

1. GLE Principles
2. The 3-step procedure
3. Download files
4. Files - description
5. Files - synoptic
6. Tutorial - 1
7. Finally

Generalised Langevin Equation GLE (1 & 2 baths) Manual and Tutorials for LAMMPS

Developers: **H. Ness and C. D. Lorenz**

Project Team: *H. Ness, L. Stella, C. D. Lorenz, L. Kantorovich*
Department of Physics, King's College London

UK EPSRC Grant No. EP/J019259/1.

London, January 2017

1. GLE Principles
2. The 3-step procedure
3. Download files
4. Files - description
5. Files - synoptic
6. Tutorial - 1
7. Finally

Outline

1. GLE Principles

1. GLE Principles
2. The 3-step procedure
3. Download files
4. Files - description
5. Files - synoptic
6. Tutorial - 1
7. Finally

Outline

1. GLE Principles
2. The 3-step procedure

1. GLE Principles
2. The 3-step procedure
3. Download files
4. Files - description
5. Files - synoptic
6. Tutorial - 1
7. Finally

Outline

1. GLE Principles
2. The 3-step procedure
3. Download files

1. GLE Principles
2. The 3-step procedure
3. Download files
4. Files - description
5. Files - synoptic
6. Tutorial - 1
7. Finally

Outline

1. GLE Principles
2. The 3-step procedure
3. Download files
4. Files - description

1. GLE Principles
2. The 3-step procedure
3. Download files
4. Files - description
5. Files - synoptic
6. Tutorial - 1
7. Finally

Outline

1. GLE Principles
2. The 3-step procedure
3. Download files
4. Files - description
5. Files - synoptic

Outline

1. GLE Principles
2. The 3-step procedure
3. Download files
4. Files - description
5. Files - synoptic
6. Tutorial - 1

Outline

- 1 1. GLE Principles
- 2 2. The 3-step procedure
- 3 3. Download files
- 4 4. Files - description
- 5 5. Files - synoptic
- 6 6. Tutorial - 1
- 7 7. Finally

1. GLE Principles
2. The 3-step procedure
3. Download files
4. Files - description
5. Files - synoptic
6. Tutorial - 1
7. Finally

Outline

1. GLE Principles
2. The 3-step procedure
3. Download files
4. Files - description
5. Files - synoptic
6. Tutorial - 1
7. Finally

1.1. GLE Principles

- Solving GLE for central region connected to $\nu = 1, 2, \dots$ bath(s):

$$\frac{dr_{i\alpha}}{dt} = \frac{p_{i\alpha}}{m_i}$$

$$\frac{dp_{i\alpha}}{dt} = F_{i\alpha}(\mathbf{r}) - \int_{-\infty}^t dt' \sum_{\nu, i'\alpha'} K_{i\alpha, i'\alpha'}^{(\nu)}(t, t'; \mathbf{r}) \dot{r}_{i'\alpha'}(t') + \sum_{\nu} \eta_{i\alpha}^{(\nu)}(t; \mathbf{r}),$$

- where $F_{i\alpha}$ is the total force (including polarisation effects of the atoms of the baths) acting on atom i , of the central region, in the direction $\alpha = x, y, z$, the stochastic forces (colored noise $\eta_{i\alpha}^{(\nu)}(t; \mathbf{r})$) are associated with each independent bath ν and $K_{i\alpha, i'\alpha'}^{(\nu)}(t, t'; \mathbf{r})$ is the friction (memory) Kernel.

1.2. GLE Principles

- The latter is related to the vibrational properties of the baths, described by their respective polarisation matrix $\Pi_{b_\nu, b'_\nu}(t - t')$ where the baths degrees of freedom (DOF) $b_\nu \equiv l_\nu \gamma$ correspond to bath atom l_ν and Cartesian coordinate γ .
- To solve the GLE, each degree of freedom $i\alpha$ in the thermostatted group (id-group) is supplemented with two sets of auxiliary degrees of freedom (aDOF) associated with the sets of parameters $\{c_{b_\nu}^{(k_\nu)}, \tau_{k_\nu}, \omega_{k_\nu}\}$. These parameters are determined from the mapping of the polarisation matrix $\Pi_{b_\nu, b'_\nu}(t - t')$ onto the following specific analytic form.

