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Multiscale Simulation Scattering Intensity Calculator (MuSSIC)

User guide

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Contents

1. Description of the Code

MuSSIC is a computational tool for calculation of neutron scattering for coarse grain (CG) systems (detailed description is provided in the Documentation). It is based on the method described by Alan Soper in his journal article on coarse-grained Empirical Potential Structure Refinement (Biochimica et Biophysica Acta 1861, 6, 2017, Pages 1652-1660). The code computes the partial pair radial distribution function and the partial pair structure factors for the trajectory provided in xyz file format. The total structure factor is the weighted sum of all partial pair structure factors. The current version of the code is available on Github page (https://github.com/disorderedmaterials/MuSSIC). Any

developments or improvements in the code/method and related examples are updated on gitpage.

2. Compilation and run

MuSSIC is written in FORTRAN and requires gfortran compiler with openmp support for parallel implementation. After downloading the source code, follow the commands on terminal

>make

copy the executable 'scattcg' to the desired location. Execute with

>./scattcg

3. Input variables

Input variables are separated into four categories. The following table shows the example variables of each category. Section 4 gives a detailed explanation of all variables by showing input files for C10TAB in water system.

Simulation parameters	**model parameters**
Title of the system box dimensions Ensemble type (NVT or NPT)	Number of species number of molecules in each species Number of atoms per molecule number of atom types
Scattering calculation parameters Binning of Q in F(Q) Binning of r in g(r) Binning regime: linear or logarithm Broadening parameters: OmegaDependentGaussian Isotopologue information	**Coarse grain representation** Number of CG bead types Label of bead beads_per_molecule Bead size Implicit atoms per bead

4. INPUT files

- input.dat - main input file
- model.dat - model parameters of the system
- trajectory - atomistic trajectory in xyz format
  (required for the run type 'atomistic or 'compare_CG_atomistic')

  InNVT case, xyz trajectory format :

```
5     # natoms
            # blank line
C   1.0   1.0   1.0   #label x   y   z   coordinates
.
.
.
.
```

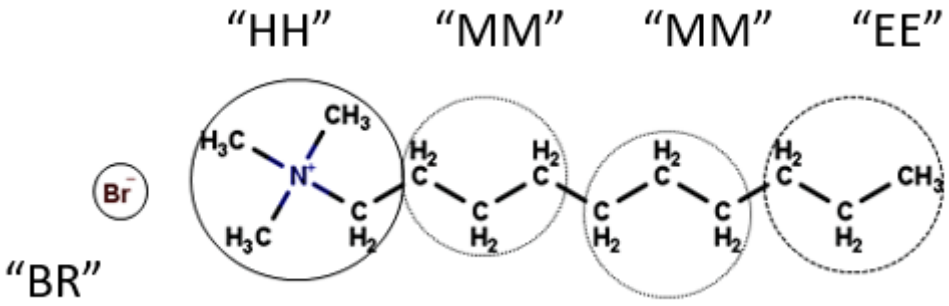
  IN NPT case, the second line reads the dimension of box for that frame

```
5     # natoms
10.0  10.0  10.0  # box dimensions in Angstroms
C   1.0   1.0   1.0   #label x   y   z   coordinates
.
.
.
.
```

Note: Please note that the user needs to re-write the trajectory to have this NPT format, which is not the standard one

- CG_trajectory - coarse grain trajectory in xyz format
  (required for the run type 'CG')

  The inputs files are explained through an example, a system consisting of C10TAB surfactants in water. The coarse-grained representation is depicted below over the atomistic one.



The labels "HH", "MM", "EE", "BR", and "WW" are the names of the CG beads in the CG_trajectory file.

The aim is to use MuSSIC to obtain the total neutron scattering cross section for two isotopologues, described in the input file as "sample_1" and "sample_2":

- Sample 1: isotopic substitution in C10TAB + H2O
- Sample 2: C10TAB with natural hydrogen + D2O

Both outputs are achieved in a single calculation.

