MagChain
User's Guide

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The MagChain package is the implementation of a Coarse-Grain (CG) simulation model for the description of the chain formation phenomena observed in dispersions of superparamagnetic nanoparticles under high magnetic fields. The main algorithm is based on a Brownian Dynamics scheme for the description of the motion of the colloidal entities (CG objects) together with an irreversible aggregation model based on the magnetic dipole-dipole interaction between particles. Further details on CG model and its implementation can be found in the original paper [1].

The original developers of the code in 2011 were Jordi S. Andreu (ICMAB-CSIC, UAB), Carles Calero (ICMAB-CSIC, UAB), Juan Camacho (UAB) and Jordi Faraudo (ICMAB-CSIC). In summer 2019, Àlex Giménez and David C. Malaspina entered the team.

The following reference to the original scientific article [1] with description of the model must be included in any published work using the MagChain program:

> J.S. Andreu, C.Calero, J. Camacho and J. Faraudo, *On-the-fly coarse-graining methodology for the simulation of chain formation of superparamagnetic colloids in strong magnetic fields*,
> Phys. Rev. E, **85**, 036709 (2012).

The MagChain program has been devised for free use in academic research within the academic community. Current license for MagChain is GNU GENERAL PUBLIC LICENSE Version 3. For details in the license information, please see the LICENSE file included with the program.

The MagChain package is distributed at the MagChain GitHub project page `https://github.com/magchainsimulationpackage/`.

The MagChain package contents are organized into four different blocks (with a repository for each block):

- The simulation code itself
- A graphical interface to generate input files and to analyze results
- A set of visualization programs to visualize trajectories
- A tutorial

We recall that each block has its own repository at GitHub with documentation. In this manual, we focus on the simulation code only. The user is advised to complete first the Tutorial and then use this Manual for further reference.

The simulation code repository contains the following folders:

src/ The source files corresponding to the MagChain application.

examples/ We provide 4 different examples of simulations performed with the MagChain program. Details on each simulation are given in the accompanying README file.

tools/ Simple C++ programs are provided in order to generate the required attraction radius file for production runs (attradius.cpp).

docs/ This manual

Chapter 1

Compilation & Execution

The MagChain program is written in C++ and it runs in any single-processor machine. The code has been successfully compiled in different platforms using the standard gnu C++ compiler. No additional libraries are required for its compilation:

- Mac OSX Leopard 10.5.8 (32bit) with g++ 4.0.1.
- Mac OSX Snow Leopard 10.6.8 (64bit) with g++ 4.2.1.
- LINUX openSUSE 11.3 2.6.34.8-0.2-desktop x86_64 with g++ 4.5.0.

In order to compile the MagChain program, download and extract the package (you can download the package from `http://www.icmab.es/softmattertheory/`. in a single zip-compressed file). Running from terminal, the program can be easily compiled by using the Makefile supplied together with the source code (the gnu makefile is required). Thus, from a terminal window, go to the source folder and type:

```
>make
```

Once the compilation is done, the binary file (magchain) is created in the same folder.

In order to run the program, we have to execute this binary file and provide the simulation parameters using an input script supplied as argument :

```
>./magchain in.script
```

Details about how to create an input script and other possible required files necessary to run the simulation are given in Chapter 3.

Chapter 2

Physical model

In this section we briefly summarize the main features of the models implemented in the MagChain program. A complete description of the models and the algorithms implemented in the MagChain package can be found in the original article [1].

2.1 Anisotropic diffusion model

The motion of any CG object (single particle or aggregate) with size s is given by the anisotropic diffusion model selected. Generally, for a single and isolated particle ($s = 1$) immersed in a fluid with viscosity η at temperature T we have:

$$D_1 = \frac{k_B T}{3\pi\eta d}, \tag{2.1}$$

Then, a chain containing $s > 1$ particles has anisotropic diffusion, characterized by a diffusion coefficient $D_s^{\parallel}$ in the direction parallel to the long axis of the chain and $D_s^{\perp}$ in the directions perpendicular to the long axis. There are several possibilities for the analytical form of these diffusion coefficients, depending on the exact geometry assumed for the chains and the degree of approximation of the calculation. We considered the following expressions (Rod model) which can be found in [3] and are valid for elongated objects of size s (slender body theory):

$$\frac{D_s^{\parallel}}{D_1} = \frac{3}{2s}[\ln(2s) - \frac{1}{2}], \tag{2.2}$$

$$\frac{D_s^{\perp}}{D_1} = \frac{3}{4s}[\ln(2s) + \frac{1}{2}]. \tag{2.3}$$

Strictly speaking, Eqs.(2.2) and (2.3) are valid for large s. We employ these equations for computing the diffusion coefficients of chains with $s > 2$. In the case of

aggregates with $s = 2$, these equations give inaccurate diffusion coefficients and we employ a simple interpolation between the diffusion coefficient D_1 corresponding to a single particle and the values given by Eqs.(2.2) and (2.3) for $s = 3$.