1.3. GLE Principles

- After Fourier transformation, the mapping is given by:

$$\Pi_{b_\nu, b'_\nu}(\omega) \rightarrow \sum_{k_\nu} c_{b_\nu}^{(k_\nu)} c_{b'_\nu}^{(k_\nu)} \left[\frac{\tau_{k_\nu}}{1 + (\omega - \omega_{k_\nu})^2 \tau_{k_\nu}^2} + \frac{\tau_{k_\nu}}{1 + (\omega + \omega_{k_\nu})^2 \tau_{k_\nu}^2} \right].$$

- Before being able to run the LAMMPS fix *gle1bath* or *gle2baths*, one has to determine the sets of coefficients $\{c_{b_\nu}^{(k_\nu)}, \tau_{k_\nu}, \omega_{k_\nu}\}$.
- For this, a 3-step procedure should be followed.

1. GLE Principles
2. The 3-step procedure
3. Download files
4. Files - description
5. Files - synoptic
6. Tutorial - 1
7. Finally

Outline

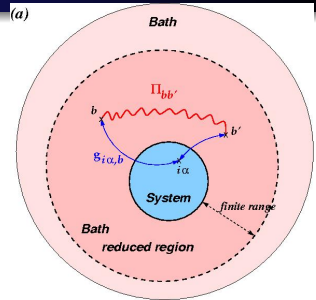
1. GLE Principles
2. The 3-step procedure
3. Download files
4. Files - description
5. Files - synoptic
6. Tutorial - 1
7. Finally

2. The 3-step procedure

- We now summarise the 3-step procedure of the case of an open system connected to a single thermal bath.
- Similar principles hold when working with the 2 baths situations

2.1. Step 1

- Build the entire system, consisting of 3 regions:
 - the central system region
 - the bath region
 - the bath reduced region, a smaller part of the bath itself



- Calculate the dynamical matrix $D_{b,b'}$ of the entire bath region from the derivatives of the forces

$$D_{b,b'} = 1/\sqrt{\mu_b \mu_{b'}} \partial f_{b'}/\partial r_b$$

- Step 1 is usually performed by using the LAMMPS code and the appropriate script (see below, and the example given in the Tutorial - 1)

2.2. Step 2

- Perform the mapping of the polarisation $\Pi_{b\nu}$,
- Fit the exact result

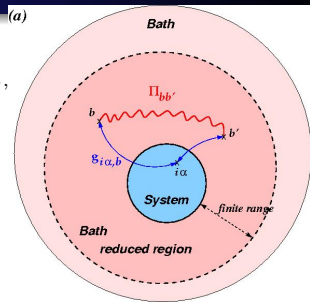
$$\Pi_{b,b'}(\omega) = -\frac{2}{|\omega|} \text{Im} [\omega^2 \mathbf{1} - \mathbf{D} + i\varepsilon]_{b,b'}^{-1}$$

onto

$$\sum_{k\nu} c_{b\nu}^{(k\nu)} c_{b'\nu}^{(k\nu)} \left[\frac{\tau_{k\nu}}{1 + (\omega - \omega_{k\nu})^2 \tau_{k\nu}^2} \right]$$

for $\omega \geq 0$.

