

---

# **magpy Documentation**

***Release 1.0***

**Oliver Laslett**

**Feb 07, 2018**



---

## Contents

---

<b>1</b>	<b>Installation</b>	<b>1</b>
1.1	Conda . . . . .	1
1.2	From source . . . . .	1
1.3	From source (Intel compilers) . . . . .	2
<b>2</b>	<b>Getting started - a single particle</b>	<b>5</b>
2.1	Simulate . . . . .	6
<b>3</b>	<b>Thermal equilibrium of a single particle</b>	<b>9</b>
3.1	Problem setup . . . . .	9
3.2	Boltzmann distribution . . . . .	9
3.3	Stoner-Wohlfarth model . . . . .	10
<b>4</b>	<b>Two particle equilibrium</b>	<b>17</b>
4.1	Metropolis MCMC . . . . .	18
4.2	Magpy - Dynamical Simulation . . . . .	21
4.3	Compare results . . . . .	22
4.4	Sanity check: no interactions . . . . .	24
<b>5</b>	<b>Convergence Tests</b>	<b>27</b>
5.1	Task 1 - 1D non-stiff SDE . . . . .	27
5.2	Task 2 - 1D stiff SDE . . . . .	28
5.3	Task 3 - 1D unstable system . . . . .	29
5.4	Task 4 - Zero-temperature LLG convergence . . . . .	30
5.5	Task 5 - stochastic LLG global convergence . . . . .	33
<b>6</b>	<b>Python API Documentation</b>	<b>37</b>
6.1	magpy.core module . . . . .	37
6.2	magpy.data module . . . . .	37
6.3	magpy.geometry package . . . . .	37
6.4	magpy.initial_conditions module . . . . .	40
6.5	magpy.model module . . . . .	40
6.6	magpy.results module . . . . .	44
<b>7</b>	<b>C++ API Documentation</b>	<b>49</b>
7.1	Namespace list . . . . .	49
7.2	File list . . . . .	65

7.3	Class list . . . . .	85
7.4	Struct list . . . . .	86
<b>8</b>	<b>Indices and tables</b>	<b>87</b>
	<b>Python Module Index</b>	<b>89</b>

The easiest way to install magpy is using the conda repositories. The only requirement is that you have anaconda or miniconda installed on your system. Alternatively, you can build the C++ and python code from source. You might want to do this if you only want the C++ library or if you would like to access the Intel accelerated code.

## 1.1 Conda

Note packages only exist for Linux and Mac OSX.

1. Go to <https://conda.io/miniconda.html> and download the Miniconda package manager
2. Create a new conda environment and install magpy into it:

```
$ conda create -n <env_name> python=3
$ source activate <env_name>
$ conda install -c owlas magpy
```

3. Launch python and import magpy

```
$ python
$ >>> import magpy
```

## 1.2 From source

The instructions below will guide you through the process of building the code from source on **Linux**.

1. Clone the magpy code

```
$ git clone https://github.com/owlas/magpy
```

2. You'll need a C++11 compatible compiler (g++>=4.9 recommended)

3. You will also the LAPACK and BLAS libraries. On Debian systems these can be obtained through the [apt repositories](#)

```
$ apt install liblapacke-dev
```

4. Build the magpy C++ library with with your compiler as <CXX>

```
$ cd magpy
$ make CXX=<CXX> libmoma.so
```

5. You can build and run the tests from the same makefile

```
$ cd magpy
$ make CXX=<CXX> run-tests
```

6. To build the python interface you'll need to obtain all the python dependencies in the `environment.yml` file. Install miniconda (see Conda, above)

```
$ conda create env -f environment.yml
$ source activate magpy
```

7. Once you have all of the dependencies you can install magpy

```
$ CXX=<CXX> pip install .
$ python
$ >>> import magpy
```

## 1.3 From source (Intel compilers)

Magpy has been optimised for Intel architectures and you can take advantage of this by taking a few extra steps:

1. Clone the magpy code

```
$ git clone https://github.com/owlas/magpy
```

2. Ensure you have the Intel compilers in your path (`icc` and `icpc`)
3. Tell magpy where to find your MKL files

```
$ export MKLROOT=/path/to/mkl/install/directory
```

4. You will also the LAPACK and BLAS libraries. On Debian systems these can be obtained through the [apt repositories](#)

```
$ apt install liblapacke-dev
```

5. Build the magpy C++ library with the intel compilers. The correct build flags should be taken care of for you

```
$ cd magpy
$ make CXX=icpc libmoma.so
```

6. You can build and run the tests from the same makefile

```
$ cd magpy
$ make CXX=icpc run-tests
```

7. To build the python interface you'll need to obtain all the python dependencies in the `environment.yml` file. Install miniconda (see Conda, above)

```
$ conda create env -f environment.yml  
$ source activate magpy
```

8. Once you have all of the dependencies you can install magpy

```
$ cd magpy  
$ CC=icc CXX=icpc pip install .  
$ python  
$ >>> import magpy
```





## CHAPTER 2

---

### Getting started - a single particle

---

In this tutorial, we'll simulate the stochastic dynamics of a single nanoparticle. We model clusters of nanoparticles using the `magpy.Model` class. In this case we only have a single particle in our cluster. The first step is to import `magpy`.

```
In [1]: import magpy as mp
```

To create our model, we need to specify the geometry and material properties of the system. The units and purpose of each property is defined below.

Name	Description	Units
Radius	The radius of the spherical particle	m
Anisotropy	Magnitude of the anisotropy	J/m <sup>3</sup>
Anisotropy axis	Unit vector indicating the direction of the anisotropy	•
Magnetisation	Saturation magnetisation of every particle in the cluster	A/m
Magnetisation direction	Unit vector indicating the initial direction of the magnetisation	•
Location	Location of the particle within the cluster	m
Damping	The damping constant of every particle in the cluster	•
Temperature	The ambient temperature of the cluster (fixed)	K

**Note:** radius, anisotropy, anisotropy\_axis, magnetisation\_direction, and location vary for each particle and must be specified as a list.

```
In [2]: single_particle = mp.Model(  
    radius = [12e-9],  
    anisotropy = [4e4],  
    anisotropy_axis = [[0., 0., 1.]],
```

```
magnetisation_direction = [[1., 0., 0.]],  
location = [[0., 0., 0.]],  
damping = 0.1,  
temperature = 300.,  
magnetisation = 400e3  
)
```

## 2.1 Simulate

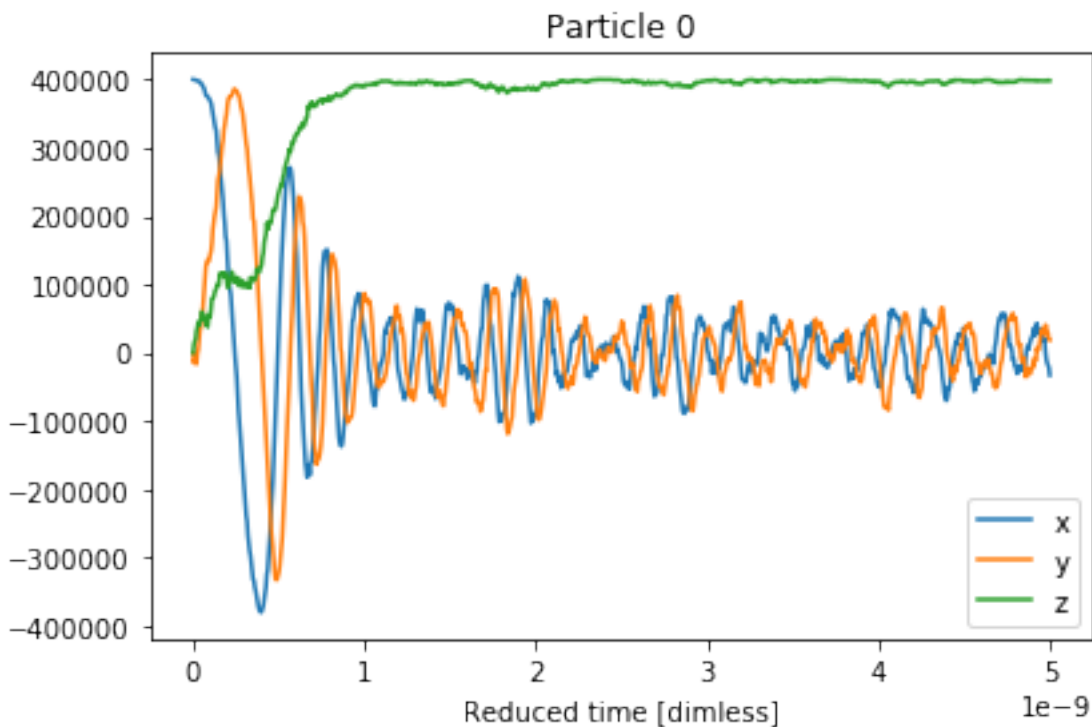
A simulation in magpy consists of simulating the magnetisation vector of the particle in time. In the model above we specified the initial magnetisation vector along the  $x$ -axis and the anisotropy along the  $z$ -axis. Since it is energetically favourable for the magnetisation to align with its anisotropy axis, we should expect the magnetisation to move toward the  $z$ -axis. With some random fluctuations.

The `simulate` function is called with the following parameters: - `end_time` the length of the simulation in seconds - `time_step` the time step of the integrator in seconds - `max_samples` in order to save memory, the output is down/upsampled as required. So if you simulate a billion steps, you can only save the state at 1000 regularly spaced intervals. - `seed` for reproducible simulations you should always choose the seed.

```
In [3]: results = single_particle.simulate(  
        end_time = 5e-9,  
        time_step = 1e-14,  
        max_samples=1000,  
        seed = 1001  
)
```

The  $x, y, z$  components of the magnetisation can be visualised with the `.plot()` function.

```
In [4]: results.plot()
```



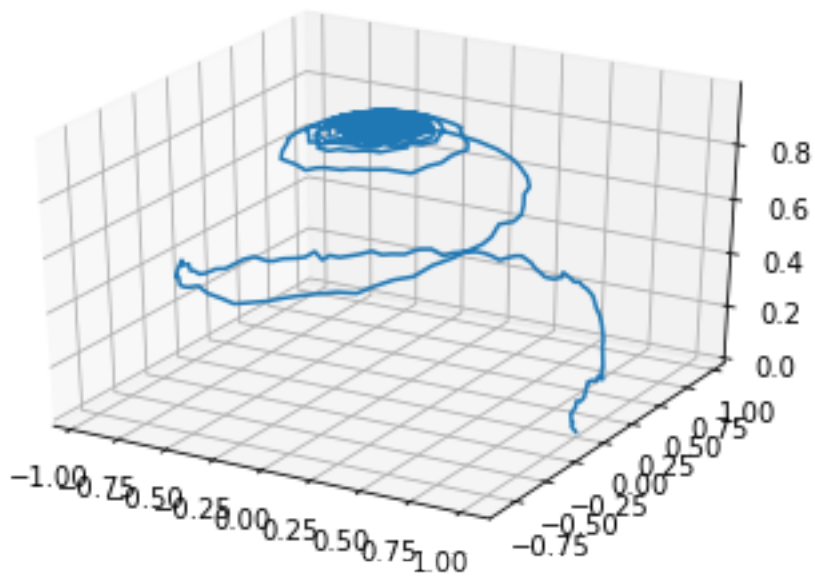
We can also access this data directly and plot it however we like! In this example, we normalise the magnetisation and plot it in 3d space.

```
In [5]: import matplotlib.pyplot as plt
        from mpl_toolkits.mplot3d import Axes3D
        %matplotlib inline

        Ms = 400e3
        time = results.time
        mx = results.x[0] / Ms # particle 0
        my = results.y[0] / Ms # particle 0
        mz = results.z[0] / Ms # particle 0

        fg = plt.figure()
        ax = fg.add_subplot(111, projection='3d')
        ax.plot3D(mx, my, mz)

Out[5]: [<mpl_toolkits.mplot3d.art3d.Line3D at 0x7f4f95319a58>]
```





---

## Thermal equilibrium of a single particle

---

In a large ensemble of identical systems each member will have a different state due to thermal fluctuations, even if all the systems were initialised in the same initial state.

As we integrate the dynamics of the ensemble we will have a distribution of states (i.e. the states of each member of the system). However, as the ensemble evolves, the distribution over the states eventually reaches a stationary distribution: the Boltzmann distribution. Even though the state of each member in the ensemble continues to fluctuate, the ensemble as a whole is in a statistical equilibrium (thermal equilibrium).

For an ensemble of single particles, we can compute the Boltzmann distribution by hand. In this example, we compare the analytical solution with the result of simulating an ensemble with Magpy.

### 3.1 Problem setup

A single particle has a uniaxial anisotropy axis  $K$  and a magnetic moment of three components (x,y,z components). The angle  $\theta$  is the angle between the magnetic moment and the anisotropy axis.

### 3.2 Boltzmann distribution

The Boltzmann distribution represents of states over the ensemble; here the state is the **solid angle**  $\phi = \sin(\theta)$  (i.e. the distribution over the surface of the sphere). The distribution is parameterised by the temperature of the system and the energy landscape of the problem.

$$p(\theta) = \frac{\sin(\theta)e^{-E(\theta)/(K_B T)}}{Z}$$

where  $Z$  is called the partition function:

$$Z = \int_{\theta} \sin(\theta)e^{-E(\theta)/(K_B T)} d\theta$$

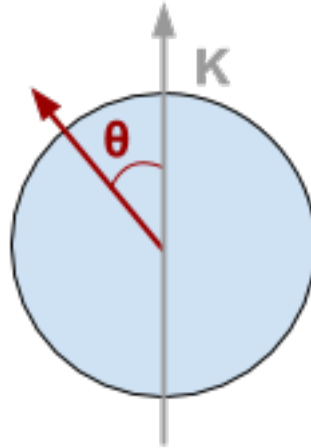


Fig. 3.1: Diagram of a single particle

## 3.3 Stoner-Wohlfarth model

The energy function for a single domain magnetic nanoparticle is given by the Stoner-Wohlfarth equation:

$$\frac{E(\theta)}{K_B T} = -\sigma \cos^2 \theta$$

where  $\sigma$  is called the normalised anisotropy strength:

$$\sigma = \frac{KV}{K_B T}$$

### 3.3.1 Functions for analytic solution

```
In [1]: import numpy as np

        # anisotropy energy of the system
        def anisotropy_e(theta, sigma):
            return -sigma*np.cos(theta)**2

In [2]: # numerator of the Boltzmann distribution
        # (i.e. without the partition function Z)
        def p_unorm(theta, sigma):
            return np.sin(theta)*np.exp(-anisotropy_e(theta, sigma))
```

We use the quadrature rule to numerically evaluate the partition function  $Z$ .

```
In [3]: from scipy.integrate import quad

        # The analytic Boltzmann distribution
        def boltzmann(thetas, sigma):
            Z = quad(lambda t: p_unorm(t, sigma), 0, thetas[-1])[0]
            distribution = np.array([
                p_unorm(t, sigma) / Z for t in thetas
            ])
            return distribution
```

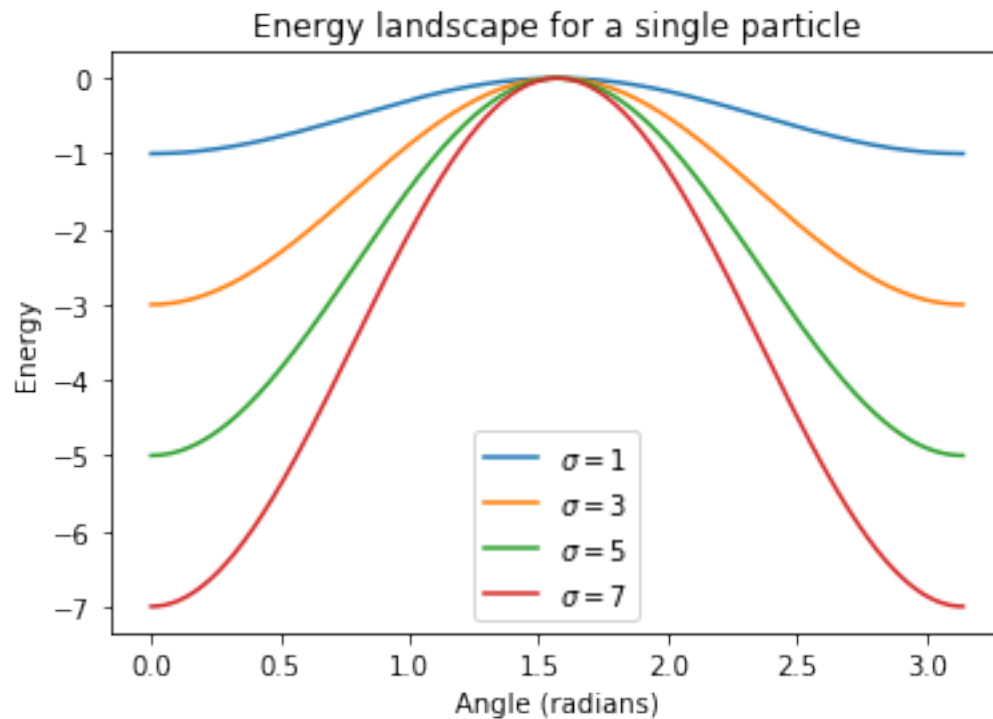
## Energy landscape

We can plot the energy landscape (energy as a function of the system variables)

```
In [4]: import matplotlib.pyplot as plt
        %matplotlib inline

In [5]: thetas = np.linspace(0, np.pi, 1000)
        sigmas = [1, 3, 5, 7]

        e_landscape = [anisotropy_e(thetas, s) for s in sigmas]
        for s, e in zip(sigmas, e_landscape):
            plt.plot(thetas, e, label='${\sigma}={}'.format(s))
        plt.legend(); plt.xlabel('Angle (radians)'); plt.ylabel('Energy')
        plt.title('Energy landscape for a single particle');
```



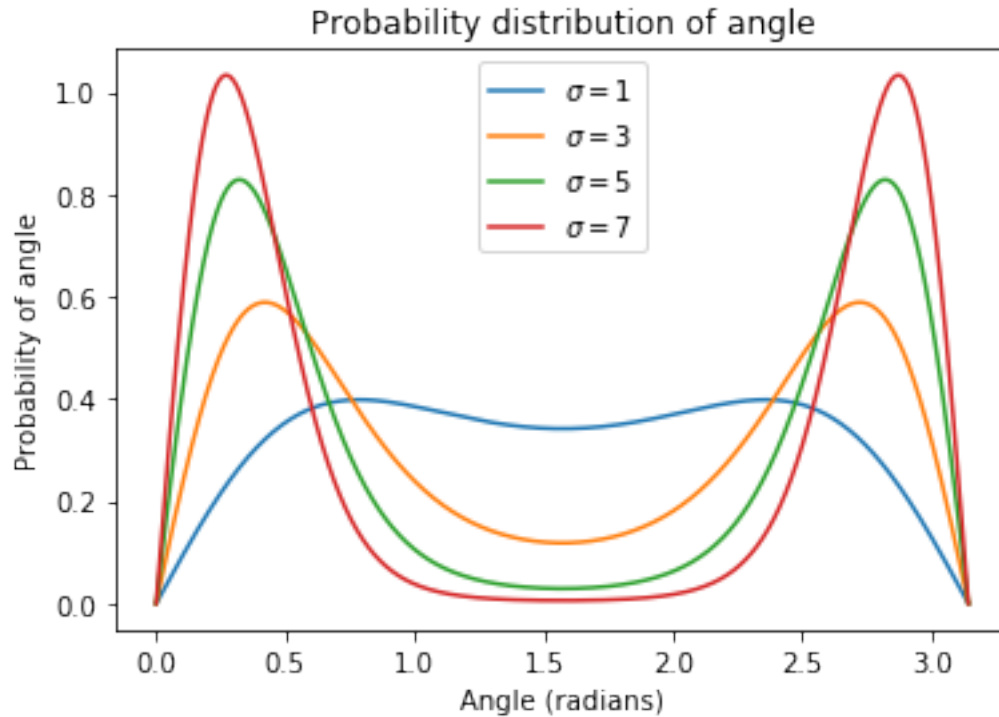
We observe that: - The energy of the system has two minima: one alongside each direction of the anisotropy axis. - The minima are separated by a maxima: perpendicular to the anisotropy axis. - Stronger anisotropy increases the size of the energy barrier between the two minima.

## Equilibrium distribution (Boltzmann)

We can also plot the equilibrium distribution of the system, which is the probability distribution over the system states in a large ensemble of systems.

```
In [6]: p_dist = [boltzmann(thetas, s) for s in sigmas]

        for s, p in zip(sigmas, p_dist):
            plt.plot(thetas, p, label='${\sigma}={}'.format(s))
        plt.legend(); plt.xlabel('Angle (radians)')
        plt.ylabel('Probability of angle')
        plt.title('Probability distribution of angle');
```



What does this mean? If we had an ensemble of single particles, the distribution of the states of those particles varies greatly depending on  $\sigma$ . Remember we can decrease  $\sigma$  by reducing the anisotropy strength or particle size or by increasing the temperature. - When  $\sigma$  is high, most of the particles in the ensemble will be found closely aligned with the anisotropy axis. - When  $\sigma$  is low, the states of the particles are more evenly distributed.

### 3.3.2 Magpy equilibrium

Using Magpy, we can simulate the dynamics of the state of a single nanoparticle. If we simulate a large ensemble of these systems for ‘long enough’, the distribution of states will reach equilibrium. If Magpy is implemented correctly, we should recover the analytical distribution from above.

#### Set up the model

Select the parameters for the single particle

```
In [7]: import magpy as mp

# These parameters will determine the distribution
K = 1e5
r = 7e-9
T = 300
kdir = [0., 0., 1.]

# These parameters affect the dynamics but
# have no effect on the equilibrium
Ms = 400e3
location = [0., 0., 0.]
alpha=1.0
initial_direction = [0., 0., 1.]
```



```

# Normalised anisotropy strength KV/KB/T
V = 4./3 * np.pi * r**3
kb = mp.core.get_KB()
sigma = K * V / kb / T
print(sigma)

```

```
34.68792671050298
```

```
In [8]: import magpy as mp
```

```

single_particle = mp.Model(
    anisotropy=[K],
    anisotropy_axis=[kdir],
    damping=alpha,
    location=[location],
    magnetisation=Ms,
    magnetisation_direction=[initial_direction],
    radius=[r],
    temperature=T
)

```

### Create an ensemble

From the single particle we create an ensemble of 10,000 identical particles.

```

In [9]: particle_ensemble = mp.EnsembleModel(
    base_model=single_particle, N=10000
)

```

### Simulate

Now we simulate! We don't need to simulate for very long because  $\sigma$  is very high and the system will reach equilibrium quickly.

```

In [10]: res = particle_ensemble.simulate(
    end_time=1e-9, time_step=1e-12, max_samples=50,
    random_state=1001, implicit_solve=True
)

```

```

[Parallel(n_jobs=1)]: Done    1 out of   1 | elapsed:    0.0s remaining:    0.0s
[Parallel(n_jobs=1)]: Done    2 out of   2 | elapsed:    0.0s remaining:    0.0s
[Parallel(n_jobs=1)]: Done    3 out of   3 | elapsed:    0.1s remaining:    0.0s
[Parallel(n_jobs=1)]: Done    4 out of   4 | elapsed:    0.1s remaining:    0.0s
[Parallel(n_jobs=1)]: Done 10000 out of 10000 | elapsed:  3.1min finished

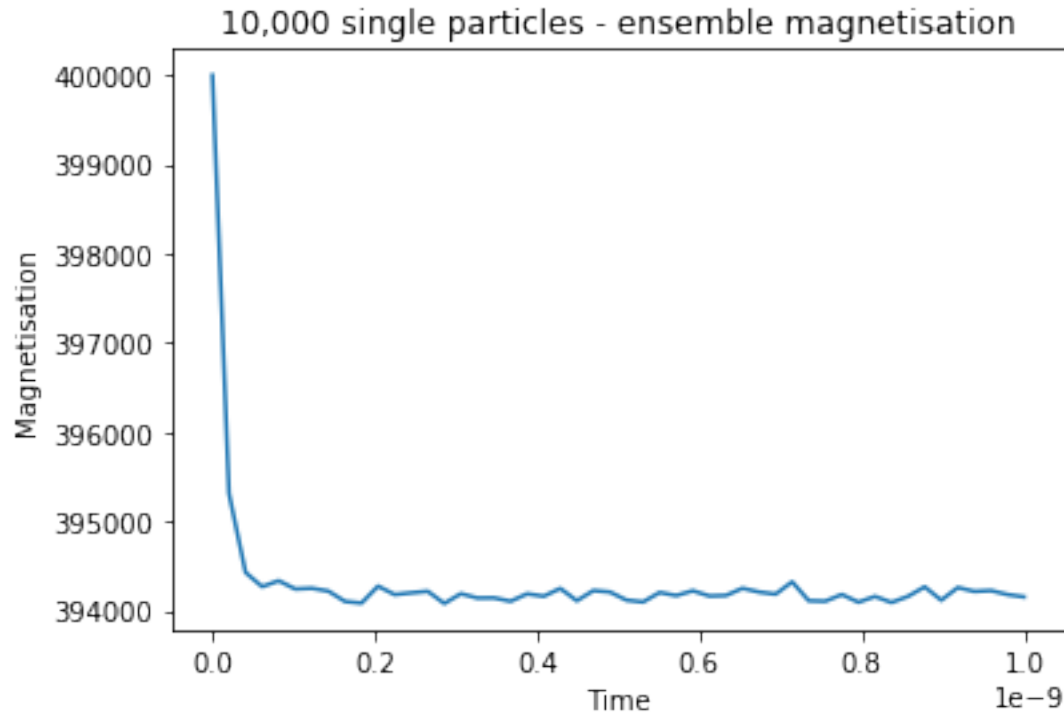
```

### Check that we have equilibrated

```

In [11]: plt.plot(res.time, res.ensemble_magnetisation())
    plt.title('10,000 single particles - ensemble magnetisation')
    plt.xlabel('Time'); plt.ylabel('Magnetisation');

```



We can see that the system has reached a local minima. We could let the simulation run until the ensemble relaxes into both minima but it would take a very long time because the energy barrier is so high in this example.

