

# Boris Computational Spintronics

## User manual, *version 2.4*

Dr. Serban Lepadatu, 17<sup>th</sup> September 2019

### Abstract

This manual describes Boris Computational Spintronics, a multi-physics research software designed to solve three-dimensional magnetization dynamics problems, coupled with a self-consistent charge and spin transport solver, heat flow solver with temperature-dependent material parameters, in arbitrary multi-layered structures and shapes. The computational routines run both on central processors and graphics processors using the CUDA platform. In addition to simple user control, advanced simulation configurations are made possible using Python scripts. The software is open source and currently runs on Windows 7 and Windows 10, 64-bit operating systems, and was programmed using C++14, CUDA C, and Python.

[boris-spintronics.uk/download](http://boris-spintronics.uk/download)

## **Disclaimer**

Boris Computational Spintronics is a freely available research, design and educational software. The author assumes no responsibility whatsoever for its use by other parties, and makes no guarantees, expressed or implied, about its quality, reliability, or any other characteristic. If using Boris for published research please use a relevant reference as given in the “Selected Publications using Boris” section (an article describing Boris, which may be used as a complete reference in the future, is pending).

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## **Installation**

An installer has been provided with the program and instructions therein should be followed. The program is designed to run on Windows 7 and Windows 10, 64 bit versions, and requires Microsoft Visual C++ 2017 Redistributable (x64) – included with the installer. On Windows 10 the executable (Boris.exe) must be run in compatibility mode – the installer sets this.

## CUDA

To enable CUDA computations Boris requires a CUDA-enabled graphics card with CUDA compute capability 5.0 or greater. If the CUDA compute version of the program exceeds the version for your GPU, then CUDA computations will not execute. If the CUDA compute version of the program is lower than that of your GPU, the program will take several minutes to launch the first time and might not work as expected. The installer detects the CUDA compute capability of the graphics card and installs the required program version.

## Known Issues

**Running DiagTrack and DPS (Diagnostic Policy Service) Windows services can in certain cases result in very poor performance. In this case these services should be stopped and disabled.**

## Overview

This manual contains a set of self-teaching tutorials that guide the user through most of its functionality. The tutorials contain a number of exercises designed for users without a background in micromagnetics, and may be skipped by more advanced users. A number of examples that accompany the tutorials have also been provided in the accompanying Examples folder.

Tutorials 1 to 7 cover the basics and it is recommended all users read through them. After these you can skip to the required tutorials as needed. Tutorial 9 covers the basics of automating simulations using Python and should be used as a starting point if required. For the transport solver Tutorials 8 and 10 should be used as a starting point. Tutorials 17 to 23 cover the spin transport solver. Tutorials 14 to 16 cover the heat solver.

The equations solved are given in the Differential Equations and Modules sections. All material parameters used in these equations have been given in the Material Parameters section.

A full list of commands has been provided in the Commands section in alphabetical order. The most commonly used commands have also been outlined.

# Tutorial 1 – Introduction

## Basics

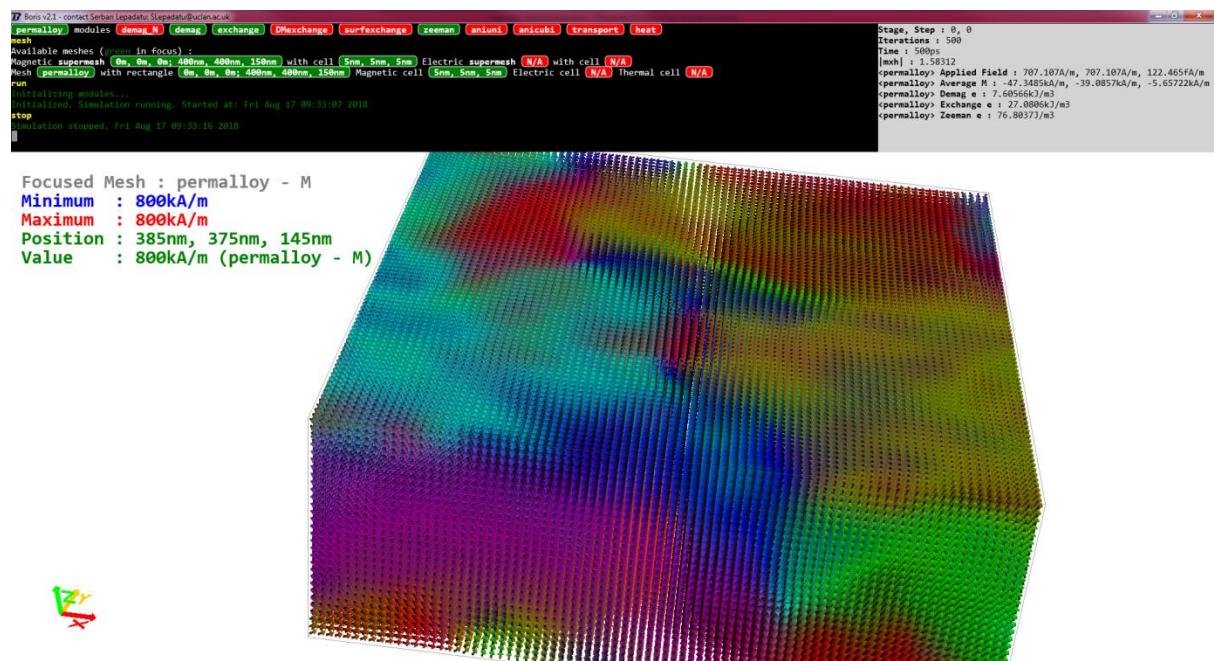
All commands are entered using the console (top-left black box) in Figure 1.1. Each console command has a case-sensitive syntax and may have a number of parameters separated by spaces. If a command is entered with wrong parameters, then a help prompt will be displayed explaining the command and full syntax. Alternatively a command may be immediately preceded by a question mark in order to display the command help. For example try it for the **run** command:

```
?run
```

Note, the program auto-completes commands entered out of the list of possible inputs – and equally stops any wrong inputs from being entered.

The main display shows the magnetization configuration (other vector and scalar quantities may be displayed, but magnetization is the default setting).

**Figure 1.1 – Boris interface**



The magnetization display may be controlled using the mouse: left-click and drag to re-position the display mesh, middle-click and move mouse to rotate the camera view about the center of the displayed (focused) mesh, right-click and move mouse up/down to zoom in/out, or left/right to rotate the camera about its axis; finally the wheel may be used to set the coarseness of magnetization representation: for large mesh dimensions, each arrow represents an average of the magnetization in that area.

Various simulation data may be displayed in the data box (top-right box) for convenience – more on these later. The displayed windows may be resized by dragging their outlines – the outline appears if you hover the mouse over the edge of a window.

The magnetization display can be reset to the default view using:

**center**

### Simulation Mesh Control

To display the current problem size enter the following command (see Figure 1.2 for expected output):

**mesh**

**Figure 1.2 – Default mesh configuration**

```
mesh
Available meshes (green in focus) :
Magnetic supermesh [0m, 0m, 0m; 80nm, 80nm, 10nm] with cell [5nm, 5nm, 5nm] Electric supermesh [N/A] with cell [N/A]
Mesh [permalloy] with rectangle [0m, 0m, 0m; 80nm, 80nm, 10nm] Magnetic cell [5nm, 5nm, 5nm] Electric cell [N/A] Thermal cell [N/A]
```

The simulation space consists of one or more named meshes – the default configuration consists of a single ferromagnetic mesh named *permalloy*. This has a rectangle with lower-left corner coordinates of (0, 0, 0) and upper-right corner coordinates of (80 nm, 80 nm, 10 nm). The magnetic discretization cellsize is a rectangular prism with dimensions ( $d_x, d_y, d_z$ ) = (5 nm, 5 nm, 5 nm) – a cubic cellsize by default. Thus the *permalloy* mesh is discretized with the integer number of cells (16, 16, 2).

To adjust the mesh dimensions you can use the **meshrect** command. An easy way to bring up this command, with current fields already entered, is to double-click on the outlined text containing the mesh rectangle dimensions: **0m, 0m, 0m; 80nm, 80nm, 10nm**

This type of outlined text is a special console text called an interactive console object, allowing a number of user interactions depending on the particular object, including left or right click, double-click, or drag. The text is also automatically updated to display currently set values. You can find out what an interactive object does by using shift-click.

Try to resize the *permalloy* mesh so it has the dimensions (300 nm, 100 nm, 15 nm). Values may be entered without specifying the units, in which case the applicable S.I. unit is assumed, or the applicable unit may be entered together with its magnitude specifier (e.g. for a meter the currently available units are designated as *am*, *fm*, *pm*, *nm*, *um*, *mm*, *m*, *km*, *Mm*, *Gm*, *Tm*, *Pm*). If entering the unit, do not leave a space between the number and unit.

The magnetic cellsize may be adjusted by double-clicking on the magnetic cell interactive object, which brings up the **cellsize** command. Try to adjust the cellsize so it has dimensions (6 nm, 6 nm, 5 nm). After changing the cellsize its dimensions are automatically adjusted in order to satisfy the requirement of integer number of discretization cells in each dimension.

Similarly the *permalloy* mesh may be renamed by double-clicking on the mesh name interactive object, which brings up the **renamemesh** command.

In Figure 1.2 you can also see an entry for the *supermesh*. Its rectangle is not controlled directly, but depends on the currently set meshes (however you can adjust the supermesh cellsize). The magnetic supermesh is the smallest simulation space containing all the currently set magnetic meshes and is useful to compute long-range interactions over several independently discretized meshes (e.g. supermesh demagnetizing field) – more on this in a dedicated tutorial.

## Basic Simulation Control

The simulation is started and stopped using:

**run**

**stop**

The stop command simply pauses the simulation without resetting it. To continue from the stop point simply type **run** again. To reset the simulation use:

**reset**

The display refresh frequency can be set using (*iter* is the number of iterations – remember you can query to command for full details: **?iterupdate**):

**iterupdate** *iter*

The simulation may be saved at any point using (do not use a termination, the .bsm termination is added by default):

**savesim** *filename*

If a directory path is not specified, the default directory path is used. To set a default directory use:

**chdir** *directory*

To load a previously saved simulation use:

**loadsim** *filename*

Alternatively a simulation file may be dragged into the console area. At any point you can return to the default program state by using:

## **default**

A uniform magnetization configuration can be set using the following (theta is the polar angle, phi is the azimuthal angle in spherical polar coordinates):

**setangle theta phi**

A uniform magnetic field can be set using (again use spherical polar coordinates):

**setfield Hmag Htheta Hphi**

## Simulation Modules

Simulation modules typically correspond to effective field terms. These can be managed using interactive objects by typing the following command:

## **modules**

The default configuration includes the demagnetizing field (*demag*), direct exchange interaction (*exchange*), and applied field (*zeeman*) – see Figure 1.3.

**Figure 1.3 – Default simulation modules**

```
Available modules (green added, red not added) :  
supermesh modules sdemag strayfield Oersted  
perm alloy modules demag_N demag exchange DMexchange surfexchange zeeman aniuni anicubi transport heat
```

Currently added modules are displayed in green. To add or remove a module left or right-click on the respective interactive object. Individual modules will be explored in future tutorials.

## Material Parameters

Default simulation parameters are set for permalloy (Ni<sub>80</sub>Fe<sub>20</sub>), as M<sub>s</sub> = 8e5 A/m, A = 1.3e-11 J/m, and α = 0.02. To see a list of currently set parameter values use the command:

## params

Values may be modified by double-clicking on the respective interactive objects. By default parameters are constant for each mesh, however they can be assigned temperature and spatial dependence for advanced simulations (more on this later).

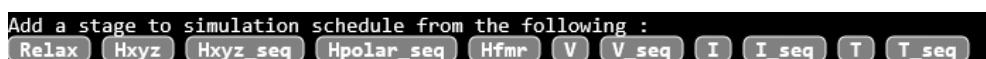
## Simulation Flow

A basic simulation flow can be programmed by setting a number of *stages*. Each stage has an identifier, parameters depending on the identifier, a stopping condition and data save condition. To show the currently set simulation stages use:

## stages

By default the *Relax* stage type is used (no simulation values changed), with a stopping condition based on the normalized torque  $|mxh| < 10^{-4}$  ( $mxh$ : 0.0001), and no data saving configured. New stages may be added by double-clicking on the interactive objects at the bottom – see Figure 1.4.

**Figure 1.4** – Simulation stage types



You can delete added stages by right-clicking on them, change the stage type by double-clicking and editing, and re-arrange the stage order by dragging.

Available stopping conditions are: *nostop*, *iter* (stop after a number of iterations), *mxh* (stop when  $|mxh|$  falls below the set threshold), *dmdt* (stop when the normalized  $|\partial\mathbf{m}/\partial t|$  value falls below the set threshold), or *time* (stop after an elapsed simulation time). When a stage reaches the stopping condition the next stage starts or the simulation finishes.

Some stage types are broken down into several sub-stages (referred to as *steps*), for example a field sequence using *Hxyz\_seq*. Try to add a field sequence stage by

double-clicking on the *Hxyz\_seq* interactive object. The default parameters for a field sequence are shown in Figure 1.5. This consists of a field sequence starting from a field of -100 kA/m along the x-axis, and stopping at +100 kA/m along the x-axis. The sequence consists of 100 field steps, thus the field step is 2 kA/m. The simulation proceeds to the next *step* when the  $|mxh| < 10^{-4}$  stopping condition is satisfied.

**Figure 1.5 – Default parameters for the *Hxyz\_seq* stage type**

```
-100kA/m, 0A/m, 0A/m; 100kA/m, 0A/m, 0A/m; 100 ]
```

### Exercise 1.1

Set a  $160 \times 80 \times 5$  nm permalloy mesh (with cubic cellsize of 5 nm) starting from a saturated magnetization state along the negative x-axis direction. Set a field sequence from -60 kA/m to +60 kA/m along the x-axis using a step of 2 kA/m and  $mxh$  stopping condition of  $10^{-4}$  (typically this threshold is too high, it should be  $10^{-5}$  or even lower for an accurate simulation depending on the problem, but this will speed up the exercise).

Display the applied field and average magnetization in the data box. To do this use the command:

**data**

You will see a list of interactive console objects representing possible output data which can be displayed in the data box or saved to a file. For now just display the applied field (*Ha*) and average magnetization (*<M>*) by right-clicking on the interactive objects (or dragging them to the data box).

Run the simulation - the magnetization should switch during this field sequence.

## Tutorial 2 – Data Output

### Saving Numerical Data

In order to save numerical simulation data (automated saving of images will be explored in a future tutorial) you need to set a data saving file, a list of output data, and a saving schedule. To set output data and a save file use the **data** command.

**Figure 2.1** – Default output data

```
data
Current file for output data : D:\Boris2\x64\Release\out_data.txt . Data save On
Current file base for images : mesh_image . Image save Off
List of output data as: dataname (<meshname>, ((box)) :
 0. sstep
 1. iter
 2. time
 3. ha <permalloy>
 4. avm <permalloy> (0m, 0m, 0m; 80nm, 80nm, 10nm)
Add data to output list from the following :
  sstep  time  stime  iter  siter  dt  mxh  ha  avm  Jc  V  I  R  e_demag
  e_exch  e_surfexch  e_zee  e_anis  dwshift  ts_iter  ts_err  Temp  heat_dT
```

The default output data file is called *out\_data.txt* and its name may be modified by double-clicking on the interactive object. The default saving directory is the path to the program executable file and may be modified by double-clicking on the interactive object.

The default output data includes *sstep* (stage and step), *iter* (iteration), *time* (simulation time), *Ha* (applied field), and *<M>* (average magnetization). This is the order the output data will appear in the output file as numerical columns. The order may be modified by dragging the respective interactive objects in the list of output data. New output data may be added by double-clicking on the interactive objects at the bottom, and set output data may be deleted by right-clicking on the respective interactive objects in the output list.

Some output data (such as *ha* and *<M>*) may be saved in a particular mesh – in this case the *permalloy* mesh which is specified using the notation *<permalloy>*, whilst other output data do not depend on any particular mesh. Some output data (such as

`<M>`) may also be saved in a particular rectangle of the named mesh (the rectangle is relative to the named mesh) – by default the entire mesh rectangle is saved, but this can be modified by double-clicking on the respective interactive object and editing.

Finally, a saving schedule may be set in the simulation stages: use the **stages** command. Each stage has a list of possible saving conditions: *none* (default – do not save), *stage* (save at the end of the stage), *step* (save at the end of each step in the current stage), *iter* (save every n iterations), and *time* (save every t simulation seconds); for *iter* and *time* the parameters may be edited by double-clicking the respective interactive objects.

### Exercise 2.1

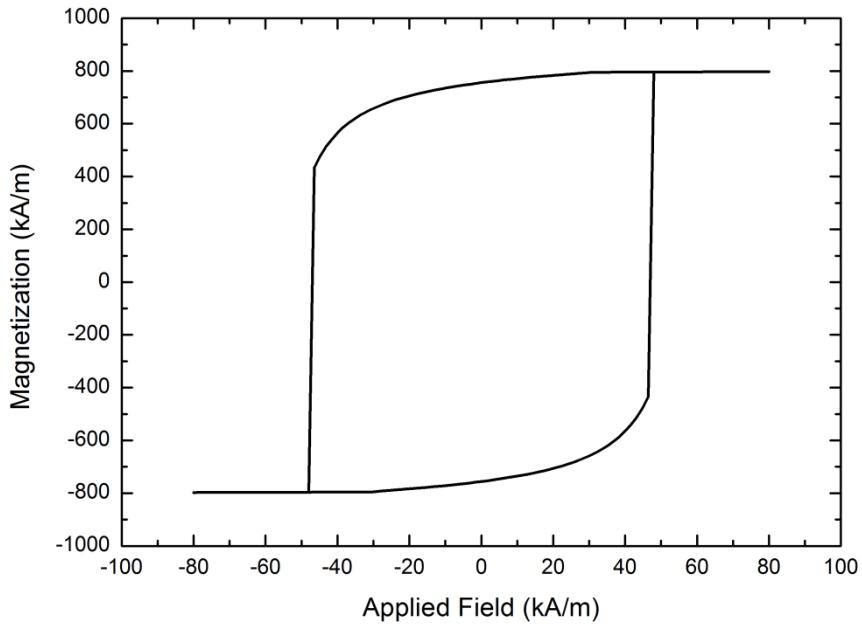
Set a  $160 \times 80 \times 10$  nm permalloy mesh (with cubic cellsize of 5 nm) starting from a saturated magnetization state along the negative x-axis direction. Set a field sequence from -100 kA/m to +100 kA/m and then back to -100 kA/m along the x-axis using a step of 2 kA/m and *mxh* stopping condition of  $10^{-4}$ .

Configure the simulation so it saves output data for a hysteresis loop (applied field and average magnetization saved after every step).

Before running the simulation save the simulation file. Once the simulation file is saved using a specified name (and directory path if needed), the next time you don't need to specify the file name – simply use **savesim** without a file name and the previously used file name will be saved. Note, correct commands previously entered in the console can be recalled using the arrow keys (invalid commands are not saved). You can also use **Ctrl^v** to paste text in the console.

Run the simulation and plot the hysteresis loop (magnetization along the applied field direction) at the end.

**Figure 2.2** – Hysteresis loop obtained in exercise 2.1



### Further Data Box Control

As introduced in the previous tutorial, output data may also be displayed in the data box for convenience. The possible output data may be listed as interactive objects by using the **data** command, and the listed interactive objects may be displayed in the data box by dragging them there, or right-clicking on them. Data box entries may be removed by right-clicking on them in the data box, and they may be re-arranged by dragging them.

If you just want to quickly see the current values of particular data without displaying them in the data box, bring up an interactive object list using the **showdata** command and double-click on the respective interactive objects.

## Exercise 2.2

In this exercise you will run the  $\mu$ MAG standard problem #4:  
<https://www.ctcms.nist.gov/~rdm/std4/spec4.html>

- a) For this problem we need a permalloy mesh with dimensions 500x125x3 nm.

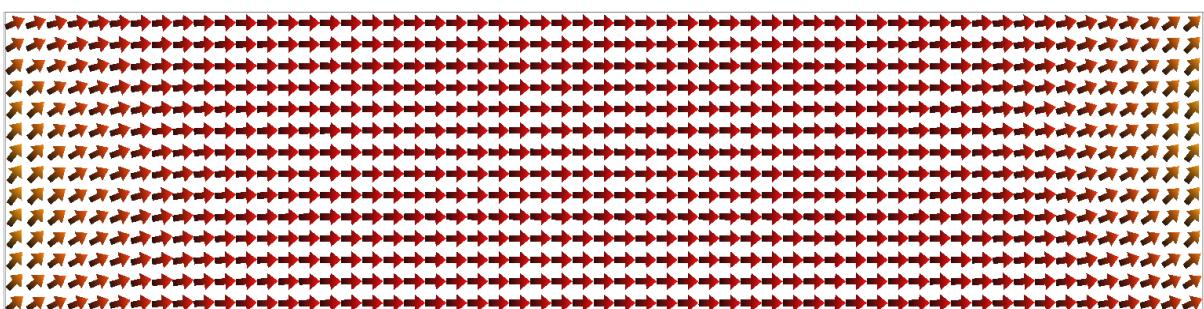
First initialize the magnetization configuration to a so-called s-state: this may be obtained by reducing a large applied field to zero along the [1,1,1] direction. For example set a field sequence starting from 1 MA/m along the [1,1,1] direction, reducing to zero in 20 steps – you should use the stricter  $|mxh| < 10^{-5}$  condition this time. Save an image of the obtained magnetization configuration – see Figure 2.3.

The easiest way to setup Exercise 2.2a is to use a polar field sequence: *Hpolar\_seq*. This specifies the starting and ending field values using polar coordinates: magnitude, polar angle and azimuthal angle – thus a starting field of 1 MA/m along the [1,1,1] direction would be specified (roughly) as 1MA/m, 55, 45. Make sure to specify the ending field value as 0, 55, 45 to keep the field values in the sequence along the same direction. You should also set the starting magnetization state along the [1,1,1] direction: **setangle 55 45**.

To save an image of the currently displayed mesh, use the command:

**savemeshimage (directory\filename)**

**Figure 2.3** – Starting s-state for micromagnetics standard problem #4



Exercise 2.2 continued

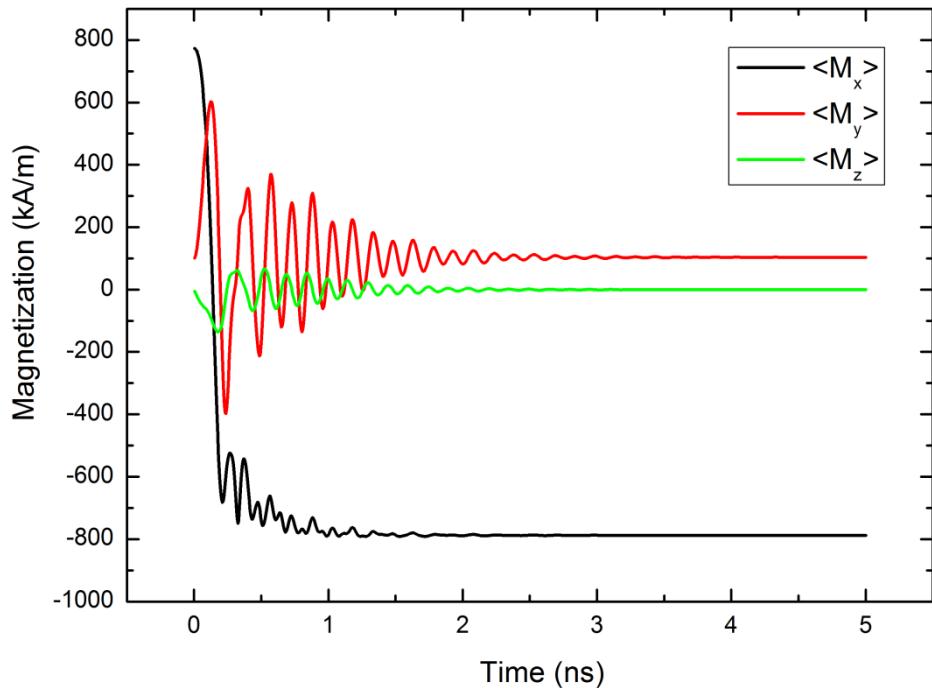
- b) Starting from the s-state, apply a fixed field with magnetic flux density (B-field) of 25 mT directed  $170^\circ$  counterclockwise from the x-axis in the x-y plane. Simulate the switching event for a duration of 5 ns, saving output data (in particular the average magnetization and simulation time are required) every 5 ps. Plot the 3 components of magnetization against time. Remember to save the simulation before starting it. How do these results compare with published solutions ?

(see <https://www.ctcms.nist.gov/~rdm/std4/results.html>)

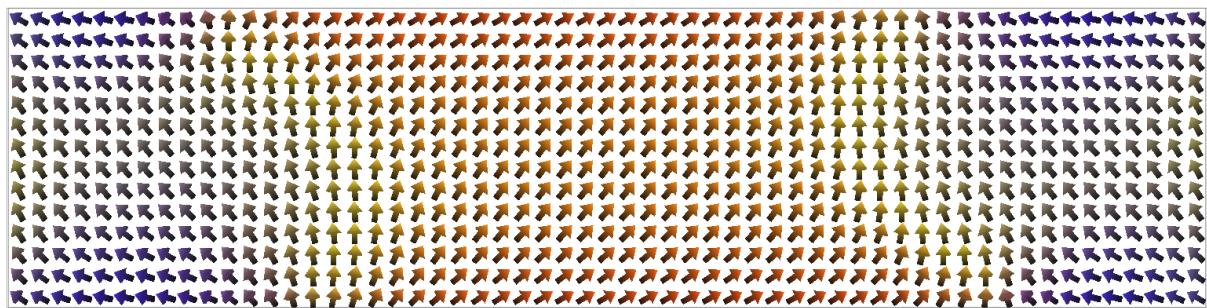
- c) Repeat part b) but this time for a B-field of 36 mT directed  $190^\circ$  degress counterclockwise from the x-axis in the x-y plane.
- d) For parts b) and c) obtain images of the magnetization configuration when the average magnetization (x component) first crosses zero – use the output data to determine the time when this occurs, then run the simulation to stop at this particular time.

**Figure 2.4** – a) Results obtained after running the  $\mu$ MAG standard problem #4 with field 1, and b) magnetization configuration when the average magnetization ( $x$  component) first crosses zero.

a)

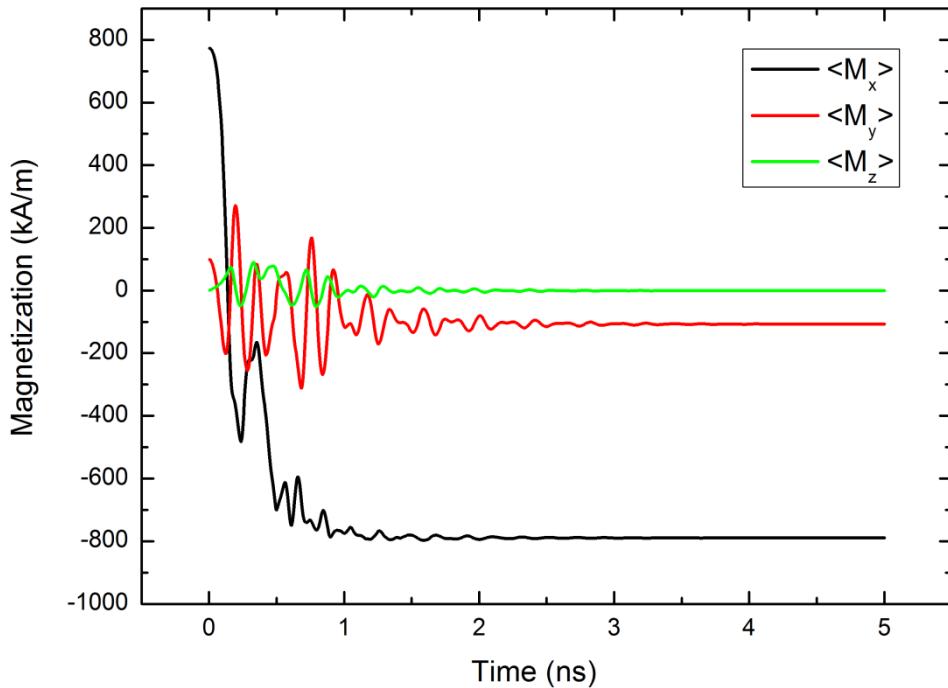


b)

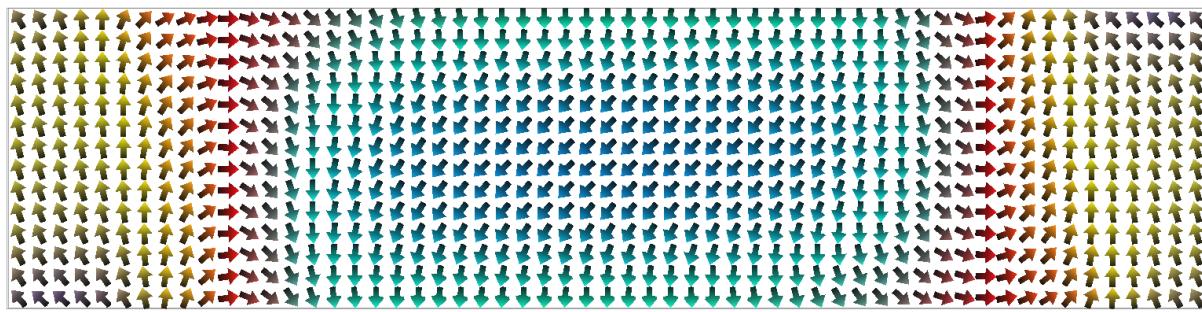


**Figure 2.5 – a)** Results obtained after running the  $\mu$ MAG standard problem #4 with field 2, and b) magnetization configuration when the average magnetization (x component) first crosses zero.

a)



b)



### Making a video from an image sequence

A video may be encoded from a sequence of .png files (e.g. as produced from a simulation with an image saving schedule) – this functionality is built into the program for convenience; for advanced image processing you should use an external program. To produce a video file from an image sequence, use:

**makevideo** (directory)\filebase *fps quality*

This makes a video from all .png files which start with the *filebase* name, including the directory, at the given *fps* (frames per second). The *quality* parameter sets the bit-rate of the output video: 0 for worst quality but smallest size, 5 for best quality but largest size. For the **makevideo** command, the files are sorted by their creation time, not alphabetically.

To enable mesh image saving, use the **data** command then click on the respective interactive object. You can also edit the mesh image filebase name. The mesh images are saved using the same save conditions as output data.

### Exercise 2.3

For the switching event in exercise 2.2b, set the problem to save mesh images every 10 ps; also reduce the simulation time to 3 ns and disable data saving. Make a video of the switching event (40 fps and quality level 3 works well).

If you want to capture only a part of the mesh display window you can set cropping factors. These are specified as normalized values and are applied whenever an image is saved (either manually or during a simulation). This is set using:

**imagecropping** *left bottom right top*

The left-bottom of the mesh display is (0, 0), whilst the right-top of the mesh display is (1,1).

## Tutorial 3 – Further Data Output

### Exercise 3.1

In this exercise you will compare coercive fields obtained using the full micromagnetics model with the predictions of the simpler Stoner-Wohlfarth model.

- a) Simulate an in-plane hysteresis loop along a 10° direction in a permalloy rectangle with dimensions 250x50x5 nm using the full micromagnetics model (*demag*, *exch*, and *zeeman* modules for permalloy) and obtain the coercive field. In order to speed up the simulation you only need to simulate one branch of the hysteresis loop, e.g. negative to positive field only, and you should also set a coarse field step up to zero field (e.g. 10 kA/m), then a fine field step in order to obtain a more accurate switching field value (use a 500 A/m fine field step or less); use the *mxh* stopping condition with a 10<sup>-5</sup> threshold.

*Solution: use two polar field sequences (Hpolar\_seq) along the (polar, azimuthal) = (90°, 10°) direction. Start at -200 kA/m and finish at 60 kA/m. This range is just enough to start from a saturated state and capture the switching field.*

i.e. : 1) *Hpolar\_seq -200kA/m 90 10 0kA/m 90 10 20*, 2) *Hpolar\_seq 0kA/m 90 10 60kA/m 90 10 120*

- b) Compute the anisotropy energy density (shape anisotropy) and hence obtain the switching field predicted by the Stoner-Wohlfarth model.

Note, the Stoner-Wohlfarth model predicts the switching field:

$$H_s = \frac{2K_u}{\mu_0 M_s} \frac{\sqrt{1-t^2+t^4}}{1+t^2}, \text{ where } t = \sqrt[3]{\tan(\theta)}$$

and  $\theta$  is the angle between the applied field and anisotropy easy axis (formula applicable for  $\theta$  between 0 and 45°).

To compute the energy density for a given magnetization orientation, set the magnetization orientation (**setangle**) and calculate the energy density terms using the command:

### **computefields**

This command runs the simulation for a single iteration and does not advance the simulation time – only the currently set simulation modules are refreshed. After running this command the required energy density term (*e\_demag*) will be available.

- c) For the same geometry and applied field direction obtain the hysteresis loop using the Stoner-Wohlfarth model. Does the coercive field agree with that obtained in part b) ?

To run this you will need to use the *demag\_N* module instead of the full *demag* module; the exchange module (*exch*) is not needed.

The *demag\_N* module computes the demagnetizing field using the simple approximation  $H_{d,i} = -N_i M_i$  ( $i = x, y, z$ ). You will need to enter correct values for the demagnetizing factors  $N_x$  and  $N_y$  (remembering that  $N_x + N_y + N_z = 1$ ). These can be entered using the command **params**, then editing the values under the *N<sub>xy</sub>* interactive object.

Calculate  $N_x$ ,  $N_y$  and  $N_z$  directly from the demagnetizing field (obtained using the full micromagnetics model) and also using the demagnetizing energy density values obtained in part b). Do the values agree, and does the relationship  $N_x + N_y + N_z = 1$  hold?

To obtain the demagnetizing field you will need to update the field using the **computefields** command with only the *demag* module enabled. After this you can display the demagnetizing field using the command:

### **display**

Using this command brings up a list of interactive objects with display options. Click on the *H<sub>eff</sub>* option under the *permalloy* mesh. This will display the computed effective field. Using the average effective field value you can obtain a value for the demagnetizing factor along the set magnetization direction using the expression  $H_d = -N M$ .

In order to obtain the average value of the demagnetizing field you can use the command:

### **dp\_averagemeshrect (sx sy sz ex ey ez)**

This command returns the average value for the displayed quantity in the currently focused mesh (the *permalloy* mesh in this case) when used without parameters. The parameters specify a mesh rectangle (start and end Cartesian coordinates) which is relative to the currently focused mesh.

- d) Repeat this exercise using the 100x25x5 nm.
- e) Repeat this exercise using the 50x25x3 nm.

Another way to calculate the demagnetizing factors is to use the formula:

$$\varepsilon_d = -\frac{\mu_0}{2} \mathbf{M} \cdot \mathbf{H}_d$$

Thus for **M** along  $i = x, y, z$ , you can obtain *e\_demag*, then use:

$$\varepsilon_{d,i} = \frac{\mu_0}{2} N_i M_s^2 \quad (i = x, y, z)$$

### Exercise 3.2

Here you will obtain the magnetization dynamics during a switching event and investigate the effect of the cellsize value on the simulation.

- a) Set a 320x160x10 nm permalloy rectangle with magnetization along the length of the rectangle (set the magnetization towards the left, thus blue coloured). Obtain the stable magnetization configuration at zero field by reducing the magnetic field from a large saturation value along x to zero in a number of steps. (e.g. from -50 kA/m to 0). For now use a cellsize of 5 nm.
- b) Starting from the magnetization configuration set-up in part a) set a single stage where you apply a large field along the x direction, opposing the magnetization – use 50 kA/m. As stopping condition using a time interval of 4 ns. Set a saving schedule to save the simulation time and average magnetization components every 10 ps. For now use a cellsize of 5 nm. From the saved data plot  $\langle M_x \rangle$  and  $\langle M_y \rangle$  versus time.
- c) Repeat the simulation in b) with cellsize values of 10 nm and 2.5 nm. Plot  $\langle M_x \rangle$  and  $\langle M_y \rangle$  versus stage time for the 3 cellsize values. How do the results compare ? Which cellsize would you recommend to use ?

## Tutorial 4 – Domain Walls

### Generating Domain Walls

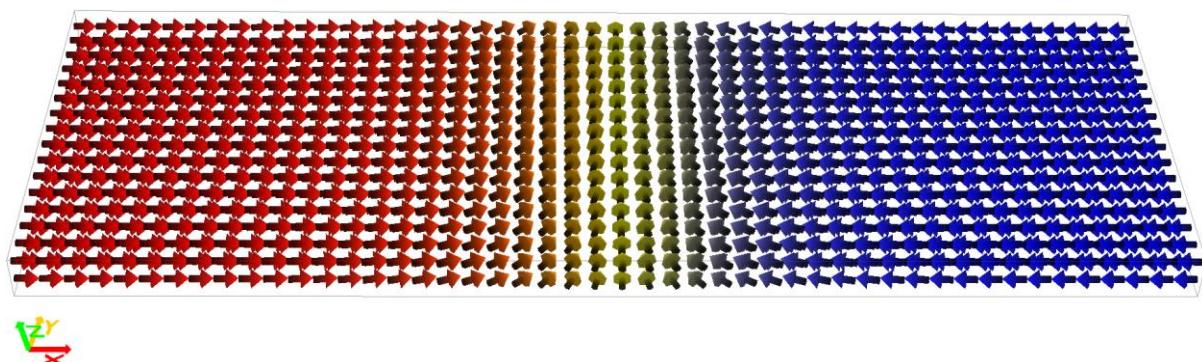
An idealized domain wall (using a tanh profile) along the  $x$  direction can be generated using:

**dwall** *longitudinal transverse width position*

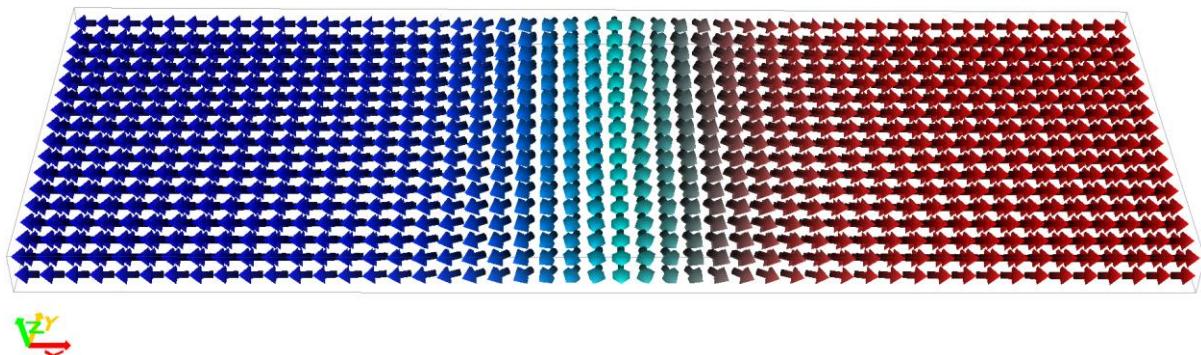
For an in-plane domain wall the longitudinal parameter determines if the wall is head-to-head (*longitudinal* =  $x$ ) or tail-to-tail (*longitudinal* =  $-x$ ); Bloch walls may be generated using  $z$  or  $-z$  for the longitudinal component. The transverse parameter determines the rotation direction through the wall – see Figure 4.1 for examples. The *width* value is the total domain wall width and *position* is the starting left-hand-side coordinate of the wall (along the  $x$  axis), relative to the focused mesh rectangle.

