Towards *Unified Micromagnetic Modelling* with Ubermag

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slides at https://s.gwdg.de/7ExWfu

Outline

Introduction

Introduction and Motivation

- Micromagnetic simulations widely used
  - OOMMF > 3500 citations
  - mumax^3 > 2800 citations

- Many *micromagnetic calculators* available, for example: OOMMF, Magpar, Nmag, MicroMagnum, Fidimag, Finmag, mumax^3, Boris, Magnum.np, ...

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Idea Unified Micromagnetic Modelling

- specify micromagnetic problem once
- can choose which micromagnetic calculator to use

Using a micromagnetic simulation

Computational research workflow (Example: OOMMF)

1. Decide what physics problem needs to be solved.
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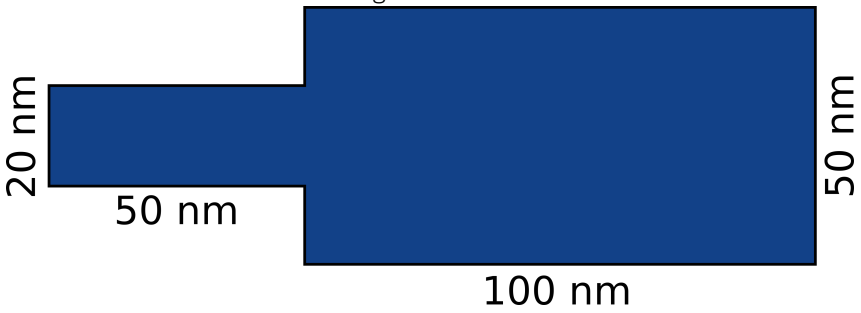
Preview: Ubermag

Ubermag automates steps 2 to 4.

Ubermag

Example: Study domain wall skyrmion conversion (Zhou and Ezawa, 2014)

1nm thick Cobalt on a substrate inducing DMI



Zhou, Y., & Ezawa, M. 2014 Nature Communications 5, 8.
`https://doi.org/10.1038/ncomms5652`

Define the problem: physics model

[2]:
```
system = mm.System(name='dw_pair_conversion')

system.energy = (mm.Exchange(A=15e-12)
                 + mm.DMI(D=3e-3, crystalclass='Cnv_z')
                 + mm.UniaxialAnisotropy(K=0.5e6, u=(0, 0, 1)))

system.energy
```

[2]:
$$-A\mathbf{m}\cdot\nabla^2\mathbf{m} + D(\mathbf{m}\cdot\nabla m_z - m_z\nabla\cdot\mathbf{m}) - K(\mathbf{m}\cdot\mathbf{u})^2$$

[3]:
```
system.dynamics = (
    mm.Precession(gamma0=mm.consts.gamma0)  # gyromagnetic ratio (m/As)
    + mm.Damping(alpha=0.3)  # Gilbert damping
    + mm.ZhangLi(u=400, beta=0.5)  # STT parameter
)

system.dynamics
```

[3]:
$$-\frac{\gamma_0}{1+\alpha^2}\mathbf{m}\times\mathbf{H}_{\text{eff}} - \frac{\gamma_0\alpha}{1+\alpha^2}\mathbf{m}\times(\mathbf{m}\times\mathbf{H}_{\text{eff}}) - \frac{1+\alpha\beta}{1+\alpha^2}\mathbf{m}\times(\mathbf{m}\times(\mathbf{u}\cdot\boldsymbol{\nabla})\mathbf{m}) - \frac{\beta-\alpha}{1+\alpha^2}\mathbf{m}\times(\mathbf{u}\cdot\boldsymbol{\nabla})\mathbf{m}$$

