

REPORT ON OpenDreamKit DELIVERABLE D2.13**Micromagnetic VRE completed and online**

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1. INTRODUCTION

The primary focus of the OpenDreamKit project is to improve e-infrastructure for research in mathematics and to provide a Jupyter project based virtual research environment. However, significant parts of these investments are of applicability to a much wider range of activities outside mathematics research.

With this deliverable we want to demonstrate the power of the (improved) Jupyter-based virtual research environment with application in the computational magnetism research domain, as a representative of the growing field of computational science and engineering.

♠TO DO: *Describe the content of the report: In section ... we ... in section ... we ...; detail a bit the description of the “implementation” section; in particular mention that best practices and sustainability are discussed.♠*

2. INTRODUCTION TO COMPUTATIONAL MICROMAGNETICS

2.1. Computational Magnetism

Magnetism underpins modern life through a number of technologies, including magnetic data storage (disk and tape, used widely in the service sector, Google, Netflix, Amazon, etc), magnetic sensors (for example to monitor steering wheel positions or rotational velocity of tires), magnetic resonance imaging in the medical sector, and permanent magnets in electric cars.

Research in this field is increasingly enabled and underpinned by computational approaches: often the appropriate equations (here time dependent partial integro-differential equations) are known but analytically impossible to solve. By discretising space and time (for example using finite differences or finite elements), problems can be computed for a particular set of initial conditions and boundary conditions.

In the following, we focus on magnetism at the nanoscale - this is technically known as micromagnetism - which is technologically relevant for data storage, sensors, and potential new storage and computing paradigms.

2.2. Object Oriented MicroMagnetic Framework (OOMMF)

The Object Oriented MicroMagnetic Framework (OOMMF) [1] is a micromagnetic simulation tool, for which development started during the 1990s at the National Institute of Science and Technology (NIST) by Michael Donahue and Don Porter. It is probably the most widely used and most trusted simulation tool in the micromagnetic scientific community, and still maintained and further developed. It was written in C++ and wrapped with Tcl, which is the language that must be used to configure simulations by the user.

2.3. Typical workflow

♠TO DO: *Original workflow?♠*

♠TO DO: *a bit of mix between past and present tense♠*

The computational workflow that had to be done by the user in order to simulate a particular micromagnetic problem was as follows:

- (1) A configuration script (`.mif`) file is written in Tcl, so that all characteristics of the micromagnetic system are specified (geometry, Hamiltonian, dynamics equation, initial configuration of magnetisation field, boundary conditions, etc.).
- (2) OOMMF is run by providing a configuration `.mif` file via Terminal/Command Prompt.
After the OOMMF run is complete, the spatially resolved vector fields are saved as `.omf` files for many time steps and scalar data is saved in an `.odt` file.
- (3) If another run with different parameters is necessary steps 1 and 2 are repeated.
- (4) Resulting files are opened and analysed by the user either using OOMMF and its GUI-driven tools or command line driven tools or different data analysis tools; typically by manually carrying out sequences of analysis steps.

We want to address several issues that are related to this particular type of workflow (which is found widely in computational science):

- It is difficult for an average user to automate the process of running many different simulations with different parameters.
- It is difficult to keep a log of all steps performed in the entire micromagnetic study.
- Postprocessing and the analysis of results is performed outside OOMMF using techniques and scripts developed by the user, or done manually.

All these issues compromise the reproducibility of the micromagnetic study because it is very difficult to convey the exact simulation procedure. They also reduce the effectiveness of the research: experts in - for example - materials science and physics have to spend time to execute computational commands repeatedly while changing parameters in input files, then search for output files, and extract the new results for the new parameter, etc.

2.4. Workflow with Jupyter notebook embedded computational research environment

TO DO: shorter title?

The main goal of this deliverable was to develop a Micromagnetic Virtual Research Environment (VRE) which would address this problem. More precisely, the goal was to develop a Python interface to OOMMF and integrate it into Jupyter notebook.

Benefits of this approach include:

- One document describes the whole study: Jupyter notebooks can contain (i) simulation and data analysis code, (ii) code output, such as numerical and visualised data, and (iii) human-readable text; see figure 1 on page 5 for an example.
- Improved reproducibility: all the necessary information required to make the study reproducible are contained in a single document which can be later shared, modified, and re-executed.
- Embedding the domain specific language (here scripting of computational micromagnetics) into Python provides a general purpose computing environment without having to invest new configuration file syntax and parses: For example, running different simulations with different parameters can be achieved by simple looping over the parameter space, which does not require the assistance from the user in terms of modifying and running individual .mif configuration files; ; see figure 2 on page 6 for an example.
- The use of the Python language allows use of Python's scientific stack for data analysis and visualisation, such as numpy, scipy, matplotlib, and pandas. This way, it is not necessary for the user to "reinvent the wheel" by writing scripts for opening .odt and .omf files as well as for performing basic data analysis and visualisation operations. Figure 3 on page 7 shows an example making use of the pandas DataFrame object.
- By integrating micromagnetic simulations in the Jupyter notebook, this makes simulations readily available to be run in the cloud via Binder.

