 rcut_oo 3.5
 rcut_oh 1.24
 acut_hoo 30

 rcut 6.5
 dr 0.01

 nx 60
 ny 40
 x0 -1.5
 y0 4.5
 dx 0.05
 dy 0.05

 func 2
#  factor 2.4783510188 #100ps
#  factor 1.2391755094 #50ps only if output=10
#  factor .6195877547 #50ps only if output=5
#  factor .3717526527 #30ps
 factor .4956702036 #40ps
#  func_b 31
```

Waterwire 2: 41

```
calculation  waterwire2
system hydroxide
geo_in_type  QE
geo_directory OH_PBE0_vdW.pos
geo_1       1
geo_2       95306
geo_interval 1
ntype       2        # number of different types of atoms.
natom       191      # total number of atoms.

natom1 64 # O
natom2 127 # H

id1 O
id2 H

celldm1 12.444655509
celldm2 12.444655509
celldm3 12.444655509

rcut_oo 3.5
rcut_oh 1.24
acut_hoo 30

rcut 6.5
dr 0.01

nx 60
ny 40
x0 -1.5
y0 4.5
dx 0.05
dy 0.05
func 2
factor .4956702036 #40ps
func_b 41
```

4.22) Waterwire compression

```
calculation  ww_compress  # hydrogen bond analysis
system hydroxide
geo_in_type  QE
geo_directory  OH_PBE0_vdW.pos
geo_1       1
geo_2       95306
geo_interval 1

ntype       2        # number of different types of atoms.
natom       191      # total number of atoms.

natom1 64 # O
natom2 127 # H

id1 O
id2 H

celldm1 12.444655509
celldm2 12.444655509
celldm3 12.444655509

rcut_oo 3.5
rcut_oh 1.24
acut_hoo 30

dr 0.05
rcut 8.0
```

3.23) Static structure factor

A. ssf_selected

The name of the code for calculating static structure factors is "'ssf_selected.cpp" in the source directory. The code can be parallerized.

1. Prepare the input file

```
calculation   ssf_selected  # command of calculating static structure
factor with selected k
geo_in_type  PROFESS  #input type of geometry file:
PROFESS/VASP/QE/ABINIT/ABACUS
geo_directory ../../md_files
geo_1        0
geo_2        999
geo_interval  2
ssf_out      Li_ssf.txt     # output static structure factor name.
ntype        1          # number of different types of atoms.
natom        6750       # total number of atoms.
struf_dgx     .1080405600   # delta G in G space, 2pi/a, a in the unit of
Angstrom
struf_dgy     .1080405600   # delta G in G space
struf_dgz     .1080405600   # delta G in G space
struf_ng      60          # number of G points with delta G described above
```

2. Prepare the "INPUT" file as described above and run CANDELA.exe. The code will generate an output file named "SSF.input0". There number of lines in the file "SSF.input0" depends on the largest G vector, each line represents one particular G vector with four numbers, namely, Gx, Gy, Gz, and |G|.

3. Use the following command to sort all G vectors in an ascending order:

sort -n -k4 SSF.input0 > SSF.input1

Next, delete some of the G vectors in this SSF.input1 file and only reserve those G vectors that you want to calculate. The principle here is that you can delete G vectors that aretoo close in values, thus the reduced number of G points will save the computational time for calculating the static structure factor.

4. Add the number of lines (the number of G vectors you want to compute) as the first line in SSF.input1 and run CANDELA again. The code will generate a new file named "SSF.input". Next, delete both SSF.input0 and SSF.input1 and only keep the "SSF.input" file.

5. Add the number of k points in the SSF.input file as the first line and now you can submit the final job to calculate the static structure factor.

B. ssf

The code for calculating the static structure factors (SSF) is ssf.cpp in the source directory.SSF is calculated partly with parallel_script.sh and averaged through collect_ssf.cpp.

1.Modify the script slurm.sh or files with other suffix names (like .bsub) to submit jobs.

2.Modify the parallel_script.sh

a. modify some parameters

```
target_dir: directory of geometry
split_to_nfile: how many parts I need
interval: geometry interval
max,min: beginning and ending geometry
addcount: restart from which part
```

b. modify INPUT in parallel_script.sh

```
calculation   ssf          # pair Distribution Function.
geo_in_type     PROFESS           #  input  type  of  geometry  file:
PROFESS/VASP/QE/ABINIT/MESIA
geo_directory $target_dir
geo_1         $start_geo       # IN PROFESS, start from file: ion.*.dat,
where * is 'geo_1'
geo_2         $stop_geo        # IN PROFESS, end at file : ion.*.dat,
where * is 'geo_2'
geo_interval  $interval    # geometry interval between geo_1 and geo_2

ssf_out       Al_ssf.txt    # output static structure factor name.
ntype         1           # number of different types of atoms.
natom         864          # total number of atoms.
struf_dgx     .2586375438   # delta G in G space, 2pi/a
struf_dgy     .2586375438   # delta G in G space
struf_dgz     .2586375438   # delta G in G space
struf_ng      18           # number of G points
```

Bold parameters should be modified.

c. Modify slurm.sh in parallel_script.sh to the right name.

3.Type: `sh parallel_script` and wait till it's over.

4. Modify collect_ssf.cpp

```
split_to_nfile: how many parts in total
line:  how many lines of each ssf_out file
```

5. Compile collect_ssf.cpp and use it to get Final_ssf.txt

3.24) Instantaneous Liquid Interface