4.1 input.dat for C10TAB system

The simulation parameters and the scattering simulation parameters are given in the input.dat file with the following format (support comments added here):

variable description

```
run:
CG        #options:'CG'  or 'atomisitc' or 'compare_CG_atomistic'
                # 'CG'  -  computes F_CG(Q) for CG trajectory
                'atomistic' - compute F(Q) for atomistic
                trajectory
                'compare_CG_atomistic' - computes F(Q) for
                atomistic trajectory provided and will compute
                F_CG(Q) for the pseudo-CG model provided in the
                model file.
```

```
nproc:          # number of the processors for openmp
20
title:          # title of the run (optional)
C10TAB+water
ntypes:         # number of atom types implicit in the system
6
box_length:     # box dimensions
159.6606d0  153.7097d0  155.2160d0
bin_width:      # bin width for rdf calculation
0.03d0
ensemble:   #Current version reads either 'NVT or 'NPT' ensemble
NVT
label_atom:     # labels for the implicit atom types
N
C
HC              # Label for H in the C10TAB surfactant
BR
OW
HW              # Label for H in the water molecule
scattering_lengths:   # scattering lengths of the atom types
9.36d0
6.646d0
-3.739d0
6.795d0
5.803d0
-3.739d0
6.671d0     #(ntypes+1) is the scattering length of deuterium
form_factor:    # density distribution within the CG bead
Gaussian
exchangeable_atoms:    # number of exchangeable atoms and the
                    label of the exchangeable atom types
1
HW
number_isotopologues: # number of isotopologues to be studied
2
```

```
isotopologues:    # ratio of the isotopes (isotope+natural=1.0)
                    in the same sequence of atom types as
                   defined above
sample_1    DH    # label for the isotopologue d-C10TAB + H2O

atom    natural    isotope

N         1.0       0.0
C         1.0       0.0
HC        0.0       1.0
BR        1.0       0.0
OW        1.0       0.0
HW        1.0       0.0

sample_2    HD    # label for the isotopologue C10TAB + D2O

atom    natural    isotope

N          1.0       0.0
C          1.0       0.0
HC         1.0       0.0
BR         1.0       0.0
OW         1.0       0.0
HW         0.0       1.0

qmin:          # minimum of Q value (usually 2*pi/box_length)

0.01d0

qdelta:        # delta in the Q scale

0.02d0

qmax:          # maximum Q value

5.0d0

binning:    # binning regime (either 'linear' or 'log_linear')

log_linear

broadening:    # type of broadening used

OmegaDependentGaussian

FWHM:          # full width at half maximum for broadening

0.02d0

windowfn:      # window function used in finding S(Q)

Lorch0

endinput
```

Note 1: the current version of the code supports only one isotope of the atoms in a bead i.e., a CG bead can have an isotopic substitution of a single atom.

Note2: In addition to the 'CG' run type, the current version can take two other run types which are 'atomistic' and 'compare_CG_atomistic'.

CG - computes F_CG(Q) for the provided CG trajectory named 'CG_trajectory'

atomistic - computes F(Q) for the provided atomistic trajectory named 'trajectory'

compare_CG_atomistic - computes F(Q) for the provided atomistic trajectory named 'trajectory' and performs CG mapping using model file parameters to compute F_CG(Q) for the same atomistic 'trajectory'

Note3: There is no need to provide 'nframes' as input in the current version. The code automatically reads the number of frames from the trajectory

4.2 model.dat for C10TAB in water

The model and CG representation parameters are given in the model.dat file:

variable description

```
num_species   # number of species/molecule types in the system
3

nmol_species     # number of molecules for each molecule type
810              # C10TA molecule
810              # Br- ions
115177           # water molecules
size_per_species     # number of implicit atoms in each molecule
44                    # atoms in C10TA molecule
1                     # number of atoms Br- ion
3                     # number of atoms in water molecule
num_CGbead_types   # number of CG bead types
5

label_bead         # label of CG bead types
1        HH
2        MM
3        EE
4        BR
```

```
5       WW
beads_per_molecule    # number of beads in each molecule
4                     # number of beads for C10TA molecule
1                     # number of beads for Br- ion
1                     # number of beads for water molecule
bead_radius       # radii of the CG beads. See notes below
6.091
2.932
3.166
0.707
0.676

num_atom_types_CGbead # Implicit atom contents in the CG beads
3      # number of atom types in CG bead 1, 'HH' (list above)

1     1     # atom type number 1, 'N' (refer to the atom type
            numbers in input.dat) and number of atoms, 1
2     4     # 4 atoms with type number 2, 'C'
3    11     # 11 atoms with type number 3, 'HC'
2            # number of atom types in CG bead 'MM'
2     3     # 3 atoms with type number 2, 'C'
3     6     # 6 atoms with type number 3, 'HC'
2            # number of atom types in CG bead 'EE'
2     3     # 3 atoms with type number 2, 'C'
3     7     # 7 atoms with type number 3, 'HC'
1            # number of atom types in CG bead 'BR'
4     1     # 1 atom with type number 4, 'BR'
2            # number of atom types in CG bead 'WW'
5     1     # 1 atom with type number 5, 'OW'
6     2     # 2 atoms with type number 6, 'HW'

#note that this section is only for the "compare_CG_atomistic"
cg_mapping #mapping model to convert atomistic traj. to CG
1            # molecule type: 1
3            #  number of segments :3
1        1        1    # segment 1: 1 bead, 1 repetition, step:1
HH      13  # bead name, take the CoM from 13 atoms
1            #indices of 13 atoms
2
3
4
5
6
7
8
9
10
11
```

```
12
13
1        2        9 # segment 2: 1 bead, 2 repetitions, step:9
MM       9       # bead name, take the CoM from 9 atoms
14                #indices of 9 atoms
15
16
17
18
19
20
21
22
1        1        1# segment 3: 1 bead, 1 repetition, step:1
EE       13         # bead name, take the CoM from 13 atoms
32                  #indices of 13 atoms
33
34
35
36
37
38
39
40
41
42
43
44
2           # molecule type: 2
1           #  number of segments: 1
1        1        1 # segment 1: 1 bead, 1 repetition, step:1
BR       1         # bead name, take the CoM from 1 atom
1                  #index of  the atom
3           # molecule type: 3
1           # number of segment : 1
1        1        1 # segment 1: 1 bead, 1 repetition, step:1
WW        3         # bead name, take the CoM from 3 atoms
1                   #indices of  3 atoms
2
3
Endinput
```

