Supporting file for reproducing results of the article: *Lanthanide molecular nanomagnets as probabilistic bits*

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This document offers a help for reproducing the graphics. As we comment in the *readme.txt*, the following modules need to be installed:

1. numpy
2. matplotlib.pyplot
3. pandas
4. scipy.optimize
5. Collections (Counter)
6. random
7. math
8. time

Moreover, the following files must be in the same folder containing the *main.py* file:

1. main.py (Part of the code where the user specifies the parameters).
2. read_data.py (Description of the system).
3. mag_relaxation.py (Relaxation Mechanisms, Total probability for spin flipping).
4. Bolztmann_distribution.py (Zeeman effect, Boltzmann distribution, single probabilities to pass from 0 to 1, and vice versa).
5. mean_matrix_state.py (For a two p-bit network, where the collective state is studied in this function).
6. association.py (For a two p-bit network, the association factor is calculated).
7. plotting.py (Graphical Representation of the results).

8. full_data_file.csv (File which contains all the information for few systems, from the work: Data-driven design of molecular nanomagnets, Nature Communications volume 13, Article number: 7626 (2022).

It is important to emphasize that the file named *main.py* contains the body of the simulator; the user could only change the configuration section at the beginning of the script (lines 25-51). In this version of STOSS we are capable to simulate three main scenarios:

1. Magnetization decays at different temperatures at constant magnetic field.

2. Magnetization decays at different temperatures at changeable magnetic field.

3. Magnetization decays at different temperatures of two p-bit networks.

Considering this idea, the user can select the type of simulation just writing the values in each variable. Figure 1 shows this part of the simulator.

```
21  #-------------------------------------------------------------------------------------------
22  #                          SETTING PARAMETERS BY THE USER
23  #-------------------------------------------------------------------------------------------
24
25  # GENERAL CONFIGURATIONS:
26  #-------------------------------------
27  N_ex = 1000                           # Number of Spins of each p-bit
28  T = 20/1000                           # Temperature, K
29  save = 0                              # 1: for saving results; 0: no
30  flag = 28                             # System to be studied from SIMDAVIS database
31  starting_mode = 0.5                   # Starting mode for all the spins (0.5 = 50% spins in the lower state of energy)
32  time_steps = 2000                     # Total time steps
33  option = 1                            # 1: changeable field; 0: constant field
34  option_2spin = 0                      # 1: yes; 0: no for the study of a p-bit network
35
36  # CONSTANT MAGNETIC FIELD:
37  #-------------------------------------
38  B_constant = 0                        # Applied magnetic field, Tesla. If only "option" = 0
39
40  # CHANGEABLE MAGNETIC FIELD:
41  #-------------------------------------
42  B_max = 0.00025                       # Maximum value for Magnetic Field, Tesla. If only "option" = 1
43  cycles = 4                            # Changeable field applied. If only "option" = 1
44
45  # TWO P-BIT NETWORK:
46  #-------------------------------------
47  B_pbit2 = 0.02                        # Applied magnetic field, Tesla. If only "option_2spin" = 1
48  factor = 100                          # Threshold for the definition of the collective state of each p-bit. If only "option_2spin" = 1
49  asociation_factor = time_steps        # How many delays the program will take into account
50  step_asociation_factor = 1            # How many steps of delay the program will take into account to reach the value of the previous variable
51
52  #-------------------------------------------------------------
```

Figure 1: Parameters that can be modified by the user.

Section 3.1. Lanthanide-based, molecular, isolated spin p-bits at constant field

As an example, we present the experiment at 80K employing $N = 10^3$ (Figure 2) and $N = 10^4$ (Figure 3) spins, respectively. In the case of 80, 40, and 2K, the program compares the results of the magnetic moment with the experimental data extracted from F.-S. Guo, B. M. Day, Y.-C. Chen, M.-L. Tong, A. Mansikkamäki and R. A. Layfield, Science, 2018, 362, 1400–1403.