Define the problem: geometry and initial magnetisation

[4]:
```python
Ms = 5.8e5  # saturation magnetisation (A/m)

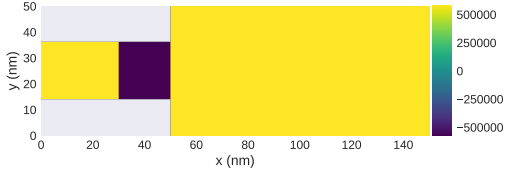
region = df.Region(p1=(0, 0, -50e-9), p2=(150e-9, 50e-9, 0))
mesh = df.Mesh(region=region, cell=(2e-9, 2e-9, 2e-9))

def Ms_fun(pos):  # Sample shape
    x, y, z = pos
    if x < 50e-9 and (y < 15e-9 or y > 35e-9):
        return 0
    else:
        return Ms

def m_init(pos):  # Magnetisation direction
    x, y, z = pos
    if 30e-9 < x < 50e-9:
        return (0.1, 0.1, -1)
    else:
        return (0.1, 0.1, 1)

system.m = df.Field(mesh, nvdim=3, value=m_init, norm=Ms_fun, valid='norm')

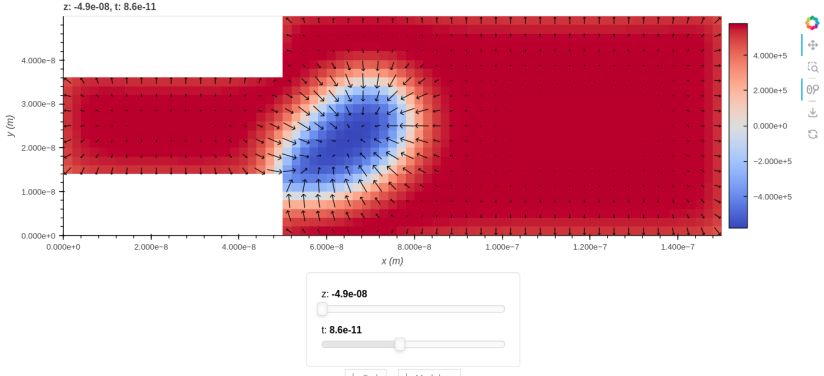
system.m.z.sel('z').mpl.scalar()
```



(Interactive) data analysis

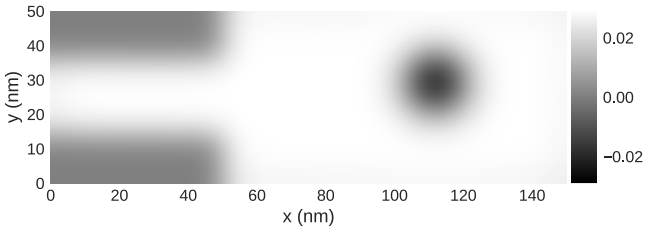
[6]:
```
import micromagneticdata as mdata
data = mdata.Data(system.name)

data[-1].hv(kdims=['x', 'y'],
            vector_kw={'n' : (45, 15)},
            scalar_kw = {'clim':(-Ms, Ms), 'cmap': 'coolwarm'})
```



Simulate experimental signature (mag2exp)

```
[7]: import mag2exp
holo_image = mag2exp.x_ray.holography(system.m, fwhm=(10e-9,10e-9))
holo_image.mpl.scalar(cmap='gray', interpolation='spline16', symmetric_clim=True)
```



→ See poster Samuel Holt et al. for **mag2exp**.

Ubermag overview (very short)

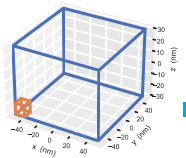
Researcher

$$E = \int_V \left[-A\mathbf{m} \cdot \nabla^2 \mathbf{m} - \mu_0 M_\mathrm{s} \mathbf{m} \cdot \mathbf{H} + w_\mathrm{d} \right] \mathrm{d}V$$