### Compute theta

The results of the simulation are x,y,z coordinates of the magnetisation of each particle in the ensemble. We need to convert these into angles.

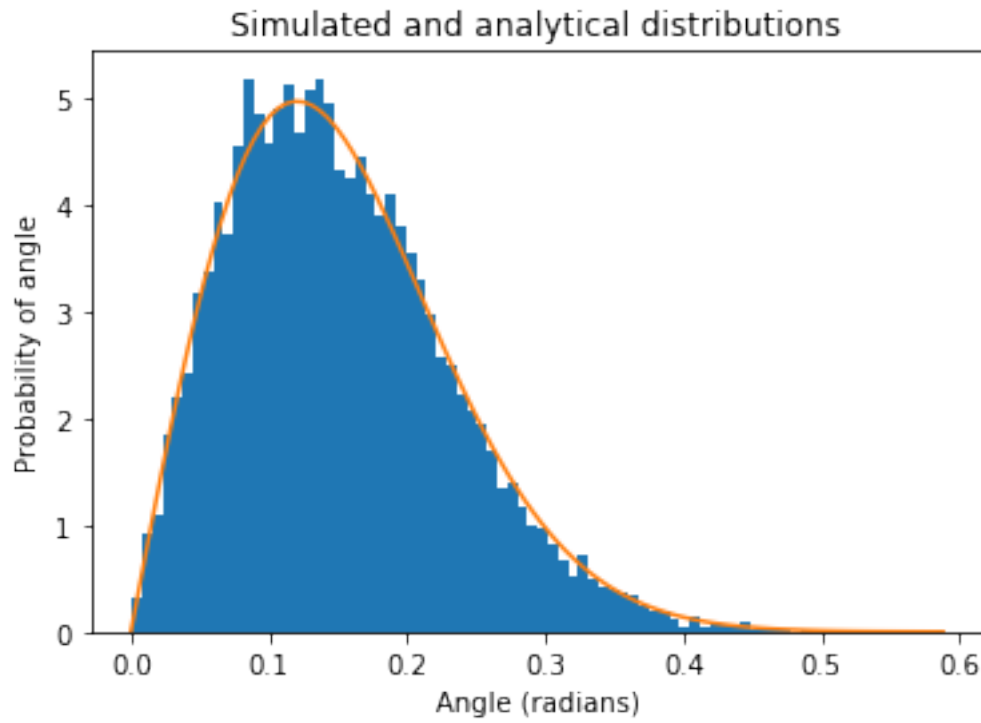
```
In [12]: M_z = np.array([state['z'][0] for state in res.final_state()])
         m_z = M_z / Ms
         simulated_thetas = np.arccos(m_z)
```

### Compare to analytical solution

Now we compare our empirical distribution of states to the analytical distribution that we computed above.

```
In [13]: theta_grid = np.linspace(0.0, simulated_thetas.max(), 100)
         analytical_probability = boltzmann(theta_grid, sigma)

         plt.hist(simulated_thetas, normed=True, bins=80, label='Simulated');
         plt.plot(theta_grid, analytical_probability, label='Analytical')
         plt.title('Simulated and analytical distributions')
         plt.xlabel('Angle (radians)'); plt.ylabel('Probability of angle');
```



The results look good! We could simulate an even bigger ensemble to produce a smoother empirical distribution.



## Two particle equilibrium

If you haven't read the `One particle equilibrium` notebook yet, go and read it now.

In the previous notebook we showed that we can use Magpy to compute the correct thermal equilibrium for a single particle. However, we also need to check that the interactions are correctly implemented by simulating the thermal equilibrium of multiple interacting particles.

In this notebook we'll simulate an ensemble of two particle systems with Magpy. Instead of computing the distribution analytically, we will use the Metropolis Markov-Chain Monte-Carlo technique to generate the correct equilibrium.

### Acknowledgements

Many thanks to [Jonathon Waters](#) for the terse python implementation of the Metropolis algorithm!

### Problem setup

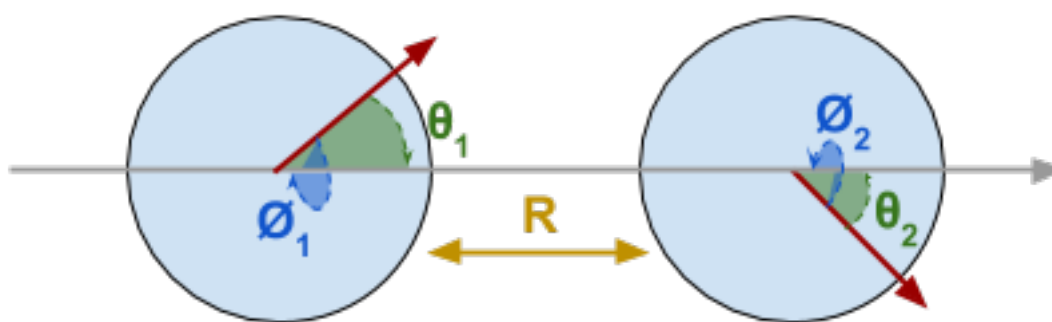


Fig. 4.1: Diagram of two anisotropy-aligned particles

In this example the system comprises two identical particles separated by a distance  $R$ . The particles have their anisotropy axes in the same direction. We are interested in the following four variables: the angle between the particle's moments and the anisotropy axis  $\theta_1, \theta_2$  and the rotational (azimuth) angle of the particles around the anisotropy axis  $\phi_1, \phi_2$

### Modules

```
In [1]: import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import axes3d
from tqdm import tqdm_notebook
#import tqdm
import magpy as mp
%matplotlib inline
```

## 4.1 Metropolis MCMC

### 4.1.1 Energy terms

#### Anisotropy

The energy contribution from the anisotropy of a single particle  $i$  is:

$$E_i^a = V_i \vec{K}_i \cdot \vec{m}_i$$

```
In [2]: def e_anisotropy(moments, anisotropy_axes, V, K, particle_id):
cos_t = np.sum(moments[particle_id, :] * anisotropy_axes[particle_id, :])
return -K * V * cos_t ** 2
```

#### Dipolar interaction energy

The energy contribution from  $N$  particles  $j = 1, 2, \dots, N$  interacting with a single particle  $i$ :

$$E_i^d = \sum_j \frac{V_i^2 M_s^2 \mu_0 (3(\vec{m}_i \cdot \vec{r}_{ij})(\vec{m}_j \cdot \vec{r}_{ij}) - \vec{m}_i \cdot \vec{m}_j)}{4\pi |r|^3}$$

```
In [3]: def e_dipole(moments, positions, Ms, V, particle_id):
mu_0 = mp.core.get_mu0()
mask = np.ones(moments.shape[0], dtype=bool)
mask[particle_id] = False
rs = positions[mask] - positions[particle_id, :]
mod_rs = np.linalg.norm(rs, axis=1)
rs[:, 0] = rs[:, 0] / mod_rs
rs[:, 1] = rs[:, 1] / mod_rs
rs[:, 2] = rs[:, 2] / mod_rs
m1_m2 = np.sum(moments[particle_id, :] * moments[mask], axis=1)
m1_r = np.sum(moments[particle_id, :] * rs, axis=1)
m2_r = np.sum(moments[mask] * rs, axis=1)
numer = (V**2) * (Ms**2) * mu_0 * (3 * m1_r * m2_r - m1_m2)
denom = 4 * np.pi * np.power(mod_rs, 3)
return -np.sum(numer / denom)
```

#### Total energy

The total energy contribution from a single particle in the ensemble is:

$$E_i = E_i^a + E_i^d$$

```
In [4]: def e_total(moments, positions, anisotropy_axes, Ms, V, K, particle_id):
        return (
            e_dipole(moments, positions, Ms, V, particle_id)
            + e_anisotropy(moments, anisotropy_axes, V, K, particle_id)
        )
```

### 4.1.2 The Monte-Carlo algorithm

1. Initialise each spin in the system
2. Randomly choose a particle in the system and change it's orientation
3. Compute  $\Delta E$  the change in total energy arising from changing the particle orientation
4. if
  - $\Delta E < 0$  then we accept the new state and store it
  - $\Delta E > 0$  we accept the new state and store it with probability  $p = e^{\Delta E/(K_B T)}$
  - otherwise we reject the new state
5. Return to 2 until desired number of samples

Once we run this loop many times, we'll have a list of accepted samples of the system state. The distribution of this ensemble of states is **guaranteed** to converge to the true distribution. Monte-Carlo is much faster than numerical integration methods when we have many particles.

```
In [5]: def sphere_point():
        theta = 2*np.pi*np.random.rand()
        phi = np.arccos(1-2*np.random.rand())
        return np.array([np.sin(phi)*np.cos(theta), np.sin(phi)*np.sin(theta), np.cos(phi)])

def MH(positions, ani_axis, spins, Neq, Nsamps, SampRate, Ms, V, K, T, seed=42):
    np.random.seed(seed)
    k_b = mp.core.get_KB()
    test = np.copy(spins)
    Ntot = Neq+Nsamps*SampRate
    Out = np.zeros([spins.shape[0], spins.shape[1], Nsamps])
    ns = 0
    for n in tqdm_notebook(range(Ntot)):
        # pick a random spin
        i = int(np.random.rand(1)*positions.shape[0])
        # pick a random dir
        test[i, :] = sphere_point()
        dE = e_total(test, positions, ani_axis, Ms, V, K, i) - \
            e_total(moments, positions, ani_axis, Ms, V, K, i)
        if(np.random.rand(1) < np.exp(-dE/(k_b*T))):
            spins[i, :] = test[i, :]
        else:
            test[i, :] = spins[i, :]
        if (n >= Neq and (n-Neq)%SampRate == 0):
            Out[:, :, ns] = np.copy(spins)
            ns += 1
    return Out
```

### 4.1.3 Parameter set up

Now we set the parameters for the two particle system. Both particles are identical and have their anisotropy axes aligned with the  $z$  direction.

```
In [6]: N = 2 # Two particles
        T = 330 # temperature
        K = 1e5 # anisotropy strength
        R = 9e-9 # distance between two particles
        r = 7e-9 # radius of the particles
        V = 4./3 * np.pi * r**3 # volume of particle
        Ms = 4e5 # saturation magnetisation

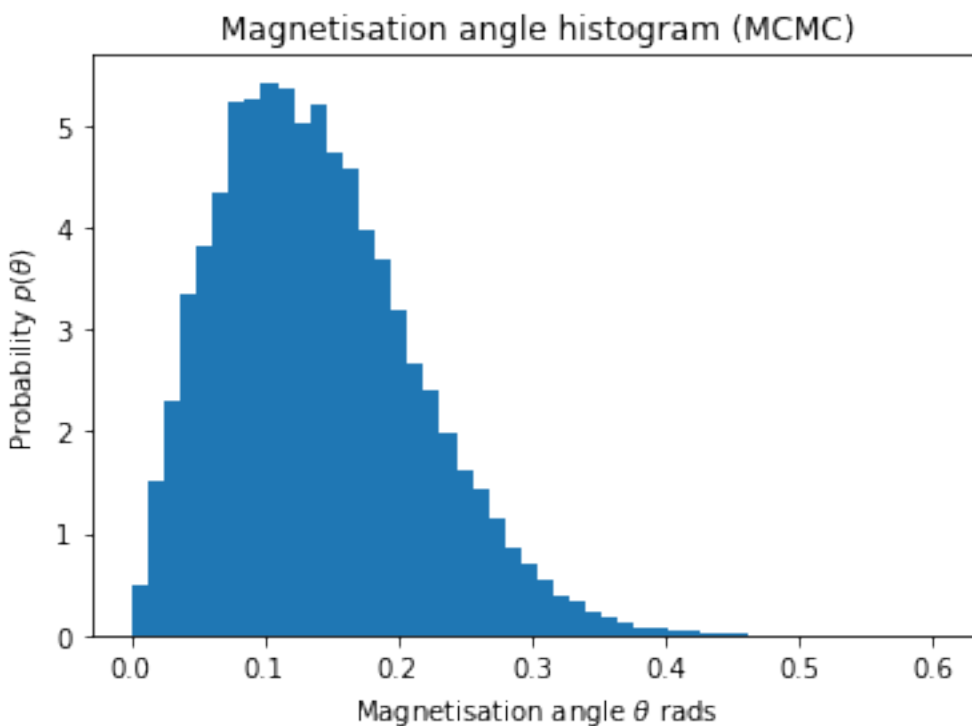
        #                particle 1    particle 2
        positions = np.array([[0., 0., 0.], [0., 0., R]])
        moments = np.array([sphere_point(), sphere_point()])
        anisotropy_axes = np.array([[0., 0., 1.], [0., 0., 1.]])
```

### 4.1.4 Run the MCMC sampler!

This will take some time

```
In [7]: output = MH(positions, anisotropy_axes, moments, 100000, 600000, 20, Ms, V, K, T, 0)
```

```
In [9]: thetas = np.arccos(output[:, 2, :])
        plt.hist(thetas[0], bins=50, normed=True)
        plt.title('Magnetisation angle histogram (MCMC)')
        plt.xlabel('Magnetisation angle  $\theta$  rads')
        plt.ylabel('Probability  $p(\theta)$ ');
```





## 4.2 Magpy - Dynamical Simulation

We now use Magpy to simulate a large ensemble of the identical two-particle system. Once the ensemble has reached a stationary distribution, we determine the distribution of magnetisation angles over the ensemble. We expect this distribution to match the equilibrium distribution determined by the MCMC sampler.

### 4.2.1 Define the Magpy model

```
In [10]: # additionally we must specify damping
        alpha = 0.1

        # We build a model of the two particles
        base_model = mp.Model(
            anisotropy=[K,K],
            anisotropy_axis=anisotropy_axes,
            damping=alpha,
            location=positions,
            magnetisation=Ms,
            magnetisation_direction=moments,
            radius=[r, r],
            temperature=T
        )

        # Create an ensemble of 50,000 identical models
        ensemble = mp.EnsembleModel(50000, base_model)
```

### 4.2.2 Simulate the ensemble!

Now we run the dynamical simulation using an implicit solver. Each model is simulated for 1ns.

```
In [11]: res = ensemble.simulate(end_time=1e-9, time_step=1e-12,
                                max_samples=500, random_state=1002,
                                n_jobs=-1, implicit_solve=True,
                                interactions=True)
```

```
[Parallel(n_jobs=-1)]: Done   2 tasks      | elapsed:    0.1s
[Parallel(n_jobs=-1)]: Done 176 tasks      | elapsed:    1.9s
[Parallel(n_jobs=-1)]: Done 536 tasks      | elapsed:    5.8s
[Parallel(n_jobs=-1)]: Done 1040 tasks     | elapsed:   11.5s
[Parallel(n_jobs=-1)]: Done 1688 tasks     | elapsed:   18.9s
[Parallel(n_jobs=-1)]: Done 2480 tasks     | elapsed:   27.4s
[Parallel(n_jobs=-1)]: Done 3416 tasks     | elapsed:   37.3s
[Parallel(n_jobs=-1)]: Done 4496 tasks     | elapsed:   48.5s
[Parallel(n_jobs=-1)]: Done 5720 tasks     | elapsed:   1.0min
[Parallel(n_jobs=-1)]: Done 7088 tasks     | elapsed:   1.3min
[Parallel(n_jobs=-1)]: Done 8600 tasks     | elapsed:   1.5min
[Parallel(n_jobs=-1)]: Done 10256 tasks    | elapsed:   1.8min
[Parallel(n_jobs=-1)]: Done 12056 tasks    | elapsed:   2.2min
[Parallel(n_jobs=-1)]: Done 14000 tasks    | elapsed:   2.5min
[Parallel(n_jobs=-1)]: Done 16088 tasks    | elapsed:   2.9min
[Parallel(n_jobs=-1)]: Done 18320 tasks    | elapsed:   3.3min
[Parallel(n_jobs=-1)]: Done 20696 tasks    | elapsed:   3.7min
[Parallel(n_jobs=-1)]: Done 23216 tasks    | elapsed:   4.1min
[Parallel(n_jobs=-1)]: Done 25880 tasks    | elapsed:   4.6min
[Parallel(n_jobs=-1)]: Done 28688 tasks    | elapsed:   5.1min
[Parallel(n_jobs=-1)]: Done 31640 tasks    | elapsed:   5.6min
```

```
[Parallel(n_jobs=-1)]: Done 34736 tasks      | elapsed: 6.2min
[Parallel(n_jobs=-1)]: Done 37976 tasks      | elapsed: 6.8min
[Parallel(n_jobs=-1)]: Done 41360 tasks      | elapsed: 7.4min
[Parallel(n_jobs=-1)]: Done 44888 tasks      | elapsed: 8.0min
[Parallel(n_jobs=-1)]: Done 48560 tasks      | elapsed: 8.7min
[Parallel(n_jobs=-1)]: Done 50000 out of 50000 | elapsed: 8.9min finished
```

### 4.2.3 Compute the final state

We use the `Results.final_state()` function to determine the state of each member of the ensemble after 1ns of simulation. The magnetisation angle is computed as the cosine of the  $z$ -axis component of magnetisation.

```
In [12]: m_z0 = np.array([state['z'][0] for state in res.final_state()])/Ms
        m_z1 = np.array([state['z'][1] for state in res.final_state()])/Ms
        theta0 = np.arccos(m_z0)
        theta1 = np.arccos(m_z1)
```

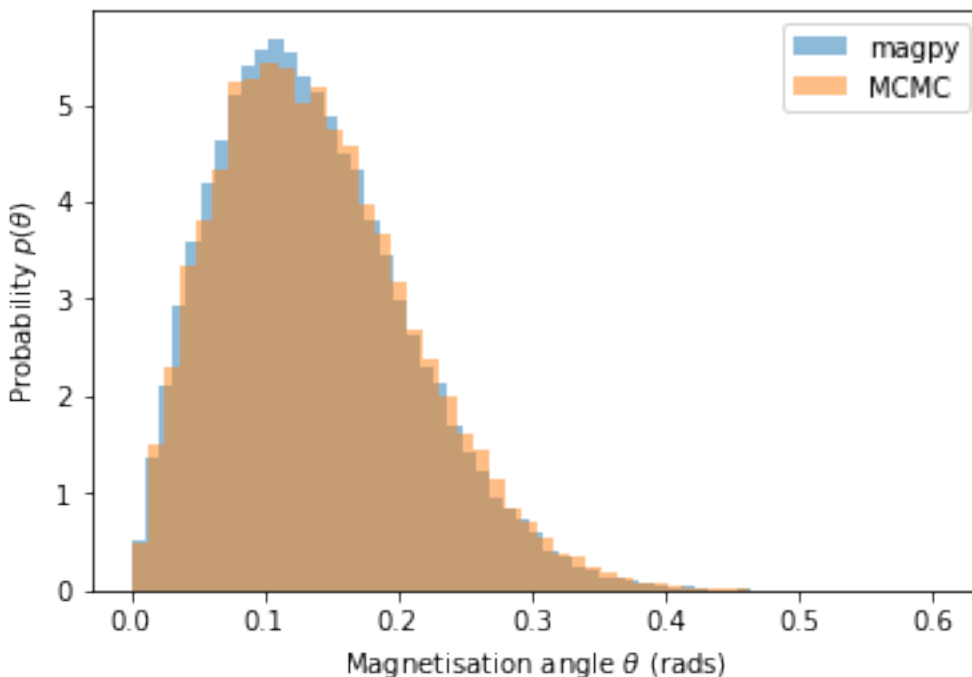
---

## 4.3 Compare results

### 4.3.1 Single variable comparison

Below we compare the magnetisation angle distribution for a single particle as simulated with Magpy and the MCMC algorithm.

```
In [13]: plt.hist(theta0, bins=50, alpha=0.5, normed=True, label='magpy')
        plt.hist(thetas[0], bins=50, alpha=0.5, normed=True, label='MCMC')
        plt.legend();
        plt.xlabel('Magnetisation angle  $\theta$  (rads)')
        plt.ylabel('Probability  $p(\theta)$ ');
```

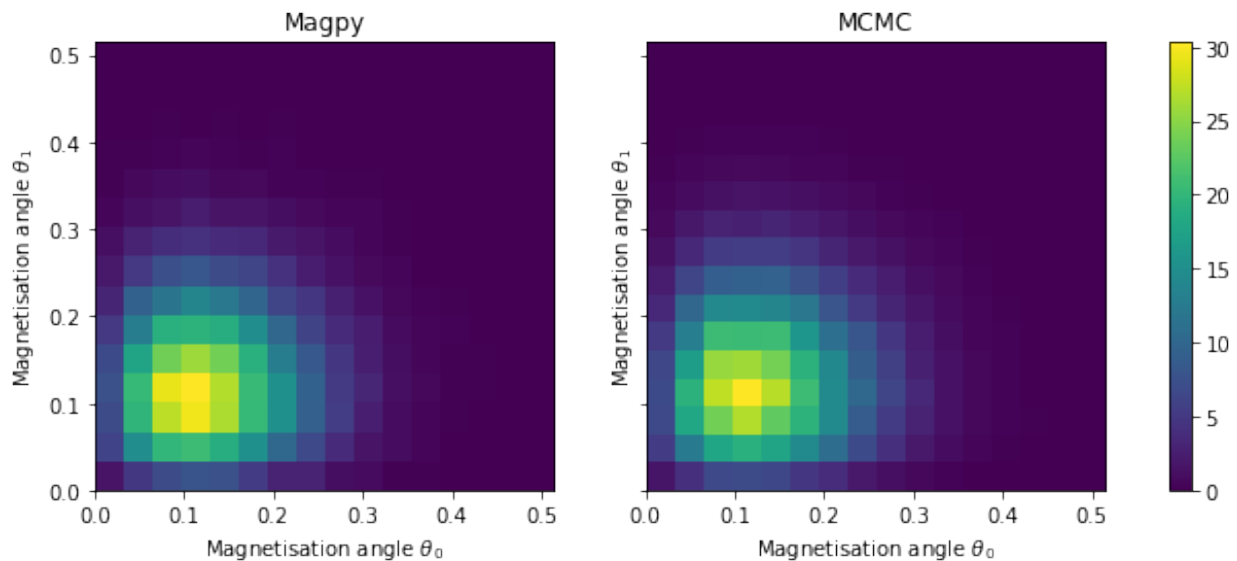


The results look to be a good match!