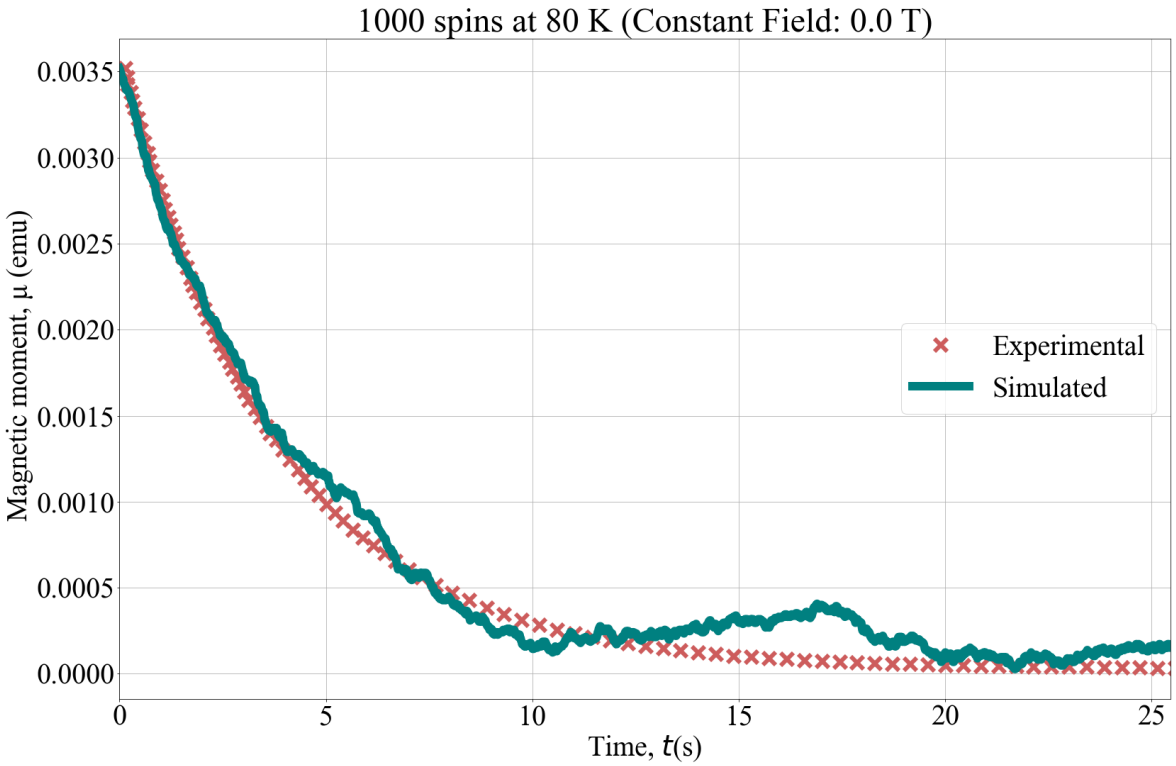

Figure 2: Relaxation plot employing $N = 10^3$ spins at 80K for $[(Cp^{iPr5})Dy(Cp^*)]^+$ (Cp^{iPr5}, penta-iso-propylcyclopentadienyl; Cp^*, pentamethylcyclopentadienyl).

Figure 4 shows the summary from the simulation process for both cases: $N = 10^3$ (a) and $N = 10^4$ (b) spins. We also present the parameters (Table 1) which must be written by the user to reproduce those results. Given the stochasticity nature of the STOSS, the results could vary slightly.