**Figure 4.1** – Domain walls generated using the **dwall** command for a mesh with 240nm length, and:

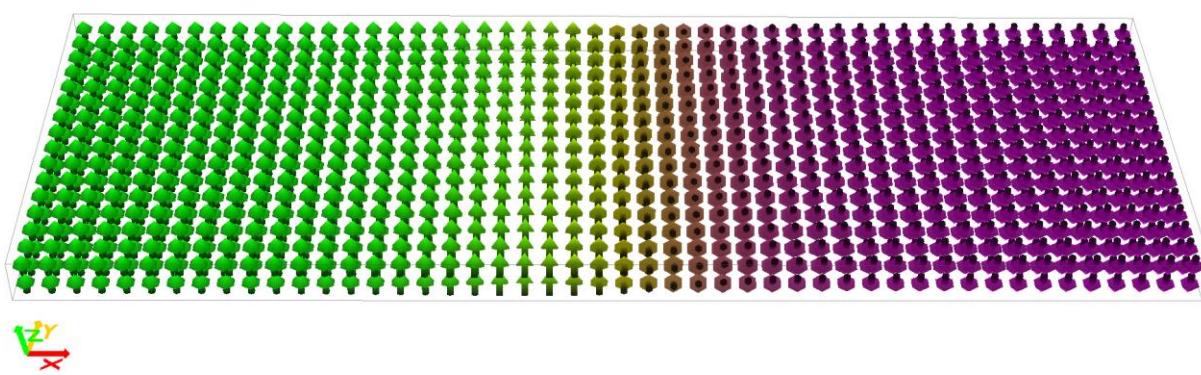
a) in-plane head-to-head transverse domain wall as **dwall**  $x$   $y$  240nm 0



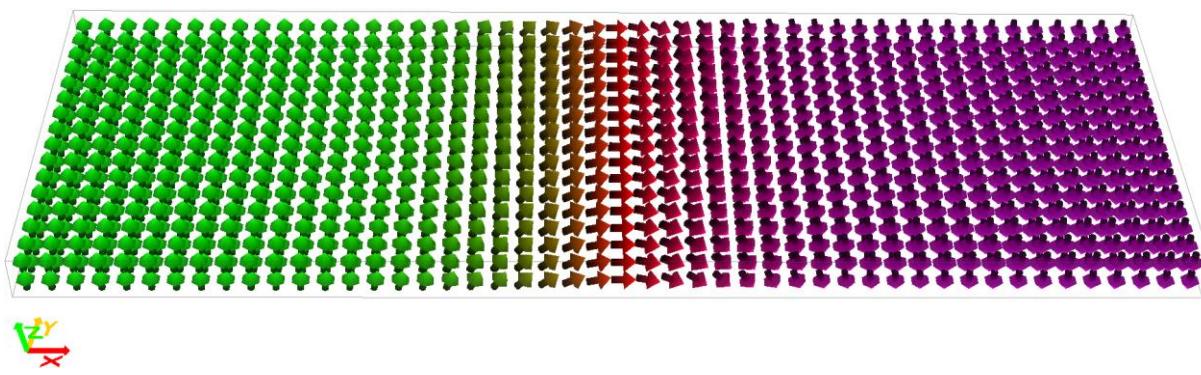
b) in-plane tail-to-tail transverse domain wall as **dwall** -x -y 240nm 0



c) Bloch domain wall as **dwall** z y 240nm 0



d) Néel domain wall as **dwall** z x 240nm 0



### Exercise 4.1

Set a mesh for a permalloy rectangle of dimensions 640x80x5 nm with 5 nm cellsize. Generate a head-to-head domain wall over this wire. Run the simulation without a stopping condition and observe how the domain wall is relaxed. You will observe the domain wall does not remain in the center, but eventually drifts towards one side until it is expelled at one of the edges. Can you explain why this happens?

### Setting Stray Fields

For domain wall mobility calculations and domain wall configuration relaxation problems in very long wires, it is possible to extend the wires outside of the ferromagnetic mesh by using external uniformly magnetized magnetic bodies, and to calculate the stray field inside the mesh, thereby allowing a smaller mesh size – this eliminates the domain wall drift problem noted in Exercise 4.1. This is done by adding dipole meshes at the left and right-hand-side of the *permalloy* mesh with magnetization direction set as a continuation of the magnetization inside the *permalloy* mesh, and enabling the *strayfield* module.

To add a dipole mesh use the following:

**adddipole name rectangle**

A dipole mesh has a uniform magnetization orientation which is not evolved by the ODE solver but may be handled in a similar manner to ferromagnetic meshes (such as the *permalloy* mesh). Thus modules may be added for computation (**modules**), mesh parameters edited (**params**), quantities displayed (**display**), etc.

You should also exchange couple the ends of the wires to the dipole meshes, thus completing the approximation of a long wire with a domain wall in the center. To enable this use the command:

**coupletodipoles**

Click on the interactive object to enable exchange coupling to the On state – with this flag turned on all magnetic cells in a ferromagnetic meshes, at the interface with a dipole mesh, are exchange coupled to the fixed dipole magnetization direction.

### Exercise 4.2

- a) Set two dipole meshes to the left and right of the *permalloy* mesh from the previous exercise, with lengths of 2.56  $\mu\text{m}$  (but same width and thickness). These dipole meshes should now be visible when using the **mesh** command – see Figure 4.2. Set their magnetization orientation in order to extend the head-to-head domain wall configuration from Exercise 4.1 (use **setangle** remembering to specify the mesh name – see **?setangle** for details) – note, the dipole meshes do not display anything by default, you will need to use the **display** command and click the *M* interactive object in order to see their magnetization orientation.

Run the simulation to relax the domain wall configuration to  $|\text{mxh}| < 10^{-5}$ . What does the stray field from the dipole meshes look like? (use the **display** command)

**Figure 4.2** – Configuration of dipole meshes for exercise 4.2

Magnetic supermesh (0m, 0m, 0m; 640nm, 80nm, 5nm) with cell (5nm, 5nm, 5nm)	Electric supermesh N/A with cell N/A
Mesh <b>permalloy</b> with rectangle (0m, 0m, 0m; 640nm, 80nm, 5nm)	Magnetic cell (5nm, 5nm, 5nm) Electric cell N/A Thermal cell N/A
Mesh <b>dip_left</b> with rectangle (-2.56um, 0m, 0m; 0m, 80nm, 5nm)	Magnetic cell N/A Electric cell N/A Thermal cell N/A
Mesh <b>dip_right</b> with rectangle (640nm, 0m, 0m; 3.2um, 80nm, 5nm)	Magnetic cell N/A Electric cell N/A Thermal cell N/A

- b) Change the *permalloy* mesh from part a) to a new size of 640x160x30 nm, making sure the dipole meshes are also scaled accordingly (to 160nm width and 30 nm thickness). For the purposes of this exercise you may use a 2D approximation by setting a cellsize of 5x5x30 nm.

Run the simulation to relax the domain wall configuration to  $|\text{mxh}| < 10^{-5}$ . What type of domain wall results?

When changing mesh dimensions with multiple meshes added to the simulation, there are two options available: i) change just the mesh rectangle required, ii) change the mesh rectangle required and resize/translate all other meshes in proportion. To change the behaviour of the program use the following command and click the interactive object to the On state:

### **scalemeshrects**

With multiple meshes, clicking on the mesh name interactive object (e.g. as displayed using the **mesh** command) changes the display focus to that mesh and resets camera orientation – try it. To quickly focus on a mesh without changing the camera orientation you can double-click on a mesh in the display window.

#### Exercise 4.3

In this exercise you will calculate the domain wall width for a symmetric transverse domain wall as a function of wire width and compare it to the values obtained using the domain wall formula ( $A$  is the exchange stiffness – see the **params** command – and  $K_u$  is the anisotropy energy density).

$$\Delta_{dw} = \pi \sqrt{\frac{A}{K_u}}$$

- a) Relax domain walls as a function of wire width for a permalloy mesh with dimensions 640 x Width x 5nm, where Width ranges from 40 nm up to 160 nm (simulate at least 4 different values of width). Obtain the domain wall width defined as the half- $M_s$  width value – i.e. the distance it takes for the longitudinal component to change from  $+M_s/2$  to  $-M_s/2$  for a head-to-head domain wall – and compare it to the value obtained using the formula above (when calculating  $K_u$  remember the longitudinal demagnetizing energy is assumed to be negligible as for a very long wire)

To obtain the domain wall profile you can use the following command:

**dp\_getprofile** *start end dp\_index*

The above command saves numerical data from the currently displayed mesh quantities (magnetization in this case) along a line starting from the *start* up to the *end* Cartesian coordinates (absolute position values, i.e. not relative to any mesh). The data is saved in internal data processing arrays – more on these in a separate tutorial. For now just obtain a magnetization profile through the middle of the wire as (e.g. for the 80nm wire width): **dp\_getprofile** 0 40nm 0 640nm 40nm 0 0.

The magnetization components are saved in the data processing arrays with indexes starting at 1 (so 1, 2, and 3), whilst data processing array 0 contains the position value. These can be saved to a file as numerical columns using the **dp\_save** command as **dp\_save** (*directory*)*filename.txt* 0 1 2 3. The file will contain the 4 columns as position along the profile (so x coordinate), Mx, My, Mz.

- b) Repeat the exercise for a thickness of 10nm using both a 3D simulation (cubic cellsize of 5x5x5 nm) and a 2D approximation (cellsize of 5x5x10 nm). How do the width values compare to those predicted by the formula and are the results obtained using the 2D and 3D model similar?

## Tutorial 5 – Domain Wall Movement and Data Processing

In this tutorial you will learn how to obtain a domain wall field-driven mobility curve.

In order to simulate domain wall movement, in addition to setting up a domain wall and dipole meshes as in the previous exercise, the moving mesh algorithm must be enabled by setting a “triggering mesh” as:

**movingmesh** *mesh\_name*

When moving mesh is enabled the magnetization is shifted either to the left or to the right by one notch at a time in order to keep the average x component of magnetization in the triggering mesh,  $\langle M_x \rangle$ , within set boundaries. This keeps the domain wall roughly in the centre of the mesh. When the mesh is shifted to the left or to the right, the data parameter *dwshift* is changed. This data parameter is available for saving to file – see list of data parameters using the **data** command, as discussed previously. Note, this can also be displayed in the console using **showdata dwshift**, or displayed in the data box. By saving the simulation time and domain wall shift, the domain wall velocity can be calculated using linear regression.

Since this type of computation is common, there is a shortcut command which sets-up everything required (adding dipole meshes with exchange coupling to the ferromagnetic mesh, enabling stray field computation, setting a domain wall and a triggering mesh):

**preparemovingmesh** (*meshname*)

### Exercise 5.1

- a) Set a  $320 \times 80 \times 20$  nm permalloy rectangle with  $5 \times 5 \times 20$  nm cellsize (2D problem). Enable the moving mesh algorithm and let the domain wall relax in zero field.
  
- b) Set a simulation stage with a field sequence starting from 500 A/m to 2000 A/m in 500 A/m steps, keeping each field step for exactly 2 ns. Set a data

save file, and make sure you save the stage time and dwshift parameters every 50 ps.

- c) For each field step extract the gradient of the dwshift vs time and plot the wall velocity as a function of field. How does the velocity compare with that predicted by the formula below? ( $K_u$  is the in-plane anisotropy energy density)

$$v_{dw} = H \frac{\gamma}{\alpha} \sqrt{\frac{A}{K_u}}, \text{ where } \gamma = \mu_0 |\gamma_e| \approx 221276 \text{ (m/As)}$$

### Console Data Processing

There are a number of built-in commands which allow for a number of operations to be performed on data processing arrays.

First of all, it is possible to load tab-spaced data from a file (such as the data files produced by a Boris simulation) into the internal data processing arrays. This is done using the following command:

```
dp_load filename filecol1 ... dp_arr1 ...
```

The above command loads entire columns from the specified file. Thus if the file has a number of tab-spaced data columns, we can load the column with number *filecol1* from the file into the internal data processing array with number *dp\_arr1* (these indexes are numbered from 0 up). Multiple columns can be loaded in one command.

Some common data processing commands are listed below.

To multiply a data processing array by a constant value use the following command:

```
dp_mul dp_source value dp_dest
```

The above command multiplies the data processing array with index *dp\_source* by the specified value and stores the result in the *dp\_dest* data processing array (this can be the same as *dp\_source*). This can be used to normalize data (e.g. a hysteresis loop).

We can use the built-in linear regression command to extract the velocity values:

**dp\_linreg** *dp\_x dp\_y (dp\_z dp\_out)*

The above command performs linear regression on the data stored in *dp\_x* and *dp\_y* data processing arrays and outputs the extracted gradient values and intercepts together with their uncertainties. If *dp\_z* is specified multiple linear regressions are performed by using the values in the *dp\_z* array to identify adjacent points to be included in a single linear regression; e.g. *dp\_z* would contain the applied field values. In this case the outputs are placed in 5 data processing arrays starting at *dp\_out* as follows: 1) unique *dp\_z* values, 2) gradient, 3) gradient error, 4) intercept, 5) intercept error.

We can also save our processed data, e.g. the domain wall velocity curve, using:

**dp\_save** *filename dp\_arr1 ...*

### Exercise 5.2

Use the console data processing commands to process the output data from Exercise 5.1 and save a domain wall velocity curve.

Other notable commands include:

**dp\_coercivity** *dp\_x dp\_y*

**dp\_remanence** *dp\_x dp\_y*

These commands can be used on data from a simulated hysteresis loop in order to extract coercivity and remanence values.

The data processing arrays may be cleared using:

**dp\_clear dp\_arr1 ...**

This clears data in the specified data processing arrays. If no parameters are included all data processing arrays are cleared.

### Exercise 5.3

Continuing Exercise 1, find the Walker breakdown threshold with a resolution of 100 A/m starting at 100 A/m. Compare the velocity values with that predicted by the formula in Exercise 5.1c for the steady domain wall movement regime. What is the Walker breakdown threshold?

### Exercise 5.4

Calculate the field-driven domain wall mobility curve for permalloy, with a resolution of 100 A/m, as a function of Gilbert damping, for values of damping 0.005, 0.01 and 0.015. How does the Walker breakdown threshold compare with the value predicted by the formula below? ( $K_{u,op}$  is the out-of-plane anisotropy energy density)

$$H_w = \frac{\alpha}{2} \frac{K_{u,op}}{\mu_0 M_s} \quad (A/m)$$

## Tutorial 6 – ODE Control and Setting Shapes

### Setting an ODE solver

The differential equation to solve and its evaluation method is configured using the following command:

#### **ode**

The default equation is the Landau-Lifshitz-Gilbert (LLG) equation which you have been using so far. Other equations may be set, e.g. LLB for temperature-dependent simulations, which will be covered in other tutorials.

There are a number of evaluation methods which you can select. The fixed-step methods available are: *Euler* (1<sup>st</sup> order), trapezoidal Euler (*TEuler* – 2<sup>nd</sup> order) and Runge-Kuta (*RK4* - 4<sup>th</sup> order). The adaptive time-step methods are the adaptive Heun (*AHeun* – 2<sup>nd</sup> order), the multi-step Adams-Bashforth-Moulton (*ABM* – 2<sup>nd</sup> order), Runge-Kutta-Bogacki-Shampine (*RK23* – 3<sup>rd</sup> order with embedded 2<sup>nd</sup> order error estimator), Runge-Kutta-Fehlberg (*RKF45* – 4<sup>th</sup> order with embedded 5<sup>th</sup> order error estimator), Runge-Kutta-Cash-Karp (*RKCK45* – 4<sup>th</sup> order with embedded 5<sup>th</sup> order error estimator), and Runge-Kutta-Dormand-Prince (*RKDP54* – 5<sup>th</sup> order with embedded 4<sup>th</sup> order error estimator).

There is also a Steepest Descent solver (*SDesc*) used for static problems where we don't need the magnetization dynamics, but are merely interested in calculating the ground state (e.g. relaxing a magnetization configuration and hysteresis loops). The steepest descent solver is only enabled for the *LLGStatic* equation, which is the LLG equation with the precession term disabled and damping value set to 1. In this case the *SDesc* solver is typically at least an order of magnitude faster in computing the ground state compared to the other methods.

For most methods the calculated *mxh* and *dmdt* stopping condition values are the maximum  $|\mathbf{mxh}|$  value (normalized torque) in any given iteration. The exceptions are

the *Euler*, *TEuler*, and *AHeun* methods, which are only ever used in practice for stochastic equations when including a thermal field (more on this later). For this reason the  $|mxh|$  values for these are the mesh averages in any given iteration. This allows using these methods with an  $mxh$  stopping condition for stochastic equations.

As an exercise we will briefly investigate here the stability of the fixed-step methods as the time step is changed. The time step may be set using:

**setdt dt**

Here  $dt$  is the time value in seconds. For the adaptive time step methods this command sets the starting time step.

### Exercise 6.1

- a) Set a  $320 \times 160 \times 20$  nm permalloy mesh with a 5 nm cubic cell and relax the magnetization to  $|mxh| < 10^{-5}$ .
- b) Set a stage with a magnetic field with components (40 kA/m, 5 kA/m, 0) for 5 ns and save data every 10 ps. Use the *RKF45* method. Record the actual computation time required to complete the simulations. Plot the magnetization switching dynamics.
- c) Repeat the simulation using the *RK4* method for fixed time steps of 0.5 ps, 0.7 ps, 0.9 ps and 1.1 ps. Record the actual computation time required to complete the simulations. Compare the results with the reference results from the *RKF45* method. How do the results change and why?
- d) Compare the computation times. Which method is more efficient whilst still maintaining accuracy?
- e) Investigate the computation time required to complete the same problem with *TEuler* with a time step of 50fs and *Euler* with a time step of 30as.

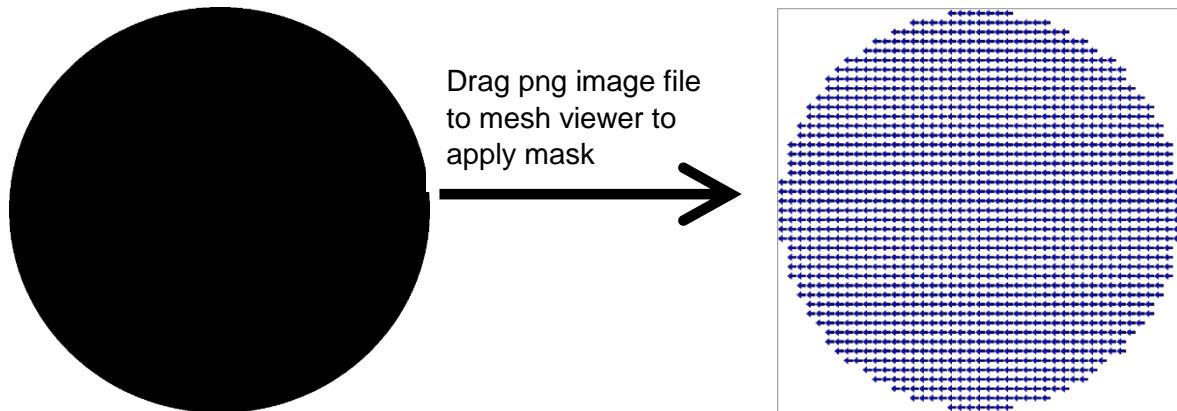
## Setting shapes

Until now we've mostly considered meshes which are filled with magnetic cells. In general, complex shapes may be generated by masking the mesh using a shape in an image file. This is achieved using the following command:

**loadmaskfile (zDepth) (directory)maskfile**

In the simplest case the image file defines a 2D shape in black and the void cells in white – see Figure 6.1 for an example. Instead of using the command you may also drag and drop the image in the mesh viewer window. The *zDepth* value defines the depth the mesh is voided to from top down (if *zDepth* > 0), or the height the mesh is voided to from bottom up (if *zDepth* < 0); this may be used to define 3D shapes with the maskfile being a grayscale image.

**Figure 6.1** – Setting a mesh shape using a mask from a png file



## Exercise 6.2

- a) Load an ellipse into a 320x160x10 nm mesh. Try not to leave void cells at the sides. You should use a circle mask as this will be stretched over the defined mesh rectangle.

- b) Obtain hysteresis loops between -50 kA/m and 50 kA/m for the ellipse along the x axis and along the y axis separately using a cellsize of 5x5x10 nm (2D simulations). You may use the relaxation condition  $|mxh| < 10^{-4}$  in order to speed up the exercise. Use the *RKF45* evaluation method. How do the two hysteresis loops compare ?
  
- c) Obtain further hysteresis loops for ellipses with dimensions 260x160x10 nm and 200x160x10 nm. Compare results for all the simulated ellipses and explain the changes in the hysteresis loops.

There is a modifier for how shapes are applied to a mesh, accessed using the **individualshape** command. By default this flag is Off, and any shape applied to the mesh is set for all relevant computational quantities. Thus **M** (magnetisation) is a computational quantity which may be shaped, but also **T** (temperature), and  **$\sigma$**  (electrical conductivity) may be shaped for the relevant solvers (micromagnetics, heat equation, and transport solver respectively). Note that in order to shape **T** and  **$\sigma$**  you need the relevant solvers enabled. If instead you only want to apply the shape to one of these quantities, or even have different shapes for all of them, you need to enable the **individualshape** flag, then apply the mask. This is useful for example if you want to include non-magnetic components (e.g. contact leads) in the magnetic mesh.

You may reset the mesh back to its solid shape using:

### **resetmesh**

This command is also useful to recover the mesh following a wrongly-posed computation – e.g. if too large a time-step is used the magnetization values will become **NaN** (not a number) and must be reset. Other methods to shape a mesh include setting and deleting rectangles using:

**delrect** *rectangle (meshname)*  
**addrct** *rectangle (meshname)*

## Tutorial 7 – Magnetocrystalline Anisotropy

In this tutorial you will learn how to use the anisotropy module and simulate hysteresis loops for different magneto-crystalline anisotropy configurations. You need to be familiar with all the basic tutorials.

There are two options available for adding magneto-crystalline anisotropy to the computations: uniaxial or cubic. These are enabled by choosing the *aniuni* or *anicubi* modules from the list displayed using the **modules** command. The modules are mutually exclusive, thus enabling one will delete the other one from the list of active modules.

The strength of the anisotropy is controlled using the *K1* and *K2* parameters (*K1* and *K2* are the anisotropy energy density constants) from the list displayed using the **params** command. These are the constants that appear in the anisotropy energy formulas:

Uniaxial anisotropy:

$$\varepsilon = K_1 \left[ 1 - (\mathbf{m} \cdot \mathbf{e}_a)^2 \right] + K_2 \left[ 1 - (\mathbf{m} \cdot \mathbf{e}_a)^2 \right]^2$$

Cubic anisotropy:

$$\varepsilon = K_1 [\alpha^2 \beta^2 + \alpha^2 \gamma^2 + \beta^2 \gamma^2] + K_2 [\alpha^2 \beta^2 \gamma^2], \text{ where}$$
$$\alpha = \mathbf{m} \cdot \mathbf{e}_1, \beta = \mathbf{m} \cdot \mathbf{e}_2, \gamma = \mathbf{m} \cdot (\mathbf{e}_1 \times \mathbf{e}_2)$$

We also need to define the anisotropy symmetry axes. For uniaxial anisotropy we only have one symmetry axis and this is set using the *ea1* parameter by giving the Cartesian components of the unit vector  $\mathbf{e}_a$  (e.g. default is 1, 0, 0 for easy axis along the x-axis). For cubic anisotropy we need two symmetry axes directions, *ea1* and *ea2* which should normally be orthogonal.

In the following you will investigate the effect of magnetocrystalline anisotropy on hysteresis loops in circular dots.

### Exercise 7.1

- a) Set a  $160 \times 160 \times 5$  nm permalloy circle with 5 nm cellsize using a mask file.  
Set a uniform magnetization along the x direction towards the left (blue state).  
Set uniaxial anisotropy with  $K_1 = 10$  kJ/m<sup>3</sup>,  $K_2 = 0$  J/m<sup>3</sup> and easy axis along x direction.
- b) Simulate hysteresis loops along the x-axis (easy axis), y-axis (hard axis) and in between along a 45° in-plane direction (remember you will need to use a polar field sequence for this). You will need to determine appropriate field sweep ranges so the loops start from a saturated magnetization state.
- c) Plot the hysteresis loops using the normalized magnetization (divide by  $M_s$  value – the saturation magnetization constant). What are the coercivity and normalized remanence values? Explain the difference between the loops.

### Exercise 7.2

Repeat the simulations in Exercise 7.1, but this time set cubic anisotropy with  $K_1 = 20$  kJ/m<sup>3</sup> and  $K_2 = 0$  J/m<sup>3</sup>, with two perpendicular easy axes in the plane (e.g. x-axis and y-axis).

Plot the resulting hysteresis loops and compare them with the previous results.

Hints:

For the 45° direction you will need to project the magnetization along the applied field direction. You can do this by taking the dot product of  $\mathbf{M}$  with the applied field direction unit vector:

$$M_H = \hat{\mathbf{h}} \cdot \mathbf{M}$$

You can do this using console data processing with the command:

```
dp_dotprod dp_vector ux uy uz dp_out
```

Here *dp\_vector* is the dp array index such that the dp arrays *dp\_vector*, *dp\_vector + 1*, *dp\_vector + 2* hold the x, y, and z components of the magnetization, (*ux*, *uy*, *uz*) are the components of a vector (dot product taken with this vector), and *dp\_out* is the dp array where the output is placed.

Finally, you can normalize the magnetization using the **dp\_div** command where you will need to divide by *Ms*. To see the value of *Ms* you can look it up in the list displayed using the **params** command.

Remember you will first need to load into dp arrays the appropriate columns for the saved hysteresis loop data file using the **dp\_load** command. You can save the contents of dp arrays after processing data using the **dp\_save** command. As always you can find more details about a command by preceding it with the ? symbol, e.g. **?dp\_load**.

## Tutorial 8 – Anisotropic Magneto-Resistance

In this tutorial you will learn how to simulate magneto-resistance loops and calculate charge current densities using the *transport* module.

### Transport Module Basics

The *transport* module is a complex spin and charge current solver (electron transport), allowing for a number of physical effects to be included in the magnetization dynamics problem, including Zhang-Li spin-transfer torques based on calculated charge currents, spin torques based on computed spin accumulations in multilayers, direct and inverse spin Hall effects (SHE and ISHE), spin pumping torques, anisotropic magneto-resistance (AMR), current-perpendicular-to-plane giant magneto-resistance (CPP-GMR), Oersted fields and Joule heating.

Here we will look at how a simple charge current density may be computed and AMR included in the simulation.

You will first need to enable the *transport* module from the list displayed using the **modules** command for the meshes where you want a charge current density to be computed. In the simplest case the computation is reduced to obtaining  $\mathbf{J}$ , the charge current density, using Ohm's law :  $\mathbf{J} = \sigma\mathbf{E}$ , where  $\sigma$  is the electrical conductivity and  $\mathbf{E} = -\nabla V$  is the electrical field with  $V$  being the electrical potential. If  $\sigma$  is constant this reduces to a Laplace equation for  $V$ .

The electrical conductivity, potential and charge current density are available as display outputs under the **display** command (*e/C*, *V* and *Jc*).

The base electrical conductivity value may be changed by editing the *e/C* mesh parameter displayed using the **params** command.

Similarly AMR may be enabled by editing the *amr* mesh parameter (0% by default which disables it). A typical value for permalloy is 2%. Enabling AMR results in a

non-uniform electrical conductivity and now the equation for  $V$  becomes a Poisson equation.

Before starting a computation you will need to define at least 2 electrodes – these set Dirichlet boundary conditions for  $V$  (fixed potential values) in the Laplace/Poisson solvers. The most common electrode configuration is to define two electrodes at the x-axis ends of the mesh (so in the y-z plane). You can do this using the command:

### **setdefaultelectrodes**

To see which electrodes have been defined use the command:

### **electrodes**

You will see two electrode rectangles. The electrode rectangles are in absolute values, so not relative to any particular mesh. You can add new electrodes but they must always be placed at the edges of a mesh rectangle – when initializing the simulation Dirichlet boundary conditions will be flagged for the boundary cells of the mesh intersecting the electrode rectangle. Each electrode has a fixed potential which may be edited. Exactly one of the electrodes has to be designated as the ground – this is the electrode where the outgoing total electrical current is calculated.

You can edit the individual electrode potential values, however a more common scenario is the set a single electrical potential drop from the ground to the other electrodes using:

### **setpotential *potential***

This sets a single inversely-symmetrical potential drop (i.e.  $+potential/2$  to  $-potential/2$ ). The inversely-symmetrical potential drop minimizes floating point errors (as opposed to setting a potential drop of *potential* to 0).

Simulations may use the constant-voltage or the constant-current mode (the interactive object displayed when using the **electrodes** command may be toggled

between these two states). Normally you would use the constant-voltage mode; with constant-current the electrode potentials are adjusted during the simulation to maintain a constant current (which may be set using the **setcurrent** command). In this tutorial we will be using the constant-voltage mode.

### Exercise 8.1

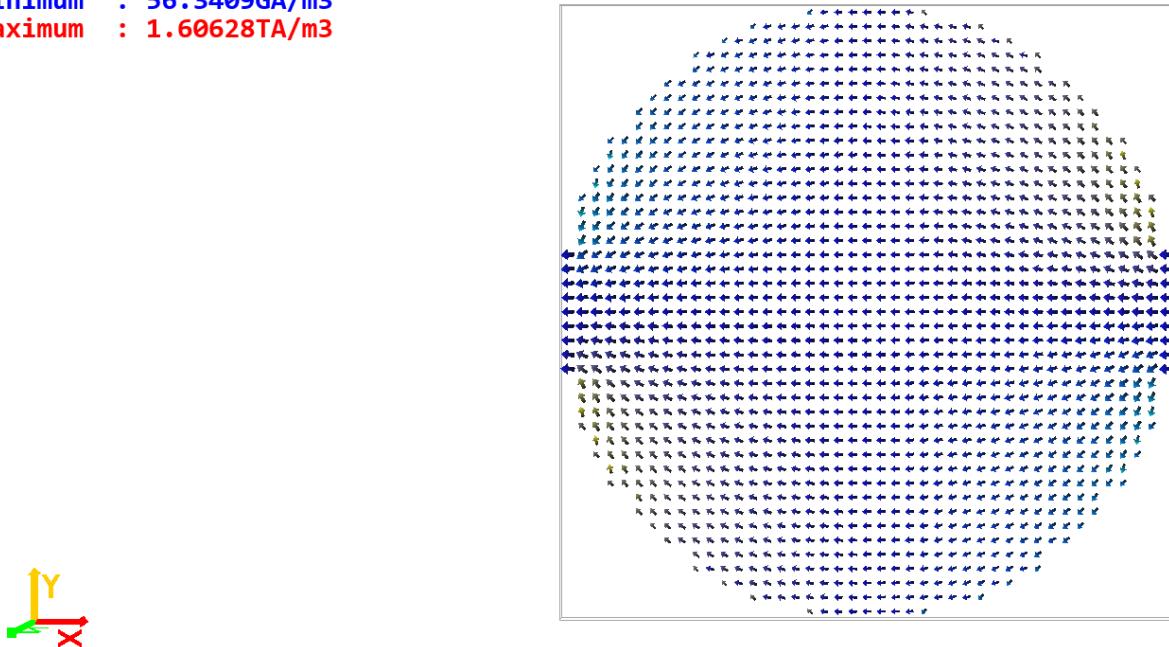
Set a permalloy mesh with dimensions 320x320x10 nm and mask it using a circle shape (in the image file make sure to not leave any white spaces at the left and right sides).

Enable the transport module, set the default electrode configuration and a potential of 10 mV.

In the data box display the average current density ( $J_c$ ), set potential ( $V$ ), total current ( $I$ ) and resistance ( $R$ ). In the mesh display the current density. Run the simulation. The calculated current density should look similar to that in Figure 8.1.

**Figure 8.1** – Computed charge current density for Exercise 8.1

Focused Mesh : permalloy -  $J_c$   
Minimum : 56.3409GA/m<sup>3</sup>  
Maximum : 1.60628TA/m<sup>3</sup>



For more advanced simulations you can add electrodes using the **addelectrode** command. Electodes may be deleted using the **delectrode** command (or more simply by right-clicking on an existing electrode in the list displayed by the **electrodes** command. All electrodes may be deleted by using the **clearelectrodes** command.

Further info:

When displaying the meshes (use the **mesh** command) you will now notice a value for the electric cell. This is the discretization cellsize used by the transport solvers. Normally this should be equal to the magnetic cellsize (default setting) but can be controlled separately for more advanced simulations (decrease computation time or increase computation accuracy as required). Multiple meshes with transport modules enabled may be configured. If the meshes are touching, composite media boundary conditions will automatically be inserted in the computation, however we still typically require 2 electrodes for a well-posed problem.

### Exercise 8.2

Set a permalloy rectangle with dimensions 300x100x20 nm. Calculate the current density for the default electrodes setting by using a potential drop of 1 V.

What is the computed sample resistance and does it agree with that predicted by the formula:

$$R = \frac{\rho l}{A},$$

where  $l$  is the length,  $A$  the cross-sectional area and  $\rho$  is the resistivity.

What is the total current, and does it agree with the expected value for a 1 V potential drop?

What is the average current density and does it agree with the expected value for the total current?

Further info:

For advanced simulations the accuracy of the transport solver may be controlled by using the command:

### **tsolverconfig**

This command displays the set convergence error (a value around  $10^{-6}$ ) is normally a good compromise between accuracy and computational speed. In this case the Laplace/Poisson solvers stop iterating when the maximum change in  $V$  from one iteration to another, normalized to the set potential drop, drops below this set convergence value. You can display the *ts\_iter* (current number of transport solver iterations) and *ts\_err* (current transport solver error) data in the data box. If the convergence error threshold is too low the transport solver will take a large number of iterations during computations – if AMR, GMR, ISHE or temperature-dependent transport parameters are enabled the transport solver must update after every magnetization and/or heat solver time step.

The transport solver may be used to calculate magneto-resistance loops when an AMR (anisotropic magneto-resistance) value is set. Since this is a static problem it is best to set the *LLGStatic* equation with the *SDesc* solver. When using the *SDesc* solver the stopping condition (*mxh* or *dmdt*) should be much lower than usual, typically at least  $10^{-6}$  or even lower. You should also set the static transport solver flag to On (see **tsolverconfig** command output). Setting this flag to On will only iterate the transport solver at the end of a schedule step, thus resulting in faster computation. In this case you should also increase the iterations timeout to at least 5000 or more to ensure the transport solver converge threshold is met.

For problems where the current density is uniform a transport solver converge threshold of  $10^{-6}$  is sufficient, however this may have to be decreased to  $10^{-8}$  or even  $10^{-9}$  if the current density is highly non-uniform.

In the following problem you should use both the static LLG equation and static transport solver as explained above.

### Exercise 8.3

Here you will obtain longitudinal and transverse magneto-resistance loops.

- a) Set a permalloy rectangle with dimensions 160x80x10 nm. You can use a 2D simulation with magnetic cellsize 5x5x10 nm, but the transport solver should be left with cubic electric cellsize of 5 nm.

Sweep the field from -100 kA/m to +100 kA/m strength and back, using a field step of at most 1 kA/m, along a nearly longitudinal direction (use  $5^\circ$  from the x-axis). You should use a *Hpolar\_seq* sequence, and an *mxh* stopping condition of  $10^{-7}$ .

Set the transport solver with default electrodes, a non-zero potential drop (e.g. 1 V), and *amr* = 2% (see **params**).

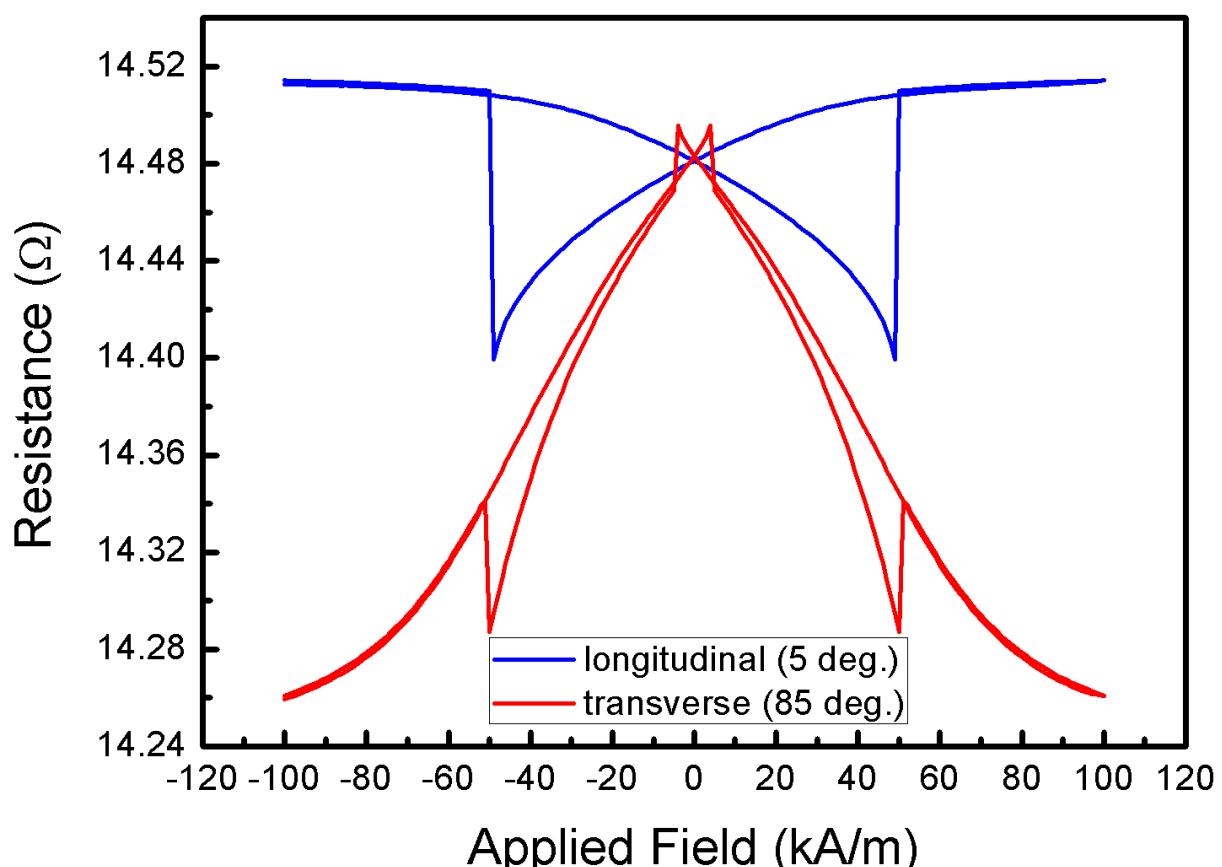
In the output data make sure to save the applied field and sample resistance every step. You should also save the transport solver error to check the converge threshold has been met at the end of each step (*ts\_err*).

Run the simulation and plot the obtained MR loop. Explain your results.

- b) Repeat the simulation along the in-plane nearly transverse direction (use  $85^\circ$  from the x-axis) by sweeping the field between -100 kA/m and +100 kA/m strength with a step of 1 kA/m.

Estimate the AMR percentage from the obtained H vs R loops from parts a) and b) – does it agree with the set 2% value?

**Figure 8.2** – Longitudinal and transverse MR loops due to AMR as calculated in Exercise 8.3.



## Tutorial 9 – Scripting using Python

In this tutorial you will learn how to use scripts to automate multiple simulations. Boris can communicate with an external program via network sockets, so both local and remote script-based control is possible. For this purpose a Python module (WinSocks) is provided, allowing use of Python scripts to communicate with Boris. This is contained in the WinSocks.py file and has been tested with **Python 2.7** (later Python versions not tested).

The scripts work by sending console commands, with syntax identical to that you would use when typing commands directly in the console. Some console commands also return values, which can be read by Python scripts. You can find out if a console command is set to return values by looking at the **USAGE** help for it. For example type the following in the console:

### **dp\_coercivity**

In the **USAGE** help you can see this command will return the calculated coercivity value (see the description “<script return values: firstcoercivityvalue>”).

### WinSocks Python Commands Usage

As an example load the attached BorisScript.py.

1. Place the WinSocks.py file in the same directory as the BorisScript.py file.
2. Next a WSClient object, ws, is created in the BorisScript.py file:

```
ws = WSClient('localhost')
```

If running the script remotely the *localhost* entry needs to be replaced by the IP address (including the port which must not be blocked in the firewall) of the computer running the Boris executable.

Now all communication is done through methods in the `ws` object.

The following methods can be used:

- `fields = ws.SendCommand(command)`

This sends a command to the console (`command` will be a string containing the exact command to run) and `fields` will contain any returned values. For example `ws.SendCommand('run')` will run the program.

Multiple commands can be sent as:

- `ws.SendCommands([command1, command2, ...])`

The above does not allow return values to be read however.

If a command has parameters, rather than including them in the string literal, these can be sent as:

- `fields = ws.SendCommand(command, [values, ...])`

In many cases the script must wait for a simulation to finish before proceeding. This is achieved by using the `Run` function:

- `ws.Run()`

This is a blocking function call, which sends the `run` command, then waits for the simulation to finish by listening to messages from the running program.

Note, some commands can return multiple values in the fields variable (`fields = ws.SendCommand(command)`). For example:

```
fields = ws.SendCommand('showdata', ['<M>'])
```

Here the 3 components of magnetization are returned in fields. To access a certain component use the Get command. For example to get the z component (3<sup>rd</sup> component thus index 2 since numbering starts from 0) of magnetization use:

```
M_z = Get(fields, 2)
```

WSClient also has a useful method for writing data to a file:

- `ws.SaveDataToFile('Results.txt', [Get(fields, 0), Get(fields, 1)])`

Continuing the example above, this command appends a new line in the Results.txt file (in the script directory) which contains two numbers: the x and y components of magnetization.