The Micromagnetic VRE serves as a demonstrator of the fact that the open source software developed as a part of the OpenDreamKit project is not only for mathematics, but also has impact on other fields of science. In addition to the development of the Python interface to OOMMF and its integration into Jupyter notebook, our goal was also to disseminate and teach the scientists to use Ubermag as well as to collect the evaluation data from the users.

3. IMPLEMENTATION DETAILS

The resulting package is called Ubermag and it is separated into several different sub-packages:

- `discretisedfield` [3] - reading, writing, analysis, and visualisation of scalar and vector fields. This package provides all the necessary functionality for reading resulting OOMMF vector and scalar field files and their analysis, such as sampling, iterating,

5. Tutorial 04: Dzyaloshinskii-Moriya energy term

Interactive online tutorial: [launch binder](#)

Dzyaloshinskii-Moriya energy density, depending on the crystallographic class, is computed as

$$\mathbf{w}_{\text{dmi}} = \begin{cases} D\mathbf{m} \cdot (\nabla \times \mathbf{m}), & \text{for } T(O) \\ D(\mathbf{m} \cdot \nabla m_z - m_z \nabla \cdot \mathbf{m}), & \text{for } C_{nv} \\ D\mathbf{m} \cdot \left(\frac{\partial \mathbf{m}}{\partial x} \times \hat{x} - \frac{\partial \mathbf{m}}{\partial y} \times \hat{y} \right), & \text{for } D_{2d} \end{cases}$$

where \mathbf{m} is the normalised ($|\mathbf{m}| = 1$) magnetisation, and D is the DM energy constant. DMI energy term tends to align neighbouring magnetic moments perpendicular to each other.

In `oommf`, \mathbf{m} is a part of the magnetisation field `system.m`. Therefore, only DMI energy constant D should be provided as an input parameter to uniquely define the Exchange energy term. D can be constant in space or spatially varying.

5.1. Spatially constant D

Let us start by assembling a simple simulation where D does not vary in space. The sample is a “one-dimensional” chain of magnetic moments. We are going to choose C_{nv} as the crystallographic class.

```
[1]: import oommfc as oc
p1 = (-10e-9, 0, 0)
p2 = (10e-9, 1e-9, 1e-9)
cell = (1e-9, 1e-9, 1e-9)
mesh = oc.Mesh(p1=p1, p2=p2, cell=cell)
```

FIGURE 1. Figure showing the beginning of one of the micromagnetic notebook tutorials provided with Ubermag. At the top, there is the Binder badge which allows to execute this example interactively in the cloud. Below, markdown with integrated LaTeX equations is used to explain a particular type of nearest neighbour interaction that has recently received lots of attention. What follows in the notebook (not shown) is a physics simulation example that makes use of this interaction).

8.2.2. Energy crossing

Now, we can plot the energies of both vortex and flower states as a function of cube edge length. This will give us an idea where the state transition occurs.

```
[6]: L_array = np.linspace(8, 9, 5) # values of L for which the system is relaxed.

vortex_energies = []
flower_energies = []

for L in L_array:
    vortex = minimise_system_energy(L, m_init_vortex)
    flower = minimise_system_energy(L, m_init_flower)

    vortex_energies.append(vortex.total_energy())
    flower_energies.append(flower.total_energy())

# Plot the energy dependences.
import matplotlib.pyplot as plt
plt.plot(L_array, vortex_energies, 'o-', label='vortex')
plt.plot(L_array, flower_energies, 'o-', label='flower')
plt.xlabel('L (lex)')
plt.ylabel('E')
plt.xlim([8.0, 9.0])
plt.grid()
plt.legend()
```