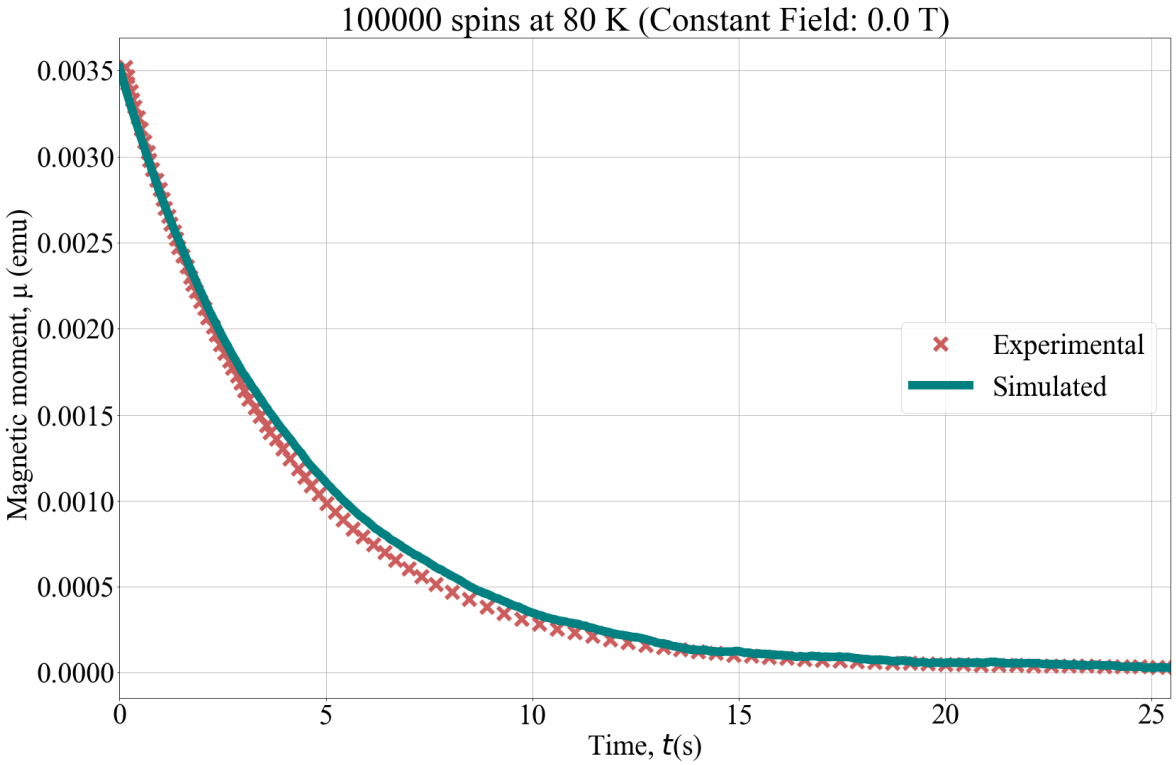

Figure 3: Relaxation plot employing $N = 10^4$ spins at 80K for $[(Cp^{iPr5})Dy(Cp^*)]^+$ (Cp^{iPr5}, penta-iso-propylcyclopentadienyl; Cp^*, pentamethylcyclopentadienyl).

Table 1: Parameters at 80K for $[(Cp^{iPr5})Dy(Cp^*)]^+$, where DNA = Does Not Apply.

Variable	Figure 2	Figure 3
N_ex	1000	10000
T	80	80
save	1	1
flag	22	22
starting_mode	0	0
time_steps	2000	2000
option	0	0
option_2spin	0	0
B_constant	0	0
B_max	DNA	DNA
cycles	DNA	DNA
B_pbit2	DNA	DNA
factor	DNA	DNA
association_factor	DNA	DNA
step_association_factor	DNA	DNA

a)

```
Sample ID:  [2.]
Relaxation Time: 4.24461 sec at 80 K
------------------------------------------------
************************************************
------------------------------------------------
First p-bit has finished
------------------------------------------------
************************************************
Time processing:  0.06571321487426758  minutes
************************************************
------------------------------------------------
Information about the simulation:
------------------------------------------------

             Name    Units     Value
0      Compound ID        -     [2.0]
1            Spins        -      1000
2      Temperature   Kelvin        80
3  Relaxation Time  seconds  4.244606
4        Time step  seconds  0.012734
5            Steps        -      2000
6  Processing time  minutes  0.065713
```

b)

```
Sample ID:  [2.]
Relaxation Time: 4.24461 sec at 80 K
------------------------------------------------
************************************************
------------------------------------------------
First p-bit has finished
------------------------------------------------
************************************************
Time processing:  5.895399037996928  minutes
************************************************
------------------------------------------------
Information about the simulation:
------------------------------------------------

             Name    Units     Value
0      Compound ID        -     [2.0]
1            Spins        -    100000
2      Temperature   Kelvin        80
3  Relaxation Time  seconds  4.244606
4        Time step  seconds  0.012734
5            Steps        -      2000
6  Processing time  minutes  5.895399
```

Figure 4: Summary file of the simulation employing $N = 10^3$ (a) and $N = 10^4$ (b) spins at 80K for $[(Cp^{iPr5})Dy(Cp^*)]^+$ (Cp^{iPr5}, penta-iso-propylcyclopentadienyl; Cp^*, pentamethylcyclopentadienyl).