- The mapping is done **only** for the bath DOF b, b' located inside the bath reduced region (because of the finite range of the interaction).
- Step 2 is performed with our home-built codes (see below, and the example given in the Tutorial - 1)

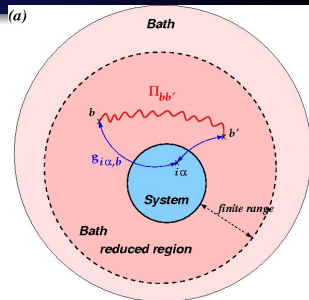


1. GLE Principles
2. The 3-step procedure
3. Download files
4. Files - description
5. Files - synoptic
6. Tutorial - 1
7. Finally

2.3. Step 3

Step 2 has generated all the necessary output files containing the parameters $\{c_{b\nu}^{(k\nu)}, \tau_{k\nu}, \omega_{k\nu}\}$ necessary for the GLE LAMMPS runs

- Run the LAMMPS *fix gle1bath*
- The system consists now of **only 2** regions: the central system region and the bath reduced region,
- The GLE MD runs are performed on the atom in the central system region (The atoms of the bath reduced region are kept at fixed position during the gle runs)



Outline

1. GLE Principles
2. The 3-step procedure
3. Download files
4. Files - description
5. Files - synoptic
6. Tutorial - 1
7. Finally

1. GLE Principles
2. The 3-step procedure
3. Download files
4. Files - description
5. Files - synoptic
6. Tutorial - 1
7. Finally

3.1. Download code for LAMMPS

Go to the following url:

<https://github.com/HerveNess/gleKCL/tree/master>

to download the files

3.2. Download code for LAMMPS

- In branch *master*
 - README file *README.md*
 - the present document *GLE1or2B_kcl.pdf*
- In branch *source_code*
 - LAMMPS codes:
 - fix_glekcl.cpp* and *fix_glekcl.h*
 - fix_gle2baths.cpp* and *fix_gle2baths.h*
 - and all the other codes for pre/post-treatment as listed in the README file
- In branch *tutorials*
 - the LAMMPS scripts *.lmp for the tutorial described from Slide [27](#)

3.3. Download code for LAMMPS

IMPORTANT REMARK:

- It is assumed that the reader has some knowledge about using Unix-based computers.
- It is assumed that the reader has some knowledge about the LAMMPS code
- i.e. how to download, compile, run LAMMPS and how to use and build elementary LAMMPS scripts.
- For simplicity of use, the GLE source codes for LAMMPS for the following tutorials are available only for serial calculations, i.e. use *make serial* to compile the LAMMPS code.

1. GLE Principles
2. The 3-step procedure
3. Download files
4. Files - description
5. Files - synoptic
6. Tutorial - 1
7. Finally

Outline

1. GLE Principles
2. The 3-step procedure
3. Download files
4. Files - description
5. Files - synoptic
6. Tutorial - 1
7. Finally

4.1. Code - description

- file name:
DynMat_from_forces_eVAng_readmass.f90
- short description:
calculate the symmetric dynamical matrix from the forces $f_{j\beta}^{(\pm, i\alpha)}$ of the displaced atoms $r_{i\alpha} \rightarrow r_{i\alpha} \pm \Delta$
- operation: compile file
gfortran DynMat_from_forces_eVAng_readmass.f90 -o DynMat_from_forces_eVAng_readmass

4.2. Code - description

- files name:
 - polar_matrix_P1bb_readdynmat_v5_fit_newinput.f90*
 - parameters_and_co_readdynmat_v5_fit_eVAng.f90*
 - makefile_readdynmat_v5_fit_newinput*
- short description:
 - perform mapping of polarisation matrix Π_{ij} for only 2 indexes i and j , need input file *input_new_rdynmat.in*
- operation:
 - cp makefile_readdynmat_v5_fit_newinput makefile*
 - then *make* compiles the fortran codes into
 - polar_matrix_P1bb_readdynmat_v5_fit_newinput*