L= 8.0, m_init_vortex 2019/08/25 21:52: Running OOMMF (stdprob3.mif) ... (3.8 s)
L= 8.0, m_init_flower 2019/08/25 21:52: Running OOMMF (stdprob3.mif) ... (2.1 s)
L= 8.25, m_init_vortex 2019/08/25 21:53: Running OOMMF (stdprob3.mif) ... (3.4 s)
L= 8.25, m_init_flower 2019/08/25 21:53: Running OOMMF (stdprob3.mif) ... (2.0 s)
L= 8.5, m_init_vortex 2019/08/25 21:53: Running OOMMF (stdprob3.mif) ... (2.9 s)
L= 8.5, m_init_flower 2019/08/25 21:53: Running OOMMF (stdprob3.mif) ... (2.2 s)
L= 8.75, m_init_vortex 2019/08/25 21:53: Running OOMMF (stdprob3.mif) ... (2.9 s)
L= 8.75, m_init_flower 2019/08/25 21:53: Running OOMMF (stdprob3.mif) ... (2.1 s)
L= 9.0, m_init_vortex 2019/08/25 21:53: Running OOMMF (stdprob3.mif) ... (3.0 s)
L= 9.0, m_init_flower 2019/08/25 21:53: Running OOMMF (stdprob3.mif) ... (2.6 s)

[6]: <matplotlib.legend.Legend at 0x1179c3110>

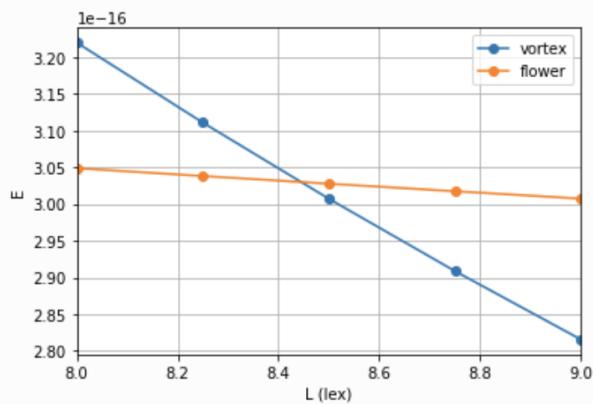


FIGURE 2. Figure showing a small part of one of the micromagnetic notebook tutorials provided with Ubermag. In this example recipe, we solve the well established micromagnetic standard problem 3. The integration of Ubermag commands with Python (i.e. the embedding of the micromagnetic domain specific language in Python [2]) allows to vary parameters (such as the parameter `L` in this example) through Python language constructs (such as a for loop), where previously these would have been done through bash scripting, and subsequent modification of OOMMF configuration files.

Finally, we can run the simulation using `TimeDriver` this time. We run the magnetisation evolution for $t = 1$ ns, during which we save the system's state $n = 200$ times.

```
[14]: t = 1e-9 # simulation time (s)
n = 200 # number of data saving steps

td = oc.TimeDriver() # create time driver
td.drive(system, t=t, n=n) # drive the system
```

2019/08/25 21:55: Running OOMMF (stdprob4.mif) ... (5.6 s)

9.4.1. Postprocessing

When we drove the system using the `TimeDriver`, we specified that we want to save the magnetisation configuration $n = 200$ times. A detailed table of all computed parameters from the last simulation can be shown from the datatable (`system.dt`), which is a `pandas` dataframe [2].

For instance, if we want to show the last 10 rows in the table, we run:

```
[15]: system.dt.tail()
```

ig	E_zeehan	iteration	stage_iteration	stage	mx	my	mz	last_time_step	t
-9	-3.624844e-18	784.0	3.0	195.0	-0.984260	-0.010971	0.033987	1.380208e-12	9.800000e-10
-9	-3.656275e-18	788.0	3.0	196.0	-0.987086	0.021592	0.039286	1.380055e-12	9.850000e-10
-9	-3.683357e-18	792.0	3.0	197.0	-0.988092	0.057824	0.042604	1.379650e-12	9.900000e-10
-9	-3.703732e-18	796.0	3.0	198.0	-0.986964	0.095870	0.043794	1.379032e-12	9.950000e-10
-9	-3.716389e-18	800.0	3.0	199.0	-0.983765	0.133793	0.042832	1.378201e-12	1.000000e-09

Finally, we want to plot the average magnetisation configuration `my` as a function of time `t`:

```
[16]: myplot = system.dt.plot('t', 'my')
```