Section 3.2. Lanthanide-based, molecular, dynamically driven spin p-bits

As we could see in the previous part, all the information to simulate this experiment is shown in the (Table 2). The result is presented in the Figure 5 with $N = 5 \cdot 10^3$ spins and $N = 2.5 \cdot 10^4$ spins in the Figure 6. Moreover, the summary of each simulation is shown in Figure 7.

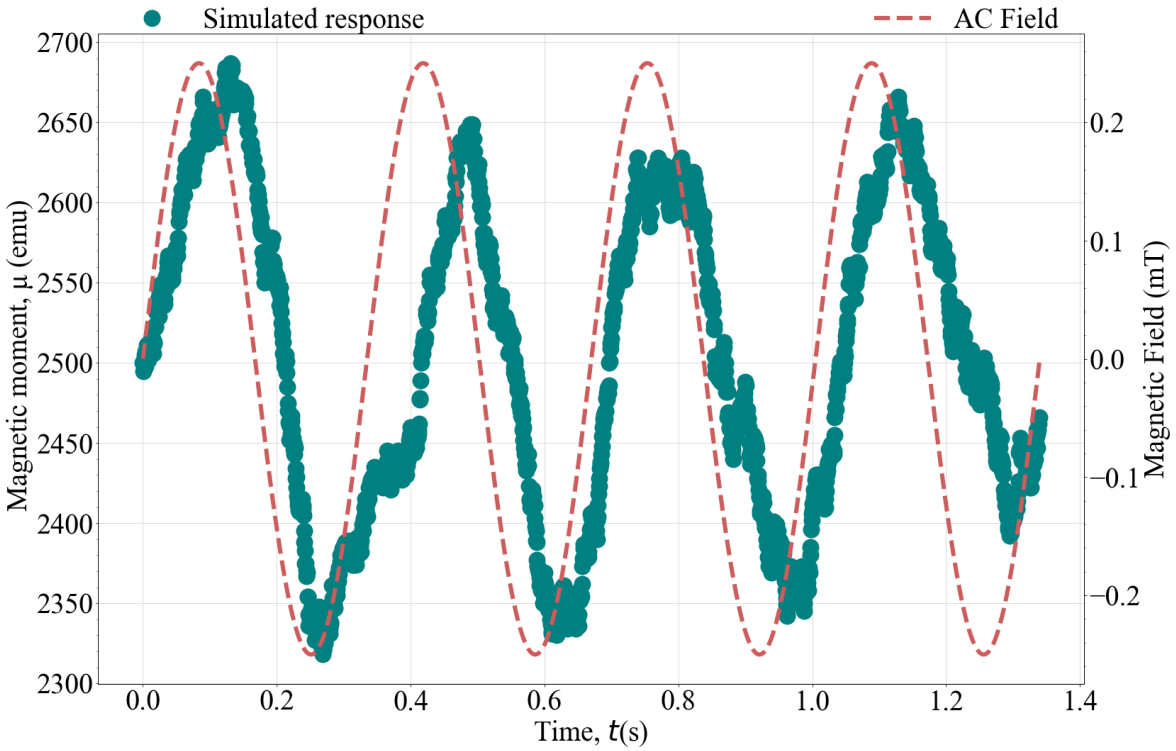

Figure 5: Relaxation plot employing $N = 5 \cdot 10^3$ spins at 20mK for $[Dy(bath)(tcpb)_3]$ and frequency 3 Hz.