4.3. Code - description

- files name:
polar_matrix_Plbb_readdynmat_v13_fit_withCregion_newinput.f90
parameters_and_co_readdynmat_v13_fit_withCregion_newinput.f90
makefile_v13_fit_withCregion_newinput
- short description:
 perform mapping of polarisation matrix Π_{ij} all indices i and j corresponding to the atoms in the bath reduced region, need input file *input_new_rdynmat.in*, and files *coord_bath_at.dat* and *coord_bathreduced_at.dat*
- operation:
cp makefile_v13_fit_withCregion_newinput makefile
 then *make* compiles the fortran codes into
polar_matrix_Plbb_readdynmat_v5_fit_newinput

4.4. Code - description

- file name:
swapDbathXred_old2new_v1.f90
- short description:
check atom coordinates and identify the LAMMPS ID index of the atoms contained in the two input files named *old_coord_bathXred_at_sort.dat* and *new_coord_bathXred_at_sort.dat*
- operation:

```
gfortran swapDbathXred_old2new_v1.f90 -o  
swapDbathXred_old2new_v1
```

1. GLE Principles
2. The 3-step procedure
3. Download files
4. Files - description
5. Files - synoptic
6. Tutorial - 1
7. Finally

Outline

1. GLE Principles
2. The 3-step procedure
3. Download files
4. Files - description
5. Files - synoptic
6. Tutorial - 1
7. Finally

5.1. What is needed:

- a LAMMPS script to (an example is given by file *get_all_forces_model_small_sys_C_withCregion.Imp* in the Tutorial):
 - build the system and bath (including the bath reduced region)
 - calculate and print out the forces $f_{j\beta}^{(\pm,i\alpha)} = f_{j\beta}[r_{i\alpha} \rightarrow r_{i\alpha} \pm \Delta]$ on each atom j (direction β) of the bath, when the atoms i in the system are moved $\rightarrow r_{i\alpha} \pm \Delta$ in the direction α
 - the forces are saved in file *forces.dat*

5.2. What is needed:

- code `DynMat_from_forces_eVAng_readmass`
calculates the dynamical matrix $D_{b,b'}$ from the forces $f_{j\beta}^{(\pm, i\alpha)}$
- input file: `forces.dat`
- output file: `dynmat_coeff.dat`

5.3. What is needed:

- code *polar_matrix_Plbb_readdynmat_v5_fit_newinput* calculates the mapping of the polarisation matrix elements (diagonal) $\Pi_{ip,ip}(\omega)$, $\Pi_{jp,jp}(\omega)$ and (off-diagonal) $\Pi_{ip,jp}(\omega)$ for **only** 2 indexes *ip*, *jp*
- input files: *dynmat_coeff.dat* and *input_new_rdynmat.in*
- output files (x-y format):
imDbbrecur_ovw.xxxx.dat to be compared with
fit_imDbbrecur_ovw_modCavtauk.xxxx.dat
 and
imDbbrecur_ovw_IJ.xxxxyyyy.dat to be compared with
fit_imDbbrecur_ovw_IJ_avtauk.xxxxyyyy.dat
 xxxx and yyyy are strings of characters of the integers *ip* and *jp*

5.4. What is needed:

- code *polar_matrix_Plbb_readdynmat_v13_fit_newinput* calculates the mapping of all the polarisation matrix elements $\Pi_{ip,jp}(\omega)$ for the indexes *ip*, *jp* corresponding to atoms located within the bath reduced region
- input files *dynmat_coeff.dat* and *input_new_rdynmat.in*
- output files (x-y format) same as for Section 5.3.
- output files:
 - fit_coef_taukomegak_Imp.dat* for the $\tau_{k_\nu}, \omega_{k_\nu}$ parameters,
 - and *fit_coef_cbk_Imp.dat* for the $c_{b_\nu}^{(k_\nu)}$ parameters.