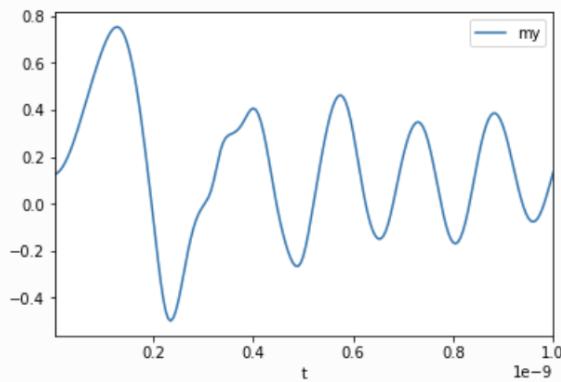


FIGURE 3. Figure showing part of the micromagnetic notebook tutorial for the micromagnetic standard problem 4: data that OOMMF is exporting into a tab-separated text file is automatically retrieved and made available in form of a pandas DataFrame. The creation of the plot (here plotting the column with data for time t against the column with the y-component of the magnetisation m_y) is a function of the DataFrame object.

computing averages and norms, and visualisation. For visualisation, we use two different approaches: (i) 2D visualisation of spacial slices of using `matplotlib` and (ii) 3D visualisation of both scalar and vector fields using `k3d`, which was developed as a part of OpenDreamKit as deliverable D4.12. The main benefit of this package is that all fields, after being created or read from files, are represented via `numpy` arrays, which enables exposing micromagnetic fields obtained from OOMMF to the Python scientific stack.

- `ubermagtable` [4] - reading and analysis of scalar table data. The main purpose of this package is to enable easy reading and analysis of OOMMF `.odt` files. This is achieved by converting the contents of an `.odt` file, created by OOMMF, to a `pandas DataFrame` object. Similar to exposing scalar and vector field data to Python's scientific stack in `discretisedfield`, in `ubermagtable`, this is achieved via `pandas DataFrame`, which enables easy analysis and visualisation of the table data, by exploiting the already existing infrastructure.
- `ubermagutil` [5] - typesystem used across all Ubermag packages. This package contains the implementation of different Python descriptors used for imposing a typesystem for individual attributes in different classes.
- `micromagneticmodel` [6] - a domain specific language (DSL) for defining a micromagnetic simulation. Details about this package are explained in Sec. 3.1.
- `oommf` [7] - OOMMF calculator. After the micromagnetic simulation is defined using `micromagneticmodel`, `oommf` translates the model into OOMMF simulation and runs it. Finally, all resulting simulation files are read by employing `discretisedfield` and `ubermagtable`. Details about this package are explained in Sec. 3.2.
- `micromagneticdata` [8] - data analysis convenience tools. This package contains code for the analysis of simulation results integrated in Jupyter notebook.

We decided to split the entire functionality of Ubermag into separate smaller packages in order to allow users to use them individually. For instance, `discretisedfield` package is a universal package - not restricted to micromagnetics - and can be used for any finite-difference field, such as in computational fluid dynamics.

3.1. `micromagneticmodel`

The motivation for the development of the domain specific language (DSL) for the definition of micromagnetic problems comes from the fact that almost all micromagnetic problems can be defined in a unified way. More precisely, in order to uniquely define a micromagnetic problem, three main components must be defined:

- (1) **Initial magnetisation.** Magnetisation is a vector field defined on a finite-difference mesh, so that one vector is associated to each discretisation cell.
- (2) **Hamiltonian.** Depending on what energies are present in the simulated sample, the Hamiltonian can contain different energy terms. More precisely, the total energy of the system can be computed as a sum of different energy terms computed for the particular magnetisation configuration.
- (3) **Dynamics equation.** This equation governs the magnetisation dynamics and, similar to Hamiltonian, it can contain different dynamics terms.

Because there is a uniform way how a micromagnetic problem can be defined, we developed a domain specific language for defining such problems. A model, defined using this domain specific language, is not aware of the particular simulation tool that is going to perform the actual micromagnetic simulation, but it is only used to describe the problem.

3.2. `oommf`

The `micromagneticmodel` described in the previous section does not contain any information on how the defined micromagnetic problem can be translated into the OOMMF configuration

file and run in OOMMF. `oommfc` inherits all the functionality of `micromagneticmodel` and specifies how all necessary elements of the micromagnetic model can be translated into the OOMMF configuration file. `oommfc` runs the simulation and after it is completed, reads the resulting files and updates the system object.

3.3. Open source code hosting and long term availability

All the code developed as a part of this deliverable is hosted in different repositories on the code hosting service GitHub as a part of the Ubermag organisation. All the code is open source and publicly available. In addition, snapshots of the repositories have been made and all their contents are hosted in Zenodo.

