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, KCL

UK EPSRC Grant No. EP/J019259/1.

London, January 2017

Outline

Outline

Outline

Outline

Outline

Outline

Outline

GLE Principles - A

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

$$\frac{dr_{i\alpha}}{dt} = \frac{p_{i\alpha}}{m_i}$$
$$\frac{dp_{i\alpha}}{dt} = F_{i\alpha}(\mathbf{r}) - \int_{-\infty}^{t} \mathrm{d}t' \sum_{\nu, i'\alpha'} K^{(\nu)}_{i\alpha, i'\alpha'}(t, t'; \mathbf{r}) \dot{r}_{i'\alpha'}(t') + \sum_{\nu} \eta^{(\nu)}_{i\alpha}(t; \mathbf{r}),$$

- 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 $\eta^{(\nu)}_{i\alpha}(t; \mathbf{r})$) are associated with each independent bath ν and $K^{(\nu)}_{i\alpha, i'\alpha'}(t, t'; \mathbf{r})$ is the friction (memory) Kernel.

GLE Principles - B

- 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) $b_\nu \equiv l_1\gamma$ 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.

GLE Principles - C

- 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.

Outline

Download code for LAMMPS

Go to the following url:
https://github.com/HerveNess/gleKCL/tree/master
to download the files

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 19

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.

Outline

Code

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

Code

- files name:
  polar_matrix_PIbb_readdynmat_v5_fit_newinput.f90
  parameters_and_co_readdynmat_v5_fit_eVAng.f90
  makefile_readdynmat_v5_fit_newinput
- operation:
  cp makefile_readdynmat_v5_fit_newinput makefile
  then *make* compiles the fortran codes into
  polar_matrix_PIbb_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*

Code

- files name:
  polar_matrix_PIbb_readdynmat_v13_fit_withCregion_newinput.f90
  parameters_and_co_readdynmat_v13_fit_withCregion_newinput.f90
  makefile_v13_fit_withCregion_newinput
- operation:
  cp makefile_v13_fit_withCregion_newinput makefile
  then *make* compiles the fortran codes into
  polar_matrix_PIbb_readdynmat_v5_fit_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*

Code

- file name:
  swapIDbathXred_old2new_v1.f90
- operation:
  gfortran swapIDbathXred_old2new_v1.f90 -o swapIDbathXred_old2new_v1
- 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*

Outline

What is needed:

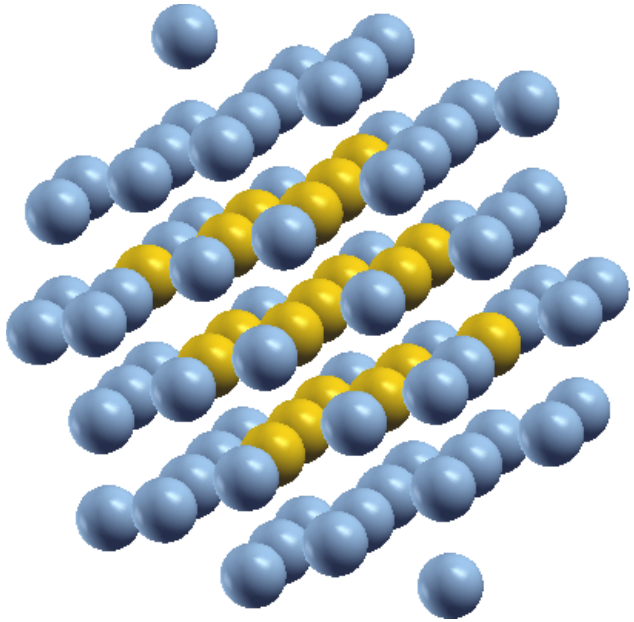
- LAMMPS script to build the system and calculate the forces
- code *DynMat_from_forces_eVAng_readmass.f90*
- code *polar_matrix_PIbb_readdynmat_v5_fit_newinput.f90* and input file *input_new_rdynmat.in*
- code *pola_matrix_PIbb_readdynmat_v13_fit_withCregion_newinput.f90* and input file *input_new_rdynmat.in*, and files *coord_bath_at.dat*, *coord_bathreduced_at.dat*
- LAMMPS script to run the GLE calculation
- code *swapIDbathXred_old2new_v1.f90*

What is needed:

- a LAMMPS script to
  - 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*
- code *DynMat_from_forces_eVAng_readmass.f90*

Outline

Tutorial - 1



- GLE with 1 bath

  for Lennard-Jones clusters
- from our paper **Physical Review B 91, 014301 (2015)**
  here

Tutorial - 1

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

  calcforce
  fitPIbb
  rungle

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).