Ubermag

Automated backend

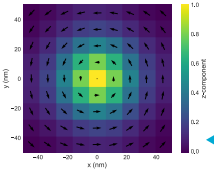
```
In [1]: system = mm.System(name='vortex')
        system.energy = mm.Exchange(A=1e-11) + mm.Demag()
        system.dynamics = (mm.Precession(c.gamma0)
                           + mm.Damping(alpha=0.2))
```




```
In [2]: mesh = df.Mesh(p1=(-50e-9, -50e-9, -30e-9),
                       p2=(50e-9, 50e-9, 30e-9),
                       cell=(10e-9, 10e-9, 10e-9))
        system.m = df.Field(mesh, dim=3, norm=4e5,
                            value=vortex_fun)
```

```
In [3]: md.drive(system)
```

```
In [4]: system.m.orientation.sel('z').mpl()
```



Ubermag design

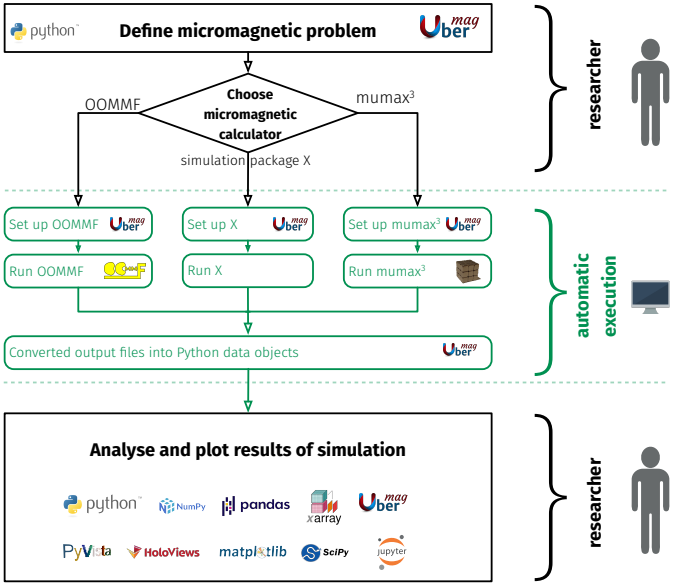
Domain-specific language for *micromagnetic problems*

- express physics problem through Python library `micromagneticmodel`
- cannot *solve* the problem (but is *machine readable*)
- *separates* the problem definition from the (numerical) solving of the problem
  - problem description is independent of simulation package syntax

Beg, Pepper, Fangohr: *User interfaces for computational science: a domain specific language for OOMMF embedded in Python*, DOI 10.1063/1.4977225, eprint pdf (2017)

Unified Micromagnetic Modelling (UMM)

Unified Micromagnetic Modelling (UMM) with Ubermag

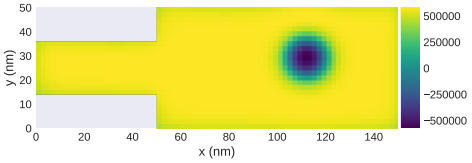


Ubermag can use different calculators (OOMMF and mumax^3)

[5]:
```
import oommfc as mc
md = mc.MinDriver()
md.drive(system)

td = mc.TimeDriver()
td.drive(system, t=0.2e-9, n=200, verbose=2)
system.m.z.sel('z').mpl.scalar()
```

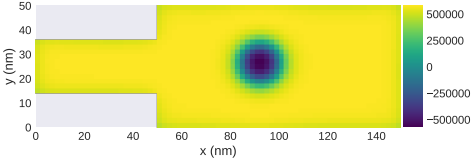
```
Running OOMMF (ExeOOMMFRunner)[2023/08/31 15:33]... (1.5 s)
Running OOMMF (ExeOOMMFRunner)[2023/08/31 15:33] took 25.8 s
```



[5]:
```
import mumax3c as mc
md = mc.MinDriver()
md.drive(system)

td = mc.TimeDriver()
td.drive(system, t=0.2e-9, n=200, verbose=2)
system.m.z.sel('z').mpl.scalar()
```

```
Running mumax3 (ExeMumax3Runner)[2023/09/05 14:59]… (0.7 s)
Running mumax3 (ExeMumax3Runner)[2023/09/05 14:59] took 3.4 s
```



