Reference manual

RISMiCal-dev

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Basic Usage

The RISMiCal package includes three basic programs: pure solvent-based, solute-solvent-based (1D), and solute-solvent-based (3D). In order to perform the calculation of the solute-solvent system, solvent susceptibility data obtained by the calculation of the pure solvent system is required. Therefore, the pure solvent system is first calculated, and then the solute solvent system is calculated.

Execution Commands

The executable binary is rismical.x. Also, it is necessary to set the environment variable RISMICALHOME before executing. RISMICALHOME specifies the path for the RISMiCal package folder. The command is

```
> rismical.x [system] [inputfile.inp]
```

Here

system : Choose from the following strings:

vv Pure solvent system, 1d Solute solvent system(1D)、 3d Solute solvent system(3D)

inputfile.inp : Input file name. The extension should be .inp.

Coupling with external programs

RISMiCal has a built-in function that can be used to couple quantum chemistry calculation programs and MD programs. (To be added in future update.)

Input References

RISM namelist

closure	Specifying a closure [string] KH … Kovalenko-Hirata closure (default) HNC … Hypernetted-chain closure MSA … Mean spherical approximation
itrmax	Maximum number of iterations [integer] (default=1000)
conv	Convergence judgment value [real] (default=1.d-8)
chargeup	Whether or not charging algorithm is used [character] on … Charging Execution (default) off … Not Charging
iguess	Specifying guess [integer] 0… Use electrostatic potential (default) 1… Read an external file (the file is specified by guessfile)
guessfile	Specifying an external file for guess [character] defaultis inputname.tuv
alp1d, alp3d	Damping factor [real] (default=1.5 for 1D, 1.0 for 3D)
grid	Grid specification [character] For 1D-RISM FINE, $N = 8192, \Delta r = 0.025$ Å LFINE, $N = 16384\ \Delta r = 0.025$ Å STANDARD(default), $N = 4096\ \Delta r = 0.05$ Å LSTANDARD, $N = 8192\ \Delta r = 0.05$ Å TEST, $N = 2048\ \Delta r = 0.1$ Å LTEST, $N = 4096\ \Delta r = 0.1$ Å USER User specification (namelist GRID1D) For 3D-RISM FINE, $N = 256\ \Delta r = 0.25$ Å LFINE, $N = 512\ \Delta r = 0.25$ Å STANDARD(default), $N = 128\ \Delta r = 0.5$ Å LSTANDARD, $N = 256\ \Delta r = 0.5$ Å TEST, $N = 64\ \Delta r = 1.0$ Å LTEST, $N = 128\ \Delta r = 1.0$ Å USER User specification (namelist GRID3D)

iolist	Output data specification [character] For solvent-solvent system g ... Radial distribution function (.gvv) h ... Fourier Space Total Correlation Function (.hvk) u ... Interaction Potential (.uvv) c ... Direct correlation function (.cvv) t ... Indirect Correlation Function (.tvv) x ... Solvent susceptibility (.xvk) For 1D solute-solvent system g ... Radial distribution function (.guv) u ... Interaction Potential (.uuv) c ... Direct correlation function (.cuv) t ... Indirect correlation function (.tuv) k ... Fourier Spatial Direct Correlation Function (.cuvk) For 3D solute-solvent system g ... Spatial distribution function (.guv) u ... Interaction Potential (.uuv) v ... Electrostatic field (.vuv) c ... Direct correlation function (.cuv) t ... Indirect correlation function (.tuv) h ... Fourier Space Total Correlation Function (.huvk) q ... Solvent charge density distribution (.qv)

RISMSOLVENT namelist

solvent	Solvent data specification [character, array] Several preset solvents can be specified. TIP3P ... TIP3P Model Water USER ... User-specified. Specified in the data list VDATA.
numspc	Number of solvent components [integer] (default=1)
temp	Temperature [real] (default=298) The unit is [K]
dens	Density [real, array] (default=55) The unit is [M]