### 4.3.2 Join distribution comparison

Below we compare the joint distribution of  $\theta_0$  and  $\theta_1$  (the magnetisation angle of both particles). In other words, this is the probability distribution over the entire state space. It is important to compare the joint distributions because the two particles interact with one another, creating a dependence between the two magnetisation angles.

```
In [26]: fg, axs = plt.subplots(ncols=2, figsize=(11,4), sharey=True)
         histdat = axs[0].hist2d(theta0, theta1, bins=16, normed=True)
         axs[1].hist2d(thetas[0], thetas[1], bins=histdat[1], normed=True);
         for ax, title in zip(axs, ['Magpy', 'MCMC']):
             ax.set_xlabel('Magnetisation angle  $\theta_0$ ')
             ax.set_ylabel('Magnetisation angle  $\theta_1$ ')
             ax.set_title(title)
         fg.colorbar(histdat[3], ax=axs.tolist());
```



#### Alternatively compare using a kernel density function

An alternative method to visually compare the two distributions is to construct a kernel density estimation one set of results and overlay it on a histogram of the other.

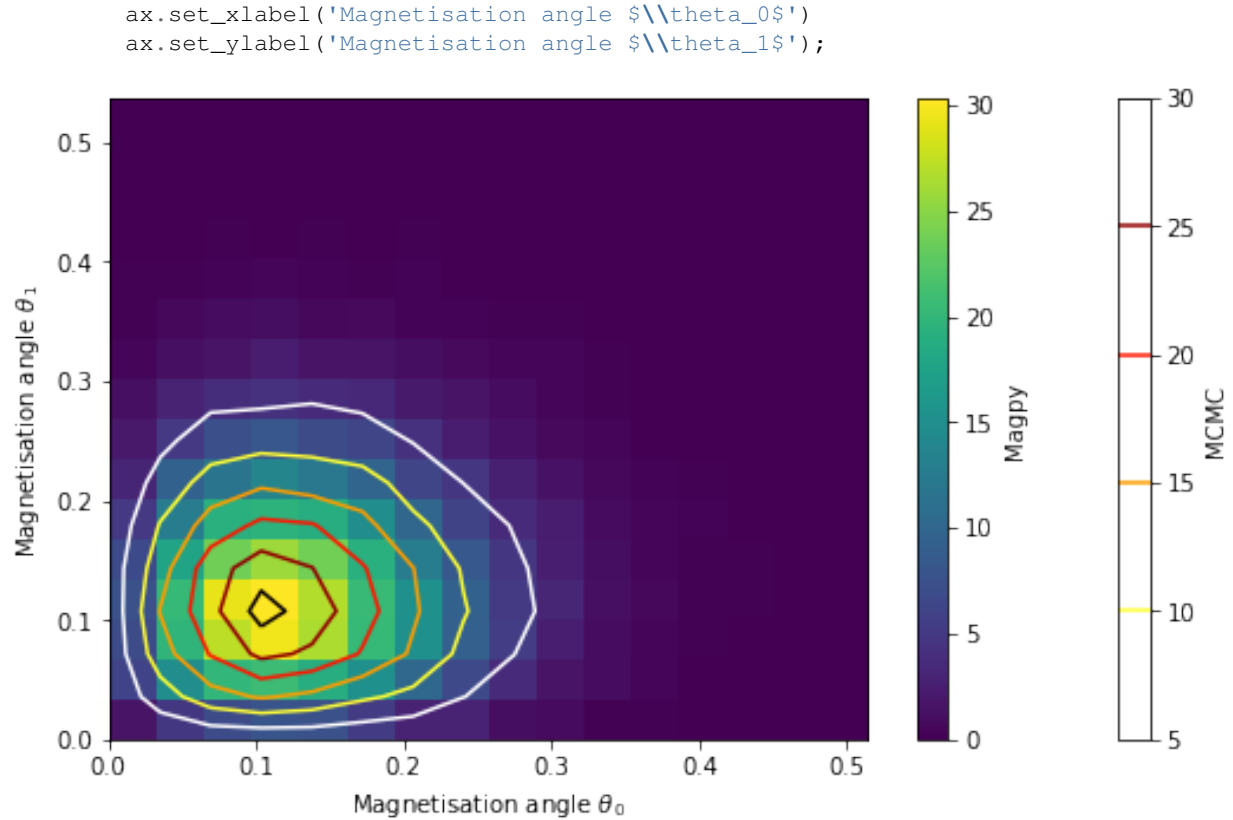
```
In [27]: from scipy.stats import gaussian_kde
         kde = gaussian_kde(thetas)

         tgrid_x = np.linspace(theta0.min(), theta0.max(), 16)
         tgrid_y = np.linspace(theta1.min(), theta1.max(), 16)
         tgrid_x, tgrid_y = np.meshgrid(tgrid_x, tgrid_y)
         Z = np.reshape(kde(np.vstack([tgrid_x.ravel(), tgrid_y.ravel()])), T, tgrid_x.shape)

In [57]: fg, ax = plt.subplots(figsize=(9,5))

         hist = ax.hist2d(theta0, theta1, bins=16, normed=True)
         contour = ax.contour(tgrid_x, tgrid_y, Z, cmap='hot_r')

         fg.colorbar(contour, label='MCMC')
         fg.colorbar(hist[3], label='Magpy')
```



## 4.4 Sanity check: no interactions

To ensure that the interactions are having a significant effect on the joint distribution, we simulate the same system but disable the interaction false (simply set `interactions=False`).

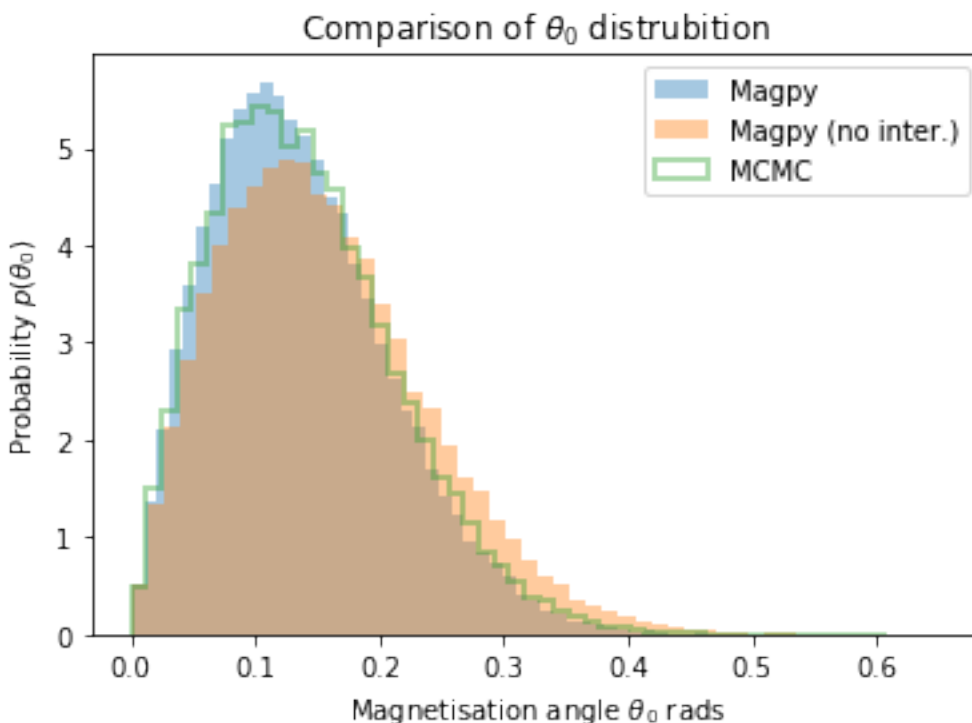
```
In [58]: res_noi = ensemble.simulate(end_time=1e-9, time_step=1e-12,
                                     max_samples=500, random_state=1002,
                                     n_jobs=-1, implicit_solve=True,
                                     interactions=False)

m_z0 = np.array([state['z'][0] for state in res_noi.final_state()])/Ms
m_z1 = np.array([state['z'][1] for state in res_noi.final_state()])/Ms
theta0_noi = np.arccos(m_z0)
theta1_noi = np.arccos(m_z1)
```

[Parallel(n_jobs=-1)]: Done 2 tasks	elapsed:	0.1s
[Parallel(n_jobs=-1)]: Done 176 tasks	elapsed:	1.6s
[Parallel(n_jobs=-1)]: Done 536 tasks	elapsed:	4.7s
[Parallel(n_jobs=-1)]: Done 1040 tasks	elapsed:	8.9s
[Parallel(n_jobs=-1)]: Done 1688 tasks	elapsed:	14.2s
[Parallel(n_jobs=-1)]: Done 2480 tasks	elapsed:	20.7s
[Parallel(n_jobs=-1)]: Done 3416 tasks	elapsed:	28.4s
[Parallel(n_jobs=-1)]: Done 4496 tasks	elapsed:	37.2s
[Parallel(n_jobs=-1)]: Done 5720 tasks	elapsed:	47.4s
[Parallel(n_jobs=-1)]: Done 7088 tasks	elapsed:	58.5s
[Parallel(n_jobs=-1)]: Done 8600 tasks	elapsed:	1.2min
[Parallel(n_jobs=-1)]: Done 10256 tasks	elapsed:	1.4min
[Parallel(n_jobs=-1)]: Done 12056 tasks	elapsed:	1.7min

```
[Parallel(n_jobs=-1)]: Done 14000 tasks      | elapsed: 2.0min
[Parallel(n_jobs=-1)]: Done 16088 tasks      | elapsed: 2.3min
[Parallel(n_jobs=-1)]: Done 18320 tasks      | elapsed: 2.6min
[Parallel(n_jobs=-1)]: Done 20696 tasks      | elapsed: 2.9min
[Parallel(n_jobs=-1)]: Done 23216 tasks      | elapsed: 3.3min
[Parallel(n_jobs=-1)]: Done 25880 tasks      | elapsed: 3.6min
[Parallel(n_jobs=-1)]: Done 28688 tasks      | elapsed: 4.0min
[Parallel(n_jobs=-1)]: Done 31640 tasks      | elapsed: 4.5min
[Parallel(n_jobs=-1)]: Done 34736 tasks      | elapsed: 4.9min
[Parallel(n_jobs=-1)]: Done 37976 tasks      | elapsed: 5.4min
[Parallel(n_jobs=-1)]: Done 41360 tasks      | elapsed: 5.9min
[Parallel(n_jobs=-1)]: Done 44888 tasks      | elapsed: 6.4min
[Parallel(n_jobs=-1)]: Done 48560 tasks      | elapsed: 6.9min
[Parallel(n_jobs=-1)]: Done 50000 out of 50000 | elapsed: 7.1min finished
```

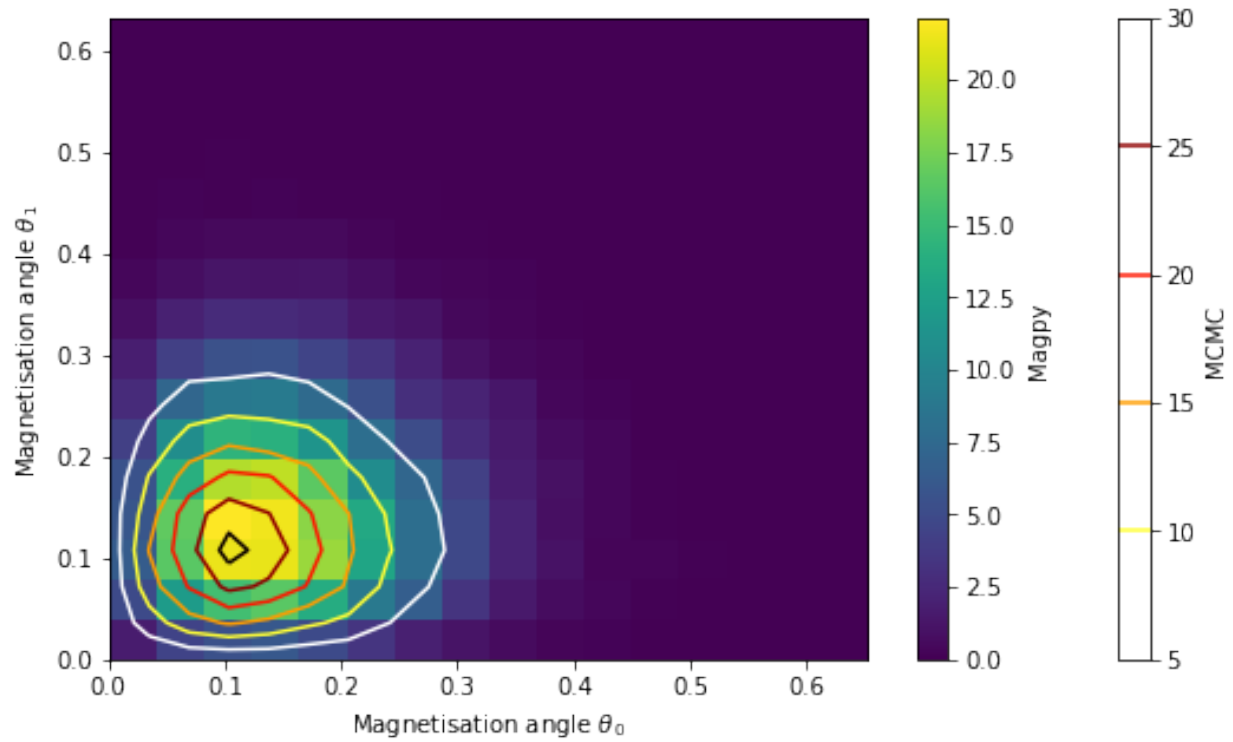
```
In [63]: plt.hist(theta0, bins=50, normed=True, alpha=0.4, label='Magpy')
plt.hist(theta0_noi, bins=50, normed=True, alpha=0.4, label='Magpy (no inter.)');
plt.hist(thetas[0], bins=50, histtype='step', lw=2, normed=True, alpha=0.4, label='MCMC')
plt.legend();
plt.xlabel('Magnetisation angle  $\theta_0$  rads')
plt.ylabel('Probability  $p(\theta_0)$ ');
plt.title('Comparison of  $\theta_0$  distrubition');
```



```
In [66]: fg, ax = plt.subplots(figsize=(9,5))

hist = ax.hist2d(theta0_noi, thetal_noi, bins=16, normed=True)
contour = ax.contour(tgrid_x, tgrid_y, Z, cmap='hot_r')

fg.colorbar(contour, label='MCMC')
fg.colorbar(hist[3], label='Magpy')
ax.set_xlabel('Magnetisation angle  $\theta_0$ ')
ax.set_ylabel('Magnetisation angle  $\theta_1$ ');
```



The results show that the distributions clearly deviate when we ignore interactions.

---

## Convergence Tests

---

In this notebook, we visualise the results from the magpy convergence tests. These tests ensure that the numerical methods are implemented correctly.

**Running the tests** Before executing this notebook, you'll need to run the convergence tests. In order to do this you must: 1. Clone the Magpy repository at <https://github.com/owlas/magpy> 2. Compile the Magpy library 3. Compile and run the convergence tests: - cd /path/to/magpy/directory - make libmoma.so - make test/convergence/run

```
In [1]: import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline

datapath = '../.../test/convergence/output/'
```

### 5.1 Task 1 - 1D non-stiff SDE

We simulate the following 1-dimensional SDE, which has an analytic solution

$$dX(t) = aX(t)dt + bX(t)dW(t)$$

- $a = -1.0$
- $b = 1.0$

```
In [2]: # load results
path = datapath + 'task1/'
files = !ls {path}
results = {name: np.fromfile(path + name) for name in files if name!='dt'}
dts = np.fromfile(path + 'dt')
```

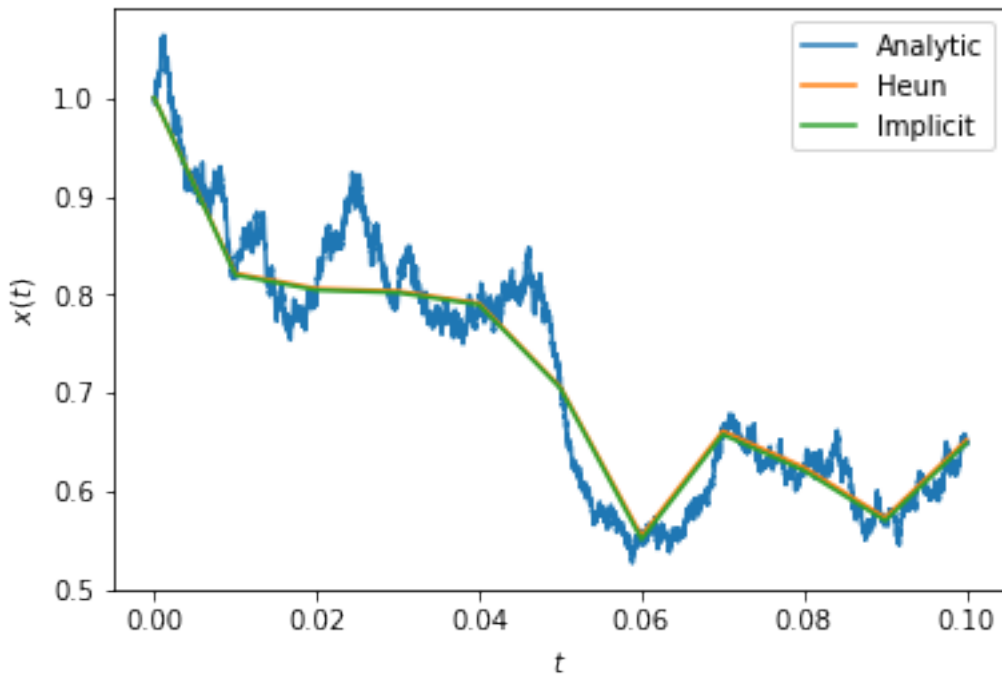
```
In [3]: tvecs = {
    i: dts[i] * np.arange(len(results['heun'+str(i)]))
    for i in range(len(dts))
}
```

The following plot shows  $x(t)$  for: - analytic - Heun with large time step - implicit with large time step

Both methods look accurate

```
In [4]: plt.plot(tvecs[0], results['true'], label='Analytic')
plt.plot(tvecs[3], results['heun3'], label='Heun')
plt.plot(tvecs[3], results['implicit3'], label='Implicit')
plt.xlabel('$t$'); plt.ylabel('$x(t)$'); plt.legend()
```

```
Out[4]: <matplotlib.legend.Legend at 0x7f58a13b4dd8>
```



## 5.2 Task 2 - 1D stiff SDE

We introduce stiffness into the 1D problem in order to compare the explicit (Heun) and implicit methods. This is done here by creating a large separation in timescales (the deterministic dynamics are fast, the random dynamics are slow).

$$dX(t) = aX(t)dt + bX(t)dW(t)$$

- $a = -20.0$
- $b = 5.0$

```
In [5]: # load results
path = datapath + 'task2/'
files = !ls {path}
results = {name: np.fromfile(path + name) for name in files if name!='dt'}
dts = np.fromfile(path + 'dt')
```

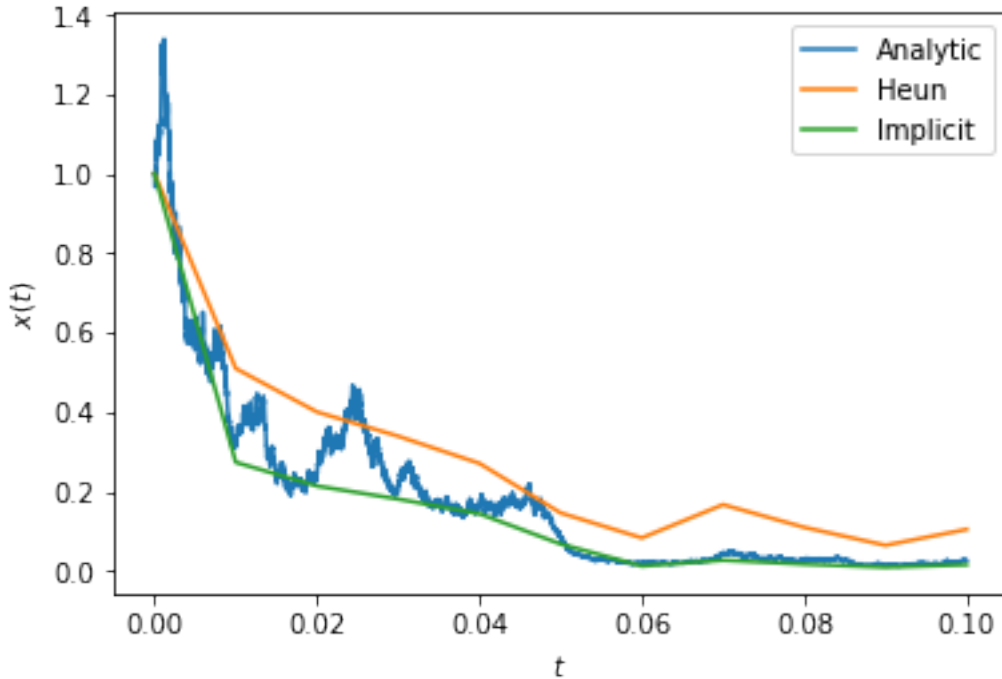
```
In [6]: tvecs = {
    i: dts[i] * np.arange(len(results['heun'+str(i)]))
    for i in range(len(dts))
}
```

The plot of  $x(t)$  shows that the explicit solver performs poorly on the stiff problem, as expected. The implicit solution looks accurate.



```
In [7]: plt.plot(tvecs[0], results['true'], label='Analytic')
plt.plot(tvecs[3], results['heun3'], label='Heun')
plt.plot(tvecs[3], results['implicit3'], label='Implicit')
plt.xlabel('$t$'); plt.ylabel('$x(t)$'); plt.legend()
```

```
Out[7]: <matplotlib.legend.Legend at 0x7f58a107c940>
```



### 5.3 Task 3 - 1D unstable system

We introduce instability by simulating a system that drifts to infinity.

$$dX(t) = aX(t)dt + bX(t)dW(t)$$

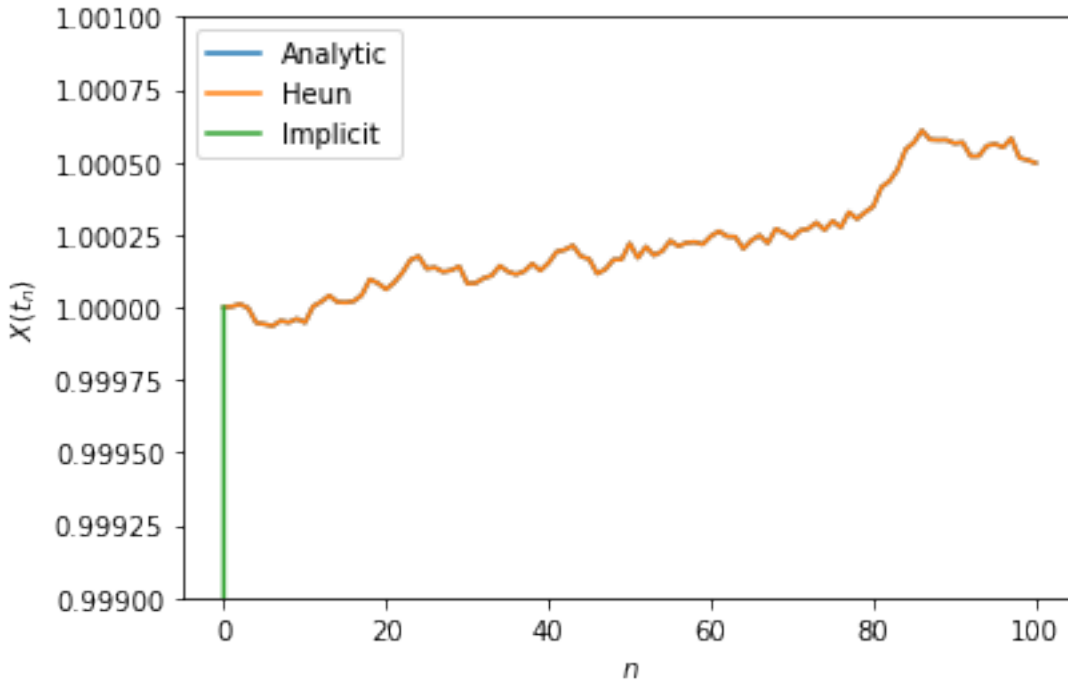
- $a = 1.0$
- $b = 0.1$

```
In [8]: # load results
path = datapath + 'task3/'
files = !ls {path}
results = {name: np.fromfile(path + name) for name in files if name!='dt'}
```