Other commands are described in the BorisScript.py file.

Run the BorisScript.py file. This script simulates a magnetization switching event, which stops as soon as the x component of magnetization switches from positive to negative.

Examples of scripted simulations will be contained in further tutorials.

## Tutorial 10 – Current-Induced Domain Wall Movement

In this tutorial you will learn how to obtain current-induced domain wall velocity curves. First we will simulate these using only console commands, including processing of output data, then we will use a Python script to more accurately determine the domain wall velocity.

The simplest available method for enabling spin torques is to use the Zhang-Li spin-transfer-torque (STT) formulation. In this formulation the calculated charge current density is used to calculate the following spin torques on the magnetization (included as additive terms in the normalised LLG equation):

$$T_{STT} = (\mathbf{u} \cdot \nabla) \mathbf{m} - \beta \mathbf{m} \times [(\mathbf{u} \cdot \nabla) \mathbf{m}]$$

where

$$\mathbf{u} = \mathbf{J}_c \frac{P}{M_s} \frac{\mu_B}{e} \frac{1}{1 + \beta^2}$$

To enable this use the **ode** command and select the *LLG-STT* equation with the *RK4* evaluation method. You will also need to enable the *transport* module (use the **modules** command and select the *transport* module). As before you need to set two electrodes (**setdefaultelectrodes**) and enable the moving mesh algorithm (**preparemovingmesh**).

In the above equation we have two new parameters:  $P$ , the charge current spin polarisation, and  $\beta$ , the STT non-adiabaticity parameter. These can be edited by using the **params** command and double-clicking on the respective interactive console objects; the default values are set for permalloy.

### Exercise 10.1

- a) Set a  $320 \times 80 \times 10$  nm permalloy rectangle with  $5 \times 5 \times 5$  nm cellsize (3D problem). Enable the moving mesh algorithm and let the domain wall relax in

zero field. Enable the transport module, set the default electrode configuration and enable the LLG-STT equation with the RK4 evaluation method.

- b) Set a simulation schedule to vary the current density from  $10^{11}$  A/m<sup>2</sup> up to  $10^{12}$  A/m<sup>2</sup> in 10 steps, saving the domain wall shift (*dwshift*), current (*I*), voltage (*V*), and charge current density (*Jc*) output data. Each current density value should be maintained for 4 ns with a data saving schedule every 50 ps.

**Hint:** You should use the *V\_seq* simulation schedule stage. This sets a sequence of voltage values with given start and stop values in a number of steps. Since we have a simple geometry you can calculate the required voltage values using the formula:

$$V = \frac{I|\mathbf{J}_c|}{\sigma}$$

where *I* is the distance between electrodes (length of the magnetic mesh) and  $\sigma$  is the electrical conductivity (see the set value using the **params** command). *Solution:* use *V\_seq* with 2.28mV; 22.8mV; 10.

**Note:** You can also vary the current density using the *I\_seq* schedule stage – this defines a sequence of current values. Setting current values directly enables the *constant current* mode, i.e. the voltage drop between electrodes is adjusted during the simulation to keep the current constant (the opposite of this is the *constant voltage* mode).

You can see the current settings using the **electrodes** command.

You can also set individual values in the console using the **setpotential** or **setCurrent** commands.

- c) Obtain and plot the domain wall velocity, *v*, using the method introduced in Tutorial 5 with **dp\_linreg**, as a function of current density. Convert the current density to spin drift velocity using the formula:

$$u = |\mathbf{J}_c| \frac{P}{M_s} \frac{\mu_B}{e} \frac{1}{1 + \beta^2}$$

Verify that the following formula holds:

$$\frac{v}{u} = \frac{\beta}{\alpha}$$

Domain wall velocity curves may also be obtained using a Python script, allowing more accurate determination of the velocity. The problem with the **dp\_linreg** method, it also includes in the regression domain wall displacement points at the start of each step. Since the domain wall requires some time to reach a steady state velocity (the acceleration is not zero at the start of each step) these initial displacement values should ideally be discarded.

With a Python script you can set a single voltage stage without saving any data (e.g. for 3 ns); this is followed by another voltage stage (e.g. again for 3 ns) during which data is saved, then a linear regression is performed to extract the velocity value for the set voltage value. The script then proceeds to set the next voltage value and so on.

### Exercise 10.2

Repeat the simulation in Exercise 10.1 but using a Python script to control the simulation flow and data output.

(*Solution: see the attached Python script*)

Note, in general you may need to adjust the stage duration times (1 – to achieve steady state motion and 2 – to generate enough data to obtain a representative velocity value using linear regression) for best results, but the suggested 3 ns, 3 ns breakdown will be sufficient for this exercise.

When setting up the Python script you will need to use the appropriate commands to edit the stage stopping and saving conditions, as well as the stage value. These commands are:

**edistagevalue**

**editstagestop**

**editdatasave**

## Tutorial 11 – Oersted Fields

In addition to spin-transfer torques, electrical currents may also interact with magnetization via the generated Oersted fields. In this tutorial we will set-up a simple bilayer mesh structure, consisting of a magnetic wire and a non-magnetic metallic capping layer, then repeat the domain wall velocity simulations from the previous tutorial but also taking into account the generated Oersted field. Since the bilayer structure has a broken mirror symmetry in the z direction we might expect the domain wall speed to be different depending on the current direction.

To enable the Oersted field you need to enable the *Oersted* module (use the **modules** command). The *Oersted* module is an electric super-mesh module, i.e. it is calculated on the electric super-mesh with a separately controlled cell-size. After enabling the *Oersted* and *transport* modules bring up the configured meshes using the **mesh** command. You should now notice the electric super-mesh rectangle with its cellsize; the electric super-mesh is simply the smallest rectangle containing all meshes with the *transport* module enabled.

To set a non-magnetic metallic capping layer you will need to add a new mesh, in particular an electrical conductor mesh. This is done using the command:

**addconductor** *name rectangle*

### Exercise 11.1

Set-up a simulation space as for Exercise 10.1. Add a metallic capping layer on top of the magnetic layer with a 5 nm thickness and enable its *transport* module (solution: use **addconductor** cap 0 0 10nm 320nm 80nm 15nm).

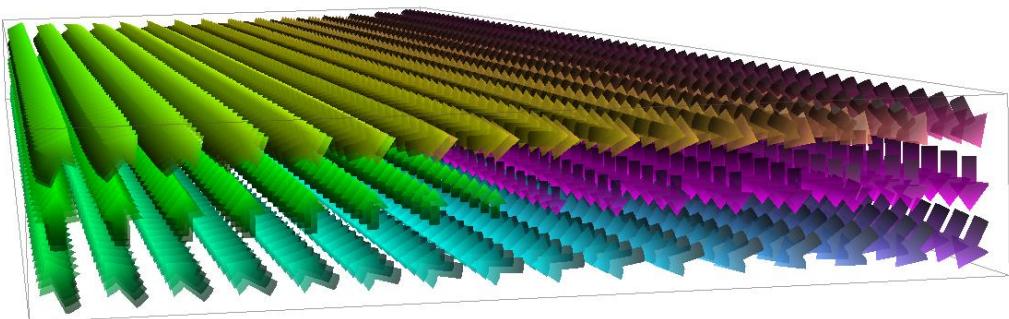
Set the electrodes to contact both meshes (use **setdefaultelectrodes** after both meshes had their *transport* module enabled).

Enable the Oersted field module and set a potential of 10mV (**setpotential** 10mV).

Compute a single iteration (**computefields**) and display the Oersted field (use the **display** command and select the Oersted display option on the super-mesh display line).

**Figure 11.1** – Computed Oersted field for Exercise 11.1.

Focused Mesh : supermesh - H0e  
Minimum : 71.7683A/m  
Maximum : 2.98761kA/m



## Exercise 11.2

Continuing from Exercise 11.1, use a Python script to simulate the domain wall velocity for both positive and negative currents in the magnitude range  $10^{11}$  A/m<sup>2</sup> to  $10^{12}$  A/m<sup>2</sup> in 10 steps. Plot the two velocity curves and compare them to the expected  $v = (\beta/\alpha)u$  relation, as well as the simulations without an Oersted field. (Solution: see the Python script in the tutorial resources).

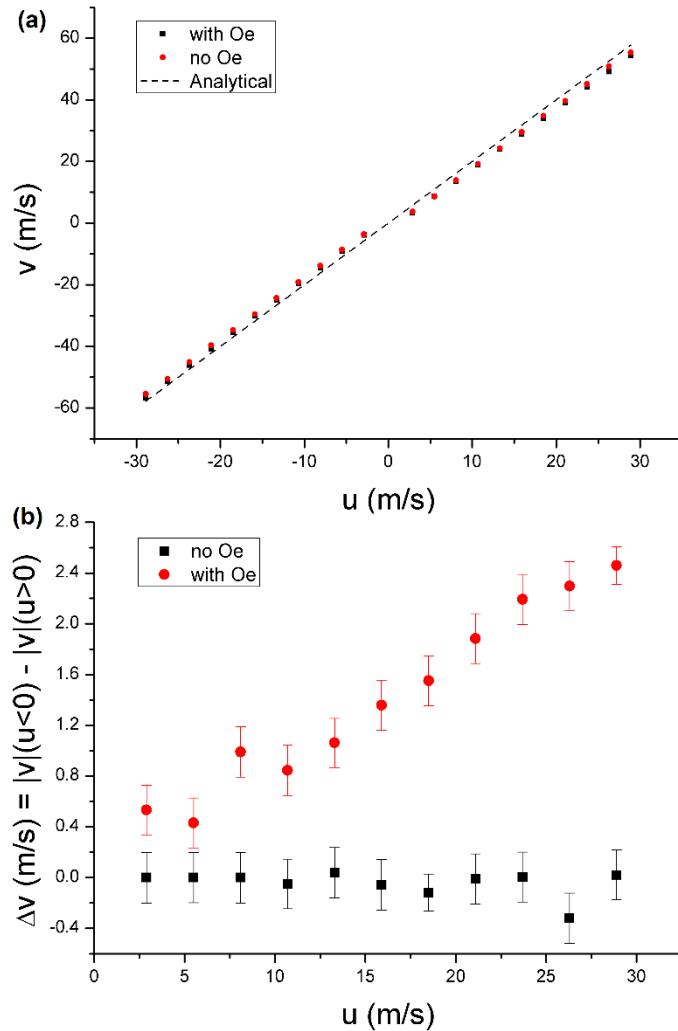
Note: when plotting  $v$  vs  $u$  you need to set the sign of  $u$  to be in the direction of electron drift, i.e. opposite sign to that of the charge current density.

In the above exercise the default electrical conductivity value of the capping layer is the same as for permalloy (this can be edited using the **params** command). In this case the current densities are the same in both layers. If you want to save output data for a particular mesh (e.g.  $J_c$ , the charge current density, which is mesh dependent) then you must focus on the required mesh first before adding that particular data to the output list.

You can focus on a particular mesh by clicking on the mesh name (bring up the list of meshes with **mesh** then click on a mesh name). Alternatively you can double click in the mesh graphical viewer on the required mesh.

Results from Exercise 11.2 are shown in Figure 11.2. The data obtained in Figure 11.2 could be improved further. The problem with using linear regression directly on the raw *dwshift* data, it contains steps due to the mesh discretisation. This is particularly problematic at low domain wall velocities where only a few steps are contained in the raw data, which can make the extracted velocity inaccurate.

**Figure 11.2** – Simulation results from Exercise 11.2 showing a) domain wall velocity plotted against spin drift velocity for cases with and without Oersted fields and also compared with the analytical formula, and b) domain wall speed difference plotted against spin drift speed for cases with and without Oersted fields.



One possibility is to collect data for a longer time, but this is inefficient. Another possibility is to assume the domain wall displacement is linear with time (in this exercise this is a valid assumption). You can then either get rid of the repeated points before using linear regression, or replace the repeated points using linear interpolation. There is a built-in command for this, and is covered in a later tutorial on skyrmion movement (**dp\_replacerepeats**).

## Tutorial 12 – Surface Exchange, Multi-Layered Demagnetization and CUDA

### Surface Exchange

Using the *surfexchange* module, two or more ferromagnetic meshes can be surface exchange coupled, allowing simulations of magnetic multilayers with RKKY interaction. The strength of the surface exchange coupling is controlled using the *J1* and *J2* material parameters: negative values result in anti-ferromagnetic coupling, positive values in ferromagnetic coupling. The *J1* parameter controls the strength of bilinear surface exchange, and *J2* controls the strength of biquadratic surface exchange.

Type **params** and have a look at *J1* and *J2*. For two meshes in surface exchange coupling, it is the top mesh *J1* and *J2* values that are used. This allows setting different coupling strength and types for the bottom and top of a mesh in a multi-layered structure. Boris allows surface exchange coupling only for xy planes, thus a multi-layered structure should be designed with the layers stacking along the z direction. Two ferromagnetic meshes will be surface exchange coupled if they both have the *surfexchange* module enabled and there's no other ferromagnetic mesh with the *surfexchange* module enabled in between them along the z direction. The coupling will only be calculated for cells which overlap in the xy plane.

### Multi-Layered Demagnetization

To add another ferromagnetic mesh use the **addmesh** command. The *demag* module for each mesh only calculates the demagnetizing field for that ferromagnetic mesh alone. When 2 or more ferromagnetic meshes are being used, if you want to compute the overall demagnetizing field you need to use the supermesh *sdemag* demagnetizing field module. In this case the individual *demag* modules are disabled and the overall demagnetizing field is computed for the collection of individual ferromagnetic meshes, including all stray field contributions. There are two ways to

do this. The default method is called multi-layered convolution, and you can see the settings for this by using the command:

### **multiconvolution**

This is an exact method of computing demagnetizing fields for a collection of computational meshes, which is able to handle arbitrary spacing and relative positioning between the layers without sacrificing accuracy or computational performance – see S. Lepadatu, Journal of Applied Physics 126, 103903 (2019) for details. In many cases you can rely on the default settings for multi-layered convolution, but for more advanced control you should read the information below.

Further info:

You can force the demagnetizing field to be computed in a 2D approximation in each mesh by clicking on the respective interactive console object (see output of the **multiconvolution** command, Force 2D : 2D meshes). This allows each mesh to have an arbitrary thickness, and is appropriate if the meshes are thin enough for the 2D approximation to hold. This option is turned off by default (Force 2D : Off), resulting in a 2D or 3D convolution in each mesh depending on their cellsizes. If the 2D approximation for each mesh is not appropriate you should use this option as long as the z cellsizes are the same in all meshes. If the z cellsizes differ the computation with Force 2D : Off may not be accurate, and in this case you should use the 2D layering option (Force 2D : 2D layered). This is similar to the 2D meshes option, however instead of forcing each mesh to be 2D, it is instead split into multiple layers, with each layer thickness set by the z cellsize in each respective mesh. This option is thus the most general case and allows exact computation of demagnetizing fields without any approximations, however it is in general more computationally expensive and should only be selected if the other 2 options are not appropriate.

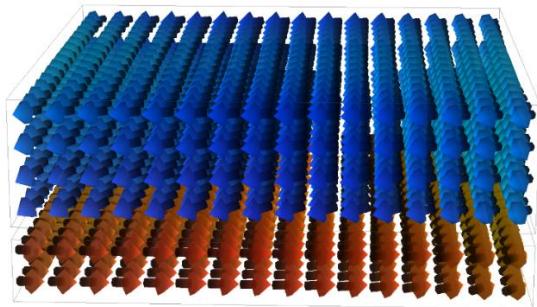
For multiple computational meshes with unequal sizes, the algorithm works by first transferring the magnetization values to scratch spaces with a common discretization. You can specify what this discretization should be, but by default it is calculated for you (see output of the **multiconvolution** command).

Another method of calculating demagnetizing fields for a collection of computational meshes is to use the so-called supermesh demagnetization. This is achieved by disabling the multi-layered convolution algorithm (see output of the **multiconvolution** command). This method calculates the demagnetizing field on the ferromagnetic supermesh by transferring magnetization and demagnetizing field values to and from the ferromagnetic supermesh using a local averaging smoother. Remember the ferromagnetic supermesh is the smallest rectangle containing all the ferromagnetic meshes and can be viewed using the **mesh** command. Computations on the ferromagnetic supermesh are done using its independent cellsize as can be seen in the console output of the **mesh** command. This cellsize will need to be carefully determined in each case to ensure accuracy of results. As a rule you should set the cellsize to be the minimum value out of the individual mesh cellsize values required to compute the demagnetizing field accurately separately. In most cases of interest, if full accuracy is required, this method is much slower than multi-layered convolution. It is also far less flexible, as it cannot accurately handle spacing between layers which cannot be exactly discretized.

Another use for the *sdemag* module without multi-layered convolution, is to calculate the demagnetizing field in an individual mesh with a different cellsize to that used for the exchange interaction. The exchange interaction typically requires a smaller cellsize to ensure accuracy, thus this method can be used to improve computational speed for larger simulations.

Starting from the **default** state, add another ferromagnetic mesh with dimensions of 80 nm × 80 nm × 20 nm, separated from the first mesh by 2 nm along the z direction. Enable the *surfexchange* module for both meshes, as well as the *sdemag* module. Now **run** the simulation and observe the result – see Figure 12.1.

**Figure 12.1** – Anti-ferromagnetic surface exchange coupled ferromagnetic meshes



You can also add a metallic spacer layer in between, using the **addconductor** command, however this will not affect magnetic computations directly; it will be needed however if charge or spin transport computations are also enabled.

#### Exercise 12.1

- a) Set-up a synthetic ferrimagnetic (SyF) Ni<sub>80</sub>Fe<sub>20</sub> bilayer with elliptical shape of 320 nm × 160 nm, thickness values of 20 nm and 10 nm respectively, and with a separation of 2 nm between layers. Simulate a hysteresis loop for this SyF structure along 1° to the x-axis direction, plotting the average magnetization for the entire bilayer against field (you will need to calculate this from the magnetization saved for the two layers separately – see notes below).

You should use the *SDesc* with *LLGStatic* solver and set a low *mxh* threshold value, in this case it is recommended to set it to 10<sup>-7</sup> (use **ode** command). The field step should not be greater than 1 kA/m.

- b) Repeat the same exercise but this time set-up a synthetic antiferromagnetic bilayer (SAF) with the same overall thickness as above – i.e. 15nm thick layers with 2 nm spacing.

When adding data to the output list, you can select the mesh for which it applies, if applicable, e.g. magnetization output. You can do this either by adding data when

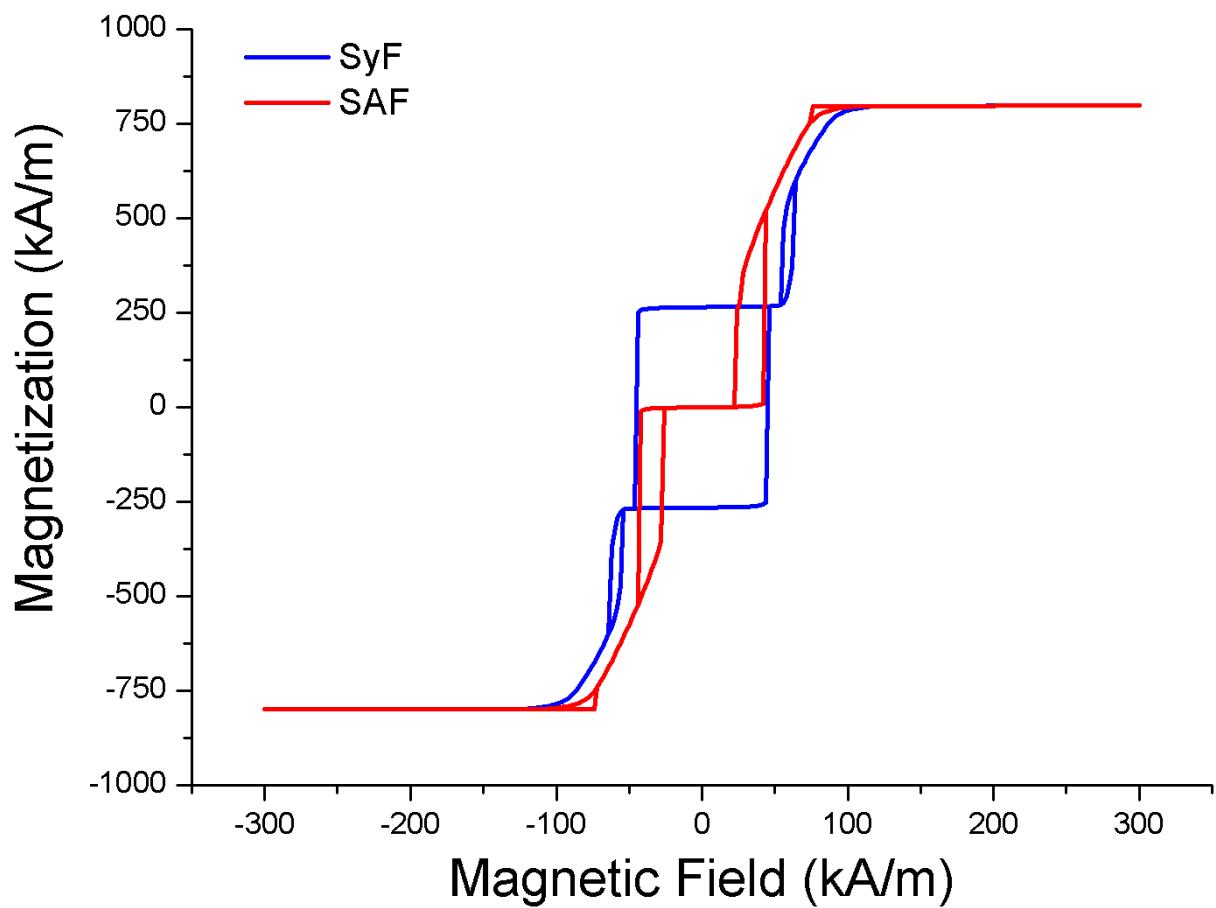
the required mesh is in focus, or editing that data entry later to change the applicable mesh name. For the exercise above you will need to add to the output the magnetization for both meshes as two separate entries (use **data** command and follow instructions therein).

You will need to apply the field for the hysteresis loop to both meshes, not just the first *permalloy* mesh. Use the **stages** command and add a *Hpolar\_seq* stage. You will see the field is set to be applied only to the current mesh in focus, e.g. *Hpolar\_seq <permalloy>*. Instead, you will need to edit this by double-clicking on the added stage entry, and changing the name from *permalloy* to *supermesh*. After this the entry should read *Hpolar\_seq <supermesh>*. The field sequence will now be applied to both ferromagnetic meshes.

When working with multiple ferromagnetic meshes, all the commands that affect changes in a ferromagnetic mesh have an optional parameter which specifies which mesh to use. If only one ferromagnetic mesh is created the mesh name doesn't need to be specified explicitly. If multiple meshes are used, unless the name is specified the settings are applied either to the current mesh in focus, or to the supermesh, depending on the command.

For example the **setangle** and **setfield** commands will make changes to all ferromagnetic meshes unless a specific name is specified – see the help for these commands (**?setangle**, **?setfield**). On the other hand the **loadmaskfile** command (remember you can just drag a .png file to the mesh viewer instead of typing this command) only applies the shape to the current mesh in focus.

**Figure 12.2** – Hysteresis loops obtained for the SyF and SAF bilayers in Exercise 12.1



## CUDA Computations

Larger simulations will benefit from using computations on the GPU, rather than the default CPU computations. If you have a CUDA-enabled graphics card you can enable GPU computations using the **cuda** command:

**cuda 1**

If CUDA computations are not available for your computer, typing the **cuda** command will show an N/A status. You can also see how much CPU and GPU-addressable memory you have by using the **memory** command.

When using CUDA computations, for optimum efficiency you will want to limit the display update frequency (use the **iterupdate** command). Boris is designed to limit memory transfers between GPU and CPU-addressable memory to an absolute minimum, as this is a critical bottleneck in performance. To display mesh data in the viewer, an average display data is computed on the GPU, then transferred to CPU-addressable memory so it can be used by graphics routines. This transfer can slow down computations, especially if the display viewing coarseness is small (remember you can use the mouse wheel to change viewing coarseness).

*If the simulation is very large you should be careful about setting too small a viewing coarseness, as this will make the program slow and less responsive when working with the console.*

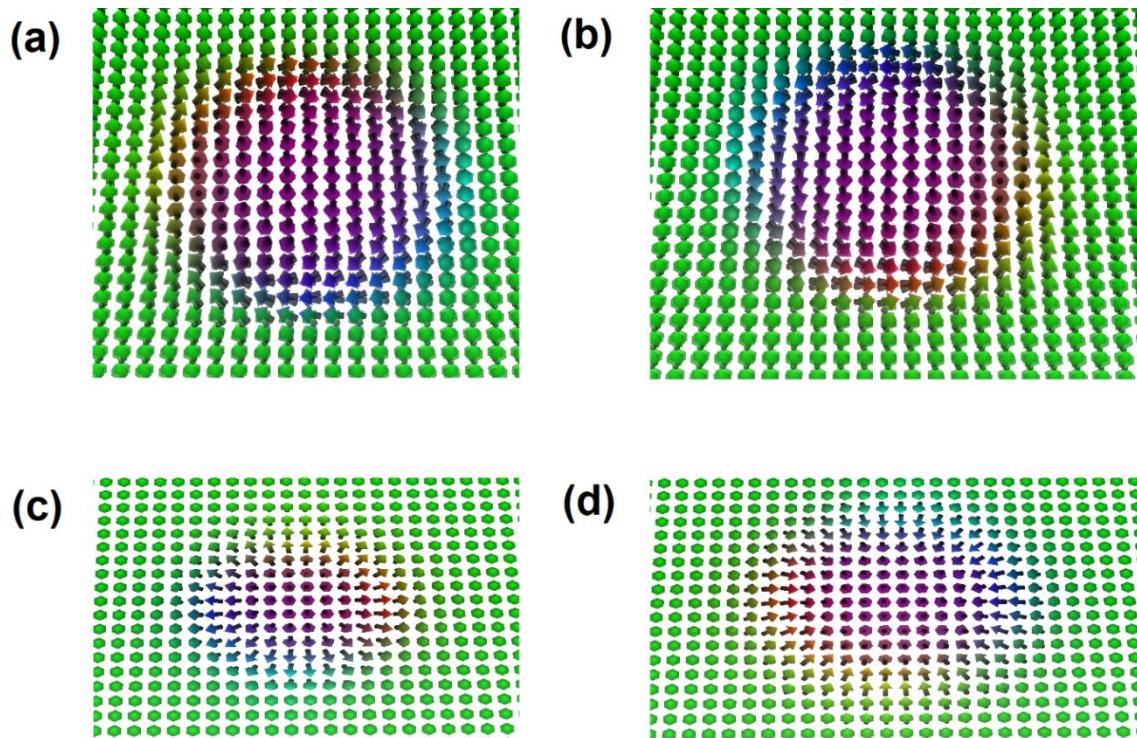
## Tutorial 13 – Dzyaloshinskii-Moriya Exchange

Dzyaloshinskii-Moriya interaction (DMI) may be included in the simulation by enabling the *DMExchange*, or the *iDMExchange* module. The former is used for bulk DMI, whilst the latter is used for interfacial DMI. The strength of the DMI interaction is controlled using the *D* material parameter (use **params** command). Néel skyrmions may be generated in the xy plane using the **skyrmion** command:

**skyrmion core chirality diameter position**

In the above command the *core* parameter sets the z direction of the skyrmion core (-1 or 1), the *chirality* parameter sets the radial direction rotation (-1 for away from core, 1 for towards core). The *diameter* and *position* may be specified using metric units, with the *position* requiring 2 components. **Figure 13.1** shows examples of relaxed Néel (*iDMExchange*) and Bloch (*DMExchange*) skyrmions for both  $D > 0$  and  $D < 0$ .

**Figure 13.1** – a) Bloch skyrmion for  $D < 0$ , b) Bloch skyrmion for  $D > 0$ , c) Néel skyrmion for  $D < 0$ , and d) Néel skyrmion for  $D > 0$ .



For the following exercises, when computing a relaxed magnetization state you should use the *SDesc* with *LLGStatic* solver, remembering to set a low *msh* convergence value (at least  $10^{-6}$ ).

### Exercise 13.1

- a) Obtain relaxed Néel skyrmions for both  $D > 0$  and  $D < 0$  in an ultrathin (1 nm) Co layer with perpendicular magnetization. You will need to use the *IDMExchange* module. Use material parameters as  $M_s = 600$  kA/m,  $A = 10$  pJ/m,  $|D| = 1.5$  mJ/m<sup>2</sup>,  $K_1 = 380$  kJ/m<sup>3</sup> for uniaxial anisotropy with easy axis along z direction. To reduce the skyrmion diameter apply an out-of-plane magnetic field opposing the skyrmion core, e.g. 15 kA/m along the 0, 0 (polar coordinates) direction.
- b) Obtain Bloch skyrmions for both  $D > 0$  and  $D < 0$ . You may use the same parameters as above, but this time set a thickness of 10 nm and use the *DMExchange* module. You will need to set a larger out-of-plane magnetic field to control the skyrmion diameter.
- c) For part a) compute the skyrmion diameter and topological charge.

To complete Exercise 13.1 c), you will need to extract a profile along the skyrmion diameter, then fit it using an analytical model for a skyrmion. Boris provides this functionality through the **dp\_fitskyrmion** command. The z component of **M** is fitted using the following formula (see X.S. Wang et al., Commun. Phys. 1, 31 (2018)):

$$M_z(x) = M_s \cos\left(2 \arctan\left(\frac{\sinh(R/w)}{\sinh(x - x_0)/w}\right)\right), \quad w = \frac{\pi D}{4K}, \quad K = K_u - \mu_0 M_s^2 / 2$$

Here  $M_s$  (saturation magnetization),  $R$  (skyrmion radius),  $x_0$  (skyrmion center position), and  $w$  are used as fitting parameters, and in particular the  $M_s$  and  $w$  values after the fit should match the expected values from the material parameters set.

Thus to obtain the skyrmion radius first use **dp\_getprofile** to extract a profile through the center of the skyrmion, then use **dp\_fitskyrmion** on the z component of **M**. The fitting works for both skyrmion topological charges, but the fitted value of  $M_s$  will change sign depending on the sign of the topological charge.

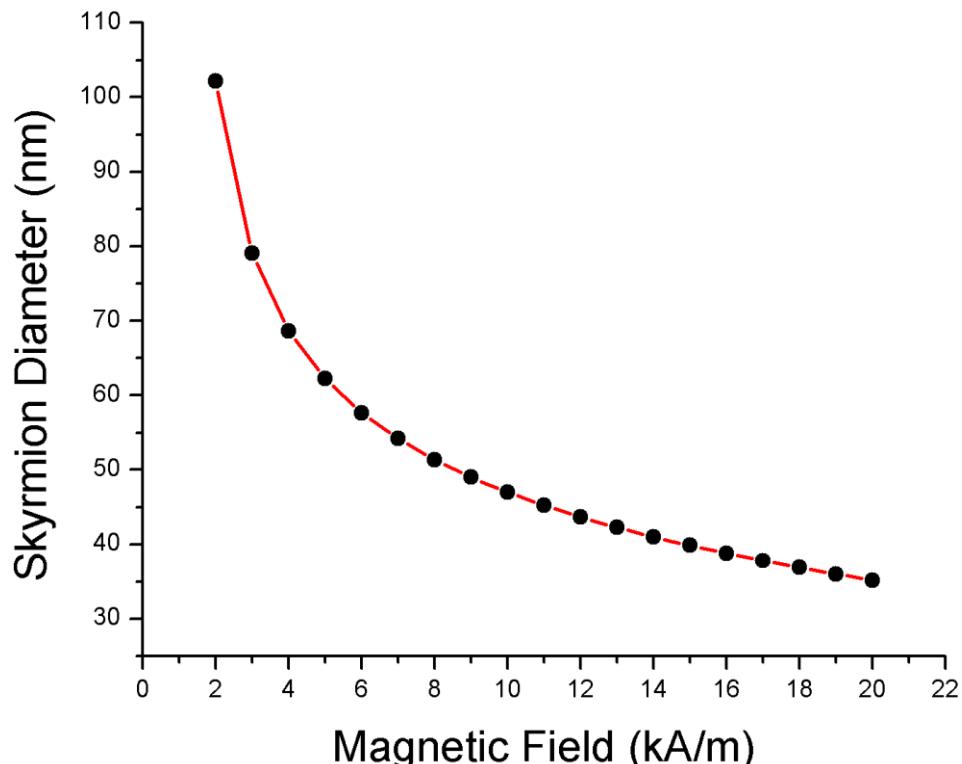
To calculate the topological charge, there is a built-in command, **dp\_topocharge**. This command solves the following formula over the xy plane S:

$$Q = \frac{1}{4\pi} \int_S \mathbf{m} \cdot \left( \frac{d\mathbf{m}}{dx} \times \frac{d\mathbf{m}}{dy} \right) dx dy$$

### Exercise 13.2

For the same parameters as in Exercise 13.1, compute the skyrmion diameter as a function of out-of-plane field strength from 2 kA/m to 20 kA/m in 1 kA/m steps. You should set-up a Python script to automate this simulation.

**Figure 13.2** – Skyrmion diameter as a function of out-of-plane field strength obtained in Exercise 13.2.



## Tutorial 14 – Simulations with non-zero temperature

### Landau-Lifshitz-Bloch equation and Curie temperature

Non-zero temperature simulations may be performed by using the Landau-Lifshitz-Bloch (LLB) equation – use the **ode** command then select the appropriate equation to solve.

With a non-zero temperature the magnetization length (saturation magnetization) is no longer a constant, but depends on the applied field strength. This is modelled via a longitudinal susceptibility included in the LLB equation. Instead, we talk about the *equilibrium magnetization*, which is the stable magnetization length at a given field. Thus at zero temperature the equilibrium magnetization coincides with the saturation magnetization. With a non-zero temperature the equilibrium magnetization gradually decreases, reaching zero at the Curie temperature. Other parameters which change with temperature include the exchange stiffness and magnetization damping. With a non-zero temperature the damping is now divided into two terms: transverse damping (coincides with the Gilbert damping at zero temperature) and longitudinal damping. For further information these articles can be used as a starting point: S. Lepadatu, Journal of Applied Physics 120, 163908 (2016) and S. Lepadatu & M.M. Vopson, Materials 10, 991 (2017).

In the simplest case the temperature inside the mesh is uniform, and is controlled using the **temperature** command, which sets the mesh *base temperature*:

**temperature value (meshname)**

When enabling the LLB equation you will also need to set appropriate temperature dependences for some material parameters, including *Ms*, *damping*, *A*, and *susrel* (the relative longitudinal susceptibility). The longitudinal damping used in the LLB equation is not available as a separate material parameter, but is automatically calculated based on the transverse damping parameter (*damping*). Default temperature dependences for these parameters may be generated based on the Curie temperature of the material – for details see S. Lepadatu, Journal of Applied

Physics 120, 163908 (2016). You can do this using the **curietemperature** command:

**curietemperature** *value* (*meshname*)

### Setting material parameters temperature dependences

#### Exercise 14.1

Set a Curie temperature of 870 K (appropriate for Ni80Fe20) and obtain plots of the temperature dependences of the *Ms*, *damping*, *A*, and *susrel* material parameters (see below).

Almost all material parameters available in Boris can be assigned a temperature dependence. This is achieved by specifying a scaling law,  $t$ . The value of a parameter at a temperature  $T$  is then obtained as  $\text{value\_at\_T\_K} = \text{value\_at\_0\_K} \times t(T)$  – any computational routine in Boris for which a parameter is used, obtains an updated value in this way, where  $T$  is either the base temperature (uniform temperature mode) or the local temperature (non-uniform temperature mode). To see the currently set temperature dependences use the **paramstemp** command. You can set a temperature dependence by assigning a pre-defined analytical formula (see console output for **paramstemp**), or by loading an array using the **setparamtemparray** command. Once a temperature dependence array has been set (e.g. after using the **curietemperature** command), you can load the set temperature dependence into an internal data processing array using the **dp\_dumptdep** command:

**dp\_dumptdep** *meshname* *paramname* *max\_temperature* *dp\_index*

For example to see the set temperature dependence for *Ms* use the following:

**dp\_dumptdep** *permalloy* *Ms* 870 0

**dp\_save** *Ms\_scaling* 0

In the file `Ms_scaling.txt` (saved under the current working directory – see **data** command) you will see a single column with the scaling coefficients. These are saved in increments of 1 K, from 0 K up to 870 K. Internally the scaling coefficients are obtained from the user loaded array at 1 K increments, irrespective of how the user specified the temperature dependence – missing temperature points are filled in using interpolation. During computations the scaling coefficients are obtained by interpolating the nearest 2 temperature scaling points. To reset all parameters temperature dependences you can use the **clearparamstemp** command.

### Field dependence of material parameters temperature dependences

With non-zero temperature simulations, the equilibrium magnetization also depends on the strength of the applied magnetic field. This dependence is enabled by setting the strength of the net atomic moment of the material, specified in Boris as multiples of the Bohr magneton. This is done using the command:

**atomicmoment (value)**

If this value is not zero, whenever the applied magnetic field changes, the temperature dependences of all the parameters affected by the Curie temperature setting (see above) are recalculated. Moreover, the longitudinal susceptibility is directly proportional to this value so must be set correctly whenever the LLB equation is used.

### Non-zero temperature simulations

#### Exercise 14.2

Simulate the hysteresis loops in a  $160 \times 160 \times 5$  nm permalloy circle at zero temperature (using the LLG equation), as well as at room temperature (297 K, using the LLB equation) and compare the two loops. With the LLB equation the time step for numerical stability is usually lower – you might need to investigate this.

## Tutorial 15 – Thermal Fields

When non-zero temperature modelling is considered, an additional effect that can be included is lattice thermal agitation. This gives rise to fluctuations in magnetic moments, and may be modelled by introducing appropriate stochastic fields and torques. In Boris thermal fields may be enabled by selecting a stochastic magnetization dynamics equation, e.g. sLLB – use the **ode** command then select the appropriate equation to solve. For further information see S. Lepadatu & M.M. Vopson, Materials 10, 991 (2017).

When solving stochastic equations, the choice of available ODE evaluation methods is more limited since they must be able to handle the stochasticity introduced. Currently the best fixed time-step method available in Boris is the trapezoidal Euler (*TEuler*) evaluation method, also known as Heun's method. Since this method is a fixed time step method you will need to investigate the time step required for numerical stability. You can use the default time step as a starting point.

There is an adaptive time-step version of this called *AHeun* which you can also use.

### Exercise 15.1

Simulate out-of-plane hysteresis loops at room temperature in a 256 nm × 256 nm Co rectangle with perpendicular magnetization, with 4 nm thickness, and cubic 4 nm cellsize. Use material parameters as  $M_s = 600$  kA/m,  $A = 10$  pJ/m, and  $K_1 = 380$  kJ/m<sup>3</sup> for uniaxial anisotropy with easy axis along z direction. You should simulate hysteresis loops with and without thermal fields for comparison.

## Tutorial 16 – Heat Flow Solver and Joule Heating

### Heat equation

Non-uniform temperature simulations may be enabled by selecting the *heat* module. Any mesh with this module enabled will solve the heat equation as a function of time. If any two meshes with the *heat* module enabled are in contact, then heat flow across the interface (also referred to as a composite media boundary) is automatically calculated based on the continuity of heat flux and temperature perpendicular to the composite media boundary.

There is a special type of mesh, referred to as an *insulator* mesh in Boris, which can be used to model substrates. You can add an insulator mesh using:

**addinsulator** *name rectangle*

When the *heat* module is enabled, the *thermal cell* discretisation cellsize becomes available in the mesh descriptions (use the **mesh** command). This can be controlled independently of the magnetic and electric cellsize (if enabled), and can also be set independently of other cellsize values in other meshes.

The heat equation time step may be set using:

**setheatdt** *value*

This value shouldn't be larger than the magnetization dynamics equation time step (**setdt**), since during computations the heat equation time is incremented only up to the current magnetization equation time (the global time, or total time – see the *time* output data). If this value is lower, the heat equation will be iterated multiple times until it catches up to the magnetization equation time.

The mesh temperature may be set as before using the **temperature** command. This sets a uniform mesh temperature as a starting point, but depending on the simulation

configuration the mesh temperature can change. This is true particularly if the mesh ambient temperature is different. For the heat equation, boundary conditions for cells not at a composite media boundary are set based on Newton's law of cooling – i.e. Robin boundary conditions are used. These require an ambient temperature (the surrounding temperature) and a heat transfer coefficient (the Robin coefficient). To adjust these values you may use the **ambient** command, then double click on the respective interactive objects to modify their values. Note, when the **temperature** command is used, setting a mesh temperature automatically sets the ambient temperature to the same value too. You may also choose to have thermally insulating boundary conditions by selecting the appropriate options displayed by the **ambient** command.