DRISM namelist

Only VV calculations are valid

idrism	Dielectric consistent RISM activation switch [integer] 0 … Do not DRISM (default) 1 … DRISM
delec	Dielectric constant [real] (default=78.5)

CHARGEUPOPT namelist

chgstep	Charging step width [real number] (default=0.1) 0<chgstep≦1
chgconv	Convergence judgment value at the time of charging [real] (default=conv*1000)

MDIIS namelist

nsub	Number of subspaces [integer] (default=10)
dumpmax	Maximum Damping Factor [real] (default=0.8)
dumpmin	Minimum Damping Factor [real] (default=0.1)
dumpnume	Damping Factor Adjustment Parameter [real] (default=0.1)

GRID1D namelist

ngrid	Number of grids for 1D calculations [integer]
rdelta	Grid width for 1D calculations [real] Unit [Å]

GRID3D namelist

ngrid3d	Number of grids for 3D calculations [integer]
rdelta3d	Grid width for 3D calculations [real] Unit [Å]

VDATA datalist

line	format	description
1	I A	Number of solvent sites (n1) Solvent name (v1)
2～(n1+2)	A I 6F	Site Name, symmetry flag, σ [Å] ε [J/mol] q[e] x[Å] y[Å] z[Å]

If there are multiple solvent species, repeat the above

example

```
 $VDATA
3    tip3p
O   1  3.150d0   636.0d0  -0.8340d0   0.0000000  0.0000000  0.0000000
H   2  0.400d0   192.5d0   0.4170d0   0.0000000  0.7566950  0.5858800
H  -2  0.400d0   192.5d0   0.4170d0   0.0000000 -0.7566950  0.5858800
1    sodium_ion
Na  1  3.328d0   11.59d0 1.0000d0   0.0000000  0.0000000  0.0000000
1    chloride_ion
Cl  1  4.401d0   418.4d0    -1.0000d0   0.0000000  0.0000000  0.0000000
 $END
```

Two hydrogen atoms have identical correlation functions due to symmetry. If the symmetry flag has a negative value, it means that the absolute value is identical to the same atom.

UDATA datalist

line	format	description
1	I A	Number of solute sites (n1) Solute name (v1)
2～(n1+1)	A 6F	Site Name σ [Å] ε [J/mol] q[e] x[Å] y[Å] z[Å]

example

```
 $UDATA
3    tip3p
O    3.150d0   636.0d0  -0.8340d0   0.0000000  0.0000000  0.0000000
H    0.400d0   192.5d0   0.4170d0   0.0000000  0.7566950  0.5858800
H    0.400d0   192.5d0   0.4170d0   0.0000000 -0.7566950  0.5858800
 $END
```

RISMSOLUTION namelist

solute	How to specify solute parameters [character] udata ... Specify by UDATA (default) Other ... Specify in external files (solutexyz, soluteesp, solutelj)
solutexyz	Atomic coordinate file of solute [character] default=inputfile.xyz
soluteesp	Effective charge and electrostatic potential file of solute [character] default=inputfile.esp
solutelj	LJ potential designation of solute [character] builtin ...Assign from parameters provided in the package (specified by ljparam) (default) And more ...External file name (default is inputfile.lj)
solvent	Solvent susceptibility data faul specification [character]
ljparam	Parameter file name [character] mm2.prm ... mm2 parameter set (default) tiny.prm ... Tinker's minimum set of parameters
esptype	Electrostatic potential type [character] PC ...Calculated from effective charge MAP ... Loading the electrostatic potential map

CURISM namelist

cuda	Whether or not to use the CUDA version of the external 3D-RISM program [logical] true … Execute external 3D-RISM programs false… Execute the built-in 3D-RISM program (default)
cupath	Folder path with CUDA version of 3D-RISM executable file [character]
ma	Number of subspaces used in the Modified Anderson method [integer] default=2
param1	Maximum value of the convergent mixing parameter used in the Modified Anderson method [real] default=0.6 The value is parm2<parm1<1.0
param2	Minimum value of the converged mixing parameter used in the Modified Anderson method [real] default=0.2 The value is 0.0<parm2<parm1