The implicit solver blows up for these unstable problems. The explicit solver is able to track the trajectory closely.

```
In [9]: plt.plot(results['true'], label='Analytic')
plt.plot(results['heun'], label='Heun')
plt.plot(results['implicit'], label='Implicit')
plt.legend(), plt.ylabel('$X(t_n)$'); plt.xlabel('$n$')
plt.ylim(0.999, 1.001)
```

```
Out[9]: (0.999, 1.001)
```



## 5.4 Task 4 - Zero-temperature LLG convergence

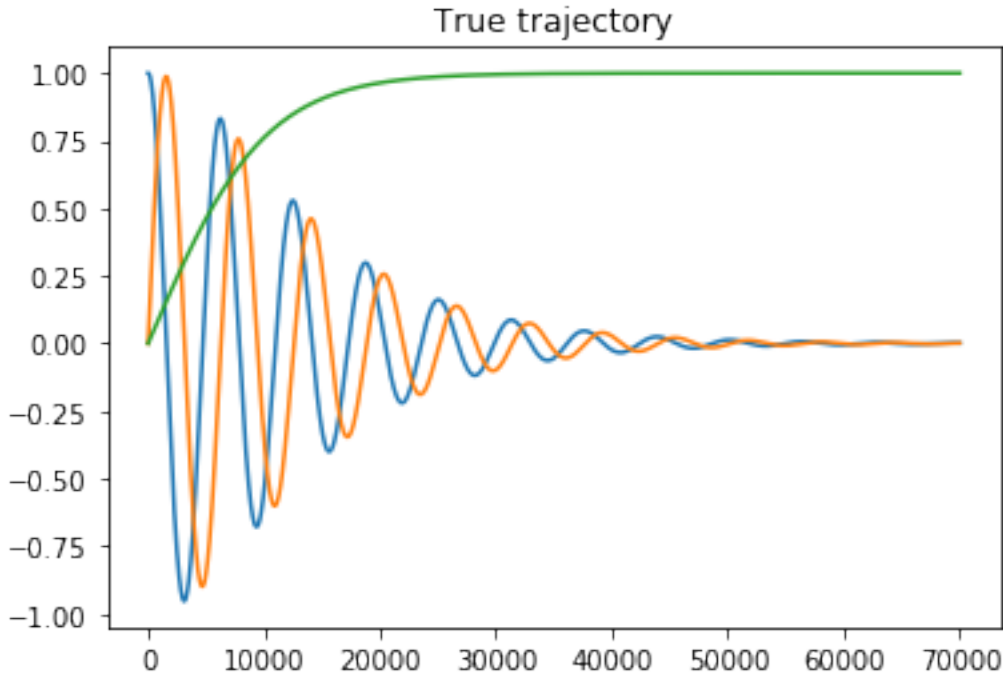
At  $T = 0$  the Landau-Lifshitz-Gilbert equation for a single particle is deterministic and has a known solution. We compare the ability of the explicit and implicit methods to integrate the LLG.

```
In [10]: # Load results
         path = datapath + 'task4/'
         files = !ls {path}
         results = {name: np.fromfile(path + name).reshape((-1,3)) for name in files if name!='dt'}
         dts = np.fromfile(path + 'dt')
```

Below is an example of the true trajectory of the x,y,z coordinates of magnetisation.

```
In [11]: plt.plot(results['true'])
         plt.title('True trajectory')

Out[11]: <matplotlib.text.Text at 0x7f58a0f334e0>
```



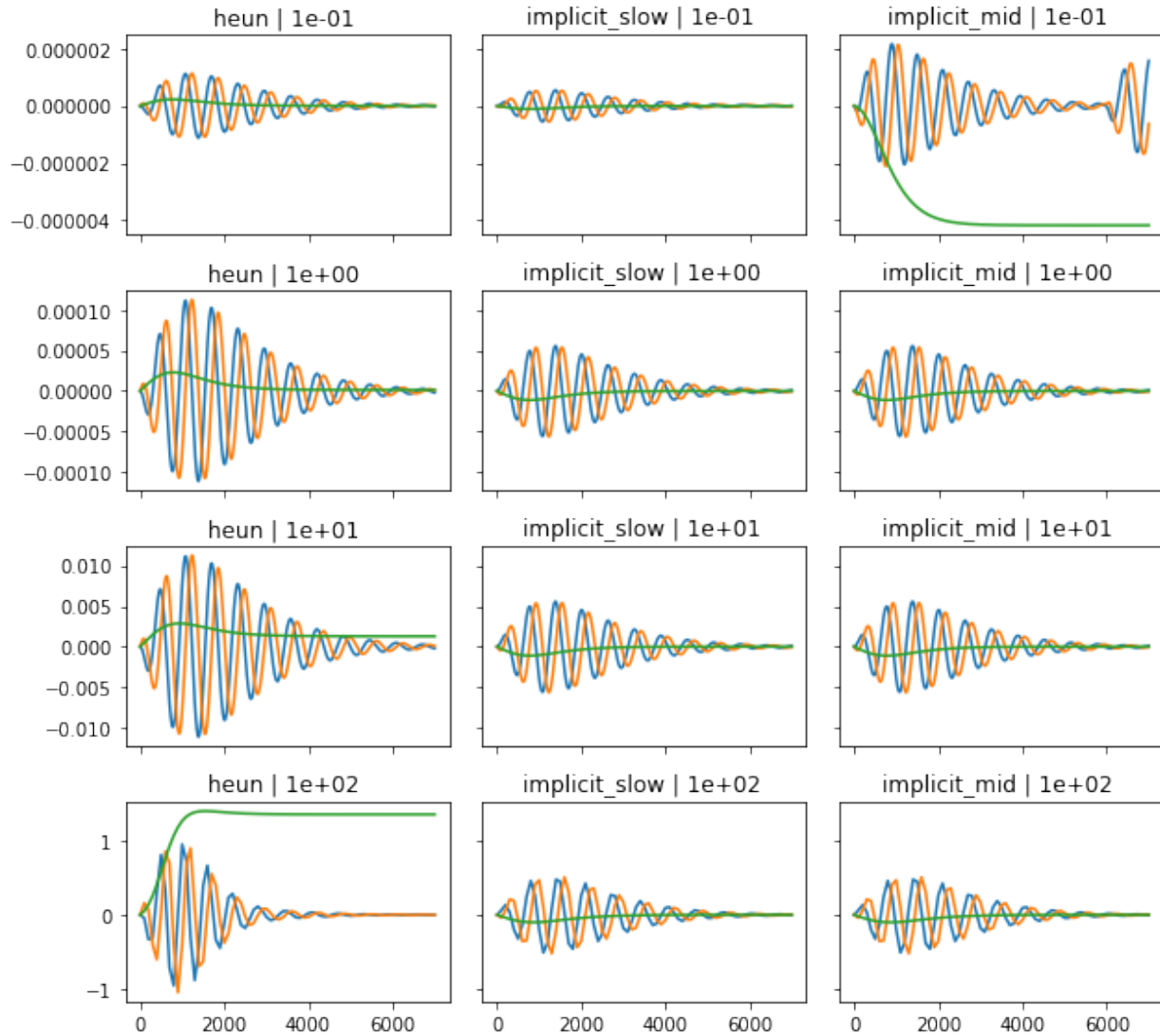
### 5.4.1 Residual plots

Below we compare three integrators: - Explicit (Heun) - Implicit slow (uses a high tolerance in the internal Quasi-newton solver) - Implicit mid (uses a medium tolerance in the internal Quasi-newton solver)

We compare the residuals (difference between the true and estimated trajectories) in x,y,z for a number of time step sizes. Note that we are using reduced time (see docs elsewhere).

```
In [12]: integ_names = ['heun', 'implicit_slow', 'implicit_mid']
         dt_indices = range(len(dts))

         fg, axs = plt.subplots(nrows=len(dts), ncols=len(integ_names),
                               sharey='row', sharex=True,
                               figsize=(3*len(integ_names), 2*len(dts)))
         for ax_row, dt_idx in zip(axs, dt_indices):
             for ax, name in zip(ax_row, integ_names):
                 mag = results[name + str(dt_idx)]
                 true = results['true'][:, 10*dt_idx:]
                 time = dts[dt_idx] * np.arange(mag.shape[0])
                 ax.plot(time, mag-true)
                 ax.set_title('{} | {:.10e} '.format(name, dts[dt_idx]))
         plt.tight_layout()
```



From the above results we make three observations: 1. For the same time step, the implicit scheme (slow) is more accurate than the explicit scheme 2. The implicit method is stable at larger time steps compared to the explicit scheme (see  $dt=1e-2$ ) 3. Guidelines for setting the implicit quasi-Newton tolerance: - As we reduce the time step, the required tolerance on the quasi-Newton solver must be smaller. - If the tolerance is not small enough the solution blows up (see top right) - If the tolerance is small enough, decreasing the tolerance further has little effect (compare 2nd and 3rd column).

### 5.4.2 Compare trajectories

We can also investigate the estimated trajectories of the x,y,z components for each solver and tolerance level.

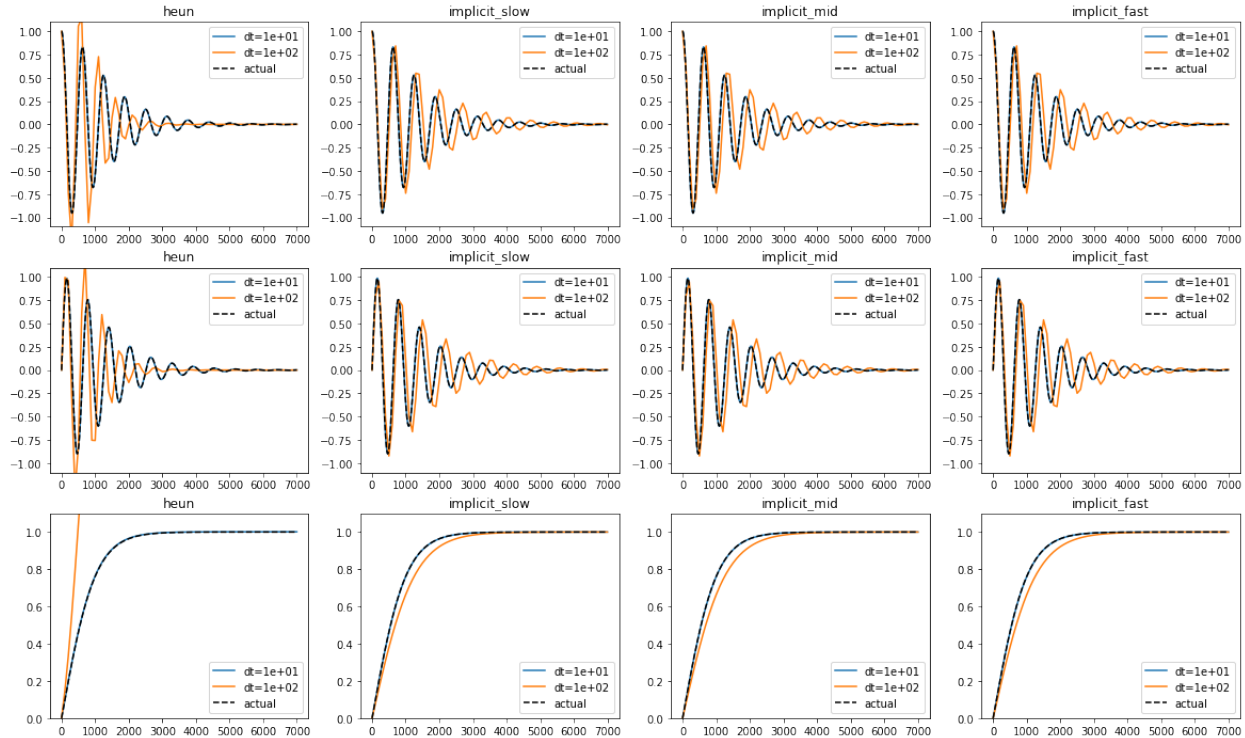
```
In [13]: intes = ['heun', 'implicit_slow', 'implicit_mid', 'implicit_fast']
         dt_indices = range(2,4)

         fg, axs = plt.subplots(nrows=3, ncols=len(intes), figsize=(5*len(intes), 12))
         for axrow, direction in zip(axs, range(3)):
             for ax, inte in zip(axrow, intes):
                 for idx in dt_indices:
                     numerical = results[inte+str(idx)][:,direction]
```

```

time = dts[idx] * np.arange(numerical.size)
ax.plot(time, numerical, label='dt={:1.0e}'.format(dts[idx]))
actual = results['true'][:,direction]
time = dts[0] * np.arange(actual.size)
ax.plot(time, actual, 'k--', label='actual')
ax.legend()
ax.set_title(inte)
ax.set_ylim(0 if direction==2 else -1.1, 1.1)

```



## 5.5 Task 5 - stochastic LLG global convergence

We now perform finite-temperature simulations of the LLG equation using the explicit and implicit scheme. We determine the global convergence (i.e. the increase in accuracy with decreasing time step).

We expect the convergence to be linear in  $\log\text{-}\log$  space and have a convergence rate (slope) of 0.5

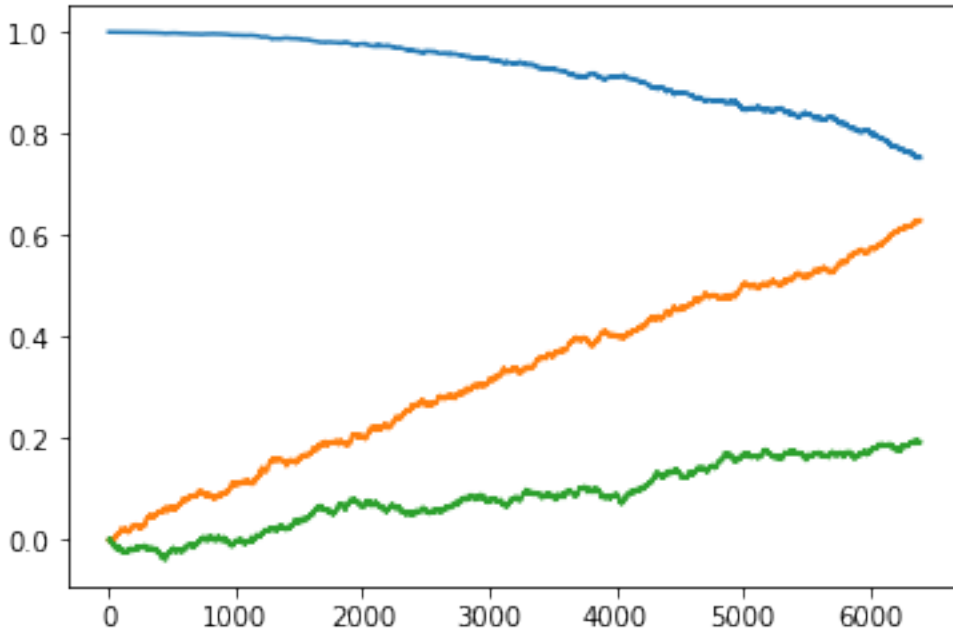
Files are ordered from smallest timestep at index 0 to lowest at index 4.

Below we show an example of the problem, which we are solving.

```

In [14]: x = np.fromfile(datapath+'task5/example_sol').reshape((-1,3))
         plt.plot(x);

```



### 5.5.1 Implicit midpoint

```
In [17]: fnames = !ls {datapath}task5/implicit*
         global_sols = [np.fromfile(fname).reshape((-1,3)) for fname in fnames]

In [18]: # Compute difference between solutions at consecutive timesteps
         diffs = np.diff(global_sols, axis=0)

         # Take err as L2 norm
         err = np.linalg.norm(diffs, axis=2)

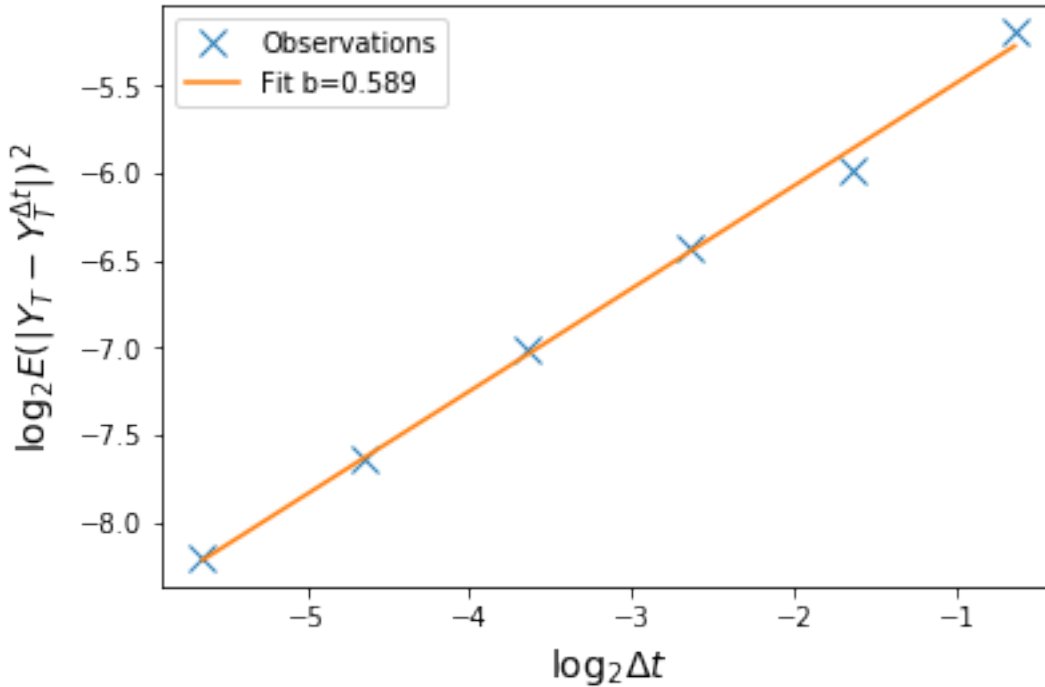
         # Compute expected error
         Eerr = np.mean(err, axis=1)

In [19]: # Load the dt values
         dts = np.fromfile(datapath+'task5/dt')[1:]

In [20]: # Fit a straight line
         a,b = np.linalg.lstsq(np.stack([np.ones_like(dts), np.log2(dts)]).T, np.log2(Eerr))[0]

In [21]: plt.plot(np.log2(dts), np.log2(Eerr), 'x', ms=10, label='Observations')
         plt.plot(np.log2(dts), a + np.log2(dts)*b, '-', label='Fit b={:.3f}'.format(b))
         plt.xlabel('$\\log_2 \\Delta t$', fontsize=14)
         plt.ylabel('$\\log_2 E (\\left| Y_T - Y_T^{\\Delta t} \\right|)^2$', fontsize=14)
         plt.legend()

Out[21]: <matplotlib.legend.Legend at 0x7f589d97e4a8>
```



### 5.5.2 Heun

```
In [22]: fnames = !ls {datapath}task5/heun*
        global_sols = [np.fromfile(fname).reshape((-1,3)) for fname in fnames]

In [23]: # Compute difference between solutions at consecutive timesteps
        diffs = np.diff(global_sols, axis=0)

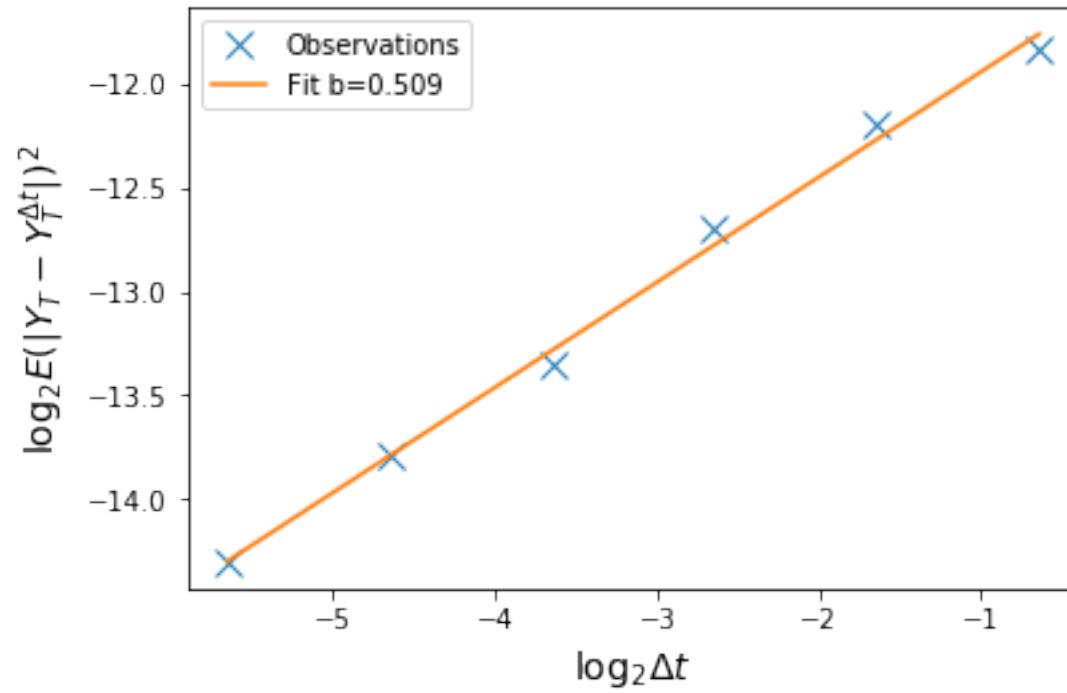
        # Take err as L2 norm
        err = np.linalg.norm(diffs, axis=2)

        # Compute expected error
        Eerr = np.mean(err, axis=1)

In [24]: # Fit a straight line
        a,b = np.linalg.lstsq(np.stack([np.ones_like(dts), np.log2(dts)]).T, np.log2(Eerr))[0]

In [25]: plt.plot(np.log2(dts), np.log2(Eerr), 'x', ms=10, label='Observations')
        plt.plot(np.log2(dts), a + np.log2(dts)*b, '-', label='Fit b={:.3f}'.format(b))
        plt.xlabel('$\\log_2 \\Delta t$', fontsize=14)
        plt.ylabel('$\\log_2 E (\\left| Y_T - Y_T^{\\Delta t} \\right|)^2$', fontsize=14)
        plt.legend()

Out[25]: <matplotlib.legend.Legend at 0x7f589d9cfb70>
```



### 5.5.3 Results

Both methods converge correctly and have a rate of 0.5. This validates the implementation of the integrators.



Detailed information on classes, methods, and functions in the magpy package.

## 6.1 magpy.core module

MagicMock is a subclass of Mock with default implementations of most of the magic methods. You can use MagicMock without having to configure the magic methods yourself.

If you use the *spec* or *spec\_set* arguments then *only* magic methods that exist in the spec will be created.

Attributes and the return value of a *MagicMock* will also be *MagicMocks*.

## 6.2 magpy.data module

```
magpy.data.grab_results(repo_path, name)
magpy.data.magpy_actor()
magpy.data.shelve_results(results, repo_path, name)
```

## 6.3 magpy.geometry package

### 6.3.1 Submodules

#### magpy.geometry.arkus module

Coordinates for Arkus cluster geometries.

This module contains the coordinates of particles arranged into Arkus cluster geometries of varying size. Arkus clusters are *minimum energy* clusters that represent tightly packed clusters of spherical particles. Their definition (and name) are derived from:

N. Arkus, V. N. Manoharan, and M. P. Brenner, *Phys. Rev. Lett.* **103**, 118303 (2009).  
<http://dx.doi.org/10.1103/PhysRevLett.103.118303>

Clusters of 1-5 particles have only one possible arrangement. Clusters of 6 or more particles have a variety of different configurations, which are accessed using a configuration id. The available configuration ranges are:

- 1-5 particles: [0]
- 6 particles: [0-1]
- 7 particles: [0-5]
- 8 particles: [0-12]

The coordinates of the particles within the cluster are normalised to a unit distance between each pair (where possible). The distance between the particles can be controlled by multiplying by a scaling factor.

`magpy.geometry.arkus.ARKUS`

*dict* – a dictionary containing the geometries of Arkus clusters of 1-8 particles. The dictionary is accessed `ARKUS[n_particles][configuration_id]` and returns an `np.ndarray` of shape `(n_particles,3)` containing the coordinates of particles in the cluster.