3.4. Automatic tests and continuous integration

All individual packages of Ubermag are tested by running different Python tests. There are three different types of tests:

- Direct testing of the source code. These tests are running individual functionalities of different Ubermag packages as well as larger micromagnetic simulations, such as standard problems. These tests are also used for computing the code coverage - the percentage of the code covered by tests.
- Jupyter notebook tests. The majority of the Ubermag's functionality is documented using Jupyter notebook. In order to make sure that the documentation is up-to-date with the newest version of the source code, they are tested using `nbval`, which was developed as a part of OpenDreamKit deliverable D4.8. More precisely, all individual code cells in a Jupyter notebook are run and their results are compared to the previous ones whenever a change is made in the source code.
- API documentation tests. As a part of different class and function implementation, docstrings were included and later used for the API documentation. These strings usually contain small examples demonstrating the usage of individual features of the code. Similar to the testing of Jupyter notebooks used for documentation, we also test these docstring examples.

All three different types of tests are run on two different continuous integration platforms: Travis CI for Linux and AppVeyor for Windows operating system. These tests are triggered automatically each time a new commit to the repository is made.

The codecov service is employed to record the coverage of the tested code.

Latest continuous integration test results and code coverage links are provided on the Readme page for every package.

3.5. Documentation

Each Ubermag package is individually documented. There are two different types of documentation: (i) API documentation, and (ii) examples of usage in Jupyter notebooks in the form of tutorials and exercises.

API documentation, implemented via docstrings, is generated by Sphinx. It contains the detailed explanation of all possible ways of using different functions and classes as well as small examples.

Jupyter notebooks provide tutorial-like documentation which explains how different functionalities of a package can be used using real-world problems to demonstrate this.

The top level documentation containing the tutorial on Ubermag, is a part of `ubermag` meta-package. All the documentation is generated as soon as a new commit is made to the repository and it is hosted on `readthedocs`. In addition, several different tutorials, in particular for the installation of Ubermag on different platforms, are recorded as videos and hosted on YouTube.

All documentation can also be interactively used via Binder (a link button is provided on every package's Readme file).

3.6. Installation

One of the main challenges scientists face in using simulation tools is their installation. Contributing factors are that (i) research software is generally not written by trained software engineers and (ii) research software may require use of less commonly used libraries which can be research products themselves, with associated behaviours such as quickly changing interfaces, lack of support, lack of robust installation procedures.

Therefore, we wanted to make the installation of Ubermag as simple as possible.

All packages are built and made available for installation on PyPI. However, installing Ubermag using pip is not going to install OOMMF, which is a C++ code. Therefore, users have to install OOMMF themselves and set the environment variable which points to the installation path. Alternatively, Docker can be installed and before the simulations are run, a Docker image will be pulled from Docker cloud, container created, simulations run inside the container, results extracted, and container destroyed. This approach allows the maximum flexibility in terms of the platforms allowed.

Alternatively, Ubermag can be installed via conda on all three major operating systems (Windows, OSX, Linux). This approach installs not only Ubermag, but also OOMMF. Detailed installation instructions are a part of documentation and videos are created and hosted on YouTube.

3.7. Ubermag in the cloud

Apart from installing Ubermag on user's machine, Ubermag can be used in the cloud. We provide this service using MyBinder where Jupyter notebooks can be run on a temporary (container based) machine that is provided in the cloud.

Running Ubermag in the cloud was particularly helpful when we delivered workshops at various international conferences. More precisely, due to the data protection rules, we were not allowed to know the participants' information in advance so that we could contact them and provide them installation instruction they should follow before they arrive to the conference. Therefore, we had to deal with a large number of simultaneous installations on different machines before the workshop. This included downloading large installation files, such as Anaconda and long waiting times for the installation to complete. This can be counteracted by bringing mass storage media with the required files available. Nevertheless, the amount of configuration and fiddling with laptops with unusual behaviour (such as: existing anaconda installation, lack of admin rights, outdated hardware, lack of RAM, lack of diskspace, ...) that was required to enable all participants to actively take part in examples using their own laptop, exceeded our resources.

Therefore, we asked all participants who were not able to install Ubermag before the workshop to use Ubermag in the cloud, where we hosted all materials we intended to cover during the workshop. All they need for this is a web browser on their laptop.

3.8. mumax3

At the beginning of the project, our main focus was to develop a Python interface to OOMMF and integrate it into Jupyter notebook. After we developed a domain specific language in `micromagneticmodel`, we decided to demonstrate its universality for other micromagnetic packages. Therefore, we chose to build another micromagnetic calculator for the mumax3 [9] simulation tool. mumax3 is another finite-difference package that is attracting increasing attention: its main advantage is that it runs on GPU and it is usually much faster than OOMMF. Accordingly, mumax3 is a simulation tool of choice when the simulation speed is an important factor. In order to implement another micromagnetic calculator, based on mumax3, we organised a workshop at European XFEL and invited 5 participants. 3 participants were from the research

group at the University of Southampton, where the OpenDreamKit project was previously hosted before moving to European XFEL. Another 2 participants are the developers of mumax3 from the University of Ghent, Belgium. After a 4-day workshop we managed to implement all the necessary functionality to run micromagnetic standard problems using Ubermag and using mumax3 as the computational backend.