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1. Can *choose* micromagnetic calculator depending on available hardware:
   - NVIDIA GPU $\rightarrow$ mumax^3
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4. Can *extend* micromagnetic calculations in (Python-based) data science environment
5. Scientist does not need to learn the syntax of each micromagnetic calculator

Issues

Design of a unified micromagnetic modelling interface

difficult if the different calculators (e.g. OOMMF and mumax^3) have different features

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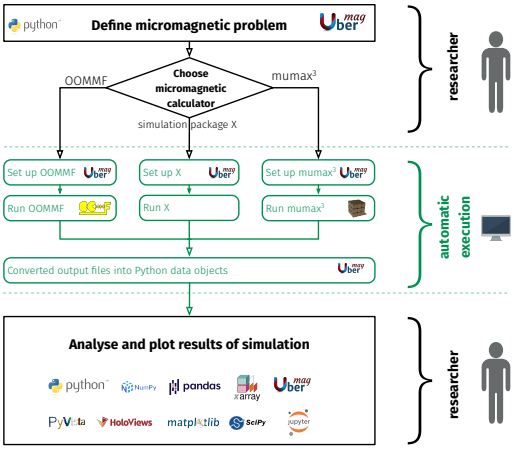
Discovering inconsistencies

ability to easily compare different simulation packages reveals discrepancies: are these important?

Summary

Summary Unified Micromagnetic Modelling (UMM)



1. UMM makes research more efficient

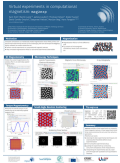
- automate what is possible
- define physics problem once, re-use in all simulation packages

2. Ubermag provides initial implementation for UMM

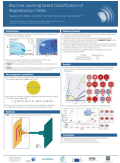
- supports* OOMMF and mumax^3
- contributions are welcome
  https://github.com/ubermag/ubermag

* compatibility overview: `https://ubermag.github.io/documentation/compatibility.html`

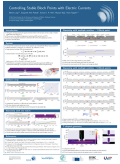
Ubermag applications in poster session



Sam Holt, Simulate experimental measurements with `mag2exp`



Swapneel Pathak, ML-based classification of magnetisation configurations



Martin Lang, Controlling stable Bloch points with electric currents

Open positions

MAgnetic Multiscale MOdelling Suite (MaMMoS)

- project January 2024 to December 2027
- modelling magnetic systems
- contribute to green power generation
- machine learning
- software engineering
- positions to be advertised in the coming months
- please get in touch if interested

Relevant Links

These slides are available at https://s.gwdg.de/7ExWfu

Ubermag software

https://ubermag.github.io/

Marijan Beg, Martin Lang and Hans Fangohr, *Ubermag: Toward More Effective Micromagnetic Workflows*, in IEEE Transactions on Magnetics, vol. 58, no. 2, pp. 1-5, Art no. 7300205, 10.1109/TMAG.2021.3078896 (2022)

Domain specific language for micromagnetic problems

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, 10.1063/1.4977225 (2017)

Acknowledgments

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Contact

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Appendix

Current status for unified micromagnetic modelling in Ubermag

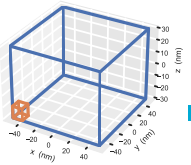
- Ubermag can use OOMMF and mumax^3 as micromagnetic calculator
  - not all features complete, see

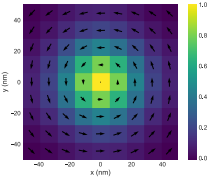
    `https://ubermag.github.io/documentation/compatibility.html`
- Ubermag design is open to include more micromagnetic calculators such as magnum.np, micromagnum, Boris, ...
- finite-difference-based discretisation is supported best