## Examples

```
>>> ARKUS[1][0]
array([[0,0,0]])
>>> ARKUS[2][0]
array([[0,0,0],
       [0,0,1]])
>>> ARKUS[2][0] * 1e-9 # apply a scaling factor
array([[0,0,0],
       [0,0,1e-9]])
```

## magpy.geometry.coordinates module

`magpy.geometry.coordinates.arkus_cluster_coordinates` (*n\_particles*, *configuration\_id*,  
*R*)

Coordinates of particles in an Arkus cluster.

Returns an array of coordinates for each particle in an Arkus cluster of size *n\_particles* with a specified *configuration\_id*. Each configuration id represents a cluster of *n\_particles* with a different arrangement.

See `magpy.geometry.arkus` for more information on Arkus geometries and available configurations.

### Parameters

- **n\_particles** (*int*) – cluster size
- **configuration\_id** (*int*) – configuration id of the Arkus cluster see [link] for more information on available configurations for each cluster size
- **R** (*float*) – distance between particles

**Returns** shape `(n_particles, 3)` array of the coordinates

**Return type** `np.ndarray`

`magpy.geometry.coordinates.arkus_cluster_random_configuration_id(n_particles)`

A randomly drawn configuration id for an Arkus cluster.

Returns a random configuration id for an Arkus cluster of a specified size. Each configuration contains *n\_particles* in a different arrangement.

See [magpy.geometry.arkus](#) for more information on Arkus geometries and available configurations.

**Parameters** *n\_particles* (*int*) – Arkus cluster size

**Returns** a random configuration id

**Return type** *int*

`magpy.geometry.coordinates.arkus_random_cluster_coordinates(n_particles, R)`

Coordinates of particles in a random Arkus cluster configuration.

Returns an array of coordinates for particles in an Arkus cluster of size *n\_particles* with a random configuration. Each configuration has a different arrangement of particles. See [\[link\]](#) for info.

See [magpy.geometry.arkus](#) for more information on Arkus geometries and possible configurations.

**Parameters**

- *n\_particles* (*int*) – Arkus cluster size
- *R* (*float*) – point to point Euclidean distance between coordinates

**Returns** shape (*n\_particles*,3) array of coordinates of particles

**Return type** *np.ndarray*

`magpy.geometry.coordinates.chain_coordinates(n_particles, R, direction=<sphinx.ext.autodoc._MockObject object>)`

Coordinates of particles along a straight chain.

Returns an array of coordinates for particles arranged in a perfectly straight chain and regularly spaced. The chain can have any direction and number of particles but will start at the origin.

## Example

..code-block:: python

```
>>> chain_coordinates(3, 2.5, direction=[1,0,0])
np.array([0,0,0],
         [2.5,0,0],
         [5,0,0])
>>> # Only unit vector of direction is used:
>>> chain_coordinates(2, 3.0, direction=[3,4,0])
np.array([0,0,0],
         [1.8, 2.4, 0])
```

**Parameters**

- *n\_particles* (*int*) – size of the particle chain
- *R* (*float*) – point to point Euclidean distance between points
- *direction* (*np.ndarray*, *optional*) – direction in 3d space to construct the chain. The magnitude of the direction is has no effect, only its unit direction. Default value is the z-axis *np.array([0,0,1])*

**Returns** shape  $(n\_particles, 3)$  array of coordinates of particles

**Return type** np.ndarray

## 6.4 magpy.initial\_conditions module

`magpy.initial_conditions.random_point_on_unit_sphere()`

Point randomly drawn from a uniform distribution on the unit sphere.

Randomly picking a point on the unit sphere requires choosing the point so that each solid angle on the sphere is equally likely.

Set `np.random.seed(seed)` for reproducible results.

**Returns** a 3d array with the x,y,z coordinates of a random point

**Return type** np.ndarray

`magpy.initial_conditions.random_quaternion()`

Random uniformly distributed quaternion

A quaternion defines an 3d axis of rotation and a corresponding angle of rotation. A random quaternion is drawn by first drawing a random rotation axis from the uniform random sphere and a uniform angle. Random quaternions are used for random rotation operations on arbitrary geometries.

**Returns** a random quaternion from a uniform distribution

**Return type** transforms3d.Quaternion

`magpy.initial_conditions.uniform_random_axes(N)`

Random 3d vectors (axes) uniformly distributed on unit sphere.

Returns  $N$  3d unit vectors drawn from a uniform distribution over the unit sphere.

Set `np.random.seed(seed)` for reproducible results.

**Parameters**  $N$  (*int*) – number of random axes to draw.

**Returns** a 2d array size  $(N \times 3)$ . Random 3d unit vectors on the uniform random sphere.

**Return type** np.ndarray

## 6.5 magpy.model module

`class magpy.model.DOModel(radius, anisotropy, initial_probabilities, magnetisation, damping, temperature, field_shape='constant', field_frequency=0.0, field_amplitude=0.0, field_n_components=1)`

Bases: object

A probabilistic model of a single particle

A magpy DOModel is a probabilistic model of a single magnetic nanoparticle with a uniaxial anisotropy axis. The model has just two possible states: up and down. The model is defined by the material properties of the particle, an external field (applied along the anisotropy axis), and an initial probability vector (length 2).

The model is simulated to solve the probability of the system being up and down over time. The particle is optionally subjected to a time-varying field along the anisotropy axis. The available field types and applicable parameters:

- *constant*: a constant (time-invariant) field. Specify *field\_amplitude*

- *sine*: a sinusoidal field. Specify *field\_amplitude* and *field\_frequency*
- *square*: a square alternating field (switching). Specify *field\_amplitude* and *field\_frequency*
- *square\_f*: a square alternating field with a finite number of cosine Fourier series terms. Specify *field\_amplitude*, *field\_frequency* and *field\_n\_components*

#### Parameters

- **radius** (*double*) – radius of the spherical particle
- **anisotropy** (*double*) – anisotropy constant for the uniaxial anisotropy axis
- **initial\_probabilities** (*ndarray[double, 2]*) – initial probability of the particle down and up state respectively.
- **magnetisation** (*double*) – saturation magnetisation of all particles in the cluster (ampres / meter). Saturation magnetisation cannot vary between particles.
- **damping** (*double*) – the damping constant for the particle.
- **temperature** (*double*) – the ambient temperature in Kelvin for the particle.
- **field\_shape** (*str, optional*) – can be either ‘constant’, ‘square’, ‘square\_f’ or ‘sine’ describing the time-varying shape of the alternating field. The field is always applied along the anisotropy axis. Default is ‘constant’
- **field\_frequency** (*double, optional*) – the frequency of the applied field in Hz. Default is 0Hz.
- **field\_amplitude** (*double, optional*) – the amplitude of the applied field in Ampres / meter. Default is 0A/m
- **field\_n\_components** (*int, optional*) – applies for *field\_shape*==‘square\_f’ only. The number of cosine Fourier series components to use for square wave. Default is 1

**simulate** (*end\_time, time\_step, max\_samples*)

Simulate the state probabilities for the particle

Simulate the time-varying probabilities of the up/down states of the particle. The system is described by a master equation, which is defined by the transition rates between the up and down state. The master equation is solved numerically using an explicit RK45 solver.

In order to save memory, the user is required to specify the *max\_samples*. The output of the time-integrator is up/downsampled to *max\_samples* regularly spaced intervals using a first-order-hold interpolation. This is useful for long simulations with very small time steps that, without downsampling, would produce GBs of data very quickly.

#### Parameters

- **end\_time** (*float*) – time to end the simulation (in seconds)
- **time\_step** (*float*) – time step for time-integration solver
- **max\_samples** (*int*) – number of regularly spaced samples of the output

#### Returns

a **magpy.results.Results** object containing the time-dependent magnetisation of the particle.

**Return type** magpy.Results

```
class magpy.model.EnsembleModel(N, base_model, **kwargs)
```

Bases: object

Ensemble of particle clusters

The EnsembleModel class represents a non-interacting ensemble of particle clusters. It aims to provide a more user-friendly alternative than handling a large number of magpy.Model instances manually.

Every member of the ensemble is copied from a base *magpy.Model* and is updated from a list of varying parameters. Parameters that are not specified as keyword arguments will be identical for every member of the ensemble and equivalent to that parameter's value in the base model.

Parameters that should vary for each particle are specified as a keyword argument whose value is a list of parameters of length *N* (where the *i*'th value of the list corresponds to the parameter's value for the *i*'th member of the cluster)

#### Parameters

- **N** (*int*) – number of clusters in the ensemble
- **base\_model** (*magpy.Model*) – the base model provides the default parameters for every member of the ensemble.
- **\*\*kwargs** – each argument may be a magpy.Model parameter and a corresponding list of *N* parameter values, which override the base model parameters for the *i*'th member of the ensemble.

```
simulate(end_time, time_step, max_samples, random_state, renorm=False, interactions=True,  
         n_jobs=1, implicit_solve=True, implicit_tol=1e-09)
```

Simulate the dynamics of an ensemble of particle clusters

Simulate the time-varying dynamics of an ensemble of particle clusters of interacting macrospins. The time-varying dynamics are described by the Landau-Lifshitz-Gilbert stochastic differential equation, which is integrated using an explicit or implicit numerical scheme.

In order to save memory, the user is required to specify the *max\_samples*. The output of the time-integrator is up/downsampled to *max\_samples* regularly spaced intervals using a first-order-hold interpolation. This is useful for long simulations with very small time steps that, without downsampling, would produce GBs of data very quickly.

**There are two time-integration schemes available:**

- a fully implicit midpoint scheme :**cpp:function:'integrator::implicit\_midpoint'**
- an explicit predictor-corrector method (Heun scheme) :**cpp:function:'integrator::heun'**

#### Parameters

- **end\_time** (*float*) – time to end the simulation (in seconds)
- **time\_step** (*float*) – time step for time-integration solver
- **max\_samples** (*int*) – number of regularly spaced samples of the output
- **random\_state** (*int, optional*) – the state is used to generate seeds for each of the individual simulations. Set for reproducible results.
- **renorm** (*bool, optional*) – default is False. If True the magnetisation of each particle is rescaled (using the 2-norm) to unity at every time step.
- **interactions** (*bool, optional*) – default is True. If False the interactions between particles are switched off.
- **implicit\_solve** (*bool, optional*) – default is True. If True a fully-implicit stochastic solver is used. If False the explicit Heun scheme is used.

- **implicit\_tol** (*float, optional*) – if using the implicit solver *implicit\_tol* sets the tolerance of the internal Newton-Raphson method. Default is 1e-9

#### Returns

a **magpy.results.Results** object containing the time-dependent magnetisation of the particle system.

**Return type** magpy.Results

```
class magpy.model.Model(radius, anisotropy, anisotropy_axis, magnetisation_direction, location, magnetisation, damping, temperature, field_shape='constant', field_frequency=0.0, field_amplitude=0.0)
```

Bases: object

A cluster of interacting magnetic nanoparticles

A magpy Model describes a cluster of magnetic nanoparticles. The cluster is defined by the material properties of the individual particles, their relative positions in 3D space, and an initial magnetisation vector. Each particle is modelled as by a single macrospin with a uniaxial anisotropy axis.

The model may be simulated to obtain the time-dependent dynamics of the magnetisation vector of the individual particles within the cluster.

The particle cluster is optionally subjected to a time-varying magnetic field, applied along the z-axis. The field can be constant or sine/square varying with a desired frequency and amplitude.

#### Parameters

- **radius** (*list of double*) – radius of each spherical particle in the ensemble in meters
- **anisotropy** (*list of double*) – anisotropy constant for the uniaxial anisotropy axis of each particle
- **anisotropy\_axis** (*list of ndarray[double, 3]*) – unit axis for the direction of the anisotropy for each particle
- **magnetisation\_direction** (*list of ndarray[double, 3]*) – initial direction of the magnetisation vector for each particle
- **location** (*list of ndarray[double, 3]*) – location of each particle in the cluster described by x,y,z coordinates
- **magnetisation** (*double*) – saturation magnetisation of all particles in the cluster (amperes / meter). Saturation magnetisation cannot vary between particles.
- **damping** (*double*) – the damping parameter for all particles in the cluster. Damping cannot vary between particles.
- **temperature** (*double*) – the ambient temperature in Kelvin for the particle cluster.
- **field\_shape** (*str, optional*) – can be either 'constant', 'square' or 'sine' describing the time-varying shape of the alternating field. The field is always applied along the z-axis. Default is 'constant'
- **field\_frequency** (*double, optional*) – the frequency of the applied field in Hz. Default is 0Hz.
- **field\_amplitude** (*double, optional*) – the amplitude of the applied field in Amperes / meter. Default is 0A/m

```
simulate(end_time, time_step, max_samples, seed=1001, renorm=False, interactions=True, implicit_solve=True, implicit_tol=1e-09)  
Simulate the dynamics of the particle cluster
```

Simulate the time-varying dynamics of the cluster of interacting macrospins. The time-varying dynamics are described by the Landau-Lifshitz-Gilbert stochastic differential equation, which is integrated using an explicit or implicit numerical scheme.

In order to save memory, the user is required to specify the *max\_samples*. The output of the time-integrator is up/downsampled to *max\_samples* regularly spaced intervals using a first-order-hold interpolation. This is useful for long simulations with very small time steps that, without downsampling, would produce GBs of data very quickly.

**There are two time-integration schemes available:**

- a fully implicit midpoint scheme :cpp:function:‘integrator::implicit\_midpoint‘
- an explicit predictor-corrector method (Heun scheme) :cpp:function:‘integrator::heun‘

#### Parameters

- **end\_time** (*float*) – time to end the simulation (in seconds)
- **time\_step** (*float*) – time step for time-integration solver
- **max\_samples** (*int*) – number of regularly spaced samples of the output
- **seed** (*int*, *optional*) – default value is 1001. The random seed for random number generation of the thermal noise. Set for reproducible results.
- **renorm** (*bool*, *optional*) – default is False. If True the magnetisation of each particle is rescaled (using the 2-norm) to unity at every time step.
- **interactions** (*bool*, *optional*) – default is True. If False the interactions between particles are switched off.
- **implicit\_solve** (*bool*, *optional*) – default is True. If True a fully-implicit stochastic solver is used. If False the explicit Heun scheme is used.
- **implicit\_tol** (*float*, *optional*) – if using the implicit solver *implicit\_tol* sets the tolerance of the internal Newton-Raphson method. Default is 1e-9

#### Returns

a *magpy.results.Results* object containing the time-dependent magnetisation of the particle system.

**Return type** *magpy.Results*

## 6.6 magpy.results module

```
class magpy.results.EnsembleResults (results)
```

Bases: object

Results from a simulation of an ensemble of particle clusters

The EnsembleResults object holds the resulting *magpy.Results* objects for an ensemble of simulated particle clusters. It provides a user-friendly alternative to handling a large collection of *magpy.Results* instances and implements methods for computing ensemble-wide properties.

**Parameters** **results** (*list* [*magpy.Results*]) – results for each particle cluster in the ensemble

**time**

(*np.ndarray*): 1d array of length *M*. Time in seconds for each sample in the ensemble results.



**field**

(np.ndarray): 1d array of length  $M$ . Field amplitude at each point in time. Field is always applied along the z-axis.

**energy\_dissipated** (*start\_time=None, end\_time=None*)

Total energy dissipated by the ensemble.

A simulation with a constant or zero applied field will dissipate no energy. The energy dissipated by an ensemble of magnetic particle clusters subjected to an alternating field is the area of the hysteresis loop (magnetisation-field plane).

The energy dissipated may be computed for the entire simulation or within a specific time window, defined by *start\_time* and *end\_time*

**Parameters**

- **start\_time** (*double, optional*) – the start of the time window for computing energy dissipated. Default value *None* uses the start of the simulation.
- **end\_time** (*double, optional*) – the end of the time window for computing energy dissipated. Default value *None* uses the end of the simulation.

**Returns** total energy dissipated by the ensemble during the time window

**Return type** double

**ensemble\_magnetisation** (*direction='z'*)

Total magnetisation of entire ensemble

The total magnetisation of an ensemble of particle clusters. The ensemble magnetisation is the average value of the magnetisation of each particle cluster in the ensemble at each point in time. The component (x, 'y', 'z') along which the magnetisation may be specified. The default value is z, which is the same direction as the applied magnetic field.

**Parameters** **direction** (*str, optional*) – direction of magnetisation x, y or z. Default value is z.

**Returns**

**1d array of length  $M$  containing the ensemble magnetisation** for each point in *self.time*

**Return type** np.ndarray

**final\_cycle\_energy\_dissipated** (*field\_frequency*)

Energy dissipated by the final cycle of the magnetic field.

A simulation with a constant or zero applied field will dissipate no energy. The energy dissipated by an ensemble of magnetic particle clusters subjected to an alternating field is the area of the hysteresis loop (magnetisation-field plane).

Use this function to compute the energy dissipated by the final cycle (i.e. period) of the applied alternating magnetic field if the total simulation time contains multiple cycles of the field (i.e. is longer than the period of the applied field). A common use case for this is to simulate a large number field cycles to reach equilibrium and then compute the energy dissipated during a single cycle of the field in equilibrium.

**Parameters** **field\_frequency** (*double*) – the frequency of the applied magnetic field

**Returns** energy dissipated during the last cycle of the applied magnetic field.

**Return type** double

**final\_state** ()

State of each ensemble member at the end of the simulation.

The final state of each particle cluster in the ensemble at the end of the simulation time. The state of each particle cluster is the value of magnetisation vector of every particle in the cluster.

**Returns** a list of nested dictionaries like  $\{ 'x': \{0: m_x, \dots, N-1: m_x\}, 'y': \dots \}$ . The dictionaries contain the final value of the magnetisation vector for each of the  $N$  particles in the cluster.

**Return type** list[dict]

**magnetisation** (*direction*='z')

Total magnetisation of each member of the ensemble

The total magnetisation of cluster is computed by summing the components of the magnetisation vector for each particle in the cluster. The component ( $x, y, z$ ) along which the magnetisation may be specified. The default value is  $z$ , which is the same direction as the applied magnetic field.

**Parameters** *direction* (*str*, *optional*) – direction of magnetisation  $x, y$  or  $z$ . Default value is  $z$ .

**Returns** list containing a length  $M$  1d array containing the total magnetisation of each particle cluster in the ensemble.

**Return type** list[np.ndarray]

**class** magpy.results.Results (*time, field, x, y, z, N*)

Bases: object

Results of a simulation of a single particle cluster

The results contain the time-varying magnetisation and field resulting from stochastic simulation of a particle cluster consisting of  $N$  particles.

#### Parameters

- **time** (*np.ndarray*) – 1d array of length  $M$ . Time in seconds for each sample in the results
- **field** (*np.ndarray*) – 1d array of length  $M$ . Field amplitude at each point in time. Field is always applied along the  $z$ -axis.
- **x** (*dict*) –  $\{0: np.ndarray, \dots, N-1: np.ndarray\}$  key, value pair is an interger particle id and a corresponding 1d array of length  $M$  for each of the  $N$  particles in the cluster. 1d array is the  $x$ -coordinate of the particle magnetisation vector at each point in time.
- **y** (*dict*) –  $\{0: np.ndarray, \dots, N-1: np.ndarray\}$  key, value pair is an interger particle id and a corresponding 1d array of length  $M$  for each of the  $N$  particles in the cluster. 1d array is the  $y$ -coordinate of the particle magnetisation vector at each point in time.
- **z** (*dict*) –  $\{0: np.ndarray, \dots, N-1: np.ndarray\}$  key, value pair is an interger particle id and a corresponding 1d array of length  $M$  for each of the  $N$  particles in the cluster. 1d array is the  $z$ -coordinate of the particle magnetisation vector at each point in time.
- **N** (*int*) – number of particles in the ensemble

**final\_state** ()

The state of the cluster at the end of the simulation.

Returns the state of the particle cluster at the end of the simulation time.

#### Returns

a nested dictionary  $\{ 'x': \{0: m_x, \dots, N-1: m_x\}, 'y': \dots \}$  containing the final value of the magnetisation vector for each of the  $N$  particles in the cluster.

**Return type** dict

**magnetisation** (*direction*='z')

Computes the total magnetisation of the cluster

Computes the total time-varying magnetisation of the cluster in a desired direction. The total magnetisation is simply the sum of the individual magnetisation vector components in the specified direction (x,y, or z).

**Parameters** **direction** (*str*, *optional*) – the direction of magnetisation *x*, *y* or *z*. Default value is *z*.

**Returns**

**1d array of length *M* the total magnetisation at each point** in *self.time*.

**Return type** np.ndarray

**plot** ()

Plots the magnetisation from the results

Plots the x,y,z coordinates of the magnetisation vector for every particle in the particle cluster.

**Returns** matplotlib figure handle containing the resulting plot axes.



The magpy C++ library powers the core functionality of the python interface. The library doesn't depend on the python features and is compiled independently of the python code. The C++ API is organised around functions in namespaces and uses classes sparingly. Use the namespace list for browsing the code base.

## 7.1 Namespace list

### 7.1.1 Namespace constants

**namespace constants**

#### Variables

```
const double KB = 1.38064852e-23
const double MU0 = 1.25663706e-6
const double GYROMAG = 1.76086e11
```

### 7.1.2 Namespace curry

**Warning:** doxygennamespace: Cannot find namespace “curry” in doxygen xml output for project “magpy-api” from directory: ../doxygen/doxyxml

### 7.1.3 Namespace distances

**namespace distances**

Compute distances between points.

Functions for computing distances between points in 3D space.

**Author** Oliver Laslett

**Date** 2017

## Functions

`std::vector<std::vector<std::array<double, 3>>> pair_wise_distance_vectors (std::vector<std::array<double, 3>>> points)`

Computes the distance vector between points in 3d space.

Given a list of x,y,z coordinates, compute the distance vector between every pair of x,y,z coordinates in the list.

**Return** NxN std::vector matrix of distances between each pair of points

### Parameters

- `points`: length N vector of arrays of x,y,z coordinates

`std::vector<std::vector<double>>> pair_wise_distance_magnitude (std::vector<std::array<double, 3>>> points)`

Computes the Euclidean distance between pairs of points.

`std::vector<std::vector<std::array<double, 3>>> pair_wise_distance_unit_vectors (std::vector<std::array<double, 3>>> points)`

Computes the unit distance vector between a list of points.

`std::vector<std::vector<double>>> pair_wise_distance_magnitude (std::vector<std::vector<std::array<double, 3>>> distance_vectors)`

Computes the Euclidean distance from a matrix of distance vectors.

Given a matrix of distance vectors, compute the 2norm of the vector corresponding to the Euclidean distance.

**Return** NxN matrix of Euclidean distance values

### Parameters

- `distance_vectors`: NxN symmetrical matrix of distance vectors (x,y,z coordinates)

`std::vector<std::vector<std::array<double, 3>>> pair_wise_distance_unit_vectors (std::vector<std::vector<std::array<double, 3>>> distance_vectors, std::vector<std::vector<double>>> distance_magnitudes)`

Computes the unit distance vectors from distance vectors and their magnitudes.

## 7.1.4 Namespace dom

### namespace dom

discrete orientation model for magnetic particles

## Functions

void **transition\_matrix** (double \*W, **const** double k, **const** double v, **const** double T, **const** double h, **const** double ms, **const** double alpha)

Compute the 2x2 transition matrix for a single particle.

Assumes uniaxial anisotropy and an applied field  $h < 1$  Only valid for large energy barriers:  $(1-h)^2 \gg 1$

### Parameters

- W: transition matrix [2x2]
- k: anisotropy strength constant for the uniaxial anisotropy
- v: volume of the particle in meter<sup>3</sup>
- T: temperature of environment in Kelvin
- h: dimensionless applied field - normalised by  $H_k = \frac{2K}{\mu_0 M_s}$
- ms: saturation magnetisation
- alpha: dimensionless damping constant

void **master\_equation\_with\_update** (double \*derivs, double \*work, **const** double k, **const** double v, **const** double T, **const** double ms, **const** double alpha, **const** double t, **const** double \*state\_probabilities, **const** std::function<double> double

> applied\_field Computes master equation for particle in time-dependent field.

Computes the applied field in the z-direction at time t. Uses the field value to compute the transition matrix and corresponding master equation derivatives for the single particle.