3.9. JOOMMF changes name to become Ubermag

After the implementation of mumax3c, we decided to rename the entire project from JOOMMF to Ubermag. The name “JOOMMF” originated from Jupyter and OOMMF, but the new functionality is more general than that.

This way, Ubermag provides the high level user interface which can currently use two different micromagnetic calculators in the background (i.e. OOMMF and mumax3).

There are some other finite difference packages that could be supported by Ubermag in the future with modest effort.

4. DISSEMINATION

During the project, we conducted several workshops at various international conferences as part of our dissemination activities. At these workshops we introduced the basics of micromagnetics and through examples demonstrated how micromagnetic simulations can be performed using Ubermag. All tutorials were followed by exercises which participants could solve. The workshops we organised are:

(1) DPG March Meeting, 19 March 2017, Dresden, Germany

This meeting is the main annual conference organised by the German Physics Society. We were invited to contribute to the mini-symposium of the conference with the main topic micromagnetics. We had about 50 attendees and we introduced the basics of micromagnetic simulations as well as the basics of running Ubermag. Unfortunately, the conference organisers did not allow us to have the details of participants or to take photos of the event due to the data protection regulations. This dissemination activity was fully funded by the OpenDreamKit grant.

(2) Institute of Physics (IOP) Magnetism conference, 04 April 2017, York, UK.

This workshop was held together with Michael Donahue, NIST, USA, who is the main developer and maintainer of OOMMF. In the first half of the workshop, Michael Donahue introduced to the participants the basics of micromagnetics as well as the main capabilities of the OOMMF simulation tool. In the second half, we introduced a Python interface to OOMMF by guiding the participants through several tutorials and letting them to complete the exercises. We had approximately 30 participants at this workshop. Unfortunately, the conference organisers did not allow us to have the details of participants or to take photos of the event due to the data protection regulations. Therefore, we had to ask the participants if they want to provide us their information personally. This workshop was co-funded with EPSRC CCP Computational Magnetism Network (EP/M022668/1).

(3) Intermag 2017 conference, 24 April 2017, Dublin, Ireland

This workshop was held at one of the major conferences in the field of magnetism research. At the workshop we had 50 registered participants, who had to register at the time of conference registration. The maximum number of allowed participants was determined by the conference organisers. The workshop was divided into two parts: (i) main workshop event and (ii) follow up session. At the main workshop event, we taught the participants the basics of micromagnetics and how they can use Ubermag in their every-day research. In the follow-up session, we talked to the participants of the main workshop event as well as to those who wanted to attend, but who could not

register due to the limited number of spaces. In the follow-up session we were able to discuss the Ubermag capabilities in more detail as well as to answer any specialised questions current or potential users might have. In both sessions we were able to receive some feedback and feature requests from users, as well as addressing their questions. This workshop was co-funded with EPSRC CCP Computational Magnetism Network (EP/M022668/1).

- (4) 62nd Annual Conference on Magnetism and Magnetic Materials, 6-10 Nov 2017, Pittsburgh, PA, USA

Similar to Intermag, this is one of the major conferences in the field of magnetism research. We were not able to organise the workshop jointly with the conference organisers. Therefore, we organised an informal workshop at the conference, comparable to a drop-in or ask-the-expert session. We invited all interested participants to come and see us at the conference using several micromagnetics oriented mailing lists. At the workshop we had both Ubermag users and researchers who could potentially start using Ubermag. We were able to introduce to all interested participants the main capabilities of OOMMF as well as the benefits of using our Python interface and Jupyter integration.

- (5) Advances in Magnetism 2017 conference, 04-07 February 2018, La Thuile, Italy

This event was organised as a tutorial session for all conference attendees by the conference organisers. This was structured as an invited talk. During the 30 min talk we explained the basics of micromagnetics as well as the benefits of Ubermag. In addition, we provided enough information for the participants to start using Ubermag on their own. At this event, we had more than 100 participants.