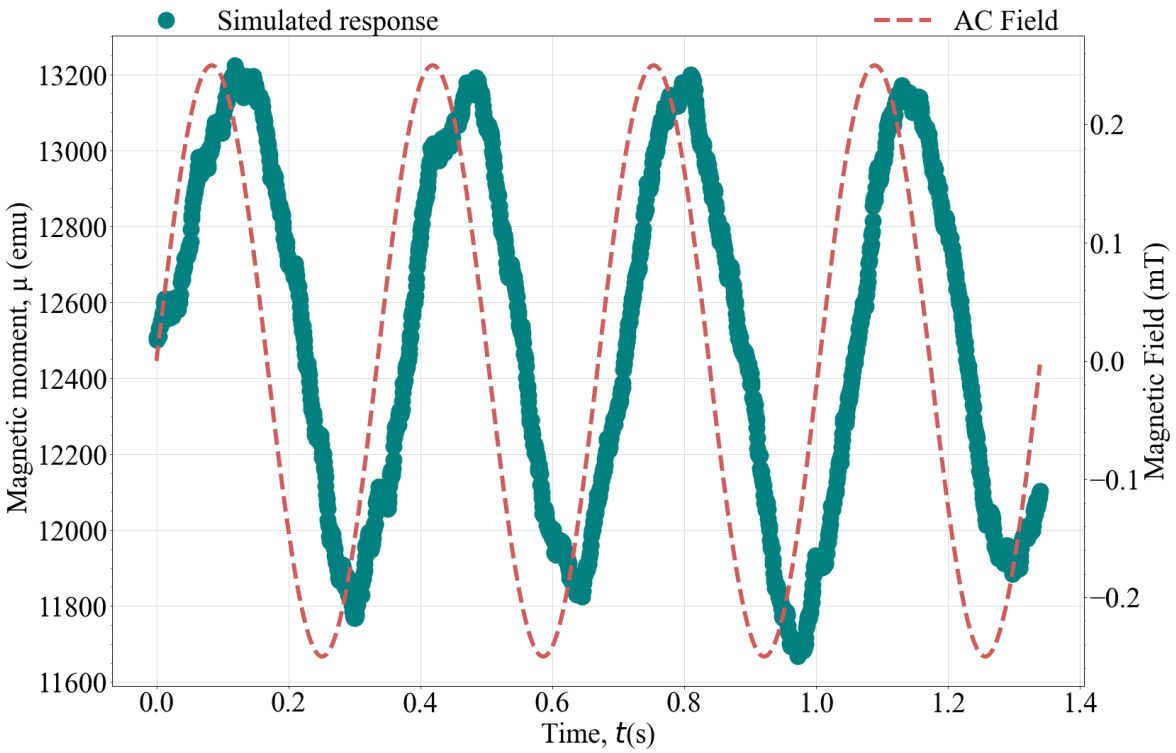

Figure 6: Relaxation plot employing $N = 2.5 \cdot 10^4$ spins at 20mK for [Dy(bath)$(tcpb)_3$] and frequency 3 Hz.

Table 2: Parameters at 20mK for [Dy(bath)$(tcpb)_3$] and frequency 3 Hz, where DNA = Does Not Apply.

Variable	Figure 5	Figure 6
N_ex	5000	25000
T	0.02	80 0.02
save	1	1
flag	26	26
starting_mode	0.5	0.5
time_steps	2000	2000
option	1	1
option_2spin	0	0
B_constant	0	0
B_max	0.00025	0.00025
cycles	4	4
B_pbit2	DNA	DNA
factor	DNA	DNA
association_factor	DNA	DNA
step_association_factor	DNA	DNA

a)

```
------------------------------------------------
Sample ID:  [1132.]
Relaxation Time: 0.06700 sec at 0.0200 K
------------------------------------------------
************************************************
------------------------------------------------
First p-bit has finished
------------------------------------------------
************************************************
Time processing:  0.30383423566818235  minutes
************************************************
------------------------------------------------
Information about the simulation:
------------------------------------------------

              Name    Units     Value
0      Compound ID        -  [1132.0]
1            Spins        -      5000
2      Temperature   Kelvin      0.02
3  Relaxation Time  seconds     0.067
4        Time step  seconds   0.00067
5            Steps        -      2000
6  Processing time  minutes  0.303834
```

b)

```
------------------------------------------------
Sample ID:  [1132.]
Relaxation Time: 0.06700 sec at 0.0200 K
------------------------------------------------
************************************************
------------------------------------------------
First p-bit has finished
------------------------------------------------
************************************************
Time processing:  1.5053065141042075  minutes
************************************************
------------------------------------------------
Information about the simulation:
------------------------------------------------

              Name    Units     Value
0      Compound ID        -  [1132.0]
1            Spins        -     25000
2      Temperature   Kelvin      0.02
3  Relaxation Time  seconds     0.067
4        Time step  seconds   0.00067
5            Steps        -      2000
6  Processing time  minutes  1.505307
```

Figure 7: Summary file of the simulation employing $N = 5 \cdot 10^3$ (a) and $N = 2.5 \cdot 10^4$ (b) spins at 20mK for [Dy(bath)$(\text{tcpb})_3$].