2.2 Aggregation model

Apart of the steric interaction between coarse grain objects, the magnetic dipole-dipole interactions between individual particles is replaced by an spherical attraction zone at the poles of each colloid or aggregate. These zones are defined by the radius of this region, r_a given by the solution of equation:

$$\frac{E_{mag}}{k_B T} = -\Gamma \sum_{n=0}^{s-1} \frac{1}{(2r_a/d + 1/2 + n)^3} = -1 \tag{2.4}$$

where s is the number of colloids in the aggregate and Γ is the magnetic coupling parameter defined as:

$$\Gamma = \frac{\mu_0 m_s^2}{2\pi d^3 k_B T} \tag{2.5}$$

where m_s is the magnetic dipole of the individual particles at saturation and d their diameter.

Chapter 3

Input files

3.1 Units

The simulation units system is defined by a typical length and time scales. In our case, the basic unit of length is the diameter d of the colloidal particle and the basic unit of time (denoted as τ) is defined by normalizing the (isotropic) diffusion coefficient D of a single isolated colloid. With this definitions, the conversion between real units and simulation units (denoted with an upper bar) for the length and time scales is:

$$\bar{r} = r/d$$
$$\bar{t} = t/\tau$$

where $\tau = d^2/D$.

3.2 Input script

In the MagChain program all the necessary parameters to setup a simulation are supplied to the main program with the help of an input script[1]. The input script is parsed line by line then, each directives (some of them mandatory and some other just optional) in the input script has to be written in a single line. All the directives are read at once and can be placed in any order within the file. This implies that each directive should be used only once. If any directive is found more than once in the input script, only the last one is used to setup the simulation. Any comment line in this input script must be preceded by the # character. Any

[1] Any of the input files required to run the simulation can be placed either in the same folder than the binary file or referenced by their relative or absolute location in the file system.

comment or blank line are skipped when reading the file.

The MagChain program allows two different simulation modes: equilibration and production. In the equilibration mode, the motion of the initial set of CG objects is performed following the diffusion model but the aggregation scheme is not applied i.e. the formation of new aggregates is not allowed. In the production mode, the aggregation scheme is switched on and the aggregation is taken into account. Only in this latter case, the different statistical quantities of interest are computed during the simulation.

The following is the complete list of directives available:

nparticles *n*
: Argument *n* is the initial number of CG objects in the simulation (single particles or aggregates). This value is skipped when restarting the simulation from a restart file.

sbox *x-value y-value z-value*
: The *x-value*, *y-value* and *z-value* specify the length (in particle diameters) of the three orthogonal axes of the simulation box. These values are skipped when restarting the simulation from a restart file.

timestep *t*
: Specifies the integration timestep (in simulation units). This is the time interval used to compute the displacement of each CG object according to the diffusion model selected.

equil *value*
: Sets an equilibration run (only diffusive motion) where *value* is the total number of time steps.

run *value*
: Sets a production run (diffusive motion + aggregation) where *value* is the total number of time steps.

attradius *filename maxvalue*
: Specifies the values of the attraction radius for each CG object. The *filename* keyword is the name of the file containing the values of attraction radius associated to each CG object according to its length. The *maxvalue* keyword

specifies the number values which will be read from the file. Then, this last value read will be used as attraction radius for CG objects with longer length.

stats_every *n*

This indicates to calculate and store *stats.dat* the statistics every n timesteps. The different quantities calculated are defined in the Output files section.
Default $n = 1$ (the statistics are stored every single time step).

restart_every *n*

Creates a restart file every n timesteps. Each file is automatically labeled as *restart.n*, where n is the corresponding timestep of this run. Every restart file contains information about the simulation box and the positions of the CG objects at a given time and can be used to restart a simulation. In this case, any information about the simulation box or about the CG objects is overwritten (except the attraction radius values, which have to be always supplied by the external file).
Default $n = 0$ (only the initial and final configurations are stored).

traj_every *n*

Creates a dump file (trajectoryCG.xyz) of the system by saving the configuration of the system every n timesteps. Each configuration is stored following a *xyz*-type format (see the Output files section for more details).
Default $n = 0$.

hist_every *n maxbin*

Creates a histogram file (histogram.dat) every n timesteps. The *maxbin* parameter limits the number of bins of the histogram. By default the *maxbin* value is 300.
Default $n = 0$.

read_restart *filename*

Specifies the name of the restart file to be used to setup a simulation. When restarting the simulation, several simulation parameters are initialized by default according to the values stored in the restart file: the actual number of aggregates and their positions, the simulation box dimensions, the integration timestep and the values for the attraction radius. Only the attraction radius and the timestep can be overwritten to different values when restarting a simulation by supplying the new values though the input script (and the corresponding additional files). Any other parameter has to be initialized again using the appropriate directives in input script.