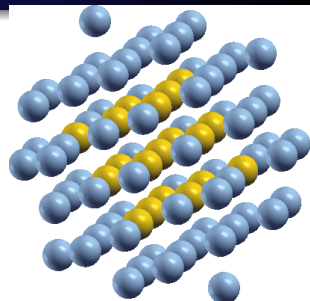
5.5. What is needed:

- Finally, a LAMMPS script to perform the GLE runs
- an example is given by file
gle_test_small_sys_C_T100_mubar32_52kts_seed2.lmp in the Tutorial
- other input files:
fit_coef_taukomegak.lmp.dat
and
fit_coef_cbk.lmp.dat
- output files are specified in the LAMMPS script
gle_test_small_sys_C_T100_mubar32_52kts_seed2.lmp
- **further intermediate steps are actually needed, they are clearly detailed in the Tutorial Section.**

Outline

1. GLE Principles
2. The 3-step procedure
3. Download files
4. Files - description
5. Files - synoptic
6. Tutorial - 1
7. Finally

6.1. Tutorial - 1



- GLE with 1 bath
for Lennard-Jones clusters
- from our paper **Physical Review B 91, 014301 (2015)**
[here](#)

6.2. Tutorial - 1

- First of all, to make things clear and neat, in your local directory,
- create 3 new sub-directories:

calcforce
fitPIbb
rungle

6.3.1. Tutorial - 1 / In sub-directory *calcforce*

In sub-directory *calcforce*

- run LAMMPS code with script
file *get_all_forces_model_small_sys_C_withCregion.lmp*
- that will create a cluster of 19 atoms for the central system (cutting out a sphere of a fcc crystal lattice) a spherical region around the central system representing the bath region (116 atoms), and another spherical region around the central system, with a small radius, representing the bath reduced region (68 atoms).

6.3.2. In sub-directory *calcforce*

- the LAMMPS script
file *get_all_forces_model_small_sys_C_withCregion.lmp*
- generates the central system (*group system_atoms*), the bath region (*group bath_atoms*), the bath reduced region (*group bath_reduced*)
- generates the necessary files for post-treatment
- calculates all the forces (stored in file named *forces.dat*) for/with the displaced atoms in order to obtain the dynamical matrix for the central region.

6.3.2. In sub-directory *calcforce*

- run code *DynMat_from_forces_eVAng_readmass*
- it calculates the dynamical matrix of the central region from the forces in file *forces.dat*
- the results are stored in file named *dynmat_coeff.dat*
- the file *dynmat_coeff_unsym.dat* can be removed, as it is now obsolete

1. GLE Principles
2. The 3-step procedure
3. Download files
4. Files - description
5. Files - synoptic
6. Tutorial - 1
7. Finally

6.3.3. In sub-directory *calcforce*

- edit the files
coord_bath_at_sort.dat and *coord_bathreduced_at_sort.dat*
in such a way that only the last TIMESTEP group of coordinates are kept,

- i.e.

```
ITEM: TIMESTEP
810
ITEM: NUMBER OF ATOMS
68
ITEM: BOX BOUNDS pp pp pp
0 96.6
0 96.6
0 96.6
ITEM: ATOMS id x y z mass
1 52.325 52.325 52.325 63.55
4 48.3 52.325 52.325 63.55
7 44.275 52.325 52.325 63.55
10 52.325 48.3 52.325 63.55
11 48.3 50.3125 54.3375 63.55
12 50.3125 48.3 54.3375 63.55
13 50.3125 50.3125 52.325 63.55
```

...

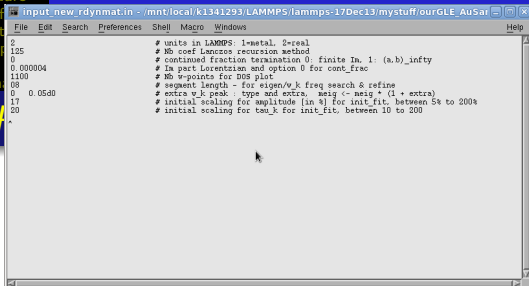
6.4.1. Tutorial - 1 / In sub-directory *fitPlbb*