### Parameters for heat transport

A few parameters are used to specify the thermal properties of the material, in particular the *thermK* (thermal conductivity) and the *shc* (specific heat capacity) material parameters – see these by using the **params** command. Additionally the *density* (mass density) parameter also enters the heat equation.

Note, all material parameters with a temperature dependence enabled will now also vary non-uniformly throughout the mesh (if *heat* module enabled), taking on the value set by the local cell temperature value.

You may obtain the mesh average temperature through the *<Temp>* output data – use **data** command. The mesh temperature may also be displayed (*Temp*) – use the **display** command.

### Joule heating

If the *transport* module is also enabled in the same mesh as the *heat* module, Joule heating is taken into account. This results in a heat source term in the heat equation due to the charge current density, **J** as:

$$C_p \frac{\partial T(\mathbf{r}, t)}{\partial t} = \nabla \cdot K \nabla T(\mathbf{r}, t) + \frac{\mathbf{J}^2}{\sigma}$$

In the next exercise you will investigate the effect of a voltage pulse on a Ni<sub>80</sub>Fe<sub>20</sub> nanowire placed on a SiO<sub>2</sub> substrate, similar to the work in S. Lepadatu, Journal of Applied Physics 120, 163908 (2016). To model a very long wire on a substrate (say the wire is oriented along the x-axis) you should set the x-axis ends of both the magnetic wire and substrate as insulating since in this case the heat flux is oriented only along the y and z directions. Similar considerations apply to the substrate if you want it to be effectively infinite in the x-y plane and depth – set insulating boundary conditions in the required directions. Note in this latter case the modelled substrate must still be large enough for the temperature evolution to be correct for the required duration – for details see S. Lepadatu, Journal of Applied Physics 120, 163908 (2016). The x-axis ends of the magnetic wire should have electrodes so a uniform current density is achieved – remember you can use the **setdefaultelectrodes** command. You can leave the Robin heat transfer coefficient (see **ambient** command output) to the default value as this is appropriate for ventilated air surrounding.

The SiO<sub>2</sub> substrate may be added by using the **addinsulator** command and enabling its *heat* module. You will also need to enter appropriate values for thermal conductivity, specific heat capacity and density, and similarly for the Ni<sub>80</sub>Fe<sub>20</sub> magnetic wire.

Note, typically the *thermal cellsize* can be greater than the magnetic (or electric) cellsize, and again can be set independently in different meshes (composite media boundary conditions do **not** require the discretizations to match on the two contacting meshes, for any computational routines used in Boris; generic composite media boundary computational routines are used which are second order accurate in space for all meshes). For the purposes of the next exercise you can use a simple cubic cellsize with a 10 nm side for all the thermal discretization lengths (note, if the mesh thickness is 10 nm then the z cellsize will be adjusted so there are at least 2 computational cells along the z direction – 3D solver used).

### Exercise 16.1

Create a Ni<sub>80</sub>Fe<sub>20</sub> nanowire with 160 nm width, 10 nm thickness and 640 nm length, centered on a SiO<sub>2</sub> substrate with 800 nm width, 640 nm length and 150 nm depth.

Enable heat equation computations in both meshes and transport module in the Ni<sub>80</sub>Fe<sub>20</sub> nanowire. By setting appropriate insulating boundary conditions for heat conduction, define the nanowire to be effectively infinite along the x axis, and the substrate elongated in the x-y plane and depth. Set the ambient temperature (as well as the base temperature – the starting temperature) to be the room temperature value (297 K). The default thermal conductivity, specific heat capacity and mass density values are appropriate for Ni<sub>80</sub>Fe<sub>20</sub>. For SiO<sub>2</sub> you should edit these as K = 1.4 W/mK (*thermK*), C = 730 J/kgK (*shc*), and ρ = 2200 kg/m<sup>3</sup>.

- a) Set a voltage step with 50 ns duration which results in a current density of 10<sup>12</sup> A/m<sup>2</sup> at T = 297 K. Use a temperature dependence for the electrical conductivity σ such that:

$$\sigma = \frac{\sigma_0}{1 + 0.025T}$$

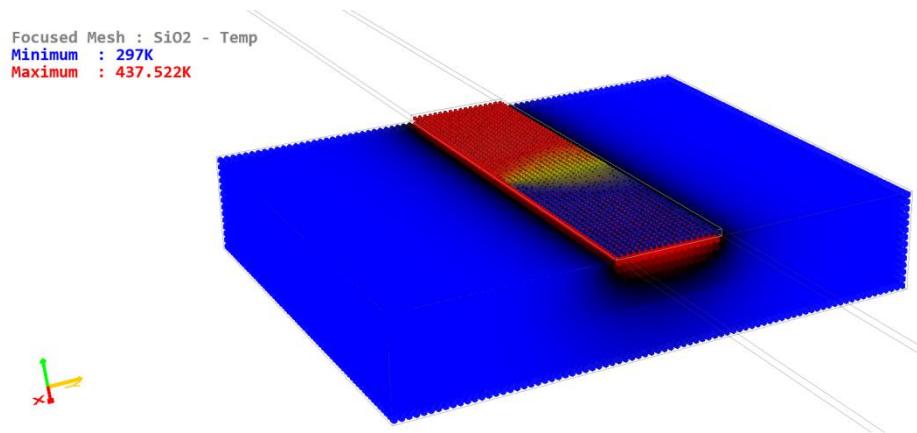
The above formula represents the default temperature dependence set for electrical conductivity - see **paramstemp** command. Obtain the average temperature and current density as a function of time in the Ni<sub>80</sub>Fe<sub>20</sub> mesh both for the heating cycle (first 50 ns), as well as the next 50 ns of the cooling cycle when the voltage is set to zero. (Note, just for this part, to speed up the computations you may want to disable any magnetic computations in the Ni<sub>80</sub>Fe<sub>20</sub> nanowire by disabling the *demag*, *exchange*, and *zeeman* modules).

- b) Set a transverse domain wall in the center of the nanowire through the **preparemovingmesh** command and relax it. Redo the simulation in part a), but this time also obtain the domain wall displacement as a function of time when using the LLG-STT equation (use the **ode** command).

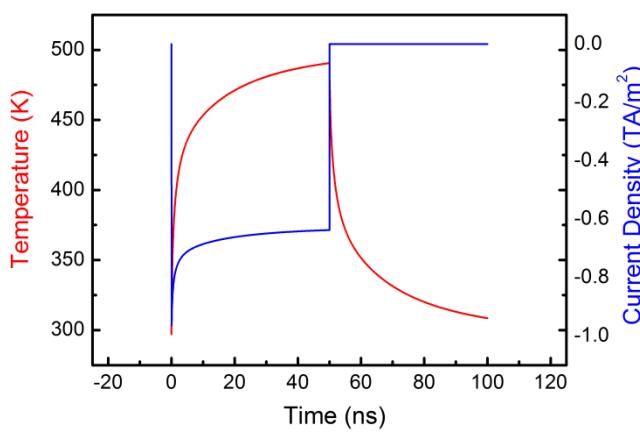
- c) Repeat part b) but this time use the LLB-STT equation with a Curie temperature of 870 K. Note, you will need to reduce the time step significantly for the LLB equation for numerical stability.

**Figure 16.1 –** a) Geometry used for Exercise 16.1, showing a magnetic wire on a SiO<sub>2</sub> substrate with Joule heating computations enabled – heat is generated in the magnetic wire due to an applied charge current density. b) Average temperature in the permalloy nanowire, also showing the current density during and after the applied voltage pulse. c) Domain wall displacement simulated using the LLG-STT and LLB-STT equations. For the latter a Curie temperature of 870 K was set.

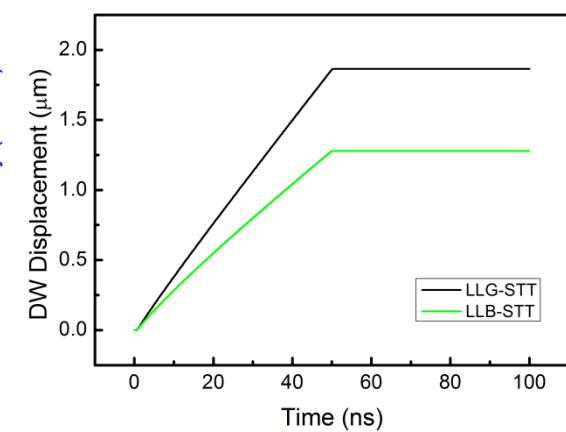
a)



b)



c)



## Tutorial 17 – Spin Transport Solver

In addition to the simple Ohm's law used to obtain the charge current density with the *transport* module, Boris also integrates a 3D spin current solver based on the spin drift-diffusion equations – see S. Lepadatu, Scientific Reports 7, 12937 (2017). This solver allows for a number of effects to be computed self-consistently in arbitrary multi-layered geometries and integrated with the magnetization dynamics solver. These include the spin Hall effect (SHE), inverse SHE, CPP-GMR, spin diffusion and non-local spin transport effects, spin pumping, as well as bulk and interfacial spin torques calculated from the spin accumulation and composite media boundary conditions.

The spin transport solver computes both the charge and spin polarisation current densities,  $\mathbf{J}_C$  and  $\mathbf{J}_s$  respectively, together with the charge potential,  $V$ , and spin accumulation,  $\mathbf{S}$ :

$$\mathbf{J}_C = \sigma \mathbf{E} + \beta_D D_e \frac{e}{\mu_B} (\nabla \mathbf{S}) \mathbf{m} + \theta_{SHA} D_e \frac{e}{\mu_B} \nabla \times \mathbf{S}$$

$$\mathbf{J}_s = -\frac{\mu_B}{e} \beta_\sigma \sigma \mathbf{E} \otimes \mathbf{m} - D_e \nabla \mathbf{S} + \theta_{SHA} \frac{\mu_B}{e} \boldsymbol{\epsilon} \sigma \mathbf{E}$$

$\mathbf{J}_s$  is a rank-2 tensor such that  $\mathbf{J}_{sij}$  signifies the flow of the  $j$  component of spin polarisation in the direction  $i$ . The electric field is given by  $\mathbf{E} = -\nabla V$  and  $\mathbf{S}$  satisfies the equation of motion:

$$\frac{\partial \mathbf{S}}{\partial t} = -\nabla \cdot \mathbf{J}_s - D_e \left( \frac{\mathbf{S}}{\lambda_{sf}^2} + \frac{\mathbf{S} \times \mathbf{m}}{\lambda_J^2} + \frac{\mathbf{m} \times (\mathbf{S} \times \mathbf{m})}{\lambda_\varphi^2} \right)$$

In the above equations we have a number of material constants which can be controlled via the **params** command:

- $D_e$  is the electron diffusion constant
- $\beta_D$  is the diffusion spin polarisation - this term leads to CPP-GMR

- $\beta_\sigma$  is the charge current spin polarisation – this term leads to Zhang-Li spin transfer torques, among other effects
- $\theta_{SHA}$  is the spin Hall angle (unitless) – the term in the equation for  $\mathbf{J}_s$  leads to SHE, whilst the term in the equation for  $\mathbf{J}_c$  leads to the inverse SHE; Note there are two related parameters available in Boris: *SHA* and *iSHA*. These represent the spin Hall angle, but may be set to different values, allowing the SHE or inverse SHE to be turned on or off in the computations by setting one or the other to zero.
- $\lambda_{sf}$  is the spin flip length
- $\lambda_J$  and  $\lambda_\varphi$  are the exchange rotation and spin dephasing lengths respectively, describing the absorption of transverse spin components (transverse to  $\mathbf{m}$ , the magnetization direction) within a ferromagnetic material

Bulk spin torques are included in the computations as:

$$\mathbf{T}_s = -\frac{D_e}{\lambda_J^2} \mathbf{m} \times \mathbf{S} - \frac{D_e}{\lambda_\varphi^2} \mathbf{m} \times (\mathbf{m} \times \mathbf{S})$$

This term is included in the implicit LLG (or LLB) equation as (in practice this term results in an effective field which is added to  $\mathbf{H}_{eff}$ ):

$$\frac{\partial \mathbf{m}}{\partial t} = -\gamma \mathbf{m} \times \mathbf{H}_{eff} + \alpha \mathbf{m} \times \frac{\partial \mathbf{m}}{\partial t} + \frac{1}{M_s} \mathbf{T}_s$$

There is a parameter in Boris, called *ts\_eff* (see **params**): This is a unitless constant which multiplies  $\mathbf{T}_s$  and is termed the spin torque efficiency, allowing bulk spin torques to be turned off (*ts\_eff* = 0) or fully on (*ts\_eff* = 1).

There are two possibilities for treating composite media boundaries. The simplest approach is to assume continuity of a flux and potential – for the spin transport solver these are  $\mathbf{J}_c$  and  $V$  for charge transport and  $\mathbf{J}_s$  and  $\mathbf{S}$  for spin transport. The continuity conditions are used when modelling interfaces between two normal metals (N) or two ferromagnets (F); they may also be used to model interfaces between a normal metal and ferromagnet (N/F) but in this case typically the second approach is more appropriate, based on interface spin conductances:

$$\begin{aligned}\mathbf{J}_c \cdot \mathbf{n} \Big|_N &= \mathbf{J}_c \cdot \mathbf{n} \Big|_F = -\left(G^{\uparrow} + G^{\downarrow}\right) \Delta V + \left(G^{\uparrow} - G^{\downarrow}\right) \Delta \mathbf{V}_s \cdot \mathbf{m} \\ \mathbf{J}_s \cdot \mathbf{n} \Big|_N - \mathbf{J}_s \cdot \mathbf{n} \Big|_F &= \frac{2\mu_B}{e} \left[ \operatorname{Re} \left\{ G^{\uparrow\downarrow} \right\} \mathbf{m} \times (\mathbf{m} \times \Delta \mathbf{V}_s) + \operatorname{Im} \left\{ G^{\uparrow\downarrow} \right\} \mathbf{m} \times \Delta \mathbf{V}_s \right] \\ \mathbf{J}_s \cdot \mathbf{n} \Big|_F &= \frac{\mu_B}{e} \left[ -\left(G^{\uparrow} + G^{\downarrow}\right) (\Delta \mathbf{V}_s \cdot \mathbf{m}) \mathbf{m} + \left(G^{\uparrow} - G^{\downarrow}\right) \Delta V \mathbf{m} \right]\end{aligned}$$

In the above equations  $G^{\uparrow}$ ,  $G^{\downarrow}$  are interface conductances for the majority and minority spin carriers respectively, and  $G^{\uparrow\downarrow}$  is the complex spin mixing conductance. Also  $\Delta V$  is the potential drop across the N/F interface ( $\Delta V = V_F - V_N$ ) and  $\Delta \mathbf{V}_s$  is the spin chemical potential drop, where  $\mathbf{V}_s = (D_e / \sigma)(e / \mu_B) \mathbf{S}$ . These interface conditions describe the absorption of transverse spin components at the interface, giving rise to interfacial spin torques:

$$\mathbf{T}_s^{\text{interface}} = \frac{g\mu_B}{ed_h} \left[ \operatorname{Re} \left\{ G^{\uparrow\downarrow} \right\} \mathbf{m} \times (\mathbf{m} \times \Delta \mathbf{V}_s) + \operatorname{Im} \left\{ G^{\uparrow\downarrow} \right\} \mathbf{m} \times \Delta \mathbf{V}_s \right]$$

There is also an associated interfacial spin torque efficiency constant –  $tsi\_eff$ . The above term is also included in the magnetization dynamics equation, much in the same way as  $\mathbf{T}_s$  is. The main difference is this torque is only included in the computational cells at the interface, where  $d_h$  is the cellsize normal to the interface – this allows correct computation of interfacial spin torques for a ferromagnetic layer of given thickness  $t$ , independent of its computational discretization, since the effect on magnetization of the interfacial spin torque is averaged over its thickness.

Spin pumping is generated at an N/F interface as:

$$\mathbf{J}_s^{pump} = \frac{\mu_B}{2\pi} \left[ \operatorname{Re} \left\{ g^{\uparrow\downarrow} \right\} \mathbf{m} \times \frac{\partial \mathbf{m}}{\partial t} + \operatorname{Im} \left\{ g^{\uparrow\downarrow} \right\} \frac{\partial \mathbf{m}}{\partial t} \right]$$

Here  $g^{\uparrow\downarrow} = (h/e^2)G^{\uparrow\downarrow}$  and the pumped spin current is used in the calculation of composite media boundary conditions by including it on the normal metal side of the equations. As with the spin torques, there's an associated spin pumping efficiency

parameter – *pump\_eff* – which allows spin pumping to be turned on or off in the computations.

When modelling N/F interfaces you may need to have different interface conductances on different sides of a ferromagnetic layer (e.g. a Pt/Co/Ta multilayer, where the Pt/Co and Co/Ta interfaces may need different spin mixing conductances). For this reason, the interface conductances ( $G^{\uparrow}$ ,  $G^{\downarrow}$ , and  $G^{\uparrow\downarrow}$ ) are not associated just with a ferromagnetic mesh, but also appear in the list of parameters for normal metal meshes (*conductor* meshes - **addconductor**). When an N/F interface is defined by the contact of two meshes, the interface conductances stored in the *upper* mesh are used – e.g. if the meshes are arranged in a multilayer structure along the z direction, the upper mesh is that with a higher z coordinate.

To turn off the interface conductance approach to modelling composite media boundaries you need to set the  $G^{\uparrow}$  and  $G^{\downarrow}$  values to zero for the appropriate mesh. In this case the computations revert to using the continuity approach described above.

To enable the spin transport solver you need to have the *transport* module active in the mesh you want spin transport computations and you must also select a magnetization dynamics equation with spin accumulation (e.g. LLG-SA, LLB-SA, etc.) – see the **ode** command.

Using the **display** command you can select to display a number of associated quantities in the mesh viewer, including **S**, bulk and interfacial spin torques, x, y, and z directions for the spin current.

With the spin transport solver enabled you will need to pay attention to the convergence constant for the spin accumulation solver. Similarly to the charge potential solver, which solves a Poisson equation to obtain V within the set convergence constant, the spin accumulation **S** is obtained by solving a vector Poisson equation – this equation is obtained from the equation of motion for **S** in the “steady state”, i.e. when  $\partial\mathbf{S}/\partial t = 0$ . The response time-scales of **m** and **S** are

separated typically by 3 orders of magnitude (ps vs fs time-scales respectively) thus we only require to obtain the “steady state” values for **S** for a given magnetization configuration. The vector Poisson equation also uses a convergence constant and a timeout for the maximum number of allowed sequential iterations, and these values may be changed by using the **tsolverconfig** command.

Further info:

Whilst each iteration taken for the Poisson equations for **V** and **S** is relatively cheap, typical problems may require a large number of iterations to reach convergence, which significantly slows down computations. This is especially true in the initialization stage when the timeout number of iterations may be reached for the first few iterations; after this, small steps in **m** should result in relatively few steps in the solution of **S** (and where appropriate **V**).

A recommended general approach is to solve for the steady state **V** and **S** values with all spin torques turned off and for a relaxed starting magnetization configuration. After this, save the simulation (which also saves the computed **V** and **S**), and re-enable the spin torques as required. From this point initialization should be quicker, with any further iterations in **V** and **S** triggered by changes in **m** (changing set electrode potential values can also trigger the Poisson solvers).

Setting the convergence factors too low may result in very slow simulations as the solvers will require a large number of iterations. You will need to determine the best compromise between computational speed and accuracy. The default normalised convergence values of  $10^{-6}$  for **V** and  $10^{-5}$  for **S** Poisson equations are set on the side of accuracy, having been found to give accurate results in all test cases, but you should still verify this for your particular simulation.

## Tutorial 18 – Spin Hall Effect

### Exercise 18.1

Consider a single Pt mesh with dimensions 320 nm x 320 nm and 40 nm thickness. Compute the spin accumulation and z-direction spin current density in response to a set potential of 10 mV with electrodes placed at the x-axis ends. Verify that **S** obeys the right-hand-rule with respect to the charge current direction.

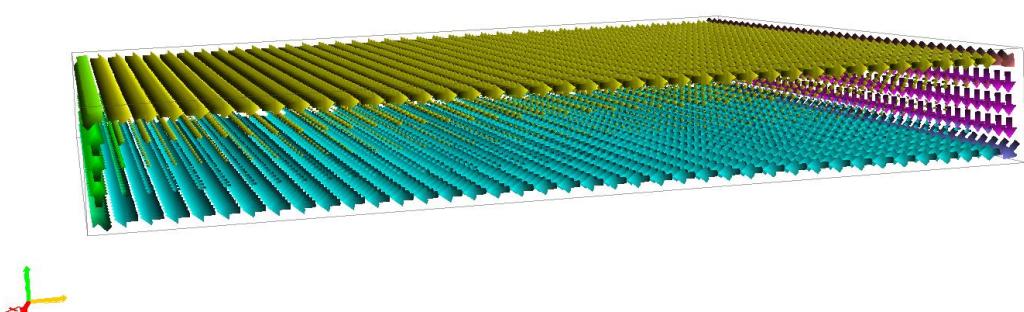
For Pt you may use  $\sigma = 7 \times 10^6$  S/m,  $\lambda_{sf} = 1.4$  nm and  $\theta_{SHA} = 0.1$ . You may use a cubic cellsize with 5 nm side.

Plot the y components of the z-direction spin current density and spin accumulation along the z-axis, through the center of the Pt slab (remember the **dp\_getprofile** command). Verify that the following relation holds, using the plotted value of the spin current at the center of the Pt slab:

$$\theta_{SHA} = -\frac{J_{sz,y}}{J_{cx}} / \frac{\mu_B}{e}$$

**Figure 18.1** – Computed spin accumulation for Exercise 18.1, where the charge current density is along the negative x direction.

Focused Mesh : Pt - S  
Minimum : 13.5814uA/m  
Maximum : 65.4158mA/m



## Exercise 18.2

- a) Continuing from Exercise 18.1, now add a Ni<sub>80</sub>Fe<sub>20</sub> layer with 20 nm thickness on top of the Pt layer. Make sure to reset to default electrodes (**setdefaultelectrodes**) so a uniform charge current density is obtained in each layer. Plot the y components of the z-direction spin current density along the z axis for both the continuous and spin-mixing conductance interface models for a) magnetization direction along the injected spin current, i.e. along the y axis, and b) magnetization direction transverse to the injected spin current, i.e. along the x axis. Explain the differences between these cases.

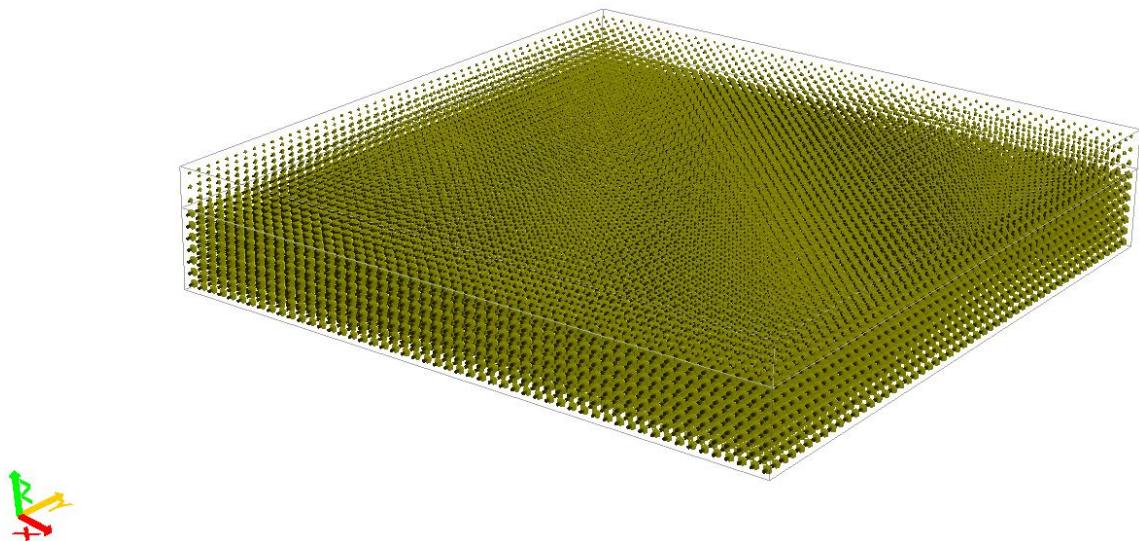
Note, for this exercise you will have to use a smaller cellsize along the z direction. This is due to the large gradients involved, and is normally the case when N / F multilayers are used. You should use a cellsize of (5 nm, 5 nm, 1 nm).

Remember you can use the **computefields** command for this exercise, instead of using **run**, since you don't want to relax the magnetization configuration. It helps to monitor the transport solver number of iterations and convergence error (in the data box display the following using the **data** command and right-clicking on the respective interactive objects: *v\_iter*, *s\_iter*, *ts\_err*).

- b) Does the relation in Exercise 18.1 hold at the N/F interface, and why not? Investigate this again with a spin flip length in Pt of 8 nm, checking the relation both at the center of the Pt layer and at the interface.

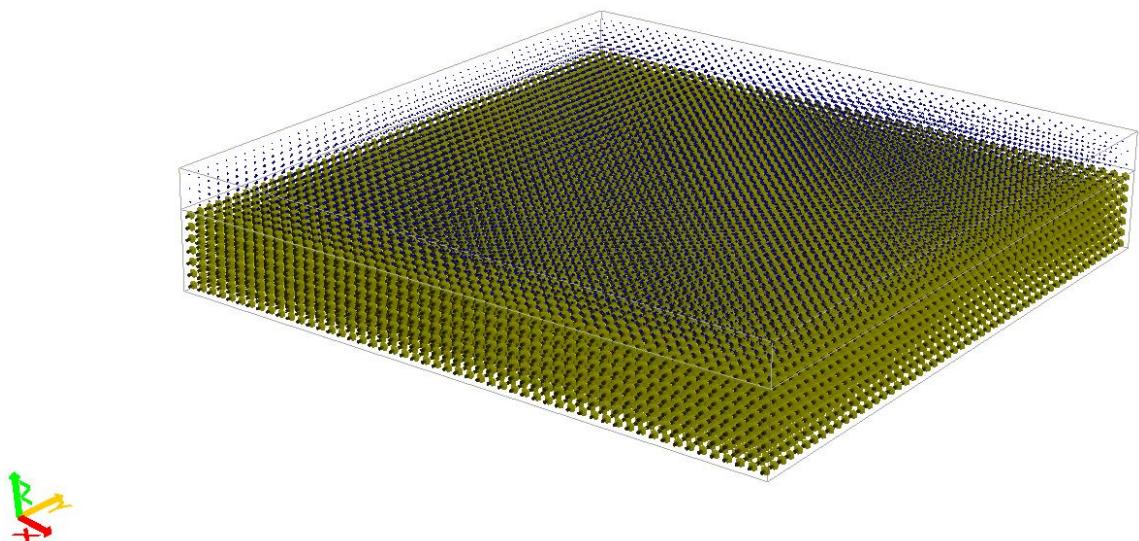
**Figure 18.2** – Spin current density in the z direction for a Pt/Ni<sub>80</sub>Fe<sub>20</sub> bilayer, where the magnetization in the permalloy mesh is along the y axis (longitudinal).

Focused Mesh : Pt - Js<sub>z</sub>  
Minimum : 1.03415MA/s  
Maximum : 1.27462MA/s



**Figure 18.3** – Spin current density in the z direction for a Pt/Ni<sub>80</sub>Fe<sub>20</sub> bilayer, where the magnetization in the permalloy mesh is along the x axis (transverse).

Focused Mesh : Pt - Js<sub>z</sub>  
Minimum : 1.03406MA/s  
Maximum : 1.27369MA/s



## Tutorial 19 – Spin Pumping and Inverse Spin Hall Effect

In this tutorial you will set-up a ferromagnetic resonance in a magnetic dot, then investigate the generated spin Hall voltage in a Pt underlayer. Due to the motion of magnetic moments in the ferromagnetic layer a spin current is pumped in the Pt underlayer, where an electrical current is generated due to the inverse SHE. This leads to charge accumulation at opposing sides of the Pt underlayer, and thus an electrical potential is generated.

### Exercise 19.1

Setup a ferromagnetic resonance (FMR) at 20 GHz excitation frequency in a Ni<sub>80</sub>Fe<sub>20</sub> circle with 80 nm diameter and 10 nm thickness, with a bias field applied in the plane of the circle along the y axis.

First, find the demagnetizing factor in the plane of the circle and set the *demag\_N* module with demagnetizing factors  $N_x = N_y = N$ . Remember you can calculate the demagnetizing energy for uniform magnetization (*e\_demag*), and the demagnetizing factor is then related to it by:

$$\varepsilon_{demag} = \frac{\mu_0}{2} NM_s^2$$

For this exercise, since you are effectively using the Stoner-Wohlfarth model you can turn off the *exchange* module. Calculate the FMR bias field required for resonance at an r.f. frequency of 20 GHz. You can use Kittel's formula applicable for elliptical shapes for a bias field  $H_0$  along the y direction:

$$f = \frac{\mu_0 |\gamma_e|}{2\pi} \sqrt{(H_0 + (N_x - N_y)M_s)(H_0 + (N_z - N_y)M_s)}$$

Using the *Hfmr* stage type, apply the excitation r.f. field (together with the calculated orthogonal bias field) in the plane of the circle for a number of cycles, and record the average magnetization. An r.f. field amplitude of 100 A/m is normally sufficient. If the r.f. field is applied for a sufficient number of cycles, the magnetization will achieve a

steady state precession at resonance. Determine the number of cycles required by examining the output average magnetization data, then **reset** and save the simulation – the next time you load the simulation the FMR precession will start directly in the steady state.

The *Hfmr* stage consists of the following parameters:  $H_{0x}$ ,  $H_{0y}$ ,  $H_{0z}$ ;  $H_{rfx}$ ,  $H_{rfy}$ ,  $H_{rfz}$ ; *r.f. steps*; *r.f. cycles*.

The bias field ( $H_0$ ) and r.f. field amplitude ( $H_{rf}$ ) are specified using Cartesian coordinates. The *r.f. steps* is the number of discretisation steps in each r.f. cycle, and the *r.f. cycles* is the number of sinusoidal oscillations the r.f. field will be applied for. To set the required 20 GHz frequency you will need to set the correct combination of *r.f. steps* and time stopping condition for each step. For example, since at 20 GHz each period takes 50 ps, if you use 20 r.f. steps per cycle, the time stopping condition for each step should be 2.5 ps (the default time stopping condition of 50 ps results in a 1 GHz frequency with 20 r.f. steps per cycle, so you will need to edit this).

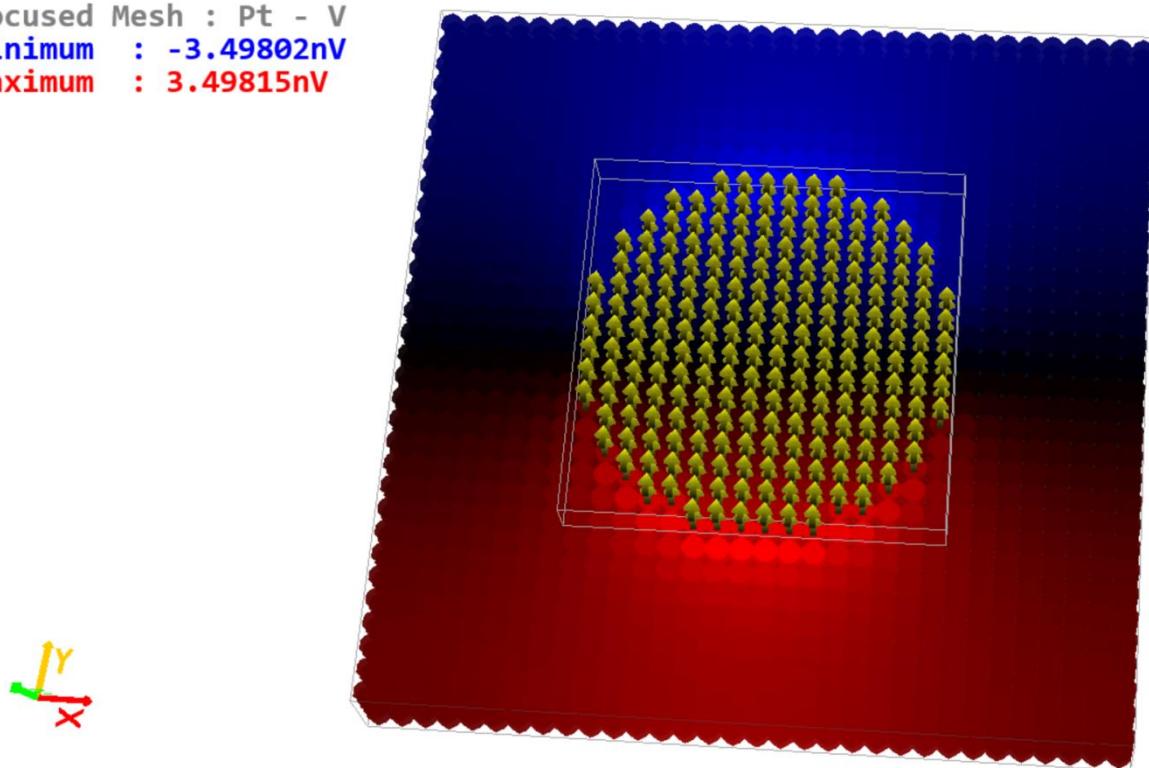
### Exercise 19.2

Using the prepared simulation from Exercise 19.1, add a Pt underlayer with dimensions 160 nm × 160 nm with the magnetic dot centered, and 20 nm depth. Enable spin pumping (*pump\_eff* = 1 in the permalloy mesh), and inverse SHE (*SHA* = *iSHA* = 0.1) in the Pt mesh. Do not set any electrodes but make sure the transport module is enabled in both the permalloy and Pt meshes, and the LLG-SA equation is selected so the spin transport solver is enabled. You will need to refine the electric cellsize in both meshes along the z direction to 1 nm. You should also relax the transport solver convergence criteria to  $10^{-4}$  for both the charge and spin solvers.

Obtain the induced spin Hall voltage at the opposing y-axis sides of the Pt mesh and plot them as a function of time for a few FMR precessions. Note, in the output data (**data**) you will have to add  $\langle V \rangle$  (the average calculated voltage) for the Pt mesh two times, editing the respective rectangles to correspond to the required two sides of the Pt mesh.

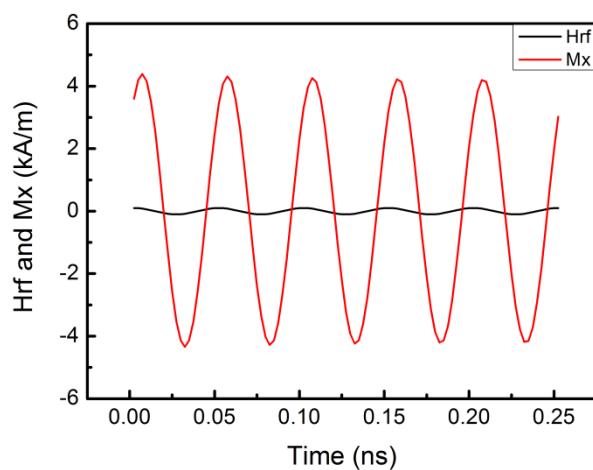
**Figure 19.1** – Inverse spin-Hall effect voltage in a Pt underlayer generated through spin pumping from a ferromagnetic dot at ferromagnetic resonance.

Focused Mesh : Pt - V  
 Minimum : -3.49802nV  
 Maximum : 3.49815nV

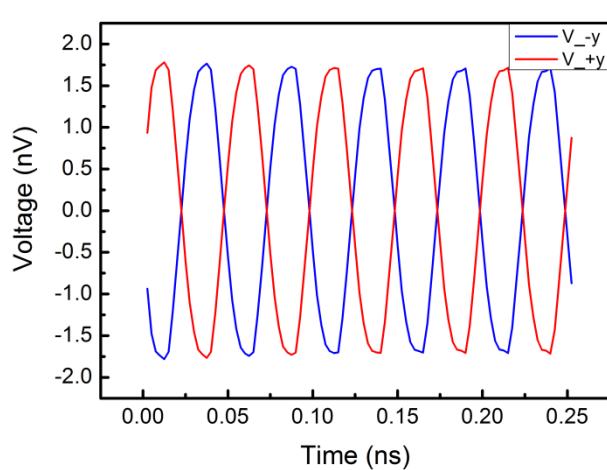


**Figure 19.2** – a) Magnetization precession at ferromagnetic resonance with a 20 GHz r.f. field, b) inverse spin-Hall effect voltage at resonance on opposing sides of the Pt mesh – see Figure 19.1.

a)



b)



## Tutorial 20 – Ferromagnetic Resonance

In this tutorial you will learn how to simulate a field-swept FMR peak, and re-produce the Gilbert damping parameter from it. Following this, in the next tutorial you will investigate how the spin torques due to spin pumping and the SHE affect the effective damping observed. An introduction to FMR simulations was given in the preceding Tutorial, and you must complete it before proceeding.

In Boris, FMR simulations are best done using a Python script. As you will note from the previous tutorial, applying an r.f. field excitation requires a number of cycles for the magnetization precession to reach steady state. For a field-swept FMR simulation, after changing the bias field you must ensure the magnetization precession is stable before obtaining output data. The simulation procedure is as follows:

- 1) Set bias field value and run the simulation for a fixed number of r.f. cycles (the “chunk” – e.g. 20 or more), but do not save any output data.
- 2) After the chunk has completed, run the simulation for a single r.f. cycle and save the output data ( $\langle M \rangle$ ).
- 3) From the saved data obtain the magnetization oscillation amplitude along the r.f. field direction.
- 4) Compare the oscillation amplitude against the previous oscillation amplitude (which is zero if this is the first chunk). If the change exceeds a set threshold (e.g. 0.5%) then repeat from step 1), otherwise proceed.
- 5) Record the oscillation amplitude and bias field. Increase bias field value and start again from step 1) until the field sweep range is completed.

A general-purpose FMR simulation Python script has been prepared and saved in the examples folder for this Tutorial.

### Exercise 20.1

Using a Ni<sub>80</sub>Fe<sub>20</sub> square of 80 nm side and 10 nm thickness simulate an FMR peak around the resonance bias field and plot the resulting magnetization oscillation amplitude against bias field data. Set the bias field along the  $-y$  direction, i.e. at 270° azimuthal angle. Use a Python script to simulate this as described above. (*You may use  $N_x = N_y = 0.12$ , with the predicted resonance field of  $H_0 \approx 367$  kA/m; aim for at least 50 kA/m either side of resonance*).

From the simulated oscillation amplitude versus bias field data, you will need to obtain a quantity proportional to the absorbed FMR power. The simplest way to do this is to square the oscillation amplitude data. The FMR power absorption peak is described by a Lorentz peak function, and you will need to fit this to your squared amplitude data.

Boris has built-in data processing command to help with processing FMR simulation data. You will need the following commands:

First load bias field and oscillation amplitude from the raw output data file (e.g. named ‘fmr\_fieldsweepFMR\_data.txt’):

```
dp_load fmr_fieldsweepFMR_data 0 1 0 1
```

Next square the magnetization oscillation amplitude data:

```
dp_muldp 1 1 1
```

Finally fit a Lorentz peak function to the data:

```
dp_fitlorentz 0 1
```

The Lorentz peak function is given as:

$$f(x) = y_0 + S \frac{w}{4(x - x_0)^2 + w^2}$$

In the above equation  $w$  is the full-width half-maximum (FWHM), and  $x_0$  is the peak center. You can obtain these values from the `dp_fitlorentz` command, including fitting uncertainties (Boris has a built-in generic Levenberg-Marquardt algorithm for curve fitting).