3.3 Attraction radius values

The values of the attraction radius have to be supplied to the MagChain program by using a plain text file. This file has to be 2-column formatted in which the first column contains a list of integer values corresponding to the length of the CG Object (i.e. the number of colloidal particles forming the aggregate) and a second column containing the corresponding attraction radius for each CG object length, according to Eq.(2.4). The first line of this file will be skipped, so it can be used as a comment line. It is assumed that the first value corresponds to $s = 1$ and that the following values correspond to CG objects with increasing consecutive length (i.e. $s = 2, 3, 4, \ldots$)

A small C++ routine is supplied within the *tools* folder to generate this file and some input scripts and attraction radius data files can be found in the examples folder.

Chapter 4

Output files

During a production run, different statistical quantities are computed such the number of aggregates, the average number of particles in a chain $\langle N \rangle$, or the so-called *cluster-size* $\langle S \rangle$, defined as in [2, 5]:

$$\langle N(t) \rangle = \frac{\sum_s s n_s(t)}{\sum_s n_s(t)}, \tag{4.1}$$

$$\langle S(t) \rangle = \frac{\sum_s s^2 n_s(t)}{\sum_s s n_s(t)}, \tag{4.2}$$

and some other can be easily calculated, like the probability of finding an aggregate of size s at a given time, defined as:

$$p(s;t) = \frac{n_s(t)}{\sum_s n_s(t)}. \tag{4.3}$$

The following is the list of all output files generated by the MagChain program and a brief description of their contents and structure:

logfile.txt: It stores a summary of the initialization stage as well as the evolution of the some statistical quantities of interest. This file is always generated by default in any mode

stats.dat: column-formatted file which stores the time evolution of several quantities (only in production mode). The file contents are (ordered by column): the dimensionless times t, the total number of aggregates A, the mean average size $\langle N \rangle$, the cluster-size $\langle S \rangle$ and the CPU elapsed time ET in seconds. This file is only generated during production runs.

histogram.dat: column-formatted file which stores the details on the distribution of aggregates as a function of time. The structure of the file is as follows: column (1) is the simulation time in dimensionless units, column 2 is the total number of CG objects (chain-like aggregates or single particles). From column 3 until the last column (3+$maxbin$), are used to store the number of CG objects of size s at that time, from $s = 1$ to $s = maxbin$.

time CG-Objects size_1 size_2 ... size_m

trajectoryCG.xyz: dump file containing different configurations of the system stored every certain timesteps. Each configuration is structured in two parts: a header and a body. The header is composed by a first line containing the total number of CG objects at that timestep and second line containing the dimensions of the simulation box. The body contains the information about the CG objects. Each line is used to specify the information of a single CG object. In each line, the first value is the *id* of the CG object, the three next values are the cartesian coordinates of its center of mass and the last two columns are its length and its diameter (fixed to 1), respectively.

n-CG-Objects
x-axis y-axis z-axis
id_1 x_1 y_1 z_1 length_1 diameter_1
id_2 x_2 y_2 z_2 length_2 diameter_2
. . .
. . .
. . .
id_n x_n y_n z_n length_n diameter_n

This is the format used for the visualization applications supplied in the tools folder.

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Bibliography

[1] J.S. Andreu, C. Calero, J. Camacho and J. Faraudo, Phys. Rev. E **85**, 036709 (2012).

[2] M. Carmen Miguel and R. Pastor-Satorras, Phys. Rev. E **59**, 826 (1999).

[3] Happel J, Brenner H (1985) Low Reynolds number hydrodynamics. Cambridge University Press, Cambridge

[4] F. Martínez-Pedrero, M. Tirado-Miranda, A. Schmitt and J. Callejas-Fernández, Phys. Rev. E **76**, 011405 (2007)

[5] P. Domínguez-García et al, Phys. Rev. E **76**, 051403 (2007)

[6] M.M. Tirado, J.G. de la Torre, J. Chem. Phys. **71**, 2581 (1979).