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.

In sub-directory *calcforce*

- run code *DynMat_from_forces_eVAng_readmass*
- it calculates the dynamical matrix of the central region rom 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

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

...

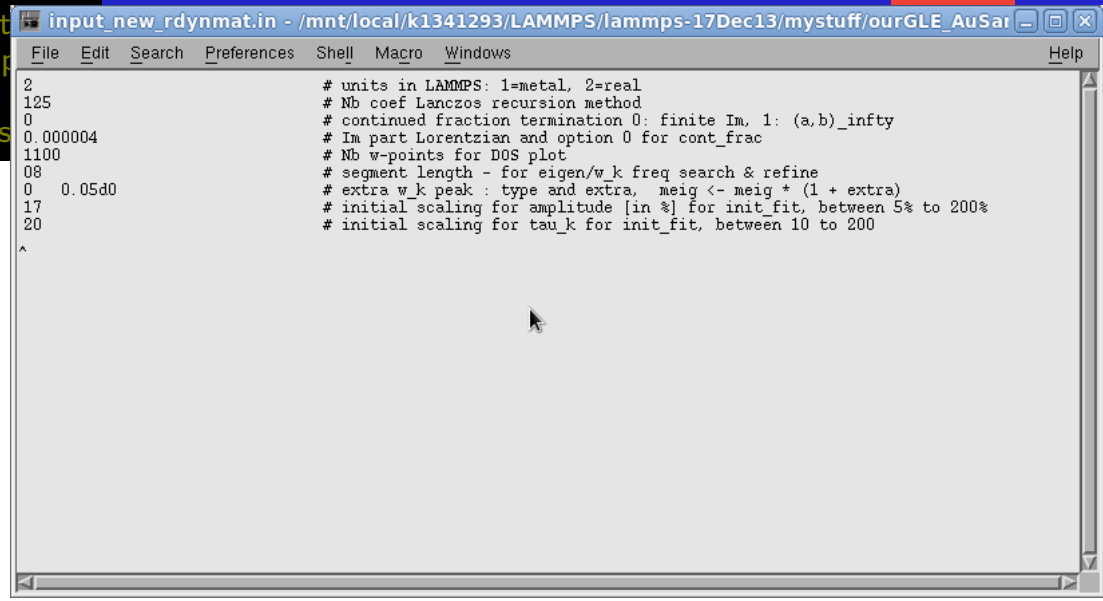
- these files will be needed later

In sub-directory *fitPIbb*

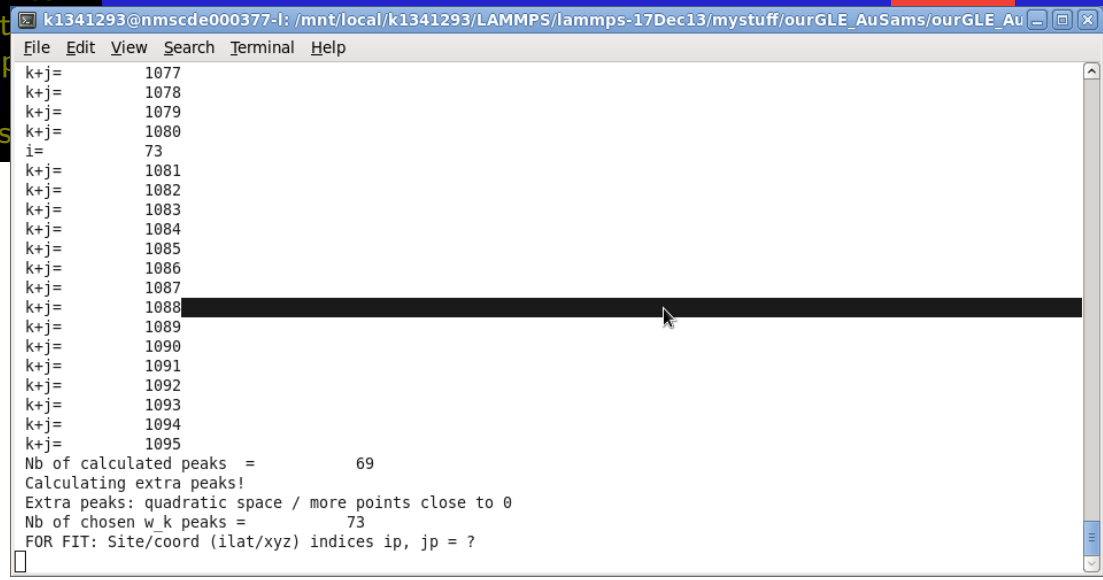
- copy the file *dynmat_coeff.dat* from sub-directory *calcforce*, or use symbolic link
- from the file *dynmat_coeff.dat*, we can start the mapping of the polarisation matrix $\Pi_{b,b'}(\omega)$