Note4: If the radii of beads not available, one can provide bead connectivity matrix as shown below.

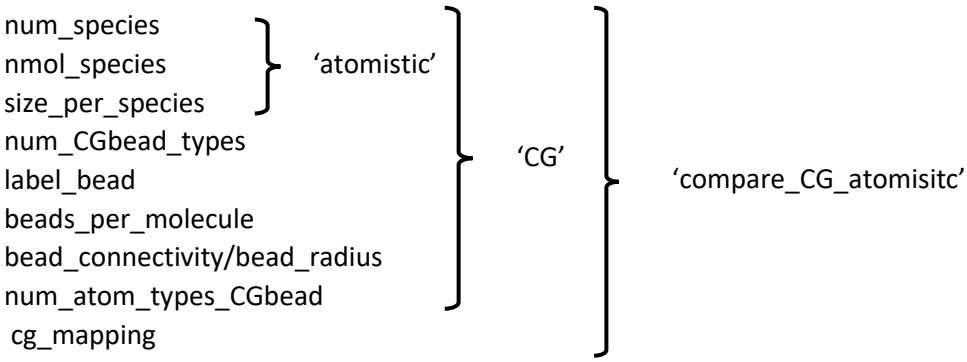
```
bead_connectivity
    HH   MM   EE   BR   WW
```

```
HH 0    1    1   0   0     # rows and columns  equal to the
MM 1    0    0   0   0     number of bead types. '1' being
EE 1    0    1   0   0     the bead pair connected and '0'
BR 0    0    0   0   0     being not connected
WW 0    0    0   0   0
```

The following inputs are not needed in the model file according to the run_type

- 'cg_mapping' is not needed if the run_type is 'CG' and you already have a CG_trajectory
- All the inputs related to bead description are not needed if the run_type is 'atomistic' like num_CG_beadtypes, label_bead, beads_per_molecule,bead_radius,num_atom_types_CGbeads,cg_mapping

model file inputs:



This diagram helps to understand the input variables needed for every run type

5. OUTPUT files

filename	description
out.log	log file printing the details of the run
CG-unweighted-*-*.gr	partial pair g_{ij}(r) (* - bead types in the pair)
CG-unweighted-*-*.sq	partial pair S_{ij}(Q) (* - bead types in the pair)
CG-unweigthed-total.gr	unweighted total G(r)
CG-unweighted-total.sq	unweighted total S(Q)

%%-weighted-*-*.sq	weighted partial pair S_{ij}(Q) (%% -isotpologue name, * - bead types in the pair)
%%-weighted-*-*.gr	weighted partial pair g_{ij}(r) (%% -isotpologue name, * - bead types in the pair)
%%-CG-weighted-total.sq	weighted S(Q) (%%-isotopologue name)
%%-weighted-total.gr	weighted G(r) (%%-isotopologue name)

6. Plotting

A gnuplot script is available for the test systems, which can be used to plot the scattering curves. Please change the file names according to the system that is being tested.

Usage:

>gnuplot plot.gnu