In sub-directory *fitPlbb*

- copy the file *dynmat_coeff.dat* from sub-directory *calcforce*, or use symbolic link
- from the file *dynmat_coeff.dat*, we can start the mapping of the polarisation matrix $\Pi_{b,b'}(\omega)$
- run code *polar_matrix_Plbb_readdynmat_v5_fit_newinput*
- input file *input_new_rdynmat.in*

6.4.2. In sub-directory *fit*

input file *input_new_rdynmat.in*



```

input_new_rdynmat.in - /mnt/local/k1341293/LAMMPS/lammps-17Dec13/mystuff/ourGLE_AuSar
File Edit Search Preferences Shell Macro Windows Help
2 # units in LAMMPS: 1=metal, 2=real
125 # Mb coef Lanczos recursion method
0 # continued fraction termination 0: finite In, 1: (a,b)_infty
0.000004 # In part Lorentzian and option 0 for cont_frac
1100 # Mb w-points for DOS plot
08 # segment length - for eigen/w_k freq search & refine
0 # extra w_k peak : type and extra. seq (-= neg * (1 + extra))
17 # initial scaling for amplitude [in %] for init_fit: between 5% to 200%
20 # initial scaling for tau_k for init_fit: between 10 to 200
^

```

- 1st line: Units used in the LAMMPS run.
- 2nd line: Number of levels in the continued fraction used in the Lanczos algorithm (max value $3N_{\text{atoms}}$).
- 3rd line: termination of the continued fraction.
- 4th line: value of the tiny imaginary part for the termination 0 of the continued fraction.
- 5th line: Number of energy grid points.
- 6th line: length of the segment (number of points) for some averages within the automatic search of the peaks ω_k in the $\Pi_{bb'}$ matrix (max value Number of energy grid points). Typical value between 5 and 20. The larger the value, the lesser number of peaks is obtained.
- 7th line: when needed, the user can add extra peaks around the origin $\omega \sim 0$. The grid spacing for these extra peaks is linear or quadratic (1,2). The value of *extra* represent the percentage of extra peaks needed.
- 8th line: initial scaling for the amplitude $c_b^{(k)}$ for starting point of the fitting procedure (typically between 5 to 20%).
- 9th line: initial scaling for τ_k for starting point of the fitting procedure (typically between 10 to 200%).

6.4.3. In sub-directory *fit*

```

k1341293@nmscde000377: /mnt/local/k1341293/LAMMPS/lammps-17Dec13/mystuff/ourGLE_AuSams/ourGLE_Au
File Edit View Search Terminal Help
k+j= 1077
k+j= 1078
k+j= 1079
k+j= 1080
i= 73
k+j= 1081
k+j= 1082
k+j= 1083
k+j= 1084
k+j= 1085
k+j= 1086
k+j= 1087
k+j= 1088
k+j= 1089
k+j= 1090
k+j= 1091
k+j= 1092
k+j= 1093
k+j= 1094
k+j= 1095
Nb of calculated peaks = 69
Calculating extra peaks!
Extra peaks: quadratic space / more points close to 0
Nb of chosen w k peaks = 73
FOR FIT: Site/coord (ilat/xyz) indices ip, jp = 7
  
```

- enter value of 2 integers i and j , they represent the indexes of 2 different bath DOFs $i\alpha$ (ip) and $j\beta$ (jp).
- integer values between 1 and $3N_{\text{atoms}}^{\text{bath}}$ correspond to the atoms in the bath region, indexed by the LAMMPS code.
- the code calculates the fitting of the matrix elements (diagonal) $\Pi_{ip,ip}(\omega)$, $\Pi_{jp,jp}(\omega)$ and (off-diagonal) $\Pi_{ip,jp}(\omega)$.