- run code *polar_matrix_PIbb_readdynmat_v5_fit_newinput*
- input file *input_new_rdynmat.in*

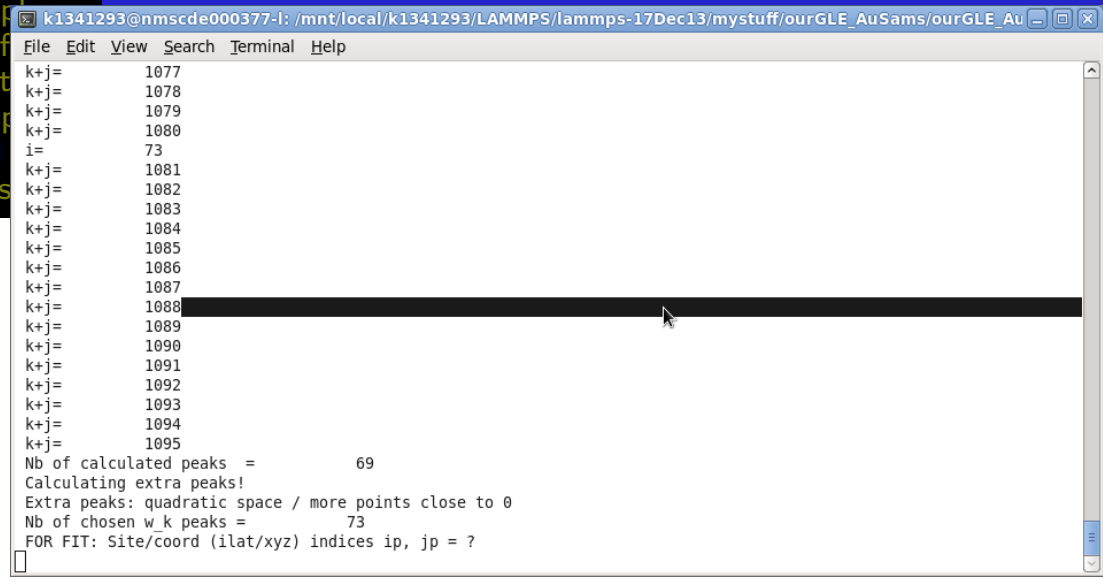
input file *input_new_rdynmat.in*



- 1st line: Units used in the LAMMPS run.
- 2nd line: Number of levels in the continued fraction used in the Lanczos algoritm (max value $3N_{\mathrm{atoms}}$).
- 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%).



- 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 calcutes the fitting of the matrix elements (diagonal) $\Pi_{ip,ip}(\omega)$, $\Pi_{jp,jp}(\omega)$ and (off-diagonal) $\Pi_{ip,jp}(\omega)$.



- 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 againts 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.

- 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_PIbb_readdynmat_v13_fit_withCregion_newinput

  with the same input file *input_new_rdynmat.in*

- 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 *./fitPIbb*

Then

- run code *polar_matrix_PIbb_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

- The file *fit_coef_taukomegak_lmp.dat* contains
  - 3 columns (of length N^{aDOF}) representing the parameters k, τ_k, ω_k (with $k = 0$ to $N^{\mathrm{aDOF}} - 1$)

    where N^{aDOF} is the number of auxilliary DOFs, i.e. the number of peaks in the fitting.

- The file *fit_coef_cbk_lmp.dat* has the following structure
  - first line: number of columns $3N_{\mathrm{atoms}}^{\mathrm{bath\ reduced}} + 3$
  - each of the following $N_{\mathrm{atoms}}^{\mathrm{bath\ reduced}}$ 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

In sub-directory *fitPIbb*

- 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.

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*

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_lmp.dat* and use the "new" indexes for the atoms in the bath reduced region

- Once this is done, the GLE LAMMPS is fully ready
- You can run the GLE LAMMPS script *./lmp*
  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

Conclusion

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

  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

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

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).