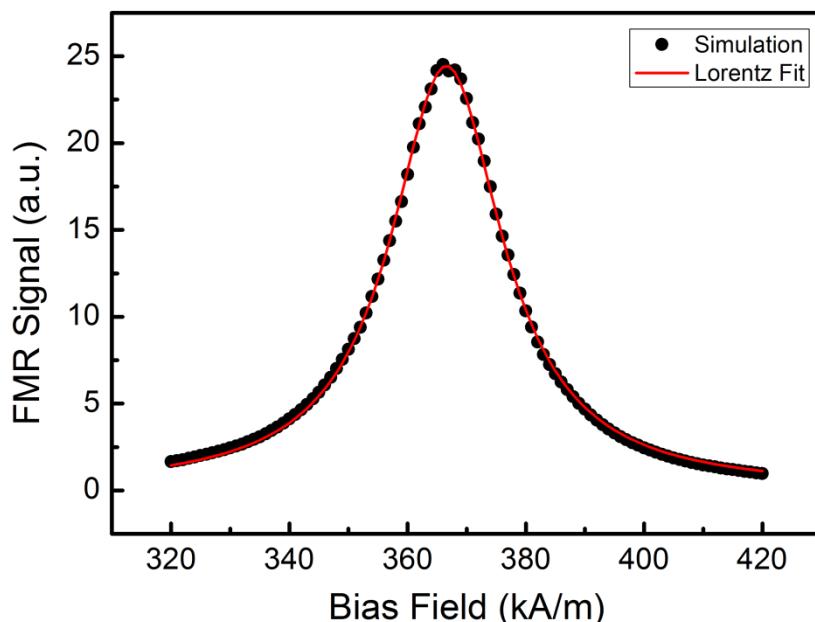
The magnetization damping value is related to the full-width half-maximum ( $\Delta H$ ) by:

$$\alpha = \frac{\mu_0 |\gamma_e| \Delta H}{4\pi f}$$

#### Exercise 20.1 continued

Process the output FMR data and verify the damping obtained from the FWHM matches the set damping value (*damping* = 0.02).

**Figure 20.1** – Simulated FMR peak with Lorentz peak function fit for Exercise 20.1.



## Tutorial 21 – Ferromagnetic Resonance with Spin Torques

Continuing from the previous tutorial, you will now investigate the effect of spin torques due to the spin-Hall effect on the magnetization damping using a Pt/Ni<sub>80</sub>Fe<sub>20</sub> bilayer. The spin current generated in the Pt underlayer is absorbed by the Ni<sub>80</sub>Fe<sub>20</sub> layer, resulting in a combination of damping-like and field-like torques. Depending on the current direction a decrease or increase of the effective damping is obtained. First the full spin transport solver is used, and following this a simpler method using an analytical form for the spin-orbit torques is introduced. Using the full spin transport solver we can also consider the effect of spin pumping on the effective damping, and this is investigated at the end of this tutorial.

The interfacial spin orbit torque added to the implicit LLG equation, as explained in Tutorial 17, is given by:

$$\mathbf{T}_s^{\text{interface}} = \frac{g\mu_B}{ed_h} \left[ \text{Re}\{G^{\uparrow\downarrow}\} \mathbf{m} \times (\mathbf{m} \times \Delta\mathbf{V}_s) + \text{Im}\{G^{\uparrow\downarrow}\} \mathbf{m} \times \Delta\mathbf{V}_s \right]$$

For an N/F interface in the x-y plane with uniform current densities we can obtain an analytical expression for this interfacial torque as (see S. Lepadatu, Scientific Reports 7, 12937 (2017)):

$$\mathbf{T}_s^{\text{interface}} = \theta_{\text{SHA, eff}} \frac{\mu_B}{e} \frac{|J_c|}{d_h} [\mathbf{m} \times (\mathbf{m} \times \mathbf{p}) + r_G \mathbf{m} \times \mathbf{p}]$$

Here  $\mathbf{p} = \mathbf{z} \times \mathbf{e}_{\mathbf{Jc}}$ , where  $\mathbf{e}_{\mathbf{Jc}}$  is the charge current direction, and:

$$\theta_{\text{SHA, eff}} = \theta_{\text{SHA}} \left( 1 - \frac{1}{\cosh(d_N / \lambda_{sf}^N)} \right) \frac{N_\lambda \text{Re}\{\tilde{G}\} + |\tilde{G}|^2}{(N_\lambda + \text{Re}\{\tilde{G}\})^2 + \text{Im}\{\tilde{G}\}^2}$$

$$r_G = \frac{N_\lambda \text{Im}\{\tilde{G}\}}{N_\lambda \text{Re}\{\tilde{G}\} + |\tilde{G}|^2}$$

In the above,  $N_\lambda = \tanh(d_N / \lambda_{sf}^N) / \lambda_{sf}^N$ ,  $F_\lambda = \tanh(d_F / \lambda_{sf}^F) / \lambda_{sf}^F$ , and  $\tilde{G} = 2G^{\uparrow\downarrow} / \sigma_N$ . Thus the interfacial torque has a damping-like and a field-like component. In the limit of abrupt interface ( $\lambda_\phi \rightarrow 0$  or equivalently  $\text{Re}\{G^{\uparrow\downarrow}\} \rightarrow \infty$ ) the field-like component tends to zero and we obtain the following expression for the torque:

$$\mathbf{T}_{SOT} = \theta_{SHA, eff} \frac{\mu_B}{e} \frac{|J_c|}{d_h} \mathbf{m} \times (\mathbf{m} \times \mathbf{p})$$

and

$$\theta_{SHA, eff} = \theta_{SHA} \left( 1 - \frac{1}{\cosh(d_N / \lambda_{sf}^N)} \right)$$

This approximation can also be used when the damping-like torque is much larger than the field-like torque. This expression is commonly used in the literature to model the spin-orbit torque resulting from the spin-Hall effect. Note however the spin-Hall angle in this expression is not the bulk (or intrinsic) spin Hall angle, but an effective spin Hall angle, scaled by transport parameters; if further the N layer thickness is many times larger than its spin flip length, we can use the approximation  $\theta_{SHA, eff} \approx \theta_{SHA}$ . In many cases this may not be true, and moreover the abrupt interface approximation may not be good either, thus to model the effect of the damping-like torque with the analytical form of the spin-orbit torque, in the expression for  $\mathbf{T}_{SOT}$  you should use the following expression to calculate the effective spin-Hall angle:

$$\theta_{SHA, eff} = \theta_{SHA} \left( 1 - \frac{1}{\cosh(d_N / \lambda_{sf}^N)} \right) \frac{N_\lambda \text{Re}\{\tilde{G}\} + |\tilde{G}|^2}{(N_\lambda + \text{Re}\{\tilde{G}\})^2 + \text{Im}\{\tilde{G}\}^2}$$

In Boris you can include this analytical spin-orbit torque using the `SOTField` module. Enabling this module in a ferromagnetic mesh introduces an additional effective field into the LLG equation which results in the  $\mathbf{T}_{SOT}$  torque given above (as it appears in the implicit LLG equation). To use it you still need to have the `transport` module enabled in order to calculate the charge current density, but instead of selecting LLG-SA (enabling the full spin transport solver) you should select just the LLG equation (`ode` command). In the material parameters for the ferromagnetic mesh

(**params** command) you need to enter the correct effective spin-Hall angle (*SHA*) to use with the *SOTField* module.

### Exercise 21.1

Using the Ni<sub>80</sub>Fe<sub>20</sub> layer from the previous tutorial, now add a Pt underlayer with the same dimensions (80 nm × 80 nm × 10 nm), using the Pt parameters from Tutorial 18. Set default electrodes (resulting in current flow along the x direction), enabling the spin transport solver both in the Ni<sub>80</sub>Fe<sub>20</sub> and Pt meshes (add *transport* modules and set the **ode** solver to LLG-SA). Make sure to disable spin pumping (*pump\_eff* = 0) and the inverse SHE (*iSHA* = 0). You should also disable bulk spin torques (*ts\_eff* = 0), only leaving interfacial spin torques enabled (*tsi\_eff* = 1). As before you may need to decrease the z-direction electrical cellsize to ensure accuracy (and numerical convergence!).

Obtain FMR peaks for charge current densities in the Pt layer of J<sub>c</sub> = ±10<sup>12</sup> A/m<sup>2</sup>. How does the damping change with current density direction?

In this case, even though you are using the Stoner-Wohlfarth model (*demag\_N* module), you should still enable the *exchange* module. The reason for this, the spin torques may not be perfectly uniform (e.g. if the permalloy and Pt layers have the same width, the spin torques will not be uniform since the spin accumulation has gradients at the sample edges), thus you do need to take the exchange interaction into consideration.

The change in damping due to a damping-like spin-orbit torque may be roughly approximated by:

$$\Delta\alpha_{SHE} \approx \theta_{SHA,eff} \frac{\mu_B}{e} \frac{J_c}{2\pi f M_s d_F}$$

Verify the change in damping obtained from simulations with the above formula.

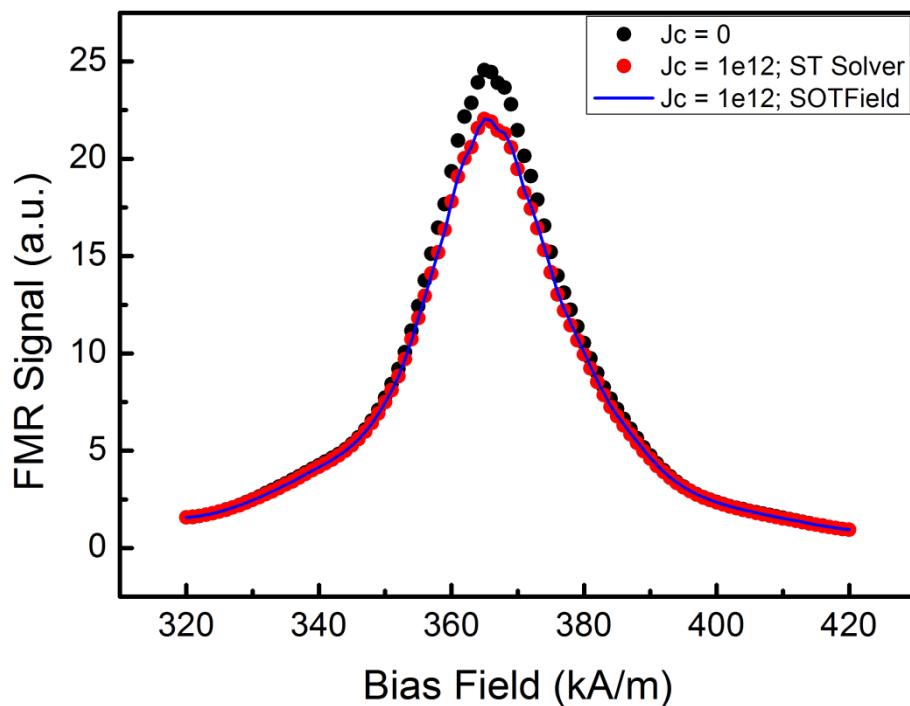
### Exercise 21.2

Repeat Exercise 21.1 but this time without the spin transport solver, only using the analytical form for the spin-orbit torque (*SOTField* module). You should delete the Pt mesh and reset the electrodes and potential to give you the correct current density. Calculate an appropriate effective spin-Hall angle to use. Compare the results with the previous exercise.

### Exercise 21.3

Repeat Exercise 21.1, using the full spin-transport solver, but now enable spin pumping (set *pump\_eff* = 1). What is the increase in damping?

**Figure 21.1** – FMR simulations with spin orbit torques for both the full spin transport solver (ST Solver) and effective field obtained from the analytical spin-orbit torque (*SOTField*).



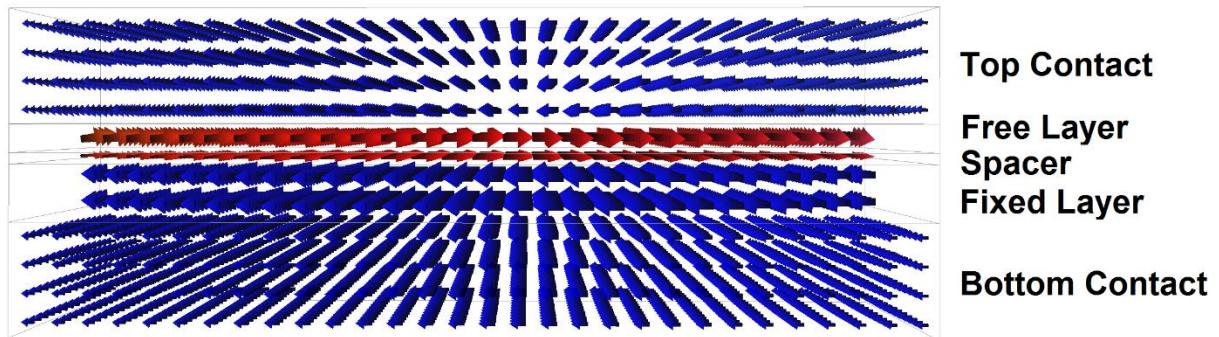
## Tutorial 22 – CPP-GMR

The spin transport solver is also able to reproduce the spin torques in a current-perpendicular to plane (CPP) giant magneto-resistance (GMR) spin valve, in addition to its magneto-resistance. Here we will investigate the current-induced switching in a simple generic spin valve between the parallel and anti-parallel states, see Figure 22.1, and plot the resistance during these switching events.

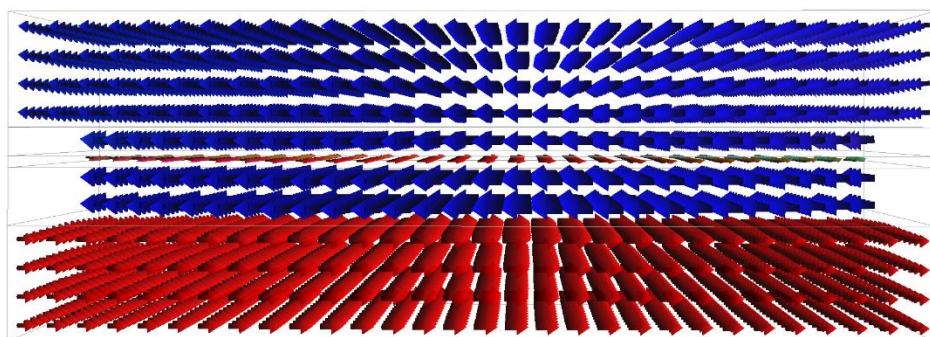
A spin valve, in its simplest form, consists of a fixed magnetic layer, a free magnetic layer which can be switched between an anti-parallel and parallel orientation with respect to the fixed layer, and a thin metallic spacer layer. The spacer layer thickness can be adjusted to give either a ferromagnetic or anti-ferromagnetic surface exchange coupling between the two magnetic layers. In the following simulation we will also add two metallic contacts, top and bottom.

**Figure 22.1** – CPP-GMR spin valve showing the spin accumulation in the spacer layer, top, and bottom contacts, and the magnetization in the elliptically shaped fixed and free layers for a) anti-parallel state, and b) parallel state.

(a)



(b)



## Exercise 22.1

Setup a generic spin valve structure (i.e. just use the default mesh parameters unless indicated otherwise) similar to that shown in Figure 22.1. This consists of:

- Bottom and top contacts (**addconductor**) with dimensions 160 nm × 80 nm × 20 nm. Disable spin-Hall effects in both ( $SHA = iSHA = 0$ ).
- Spacer layer with dimensions 160 nm × 80 nm × 2 nm and set it to an elliptical shape (drag a .png file with a circle shape to the mesh viewer when the spacer layer mesh is in focus). Disable spin-Hall effects.
- Fixed layer (**addmesh**) with dimensions 160 nm × 80 nm × 10 nm and elliptical shape. Disable spin torques and spin pumping in this mesh ( $ts\_eff = tsi\_eff = ts\_pump = 0$ ). You should also disable magnetization dynamics in this mesh so the magnetization is fixed. You can do this by setting the relative gyromagnetic factor to zero ( $grel = 0$  in **params**).
- Free layer with dimensions 160 nm × 80 nm × 5 nm and elliptical shape. Disable spin pumping and bulk spin torques only, in this mesh (i.e. keep  $tsi\_eff = 1$ ).

You will need to add the following modules:

- super-mesh demagnetization with a cellsize of 5 nm × 5 nm × 4.25 nm (**sdemag**).
- *surfexchange* modules in both magnetic meshes. Edit the  $J1$  (bilinear surface exchange energy density) value in the free layer to give you a weak ferromagnetic coupling; set  $J1 = 0.1 \text{ mJ/m}^2$ .
- *transport* modules in all meshes. Set the electrical cellsize to 5 nm × 5 nm × 1 nm everywhere except in the spacer layer where you should set it to 5 nm × 5 nm × 0.5 nm.

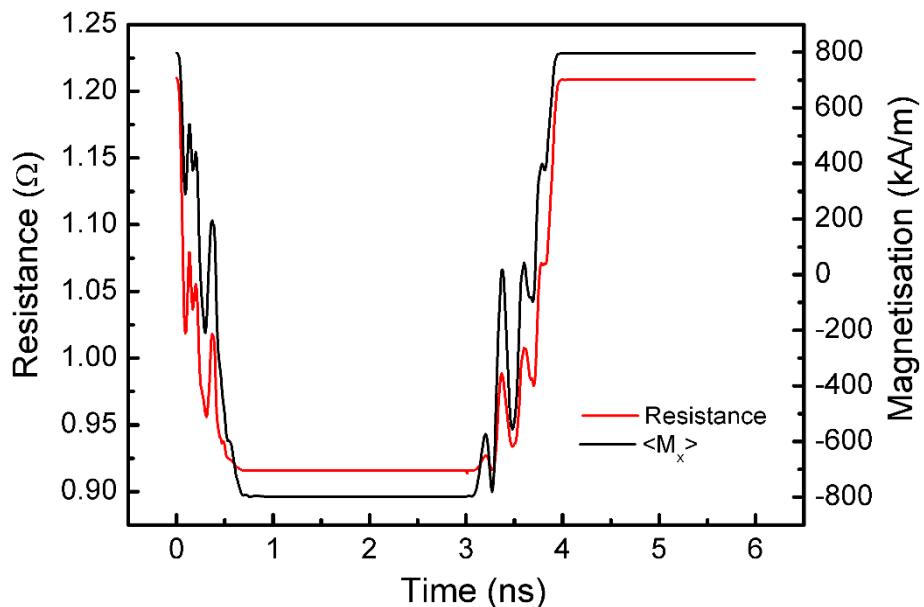
For the **ode** solver you should set the LLG-SA equation (thus enabling the spin-transport solver) with RKF45 evaluation. For output **data** you should have *time*, *R* (resistance), and  $\langle M \rangle$  (average magnetization) in the free layer. Set electrodes top and bottom (**addelectrode**), designating the bottom electrode to be the ground

electrode (**electrodes**). You need to simulate switching starting from the anti-parallel state (see Figure 22.1) using a +15 mV pulse for 3 ns, then back to this state with a further -15 mV pulse for 3 ns. Save data every 10 ps for both stages. Before starting the simulation you should relax the starting state as follows:

- 1) Set all spin torques to zero and insert a *Relax* stage with *nostop* condition at the start.
- 2) First relax the magnetization in the anti-parallel state without the spin-transport solver (set **ode** to LLG).
- 3) Next enable the spin-transport solver and relax it (run it until the solver no longer iterates, monitoring *v\_iter* and *s\_iter* **data**).
- 4) Re-enable the appropriate spin torques (*tsi\_eff* = 1 in the free layer only), **reset**, delete the *Relax* stage, then save the simulation (**savesim**).

Explain the resistance change observed by comparing it with the magnetization in the free layer as a function of time – see Figure 22.2 for expected results.

**Figure 22.2** – Change in resistance for the CPP-GMR spin valve of Exercise 22.1, together with the magnetization along the longitudinal direction in the free layer.



## Tutorial 23 – Skyrmion Movement with Spin Currents

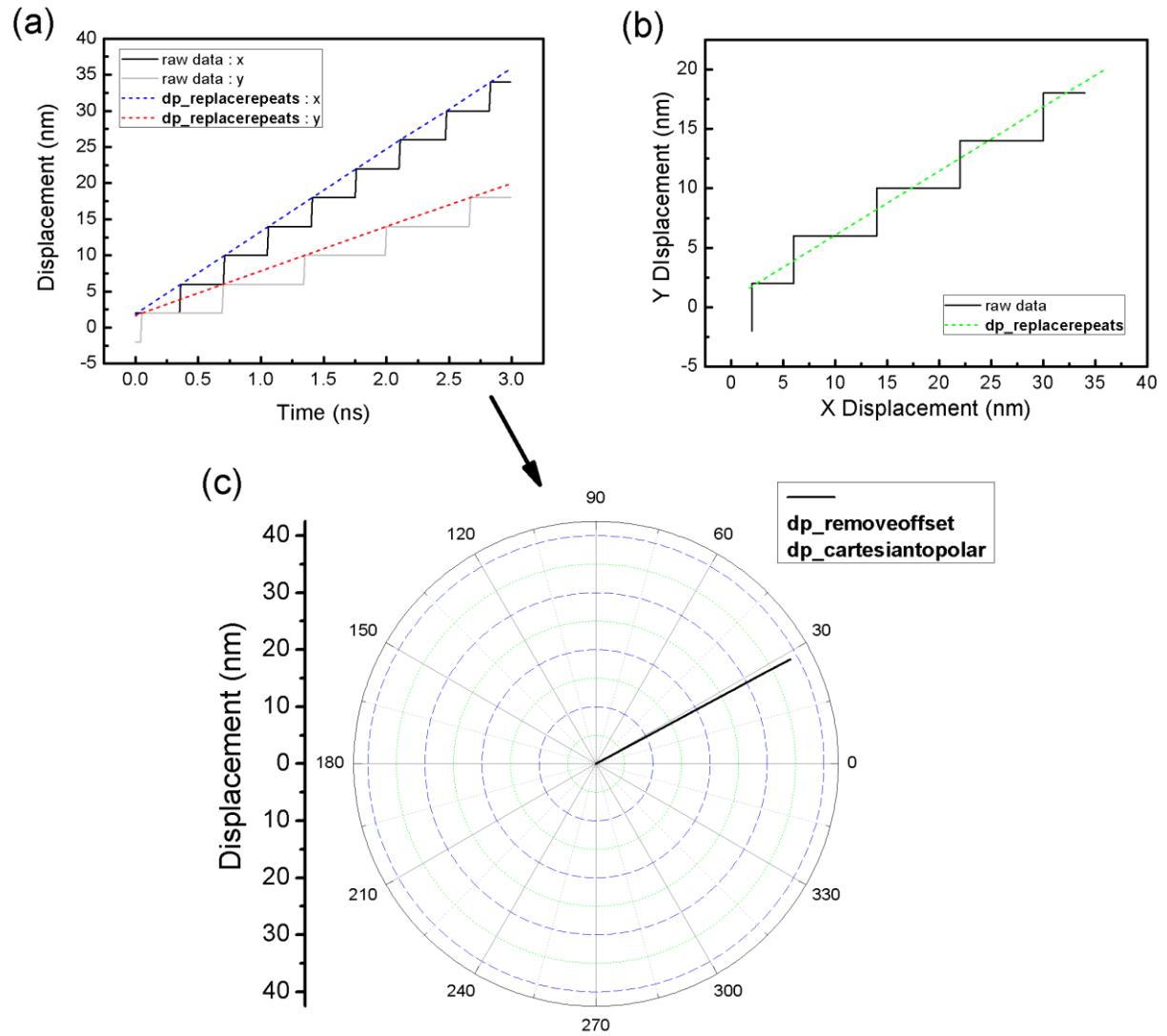
Skyrmions may be displaced efficiently using charge and spin currents. To study their movement a skyrmion tracking window can be used in Boris. There are two methods available for tracking a skyrmion, discussed below, both available as data outputs: *skyshift* and *skypos* (use **data** command).

The *skyshift* entry needs a rectangle defined, which should be set around the initial position of a skyrmion, making sure to fully contain it, but don't leave excessive space around it; the thickness of this rectangle should be set to the thickness of the ferromagnetic mesh containing the skyrmion. During a simulation a x-y shift is recorded and saved in the output data file. This shift is determined by comparing the average magnetization magnitude in the 4 quadrants of the skyrmion tracking window – e.g. if the skyrmion shifts to the right, the average magnetization magnitude in the 2 right-hand-side quadrants will decrease compared to the left, thus a right single-cell shift is recorded. Multiple *skyshift* entries can be defined, with different rectangles, to track multiple skyrmions. Note, the *skyshift* entry only works with data file output, and not in the data box or with the **showdata** command.

The raw output *skyshift* data will contain staircase steps due to mesh discretisation. It is possible to obtain a more natural skyrmion movement path by assuming linear displacement in between the staircase steps – this is illustrated in Figure 23.1. Here skyrmion displacement was simulated for 3 ns and the individual x and y *skyshift* raw data are shown in Figure 23.1(a). To remove the stair steps and replace them using linear interpolation you can use the **dp\_replacerepeats** command on both the x and y *skyshift* data columns. The x, y data can then be plotted directly in Cartesian coordinates. You will notice this path doesn't start from (0, 0). To display the skyrmion displacement path relative to its starting position you should remove this offset using the **dp\_removeoffset** command on both the x and y data. Finally, if you want to plot this path using polar coordinates you can use the **dp\_cartesiantopolar** command, included in Boris for convenience. Note, especially when converting to polar coordinates you should check the processed data correctly represents the raw data. Problems may occur due to blips in the raw data, especially if the tracking

window was not defined well or the starting state is not sufficiently relaxed, thus the results from this procedure must be carefully compared with the raw data.

**Figure 23.1** – Skyrmion movement raw data processing, showing (a) individual x and y displacements, (b) Cartesian coordinates path, and (c) polar coordinates path.



The second method uses the *skypos* data output. Again this needs an initial rectangle defined around the skyrmion as for the *skyshift* data output. *Skypos* uses a far more computationally expensive algorithm to track the skyrmion, but is able to obtain the exact skyrmion center position, as well as skyrmion diameters along the x and y axes, without being affected by staircase discretisation artifacts. It is also able to adjust the tracking window size if the skyrmion diameter changes significantly. The

algorithm works by fitting the skyrmion using an analytical function (the same one used for the **dp\_fitskyrmion** command) in three steps: 1) Skyrmion is fitted along the x axis through the center of the skyrmion tracking window in order to find the center position. The tracking window x position is adjusted to center it. 2) Skyrmion is fitted along the y axis through the center of the skyrmion tracking window in order to find the center position. The tracking window y position is adjusted to center it. The y diameter is also recorded at this step. 3) The skyrmion is again fitted along the x axis to obtain its x diameter.

For the following exercises you should first use the *skyshift* method of tracking the skyrmion, then repeat them using the *skypos* method. Note, you should not use both methods simultaneously on the same skyrmion.

### Exercise 23.1

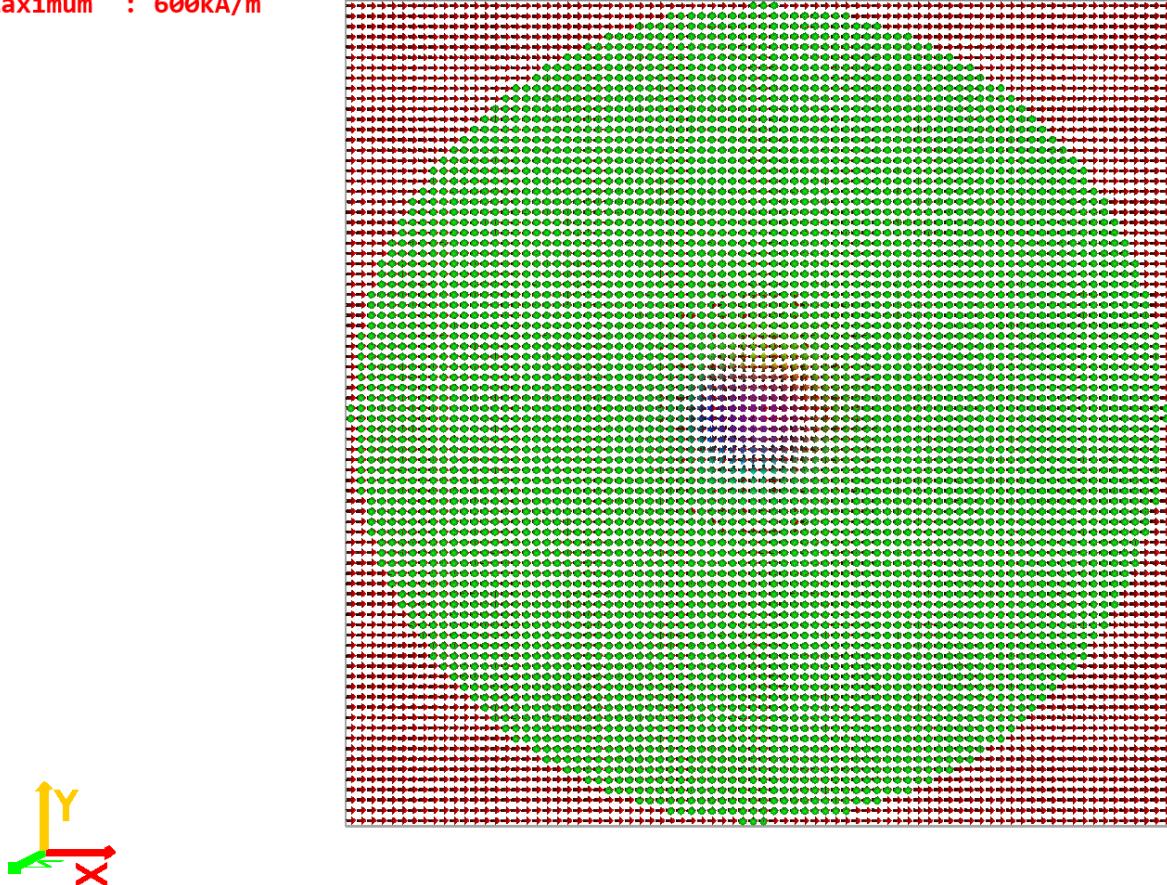
- a) Setup a Pt/Co bilayer with a skyrmion relaxed at the center of the Co layer under a 15 kA/m out-of-plane magnetic field as shown in Figure 23.2. The Pt layer should be a 320 nm × 320 nm × 3 nm rectangle, whilst the Co layer should be a 320 nm diameter disk with a 1 nm thickness. Relax this magnetization configuration.

For Pt you should use  $\sigma = 7 \times 10^6$  S/m,  $\lambda_{sf} = 1.4$  nm and  $\theta_{SHA} = 0.19$ . Use a discretisation cellsize of (4 nm, 4 nm, 0.5 nm). Set *iSHA* to zero.

For Co you should use  $\sigma = 5 \times 10^6$  S/m,  $\lambda_{sf} = 38$  nm,  $\lambda_J = 2$  nm,  $\lambda_\varphi = 4$  nm,  $G_{mix} = 1.5$  PS/m<sup>2</sup>,  $g_{rel} = 1.3$ ,  $\alpha = 0.03$ ,  $M_s = 600$  kA/m,  $A = 10$  pJ/m,  $D = -1.5$  mJ/m<sup>2</sup>,  $K_1 = 380$  kJ/m<sup>3</sup> with uniaxial anisotropy perpendicular to the plane. You should also enable the interfacial DM exchange module. Use a discretisation cellsize of (4 nm, 4 nm, 1 nm) for magnetic computations and (4 nm, 4 nm, 0.25 nm) for spin transport computations. In the Co mesh only enable the interfacial spin torques, not the bulk spin torques or spin pumping.

**Figure 23.2** – Skyrmion in a Co disk on a Pt underlayer.

Focused Mesh : Co - M  
 Minimum : 600kA/m  
 Maximum : 600kA/m

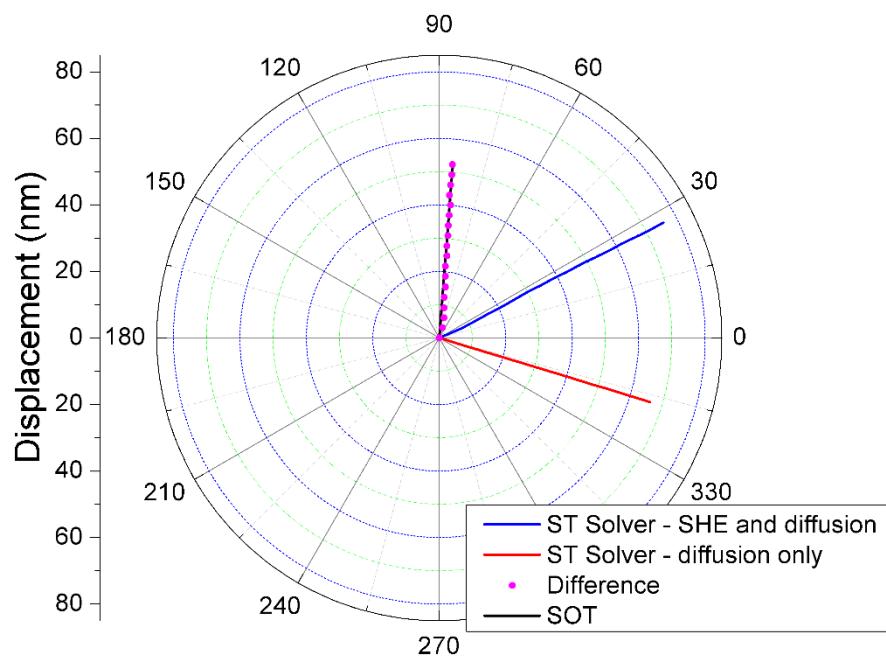


- b) Enable the spin transport solver in both meshes and set electrodes at the x-axis ends of the Pt mesh only. Set a -20 mV potential for 3 ns and save the *time* and *skyshift* (or *skypos*) data every 10 ps. (for *skyshift* and *skypos* define a rectangle around the initial position of the skyrmion). Simulate the skyrmion movement path with SHE enabled (*SHA* = 0.19 in the Pt mesh), as well as without SHE (*SHA* = 0 in the Pt mesh), and plot them in polar coordinates.
- c) Simulate the skyrmion movement path without the spin transport solver but with the *SOTfield* module enabled. Still keep the *transport* module enabled to calculate the charge current density. For the *SOTfield* module set a suitable effective spin Hall angle in the Co mesh (*SHA*). You can use the effective spin Hall angle formula from Tutorial 21, but note this is only strictly applicable for

uniform magnetization and spin currents. You can use this as a starting point, but will need to adjust the effective spin Hall angle.

Plot the skyrmion path in polar coordinates and compare it with the path obtained as the difference between the SHE and no SHE simulations above – see Figure 23.3 for expected results.

**Figure 23.3** – Skyrmion movement paths obtained in Exercise 23.1.



## Tutorial 24 – Roughness and Staircase Corrections

### Staircase Corrections

With finite difference discretisation, errors can arise due to a staircase effect when discretising curved boundaries. In micromagnetics the largest errors arise in the demagnetizing field and may be reduced by decreasing the discretisation cellsize. This method is inefficient however since for most problems the results converge when the discretisation cellsize is close to the exchange length of the material – thus to further reduce this everywhere just to improve the discretisation accuracy at a boundary is very inefficient. Note, for materials where the demagnetizing energy dominates the exchange length may be defined as:

$$l_{ex} = \sqrt{\frac{2A}{\mu_0 M_s^2}}$$

For systems where the anisotropy energy dominates ( $K_u > \mu_0 M_s^2 / 2$ ), the exchange length may be defined as:

$$l_{ex} = \sqrt{\frac{A}{K_u}}$$

Instead of refining this, a good approximation may be achieved by computing a correction field using a finely discretised demagnetization kernel, but applying it at run-time to the coarsely discretised mesh, as described in S. Lepadatu, Journal of Applied Physics 118, 243908 (2015). This correction field is typically similar to an uniaxial anisotropy field when averaged.

To enable staircase corrections in a particular magnetic mesh you must enable its *Roughness* module. When applying a mask shape to the mesh, staircase corrections will now automatically be taken into account. You must enable the *Roughness* module and reset the mesh shape before applying the mask to correctly enable

staircase corrections. You must also set the required refinement using the **refineroughness** command:

**refineroughness**  $m_x\ m_y\ m_z$

When calculating the correction field factors, the shape is first discretised on a fine mesh as set by the **refineroughness** parameters. Thus if the coarse mesh has cellsize ( $h_x, h_y, h_z$ ), the fine mesh used for correction field initialization has cellsize ( $h_x / m_x, h_y / m_y, h_z / m_z$ ). Typically the improvement in accuracy is small above  $m > 10$ , so the refinement set should not be excessive. Since a demagnetizing kernel must be computed for the fine mesh, the initialisation time may become very long, and the available memory may be exceeded if the  $m$  factors are set too large. You must also set them before applying the mask shape.

With the *Roughness* module enabled, setting a mask shape may result in a slightly different shape than without. This is because a fine shape is internally obtained first, then the coarse mesh shape is calculated to be the smallest shape which includes the fine shape on the coarse mesh – this is a requirement of the corrections calculation method. To clear the staircase corrections, effectively setting the fine mesh shape to the coarse mesh shape you can use:

**clearroughness**

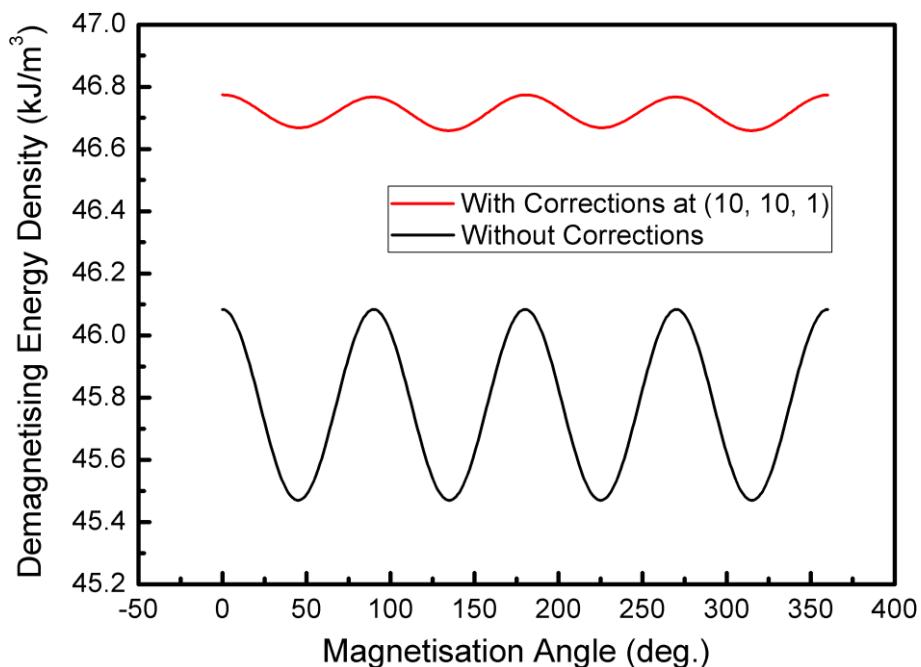
There's an energy density term associated with the correction fields, and this is available as a **data** parameter: *e\_rough*. The demagnetizing energy density, *e\_demag*, still corresponds to the coarse mesh shape; the sum of *e\_rough* and *e\_demag* is the approximated demagnetizing energy for the fine mesh shape.

### Exercise 24.1

Set a 80 nm diameter  $\text{Ni}_{80}\text{Fe}_{20}$  disk with 10 nm thickness. Calculate the demagnetizing energy density as a function of in-plane uniform magnetization orientation from  $0^\circ$  through  $360^\circ$  by saturating in a strong magnetic field ( $10^6 \text{ A/m}$ ). Repeat this computation but now set the shape with the *Roughness* module enabled and a refinement of (10, 10, 1) – **refineroughness**. Compare the demagnetizing energies for the coarse mesh and the approximated demagnetizing energy for the fine mesh ( $e_{\text{rough}} + e_{\text{demag}}$ ).

For the above exercise, in theory the demagnetizing energy should be constant for a circle as the field rotates. In practice, due to discretisation errors a shape anisotropy effect is observed (the magnetization is not fully saturated even at  $10^6 \text{ A/m}$ , so some non-uniformity persists). With staircase corrections enabled this anisotropy should be significantly reduced, thus closer to the ideal uniform demagnetizing energy – see Figure 24.1. The refinement can be increased but further improvement is small.