### Parameters

- derivs: master equation derivatives [length 2]
- work: vector [length 4]
- k: anisotropy strength constant for the uniaxial anisotropy
- v: volume of the particle in meter<sup>3</sup>
- T: temperature of environment in Kelvin
- ms: saturation magnetisation
- alpha: dimensionless damping constant
- t: time at which to evaluate the external field
- state\_probabilities: the current state probabilities for each of the 2 states (up and down) [length 2]
- applied\_field: a scalar function takes a double and returns a double. Given the current time should return normalised field  $h = (t)$  where the field is normalised by  $H_k$

double **single\_transition\_energy** (double K, double V, double h)

Compute the energy dissipated during one transition of the particle.

**Return** the energy dissipated in one transition

### Parameters

- K: anisotropy constant of the particle

- V: volume of the particle
- h: applied field on the particle, reduced by the anisotropy field  $H_k = \frac{2K}{\mu_0 M_s}$

### 7.1.5 Namespace driver

#### namespace driver

High level interface to differential equation integrators.

Drivers wrap the single step integrators and provide an interface for simulating differential equations for multiple steps from the initial condition. Drivers also handle memory management of the work arrays needed by the integrators.

**Author** Oliver Laslett

**Date** 2017

#### Functions

```
void rk4 (double *states, const double *initial_state, const std::function<void> double *, const
         double *, const double
         > derivs, const size_t n_steps, const size_t n_dims, const double step_size

void eulerm (double *states, const double *initial_state, const double *wiener_process, const
            std::function<void> double *, const double *, const double
            > drift, const std::function<void> double *, const double *, const double > diffusion, const size_t
            n_steps, const size_t n_dims, const size_t n_wiener, const double step_size

void heun (double *states, const double *initial_state, const double *wiener_process, const
          std::function<void> double *, double *, const double *, const double
          > sde, const size_t n_steps, const size_t n_dims, const size_t n_wiener, const double step_size

void implicit_midpoint (double *x, const double *x0, const double *dw, const
                      std::function<void> double *, double *, double *, double *, const double
                      *, const double, const double
                      > sde, const size_t n_dim, const size_t w_dim, const size_t n_steps, const double t0, const
                      double dt, const double eps, const size_t max_iter
```

### 7.1.6 Namespace energy

#### namespace energy

#### Functions

```
double anisotropy_r ()

double zeeman_r ()

double dipolar_r ()
```



## 7.1.7 Namespace field

### namespace field

Contains functions for computing magnetic fields.

Functions for computing effective fields from anistoropy and a range of time-varying applied fields.

**Author** Oliver Laslett

**Date** 2017

### Enums

#### enum options

*Values:*

**SINE**

**SQUARE**

**CONSTANT**

### Functions

**template** <typename... *T*>

std::function<double (double)> **bind\_field\_function**

std::function<doubledouble, T...> *func*, T... *bind\_args* Bind field parameters into a field function.

Field functions are of the form `std::function (double<double>)` This function allows additional arguments to be bound to functions and returns the function as a field function.

**Return** field function

#### Parameters

- *func*: function to bind
- *bind\_args*: arguments to bind

double **constant** (**const** double *t*, **const** double *h*)

A constant applied field.

A simple placeholder function representing a constant field. Always returns the same value.

**Return** the constant field amplitude at all values of time

#### Parameters

- *t*: time (parameter has no effect)
- *h*: applied field amplitude

double **sinusoidal** (**const** double *t*, **const** double *h*, **const** double *f*)

A sinusoidal alternating applied field.

Returns the value of a sinusoidally varying field at any given time.

**Return** the value of the varying applied field at time *t*

#### Parameters

- *t*: time

- `h`: applied field amplitude
- `f`: applied field frequency

double **square** (**const** double `t`, **const** double `h`, **const** double `f`)

A square wave switching applied field.

An alternating applied field with a square shape centred around zero. i.e. it alternates between values  $-h$  and  $h$

**Return** the value of the square wave applied field at time `t`

**Parameters**

- `t`: time
- `h`: applied field amplitude
- `f`: applied field frequency

double **square\_fourier** (**const** double `t`, **const** double `h`, **const** double `f`, **const** size\_t `n_components`)

A square wave applied field of finite Fourier components.

An approximate square wave is computed from a finite number of Fourier components. The square wave alternates between  $-h$  and  $h$ .

**Return** the value of the square wave applied field at time `t`

**Parameters**

- `t`: time
- `h`: applied field amplitude
- `f`: applied field frequency
- `n_components`: number of Fourier components to compute

void **multi\_add\_applied\_z\_field\_function** (double `*heff`, **const** std::function<double> `func`, **const** double `t`, **const** size\_t `N`)  
Add the applied field in the z direction.

void **uniaxial\_anisotropy** (double `*h_anis`, **const** double `*magnetisation`, **const** double `*anis_axis`)  
Effective field contribution from uniaxial anisotropy.

The effective field experienced by a single particle with a uniaxial anisotropy.

**Parameters**

- `h_anis`: effective field [length 3]
- `mag`: the magnetisation of the particle of [length 3]
- `axis`: the anisotropy axis of the particle [length 3]

void **multi\_add\_uniaxial\_anisotropy** (double `*h`, **const** double `*states`, **const** double `*axes`, **const** double `*k_reduced`, **const** size\_t `N`)  
Add the uniaxial anisotropy term term to the field of `N` particles.

**Parameters**

- `h`: effective field incremented with the anisotropy term
- `states`: magnetic state of the particles (length 3N)

- `axes`: anisotropy axis of each particle (length 3N)
- `k_reduced`: the reduced anisotropy constant for each particle (length N)
- `N`: number of particles

void **uniaxial\_anisotropy\_jacobian** (double *\*jac*, **const** double *\*axis*)  
 Jacobian of the uniaxial anisotropy effective field term.

The Jacobian of a particle's uniaxial anisotropy with respect to it's magnetisation value.  $J_h(m) = \frac{\partial h(m)}{\partial m}$

#### Parameters

- `jac`: the jacobian of the effective field [length 3x3]
- `axis`: the anisotropy axis of the particle [length 3]

void **multi\_add\_uniaxial\_anisotropy\_jacobian** (double *\*jac*, **const** double *\*axes*,  
**const** double *\*anis*, **const** size\_t *N*)  
 Jacobian of the uniaxial anisotropy effective field term for many particles.

The Jacobian of a particle's uniaxial anisotropy with respect to it's magnetisation value.  $J_h(m) = \frac{\partial h(m)}{\partial m}$

#### Parameters

- `jac`: the jacobian of the effective field [length 3Nx3N]
- `axes`: the anisotropy axis of the particle [length 3N]
- `N`: number of particles

void **multi\_add\_dipolar** (double *\*field*, **const** double *ms*, **const** double *k\_av*, **const** double  
*\*v\_reduced*, **const** double *\*mag*, **const** double *\*dists*, **const** double  
*\*dist\_cubes*, **const** size\_t *N*)

`field` is Nx3 and is the effective field on each particle `ms` is the same for all particles `k_av` is the average anisotropy constant for all particles `v_reduced` is the reduced volume of each particle `v_av` is the average volume for all particles `mag` is Nx3 long and is the magnetic state of each of the N particles `dists` is NxNx3 long and is the distance between each pair of particles `N` is the number of particles `dist_cubes` is NxN and is the reduced cubed distance between each pair

double **dipolar\_prefactor** (**const** double *ms*, **const** double *k\_av*)  
 Prefactor term (helper for `field::dipolar`)

prefactor is  $\frac{\mu_0 M_s^2}{8\pi K}$

**Return** prefactor term

#### Parameters

- `ms`: saturation magnetisation
- `k_av`: average anisotropy constant for system

void **dipolar\_add\_p2p\_term** (double *\*out*, **const** double *vj*, **const** double *rij3*, **const** double  
*\*mj*, **const** double *\*dist*, **const** double *prefactor*)

void **zero\_all\_field\_terms** (double *\*h*, **const** size\_t *N*)  
 Set all N values of the field to zero.

#### Parameters

- `h`: pointer to array of N doubles will all be set to zero
- `N`: number of elements in array

## 7.1.8 Namespace integrator

### namespace integrator

Numerical methods for differential equations.

Numerical methods for simulating the time evolution of deterministic and stochastic ordinary nonlinear differential equations. All integrators compute a single step of the solution.

**Author** Oliver Laslett

**Date** 2017

### Functions

```
void rk4 (double *next_state, double *k1, double *k2, double *k3, double *k4, const double *current_state, const std::function<void> double *, const double *, const double > derivs, const size_t n_dims, const double t, const double h

void heun (double *next_state, double *drift_arr, double *trial_drift_arr, double *diffusion_matrix, double *trial_diffusion_matrix, const double *current_state, const double *wiener_steps, const std::function<void> double *, double *, const double *, const double > sde, const size_t n_dims, const size_t wiener_dims, const double t, const double step_size

void eulerm (double *states, double *diffusion_matrix, const double *initial_state, const double *wiener_process, const std::function<void> double *, const double *, const double > drift, const std::function<void> double *, const double *, const double > diffusion, const size_t n_dims, const size_t n_wiener, const double t, const double step_size

template <class CSTATES, class CDIFF>
void milstein (CSTATES &next_state, const CSTATES &current_state, const CSTATES &drift, const CDIFF &diffusion, const CSTATES &wiener_increments, const double step_size)

int implicit_midpoint (double *x, double *dwm, double *a_work, double *b_work, double *adash_work, double *bdash_work, double *x_guess, double *x_opt_tmp, double *x_opt_jac, lapack_int *x_opt_ipiv, const double *x0, const double *dw, const std::function<void> double *, double *, double *, double *, const double *, const double *, const double, const double > sde, const size_t n_dim, const size_t w_dim, const double t, const double dt, const double eps, const size_t max_iter

void rk45 (double *next_state, double *temp_state, double *k1, double *k2, double *k3, double *k4, double *k5, double *k6, double *h_ptr, double *t_ptr, const double *current_state, const std::function<void> double *, const double *, const double > ode, const size_t n_dims, const double epsRK45 Cash-Karp adaptive step deterministic ODE solver.
```

Solves ODEs :) returns the next state and the time step to be used in the next instance what about the actual time step that it used? That's also important!

### namespace ck\_butcher\_table

Cash-Karp parameter table for RK45.

### Variables

```
constexpr double c11 = 0.2
```

```
constexpr double c21 = 3.0/40.0
```

```

constexpr double c22 = 9.0/40.0
constexpr double c31 = 3.0/10.0
constexpr double c32 = -9.0/10.0
constexpr double c33 = 6.0/5.0
constexpr double c41 = -11.0/54.0
constexpr double c42 = 2.5
constexpr double c43 = -70.0/27.0
constexpr double c44 = 35.0/27.0
constexpr double c51 = 1631.0/55296.0
constexpr double c52 = 175.0/512.0
constexpr double c53 = 575.0/13824.0
constexpr double c54 = 44275.0/110592.0
constexpr double c55 = 253.0/4096.0
constexpr double hc1 = 0.2
constexpr double hc2 = 0.3
constexpr double hc3 = 0.6
constexpr double hc4 = 1.0
constexpr double hc5 = 7.0/8.0
constexpr double x11 = 37.0/378.0
constexpr double x13 = 250.0/621.0
constexpr double x14 = 125.0/594.0
constexpr double x16 = 512.0/1771.0
constexpr double x21 = 2825.0/27648.0
constexpr double x23 = 18575.0/48384.0
constexpr double x24 = 13525.0/55296.0
constexpr double x25 = 277.0/14336.0
constexpr double x26 = 0.25

```

### 7.1.9 Namespace `integrator::ck_butcher_table`

**namespace** `integrator::ck_butcher_table`  
 Cash-Karp parameter table for RK45.

#### Variables

```

constexpr double c11 = 0.2
constexpr double c21 = 3.0/40.0
constexpr double c22 = 9.0/40.0

```

```
constexpr double c31 = 3.0/10.0
constexpr double c32 = -9.0/10.0
constexpr double c33 = 6.0/5.0
constexpr double c41 = -11.0/54.0
constexpr double c42 = 2.5
constexpr double c43 = -70.0/27.0
constexpr double c44 = 35.0/27.0
constexpr double c51 = 1631.0/55296.0
constexpr double c52 = 175.0/512.0
constexpr double c53 = 575.0/13824.0
constexpr double c54 = 44275.0/110592.0
constexpr double c55 = 253.0/4096.0
constexpr double hc1 = 0.2
constexpr double hc2 = 0.3
constexpr double hc3 = 0.6
constexpr double hc4 = 1.0
constexpr double hc5 = 7.0/8.0
constexpr double x11 = 37.0/378.0
constexpr double x13 = 250.0/621.0
constexpr double x14 = 125.0/594.0
constexpr double x16 = 512.0/1771.0
constexpr double x21 = 2825.0/27648.0
constexpr double x23 = 18575.0/48384.0
constexpr double x24 = 13525.0/55296.0
constexpr double x25 = 277.0/14336.0
constexpr double x26 = 0.25
```

### 7.1.10 Namespace io

namespace io

#### Functions

```
template <typename T>
int write_array (const std::string fname, T const *arr, const size_t len)
```

### 7.1.11 Namespace llg

#### namespace llg

Functions for evaluating the Landau-Lifshitz-Gilbert equation.

Includes the basic equation as well as Jacobians and combined functions to update fields during integration.

**Author** Oliver Laslett

**Date** 2017

#### Functions

void **drift** (double *\*deriv*, **const** double *\*state*, **const** double *time*, **const** double *alpha*, **const** double *\*heff*)

Deterministic drift component of the stochastic LLG.

##### Parameters

- *deriv*: drift derivative of the deterministic part of the stochastic llg [length 3]
- *state*: current state of the magnetisation vector [length 3]
- *t*: time (has no effect)
- *alpha*: damping ratio
- *the*: effective field on the magnetisation [length 3]

void **drift\_jacobian** (double *\*deriv*, **const** double *\*state*, **const** double *time*, **const** double *alpha*, **const** double *\*heff*, **const** double *\*heff\_jac*)

Jacobian of the deterministic drift component of the stochastic LLG. Since, in the general case, the effective field is a function of the magnetisation, the Jacobian of the effective field must be known in order to compute the Jacobian of the drift component.

##### Parameters

- *jac*: Jacobian of the drift [length 3x3]
- *m*: state of the magnetisation vector [length 3]
- *t*: time (has no effect)
- *a*: damping ratio  $\alpha$
- *h*: effective field acting on the magnetisation [length 3]
- *h\_j*: Jacobian of the effective field evaluated at the current value of *m* [length 3x3]

void **diffusion** (double *\*deriv*, **const** double *\*state*, **const** double *time*, **const** double *sr*, **const** double *alpha*)

The stochastic diffusion component of the stochastic LLG.

##### Parameters

- *deriv*: diffusion derivatives [length 3x3]
- *state*: current state of the magnetisation [length 3]
- *t*: time (has no effect)
- *sr*: normalised noise power of the thermal field (see notes on LLG normalisation for details)

- `alpha`: damping ratio

void **diffusion\_jacobian** (double *\*jacobian*, **const** double *\*state*, **const** double *time*, **const** double *sr*, **const** double *alpha*)  
Jacobian of the stochastic diffusion component of the LLG.

#### Parameters

- `jacobian`: Jacobian of the LLG diffusion [length 3x3]
- `state`: current state of the magnetisation vector [length 3]
- `t`: time (has no effect)
- `sr`: normalised noise power of the thermal field (see notes on LLG normalisation for details)
- `alpha`: damping ratio

void **sde\_with\_update** (double *\*drift*, double *\*diffusion*, double *\*heff*, **const** double *\*current\_state*, **const** double *drift\_time*, **const** double *diffusion\_time*, **const** double *\*happ*, **const** double *\*anisotropy\_axis*, **const** double *alpha*, **const** double *noise\_power*)

Computes drift and diffusion of LLG after updating the field.

The effective field is first computed based on the applied field and current state of the magnetisation. This is then used to compute the current drift and diffusion components of the LLG. Assumes uniaxial anisotropy.

#### Parameters

- `drift`: deterministic component of the LLG [length 3]
- `diffusion`: stochastic component of the LLG [length 3x3]
- `heff`: effective field including the applied field contribution [length 3]
- `state`: current state of the magnetisation [length 3]
- `a_t`: time at which to evaluate the drift
- `b_t`: time at which to evaluate the diffusion
- `happ`: the applied field at time `a_t` [length 3]
- `aaxis`: the anisotropy axis of the particle [length 3]
- `alpha`: damping ratio
- `sr`: normalised noise power of the thermal field (see notes on LLG normalisation for details)

void **jacobians\_with\_update** (double *\*drift*, double *\*diffusion*, double *\*drift\_jac*, double *\*diffusion\_jac*, double *\*heff*, double *\*heff\_jac*, **const** double *\*current\_state*, **const** double *drift\_time*, **const** double *diffusion\_time*, **const** double *\*happ*, **const** double *\*anisotropy\_axis*, **const** double *alpha*, **const** double *noise\_power*)

Computes effective field, drift, diffusion and Jacobians of LLG.

The effective field is first computed based on the applied field and current state of the magnetisation. This is then used to compute the drift, diffusion, and their respective Jacobians. Assumes uniaxial anisotropy.

#### Parameters

- `drift`: deterministic component of the LLG [length 3]
- `diffusion`: stochastic component of the LLG [length 3x3]



- `drift_jac`: Jacobian of the deterministic component [length 3x3]
- `diffusion_jac`: Jacobian of the diffusion component [length 3x3x3]
- `heff`: effective field including the applied field contribution [length 3]
- `heff_jac`: Jacobian of the effective field [length 3x3]
- `state`: current state of the magnetisation [length 3]
- `a_t`: time at which to evaluate the drift
- `b_t`: time at which to evaluate the diffusion
- `happ`: the applied field at time `a_t` [length 3]
- `aaxis`: the anisotropy axis of the particle [length 3]
- `alpha`: damping ratio
- `s`: normalised noise power of the thermal field (see notes on LLG normalisation for details)

void **multi\_drift** (double *\*deriv*, **const** double *\*state*, **const** double *\*alphas*, **const** double *\*heff*,  
**const** size\_t *N\_particles*)  
 Deterministic drift component of the stochastic LLG for many particles.

#### Parameters

- `deriv`: drift derivative of the deterministic part of the stochastic llg for each particle [length 3xN]
- `state`: current state of the magnetisation vectors [length 3xN]
- `t`: time (has no effect)
- `alpha`: damping ratio
- `heff`: the effective field on each particle [length 3xN]
- `N_particles`: the number of particles

void **multi\_diffusion** (double *\*deriv*, **const** double *\*state*, **const** double *\*field\_strengths*,  
**const** double *\*alphas*, **const** size\_t *N\_particles*)  
 Compute 3x3 block diagonal multi diffusion.

Note zero terms are not written.

void **multi\_stochastic\_llg\_field\_update** (double *\*drift*, double *\*diffusion*, double *\*heff*,  
**const** std::function<void> double *\**, **const**  
 double *\**, **const** double  
 > *heff\_func*, **const** double *\*state*, **const** double *t*, **const** double *\*alphas*, **const** double  
*\*field\_strengths*, **const** size\_t *N\_particles*) Updates field and computes LLG for N interacting particles.

`heff_fuc` is a function that returns the effective field given the current state and the current time. This can be whatever you want e.g. cubic anisotropy terms and interactions. EZEZE.

void **multi\_drift\_quasijacobian** (double *\*jac*, **const** double *\*m*, **const** double *\*alphas*,  
**const** double *\*h*, **const** double *\*hj*, size\_t *N\_particles*)  
 Computes the Jacobian of the drift for N interacting particles.

Assumes that `jac` is zero'd (i.e. function will not fill in 0 entries)

```
void multi_diffusion_jacobian(double *jacobian, const double *state, const double
                             *therm_field_strengths, const double *alphas, const size_t
                             N_particles)
```

Computes the Jacobian of the diffusion for N interacting particles.

Only computes non-zero values. jacobian must be 0 initialised before function call.

```
void multi_stochastic_llg_jacobians_field_update(double *drift, double *diffu-
                                                  sion, double *drift_jac, double
                                                  *diffusion_jac, double *heff,
                                                  double *heff_jac, const dou-
                                                  ble *state, const double t,
                                                  const double *alphas, const
                                                  double *field_strengths, const
                                                  size_t N_particles, const
                                                  std::function<void> double *,
                                                  const double *, const double
> heff_func, const std::function<void> double *, const double *, const double>
heff_jac_func
```

Computes all fields, drift/diffusion, jacobians for N particles.

The effective field is first computed based on the applied field and current state of the magnetisation. This is then used to compute the drift, diffusion, and their respective Jacobians. Assumes uniaxial anisotropy.

#### Parameters

- drift: deterministic component of the LLG [length 3]
- diffusion: stochastic component of the LLG [length 3x3]
- drift\_jac: Jacobian of the deterministic component [length 3x3]
- diffusion\_jac: Jacobian of the diffusion component [length 3x3x3]
- heff: effective field including the applied field contribution [length 3]
- heff\_jac: Jacobian of the effective field [length 3x3]
- state: current state of the magnetisation [length 3]
- a\_t: time at which to evaluate the drift
- b\_t: time at which to evaluate the diffusion
- happ: the applied field at time a\_t [length 3]
- aaxis: the anisotropy axis of the particle [length 3]
- alpha: damping ratio
- s: normalised noise power of the thermal field (see notes on LLG normalisation for details)

### 7.1.12 Namespace mnp

namespace mnp

#### Typedefs

```
using mnp::axis = typedef std::array<double, 3>
```

### 7.1.13 Namespace moma\_config

**Warning:** doxygennamespace: Cannot find namespace “moma\_config” in doxygen xml output for project “magpy-api” from directory: ../doxygen/doxyxml

### 7.1.14 Namespace optimisation

namespace optimisation

#### Functions

```
int newton_raphson_1 (double *x_root, const std::function<double> const double
    > f, const std::function<double> const double> fdash, const double x0, const double eps = 1e-7,
    const size_t max_iter = 1000

int newton_raphson_noinv (double *x_root, double *x_tmp, double *jac_out, lapack_int *ipiv,
    int *lapack_err_code, const std::function<void> double *, double *,
    const double *
    > func_and_jacobian, const double *x0, const lapack_int dim, const double eps = 1e-7, const
    size_t max_iter = 1000
```

#### Variables

```
const int SUCCESS = 0
    Optimisation success return code.

const int MAX_ITERATIONS_ERR = 1
    Optimisation maximum iterations reached error code.

const int LAPACK_ERR = 2
    Optimisation internal LAPACK error code.

    This error code indicates an error occurred in an internal LAPACK call. Further investigation will be needed
    to determine the cause.
```

### 7.1.15 Namespace simulation

namespace simulation

## Functions

```
std::vector<struct results> full_dynamics (const          std::vector<double>          ther-  
                                          mal_field_strengths, const std::vector<double>  
                                          reduced_anisotropy_constants,          const  
                                          std::vector<double>          reduced_particle_volumes,  
                                          const std::vector<d3>          anisotropy_unit_axes,  
                                          const std::vector<d3>          initial_magnetisations,  
                                          const          std::vector<std::vector<d3>>  
                                          interparticle_unit_distances,          const  
                                          std::vector<std::vector<double>>          interparti-  
                                          cle_reduced_distance_magnitudes,          const  
                                          std::function<double> const double  
> applied_field, const double average_anisotropy, const double average_volume, const double  
damping_constant, const double saturation_magnetisation, const double time_step, const double  
end_time, Rng &rng, const bool renorm, const bool interactions, const bool use_implicit, const  
double eps, const int max_samples
```

```
std::vector<results> full_dynamics (const          std::vector<double>          radius,          const  
                                  std::vector<double>          anisotropy, const std::vector<d3>  
                                  anisotropy_axes,          const std::vector<d3>          magnetisa-  
                                  tion_direction, const std::vector<d3>          location, const  
                                  double magnetisation, const double damping, const  
                                  double temperature, const bool renorm, const bool  
                                  interactions, const bool use_implicit, const double  
                                  eps, const double time_step, const double end_time,  
                                  const size_t max_samples, const long seed, const  
                                  field::options field_option = field::CONSTANT, const double  
                                  field_amplitude = 0.0, const double field_frequency = 0.0)
```

```
struct results dom_ensemble_dynamics (const double volume, const double anisotropy,  
                                     const double temperature, const double  
                                     magnetisation, const double alpha, const  
                                     std::function<double> double  
> applied_field, const std::array<double, 2> initial_mags, const double time_step, const double  
end_time, const int max_samples
```

```
void save_results (const std::string fname, const struct results &res)  
    Save results to disk.
```

Saves the contents of a results struct to disk. Given a file name ‘foo’ the following files are written to disk ‘foo.mx’, ‘foo.my’, ‘foo.mz’, ‘foo.field’, ‘foo.time’, ‘foo.energy’.