- (6) International Conference on Magnetism, 14-20 July 2018, San Francisco, USA

This workshop was a part of the official conference programme. Jointly with the conference organisers, we organised a workshop which was offered to all conference participants. No limitation on the number of available places was imposed by the organisers. The conference attendees were offered to register for the workshop at the time of conference registration. Similar to the previous events, we were not allowed to have the details of the participants. At the workshop, we had more than 70 participants. At the workshop we had both Ubermag users and researchers who could potentially start using Ubermag. The workshop was divided into two parts: (i) main workshop event and (ii) follow up session. At the main workshop event, we taught the participants the basics of micromagnetics and how they can use Ubermag in their every-day research. In the follow-up session, we talked to the participants of the main workshop event as well as to those who were not able to attend on the first day of the conference. In the follow-up session we were able to discuss the Ubermag capabilities in more detail as well as to answer any specialised questions current or potential users might have. In Fig. 4 we show the photo taken at the workshop.

- (7) Joint Magnetism and Magnetic Materials - Intermag conference, 14-18 Jan 2019, Washington DC, USA

Similar to other MMM conferences, we could not organise the workshop jointly with the conference organisers. Therefore, we invited all interested participants to come and see us at the conference using several micromagnetics oriented mailing lists. At the workshop we had both Ubermag users and researchers who could potentially start using Ubermag. We were able to introduce to all interested participants the main capabilities of OOMMF as well as the benefits of using our Python interface and Jupyter integration. As before, we received valuable feedback from the participants.

Due to the restrictions imposed by the conference organisers, we were not able to take photos and get personal information from the participants. Therefore, we asked them to voluntarily do our online survey.



FIGURE 4. Computational micromagnetics with JOOMMF workshop at the International Conference on Magnetism, 14-20 July 2018, San Francisco, USA

In addition to the workshops listed above, we have delivered some conference talks on Ubermag (which was called JOOMMF at the time) addressing 3 different audience groups:

- Hans Fangohr: A case study of computational science in Jupyter notebooks: JOOMMF, Computational Mathematics with Jupyter Workshop, Edinburgh (UK), 20 Jan 2017
- Hans Fangohr: User interfaces for computational science: a domain specific language for OOMMF embedded in Python , Magnetism and Magnetic Materials Conference, New Orleans, Louisiana (US), 2 Nov 2016
- Hans Fangohr: Driving Simulation and Data analysis of magnetic nanostructures through Jupyter notebooks. PyCon.DE 2018, Karlsruhe, (Germany), 24 October 2018

A publication on the micromagnetic abstraction of Ubermag is available: Marijan Beg, Ryan A. Pepper, Hans Fangohr. *User interfaces for computational science: a domain specific language for OOMMF embedded in Python*, AIP Advances 7, 056025 (2017), <https://doi.org/10.1063/1.4977225>

5. EVALUATION

We evaluated Ubermag by asking users as well as the participants at different workshops to complete our online survey. Basic conclusions about our users/participants and their previous experiences we got from the survey are:

- The majority of our users/participants are students (56.1%), whereas 43.9% of them are employed. Similarly, the vast majority of them are employed in academia (90.2%) - much more than in industry and government laboratories. The age of our participants is 18-34 (78%) and 35-54 (22%).
- Firstly, we asked both current and potential Ubermag users whether they are active in the field of magnetism research. 92.7% of participants answered they are. However, from another question if they have ever performed a micromagnetic simulation 65.9% of participants answered that they have not. Accordingly, we concluded that the majority of participants at our workshops had no previous experience of running micromagnetic

simulations and they attended our workshops not only to learn a new simulation tool, but to learn general micromagnetic simulation techniques. After we learned this information, we restructured our future workshops and taught users for the first half of the workshop the basics of micromagnetics. In the second half of the workshop we focused on Ubermag.