**Figure 24.1** – Demagnetizing energy computed for a circle with and without staircase corrections.

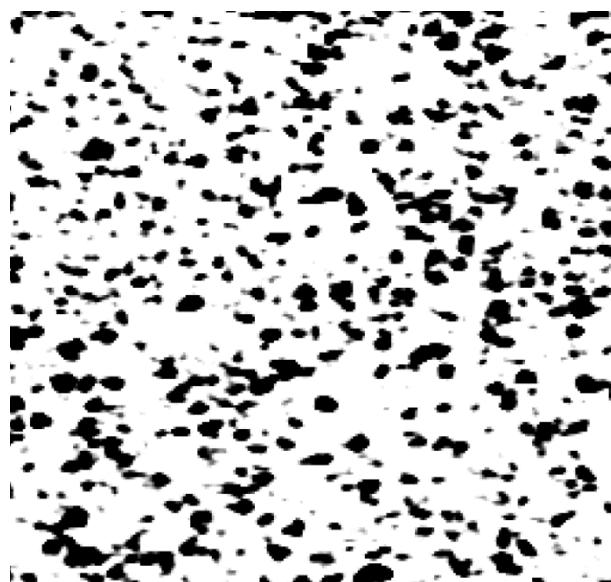


## Edge and Surface Roughness

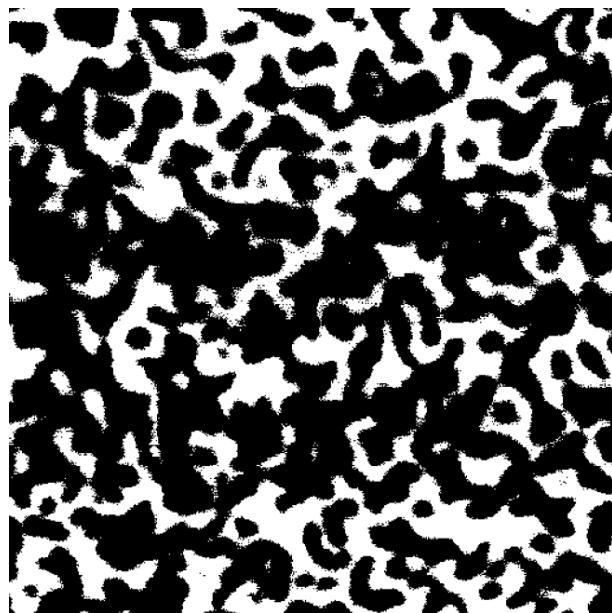
The same model used to reduce staircase corrections may be applied to compute the effect of topological roughness with variations below the exchange length of the material. As before, coefficients for a roughness field are computed at initialisation depending on the shape of a finely discretised mesh (the mesh with topological roughness applied), and that of the coarse mesh (the actual mesh used in computations but without roughness).

A roughness profile may be applied using a built-in algorithm, or alternatively a mask may be used. See Figures 24.2 – 4 for examples of real surface scans, processed into a grayscale image suitable for use as masks. These may be found in the Examples folder for this tutorial.

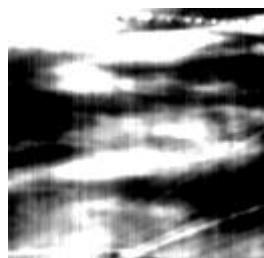
**Figure 24.2** – Granular surface roughness profile



**Figure 24.3** – Maze-like surface roughness profile.



**Figure 24.4** – Elongated defects, or stripes, surface roughness profile.



To apply a roughness profile using a mask, instead of simply dragging the file to the mesh viewer (as you would do when applying a shape), you should also specify the depth to which you want to apply the profile. For example, with the mask shown in Figure 24.4, to apply it to a 4.5 nm depth (the coarse discretisation cellsize is 5 nm so this keeps the coarse mesh shape intact) you need to use:

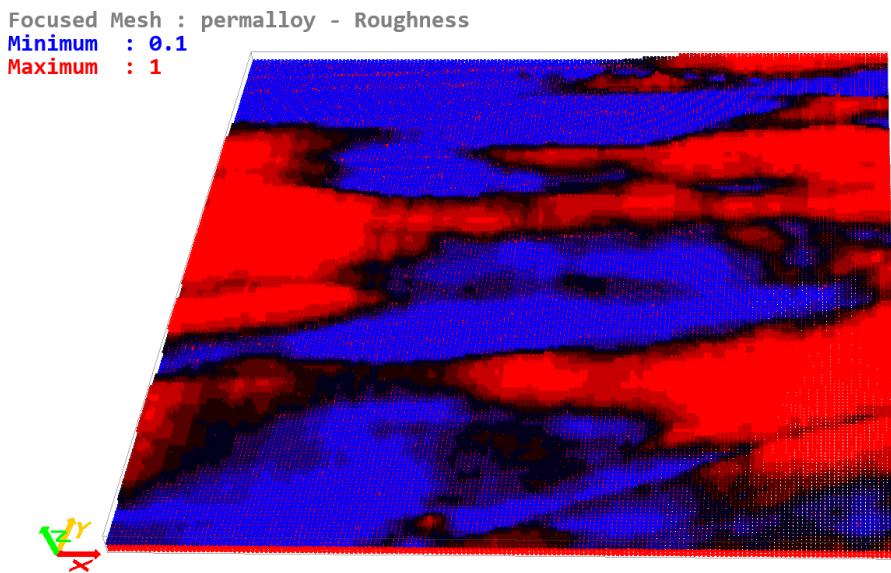
```
loadmaskfile 4.5nm (directory)\Stripes
```

This will apply a surface roughness profile on the top face up to 4.5 nm depth – black results in 0 depth cut, whilst white results in full depth cut (i.e. 4.5 nm); values on the

greyscale in between are correlated linearly with the depth cut. For the actual surface roughness profile obtained see Figure 24.5.

In this example the starting mesh has dimensions of 320 nm × 320 nm × 10 nm, and the roughness refinement was set to (4, 4, 10) – **refineroughness**. To view the set roughness, under **display** select the *Roughness* option for the respective mesh. To apply the surface roughness to the bottom face, negative values need to be set for the depth value – see help for **loadmaskfile** command.

**Figure 24.5** – Applied surface roughness using the mask in Figure 24.4.



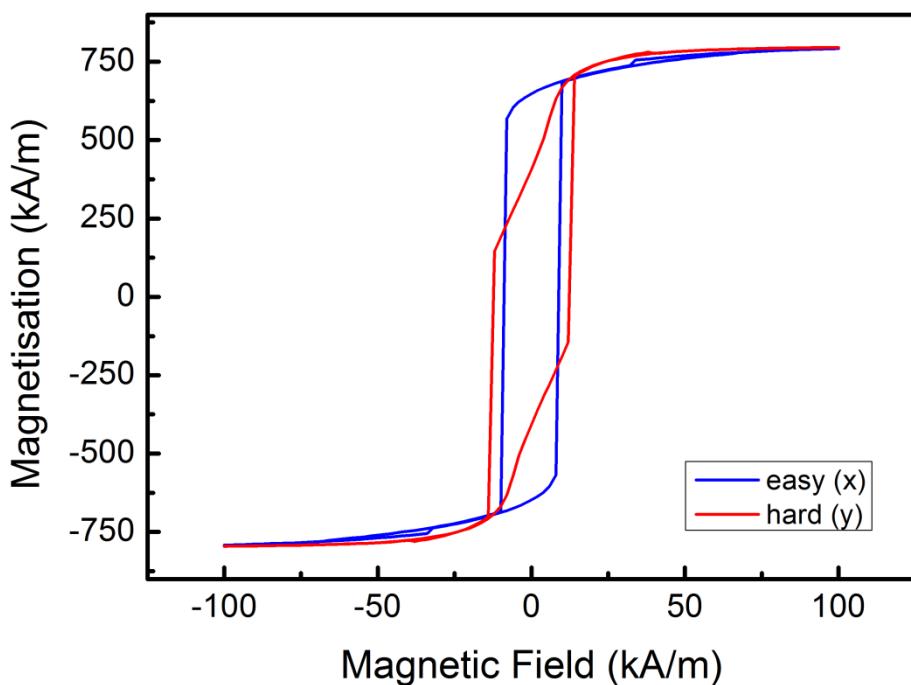
You can also apply edge and surface roughness using a built-in console command. Currently two methods are available: **roughenmesh**, **surfroughenjagged**. The **roughenmesh** command applies a completely random roughness profile to one of the 6 faces as indicated – see help for this command. The **surfroughenjagged** command applies a jagged profile to either the top, bottom, or both, faces – see help for this command.

### Exercise 24.2

Set a 160 nm × 160 nm × 10 nm permalloy rectangle and apply the Stripes roughness profile from Figure 24.4 (use file in Examples folder) to a depth of 4.5 nm. Use a roughness refinement of (4, 4, 10). Simulate the hysteresis loops along the x and y directions and compare them. (*You should apply the field at a slight angle to the x and y directions to avoid artifacts associated with a finite geometry – in particular for the easy axis you want to avoid the “U” shape configuration at zero field which can happen if the field is perfectly along the x axis.*)

Since permalloy does not have a magneto-crystalline anisotropy, without roughness it is expected the two hysteresis loops will be identical. With roughness applied an effective anisotropy is observed, due to the orientation of the surface roughness stripes as seen in Figure 24.5.

**Figure 24.6** – Hysteresis loops for Exercise 24.2, showing a roughness-induced anisotropy effect.



## Tutorial 25 – Defects and Impurities

Material parameters in Boris may also be assigned a spatial variation, in addition to a temperature dependence. This spatial variation will be taken into account in all routines where the material parameters appear, allowing inclusion of material defects and impurities in simulations as appropriate.

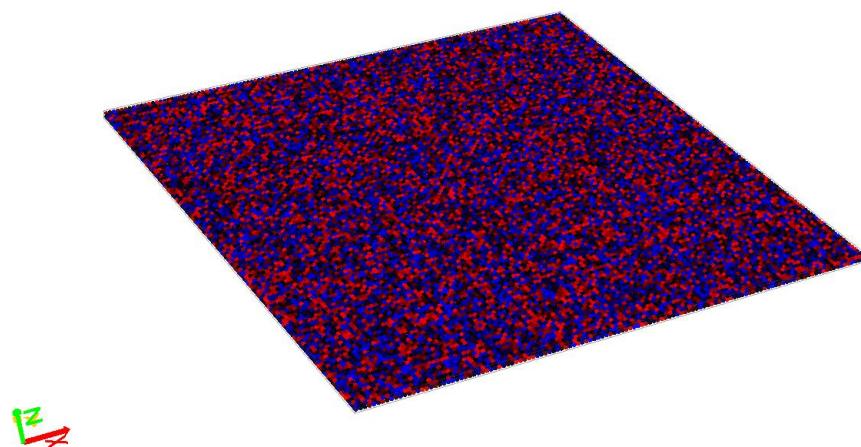
To see the currently set parameters spatial variation use the command:

**paramsvar**

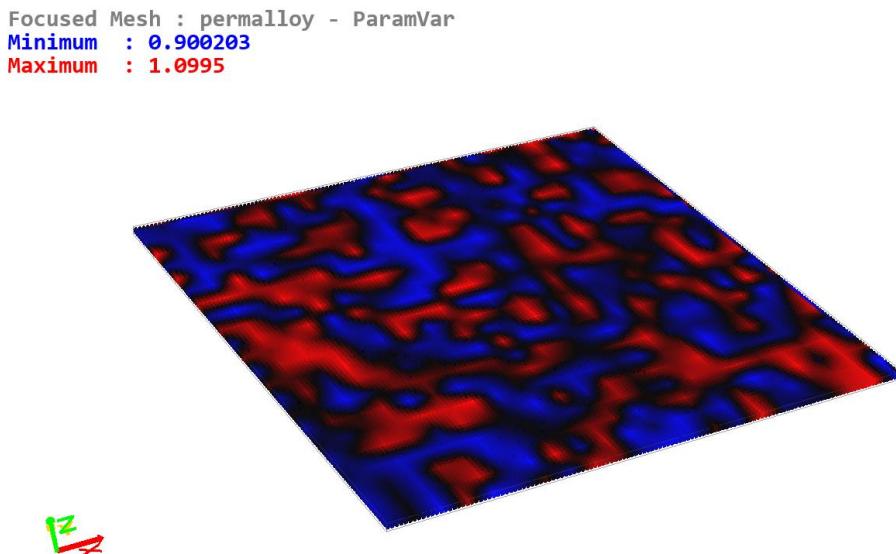
You can use a pre-defined method of generating defects by following the instructions displayed after using the **paramsvar** command. Currently these include: *random*, *jagged*, *defects*, *faults*. To see the spatial variation generated, under **display** select the *ParamVar* option, making sure to select the required parameter under the **paramvar** list. The generated spatial variation is stored as an array of coefficients, multiplying the base parameter value. For examples of these profiles see Figures 25.1 – 4.

**Figure 25.1** – *Random* parameter variation between 0.9 and 1.1 with generator seed 1.

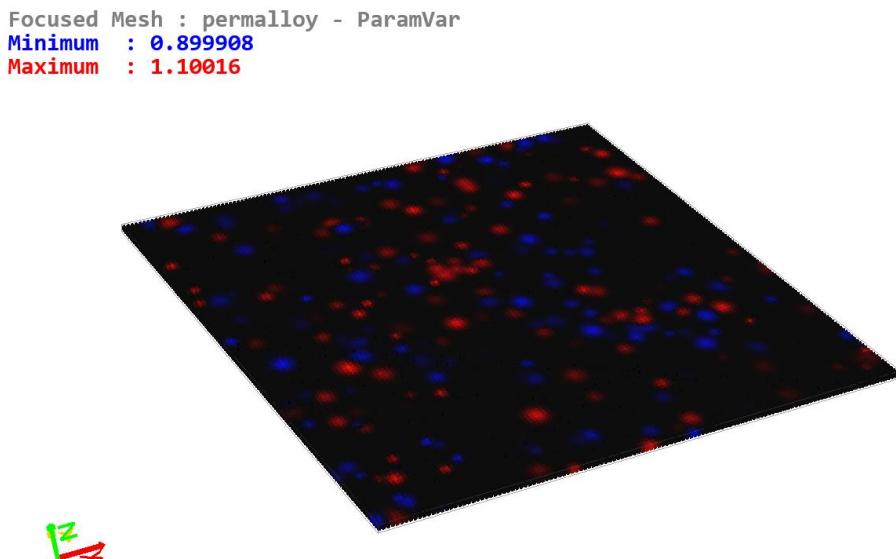
```
Focused Mesh : permalloy - ParamVar
Minimum   : 0.900002
Maximum   : 1.1
```



**Figure 25.2** – Jagged parameter variation between 0.9 and 1.1 with 30 nm average spacing and generator seed 1.

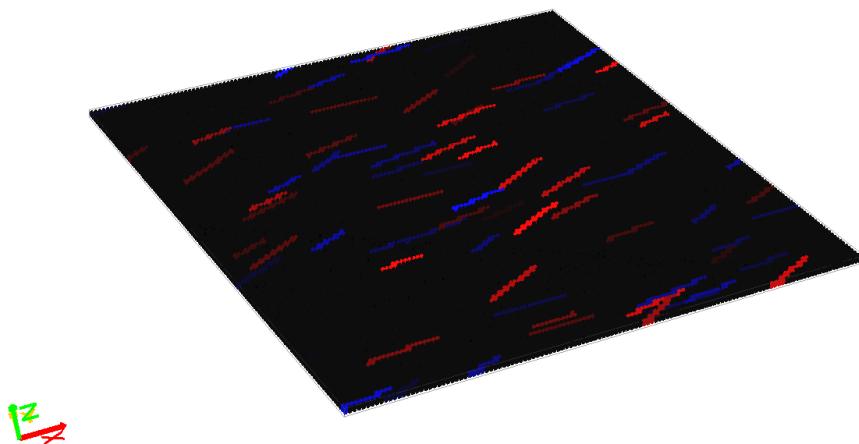


**Figure 25.3** – Defects parameter variation between 0.9 and 1.1 with diameters in the range 20 nm to 50 nm, and 40 nm average spacing with generator seed 1.



**Figure 25.4** – *Faults* parameter variation between 0.9 and 1.1 with 20 nm to 50 nm fault length, -30° to 30° fault orientation and 50 nm average spacing with generator seed 1.

```
Focused Mesh : permalloy - ParamVar
Minimum : 0.904194
Maximum : 1.09685
```



### Exercise 25.1

Generate Ms defects in a 640 nm × 640 nm × 10 nm mesh as shown in Figures 25.1 – 4.

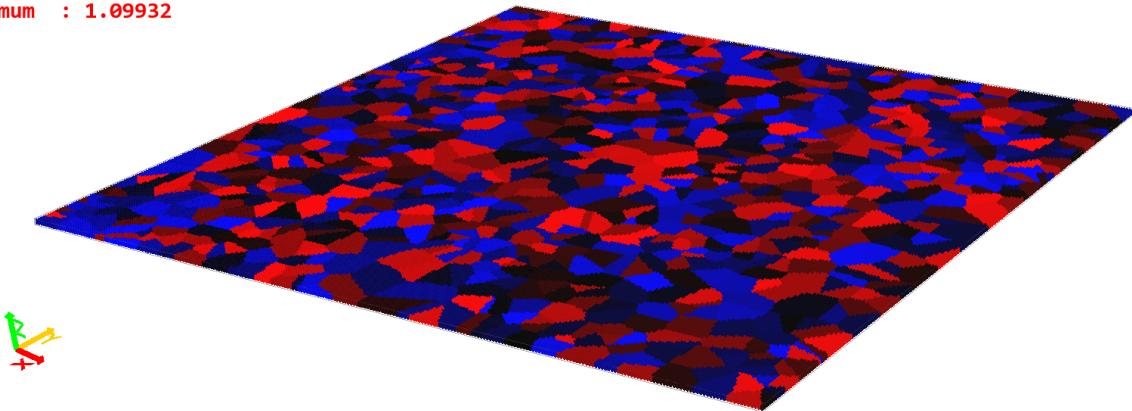
You can also set a custom parameter variation using an image as a mask file. To do this, drag the *custom* spatial variation generator to the required parameter. After this, double click on the required parameter to bring up a console command with parameters you can edit. Here, you can edit the image file to give the required image file together with path. The image file should be in grayscale, with black setting a value of 0, and white setting a value of 1. You can modify this by changing the offset and scaling values in the command parameters, which are by default 0 and 1 respectively. You need to give the full path for the file as the default working directory is not used.

## Tutorial 26 – Polycrystalline and Granular Films

Boris includes a Voronoi tessellation generator, both 2D and 3D, which can be used to generate polycrystalline and granular films.

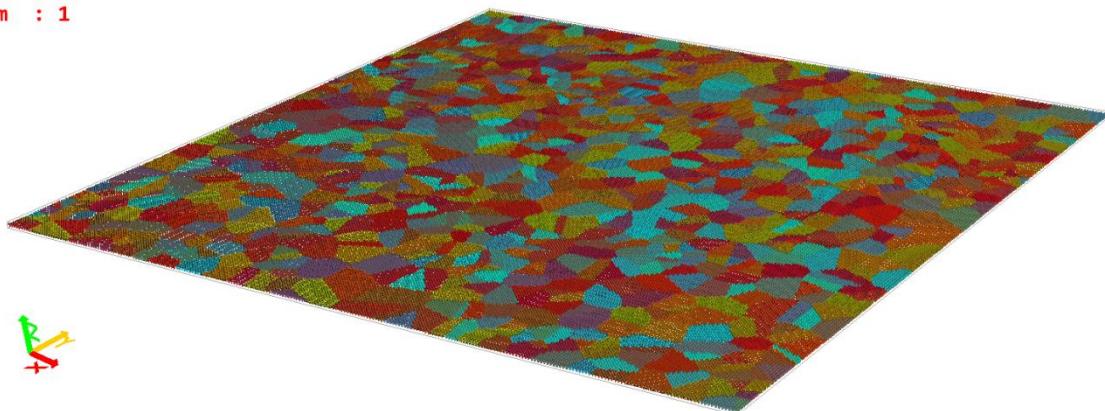
**Figure 26.1** – Polycrystalline film showing *K1* parameter variation generated using **vor2D** generator between 0.9 and 1.1 with 40 nm spacing and generator seed 1.

```
Focused Mesh : permalloy - ParamVar  
Minimum : 0.900115  
Maximum : 1.09932
```



**Figure 26.2** – Polycrystalline film showing easy axis (*ea1*) parameter variation generated using **vorrot2D** generator with polar angle range 70° to 110°, azimuthal angle range -90° to 90°, with 40 nm spacing and generator seed 1.

```
Focused Mesh : permalloy - ParamVar  
Minimum : 1  
Maximum : 1
```



Polycrystalline films may be simulated by generating parameter variations using one of the Voronoi tessellation generators under the **paramsvar** command. These include:

**vor2d** *min, max; spacing; seed* – Used for 2d crystallites in the xy plane.

**vor3d** *min, max; spacing; seed* – Used for 3d crystallites.

**vorbnd2d** *min, max; spacing; seed* – Used for 2d crystallites in the xy plane, but parameter variation generated randomly only at Voronoi cell boundaries.

**vorbnd3d** *min, max; spacing; seed* – Used for 3d crystallites, but parameter variation generated randomly only at Voronoi cell boundaries.

**vorrot2d** *min\_polar, max\_polar; min\_azimuthal, max\_azimuthal, spacing; seed* – Used for 2d crystallites in the xy plane, specifically magneto-crystalline anisotropy easy axes.

**vorrot3d** *min\_polar, max\_polar; min\_azimuthal, max\_azimuthal, spacing; seed* – Used for 3d crystallites, specifically magneto-crystalline anisotropy easy axes.

Both 2D and 3D crystallites may be generated using the generators listed above. For an example of a 2D polycrystalline film with *K1* (magneto-crystalline anisotropy) variation see Figure 26.1. In order to generate crystallites with a varying magneto-crystalline anisotropy easy axis orientation you can use either the **vorrot2d** or **vorrot3d** generator – for example see Figure 26.2 for the *ea1* parameter having the same polycrystalline structure as in Figure 26.1. Figure 26.2 shows the rotation to be applied, as a vector quantity. For an easy axis base value set along the x-axis this coincides with the resulting easy axis orientation.

You can also generate a parameter variation at the Voronoi cell boundaries rather than in the cells themselves. This can be done using the **vorbnd2d** and **vorbnd3d** generators. This could be useful for example to modify the electrical conductivity at the grain boundaries only.

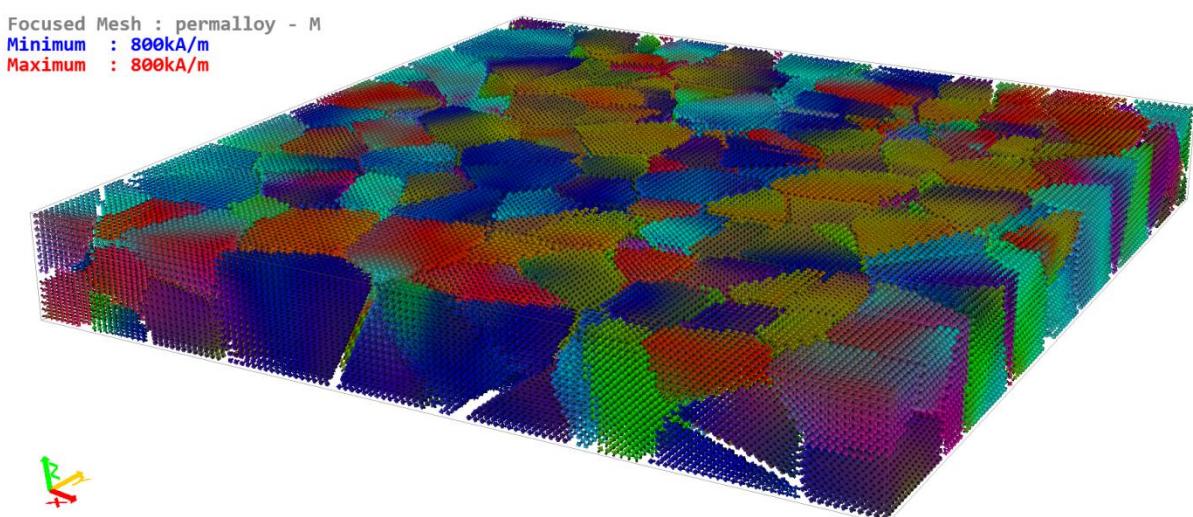
In order to generate a granular film with non-magnetic phase separation you can use one of the following commands:

```
generate2dgrains spacing (seed)  
generate3dgrains spacing (seed)
```

These commands generate granular films directly on the magnetization mesh – see for example Figure 26.3. You can also combine this with parameter variations generated using the same generator seed and sizes (e.g. grains with varying  $M_s$  values).

When generating grains for the magnetic mesh you can choose to generate grains for the electrical conductivity mesh also. To carry the grain structure over you should generate the grains first without the *Transport* module enabled. After enabling the *Transport* module the granular structure is also applied to the electrical conductivity mesh. This could be useful for example in a multi-layered structure. If you apply the grain structure with the *Transport* module already enabled, the grains are not generated for the electrical conductivity also. You could combine this with a Voronoi generator for the e/C material parameter however (e.g. **vorbnd2d** or **vorbnd3d**, or even **vor2d** or **vor3d**) as mentioned above.

**Figure 26.3** – Granular film (80 nm thick) with non-magnetic phase separation, generated using **generate3dgrains** command with 50 nm spacing and generator seed 1. The image shows a magnetization configuration at zero field.



## Tutorial 27 – Periodic Boundary Conditions

Periodic boundary conditions (PBC) may be applied when computing demagnetizing fields. Enabling this setting also affects exchange coupling (e.g. *Exchange*, *DMExchange*, *iDMExchange*), resulting in a wrap-around effect. PBCs are useful to simulate periodic arrays, or to approximate effectively infinite thin films or tracks using only a finite simulation window. PBCs are applicable to both single mesh demagnetization (*Demag*), as well as supermesh demagnetization (*SDemag*), including multi-layered demagnetization. Moreover, when enabling the *Roughness* module, PBCs are also taken into account when calculating an effective roughness field.

To enable PBCs use the command:

**pbc**

The configuration for all meshes, or the supermesh if applicable, will be shown. You can enable PBCs in any direction by setting a number of images using the interactive console objects (10 images are set by default when enabled, which can be edited if required; the default setting is for no PBCs). If the *SDemag* module is enabled you can edit the PBC settings on the supermesh, otherwise you need to edit them for the individual meshes.

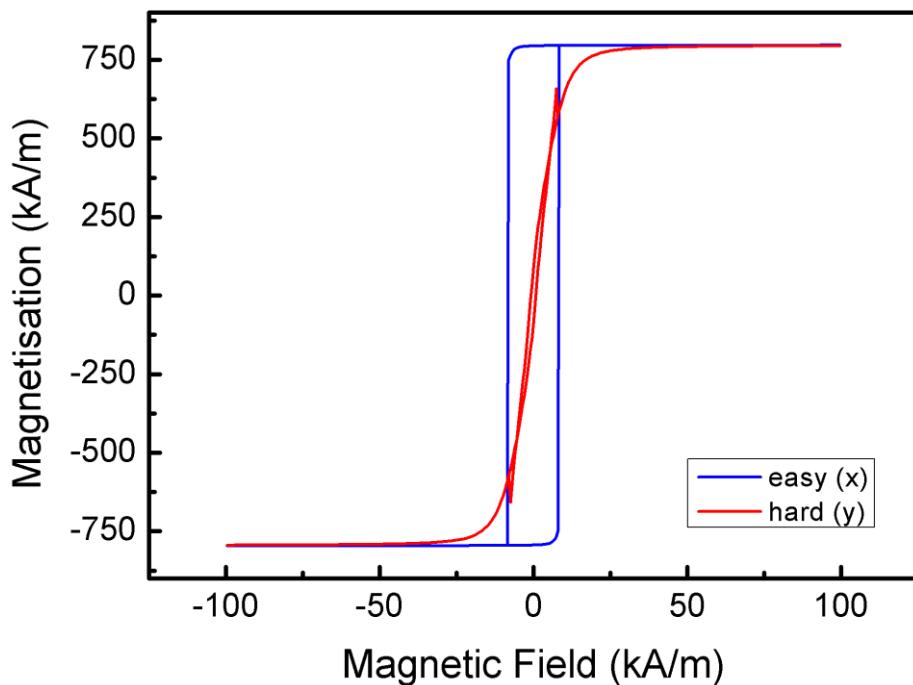
When using PBCs with multi-layered convolution you need to ensure the problem is physically meaningful. For example the recommended approach is to use a z direction stacking of layers, then either x or y PBCs are fine, but z PBCs will not lead to physically meaningful results in this case.

### Exercise 27.1

Repeat Exercise 24.2, but this time set default PBCs along both x and y. Compare the hysteresis loops.

When using PBCs with the *Roughness* module enabled, you should be careful about setting a combination of a large number of PBC images and fine roughness refinement (**refineroughness**). This can result in excessive initialization time due to the large demag kernel calculated by the *Roughness* module.

**Figure 27.1** – Hysteresis loops obtained for Exercise 27.1. The small peaks in the hard axis loop are artifacts resulting from the finite simulation mesh size, and could be decreased by increasing the simulation mesh rectangle.



## Tutorial 28 – Spatially Non-Uniform Stimuli

A spatial variation may be assigned to stimuli used in a simulation schedule, or when set through a console command. These include the applied field (thus any stage type setting a field, e.g. *Hxyz*, *Hxyz\_seq*, *Hfmr* etc.) set temperature (*T*, *T\_seq*) and heat source in the heat equation (*Q*, *Q\_seq*). The spatial variation is defined through a material parameter, in exactly the same way as any normal material parameter can be assigned a spatial variation.

Use **paramsvar** command. These are: *cHa* for applied field, *cT* for set temperature, and *Q* for heat sources. When setting a spatial variation for *T* or *Q* you need the *Heat* module enabled for it to take effect. If you want to set a fixed non-uniform temperature, you then need to prevent the heat solver from iterating, as any gradients in temperature will result in a heat flux. You can do this by setting the heat equation time step to zero: **setheatdt** 0.

To set a spatial variation for *Q* from a mask file, drag the *custom* spatial variation generator to *Q* (use **paramsvar** command to display the options). You will see the following:

*Q: custom; 0; 1; pngfile.*

The numbers specify the *offset* and *scale*. For a grayscale png file this means black is zero (the offset), and white is 1 (offset + scale). For example if you want the spatial variation to be between 1 (black) and 2 (white), you would have to set *offset* = 1, *scale* = 1. Double click on the *Q* interactive object to edit it. To load the mask file specify its name together with the full path. You can view the effect by selecting *ParamVar* under the **display** (console command) options.

Remember the spatial variation merely acts as a multiplier on the actual parameter value. To set a base heat source value you have to edit the *Q* value (in W/m<sup>3</sup>) found under the **params** console command.

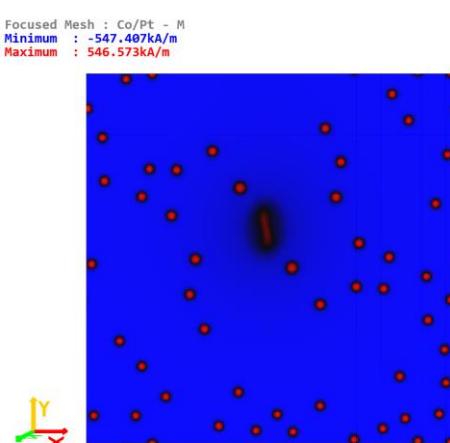
In the next exercise you will simulate the effect of a focused laser pulse on a Co/Pt/MgO structure with interfacial DMI enabled, and investigate the creation of skyrmions by heat-assisted reversal under a small magnetic field. The materials should be added from the materials database using the **addmaterial** command (for Co use the Co/Pt material, i.e. Co interfaced to Pt), and should have the appropriate modules enabled (including *iDMEchange*, *Aniuni*, and *Heat*).

### Exercise 28.1

Set up a Co (1 nm)/Pt (4 nm)/MgO (50 nm) structure, enabling the *iDMEchange* and *Aniuni* modules for Co, and the *Heat* module for all layers. Use xy dimensions of 1024 nm × 1024 nm and enable PBCs for both x and y. Start from uniform magnetization along the (0, 0) direction and apply a reversal field of 70 kA/m along the (180, 0) direction. Simulate using a Q stage with  $Q = 3 \times 10^{20}$  W/m<sup>3</sup> for 5 ns, and a spatial dependence for Q similar to that observed in Figure 28.1. Start from a uniform temperature of 300 K, enabling the indicative material Curie temperature for Co.

Use a 4nm in-plane cellsize for the Co layer for both magnetization and heat equation solvers. For the Pt and MgO layers you can use a 8 nm in-plane cellsize for the heat equation solver; for MgO you can set the z cellsize to 5 nm. Solve the LLG equation with RK4 set to 500 fs time step. For the heat equation you will have to use a low 50 fs time step. You should enable CUDA computations for this simulation.

**Figure 28.1 –** Skyrmions obtained in Exercise 28.1, showing the z component of magnetization. The dark spot in the middle is due to reduced magnetization magnitude at the focused laser heat source site.



## Materials Database

Material definitions can be saved in a materials database. This includes base material parameter values. The default database is called BorisMDB.txt. You can see this using the command:

### **materialsdatabase**

The default materials database can be updated from a shared database stored on a server. The shared database can be seen at: <https://boris-spintronics.uk/online-materials-database>. To update your local BorisMDB database using the latest material parameter definitions, use the command:

### **updatemdb**

You can also switch to an alternative custom database using the **materialsdatabase** command. To add a new computational mesh with given material parameters you can use the **addmaterial** command. The type of material will determine the type of computational mesh generated. For example the *ferromagnetic* type will generate a computational mesh with LLG/LLB solvers enabled. The *conductor* mesh type will generate a computational mesh with only the transport and heat solvers enabled, while the *insulator* mesh will only have the heat solver enabled (e.g. a substrate material).

Users can also send in entries to be added to the centrally stored database. This can be done using the **requestmdbsync** command. Before sending entries, you must properly format the material entry. The procedure is described as follows.

1. Add a new entry to your local BorisMDB file.

Suppose you want to enter a new ferromagnetic material. First create a ferromagnetic mesh in Boris (**addmesh**), and set as many parameter values as possible. Next, add the entry to your local BorisMDB file using:

**addmdbentry** *meshname (materialname)*

Here *meshname* is the name of the mesh as it appears in Boris (the one you created using **addmesh**), and *materialname* is the name of the material, or entry, you want to create, if different.

## 2. Edit the material description fields in BorisMDB.txt

There are 5 description fields for the entry:

*Name, Formula, Type, Description, Contributor*

*Name* is the name of your new material entry, which should not already be in the shared online database. This should already be filled.

*Formula* is the symbolic formula for the material. Make sure to fill this.

*Type* is already filled for you, and is the type of computational mesh for which the material applies.

*Description* should have a very brief description for the material entry, with any useful information. Make sure to fill this.

*Contributor* is the name of the entry contributor; leave as N/A if you don't want to specify this.

There is another field called *State*. This specifies if the entry was taken from the online database (SHARED) or if it's a new user-created entry (LOCAL). You don't need to change this.

### 3. Set references for the parameters

After each parameter there is a column called DOI. This must hold a DOI reference for where the material parameter value was taken from, or derived. You can leave it as N/A only if not applicable, but in most cases should be properly referenced.

### 4. Unspecified material parameters

If you cannot reasonably give an entry for a material parameter value then override it as “N/A”.

### 5. Send in the entry

After properly formatting the entry, you can upload it to a holding database using the **requestmdbsync** command:

**requestmdbsync** *materialname (email)*

*Materialname* is the name of the material you've just created. If you specify an email address you will receive feedback about whether the entry was added to the shared database or not – the entry will be verified for validity before being added to the online materials database. Once entered there, it will be visible at <https://boris-spintronics.uk/online-materials-database>, and other users can update their databases with it.

## Differential Equations

This section outlines the magnetization dynamics equations solved as selected using the **ode** command. For descriptions of parameters used see the Material Parameters section.

A number of evaluation methods are available for the magnetization dynamics equations. These are fixed step methods *Euler* (1<sup>st</sup> order), trapezoidal Euler (*TEuler* – 2<sup>nd</sup> order) and Runge-Kuta (*RK4* - 4<sup>th</sup> order). Adaptive time-step methods are the adaptive Heun (*AHeun* – 2<sup>nd</sup> order), the multi-step Adams-Basforth-Moulton (*ABM* – 2<sup>nd</sup> order), Runge-Kutta-Bogacki-Shampine (*RK23* – 3<sup>rd</sup> order with embedded 2<sup>nd</sup> order error estimator), Runge-Kutta-Fehlberg (*RKF45* – 4<sup>th</sup> order with embedded 5<sup>th</sup> order error estimator), Runge-Kutta-Cash-Karp (*RKCK45* – 4<sup>th</sup> order with embedded 5<sup>th</sup> order error estimator), and Runge-Kutta-Dormand-Prince (*RKDP54* – 5<sup>th</sup> order with embedded 4<sup>th</sup> order error estimator). For static problems a steepest descent solver is available, *SDesc*, using Barzilai-Borwein stepsize selection formulas.

### Landau-Lifshitz-Gilbert (LLG)

The normalised LLG equation in implicit form is given by:

$$\frac{\partial \mathbf{m}}{\partial t} = -\gamma \mathbf{m} \times \mathbf{H} + \alpha \mathbf{m} \times \frac{\partial \mathbf{m}}{\partial t}$$

Here  $\gamma = \mu_0 g_{rel} |\gamma_e|$ , where  $\gamma_e = -g\mu_B/\hbar$  is the electron gyromagnetic ratio and  $g_{rel}$  is a relative g-factor ( $g_{rel} = 1$  by default giving  $\gamma = 2.212761569 \times 10^5$  m/As).

In explicit form the normalised LLG equation is given by:

$$\frac{\partial \mathbf{m}}{\partial t} = -\frac{\gamma}{1+\alpha^2} \mathbf{m} \times \mathbf{H} - \frac{\alpha\gamma}{1+\alpha^2} \mathbf{m} \times \mathbf{m} \times \mathbf{H}$$

### Landau-Lifshitz-Gilbert with Spin-Transfer Torques (LLG-STT)

The LLG equation can be complemented by Zhang-Li spin-transfer torques. In implicit form this becomes:

$$\frac{\partial \mathbf{m}}{\partial t} = -\gamma \mathbf{m} \times \mathbf{H} + \alpha \mathbf{m} \times \frac{\partial \mathbf{m}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{m} - \beta \mathbf{m} \times (\mathbf{u} \cdot \nabla) \mathbf{m}$$

The spin-drift velocity  $\mathbf{u}$  is given by:

$$\mathbf{u} = \mathbf{J} \frac{Pg\mu_B}{2eM_s} \frac{1}{1+\beta^2}$$

The LLG-STT equation in explicit form is given by:

$$\begin{aligned} \frac{\partial \mathbf{m}}{\partial t} = & -\frac{\gamma}{1+\alpha^2} \mathbf{m} \times \mathbf{H} - \frac{\alpha\gamma}{1+\alpha^2} \mathbf{m} \times (\mathbf{m} \times \mathbf{H}) + \\ & \frac{1}{1+\alpha^2} [(1+\alpha\beta)(\mathbf{u} \cdot \nabla) \mathbf{m} - (\beta - \alpha) \mathbf{m} \times (\mathbf{u} \cdot \nabla) \mathbf{m} - \alpha(\beta - \alpha)(\mathbf{m} \cdot (\mathbf{u} \cdot \nabla) \mathbf{m}) \mathbf{m}] \end{aligned}$$

### Landau-Lifshitz-Bloch (LLB)

For non-zero temperature simulations the LLB equation should be used and in implicit form is given by (un-normalised):

$$\frac{\partial \mathbf{M}}{\partial t} = -\gamma \mathbf{M} \times \mathbf{H} + \frac{\tilde{\alpha}_\perp}{|\mathbf{M}|} \mathbf{M} \times \frac{\partial \mathbf{M}}{\partial t} + \frac{\gamma \tilde{\alpha}_\parallel}{|\mathbf{M}|} (\mathbf{M} \cdot \mathbf{H}) \mathbf{M}$$

Here for  $T < T_C$  ( $T_C$  is the Curie temperature)  $\alpha_\perp = \alpha(1 - T/3T_C)$ ,  $\alpha_\parallel = \alpha 2T/3T_C$  and  $\tilde{\alpha}_\perp = \alpha_\perp/m$ ,  $\tilde{\alpha}_\parallel = \alpha_\parallel/m$ , where  $m$  is the magnetization length normalised to its zero temperature value, i.e.  $m = |\mathbf{M}| / M_s^0$ . For  $T > T_C$   $\alpha_\perp = \alpha_\parallel$ .

The effective field  $\mathbf{H}$  must be complemented by a longitudinal susceptibility field given by:

$$\mathbf{H}_l = \begin{cases} \left(1 - \frac{m^2}{m_e^2}\right) \frac{\mathbf{m}}{2\mu_0\chi_{\parallel}}, & T \leq T_c \\ -\left(1 + \frac{3}{5} \frac{T_c m^2}{T - T_c}\right) \frac{\mathbf{m}}{\mu_0\chi_{\parallel}}, & T > T_c \end{cases}$$

The field and temperature-dependent equilibrium magnetization,  $m_e$ , is given by:

$$m_e(T) = B \left[ m_e \frac{3T_c}{T} + \frac{\mu\mu_0 H_{ext}}{k_B T} \right]$$

where  $B(x) = \coth(x) - 1/x$  is the Langevin function,  $\mu$  is the atomic moment, and:

$$\chi_{\parallel}(T) = \frac{\mu}{k_B T} \frac{B'(x)}{1 - B'(x)(3T_c/T)}, \quad \text{with } x = m_e 3T_c / T$$

Further, we have the temperature dependences  $M_s(T) = M_s^0 m_e(T)$ , and  $A(T) = A_0 m_e^2(T)$  for the exchange stiffness.