### Parameters

- *fname*: /path/to/filename prefix for files
- *res*: results struct to save

```
void zero_results (struct results &res)  
    Initialise results memory to zero.
```

### Parameters

- *res*: results struct to zero

```
void reduce_to_system_magnetisation (double *mag, const double *particle_mags, const  
size_t N_particles)
```

## 7.1.16 Namespace stochastic

**namespace stochastic**

### Functions

void **master\_equation** (double \*derivs, **const** double \*transition\_matrix, **const** double \*current\_state, **const** size\_t dim)

Evaluates the derivatives of the master equation given a transition matrix.

The master equation is simply a linear system of ODEs, with coefficients described by the transition matrix.

$$\frac{dx}{dt} = Wx$$

### Parameters

- derivs: the master equation derivatives [length dim]
- transition\_matrix: the [dim x dim] transition matrix (row-major)  $W$
- current\_state: values of the state vector  $x$

## 7.1.17 Namespace trap

**namespace trap**

numerical schemes for computing the area under curves

**Author** Oliver Laslett

### Functions

double **trapezoidal** (double \*x, double \*y, size\_t  $N$ )

double **one\_trapezoid** (double  $x1$ , double  $x2$ , double  $fx1$ , double  $fx2$ )

## 7.2 File list

### 7.2.1 File constants.hpp

**namespace constants**

### Variables

**const** double **KB** = 1.38064852e-23

**const** double **MU0** = 1.25663706e-6

**const** double **GYROMAG** = 1.76086e11

## 7.2.2 File curry.hpp

**Warning:** doxygenfile: Cannot find file “curry.hpp”

## 7.2.3 File distances.cpp

### Functions

`std::vector<std::vector<double>>> pair_wise_distance_magnitude` (`std::vector<std::array<double, 3>>> points`)

Computes the Euclidean distance between pairs of points.

#### **namespace distances**

Compute distances between points.

Functions for computing distances between points in 3D space.

**Author** Oliver Laslett

**Date** 2017

## 7.2.4 File distances.hpp

#### **namespace distances**

Compute distances between points.

Functions for computing distances between points in 3D space.

**Author** Oliver Laslett

**Date** 2017

### Functions

`std::vector<std::vector<std::array<double, 3>>> pair_wise_distance_vectors` (`std::vector<std::array<double, 3>>> points`)

Computes the distance vector between points in 3d space.

Given a list of x,y,z coordinates, compute the distance vector between every pair of x,y,z coordinates in the list.

**Return** NxN `std::vector` matrix of distances between each pair of points

#### **Parameters**

- `points`: length N vector of arrays of x,y,z coordinates

`std::vector<std::vector<double>>> pair_wise_distance_magnitude` (`std::vector<std::array<double, 3>>> points`)

Computes the Euclidean distance between pairs of points.

`std::vector<std::vector<std::array<double, 3>>> pair_wise_distance_unit_vectors` (`std::vector<std::array<double, 3>>> points`)

Computes the unit distance vector between a list of points.

`std::vector<std::vector<double>>> pair_wise_distance_magnitude` (`std::vector<std::vector<std::array<double, 3>>> distance_vectors`)

Computes the Euclidean distance from a matrix of distance vectors.

Given a matrix of distance vectors, compute the 2norm of the vector corresponding to the Euclidean distance.

**Return** NxN matrix of Euclidean distance values

#### Parameters

- `distance_vectors`: NxN symmetrical matrix of distance vectors (x,y,z coordinates)

`std::vector<std::vector<std::array<double, 3>>> pair_wise_distance_unit_vectors` (`std::vector<std::vector<std::array<double, 3>>> distance_vectors, std::vector<std::vector<double>>> distance_magnitudes`)

Computes the unit distance vectors from distance vectors and their magnitudes.

## 7.2.5 File dom.cpp

## 7.2.6 File dom.hpp

### namespace dom

discrete orientation model for magnetic particles

### Functions

void **transition\_matrix** (`double *W, const double k, const double v, const double T, const double h, const double ms, const double alpha`)

Compute the 2x2 transition matrix for a single particle.

Assumes uniaxial anisotropy and an applied field  $h < 1$  Only valid for large energy barriers:  $(1-h)^2 \gg 1$

#### Parameters

- `W`: transition matrix [2x2]
- `k`: anisotropy strength constant for the uniaxial anisotropy
- `v`: volume of the particle in meter<sup>3</sup>
- `T`: temperature of environment in Kelvin
- `h`: dimensionless applied field - normalised by  $H_k = \frac{2K}{\mu_0 M_s}$
- `ms`: saturation magnetisation
- `alpha`: dimensionless damping constant

void **master\_equation\_with\_update** (`double *derivs, double *work, const double k, const double v, const double T, const double ms, const double alpha, const double t, const double *state_probabilities, const std::function<double> double > applied_field`)

Computes master equation for particle in time-dependent field.

Computes the applied field in the z-direction at time t. Uses the field value to compute the transition matrix and corresponding master equation derivatives for the single particle.

**Parameters**

- `derivs`: master equation derivatives [length 2]
- `work`: vector [length 4]
- `k`: anisotropy strength constant for the uniaxial anisotropy
- `v`: volume of the particle in meter<sup>3</sup>
- `T`: temperature of environment in Kelvin
- `ms`: saturation magnetisation
- `alpha`: dimensionless damping constant
- `t`: time at which to evaluate the external field
- `state_probabilities`: the current state probabilities for each of the 2 states (up and down) [length 2]
- `applied_field`: a scalar function takes a double and returns a double. Given the current time should return normalised field  $h = (t)$  where the field is normalised by  $H_k$

double **single\_transition\_energy** (double *K*, double *V*, double *h*)

Compute the energy dissipated during one transition of the particle.

**Return** the energy dissipated in one transition

**Parameters**

- *K*: anisotropy constant of the particle
- *V*: volume of the particle
- *h*: applied field on the particle, reduced by the anisotropy field  $H_k = \frac{2K}{\mu_0 M_s}$

## 7.2.7 File energy.hpp

namespace **energy**

**Functions**

double **anisotropy\_r** ()

double **zeeman\_r** ()

double **dipolar\_r** ()

## 7.2.8 File field.cpp

**Defines**

**\_USE\_MATH\_DEFINES**



**namespace field**

Contains functions for computing magnetic fields.

Functions for computing effective fields from anistoropy and a range of time-varying applied fields.

**Author** Oliver Laslett

**Date** 2017

## 7.2.9 File field.hpp

**namespace field**

Contains functions for computing magnetic fields.

Functions for computing effective fields from anistoropy and a range of time-varying applied fields.

**Author** Oliver Laslett

**Date** 2017

### Enums

**enum options**

*Values:*

**SINE**

**SQUARE**

**CONSTANT**

### Functions

**template** <typename... *T*>

std::function<double (double)> **bind\_field\_function**

std::function<doubledouble, T...> *func*, T... *bind\_args* Bind field parameters into a field function.

Field functions are of the form `std::function<double<double>>` This function allows additional arguments to be bound to functions and returns the function as a field function.

**Return** field function

**Parameters**

- *func*: function to bind
- *bind\_args*: arguments to bind

double **constant** (**const** double *t*, **const** double *h*)

A constant applied field.

A simple placeholder function representing a constant field. Always returns the same value.

**Return** the constant field amplitude at all values of time

**Parameters**

- *t*: time (parameter has no effect)
- *h*: applied field amplitude

double **sinusoidal** (**const** double *t*, **const** double *h*, **const** double *f*)

A sinusoidal alternating applied field.

Returns the value of a sinusoidally varying field at any given time.

**Return** the value of the varying applied field at time *t*

**Parameters**

- *t*: time
- *h*: applied field amplitude
- *f*: applied field frequency

double **square** (**const** double *t*, **const** double *h*, **const** double *f*)

A square wave switching applied field.

An alternating applied field with a square shape centred around zero. i.e. it alternates between values  $-h$  and  $h$

**Return** the value of the square wave applied field at time *t*

**Parameters**

- *t*: time
- *h*: applied field amplitude
- *f*: applied field frequency

double **square\_fourier** (**const** double *t*, **const** double *h*, **const** double *f*, **const** size\_t *n\_components*)

A square wave applied field of finite Fourier components.

An approximate square wave is computed from a finite number of Fourier components. The square wave alternates between  $-h$  and  $h$ .

**Return** the value of the square wave applied field at time *t*

**Parameters**

- *t*: time
- *h*: applied field amplitude
- *f*: applied field frequency
- *n\_components*: number of Fourier components to compute

void **multi\_add\_applied\_Z\_field\_function** (double *heff*, **const** std::function<double> *hfunc*, **const** double *t*, **const** size\_t *N*) Add the applied field in the z direction.

void **uniaxial\_anisotropy** (double *h\_anis*, **const** double *magnetisation*, **const** double *anis\_axis*)

Effective field contribution from uniaxial anisotropy.

The effective field experienced by a single particle with a uniaxial anisotropy.

**Parameters**

- *h\_anis*: effective field [length 3]
- *mag*: the magnetisation of the particle of [length 3]
- *axis*: the anisotropy axis of the particle [length 3]

void **multi\_add\_uniaxial\_anisotropy** (double \*h, **const** double \*states, **const** double \*axes, **const** double \*k\_reduced, **const** size\_t N)  
Add the uniaxial anisotropy term to the field of N particles.

#### Parameters

- h: effective field incremented with the anisotropy term
- states: magnetic state of the particles (length 3N)
- axes: anisotropy axis of each particle (length 3N)
- k\_reduced: the reduced anisotropy constant for each particle (length N)
- N: number of particles

void **uniaxial\_anisotropy\_jacobian** (double \*jac, **const** double \*axis)  
Jacobian of the uniaxial anisotropy effective field term.

The Jacobian of a particle's uniaxial anisotropy with respect to it's magnetisation value.  $J_h(m) = \frac{\partial h(m)}{\partial m}$

#### Parameters

- jac: the jacobian of the effective field [length 3x3]
- axis: the anisotropy axis of the particle [length 3]

void **multi\_add\_uniaxial\_anisotropy\_jacobian** (double \*jac, **const** double \*axes, **const** double \*anis, **const** size\_t N)  
Jacobian of the uniaxial anisotropy effective field term for many particles.

The Jacobian of a particle's uniaxial anisotropy with respect to it's magnetisation value.  $J_h(m) = \frac{\partial h(m)}{\partial m}$

#### Parameters

- jac: the jacobian of the effective field [length 3Nx3N]
- axis: the anisotropy axis of the particle [length 3N]
- N: number of particles

void **multi\_add\_dipolar** (double \*field, **const** double ms, **const** double k\_av, **const** double \*v\_reduced, **const** double \*mag, **const** double \*dists, **const** double \*dist\_cubes, **const** size\_t N)  
field is Nx3 and is the effective field on each particle ms is the same for all particles k\_av is the average anisotropy constant for all particles v\_reduced is the reduced volume of each particle v\_av is the average volume for all particles mag is Nx3 long and is the magnetic state of each of the N particles dists is NxNx3 long and is the distance between each pair of particles N is the number of particles dist\_cubes is NxN and is the reduced cubed distance between each pair

double **dipolar\_prefactor** (**const** double ms, **const** double k\_av)  
Prefactor term (helper for field::dipolar)

prefactor is  $\frac{\mu_0 M_s^2}{8\pi K}$

**Return** prefactor term

#### Parameters

- ms: saturation magnetisation
- k\_av: average anisotropy constant for system

void **dipolar\_add\_p2p\_term** (double \*out, **const** double vj, **const** double rij3, **const** double \*mj, **const** double \*dist, **const** double prefactor)

void **zero\_all\_field\_terms** (double \**h*, **const** size\_t *N*)  
Set all *N* values of the field to zero.

#### Parameters

- *h*: pointer to array of *N* doubles will all be set to zero
- *N*: number of elements in array

## 7.2.10 File integrators.cpp

Integrator implementation

### Typedefs

```
using sde_function = std::function<void (double *, const double *, const double) >  
using sde_func = std::function<void (double *, double *, const double *, const double) >  
using sde_jac = std::function<void (double *, double *, double *, double *, const double *, const  
double, const double) >
```

#### namespace integrator

Numerical methods for differential equations.

Numerical methods for simulating the time evolution of deterministic and stochastic ordinary nonlinear differential equations. All integrators compute a single step of the solution.

**Author** Oliver Laslett

**Date** 2017

#### namespace driver

High level interface to differential equation integrators.

Drivers wrap the single step integrators and provide an interface for simulating differential equations for multiple steps from the initial condition. Drivers also handle memory management of the work arrays needed by the integrators.

**Author** Oliver Laslett

**Date** 2017

## 7.2.11 File integrators.hpp

Header includes various numerical methods for estimating solutions to stochastic and deterministic ODEs. Methods included in this are: -ODEs: RK4 -SDEs: Euler, Heun

#### namespace driver

High level interface to differential equation integrators.

Drivers wrap the single step integrators and provide an interface for simulating differential equations for multiple steps from the initial condition. Drivers also handle memory management of the work arrays needed by the integrators.

**Author** Oliver Laslett

**Date** 2017

## Functions

```
void rk4 (double *states, const double *initial_state, const std::function<void> double *, const
        double *, const double
        > derivs, const size_t n_steps, const size_t n_dims, const double step_size)

void eulerm (double *states, const double *initial_state, const double *wiener_process, const
        std::function<void> double *, const double *, const double
        > drift, const std::function<void> double *, const double *, const double > diffusion, const size_t
        n_steps, const size_t n_dims, const size_t n_wiener, const double step_size)

void heun (double *states, const double *initial_state, const double *wiener_process, const
        std::function<void> double *, double *, const double *, const double
        > sde, const size_t n_steps, const size_t n_dims, const size_t n_wiener, const double step_size)

void implicit_midpoint (double *x, const double *x0, const double *dw, const
        std::function<void> double *, double *, double *, double *, const double
        *, const double, const double
        > sde, const size_t n_dim, const size_t w_dim, const size_t n_steps, const double t0, const
        double dt, const double eps, const size_t max_iter)
```

### namespace integrator

Numerical methods for differential equations.

Numerical methods for simulating the time evolution of deterministic and stochastic ordinary nonlinear differential equations. All integrators compute a single step of the solution.

**Author** Oliver Laslett

**Date** 2017

## Functions

```
void rk4 (double *next_state, double *k1, double *k2, double *k3, double *k4, const double *cur-
        rent_state, const std::function<void> double *, const double *, const double
        > derivs, const size_t n_dims, const double t, const double h)

void heun (double *next_state, double *drift_arr, double *trial_drift_arr, double *diffusion_matrix, dou-
        ble *trial_diffusion_matrix, const double *current_state, const double *wiener_steps,
        const std::function<void> double *, double *, const double *, const double
        > sde, const size_t n_dims, const size_t wiener_dims, const double t, const double step_size)

void eulerm (double *states, double *diffusion_matrix, const double *initial_state, const double
        *wiener_process, const std::function<void> double *, const double *, const double
        > drift, const std::function<void> double *, const double *, const double > diffusion, const size_t
        n_dims, const size_t n_wiener, const double t, const double step_size)

template <class CSTATES, class CDIFF>
void milstein (CSTATES &next_state, const CSTATES &current_state, const CSTATES &drift,
        const CDIFF &diffusion, const CSTATES &wiener_increments, const double
        step_size)

int implicit_midpoint (double *x, double *dwm, double *a_work, double *b_work, double
        *adash_work, double *bdash_work, double *x_guess, double *x_opt_tmp,
        double *x_opt_jac, lapack_int *x_opt_ipiv, const double *x0, const
        double *dw, const std::function<void> double *, double *, double *, dou-
        ble *, const double *, const double, const double
        > sde, const size_t n_dim, const size_t w_dim, const double t, const double dt, const double
        eps, const size_t max_iter)
```

```
void rk45 (double *next_state, double *temp_state, double *k1, double *k2, double *k3, double *k4,  
          double *k5, double *k6, double *h_ptr, double *t_ptr, const double *current_state, const  
          std::function<void> double *, const double *, const double  
          > ode, const size_t n_dims, const double epsRK45) Cash-Karp adaptive step deterministic ODE solver.
```

Solves ODEs :) returns the next state and the time step to be used in the next instance what about the actual time step that it used? That's also important!

**namespace ck\_butcher\_table**

Cash-Karp parameter table for RK45.

### Variables

```
constexpr double c11 = 0.2  
constexpr double c21 = 3.0/40.0  
constexpr double c22 = 9.0/40.0  
constexpr double c31 = 3.0/10.0  
constexpr double c32 = -9.0/10.0  
constexpr double c33 = 6.0/5.0  
constexpr double c41 = -11.0/54.0  
constexpr double c42 = 2.5  
constexpr double c43 = -70.0/27.0  
constexpr double c44 = 35.0/27.0  
constexpr double c51 = 1631.0/55296.0  
constexpr double c52 = 175.0/512.0  
constexpr double c53 = 575.0/13824.0  
constexpr double c54 = 44275.0/110592.0  
constexpr double c55 = 253.0/4096.0  
constexpr double hc1 = 0.2  
constexpr double hc2 = 0.3  
constexpr double hc3 = 0.6  
constexpr double hc4 = 1.0  
constexpr double hc5 = 7.0/8.0  
constexpr double x11 = 37.0/378.0  
constexpr double x13 = 250.0/621.0  
constexpr double x14 = 125.0/594.0  
constexpr double x16 = 512.0/1771.0  
constexpr double x21 = 2825.0/27648.0  
constexpr double x23 = 18575.0/48384.0  
constexpr double x24 = 13525.0/55296.0
```

```
constexpr double x25 = 277.0/14336.0
```

```
constexpr double x26 = 0.25
```

## 7.2.12 File io.hpp

```
namespace io
```

### Functions

```
template <typename T>
int write_array (const std::string fname, T const *arr, const size_t len)
```

## 7.2.13 File llg.cpp

## 7.2.14 File llg.hpp

```
namespace llg
```

Functions for evaluating the Landau-Lifshitz-Gilbert equation.

Includes the basic equation as well as Jacobians and combined functions to update fields during integration.

**Author** Oliver Laslett

**Date** 2017

### Functions

```
void drift (double *deriv, const double *state, const double time, const double alpha, const
            double *heff)
```

Deterministic drift component of the stochastic LLG.

#### Parameters

- `deriv`: drift derivative of the deterministic part of the stochastic llg [length 3]
- `state`: current state of the magnetisation vector [length 3]
- `t`: time (has no effect)
- `alpha`: damping ratio
- `the`: effective field on the magnetisation [length 3]

```
void drift_jacobian (double *deriv, const double *state, const double time, const double al-
                    pha, const double *heff, const double *heff_jac)
```

Jacobian of the deterministic drift component of the stochastic LLG Since, in the general case, the effective field is a function of the magnetisation, the Jacobian of the effective field must be known in order to compute the Jacobian of the drift component.

#### Parameters

- `jac`: Jacobian of the drift [length 3x3]
- `m`: state of the magnetisation vector [length 3]
- `t`: time (has no effect)

- a: damping ratio  $\alpha$
- h: effective field acting on the magnetisation [length 3]
- h<sub>j</sub>: Jacobian of the effective field evaluated at the current value of m [length 3x3]

void **diffusion** (double \*deriv, **const** double \*state, **const** double time, **const** double sr, **const** double alpha)

The stochastic diffusion component of the stochastic LLG.

#### Parameters

- deriv: diffusion derivatives [length 3x3]
- state: current state of the magnetisation [length 3]
- t: time (has no effect)
- sr: normalised noise power of the thermal field (see notes on LLG normalisation for details)
- alpha: damping ratio

void **diffusion\_jacobian** (double \*jacobian, **const** double \*state, **const** double time, **const** double sr, **const** double alpha)

Jacobian of the stochastic diffusion component of the LLG.

#### Parameters

- jacobian: Jacobian of the LLG diffusion [length 3x3]
- state: current state of the magnetisation vector [length 3]
- t: time (has no effect)
- sr: normalised noise power of the thermal field (see notes on LLG normalisation for details)
- alpha: damping ratio

void **sde\_with\_update** (double \*drift, double \*diffusion, double \*heff, **const** double \*current\_state, **const** double drift\_time, **const** double diffusion\_time, **const** double \*happ, **const** double \*anisotropy\_axis, **const** double alpha, **const** double noise\_power)

Computes drift and diffusion of LLG after updating the field.

The effective field is first computed based on the applied field and current state of the magnetisation. This is then used to compute the current drift and diffusion components of the LLG. Assumes uniaxial anisotropy.

#### Parameters

- drift: deterministic component of the LLG [length 3]
- diffusion: stochastic component of the LLG [length 3x3]
- heff: effective field including the applied field contribution [length 3]
- state: current state of the magnetisation [length 3]
- a\_t: time at which to evaluate the drift
- b\_t: time at which to evaluate the diffusion
- happ: the applied field at time a\_t [length 3]
- aaxis: the anisotropy axis of the particle [length 3]
- alpha: damping ratio



- `sr`: normalised noise power of the thermal field (see notes on LLG normalisation for details)

void **jacobians\_with\_update** (double *\*drift*, double *\*diffusion*, double *\*drift\_jac*, double *\*diffusion\_jac*, double *\*heff*, double *\*heff\_jac*, **const** double *\*current\_state*, **const** double *drift\_time*, **const** double *diffusion\_time*, **const** double *\*happ*, **const** double *\*anisotropy\_axis*, **const** double *alpha*, **const** double *noise\_power*)

Computes effective field, drift, diffusion and Jacobians of LLG.

The effective field is first computed based on the applied field and current state of the magnetisation. This is then used to compute the drift, diffusion, and their respective Jacobians. Assumes uniaxial anisotropy.

#### Parameters

- `drift`: deterministic component of the LLG [length 3]
- `diffusion`: stochastic component of the LLG [length 3x3]
- `drift_jac`: Jacobian of the deterministic component [length 3x3]
- `diffusion_jac`: Jacobian of the diffusion component [length 3x3x3]
- `heff`: effective field including the applied field contribution [length 3]
- `heff_jac`: Jacobian of the effective field [length 3x3]
- `state`: current state of the magnetisation [length 3]
- `a_t`: time at which to evaluate the drift
- `b_t`: time at which to evaluate the diffusion
- `happ`: the applied field at time `a_t` [length 3]
- `aaxis`: the anisotropy axis of the particle [length 3]
- `alpha`: damping ratio
- `s`: normalised noise power of the thermal field (see notes on LLG normalisation for details)

void **multi\_drift** (double *\*deriv*, **const** double *\*state*, **const** double *\*alphas*, **const** double *\*heff*, **const** size\_t *N\_particles*)

Deterministic drift component of the stochastic LLG for many particles.

#### Parameters

- `deriv`: drift derivative of the deterministic part of the stochastic llg for each particle [length 3xN]
- `state`: current state of the magnetisation vectors [length 3xN]
- `t`: time (has no effect)
- `alpha`: damping ratio
- `heff`: the effective field on each particle [length 3xN]
- `N_particles`: the number of particles

void **multi\_diffusion** (double *\*deriv*, **const** double *\*state*, **const** double *\*field\_strengths*, **const** double *\*alphas*, **const** size\_t *N\_particles*)

Compute 3x3 block diagonal multi diffusion.

Note zero terms are not written.

```
void multi_stochastic_llg_field_update (double *drift, double *diffusion, double *heff,
                                         const std::function<void> double *, const
                                         double *, const double
> heff_func, const double *state, const double t, const double *alphas, const double
*field_strengths, const size_t N_particles)Updates field and computes LLG for N interacting particles.
```

heff\_fuc is a function that returns the effective field given the current state and the current time. This can be whatever you want e.g. cubic anisotropy terms and interactions. EZEZE.

```
void multi_drift_quasijacobian (double *jac, const double *m, const double *alphas,
                                const double *h, const double *hj, size_t N_particles)
Computes the Jacobian of the drift for N interacting particles.
```

Assumes that jac is zero'd (i.e. function will not fill in 0 entries)

```
void multi_diffusion_jacobian (double *jacobian, const double *state, const double
*therm_field_strengths, const double *alphas, const size_t
N_particles)
Computes the Jacobian of the diffusion for N interacting particles.
```

Only computes non-zero values. jacobian must be 0 initialised before function call.

```
void multi_stochastic_llg_jacobians_field_update (double *drift, double *diffu-
sion, double *drift_jac, double
*diffusion_jac, double *heff,
double *heff_jac, const dou-
ble *state, const double t,
const double *alphas, const
double *field_strengths, const
size_t N_particles, const
std::function<void> double *,
const double *, const double
> heff_func, const std::function<void>double *, const double *, const double>
heff_jac_func)Computes all fields, drift/diffusion, jacobians for N particles.
```

The effective field is first computed based on the applied field and current state of the magnetisation. This is then used to compute the drift, diffusion, and their respective Jacobians. Assumes uniaxial anisotropy.