- For those participants, who have performed micromagnetic simulations before, we asked them what simulation tool they have used. More than two thirds answered that they have used or are actively using OOMMF. This confirmed our initial prediction that OOMMF is the most widely used simulation tool at the moment of the project proposal. In the second place (37.5%) was mumax3, which reflects our decision to demonstrate the universality of our domain based language for the description of micromagnetic problems by adding mumax3 as another computational back-end.
- We wanted to know what computational science tools they have used in the past and how familiar they are with the state-of-the art tools we used to develop our Python interface to OOMMF. The majority (more than two thirds - 68.3%) of users are working on Windows operating system. In the second place was MacOS (31.7%) and Linux (24.4%). These results confirmed our idea of making the installation simple on all three major operating systems by building conda packages. All participants have heard previously about Python and 70.7% of them have used it before. However, 60% of all participants do not have enough experience in using Python and consider themselves to be beginners. Only 12.2% of users think they are advanced users of Python. These findings confirmed several of our observations at the workshops. Although we built a much simpler to use interface to OOMMF and integrated it into Jupyter notebook, for new users learning Ubermag is still a steep learning curve. This is partly because they are new to Python, but mostly due to the fact that they have no prior programming experience.
- In terms of Jupyter notebooks, 63.2% of our participants have heard about the Jupyter notebook, but only 26.8% are actively using it. On the other hand, 36.6% of users have never heard of it.
- The questions regarding the use of more advanced tools in computational science, such as Docker and Anaconda, the vast majority have never heard of it.
- We asked users to give us an overview of what expectation do they have from a new simulation tool they want to employ in their every-day research. In the first place is the ease of use, which confirmed our initial predictions that it is necessary to have a simple, intuitive, and understandable user interface. This was what guided us in the development of Ubermag. Secondly, simple installation was marked as a second most important factor. This, in combination with the computational habits of our users motivated us to make a simple installation procedure based on Anaconda. Last but not least, documentation, visualisation capabilities, and speed were mentioned and some of the factors users consider before they decide to use a micromagnetic simulation tool.

In addition to general questions we asked users about their previous experiences in computational science and micromagnetics, we asked users to give a direct feedback on what they like and do not like about Ubermag. The vast majority of participants answered that they think Ubermag is user friendly and simple to use. Among the things they do not like, they say that documentation was not complete which comes from the fact that most of the workshops were held early on in the project and not all documentation was complete at that point. Secondly, users complained about the installation due to certain limitations they experienced on their machines.

6. ADMINISTRATION

6.1. Move from the University of Southampton to European XFEL

The OpenDreamKit project with principal investigator Hans Fangohr and postdoctoral researcher Marijan Beg moved from the University of Southampton (UK) to European XFEL (Germany) on 1st September 2017. The last day of OpenDreamKit at the University of Southampton was 31st August 2017. The move was initiated by the offer and acceptance of a new position for Hans Fangohr at European XFEL. There were no problems encountered in the relocation process. The facilities at European XFEL are suitable for the completion of OpenDreamKit and the administrative support is provided. Tasks started at Southampton will be continued at European XFEL. There are no parts of OpenDreamKit left at the University of Southampton.

6.2. Sergii Mamedov

In addition to Marijan Beg, who was fully employed on the OpenDreamKit project, between Oct 2.18 and February 2019 Sergii Mamedov was employed. The reported work contains additional contributions from Ryan Pepper and Thomas Kluyver.

7. SUMMARY

Above, we have summarised the creation of the Ubermag micromagnetic simulation environment. Although we know of some publications that make use of Ubermag (at the time it was still called JOOMMF), such as [10], [11] and [12], it is too early to comment on uptake of this technology/tool in the community.

From interactions with users we have seen, however, that the model of directing and coordinating computational science studies from inside the Jupyter Notebook environment is popular with scientists - a key feature is the integration of code (i.e. the detailed and exact description of the computational process) with the outcome in one document. Another import point is that the people doing the technical work can convert the notebook to html or pdf and send it/show it to collaborators and supervisors who can then enjoy the document including its multimedia components within their webbrowser (but importantly without having to install software).

The integration of elements similar to graphical user interfaces (that can be realised with ipywidgets) has also been welcomed and allows blending of command driven and GUI-supported data analysis.

Another item of feedback from interactions with power users and decision makers in computational science projects was that the creation and maintenance of nbdime and nbval was highly welcome and allows to use Notebook-driven projects more effectively.

A technical difficulty we encountered is that some packages (IPywidgets, k3d) do not work reliably for all major browsers for both the classic Jupyter Notebook and the next generation JupyterLab. This is maybe not unexpected given the high rate of change in these community driven projects but affects robustness of tools based on these infrastructures.

♠**TO DO:** mention that this is likely to get better very soon as those packages mature and the transition to JupyterLab happens♠

For completeness, we'd like to mention that during this work, we have become aware of a related initiative[13] that provides an *atomic simulation environment* and provides a high level user interface to a number of atomic simulation tools, similar to the way that Ubermag provides a high level user interface to some micromagnetic tools.

Looking beyond the area of micromagnetism, we can see that the model of virtual research environments based on the Jupyter project and developed and demonstrated here have already affected the provision of data analysis software environments, for example at the European

X-ray Free Electron Laser facility in Germany and its partners in the PaNOSC project¹, which we expect to also feature in (parts of) the European Open Science Cloud user interface and capabilities.

¹Photon And Neutron Open Science Cloud, EC research and innovation programme grant agreement No 823852, <http://panosc.eu>

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