In explicit form the LLB equation becomes:

$$\frac{\partial \mathbf{M}}{\partial t} = -\frac{\gamma}{1 + \tilde{\alpha}_{\perp}^2} \mathbf{M} \times \mathbf{H} - \frac{\tilde{\alpha}_{\perp} \gamma}{1 + \tilde{\alpha}_{\perp}^2} \frac{1}{|\mathbf{M}|} \mathbf{M} \times (\mathbf{M} \times \mathbf{H}) + \frac{\gamma \tilde{\alpha}_{\parallel}}{|\mathbf{M}|} (\mathbf{M} \cdot \mathbf{H}) \mathbf{M}$$

### Landau-Lifshitz-Bloch with Spin-Transfer Torques (LLB-STT)

In implicit form we have the LLB-STT equation as:

$$\frac{\partial \mathbf{M}}{\partial t} = -\gamma \mathbf{M} \times \mathbf{H} + \frac{\tilde{\alpha}_{\perp}}{|\mathbf{M}|} \mathbf{M} \times \frac{\partial \mathbf{M}}{\partial t} + \frac{\gamma \tilde{\alpha}_{\parallel}}{|\mathbf{M}|} (\mathbf{M} \cdot \mathbf{H}) \mathbf{M} + (\mathbf{u} \cdot \nabla) \mathbf{M} - \frac{\beta}{|\mathbf{M}|} \mathbf{M} \times (\mathbf{u} \cdot \nabla) \mathbf{M}$$

In this case the spin-drift velocity is given by:

$$\mathbf{u} = \mathbf{J} \frac{P^0 g \mu_B}{2eM_s^0} \frac{1}{1+\beta^2}$$

Note, this is the same as the previous definition of the spin-drift velocity with  $P$  having the same temperature dependence as  $M_s$ , i.e.  $P(T) = P^0 m_e(T)$ . In Boris this latter approach is used, allowing custom definitions of  $P(T)$  temperature scaling.

In explicit form the LLB-STT equation becomes:

$$\begin{aligned} \frac{\partial \mathbf{M}}{\partial t} = & -\frac{\gamma}{1+\tilde{\alpha}_\perp^2} \mathbf{M} \times \mathbf{H} - \frac{\tilde{\alpha}_\perp \gamma}{1+\tilde{\alpha}_\perp^2} \frac{1}{|\mathbf{M}|} \mathbf{M} \times (\mathbf{M} \times \mathbf{H}) + \frac{\gamma \tilde{\alpha}_\parallel}{|\mathbf{M}|} (\mathbf{M} \cdot \mathbf{H}) \mathbf{M} + \\ & \frac{1}{(1+\tilde{\alpha}_\perp^2)} \left[ (1+\tilde{\alpha}_\perp \beta) (\mathbf{u} \cdot \nabla) \mathbf{M} - \frac{(\beta - \tilde{\alpha}_\perp)}{|\mathbf{M}|} \mathbf{M} \times (\mathbf{u} \cdot \nabla) \mathbf{M} - \frac{\tilde{\alpha}_\perp (\beta - \tilde{\alpha}_\perp)}{|\mathbf{M}|^2} (\mathbf{M} \cdot (\mathbf{u} \cdot \nabla) \mathbf{M}) \mathbf{M} \right] \end{aligned}$$

### Stochastic Landau-Lifshitz-Gilbert (sLLG)

The LLG equation with a stochastic thermal field is available in Boris for comparisons, but should normally not be used. Instead the stochastic LLB equation should be used. The explicit sLLG equation is given as:

$$\frac{\partial \mathbf{m}}{\partial t} = -\frac{\gamma}{1+\alpha^2} \mathbf{m} \times \mathbf{H} - \frac{\alpha \gamma}{1+\alpha^2} \mathbf{m} \times \mathbf{m} \times (\mathbf{H} + \mathbf{H}_{thermal})$$

The thermal field varies randomly both in magnitude and direction, and has maximum magnitude given by:

$$|\mathbf{H}_{thermal}|_{max} = \sqrt{\frac{2k_B T}{\alpha \gamma \mu_0 M_s^0 V \Delta t}}$$

$V$  is the volume of the computational cell, and  $\Delta t$  is the time step used by the stochastic differential equation evaluation method.

### Stochastic Landau-Lifshitz-Bloch (sLLB)

For the stochastic LLB equation we have both a thermal field and thermal torque, and is given by:

$$\frac{\partial \mathbf{M}}{\partial t} = -\frac{\gamma}{1 + \tilde{\alpha}_\perp^2} \mathbf{M} \times \mathbf{H} - \frac{\tilde{\alpha}_\perp \gamma}{1 + \tilde{\alpha}_\perp^2} \frac{1}{|\mathbf{M}|} \mathbf{M} \times (\mathbf{M} \times (\mathbf{H} + \mathbf{H}_{thermal})) + \frac{\gamma \tilde{\alpha}_\parallel}{|\mathbf{M}|} (\mathbf{M} \cdot \mathbf{H}) \mathbf{M} + \boldsymbol{\eta}_{thermal}$$

The thermal field and torque vary randomly both in magnitude and direction, and have maximum magnitude given by:

$$|\mathbf{H}_{thermal}|_{max} = \frac{1}{\alpha_\perp} \sqrt{\frac{2k_B T(\alpha_\perp - \alpha_\parallel)}{\gamma \mu_0 M_s^0 V \Delta t}}$$
$$|\boldsymbol{\eta}_{thermal}|_{max} = \sqrt{\frac{2k_B T \alpha_\parallel \gamma M_s^0}{\mu_0 V \Delta t}}$$

### Stochastic Landau-Lifshitz-Gilbert with Spin-Transfer Torques (sLLG-STT)

This is similar to the LLG-STT equation, but also has the thermal field from the sLLG equation added to the damping torque term.

### Stochastic Landau-Lifshitz-Bloch with Spin-Transfer Torques (sLLB-STT)

This is similar to the LLB-STT equation, but also has the thermal field from the sLLB equation added to the damping torque term, as well as the additional thermal torque term.

## Equations with Spin Accumulation

The LLG, LLB, sLLG, and sLLB equations also appear in the forms LLG-SA, LLB-SA, sLLG-SA, and sLLB-SA. When using these equations the spin transport solver is enabled and a spin accumulation  $\mathbf{S}$  is calculated. This gives rise to bulk and interfacial torques which are added to the respective equation. For example for the LLG equation we obtain the LLG-SA equation as:

$$\frac{\partial \mathbf{M}}{\partial t} = -\gamma \mathbf{M} \times \mathbf{H} + \frac{\alpha}{|\mathbf{M}|} \mathbf{M} \times \frac{\partial \mathbf{M}}{\partial t} + \mathbf{T}_s$$

The bulk spin-accumulation torque is given by:

$$\mathbf{T}_s = -\frac{D_e}{\lambda_J^2} \mathbf{m} \times \mathbf{S} - \frac{D_e}{\lambda_\varphi^2} \mathbf{m} \times (\mathbf{m} \times \mathbf{S})$$

This is included as an additional effective field in the explicit forms of the equations:

$$\mathbf{H}_s = \frac{D_e}{\gamma |\mathbf{M}|} \left( \frac{\mathbf{S}}{\lambda_J^2} + \frac{\mathbf{m} \times \mathbf{S}}{\lambda_\varphi^2} \right)$$

Note there are no SA version for the STT equations. This is because the Zhang-Li STTs result from the bulk  $\mathbf{T}_s$  torque as a special case (see e.g. S. Lepadatu, Scientific Reports 7, 12937 (2017)).

Interfacial spin-accumulation torques are also present when N/F interfaces are used:

$$\mathbf{T}_s^{interface} = \frac{g\mu_B}{ed_h} \left[ \text{Re}\{G^{\uparrow\downarrow}\} \mathbf{m} \times (\mathbf{m} \times \Delta\mathbf{V}_s) + \text{Im}\{G^{\uparrow\downarrow}\} \mathbf{m} \times \Delta\mathbf{V}_s \right]$$

where  $\Delta\mathbf{V}_s = \mathbf{V}_{s,F} - \mathbf{V}_{s,N}$  and  $\mathbf{V}_s = (D_e/\sigma)(e/\mu_B)\mathbf{S}$ .

This is included as an additional effective field in the explicit forms of the equations:

$$\mathbf{H}_s = \frac{-1}{\gamma |\mathbf{M}|} \frac{g\mu_B}{ed_h} \left( \text{Re}\{G^{\uparrow\downarrow}\} \mathbf{m} \times \Delta\mathbf{V}_s + \text{Im}\{G^{\uparrow\downarrow}\} \Delta\mathbf{V}_s \right)$$

### Static Landau-Lifshitz-Gilbert (*LLGStatic*)

This equation is used for static problems, i.e. where only the relaxed magnetization state is required. It is the explicit LLG equation without the precession term, and with the damping factor set to 1. This is given by:

$$\frac{\partial \mathbf{m}}{\partial t} = -\frac{\gamma}{2} \mathbf{m} \times \mathbf{m} \times \mathbf{H}$$

## Modules

Modules typically correspond to an additive field in the total effective field  $\mathbf{H}$  appearing in the equations shown in the Differential Equations section:

$$\mathbf{H} = \mathbf{H}_{\text{eff}} = \mathbf{H}_1 + \mathbf{H}_2 + \dots$$

Most modules also have an energy density term associated with their effective field contributions, available as an output data parameter.

All contributions are evaluated on a cell-centered uniform finite difference mesh, with all differential operators evaluated to second order accuracy.

### Aniuni – Uniaxial Magneto-Crystalline Anisotropy

Effective field contribution:

$$\mathbf{H} = \frac{2K_1}{\mu_0 M_S} (\mathbf{m} \cdot \mathbf{e}_A) \mathbf{e}_A + \frac{4K_2}{\mu_0 M_S} [1 - (\mathbf{m} \cdot \mathbf{e}_A)^2] (\mathbf{m} \cdot \mathbf{e}_A) \mathbf{e}_A$$

Energy density term (output data parameter:  $e\_anis$ ):

$$\varepsilon = K_1 [1 - (\mathbf{m} \cdot \mathbf{e}_A)^2] + K_2 [1 - (\mathbf{m} \cdot \mathbf{e}_A)^2]^2$$

## **Anicubi** – Cubic Magneto-Crystalline Anisotropy

Effective field contribution:

$$\begin{aligned}\mathbf{H} = & -\frac{2K_1}{\mu_0 M_s} [\mathbf{e}_1 \alpha (\beta^2 + \gamma^2) + \mathbf{e}_2 \beta (\alpha^2 + \gamma^2) + \mathbf{e}_3 \gamma (\alpha^2 + \beta^2)] \\ & -\frac{2K_2}{\mu_0 M_s} [\mathbf{e}_1 \alpha \beta^2 \gamma^2 + \mathbf{e}_2 \alpha^2 \beta \gamma^2 + \mathbf{e}_3 \alpha^2 \beta^2 \gamma]\end{aligned}$$

Here  $\alpha = \mathbf{m} \cdot \mathbf{e}_1$ ,  $\beta = \mathbf{m} \cdot \mathbf{e}_2$ , and  $\gamma = \mathbf{m} \cdot \mathbf{e}_3$ , where  $\mathbf{e}_3 = \mathbf{e}_1 \times \mathbf{e}_2$ .

Energy density term (output data parameter: *e\_anis*):

$$\varepsilon = K_1 [\alpha^2 \beta^2 + \alpha^2 \gamma^2 + \beta^2 \gamma^2] + K_2 \alpha^2 \beta^2 \gamma^2$$

## **Demag\_N** – Stoner-Wohlfarth Magnetostatic Interaction

Effective field contribution:

$$H_i = -N_i M_i \quad (i = x, y, z)$$

Here  $N_z = 1 - N_x - N_y$ .

Energy density term (output data parameter: *e\_demag*):

$$\varepsilon = -\frac{\mu_0}{2} \mathbf{M} \cdot \mathbf{H}$$

## **Demag** - Magnetostatic Interaction

Effective field contribution:

$$\mathbf{H}(\mathbf{r}_0) = - \int_{\mathbf{r} \in V} \mathbf{N}(\mathbf{r} - \mathbf{r}_0) \mathbf{M}(\mathbf{r}) d\mathbf{r}$$

Here **N** is a rank-2 tensor with the following symmetry:

$$\mathbf{N} = \begin{pmatrix} N_{xx} & N_{xy} & N_{xz} \\ N_{xy} & N_{yy} & N_{yz} \\ N_{xz} & N_{yz} & N_{zz} \end{pmatrix}$$

**N** is computed using the formulas in A.J. Newell et al., "A Generalization of the Demagnetizing Tensor for Nonuniform Magnetization" J. Geophys. Res. **98**, 9551 (1993).

Energy density term (output data parameter: *e\_demag*):

$$\varepsilon = -\frac{\mu_0}{2} \mathbf{M} \cdot \mathbf{H}$$

The convolution function is evaluated using the convolution theorem, i.e. both **N** and **M** are transformed using an FFT algorithm, multiplied in the transform space, then **H** is obtained using the inverse FFT; **M** is zero-padded before computing the FFT.

## **DMExchange** – Dzyaloshinskii-Moriya Bulk Exchange Interaction

Effective field contribution:

$$\mathbf{H} = -\frac{2D}{\mu_0 M_s^2} \nabla \times \mathbf{M}$$

Non-homogeneous Neumann boundary conditions are used to evaluate the curl operator:

$$\frac{\partial \mathbf{M}}{\partial \mathbf{n}} = \frac{D}{2A} \mathbf{n} \times \mathbf{M}$$

The DM exchange field adds to the direct exchange field.

Energy density term (output data parameter: *e\_exch*):

$$\varepsilon = -\frac{\mu_0}{2} \mathbf{M} \cdot \mathbf{H}$$

## **Exchange** – Direct Exchange Interaction

Effective field contribution:

$$\mathbf{H} = \frac{2A}{\mu_0 M_s^2} \nabla^2 \mathbf{M}$$

Homogeneous Neumann boundary conditions are used to evaluate the Laplacian operator.

Energy density term (output data parameter: *e\_exch*):

$$\varepsilon = -\frac{\mu_0}{2} \mathbf{M} \cdot \mathbf{H}$$

## Heat – Heat Equation Solver

The heat equation with Joule heating is given by:

$$C\rho \frac{\partial T(\mathbf{r}, t)}{\partial t} = \nabla \cdot K \nabla T(\mathbf{r}, t) + \frac{\mathbf{J}^2}{\sigma}$$

Robin boundary conditions are used to evaluate the differential operators.

The heat equation is evaluated using the simple forward-time centered-space method. The heat equation time-step is normally comparable to the magnetization equation time-step thus a more time-efficient method (e.g. Crank-Nicolson) is not normally required.

## iDMEexchange – Dzyaloshinskii-Moriya Interfacial Exchange Interaction

Effective field contribution for thin film in xy plane:

$$\mathbf{H} = -\frac{2D}{\mu_0 M_s^2} \left( \frac{\partial M_z}{\partial x}, \frac{\partial M_z}{\partial y}, -\frac{\partial M_x}{\partial x} - \frac{\partial M_y}{\partial y} \right)$$

Non-homogeneous Neumann boundary conditions are used to evaluate the differential operators:

$$\frac{\partial \mathbf{M}}{\partial \mathbf{n}} = \frac{D}{2A} (\hat{\mathbf{z}} \times \mathbf{n}) \times \mathbf{M}$$

The iDM exchange field adds to the direct exchange field.

Energy density term (output data parameter: `e_exch`):

$$\varepsilon = -\frac{\mu_0}{2} \mathbf{M} \cdot \mathbf{H}$$

### Oersted – Oersted Field

Effective field contribution:

$$\mathbf{H}(\mathbf{r}_0) = \int_{\mathbf{r} \in V} \mathbf{K}(\mathbf{r} - \mathbf{r}_0) \mathbf{J}_C(\mathbf{r}) d\mathbf{r}$$

Here  $\mathbf{K}$  is a rank-2 tensor with the following symmetry:

$$\mathbf{K} = \begin{pmatrix} 0 & K_{xy} & K_{xz} \\ -K_{xy} & 0 & K_{yz} \\ -K_{xz} & -K_{yz} & 0 \end{pmatrix}$$

$\mathbf{K}$  is computed using the formulas in B. Krüger, “Current-Driven Magnetization Dynamics: Analytical Modeling and Numerical Simulation”, PhD Dissertation, University of Hamburg (2011) – Appendix D, page 118.

### Roughness – Roughness Field and Staircase Magnetostatic Corrections

Effective field contribution computed on the coarse mesh (i.e. the actual mesh discretisation used at run-time with  $N_V$  number of discretisation cells):

$$\mathbf{H}(\mathbf{r}_0) = - \left[ \sum_{\mathbf{r} \in V} \mathbf{N}(\mathbf{r} - \mathbf{r}_0) G(\mathbf{r}, \mathbf{r}_0) \right] \mathbf{M}(\mathbf{r}_0) \quad (\mathbf{r}_0 \in V)$$

Here  $\mathbf{N}$  is the demagnetizing tensor computed on the fine mesh with  $N_{V_f}$  number of discretisation cells, and:

$$G(\mathbf{r}, \mathbf{r}_0) = \begin{cases} \frac{N_V}{N_{V_r}} - 1 & \mathbf{r} \wedge \mathbf{r}_0 \in V_R \\ -1 & \mathbf{r} \vee \mathbf{r}_0 \in V - V_R \end{cases}$$

$V$  is the smooth body without roughness and  $V_R$  is the mesh with roughness, and we require  $V_R \subseteq V$ . If the coarse cellsize has dimensions  $(h_x, h_y, h_z)$ , the fine cellsize must have dimensions  $(h_x / m_x, h_y / m_y, h_z / m_z)$ , where the  $m$  factors are integers. The function  $\sum_{\mathbf{r} \in V} \mathbf{N}(\mathbf{r} - \mathbf{r}_0) G(\mathbf{r}, \mathbf{r}_0)$  is computed at initialisation on the finely discretised mesh then averaged up to the coarse mesh (each coarse cellsize value is obtained as an average of its contained fine cellsize values).

Energy density term (output data parameter: *e\_rough*):

$$\varepsilon = -\frac{\mu_0}{2} \mathbf{M} \cdot \mathbf{H}$$

Details can be found in: S. Lepadatu, “Effective field model of roughness in magnetic nano-structures” J. Appl. Phys. **118**, 243908 (2015).

## **SDemag** – Supermesh Magnetostatic Interaction

### I. Supermesh demagnetization (**multiconvolution 0**).

The same formulas as for the *Demag* module are used when computing demagnetizing fields on the uniformly discretised super-mesh. The ferromagnetic super-mesh may have a cellsize which differs from that of the individual ferromagnetic meshes. In this case a weighted average smoother is used to transfer magnetization to the super-mesh and demagnetizing field values back from the super-mesh.

Consider a discrete distribution of magnetization values  $\mathbf{M}$  at points  $V = \{\mathbf{r}_i; i \in P\}$ . Let  $\mathbf{h}$  be the cellsize of the input mesh, with the set of cells  $\{c_i; i \in P\}$  centered around the

points  $\mathbf{r}_i$ . To obtain the magnetization value at a point  $\mathbf{r}'$  in a cell  $c$  with dimensions  $\mathbf{h}'$  we introduce the definitions  $d_i = |\mathbf{r}' - \mathbf{r}_i|$ ,  $d_V = |\mathbf{h}' + \mathbf{h}|/2$ , and  $\tilde{d}_i = d_V - d_i$ . The weighted average is given as:

$$\mathbf{M}(\mathbf{r}') = \sum_{i \in P} w_i \mathbf{M}(\mathbf{r}_i),$$

where

$$w_i = \frac{\tilde{d}_i \delta_i}{\tilde{d}_T}$$

$$\delta_i = \begin{cases} 1, & c_i \cap c \neq \emptyset \\ 0, & \text{otherwise} \end{cases}$$

$$\tilde{d}_T = \sum_{i \in P} \tilde{d}_i \delta_i$$

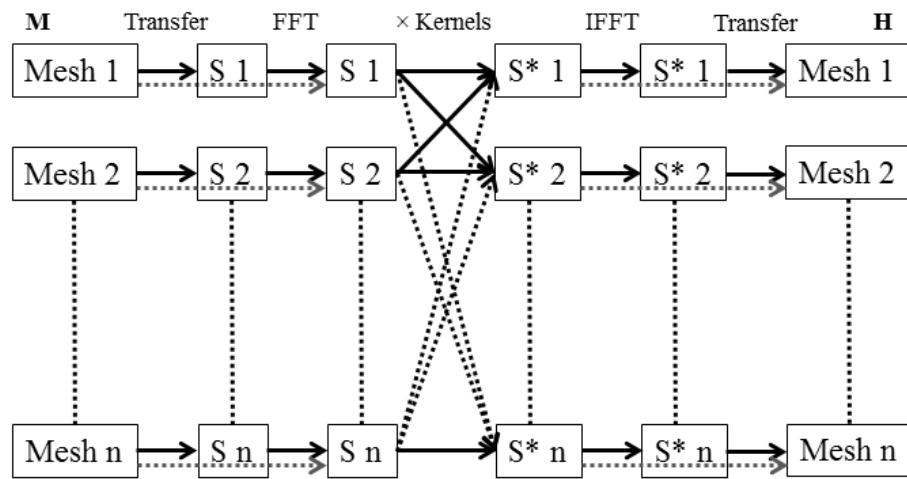
## II. Multi-Layered convolution (**multiconvolution 1**)

A generalisation of the single layer convolution algorithm is used here. We can write the convolution sum as:

$$\mathbf{H}(\mathbf{r}'_{kl}) = - \sum_{\substack{i=1, \dots, n \\ \mathbf{r}'_i \in V_i}} \mathbf{N}(\mathbf{r}'_{kl} - \mathbf{r}'_i, \mathbf{h}_k, \mathbf{h}_i) \mathbf{M}(\mathbf{r}'_i), \quad k = 1, \dots, n; \quad \mathbf{r}'_{kl} \in V_k$$

In the demagnetizing tensor for the equation above we explicitly specify the cellsize,  $\mathbf{h}$ , of the two computational meshes the tensor relates. Since we have  $n$  terms of the form appearing in the single layer convolution sum, we can again apply the convolution theorem. This time for each output mesh ( $\mathbf{H}$ ) we have  $n$  input meshes ( $\mathbf{M}$ ), together with  $n$  kernels. Thus to calculate the outputs in all  $n$  meshes we require a total of  $n^2$  sets of kernel multiplications in the transform space. This is illustrated in the figure below.

**Multi-Layered convolution algorithm** for  $n$  computational meshes. The magnetization input of each mesh is transformed separately using a FFT algorithm, either directly (dotted line), or by first transferring to a scratch space with a common discretisation cellsize, using a weighted average smoother (solid lines). In the transform space the inputs are multiplied with pre-computed kernels for a total of  $n^2$  sets of point-by-point multiplications. Finally the output demagnetizing fields are obtained using an inverse FFT algorithm, which are set directly in the output meshes (dotted line), or transferred using a weighted average smoother if the discretisation cellsizes differ (solid lines).



## SOTField – Spin-Orbit Torque Field

The spin-orbit torque is given by:

$$\mathbf{T}_{SOT} = \theta_{SHA,eff} \frac{\mu_B}{e} \frac{|J_c|}{d_h} (\mathbf{m} \times (\mathbf{m} \times \mathbf{p}) + r_G \mathbf{m} \times \mathbf{p})$$

Here  $\mathbf{p} = \mathbf{z} \times \mathbf{e}_{Jc}$ . This results in an effective field in the magnetization dynamics equation given by:

$$\mathbf{H}_{SOT} = -\frac{1}{M_s} \theta_{SHA,eff} \frac{\mu_B}{e} \frac{|J_c|}{d_h} (\mathbf{m} \times \mathbf{p} + r_G \mathbf{p})$$

## **Strayfield** – Stray field from magnetic dipoles

If  $\mathbf{M}_d$  is the magnetization of a uniformly magnetized prism with dimensions  $\mathbf{d}$ , then the magnetic field (stray field) at a distance  $\mathbf{r}$  from the centre of the prism is given by:

$$\mathbf{H} = \mathbf{N}_d(\mathbf{r}, \mathbf{d})\mathbf{M}_d$$

Here  $\mathbf{N}_d$  is a rank-2 tensor with the following symmetry:

$$\mathbf{N}_d = \begin{pmatrix} N_{xx} & N_{xy} & N_{xz} \\ N_{xy} & N_{yy} & N_{yz} \\ N_{xz} & N_{yz} & N_{zz} \end{pmatrix}$$

$\mathbf{N}_d$  is computed using the formulas in A. Andreev et al., “Universal Method for the Calculation of Magnetic Microelectronic Components: the Saturated Ferromagnetic Rectangular Prism and the Rectangular Coil.” ICSE2000 Proceedings, Nov. 2000, 187.

## **Surfexchange** – Surface Exchange Interaction

Let  $\mathbf{m}_i$  and  $\mathbf{m}_j$  be the normalised magnetization values of two cells,  $i$  and  $j$ , which are surface exchange coupled across a gap between two ferromagnetic meshes with thicknesses  $t_1$  and  $t_2$ . Let  $\Delta = 2t_1t_2 / (t_1 + t_2)$ . The surface exchange field at cell  $i$ , from cell  $j$ , is given as:

$$\mathbf{H}_i = \frac{J_1}{\mu_0 M_s \Delta} \mathbf{m}_j + \frac{2J_2}{\mu_0 M_s \Delta} (\mathbf{m}_i \cdot \mathbf{m}_j) \mathbf{m}_j$$

Energy density term (output data parameter:  $e\_surfexch$ ):

$$\epsilon = -\frac{J_1}{\Delta} \mathbf{m}_i \cdot \mathbf{m}_j - \frac{J_2}{\Delta} (\mathbf{m}_i \cdot \mathbf{m}_j)^2$$

## Transport – Charge and Spin-Transport Solver

### Charge Transport

When solving only for the charge current density, a Poisson-type equation for V is solved as:

$$\nabla^2 V = -\frac{(\nabla V) \cdot (\nabla \sigma)}{\sigma}$$

For V Dirichlet boundary conditions are used at boundaries containing a fixed potential electrode, otherwise Neumann boundary conditions are used. The conductivity may have an AMR contribution (AMR given as a percentage value) calculated as:

$$\sigma = \frac{\sigma_0}{1 + (AMR/100)\mathbf{d}^2},$$

where

$$\mathbf{d} = \frac{\mathbf{J}_c \cdot \mathbf{M}}{|\mathbf{J}_c| |\mathbf{M}|}.$$

From V the charge current density is obtained as  $\mathbf{J}_c = -\sigma \nabla V$ , and is used for Joule heating computations and to obtain spin torques (Zhang-Li STT and SOT).

The Poisson equation is evaluated using the successive over-relaxation (SOR) algorithm with black-red ordering for parallelization.

### Charge and Spin Transport

Charge and spin current densities are given as (see S. Lepadatu, “Unified treatment of spin torques using a coupled magnetization dynamics and three-dimensional spin current solver” Scientific Reports 7, 12937 (2017) for details):

$$\mathbf{J}_c = \sigma \mathbf{E} + \beta_D D_e \frac{e}{\mu_B} (\nabla \mathbf{S}) \mathbf{m} + \theta_{SHA} D_e \frac{e}{\mu_B} \nabla \times \mathbf{S}$$

$$\mathbf{J}_s = -\frac{\mu_B}{e} P \sigma \mathbf{E} \otimes \mathbf{m} - D_e \nabla \mathbf{S} + \theta_{SHA} \frac{\mu_B}{e} \boldsymbol{\epsilon} \sigma \mathbf{E}$$

With the full spin transport solver enabled both  $V$  and  $\mathbf{S}$  are computed using Poisson-type equations as:

$$\nabla^2 V = -\frac{(\nabla V)(\nabla \sigma)}{\sigma} + \frac{\beta_D D_e}{\sigma} \frac{e}{\mu_B} \nabla \cdot (\nabla \mathbf{S}) \mathbf{m}$$

and

$$\begin{aligned} \nabla^2 \mathbf{S} = & -\frac{P}{D_e} \frac{\mu_B}{e} (\mathbf{J}_c \cdot \nabla) \mathbf{m} + P \beta_D \{ [(\nabla \mathbf{S}) \mathbf{m} \cdot \nabla] \mathbf{m} + \mathbf{m} \nabla \cdot (\nabla \mathbf{S}) \mathbf{m} \} \\ & + \frac{\theta_{SHA}}{D_e} \frac{\mu_B}{e} \nabla \cdot (\boldsymbol{\epsilon} \mathbf{J}_c) + \frac{\mathbf{S}}{\lambda_{sf}^2} + \frac{\mathbf{S} \times \mathbf{m}}{\lambda_J^2} + \frac{\mathbf{m} \times (\mathbf{S} \times \mathbf{m})}{\lambda_\varphi^2} \end{aligned}$$

For boundaries containing an electrode with a fixed potential, differential operators applied to  $V$  use a Dirichlet boundary condition. For other external boundaries the following non-homogeneous Neumann boundary conditions are used:

$$\nabla V \cdot \mathbf{n} = \theta_{SHA} \frac{D_e}{\sigma} \frac{e}{\mu_B} (\nabla \times \mathbf{S}) \cdot \mathbf{n}$$

$$(\nabla \mathbf{S}) \cdot \mathbf{n} = \theta_{SHA} \frac{\sigma}{D_e} \frac{\mu_B}{e} (\boldsymbol{\epsilon} \mathbf{E}) \cdot \mathbf{n}$$

At N/F composite media boundaries the following conditions are applied:

$$\begin{aligned} \mathbf{J}_c \cdot \mathbf{n}|_N &= \mathbf{J}_c \cdot \mathbf{n}|_F = -\left(G^\uparrow + G^\downarrow\right) \Delta V + \left(G^\uparrow - G^\downarrow\right) \Delta \mathbf{V}_s \cdot \mathbf{m} \\ \mathbf{J}_s \cdot \mathbf{n}|_N - \mathbf{J}_s \cdot \mathbf{n}|_F &= \frac{2\mu_B}{e} \left[ \operatorname{Re}\{G^{\uparrow\downarrow}\} \mathbf{m} \times (\mathbf{m} \times \Delta \mathbf{V}_s) + \operatorname{Im}\{G^{\uparrow\downarrow}\} \mathbf{m} \times \Delta \mathbf{V}_s \right] \\ \mathbf{J}_s \cdot \mathbf{n}|_F &= \frac{\mu_B}{e} \left[ -\left(G^\uparrow + G^\downarrow\right) (\Delta \mathbf{V}_s \cdot \mathbf{m}) \mathbf{m} + \left(G^\uparrow - G^\downarrow\right) \Delta V \mathbf{m} \right] \end{aligned}$$

Spin pumping is included on the N side of the above equations as:

$$\mathbf{J}_s^{pump} = \frac{\mu_B \hbar}{e^2} \left[ \operatorname{Re}\{G^{\uparrow\downarrow}\} \mathbf{m} \times \frac{\partial \mathbf{m}}{\partial t} + \operatorname{Im}\{G^{\uparrow\downarrow}\} \frac{\partial \mathbf{m}}{\partial t} \right]$$

At N/F interfaces, interfacial spin torques are obtained as ( $h_F$  is the discretisation cellsize of the F layer in the direction normal to the composite media boundary) :

$$\mathbf{T}_s = \frac{g\mu_B}{eh_F} \left[ \operatorname{Re}\{G^{\uparrow\downarrow}\} \mathbf{m} \times (\mathbf{m} \times \Delta \mathbf{V}_s) + \operatorname{Im}\{G^{\uparrow\downarrow}\} \mathbf{m} \times \Delta \mathbf{V}_s \right]$$

From  $\mathbf{S}$ , bulk spin torques are obtained as:

$$\mathbf{T}_s = -\frac{D_e}{\lambda_J^2} \mathbf{m} \times \mathbf{S} - \frac{D_e}{\lambda_\varphi^2} \mathbf{m} \times (\mathbf{m} \times \mathbf{S})$$

Both Poisson equations are evaluated using the SOR algorithm with black-red ordering for parallelization. Note, whilst the SOR algorithm is robust in evaluating the spin transport equations in arbitrary multi-layers with composite media boundary conditions, it does suffer from slow convergence in particular for lower target solver errors. This algorithm is due to be replaced with a more efficient method in the next version. Currently the alternating direction implicit method with parallelized Thomas algorithm, as well as a FFT-based Poisson solver are being evaluated. Another possibility is a bi-conjugate gradient method.

## Zeeman – Applied Magnetic Field

Effective field contribution:

$$\mathbf{H} = \mathbf{H}_{ext}$$

Energy density term (output data parameter: `e_zee`):

$$\varepsilon = -\mu_0 \mathbf{M} \cdot \mathbf{H}$$

## Material Parameters

**A:**  $A$  (J/m)

Exchange stiffness.

**amr:**  $AMR$  (%)

Anisotropic magneto-resistance as a percentage of base resistance.

**beta:**  $\beta$  (unitless)

Spin-transfer torque non-adiabaticity parameter.

**betaD:**  $\beta_D$  (unitless)

Diffusion spin polarisation.

**cHA:**  $cHA$  (unitless)

Applied field spatial variation parameter, which multiplies the applied field value.

**cT:**  $cT$  (unitless)

Set temperature spatial variation parameter, which multiplies the set temperature value. To enable spatial variation of temperature you need to have the *heat* module enabled. If you want the set temperature to remain constant you need to disable the heat equation by using **setheatdt** 0.

**D:**  $D$  (J/m<sup>2</sup>)

Dzyaloshinskii-Moriya exchange constant.

**damping:**  $\alpha$  (unitless)

Gilbert magnetization damping.

**De:**  $De$  (m<sup>2</sup>/s)

Electron diffusion constant.

**density:**  $\rho$  (kg/m<sup>3</sup>)

Mass density.

**ea1:**  $\mathbf{e}_{a1}$  (unit vector)

Uniaxial magneto-crystalline anisotropy symmetry axis, or first cubic magneto-crystalline anisotropy symmetry axis.

**ea2:**  $\mathbf{e}_{a2}$  (unit vector)

Second cubic magneto-crystalline anisotropy symmetry axis ( $\mathbf{e}_{a3} = \mathbf{e}_{a1} \times \mathbf{e}_{a2}$ ).

**eIC:**  $\sigma$  (S/m)

Base electrical conductivity.

**fISOT:**  $r_G$  (unitless)

Field-like spin orbit torque coefficient.

**Gi:**  $G^\uparrow, G^\downarrow$  (S/m<sup>2</sup>)

Interface spin-dependent conductivity (for majority and minority carriers). The top contacting mesh sets the interface value, thus  $Gi$  is available in both magnetic and non-magnetic meshes.

**Gmix:**  $G^{\uparrow\downarrow} = Re\{G\} + i Im\{G\}$  (S/m<sup>2</sup>)

interface spin-mixing conductivity (real and imaginary parts). The top contacting mesh sets the interface value, thus  $Gmix$  is available in both magnetic and non-magnetic meshes.

**grel:**  $g_{rel}$  (unitless)

Relative electron gyromagnetic ratio.

**iSHA:**  $\theta_{SHA}$  (unitless)

Spin Hall angle used for the inverse spin Hall effect.

**J1:**  $J_1$  (J/m<sup>2</sup>)

Bilinear surface exchange coupling. For coupled meshes it is the top mesh that sets the J values.

**J2:**  $J_2$  (J/m<sup>2</sup>)

Biquadratic surface exchange coupling. For coupled meshes it is the top mesh that sets the J values.

**K1:**  $K_1$  (J/m<sup>3</sup>)

Magneto-crystalline anisotropy energy.

**K2:**  $K_2$  (J/m<sup>3</sup>)

Magneto-crystalline anisotropy energy, higher order.

**I\_J:**  $\lambda_J$  (m)

Spin exchange rotation length.

**I\_phi:**  $\lambda_\phi$  (m)

Spin dephasing length.

**I\_sf:**  $\lambda_{sf}$  (m)

Spin-flip length.

**Ms:**  $M_s$  (A/m)

Saturation magnetization.

**Nx, Ny:**  $N_{xy}$  (unitless)

In-plane demagnetizing factors (used by demag\_N module)

**P:**  $P$  or  $\beta_\sigma$  (unitless)

Charge current spin polarization.

**pump\_eff:**  $\eta_{pump}$  (unitless)

Spin pumping efficiency.

**Q:** Q (W/m<sup>3</sup>)

Heat source added to the heat equation. Can be non-uniform by setting a spatial variation.

**SHA:**  $\theta_{SHA}$  (unitless)

Spin Hall angle used for the spin Hall effect.

**shc:** C (J/kgK).

Specific heat capacity.

**susrel:**  $\chi_{\perp}$  (As<sup>2</sup>/kg)

Transverse (perpendicular) susceptibility divided by  $\mu_0 M_s$ . Not currently used, reserved for next version.

**susrel:**  $\chi_{\parallel}$  (As<sup>2</sup>/kg)

Longitudinal (parallel) susceptibility divided by  $\mu_0 M_s$ .

**thermK:** K (W/mK)

Thermal conductivity.

**ts\_eff:**  $\eta_{ts}$  (unitless)

Spin accumulation torque efficiency in the bulk.

**tsi\_eff:**  $\eta_{tsi}$  (unitless)

Spin accumulation torque efficiency at interfaces.

## Commands – Essential

Essential commands only. These commands are used most often, or unlock a large part of the functionality through interactive objects console output. For descriptions see Commands – All section or type them in the console.

<b>addconductor</b>	<b>modules</b>
<b>addinsulator</b>	<b>multiconvolution</b>
<b>addmesh</b>	<b>ode</b>
<b>center</b>	<b>params</b>
<b>chdir</b>	<b>pbc</b>
<b>computefields</b>	<b>reset</b>
<b>cuda</b>	<b>run</b>
<b>data</b>	<b>savesim</b>
<b>default</b>	<b>setangle</b>
<b>display</b>	<b>setfield</b>
<b>loadsim</b>	<b>stages</b>
<b>mesh</b>	<b>stop</b>

## Commands – Important

Important commands for more advanced users, but might not be used as often as the essential commands. For descriptions see Commands – All section or type them in the console.

<b>ambient</b>	<b>savemeshimage</b>
<b>curietemperature</b>	<b>setcurrent</b>
<b>dwall</b>	<b>setdefaultelectrodes</b>
<b>electrodes</b>	<b>setdt</b>
<b>dp_getprofile</b>	<b>setheatdt</b>
<b>iterupdate</b>	<b>setpotential</b>
<b>paramstemp</b>	<b>skyrmion</b>
<b>paramsvar</b>	<b>showdata</b>
<b>preparemovingmesh</b>	<b>temperature</b>
<b>resetmesh</b>	<b>tsolverconfig</b>

## Commands – Useful

Other useful commands. For descriptions see Commands – All section or type them in the console.

<b>addirpole</b>	<b>loadmaskfile</b>
<b>addelectrode</b>	<b>makevideo</b>
<b>clearelectrodes</b>	<b>refineroughness</b>
<b>clearroughness</b>	<b>roughenmesh</b>
<b>copymeshdata</b>	<b>scalemeshrects</b>
<b>copyparams</b>	<b>setparamtemparray</b>
<b>dp_averagemeshrect</b>	<b>surfroughenjagged</b>

## Commands – All (Alphabetical)

### **2dmulticonvolution**

**USAGE :** **2dmulticonvolution** *status*

Switch to multi-layered convolution and force it to 2D layering in each mesh (2), or 2D convolution for each mesh (1), or allow 3D (0).

### **addconductor**

**USAGE :** **addconductor** *name rectangle*

Add a normal metal mesh with given name and rectangle (m). The rectangle can be specified as: sx sy sz ex ey ez for the start and end points in Cartesian coordinates, or as: ex ey ez with the start point as the origin.

### **adddata**

**USAGE :** **adddata** *dataname (meshname, (rectangle))*

Add dataname to list of output data. If applicable specify meshname and rectangle (m) in mesh. If not specified and required, active mesh is used with entire mesh rectangle.

### **adddipole**

**USAGE :** **adddipole** *name rectangle*

Add a rectangular dipole with given name and rectangle (m). The rectangle can be specified as: sx sy sz ex ey ez for the start and end points in Cartesian coordinates, or as: ex ey ez with the start point as the origin.

## **addelectrode**

**USAGE** : **addelectrode** *electrode\_rect*

Add an electrode in given rectangle (m).

## **addinsulator**

**USAGE** : **addinsulator** *name rectangle*

Add an insulator mesh with given name and rectangle (m). The rectangle can be specified as: sx sy sz ex ey ez for the start and end points in Cartesian coordinates, or as: ex ey ez with the start point as the origin.