#### Parameters

- drift: deterministic component of the LLG [length 3]
- diffusion: stochastic component of the LLG [length 3x3]
- drift\_jac: Jacobian of the deterministic component [length 3x3]
- diffusion\_jac: Jacobian of the diffusion component [length 3x3x3]
- heff: effective field including the applied field contribution [length 3]
- heff\_jac: Jacobian of the effective field [length 3x3]
- state: current state of the magnetisation [length 3]
- a\_t: time at which to evaluate the drift
- b\_t: time at which to evaluate the diffusion
- happ: the applied field at time a\_t [length 3]
- aaxis: the anisotropy axis of the particle [length 3]
- alpha: damping ratio
- s: normalised noise power of the thermal field (see notes on LLG normalisation for details)

### 7.2.15 File mnps.hpp

```
namespace mnp
```

#### Typedefs

```
using mnp::axis = typedef std::array<double,3>
```

```
struct norm_params
```

#### Public Members

```
double gamma
```

```
double alpha
```

```
double stability
```

```
double volume
```

```
double temperature
```

```
axis anisotropy_axis
```

```
struct params
```

#### Public Members

```
double gamma
```

```
double alpha
```

```
double saturation_mag
```

```
double diameter
```

```
double anisotropy
```

```
axis anisotropy_axis
```

### 7.2.16 File moma\_config.cpp

**Warning:** doxygenfile: Cannot find file “moma\_config.cpp”

### 7.2.17 File moma\_config.hpp

**Warning:** doxygenfile: Cannot find file “moma\_config.hpp”

### 7.2.18 File optimisation.cpp

Numerical methods for optimisation and root finding.

Contains Newton Raphson methods for root finding.

### 7.2.19 File optimisation.hpp

Contains numerical methods for optimisation and root-finding.

**Author** Oliver W. Laslett

**Date** 2016

**namespace** `optimisation`

#### Functions

```
int newton_raphson_1 (double *x_root, const std::function<double> const double  
    > f, const std::function<double> const double> fdash, const double x0, const double eps = 1e-7,  
    const size_t max_iter = 1000  
  
int newton_raphson_noinv (double *x_root, double *x_tmp, double *jac_out, lapack_int *ipiv,  
    int *lapack_err_code, const std::function<void> double *, double *,  
    const double *  
    > func_and_jacobian, const double *x0, const lapack_int dim, const double eps = 1e-7, const  
    size_t max_iter = 1000
```

#### Variables

```
const int SUCCESS = 0  
    Optimisation success return code.  
  
const int MAX_ITERATIONS_ERR = 1  
    Optimisation maximum iterations reached error code.  
  
const int LAPACK_ERR = 2  
    Optimisation internal LAPACK error code.  
  
    This error code indicates an error occurred in an internal LAPACK call. Further investigation will be needed  
    to determine the cause.
```

### 7.2.20 File rng.cpp

Class for holding different random number generators.

### 7.2.21 File rng.hpp

Class for holding different random number generators.

**Author** Oliver W. Laslett

```
class Rng  
    #include <rng.hpp> Abstract class for random number generators.  
    Subclassed by RngArray, RngMtDownsample, RngMtNorm
```

## Public Functions

**virtual double get () = 0**

Get a single random number.

**Return** a single draw from the random number generator

**class RngMtNorm**

*#include <rng.hpp>* Uses Mersenne Twister to generate normally distributed values.

Random numbers have a mean of zero and a user specified standard deviation.

Inherits from *Rng*

## Public Functions

**RngMtNorm (const unsigned long int seed, const double std)**

Default constructor for *RngMtNorm*.

### Parameters

- seed: seed for random number generator
- std: the standard deviation of the normally distributed numbers

**double get ()**

Draw a single normally distributed value from the RNG.

**Return** single normally distributed number

## Private Members

**std::mt19937\_64 generator**

A Mersenne twister generator instance.

**std::normal\_distribution<double> dist**

A normal distribution instance.

**class RngMtDownsample**

*#include <rng.hpp>* Generate normally distributed values with downsampling.

Uses the Mersenne Twister to generate normally distributed random numbers. Down-samples the stream of random numbers by summing consecutive draws along each dimension. Function is usually used for generating coarse Wiener processes

Inherits from *Rng*

## Public Functions

**RngMtDownsample (const unsigned long int seed, const double std, const size\_t dim, const size\_t down\_factor)**

Default constructor for *RngMtDownsample*.

double **get** ()

Get a single downsampled value from the random number generator.

## Private Functions

void **downsample\_draw** ()

## Private Members

std::mt19937\_64 **generator**

A Mersenne Twister generator instance.

std::normal\_distribution<double> **dist**

A normal distribution instance.

size\_t **current\_dim**

Stores the current state of the output dimension.

std::vector<double> **store**

Stores consecutive random numbers.

**const** size\_t **D**

The number of dimensions required.

**const** size\_t **F**

The number of consecutive random numbers to downsample.

**class RngArray**

*#include <rng.hpp>* Provides an *Rng* interface to a predefined array of numbers.

Inherits from *Rng*

## Public Functions

**RngArray** (**const** double \**arr*, size\_t *arr\_length*, size\_t *stride* = 1)

Default constructor for *RngArray*.

### Parameters

- *\_arr*: a predefined array of random numbers
- *\_arr\_length*: length of the predefined array
- *\_stride*: the number of consecutive elements to stride for each call to *.get()*

double **get** ()

Get the next (possibly stridden) value from the array.

The first call will always return the value at the 0th index. Each subsequent call will stride the array (default value is 1) and return that value. A call that extends beyond the end of the array will result in an error.

### Exceptions

- `std::out_of_range`: when a call attempts to get a value beyond the maximum length of the predefined array.

## Private Members

unsigned int **i** =0  
Internal state.

**const** size\_t **max**  
Maximum number of draws available.

**const** double \***arr**  
Pointer to the predefined array of numbers.

**const** size\_t **stride**  
Number of values to stride for each draw.

## 7.2.22 File simulation.cpp

## 7.2.23 File simulation.hpp

### Typedefs

```
using d3 = std::array<double, 3>
using rng_vec = std::vector<std::shared_ptr<Rng>, std::allocator<std::shared_ptr<Rng>>>
using sde_jac = std::function<void (double *, double *, double *, double *, const double *, const
double, const double) >
namespace simulation
```

### Functions

```
std::vector<struct results> full_dynamics (const std::vector<double> thermal_field_strengths, const std::vector<double>
reduced_anisotropy_constants, const std::vector<double> reduced_particle_volumes,
const std::vector<d3> anisotropy_unit_axes,
const std::vector<d3> initial_magnetisations,
const std::vector<std::vector<d3>> interparticle_unit_distances, const
std::vector<std::vector<double>> interparticle_reduced_distance_magnitudes, const
std::function<double>) const double
> applied_field, const double average_anisotropy, const double average_volume, const double
damping_constant, const double saturation_magnetisation, const double time_step, const double
end_time, Rng &rng, const bool renorm, const bool interactions, const bool use_implicit, const
double eps, const int max_samples
```

```
std::vector<results> full_dynamics (const      std::vector<double>      radius,      const
                                   std::vector<double> anisotropy,      const std::vector<d3>
                                   anisotropy_axes,      const std::vector<d3> magnetisa-
                                   tion_direction,      const std::vector<d3> location,      const
                                   double magnetisation,      const double damping,      const
                                   double temperature,      const bool renorm,      const bool
                                   interactions,      const bool use_implicit,      const double
                                   eps,      const double time_step,      const double end_time,
                                   const size_t max_samples,      const long seed,      const
                                   field::options field_option = field::CONSTANT,      const double
                                   field_amplitude = 0.0,      const double field_frequency = 0.0)

struct results dom_ensemble_dynamics (const double volume,      const double anisotropy,
                                       const double temperature,      const double
                                       magnetisation,      const double alpha,      const
                                       std::function<double> double
                                       > applied_field,      const std::array<double, 2> initial_mags,      const double time_step,      const double
                                       end_time,      const int max_samples
```

```
void save_results (const std::string fname,      const struct results &res)
    Save results to disk.
```

Saves the contents of a results struct to disk. Given a file name ‘foo’ the following files are written to disk ‘foo.mx’, ‘foo.my’, ‘foo.mz’, ‘foo.field’, ‘foo.time’, ‘foo.energy’.

#### Parameters

- `fname`: /path/to/filename prefix for files
- `res`: results struct to save

```
void zero_results (struct results &res)
    Initialise results memory to zero.
```

#### Parameters

- `res`: results struct to zero

```
void reduce_to_system_magnetisation (double *mag,      const double *particle_mags,      const
                                     size_t N_particles)
```

```
struct results
```

### Public Functions

```
results (size_t _N)
```

### Public Members

```
std::unique_ptr<double[]> mx
std::unique_ptr<double[]> my
std::unique_ptr<double[]> mz
std::unique_ptr<double[]> field
std::unique_ptr<double[]> time
```



size\_t *N*

## 7.2.24 File stochastic\_processes.cpp

## 7.2.25 File stochastic\_processes.hpp

namespace stochastic

### Functions

void **master\_equation** (double \**derivs*, **const** double \**transition\_matrix*, **const** double \**current\_state*, **const** size\_t *dim*)

Evaluates the derivatives of the master equation given a transition matrix.

The master equation is simply a linear system of ODEs, with coefficients described by the transition matrix.

$$\frac{dx}{dt} = Wx$$

#### Parameters

- *derivs*: the master equation derivatives [length *dim*]
- *transition\_matrix*: the [*dim* x *dim*] transition matrix (row-major) *W*
- *current\_state*: values of the state vector *x*

## 7.2.26 File trap.cpp

Implementation of trapezoidal integration scheme.

**Author** Oliver W. Laslett (2016)

## 7.2.27 File trap.hpp

namespace trap

numerical schemes for computing the area under curves

**Author** Oliver Laslett

### Functions

double **trapezoidal** (double \**x*, double \**y*, size\_t *N*)

double **one\_trapezoid** (double *x1*, double *x2*, double *fx1*, double *fx2*)

## 7.3 Class list

### 7.3.1 Class Rng

class Rng

Abstract class for random number generators.

Subclassed by *RngArray*, *RngMtDownsample*, *RngMtNorm*

### 7.3.2 Class RngArray

**class RngArray**

Provides an *Rng* interface to a predefined array of numbers.

Inherits from *Rng*

### 7.3.3 Class RngMtDownsample

**class RngMtDownsample**

Generate normally distributed values with downsampling.

Uses the Mersenne Twister to generate normally distributed random numbers. Down-samples the stream of random numbers by summing consecutive draws along each dimension. Function is usually used for generating coarse Wiener processes

Inherits from *Rng*

### 7.3.4 Class RngMtNorm

**class RngMtNorm**

Uses Mersenne Twister to generate normally distributed values.

Random numbers have a mean of zero and a user specified standard deviation.

Inherits from *Rng*

## 7.4 Struct list

### 7.4.1 Struct mnp::norm\_params

```
struct mnp::norm_params
```

### 7.4.2 Struct mnp::params

```
struct mnp::params
```

### 7.4.3 Struct simulation::results

```
struct simulation::results
```

## CHAPTER 8

---

### Indices and tables

---

- `genindex`
- `modindex`
- `search`



### m

- `magpy.core`, [37](#)
- `magpy.data`, [37](#)
- `magpy.geometry`, [37](#)
- `magpy.geometry.arkus`, [37](#)
- `magpy.geometry.coordinates`, [38](#)
- `magpy.initial_conditions`, [40](#)
- `magpy.model`, [40](#)
- `magpy.results`, [44](#)



## Symbols

`_USE_MATH_DEFINES` (C macro), 68

## A

ARKUS (in module `magpy.geometry.arkus`), 38  
`arkus_cluster_coordinates()` (in module `magpy.geometry.coordinates`), 38  
`arkus_cluster_random_configuration_id()` (in module `magpy.geometry.coordinates`), 38  
`arkus_random_cluster_coordinates()` (in module `magpy.geometry.coordinates`), 39

## C

`chain_coordinates()` (in module `magpy.geometry.coordinates`), 39  
`constants` (C++ type), 49, 65  
`constants::GYROMAG` (C++ member), 49, 65  
`constants::KB` (C++ member), 49, 65  
`constants::MU0` (C++ member), 49, 65

## D

`d3` (C++ type), 83  
`distances` (C++ type), 49, 66  
`distances::pair_wise_distance_magnitude` (C++ function), 50, 66  
`distances::pair_wise_distance_unit_vectors` (C++ function), 50, 66, 67  
`distances::pair_wise_distance_vectors` (C++ function), 50, 66  
`dom` (C++ type), 50, 67  
`dom::master_equation_with_update` (C++ function), 51, 67  
`dom::single_transition_energy` (C++ function), 51, 68  
`dom::transition_matrix` (C++ function), 51, 67  
`DOModel` (class in `magpy.model`), 40  
`driver` (C++ type), 52, 72  
`driver::eulerm` (C++ function), 52, 73  
`driver::heun` (C++ function), 52, 73  
`driver::implicit_midpoint` (C++ function), 52, 73

`driver::rk4` (C++ function), 52, 73

## E

`energy` (C++ type), 52, 68  
`energy::anisotropy_r` (C++ function), 52, 68  
`energy::dipolar_r` (C++ function), 52, 68  
`energy::zeeman_r` (C++ function), 52, 68  
`energy_dissipated()` (`magpy.results.EnsembleResults` method), 45  
`ensemble_magnetisation()` (`magpy.results.EnsembleResults` method), 45  
`EnsembleModel` (class in `magpy.model`), 41  
`EnsembleResults` (class in `magpy.results`), 44

## F

`field` (C++ type), 53, 68, 69  
`field` (`magpy.results.EnsembleResults` attribute), 44  
`field::bind_field_function` (C++ function), 53, 69  
`field::CONSTANT` (C++ enumerator), 53, 69  
`field::constant` (C++ function), 53, 69  
`field::dipolar_add_p2p_term` (C++ function), 55, 71  
`field::dipolar_prefactor` (C++ function), 55, 71  
`field::multi_add_applied_Z_field_function` (C++ function), 54, 70  
`field::multi_add_dipolar` (C++ function), 55, 71  
`field::multi_add_uniaxial_anisotropy` (C++ function), 54, 70  
`field::multi_add_uniaxial_anisotropy_jacobian` (C++ function), 55, 71  
`field::options` (C++ type), 53, 69  
`field::SINE` (C++ enumerator), 53, 69  
`field::sinusoidal` (C++ function), 53, 69  
`field::SQUARE` (C++ enumerator), 53, 69  
`field::square` (C++ function), 54, 70  
`field::square_fourier` (C++ function), 54, 70  
`field::uniaxial_anisotropy` (C++ function), 54, 70  
`field::uniaxial_anisotropy_jacobian` (C++ function), 55, 71

field::zero\_all\_field\_terms (C++ function), 55, 72  
 final\_cycle\_energy\_dissipated()  
     (magpy.results.EnsembleResults method), 45  
 final\_state() (magpy.results.EnsembleResults method), 45  
 final\_state() (magpy.results.Results method), 46

## G

grab\_results() (in module magpy.data), 37

## I

integrator (C++ type), 56, 72, 73  
 integrator::ck\_butcher\_table (C++ type), 56, 57, 74  
 integrator::ck\_butcher\_table::c11 (C++ member), 56, 57, 74  
 integrator::ck\_butcher\_table::c21 (C++ member), 56, 57, 74  
 integrator::ck\_butcher\_table::c22 (C++ member), 56, 57, 74  
 integrator::ck\_butcher\_table::c31 (C++ member), 57, 74  
 integrator::ck\_butcher\_table::c32 (C++ member), 57, 58, 74  
 integrator::ck\_butcher\_table::c33 (C++ member), 57, 58, 74  
 integrator::ck\_butcher\_table::c41 (C++ member), 57, 58, 74  
 integrator::ck\_butcher\_table::c42 (C++ member), 57, 58, 74  
 integrator::ck\_butcher\_table::c43 (C++ member), 57, 58, 74  
 integrator::ck\_butcher\_table::c44 (C++ member), 57, 58, 74  
 integrator::ck\_butcher\_table::c51 (C++ member), 57, 58, 74  
 integrator::ck\_butcher\_table::c52 (C++ member), 57, 58, 74  
 integrator::ck\_butcher\_table::c53 (C++ member), 57, 58, 74  
 integrator::ck\_butcher\_table::c54 (C++ member), 57, 58, 74  
 integrator::ck\_butcher\_table::c55 (C++ member), 57, 58, 74  
 integrator::ck\_butcher\_table::hc1 (C++ member), 57, 58, 74  
 integrator::ck\_butcher\_table::hc2 (C++ member), 57, 58, 74  
 integrator::ck\_butcher\_table::hc3 (C++ member), 57, 58, 74  
 integrator::ck\_butcher\_table::hc4 (C++ member), 57, 58, 74  
 integrator::ck\_butcher\_table::hc5 (C++ member), 57, 58, 74  
 integrator::ck\_butcher\_table::x11 (C++ member), 57, 58, 74

integrator::ck\_butcher\_table::x13 (C++ member), 57, 58, 74  
 integrator::ck\_butcher\_table::x14 (C++ member), 57, 58, 74  
 integrator::ck\_butcher\_table::x16 (C++ member), 57, 58, 74  
 integrator::ck\_butcher\_table::x21 (C++ member), 57, 58, 74  
 integrator::ck\_butcher\_table::x23 (C++ member), 57, 58, 74  
 integrator::ck\_butcher\_table::x24 (C++ member), 57, 58, 74  
 integrator::ck\_butcher\_table::x25 (C++ member), 57, 58, 74  
 integrator::ck\_butcher\_table::x26 (C++ member), 57, 58, 75  
 integrator::eulerm (C++ function), 56, 73  
 integrator::heun (C++ function), 56, 73  
 integrator::implicit\_midpoint (C++ function), 56, 73  
 integrator::milstein (C++ function), 56, 73  
 integrator::rk4 (C++ function), 56, 73  
 integrator::rk45 (C++ function), 56, 74  
 io (C++ type), 58, 75  
 io::write\_array (C++ function), 58, 75

## L

llg (C++ type), 59, 75  
 llg::diffusion (C++ function), 59, 76  
 llg::diffusion\_jacobian (C++ function), 60, 76  
 llg::drift (C++ function), 59, 75  
 llg::drift\_jacobian (C++ function), 59, 75  
 llg::jacobians\_with\_update (C++ function), 60, 77  
 llg::multi\_diffusion (C++ function), 61, 77  
 llg::multi\_diffusion\_jacobian (C++ function), 61, 78  
 llg::multi\_drift (C++ function), 61, 77  
 llg::multi\_drift\_quasijacobian (C++ function), 61, 78  
 llg::multi\_stochastic\_llg\_field\_update (C++ function), 61, 77  
 llg::multi\_stochastic\_llg\_jacobians\_field\_update (C++ function), 62, 78  
 llg::sde\_with\_update (C++ function), 60, 76

## M

magnetisation() (magpy.results.EnsembleResults method), 46  
 magnetisation() (magpy.results.Results method), 46  
 magpy.core (module), 37  
 magpy.data (module), 37  
 magpy.geometry (module), 37  
 magpy.geometry.arkus (module), 37  
 magpy.geometry.coordinates (module), 38  
 magpy.initial\_conditions (module), 40  
 magpy.model (module), 40  
 magpy.results (module), 44



magpy\_actor() (in module magpy.data), 37  
 mnp (C++ type), 62, 79  
 mnp::norm\_params (C++ class), 79, 86  
 mnp::norm\_params::alpha (C++ member), 79  
 mnp::norm\_params::anisotropy\_axis (C++ member), 79  
 mnp::norm\_params::gamma (C++ member), 79  
 mnp::norm\_params::stability (C++ member), 79  
 mnp::norm\_params::temperature (C++ member), 79  
 mnp::norm\_params::volume (C++ member), 79  
 mnp::params (C++ class), 79, 86  
 mnp::params::alpha (C++ member), 79  
 mnp::params::anisotropy (C++ member), 79  
 mnp::params::anisotropy\_axis (C++ member), 79  
 mnp::params::diameter (C++ member), 79  
 mnp::params::gamma (C++ member), 79  
 mnp::params::saturation\_mag (C++ member), 79  
 Model (class in magpy.model), 43

## O

optimisation (C++ type), 63, 80  
 optimisation::LAPACK\_ERR (C++ member), 63, 80  
 optimisation::MAX\_ITERATIONS\_ERR (C++ member), 63, 80  
 optimisation::newton\_raphson\_1 (C++ function), 63, 80  
 optimisation::newton\_raphson\_noinv (C++ function), 63, 80  
 optimisation::SUCCESS (C++ member), 63, 80

## P

pair\_wise\_distance\_magnitude (C++ function), 66  
 plot() (magpy.results.Results method), 47

## R

random\_point\_on\_unit\_sphere() (in module magpy.initial\_conditions), 40  
 random\_quaternion() (in module magpy.initial\_conditions), 40  
 Results (class in magpy.results), 46  
 Rng (C++ class), 80, 85  
 Rng::get (C++ function), 81  
 rng\_vec (C++ type), 83  
 RngArray (C++ class), 82, 86  
 RngArray::arr (C++ member), 83  
 RngArray::get (C++ function), 82  
 RngArray::i (C++ member), 83  
 RngArray::max (C++ member), 83  
 RngArray::RngArray (C++ function), 82  
 RngArray::stride (C++ member), 83  
 RngMtDownsample (C++ class), 81, 86  
 RngMtDownsample::current\_dim (C++ member), 82  
 RngMtDownsample::D (C++ member), 82  
 RngMtDownsample::dist (C++ member), 82  
 RngMtDownsample::downsample\_draw (C++ function), 82

RngMtDownsample::F (C++ member), 82  
 RngMtDownsample::generator (C++ member), 82  
 RngMtDownsample::get (C++ function), 81  
 RngMtDownsample::RngMtDownsample (C++ function), 81  
 RngMtDownsample::store (C++ member), 82  
 RngMtNorm (C++ class), 81, 86  
 RngMtNorm::dist (C++ member), 81  
 RngMtNorm::generator (C++ member), 81  
 RngMtNorm::get (C++ function), 81  
 RngMtNorm::RngMtNorm (C++ function), 81

## S

sde\_func (C++ type), 72  
 sde\_function (C++ type), 72  
 sde\_jac (C++ type), 72, 83  
 shelve\_results() (in module magpy.data), 37  
 simulate() (magpy.model.DOModel method), 41  
 simulate() (magpy.model.EnsembleModel method), 42  
 simulate() (magpy.model.Model method), 43  
 simulation (C++ type), 63, 83  
 simulation::dom\_ensemble\_dynamics (C++ function), 64, 84  
 simulation::full\_dynamics (C++ function), 64, 83  
 simulation::reduce\_to\_system\_magnetisation (C++ function), 64, 84  
 simulation::results (C++ class), 84, 86  
 simulation::results::field (C++ member), 84  
 simulation::results::mx (C++ member), 84  
 simulation::results::my (C++ member), 84  
 simulation::results::mz (C++ member), 84  
 simulation::results::N (C++ member), 84  
 simulation::results::results (C++ function), 84  
 simulation::results::time (C++ member), 84  
 simulation::save\_results (C++ function), 64, 84  
 simulation::zero\_results (C++ function), 64, 84  
 stochastic (C++ type), 65, 85  
 stochastic::master\_equation (C++ function), 65, 85

## T

time (magpy.results.EnsembleResults attribute), 44  
 trap (C++ type), 65, 85  
 trap::one\_trapezoid (C++ function), 65, 85  
 trap::trapezoidal (C++ function), 65, 85

## U

uniform\_random\_axes() (in module magpy.initial\_conditions), 40