6.4.4. In sub-directory *fit*

```

k1341293@nmmscde000377: /mnt/local/k1341293/LAMMPS/lammps-17Dec13/mystuff/ourGLE/AuSams.ourGLE.Au
File Edit View Search Terminal Help
k+j= 1077
k+j= 1078
k+j= 1079
k+j= 1080
i= 73
k+j= 1081
k+j= 1082
k+j= 1083
k+j= 1084
k+j= 1085
k+j= 1086
k+j= 1087
k+j= 1088
k+j= 1089
k+j= 1090
k+j= 1091
k+j= 1092
k+j= 1093
k+j= 1094
k+j= 1095
Nb of calculated peaks = 69
Calculating extra peaks!
Extra peaks: quadratic space / more points close to 0
Nb of chosen w k peaks = 73
FOR FIT: Site/coord (ilat/xyz) indices ip, jp = ?
  
```

- output files named:
 - fit_imDbbrecur_ovw_modCavtauk.xxxx.dat*
 - fit_imDbbrecur_IJ_ovw_min2.xxxxyyyy.dat* or
 - fit_imDbbrecur_IJ_ovw_min3.xxxxyyyy.dat*
 to be compared against the exact results in files named
 - imDbbrecur_ovw.xxxx.dat* and
 - imDbbrecur_ovw_IJ.xxxxyyyy.dat*
- *xxxx* and *yyyy* are strings of characters of the integers *ip* and *jp*
- change the different parameters in input file *input_new_rdynmat.in*, i.e. number of peaks, type of grid, imaginary part, numbers of levels in the continued fraction, ...
- until the fitting is considered to be sufficiently good.

6.4.5. In sub-directory *fitPlbb*

- Once the parameters in input file *input_new_rdynmat.in* are considered good enough for the fitting, we can start the whole mapping procedure of the polarisation matrix for all atoms in the **bath reduced region** for that
- run code *polar_matrix_Plbb_readdynmat_v13_fit_withCregion_newinput* with the same input file *input_new_rdynmat.in*

6.4.6. In sub-directory *fitPlbb*

- in the local directory where the code is launched, one also needs two supplementary files, giving information of the atoms in the bath region, and atoms in the bath reduced region.
- they were already generated by the LAMMPS script for the calculation of the forces in sub-directory *calcforce*
- copy (link) files *coord_bath_at_sort.dat* and *coord_bathreduced_at_sort.dat* from *../calcforce/* into *./fitPlbb*

6.4.7. In sub-directory *fitPlbb*

Then

- run code *polar_matrix_Plbb_readdynmat_v13_fit_newinput* with the same input file *input_new_rdynmat.in*
- the mapping (fitting) procedure is then performed for all atoms ($N_{\text{atoms}}^{\text{bath reduced}}$) contained in the **bath reduced region**
- The fitting procedure may run for a “long” time
- the output files for the mapping coefficients are named:
fit_coef_taukomegak_lmp.dat
and
fit_coef_cbk_lmp.dat

6.4.8. In sub-directory *fitPlbb*

- The file *fit_coef_taukomegak_imp.dat* contains
 - 3 columns (of length N^{aDOF}) representing the parameters k, τ_k, ω_k (with $k = 0$ to $N^{\text{aDOF}} - 1$)
 where N^{aDOF} is the number of auxilliary DOFs, i.e. the number of peaks in the fitting.

- The file *fit_coef_cbk_imp.dat* has the following structure
 - first line: number of columns $3N_{\text{atoms}}^{\text{bath reduced}} + 3$
 - each of the following $N_{\text{atoms}}^{\text{bath reduced}}$ line contains
 index i , LAMMPS ID index of the atom i , mass of atom i , vector of the coefficients $c_b^{(k)}$

- These 2 files will be input files for running the subsequent GLE-LAMMPS scripts

1. GLE Principles
2. The 3-step procedure
3. Download files
4. Files - description
5. Files - synoptic
6. Tutorial - 1
7. Finally

6.4.9. In sub-directory *fitPlbb*

- The mapping procedure also generate 3 huge files (only needed in case of failure of the fitting process).
- These 3 files (*SignMixedCoef.dat*, *SignEachCoef.dat* and *SignPMONE_EachCoef.dat*) can be removed to save disk-space

