README FOR C++ CODE FOR COMPUTING DIFFUSIVITIES FROM PARTICLE MODELS OUT OF EQUILIBRIUM: ZRP CODE

This file explains the C++ code used to generate the data for the Zero Range Processes presented in Figures 4-7 in

Embacher, P., Dirr, N., Zimmer, J., Reina, C.: Computing diffusivities from particle models out of equilibrium, Proc. R. Soc. A DOI 10.1098/rspa.2017.0694 (arXiv:1710.03680).

1. Overview of the code: Main file and functions

The code is composed of the following files

Main.cpp: Main file to be launched where parameters are set and options are selected (see next section for details).
SavingParameters.h/.cpp: Function that saves the parameters set in the Main file.
InitialProfile.h/.cpp: Function that generates the initial density profile according to the parameters and options selected.
ZRP_KMC_new.h/cpp: Functions that advances the density profile using a Lattice Kinetic Monte Carlo algorithm, and considering periodic boundary conditions.
Postprocessing.h/cpp: Function that evaluates and saves $\langle \rho^L(t_0), \gamma_1 \rangle, \langle \rho^L(t_0 + h), \gamma_1 \rangle, \langle \rho^L(t_0), \gamma_2 \rangle, \langle \rho^L(t_0 + h), \gamma_2 \rangle, \ldots$ for each realization.

2. Parameters and options of the code

The following variables and options can be adjusted in the Main file. Their equivalent name in the paper and their meaning is provided below.

Configuration and process parameters:

Nbin	L, number of bins
Npart	$\sim N$, number of particles
profile	this option can be set as "flat", "sin" or "cos" to generate a flat profile, a sine shaped profile or a cosine shaped profile. Note that the profile is randomly perturbed in InitialProfile.cpp.
process	this option can only be set to "ZR".

Time parameters:

t_equilibration	$t_{prep} - t_{ini}$, time of equilibration
t_randomized	$t_0 - t_{prep}$, time to prepare the system for a new realization
dt	h, simulation time for actual measurements.

Sampling parameters:

Req	R_1
R	R_2

Filter function parameters:

x0_range	position of the center points of the functions γ over the domain [0,1].
a1	parameter a_1 of the functions γ
a2	parameter a_2 of the functions γ

Output options:

file_path Directory where the user wants the save the output of the code.

In addition, the type of Zero Range Process, can be set inside the function ZRP_KMC_new.cpp, by adjusting the parameter power to 1.0 or 2.0, for g(k)=k and g(k)=k^2, respectively.

3. Running the code

The following commands may be typed on the terminal to compile the code

```
>> module load gcc/6.3.0
>> g++ -std=gnu++0x -O3 Main.cpp InitialProfile.cpp ZRP_KMC_new.cpp Postprocessing.cpp
SavingParameters.cpp -o executable_name
```

where the first command is needed to load version C++11 in order to use the random variable generator used in the code.

4. Output of the code and postprocessing

After running the executable, the code generates in the specified filename path, 1 summary file and Req data files. Their names depend on the set values of Nbin and Npart set in the Main file as follows

Summary_Nbin_5000_Npart_79616.m: contains all the parameters prescribed in the Main file.

Data_Nbin_5000_Npart_79616_req_1.m: each row contains $\langle \rho^L(t_0), \gamma_1 \rangle, \langle \rho^L(t_0+h), \gamma_1 \rangle, \langle \rho^L(t_0), \gamma_2 \rangle, \langle \rho^L(t_0+h), \gamma_2 \rangle, \ldots$ for each realization $r \in [1:R]$. The number following req ranges from 1 to Req.

This data can be further postprocessed using the file **Postprocessing_m.m** to deliver the expected values of ρ, m and the standard deviation of m associated to each function γ. This file will also include the values of the all parameters. Note that m in the code is equivalent to $2m$ in the paper.

5. Parameters used to generate the figures in the paper

The default parameters for figures 4-7 are:

Nbin	Npart	t_equilibration	t_randomize	dt	Req	R	x0_range	a1	a2
5000	79616	4e-06	4e-09	4e-11	50	2000	[0.025:0.025:0.975]	160	2

and their specific parameters are:

Figure 4	none
Figure 5	Nbin=[100,200,500,1000,2000,5000,10000] Npart=[1592,3184,7962,15923,31846,79616,159232]
Figure 6	dt=[4e-8,4e-9,4e-10,4e-11,4e-12,4e-13,4e-14]
Figure 7	R=[20,50,100,200,500,1000,5000]