```
calculation  ili  # instantaneous liquid interfaces
geo_in_type  QE
geo_directory ../60.pos
geo_out     ili.dat
geo_1       1
geo_2       7441
geo_interval 1
ntype       3        # number of different types of atoms.
natom       407      # total number of atoms.

natom1 96 # O
natom2 275 # H
natom3 36 # C
id1 O
id2 H
id3 C

celldm1 12.444655509
celldm2 12.444655509
celldm3 26.9617536455 # celldm3 in Angstrom

zeta 2.4
d 3
nx 30
ny 30

ntry 20
z0 24
dz -0.5

ele1 O
ref_den 0.016
```

3.25) Infrared Spectra

Step1: use ‘calculation wannier’ to generate all_dipole.dat and all_vdipole.dat files

Step2: obtain the above two files and change calculation to `infrared`

```
calculation  infrared wannier  # step 1: wannier step2: infrared
system water         # system is water
geo_in_type  QE
geo_directory  ./reorganize10/new.pos
wannier_file ./reorganize10/new.wfc
cell_file ./reorganize10/new.cel
geo_1       1      # starting geometry index
geo_2       39411   # ending geometry index
geo_interval 1      # interval between starting and ending geometries
geo_ignore   0      # ignore the first xxx geometries

ntype       2       # number of different types of atoms.
natom       192     # total number of atoms.
natom1      64
natom2      128
id1 O
id2 H

ele1 O  # please do not change this value

nbands 256 # number of bands for the system

factor 0.05 // only for func_b=2 in infrared mode
bdf_rcut 0.1 // only for func_b=2 in infrared mode

dr 0.001 # for MLWF distribution
rcut 1.00 # for MLWF distribution

dz 0.02  # for dipole moment distribution (in Debye)
rcut1 10.0 # for dipole moment range (in Deybe)

tcor 600 # correlation with 'tcor' snapshots for  correlation function
dt_snapshots # the delta_t of two snapshots, unit is ps
func_b  2
```

3.26) Dynamic Structure Factor

Step 1 ： Calculate intermediate scattering function.

```
calculation    isf2 # Pair Distribution Function.
geo_in_type    PROFESS
geo_directory   ../out/
isf_outfile 2.00864isf.txt #outfile for isf

geo_1         10000  #(make sure: interval*(nt+nT)<=geo_2-geo_1)
geo_2         100000
geo_interval   1

natom         864     # total number of atoms.
natom1     864
ntype      1
isf_nt1    10000  #The range of time for ISF.
isf_nt2    80000  #The number of time for averaging ISF.
dt_snapshots    0.00025 #The time between two continuous snapshots.

isf_target_q   2.00 # The target q of ISF. (in A^-1)
isf_ngx    20     # The number of dg in x-direction for searching
target_q
isf_ngy    20
isf_ngz    20
isf_dgx    0.25863754383  #(in A^-1) The minimal step of q.
isf_dgy    0.25863754383
isf_dgz    0.25863754383
```

Step 2 : Calculate DSF and get maximam.

Modify tcut,dw,nwt,interval in onedsf.sh

tcut : The cut time for ISF. After this cut time, the ISF will decay exponentially.

dw : the minimal energy step for DSF (in eV)

nwt : the maximal number of dw for DSF

interval : dt_snapshots in INPUT

sh onedsf.sh

3.27) Electric Conductivity

Step 1: Create directories containing different snapshots. (The order of folders should be 1,2,3…)

```
calculation write
write_cartesian 0
geo_in_type PWmat
geo_directory MOVEMENT
geo_1 1
geo_2 9000
geo_ignore 7100
geo_interval 100
headfile       headqe.txt
tailfile       tailqe.txt
geo_out        al.md.in
ntype     1
id1 Al
natom     64
natom1    64
```

Step 2: Calculate electric conductivity.

```
calculation     ele_conductivity
wf_in_type      PWmat/QE1/QE2/ABACUS
multi_directory path_to_multi_files #the directory of multiple
snapshots files. (only valid when nscf > 0)
wfdirectory     path_to_wfs #(if nscf==0, then we read wf in
path_to_wfs; else if nscf=Nfolders(Nfolders>0), then we read wf in
path_to_multi_files/[1,2,…,Nfolders]/path_to_wfs)

wcut    12    #maximal energy (in eV) for conductivity
dw      0.9   #minimla energy step (in eV) for conductivity
fwhm    0.1   #Full Width at Half Maximam of Gauss or Lorentz
function. Only useful when smear is 1 or 2
(or   n_fwhm  2
fwhm    0.1 0.2 #use it if we want to print results with different
fwhm at the same time.)
smear   0     #0(default) for linear approx.; 1 for Gauss approx.;
2 for Lorentz approx.
nscf          #0(default, only calculate one snapshot) or the number
of snapshots used
temperature 10000 # in K
error_con    0/1 #if print the std of multi snapshots (only valid
when nscf > 0)
tpk         1  #a factor convert student distribution to normal
distribution
```

Key words

The units of input atomic coordinates depend on the package you used for molecular dynamics simulations. For example, the output files of QE are all in Bohr, and the output files of LAMMPS are typically in Angstroms. We design specific interfaces for different simulation packages, and all data once read into CANDELA, are transformed into data with Angstroms.