- Before being able to run the subsequent GLE LAMMPS scripts one needs to edit the content of the file *fit_coef_cbk_lmp.dat* to modify the list of LAMMPS ID index of the atom i
- Why?
- In the GLE LAMMPS runs, we need to have ONLY the atoms in the bath reduced region, while in the calculations of the dynamical matrix, we were using all the atom in the bath region
- In the GLE LAMMPS runs, the atoms in the bath region outside the bath reduced region will be removed, and consequently there might be a modification of the LAMMPS ID index for some of the atoms present in the bath reduced region.

6.5.1. Tutorial - 1 / In sub-directory *rungle*

In sub-directory *rungle*

- copy (or symbolic link) the files *fit_coef_taukomegak_lmp.dat* and *fit_coef_cbk_lmp.dat* from sub-directory *fitPIbb*,
- run LAMMPS with the script *gle_test_small_sys_C_T100_mubar32_52kts_seed2.lmp* for 0 timestep
- Then compared the LAMMPS ID index of the atoms in the generated file *coord_bathreduced_at_sort.dat* against the LAMMPS ID index in the file with the same name in the sub-directory *calcforce*

6.5.2. In sub-directory *rungle*

- The one-to-one correspondence between the “old” and “new” LAMMPS ID indexes can be done automatically by using the code *swapIDbathXred_old2new_v1.f90*
- ```
cp ../calcforce/coord_bathreduced_at_sort.dat
./old_coord_bathXred_at_sort.dat
cp ./coord_bathreduced_at_sort.dat
./new_coord_bathXred_at_sort.dat
```
- edit file *new\_coord\_bathXred\_at\_sort.dat* such that it has the same format as file *old\_coord\_bathXred\_at\_sort.dat*
- run code *swapIDbathXred\_old2new\_v1*
- Then simply edit the file *fit\_coef\_cbk\_imp.dat* and use the “new” indexes for the atoms in the bath reduced region

## 6.5.3. In sub-directory *rungle*

- Once this is done, the GLE LAMMPS is fully ready
- You can run the GLE LAMMPS script *.Imp* for as many timesteps needed
- and do GLE MD runs and extract forces, velocities, autocorrelation, thermodynamical properties, ... as usual done for any other LAMMPS calculation.

# Outline

1. GLE Principles
2. The 3-step procedure
3. Download files
4. Files - description
5. Files - synoptic
6. Tutorial - 1
7. Finally

1. GLE Principles
2. The 3-step procedure
3. Download files
4. Files - description
5. Files - synoptic
6. Tutorial - 1
7. Finally

## 7.1. Contacts & Support

- For further information and/or help, contact us at

**[gle.at.kcl@gmail.com](mailto:gle.at.kcl@gmail.com)**

- We are welcoming any suggestions for further development of our codes,
- We are open to develop fruitful collaborations on research projects using our GLE codes

## 7.2. Papers

- L. Kantorovich, Phys. Rev. B **78** 094304 (2008).
- L. Stella, C. D. Lorenz and L. Kantorovich, Phys. Rev. B **89**, 134303 (2014).
- H. Ness, L. Stella, C. D. Lorenz and L. Kantorovich, Phys. Rev. B **91**, 014301 (2015).
- H. Ness, A. Genina, L. Stella, C. D. Lorenz and L. Kantorovich, Phys. Rev. B **93**, 174303 (2016).
- H. Ness, L. Stella, C. D. Lorenz and L. Kantorovich, arXiv:1612.00990

## 7.3. Miscellaneous

- The GLE source codes for LAMMPS for the present tutorials are available only for serial calculations, i.e. use *make serial* to compile the LAMMPS code
- The full MPI versions are under last optimisation steps.
- They are available upon request and within the frame of developing new collaborations (at least, at the present stage of the development of our GLE codes).