## **addmaterial**

**USAGE** : **addmaterial** *name rectangle*

Add a new mesh with material parameters loaded from the materials database. The name is the material name as found in the mdb file (see materialsdatabase command); this also determines the type of mesh to create, as well as the created mesh name. The rectangle (m) can be specified as: sx sy sz ex ey ez for the start and end points in Cartesian coordinates, or as: ex ey ez with the start point as the origin.

**Script return values:** *meshname* - return name of mesh just added (can differ from the material name).

## **addmdbentry**

**USAGE** : **addmdbentry** *meshname (materialname)*

Add new entry in the local materials database from parameters in the given mesh. The name of the new entry is set to materialname if specified, else set to meshname.

For a complete entry you should then edit the mdb file manually with all the appropriate fields shown there.

### **addmesh**

**USAGE** : **addmesh** *name rectangle*

Add a ferromagnetic mesh with given name and rectangle (m). The rectangle can be specified as: sx sy sz ex ey ez for the start and end points in Cartesian coordinates, or as: ex ey ez with the start point as the origin.

### **addmodule**

**USAGE** : **addmodule** *meshname handle*

Add module with given handle to named mesh.

### **addpinneddata**

**USAGE** : **addpinneddata** *dataname (meshname)*

Add new entry in data box (at the end) with given dataname and meshname if applicable.

### **addrct**

**USAGE** : **addrct** *rectangle (meshname)*

Fill rectangle (m) within given mesh (active mesh if name not given). The rectangle coordinates are relative to specified mesh.

## **addstage**

**USAGE** : **addstage** *stagetype* (*meshname*)

Add a generic stage type to the simulation schedule with name *stagetype*, specifying a *meshname* if needed (if not specified and required, active mesh is used).

## **ambient**

**USAGE** : **ambient** *ambient\_temperature* (*meshname*)

Set mesh ambient temperature (all meshes if *meshname* not given) for Robin boundary conditions : flux normal = alpha \* (T\_boundary - T\_ambient).

**Script return values:** *ambient\_temperature* - ambient temperature for mesh in focus.

## **astepctrl**

**USAGE** : **astepctrl** *err\_fail* *err\_high* *err\_low* *dT\_incr* *dT\_min* *dT\_max*

Set parameters for adaptive time step control: *err\_fail* - repeat step above this, *err\_high* - decrease *dT* above this, *err\_low* - increase *dT* below this, *dT\_incr* - increase *dT* using fixed multiplier, *dT\_min*, *dT\_max* - *dT* bounds.

## **atomicmoment**

**USAGE** : **atomicmoment** *ub\_multiple* (*meshname*)

Set atomic moment as a multiple of Bohr magnetons (all ferromagnetic meshes if *meshname* not given) for ferromagnetic mesh. This affects the temperature dependence of 'me' (see curietemperature command). A non-zero value will result in *me(T)* being dependent on the applied field.

**Script return values:** *ub\_multiple* - atomic moment multiple of Bohr magneton for mesh in focus.

## **benchtime**

**USAGE** : **benchtime**

Show the last simulation duration time in ms, between start and stop; used for performance becnmarking.

Script return values: *value*

## **blochpreparemovingmesh**

**USAGE** : **blochpreparemovingmesh** (*meshname*)

Setup the named mesh (or active mesh) for moving Bloch domain wall simulations:  
1) set movingmesh trigger, 2) set domain wall structure, 3) set dipoles left and right to remove end magnetic charges, 4) enable strayfield module.

## **cellsize**

**USAGE** : **cellsize** *value*

Change cellsize of mesh in focus (m). The cellsize can be specified as: hx hy hz, or as: hxyz

Script return values: *cellsize* - return cellsize of mesh in focus.

## **center**

**USAGE** : **center**

Center mesh view and scale to fit window size.

## **chdir**

**USAGE** : **chdir** *directory*

Change working directory.

**Script return values:** *directory*

## **clearelectrodes**

**USAGE** : **clearelectrodes**

Delete all currently set electrodes.

## **clearmovingmesh**

**USAGE** : **clearmovingmesh**

Clear moving mesh settings made by a prepare command.

## **clearparamstemp**

**USAGE** : **clearparamstemp** (*meshname*)

Clear all material parameters temperature dependence in given mesh. If *meshname* not given clear temperature dependence in all meshes.

## **clearparamsvar**

**USAGE** : **clearparamsvar** (*meshname*)

Clear all material parameters spatial dependence in given mesh. If *meshname* not given clear spatial dependence in all meshes.

## **clearparamvar**

**USAGE** : **clearparamvar** *meshname paramname*

Clear parameter spatial dependence in given mesh.

## **clearroughness**

**USAGE** : **clearroughness** (*meshname*)

Clear roughness by setting the fine shape same as the coarse M shape.

## **clearscreen**

**USAGE** : **clearscreen**

Clear all console text.

## **computefields**

**USAGE** : **computefields**

Run simulation from current state for a single iteration without advancing the simulation time.

## **copymeshdata**

**USAGE** : **copymeshdata** *meshname\_from* *meshname\_to* (...)

Copy all primary mesh data (e.g. magnetization values and shape) from first mesh to all other meshes given - all meshes must be of same type.

## **copyparams**

**USAGE** : **copyparams** *meshname\_from* *meshname\_to* (...)

Copy all mesh parameters from first mesh to all other meshes given - all meshes must be of same type.

## **coupletodipoles**

**USAGE** : **coupletodipoles** *status*

Set/unset coupling to dipoles : if ferromagnetic meshes touch a dipole mesh then interface magnetic cells are exchange coupled to the dipole magnetization direction.

## **cuda**

**USAGE** : **cuda** *status*

Switch CUDA GPU computations on/off.

**Script return values:** *status*

## **curietemperature**

**USAGE** : **curietemperature** *curie\_temperature* (*meshname*)

Set Curie temperature (all ferromagnetic meshes if meshname not given) for ferromagnetic mesh. This will set default temperature dependencies as:  $Ms = Ms_0 \times me$ ,  $A = A_0 \times me^2$ ,  $D = D_0 \times me^2$ ,  $K = K_0 \times me^3$  (K1 and K2),  $\alpha = \alpha_0 \times (1-T/3T_c)$   $T < T_c$ ,  $\alpha = \alpha_0 \times 2T/3T_c$   $T \geq T_c$ ,  $\chi_{rel} = dm_e/d(\mu_0 H_{ext})$ . Setting the Curie temperature to zero will disable temperature dependence for these parameters.

**Script return values:** *curie\_temperature* - Curie temperature for mesh in focus.

**data****USAGE : data**

Shows list of currently set output data and available data.

**Script return values:** number of set output data fields

**default****USAGE : default**

Reset program to default state.

**deldata****USAGE : deldata *index***

Delete data from list of output data at index number. If index number is -1 then delete all data fields, leaving just a default time data field - there must always be at least 1 output data field.

**delectrode****USAGE : delectrode *index***

Delete electrode with given index.

**delmdbentry****USAGE : delmdbentry *materialname***

Delete entry in the local materials database (see materialsdatabase for current selection).

## **delmesh**

**USAGE** : **delmesh** *name*

Delete mesh with given name.

## **delmodule**

**USAGE** : **delmodule** *meshname handle*

Delete module with given handle from named mesh.

## **delpinneddata**

**USAGE** : **delpinneddata** *index*

Delete entry in data box at given index (index in order of appearance in data box from 0 up).

## **delrect**

**USAGE** : **delrect** *rectangle (meshname)*

Void rectangle (m) within given mesh (active mesh if name not given). The rectangle coordinates are relative to specified mesh.

## **delstage**

**USAGE** : **delstage** *index*

Delete stage from simulation schedule at index number. If index number is -1 then delete all stages, leaving just a default Relax stage - there must always be at least 1 stage set.

## **designateground**

**USAGE** : **designateground** *electrode\_index*

Change ground designation for electrode with given index.

## **display**

**USAGE** : **display** *name (meshname)*

Change quantity to display for given mesh (active mesh if name not given).

## **dp\_add**

**USAGE** : **dp\_add** *dp\_source value (dp\_dest)*

Add value to dp array and place it in destination (or at same position if destination not specified).

## **dp\_adddp**

**USAGE** : **dp\_adddp** *dp\_x1 dp\_x2 dp\_dest*

Add dp arrays :  $dp\_dest = dp\_x1 + dp\_x2$

## **dp\_append**

**USAGE** : **dp\_append** *dp\_original dp\_new*

Append data from *dp\_new* to the end of *dp\_original*.

## **dp\_averagemeshrect**

**USAGE** : **dp\_averagemeshrect** (*rectangle*)

Calculate the average value for the quantity displayed in the focused mesh. If specified the rectangle is relative to the focused mesh, otherwise average the entire focused mesh.

## **dp\_cartesiantopolar**

**USAGE** : **dp\_cartesiantopolar** *dp\_in\_x dp\_in\_y (dp\_out\_r dp\_out\_theta)*

Convert from Cartesian coordinates (x,y) to polar (r, theta).

## **dp\_clear**

**USAGE** : **dp\_clear** *indexes...*

Clear dp arrays with specified indexes.

## **dp\_clearall**

**USAGE** : **dp\_clearall**

Clear all dp arrays.

## **dp\_coercivity**

**USAGE** : **dp\_coercivity** *dp\_index\_x dp\_index\_y*

Obtain coercivity from x-y data: find first crossings of x axis in the two possible directions, with uncertainty obtained from step size.

**Script return values:** *Hc\_up Hc\_up\_err- Hc\_up\_err+ Hc\_dn Hc\_dn\_err- Hc\_dn\_err+*.

## **dp\_completehysteresis**

**USAGE :** *dp\_completehysteresis dp\_index\_x dp\_index\_y*

For a hysteresis loop with only one branch continue it by constructing the other direction branch (invert both x and y data and add it in continuation) - use only with hysteresis loops which are expected to be symmetric.

## **dp\_div**

**USAGE :** **dp\_div** *dp\_source value (dp\_dest)*

Divide dp array by value and place it in destination (or at same position if destination not specified).

## **dp\_divdp**

**USAGE :** **dp\_divdp** *dp\_x1 dp\_x2 dp\_dest*

Divide dp arrays :  $dp\_dest = dp\_x1 / dp\_x2$

## **dp\_dotprod**

**USAGE :** **dp\_dotprod** *dp\_vector ux uy uz dp\_out*

Take dot product of (ux, uy, uz) with vectors in dp arrays *dp\_vector*, *dp\_vector + 1*, *dp\_vector + 2* and place result in *dp\_out*.

## **dp\_dotproddp**

**USAGE :** **dp\_dotproddp** *dp\_x1 dp\_x2*

Take dot product of dp arrays :  $value = dp\_x1.dp\_x2$

## **dp\_dumptdep**

**USAGE :** **dp\_dumptdep** *meshname paramname max\_temperature dp\_index*

Get temperature dependence of named parameter from named mesh up to max\_temperature, at dp\_index - temperature scaling values obtained.

## **dp\_erase**

**USAGE :** **dp\_erase** *dp\_index start\_index length*

From dp\_index array erase a number of points - length - starting at start\_index.

## **dp\_extract**

**USAGE :** **dp\_extract** *dp\_in dp\_out start\_index (length)*

From dp\_in array extract a number of points - length - starting at start\_index, and place them in dp\_out.

## **dp\_fitlorentz**

**USAGE :** **dp\_fitlorentz** *dp\_x dp\_y*

Fit Lorentz peak function to x y data :  $f(x) = y_0 + S \frac{dH}{(4(x-H_0)^2 + dH^2)}$ .

**Script return values:** *S, H0, dH, y0, std\_S, std\_H0, std\_dH, std\_y0*.

## **dp\_fitskyrmion**

**USAGE :** **dp\_fitskyrmion** *dp\_x dp\_y*

Fit skyrmion z component to obtain radius and center position :  $M_z(x) = M_s * \cos(2 * \arctan(\sinh(R/w)/\sinh((x-x_0)/w)))$ .

**Script return values:** *R, x0, Ms, w, std\_R, std\_x0, std\_Ms, std\_w*.

## **dp\_get**

**USAGE** : **dp\_get** *dp\_arr index*

Show value in dp\_arr at given index - the index must be within the dp\_arr size.

**Script return values:** *value*

## **dp\_getampli**

**USAGE** : **dp\_getampli** *dp\_source pointsPeriod*

Obtain maximum amplitude obtained every pointsPeriod points.

**Script return values:** *amplitude*.

## **dp\_getprofile**

**USAGE** : **dp\_getprofile** *start end dp\_index*

Extract profile of physical quantity displayed on screen along the line specified with given start and end cartesian absolute coordinates (m). Place profile in given dp arrays: 4 consecutive dp arrays are used, first for distance along line, the next 3 for physical quantity so allow space for these starting at dp\_index.

## **dp\_linreg**

**USAGE** : **dp\_linreg** *dp\_index\_x dp\_index\_y (dp\_index\_z dp\_index\_out)*

Fit using linear regression to obtain gradient and intercept with their uncertainties. If dp\_index\_z is specified multiple linear regressions are performed on adjacent data points with same z value; output in 5 dp arrays starting at dp\_index\_out as: z g g\_err c c\_err.

**Script return values:** *g g\_err c c\_err*.

## **dp\_load**

**USAGE** : **dp\_load** (*directory\filename* *file\_indexes...* *dp\_indexes...*)

Load data columns from filename into dp arrays. file\_indexes are the column indexes in filename (.txt termination by default), dp\_indexes are used for the dp arrays; count from 0. If directory not specified, the default one is used.

## **dp\_mean**

**USAGE** : **dp\_mean** *dp\_index*

Obtain mean value with standard deviation.

**Script return values:** *mean stdev*.

## **dp\_minmax**

**USAGE** : **dp\_minmax** *dp\_index*

Obtain absolute minimum and maximum values, together with their index position.

**Script return values:** *min\_value min\_index max\_value max\_index*.

## **dp\_mul**

**USAGE** : **dp\_mul** *dp\_source* *value* (*dp\_dest*)

Multiply dp array with value and place it in destination (or at same position if destination not specified).

## **dp\_muldp**

**USAGE** : **dp\_muldp** *dp\_x1* *dp\_x2* *dp\_dest*

Multiply dp arrays : *dp\_dest* = *dp\_x1* \* *dp\_x2*

## **dp\_rarefy**

**USAGE** : **dp\_rarefy** *dp\_in dp\_out (skip = 1)*

Pick elements from *dp\_in* using the *skip* value (1 by default) and set them in *dp\_out*; e.g. with *skip* = 2 every 3rd data point is picked. The default *skip* = 1 picks every other point.

## **dp\_remanence**

**USAGE** : **dp\_remanence** *dp\_index\_x dp\_index\_y*

Obtain remanence from x-y data: find values at zero field in the two possible directions.

**Script return values:** *Mr\_up Mr\_dn*.

## **dp\_removeoffset**

**USAGE** : **dp\_removeoffset** *dp\_index (dp\_index\_out)*

Subtract the first point (the offset) from all the points in *dp\_index*. If *dp\_index\_out* not specified then processed data overwrites *dp\_index*.

## **dp\_replacerepeats**

**USAGE** : **dp\_replacerepeats** *dp\_index (dp\_index\_out)*

Replace repeated points from data in *dp\_index* using linear interpolation: if two adjacent sets of repeated points found, replace repeats between the mid-points of the sets. If *dp\_index\_out* not specified then processed data overwrites *dp\_index*.

## **dp\_save**

**USAGE** : **dp\_save** (*directory*)*filename dp\_indexes...*

Save specified dp arrays in filename (.txt termination by default). If directory not specified, the default one is used. dp\_indexes are used for the dp arrays; count from 0.

## **dp\_sequence**

**USAGE** : **dp\_sequence** *dp\_index start\_value increment points*

Generate a sequence of data points in dp\_index from start\_value using increment.

## **dp\_set**

**USAGE** : **dp\_set** *dp\_arr index value*

Set value in dp\_arr at given index - the index must be within the dp\_arr size.

## **dp\_showsizes**

**USAGE** : **dp\_showsizes** (*dp\_arr*)

List sizes of all non-empty dp arrays, unless a specific dp\_arr index is specified, in which case only show the size of dp\_arr.

**Script return values:** *dp\_arr size if specified*

## **dp\_smooth**

**USAGE** : **dp\_smooth** *dp\_in dp\_out window\_size*

Smooth data in dp\_in using nearest-neighbor averaging with given window size, and place result in dp\_out (must be different).

## **dp\_sub**

**USAGE :** **dp\_sub** *dp\_source value (dp\_dest)*

Subtract value from dp array and place it in destination (or at same position if destination not specified).

## **dp\_subdp**

**USAGE :** **dp\_subdp** *dp\_x1 dp\_x2 dp\_dest*

Subtract dp arrays :  $dp_{dest} = dp_{x1} - dp_{x2}$

## **dp\_topocharge**

**USAGE :** *dp\_topocharge (x y radius)*

Calculate the topological charge for focused mesh (must be ferromagnetic), optionally in the given circle with radius and centered at x y (relative values).  $Q = \text{Integral}(m.(dm/dx \times dm/dy) dx dy) / 4\pi$ .

**Script return values:** Q - the calculated topological charge.

## **dwall**

**USAGE :** **dwall** *longitudinal transverse width position (meshname)*

Create an idealised domain wall (tanh profile for longitudinal component, 1/cosh profile for transverse component) along the x-axis direction in the given mesh (active mesh if name not specified). For longitudinal and transverse specify the components of magnetization as x, -x, y, -y, z, -z, i.e. specify using these string literals. For width and position use metric units.

## **ecellsizes**

**USAGE** : **ecellsizes** *value*

Change cellsize of mesh in focus for electrical conduction (m). The cellsize can be specified as: hx hy hz, or as: hxyz

**Script return values:** *cellsize* - return electrical conduction cellsize of mesh in focus.

## **editdata**

**USAGE** : **editdata** *index dataname (meshname, (rectangle))*

Edit entry in list of output data at given index in list. If applicable specify meshname and rectangle (m) in mesh. If not specified and required, active mesh is used with entire mesh rectangle.

## **editdatasave**

**USAGE** : **editdatasave** *index savetype (savevalue)*

Edit data saving condition in simulation schedule. Use index < 0 to set condition for all stages.

## **editstage**

**USAGE** : **editstage** *index stagetype (meshname)*

Edit stage type from simulation schedule at index number.

## **editstagestop**

**USAGE** : **editstagestop** *index stoptype (stopvalue)*

Edit stage/step stopping condition in simulation schedule. Use index < 0 to set condition for all stages.

## **editstagevalue**

**USAGE** : **editstagevalue** *index value*

Edit stage setting value in simulation schedule. The value type depends on the stage type.

## **electrodes**

**USAGE** : **electrodes**

Show currently configured electrodes.

## **escellsize**

**USAGE** : **escellsize** *value*

Change cellsize for electric super-mesh (m). The cellsize can be specified as: hx hy hz, or as: hxyz

**Script return values:** *cellsize* - return cellsize for electric super-mesh.

## **exchangeCoupledMeshes**

**USAGE :** `exchangecoupledmeshes status (meshname)`

Set/unset direct exchange coupling to neighboring meshes : if neighboring ferromagnetic meshes touch the named mesh (set for focused mesh if meshname not given) then interface magnetic cells are direct exchange coupled to them.

Script return values: status

## **fmscellsize**

**USAGE :** `fmscellsize value`

Change cellsize for ferromagnetic super-mesh (m). The cellsize can be specified as:  
hx hy hz, or as: hxyz

Script return values: `cellsize` - return cellsize for ferromagnetic super-mesh.

## **generate2dgrains**

**USAGE :** `generate2dgrains spacing (seed)`

Generate 2D Voronoi cells in the xy plane at given average spacing. The seed is used for the pseudo-random number generator, 1 by default.

## **generate3dgrains**

**USAGE :** `generate3dgrains spacing (seed)`

Generate 3D Voronoi cells at given average spacing. The seed is used for the pseudo-random number generator, 1 by default.

## **imagecropping**

**USAGE :** *imagecropping left bottom right top*

Set cropping of saved mesh images using normalized left, bottom, right, top values: 0, 0 point is left, bottom of mesh window and 1, 1 is right, top of mesh window.

## **individualshape**

**USAGE :** *individualmaskshape status*

When changing the shape inside a mesh, e.g. through a mask file, set this flag to true so the shape is applied only to the primary displayed physical quantity. If set to false then all relevant physical quantities are shaped.

Script return values: status

## **insulatingside**

**USAGE :** *insulatingside side\_literal status (meshname)*

Set temperature insulation (Neumann boundary condition) for named mesh side (active mesh if not given). side\_literal : x, -x, y, -y, z, -z.

Script return values: *status\_x status\_-x status\_y status\_-y status\_z status\_-z* - insulating sides status for mesh in focus.

## **invertmag**

**USAGE :** *invertmag (meshname)*

Invert magnetization direction. If mesh name not specified, the active mesh is used.

## **isrunning**

**USAGE** : **isrunning**

Checks if the simulation is running and sends state value to the calling script.

**Script return values:** *state* - return simulation running state.

## **iterupdate**

**USAGE** : **iterupdate** *iterations*

Update mesh display every given number of iterations during a simulation.

**Script return values:** *iterations* - return number of iterations for display update.

## **loadmaskfile**

**USAGE** : **loadmaskfile** (*z-depth*) (*directory\filename*)

Apply .png mask file to magnetization in active mesh (i.e. transfer shape from .png file to mesh - white means empty cells). If image is in grayscale then void cells up to given depth top down (*z-depth* > 0) or down up (*z-depth* < 0). If *z-depth* = 0 then void top down up to all z cells.

## **loadovf2mag**

**USAGE** : **loadovf2mag** (*renormalize\_value*) (*directory\filename*)

Load an OOMMF-style OVF 2.0 file containing magnetisation data, into the currently focused mesh (which must be ferromagnetic). The mesh dimensions will be changed using the settings in the OVF file. By default the loaded data will not be renormalized: *renormalize\_value* = 0. If a value is specified for *renormalize\_value*, the loaded data will be renormalized to it (e.g. this would be an Ms value).

## **loadovf2mesh**

**USAGE :** *loadovf2mesh (renormalize\_value) (directory\filename)*

Load an OOMMF-style OVF 2.0 file containing 3-component vector data. This will create a new permalloy ferromagnetic mesh with dimensions and magnetization data obtained from the OVF 2.0 file. By default the loaded data will not be renormalized: renormalize\_value = 0. If a value is specified for renormalize\_value, the loaded data will be renormalized to it (e.g. this would be an Ms value).

## **loadsim**

**USAGE :** **loadsim** *(directory\filename)*

Load simulation with given name.

## **makevideo**

**USAGE :** **makevideo** *(directory\filebase fps quality)*

Make a video from .png files sharing the common filebase name. Make video at given fps and quality (0 to 5 worst to best).

## **manual**

**USAGE :** **manual**

Opens Boris manual for current version.

## **matcurietemperature**

**USAGE** : **matcurietemperature** *curie\_temperature (meshname)*

Set indicative material Curie temperature for ferromagnetic mesh (focused ferromagnetic mesh if meshname not given). This is not used in calculations, but serves as an indicative value - set the actual Tc value with the curietemperature command.

**Script return values:** curie\_temperature - Indicative material Curie temperature for mesh in focus.

## **materialsdatabase**

**USAGE** : **materialsdatabase** (*mdbname*)

Switch materials database in use. This setting is not saved by savesim, so using loadsim doesn't affect this setting; default mdb set on program start.

## **memory**

**USAGE** : **memory**

Show CPU and GPU-addressable memory information (total and free).

## **mesh**

**USAGE** : **mesh**

Display information for all meshes.

## **meshfocus**

**USAGE** : **meshfocus** *meshname*

Change mesh focus to given mesh name.

**Script return values:** *meshname* - return name of mesh in focus.

## **meshfocus2**

**USAGE** : **meshfocus2** *meshname*

Change mesh focus to given mesh name but do not change camera orientation.

**Script return values:** *meshname* - return name of mesh in focus.

## **meshrect**

**USAGE** : **meshrect** *rectangle*

Change rectangle of mesh in focus (m). The rectangle can be specified as: sx sy sz ex ey ez for the start and end points in Cartesian coordinates, or as: ex ey ez with the start point as the origin.

**Script return values:** *rectangle* - return rectangle of mesh in focus.

## **modules**

**USAGE** : **modules**

Show interactive list of available and currently set modules.

## **movingmesh**

**USAGE** : **movingmesh** *status\_or\_meshname*

Set/unset trigger for movingmesh algorithm. If *status\_or\_meshname* = 0 then turn off, if *status\_or\_meshname* = 1 then turn on with trigger set on first ferromagnetic mesh, else *status\_or\_meshname* should specify the mesh name to use as trigger.

## **movingmeshasym**

**USAGE** : **movingmeshasym** *status*

Change symmetry type for moving mesh algorithm: 1 for antisymmetric (domain walls), 0 for symmetric (skyrmions).

**Script return values:** *status*

## **movingmeshthresh**

**USAGE** : **movingmeshthresh** *value*

Set threshold used to trigger a mesh shift for moving mesh algorithm - normalised value between 0 and 1.

**Script return values:** *threshold*

## **multiconvolution**

**USAGE** : **multiconvolution** *status*

Switch between multi-layered convolution (true) and supermesh convolution (false).

## **ncommon**

**USAGE** : **ncommon** *sizes*

Switch to multi-layered convolution and force it to user-defined discretisation, specifying sizes as nx ny nz.

## **ncommonstatus**

**USAGE** : **ncommonstatus** *status*

Switch to multi-layered convolution and force it to user-defined discretisation (status = true), or default discretisation (status = false).

## **neelpreparemovingmesh**

**USAGE** : **neelpreparemovingmesh** (*meshname*)

Setup the named mesh (or active mesh) for moving Neel domain wall simulations: 1) set movingmesh trigger, 2) set domain wall structure, 3) set dipoles left and right to remove end magnetic charges, 4) enable strayfield module.

## **ode**

**USAGE** : **ode**

Show interactive list of available and currently set ODEs and evaluation methods.

## **params**

**USAGE** : **params** (*meshname*)

List all material parameters. If meshname not given use the active mesh.

## **paramstemp**

**USAGE** : **paramstemp** (*meshname*)

List all material parameters temperature dependence. If *meshname* not given use the active mesh.

## **paramsvar**

**USAGE** : **paramsvar** (*meshname*)

List all material parameters spatial variation. If *meshname* not given use the active mesh.

## **pbc**

**USAGE** : *pbc* *meshname* *flag* *images*

Set periodic boundary conditions for magnetization in given mesh (must be ferromagnetic). Flags specify types of perodic boundary conditions: x, y, or z; images specify the number of mesh images to use either side for the given direction when calculating the demagnetising kernel - a value of zero disables pbc. e.g. *pbc* x 10 sets x periodic boundary conditions with 10 images either side for the focused mesh; *pbc* x 0 clears pbc for the x axis.

## **preparemovingmesh**

**USAGE** : **preparemovingmesh** (*meshname*)

Setup the named mesh (or active mesh) for moving transverse (or vortex) domain wall simulations: 1) set movingmesh trigger, 2) set domain wall structure, 3) set dipoles left and right to remove end magnetic charges, 4) enable strayfield module.

## **random**

**USAGE :** *random (meshname)*

Set random magnetisation distribution in mesh. If mesh name not specified, set for focused mesh.

## **refineroughness**

**USAGE :** **refineroughness** *value (meshname)*

Set roughness refinement cellsize divider in given mesh, i.e. cellsize used for roughness initialization is the ferromagnetic cellsize divided by value (3 components, so divide component by component).

**Script return values:** *value* - roughness refinement.

## **refreshmdb**

**USAGE :** **refreshmdb**

Reload the local materials database (see `materialsdatabase` for current selection). This is useful if you modify the values in the materials database file externally.

## **refreshscreen**

**USAGE :** **refreshscreen**

Refreshes entire screen.

## **renamemesh**

**USAGE :** **renamemesh** (*old\_name*) *new\_name*

Rename mesh. If *old\_name* not specified then the mesh in focus is renamed.

## **requestmdbsync**

**USAGE :** **requestmdbsync** *materialname (email)*

Request the given entry in the local materials database is added to the online shared materials database. This must be a completed entry - see manual for instructions. The entry will be checked before being made available to all users through the online materials database. If you want to receive an update about the status of this request include an email address.

## **reset**

**USAGE :** **reset**

Reset simulation state to the starting state.

## **resetmesh**

**USAGE :** **resetmesh** *(meshname)*

Reset to constant magnetization in given mesh (active mesh if name not given).

## **robinalpha**

**USAGE :** **robinalpha** *robin\_alpha (meshname)*

Set alpha coefficient (all meshes if meshname not given) for Robin boundary conditions : flux normal = alpha \* (T\_boundary - T\_ambient).

**Script return values:** *robin\_alpha* - Robin alpha value for mesh in focus.

## **roughenmesh**

**USAGE** : **roughenmesh** *depth (axis, (seed))*

Roughen active mesh to given depth (m) along a named axis (use axis = x, y, or z as literal, z by default). The seed is used for the pseudo-random number generator, 1 by default.

## **run**

**USAGE** : **run**

Run simulation from current state.

## **savecomment**

**USAGE** : **savecomment** (*directory\filename comment*)

Save comment in given file by appending to it.

## **savedatafile**

**USAGE** : **savedatafile** (*directory\filename*)

Change output data file (and working directory if specified).

Script return values: *filename*

## **savedataflag**

**USAGE** : **savedataflag** *status*

Set data saving flag status.

Script return values: *status*

## **saveimagefile**

**USAGE** : **saveimagefile** (*directory\filename*)

Change image file base (and working directory if specified).

**Script return values:** *filename*

## **saveimageflag**

**USAGE** : **saveimageflag** *status*

Set image saving flag status.

**Script return values:** *status*

## **savemeshimage**

**USAGE** : **savemeshimage** ((*directory\filename*)

Save currently displayed mesh image to given file (as .png). If directory not specified then default directory is used. If filename not specified then default image save file name is used.

## **savesim**

**USAGE** : **savesim** (*directory\filename*)

Save simulation with given name. If no name given, the last saved/loaded file name will be used.

## **scalemeshrects**

**USAGE** : **scalemeshrects** *status*

When changing a mesh rectangle scale and shift all other mesh rectangles in proportion if status set.

**Script return values:** *status*

## **setangle**

**USAGE** : **setangle** *polar azimuthal (meshname)*

Set magnetization angle in mesh uniformly using polar coordinates. If mesh name not specified, this is set for all ferromagnetic meshes.

## **setcurrent**

**USAGE** : **setcurrent** *current*

Set a constant current source with given value. The potential will be adjusted to keep this constant current.

**Script return values:** *current*

## **setdefaultelectrodes**

**USAGE** : **setdefaultelectrodes**

Set electrodes at the x-axis ends of the given mesh, both set at 0V. Set the left-side electrode as the ground. Delete all other electrodes.

## **setdisplayedparamsvar**

**USAGE** : **setdisplayedparamsvar** *meshname paramname*

Set param to display for given mesh when ParamVar display is enabled (to show spatial variation if any).

## **setdt**

**USAGE** : **setdt** *value*

Set differential equation time-step (only applicable to fixed time-step methods).

**Script return values:** *dT*

## **setelectrodepotential**

**USAGE** : **setelectrodepotential** *electrode\_index potential*

Set potential on electrode with given index.

**Script return values:** *potential*

## **setelectroderect**

**USAGE** : **setelectroderect** *electrode\_index electrode\_rect*

Edit rectangle (m) for electrode with given index.

## **setfield**

**USAGE** : **setfield** *magnitude polar azimuthal (meshname)*

Set uniform magnetic field (A/m) using polar coordinates. If mesh name not specified, this is set for all ferromagnetic meshes - must have Zeeman module added.

**Script return values:** <*Ha\_x, Ha\_y, Ha\_z*> - applied field in Cartesian coordinates for mesh in focus.

## **setfixedsor**

**USAGE** : **setfixedsor** *status*

Set damping type for SOR algorithm (adaptive or fixed) used for transport solver Poisson equations.

**Script return values:** *status*

## **setheatdt**

**USAGE** : **setheatdt** *value*

Set heat equation solver time step.

**Script return values:** *value* - heat equation time step.

## **setmaterial**

**USAGE** : **setmaterial** *name*

Copy material parameter values to the focused mesh, from the materials database entry with given name (see materialsdatabase command). This works even if there is a mismatch between the material types.

## **setode**

**USAGE** : **setode** *equation evaluation*

Set differential equation to solve, and method used to solve it.

## **setparam**

**USAGE** : **setparam** (*meshname*) *paramname value*

Set the named parameter to given value. If meshname not given use the active mesh.

**Script return values:** *value* - return value of named parameter for the mesh in focus only.

## **setparamtemp**

**USAGE** : **setparamtemp** *meshname paramname formulaname (coefficients...)*

Set the named parameter temperature dependence formula for the named mesh (including any required coefficients for the formula - if not given default values are used).

## **setparamtemparray**

**USAGE** : **setparamtemparray** *paramname [filename / dp\_arr\_T dp\_arr\_c]*

Set the named parameter temperature dependence using an array. This must contain temperature values and scaling coefficients. Load directly from a file (tab spaced) or internal dp arrays.

## **setparamvar**

**USAGE** : **setparamvar** *meshname paramname generatormame (arguments...)*

Set the named parameter spatial dependence for the named mesh using the given generator (including any required arguments for the generator - if not given default values are used).

## **setpotential**

**USAGE** : **setpotential** *potential*

Set a symmetric potential drop : -potential/2 for ground electrode, +potential/2 on all other electrodes.

**Script return values:** *potential*

## **setrect**

**USAGE** : **setrect** *polar azimuthal rectangle (meshname)*

Set magnetization angle in given rectangle of mesh (relative coordinates) uniformly using polar coordinates. If mesh name not specified, the active mesh is used.

## **setsordamping**

**USAGE** : **setsordamping** *damping\_v damping\_s*

Set fixed damping values for SOR algorithm used to solve the Poisson equation for V (electrical potential) and S (spin accumulation) respectively.

**Script return values:** *damping\_v damping\_s*

## **showdata**

**USAGE** : **showdata** *dataname (meshname, (rectangle))*

Show value(s) for dataname. If applicable specify meshname and rectangle (m) in mesh. If not specified and required, active mesh is used with entire mesh rectangle.

**Script return values:** varies

## **showlengths**

**USAGE** : *showlengths*

Calculate a number of critical lengths for the focused mesh (must be ferromagnetic) to inform magnetisation cellsize selection.  $l_{ex} = \sqrt{2 A / \mu_0 M_s^2}$  : exchange length,  $l_{Bloch} = \sqrt{A / K_1}$  : Bloch wall width,  $l_{sky} = \pi D / 4 K_1$  : Neel skyrmion wall width.

## **showmcells**

**USAGE** : *showmcells*

Show number of discretisation cells for magnetisation for focused mesh (must be ferromagnetic).

**Script return values:** *n*

## **skyrmion**

**USAGE** : **skyrmion** *core chirality diameter position (meshname)*

. Create an idealised Neel-type skyrmion with given diameter and centre position in the x-y plane (2 relative coordinates needed only) of the given mesh (active mesh if name not specified). Core specifies the skyrmion core direction: -1 for down, 1 for up. Chirality specifies the radial direction rotation: 1 for towards core, -1 away from core. For diameter and position use metric units.

## **skyrmionbloch**

**USAGE** : **skyrmionbloch** *core chirality diameter position (meshname)*

. Create an idealised Bloch-type skyrmion with given diameter and centre position in the x-y plane (2 relative coordinates needed only) of the given mesh (active mesh if name not specified). Core specifies the skyrmion core direction: -1 for down, 1 for up. Chirality specifies the radial direction rotation: 1 for clockwise, -1 for anti-clockwise. For diameter and position use metric units.

## **skyrmionpreparemovingmesh**

**USAGE** : **skyrmionpreparemovingmesh** (*meshname*)

Setup the named mesh (or active mesh) for moving skyrmion simulations: 1) set movingmesh trigger, 2) set domain wall structure, 3) set dipoles left and right to remove end magnetic charges, 4) enable strayfield module.

## **ssolverconfig**

**USAGE** : **ssolverconfig** *s\_convergence\_error (s\_iters\_timeout)*

Set spin-transport solver convergence error and iterations for timeout (if given, else use default).

**Script return values:** *s\_convergence\_error s\_iters\_timeout*

## **stages**

**USAGE** : **stages**

Shows list of currently set simulation stages and available stage types.

**Script return values:** number of set stages

## **statictransportsolver**

**USAGE :** *statictransportsolver status*

If static transport solver is set, the transport solver is only iterated at the end of a stage or step. You should set a high iterations timeout if using this mode.

Script return values: status

## **stop**

**USAGE :** **stop**

Stop simulation without resetting it.

## **surfroughenjagged**

**USAGE :** **surfroughenjagged** *depth spacing (seed, (sides))*

Roughen active mesh surfaces using a jagged pattern to given depth (m) and peak spacing (m). Roughen both sides by default, unless sides is specified as -z or z (string literal). The seed is used for the pseudo-random number generator, 1 by default.

## **tcellsize**

**USAGE :** **tcellsize** *value*

Change cellsize of mesh in focus for thermal conduction (m). The cellsize can be specified as: hx hy hz, or as: hxyz

Script return values: *cellsize* - return thermal conduction cellsize of mesh in focus.

## **temperature**

**USAGE** : **temperature** *value (meshname)*

Set mesh base temperature (all meshes if meshname not given) and reset temperature. Also set ambient temperature if Heat module added. If the base temperature setting has a spatial dependence specified through cT, this command will take it into account but only if the Heat module is added. If you want the temperature to remain fixed you can still have the Heat module enabled but disable the heat equation by setting the heat dT to zero (**setheatdt** 0).

**Script return values:** *value* - temperature value for mesh in focus.

## **tsolverconfig**

**USAGE** : **tsolverconfig** *convergence\_error (iters\_timeout)*

Set transport solver convergence error and iterations for timeout (if given, else use default).

**Script return values:** *convergence\_error iters\_timeout*

## **updatemdb**

**USAGE** : **updatemdb**

Switch to, and update the local materials database from the online shared materials database.

## **updatescreen**

**USAGE** : **updatescreen**

Updates all displayed values on screen and also refreshes.

**vecrep**

**USAGE :** *vecrep meshname vecreptype*

Set representation type for vectorial quantities in named mesh (or supermesh).  
vecreptype = 0 (full), vecreptype = 1 (x component), vecreptype = 2 (y component),  
vecreptype = 3 (z component), vecreptype = 4 (direction only).

## **Selected Publications using Boris**

1. S. Lepadatu, "Efficient computation of demagnetizing fields for magnetic multilayers using multi-layered convolution" *Journal of Applied Physics* **126**, 103903 (2019)
2. M. Belusky, S. Lepadatu, J. Naylor, M.M. Vopson, "Study of roughness effect in Fe and Co thin films prepared by plasma magnetron sputtering" *Physica B* **574**, 411666 (2019)
3. S. Lepadatu, "Effect of inter-layer spin diffusion on skyrmion motion in magnetic multilayers" *Scientific Reports* **9**, 9592 (2019)
4. M. Belusky, S. Lepadatu, J. Naylor, M.M. Vopson, "Evidence of substrate roughness surface induced magnetic anisotropy in Ni<sub>80</sub>Fe<sub>20</sub> flexible thin films" *J. Magn. Magn. Mater.* **478**, 77 (2019)
5. S. Lepadatu, "Unified treatment of spin torques using a coupled magnetization dynamics and three-dimensional spin current solver" *Scientific Reports* **7**, 12937 (2017)
6. M.M. Vopson, J. Naylor, T. Saengow, E.G.Rogers, S. Lepadatu, Y.K. Fetisov, "Development of flexible Ni<sub>80</sub>Fe<sub>20</sub> magnetic nano-thin films" *Physica B* **525**, 12 (2017)
7. S. Lepadatu, M.M. Vopson, "Heat assisted multiferroic solid-state memory" *Materials* **10**, 991 (2017)
8. S. Lepadatu, H. Saarikoski, R. Beacham, M.J.B. Romero, T.A. Moore, G. Burnell, S. Sugimoto, D. Yesudas, M.C. Wheeler, J. Miguel, S.S. Dhesi, D. McGrouther, S. McVitie, G. Tatara, and C.H. Marrows, "Very low critical current density for motion of coupled domain walls in synthetic ferrimagnet nanowires" *Scientific Reports* **7**, 1640 (2017)
9. S. Lepadatu, "Interaction of Magnetization and Heat Dynamics for Pulsed Domain Wall Movement with Joule Heating" *Journal of Applied Physics* **120**, 163908 (2016)

10. S. Lepadatu, "Effective field model of roughness in magnetic nano-structures"  
Journal of Applied Physics **118**, 243908 (2015)
11. M.M. Vopson, S. Lepadatu, "Solving the electrical control of magnetic coercive field paradox" Appl. Phys. Lett. **105**, 122901 (2014)