Section 3.3. Lanthanide-based, molecular spin p-bit network

This part of the simulator follows the calculations of two p-bit network. To reproduce the result, we present the Table 3 with all the necessary values and its simulation. In contrast, Figure 8 shows the summary part where we could see the computational cost when we increase the number of spins of each p-bit to 1 million with 10,000 total time steps.

Variable	Figure 8
N_ex	1000000
T	4
save	1
flag	25
starting_mode	0.5
time_steps	10000
option	0
option_2spin	1
B_constant	0
B_max	DNA
cycles	DNA
B_pbit2	0.02
factor	1000
association_factor	time_steps
step_association_factor	1

Table 3: Parameters at 4 K to analyze the effect of a p-bit to another, for $[Dy(obPc)_2]$ $Cd[Dy(obPc)_2]$.

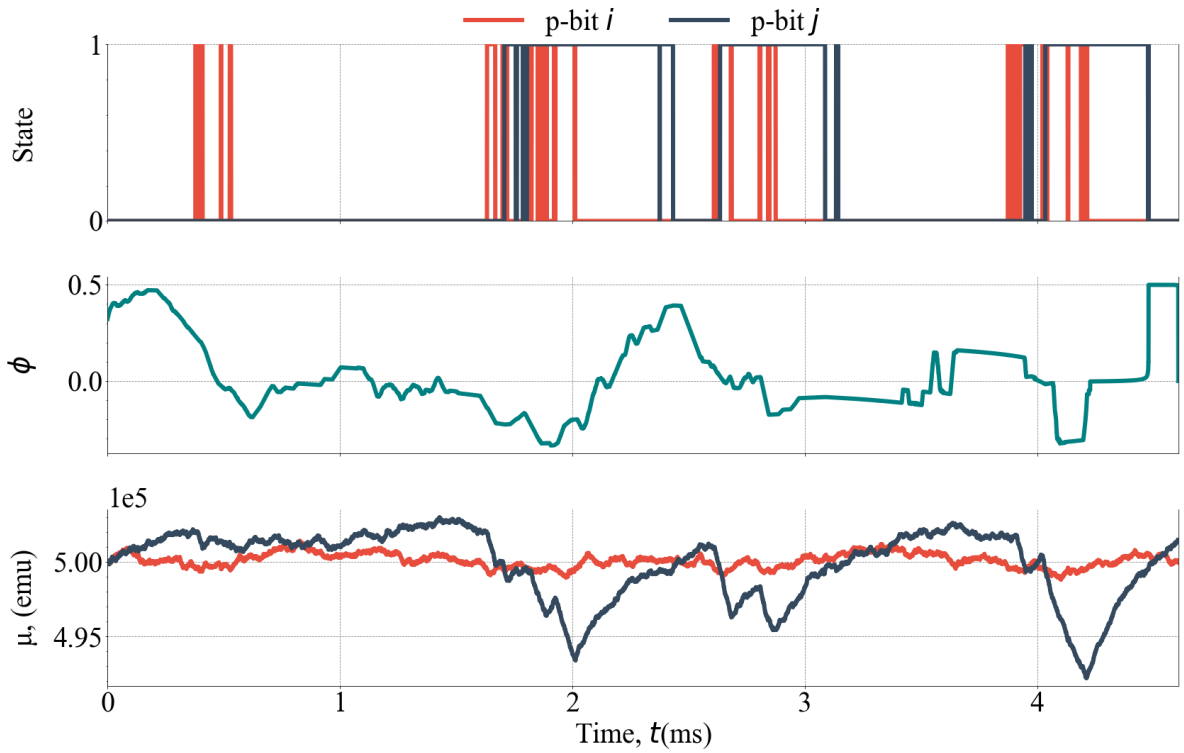

Figure 8: Simulation employing $N = 10^6$ spins per p-bit at 4 K for $[Dy(obPc)_2]$ $Cd[Dy(obPc)_2]$. Where part a) represents the state of each p-bit, b) the association factor, and c) the relaxation behaviour.