Ubermag overview (very short)

Researcher

$$E = \int_V \left[-A\mathbf{m} \cdot \nabla^2 \mathbf{m} - \mu_0 M_\mathrm{s} \mathbf{m} \cdot \mathbf{H} + w_\mathrm{d} \right] \mathrm{d}V$$





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In [3]: md.drive(system)

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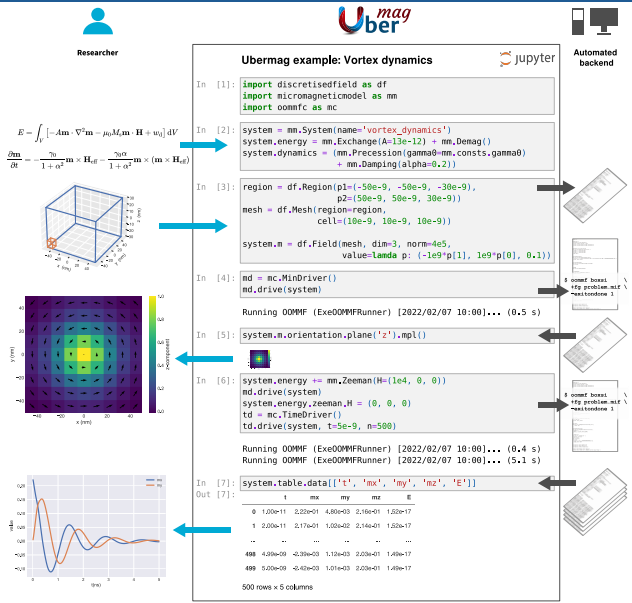
```

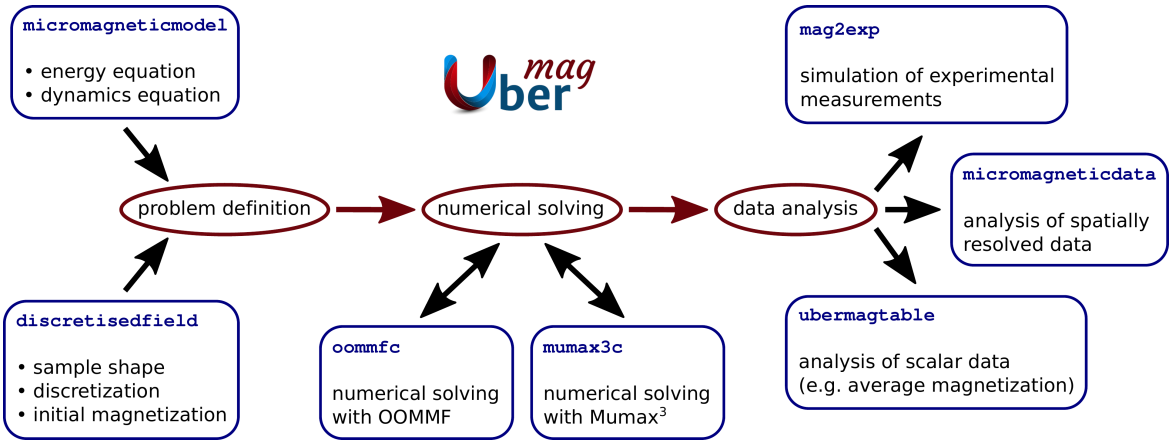
Automated backend

```
$ oommf boxsi  \
  +fg problem.mif \
  -exitondone 1
```

Ubermag overview (longer)



Ubermag workflow and packages



Installation options

- Ubermag:
  - `pip install ubermag` (Python only, needs separate install of OOMMF)
  - `conda install -c conda-forge ubermag` (contains OOMMF)
- OOMMF:
  - install binary package (Windows) from NIST
  - compile from source (Linux, OSX) from NIST
  - conda (`conda install -c conda-forge oommf`)
  - Docker (`docker pull oommf/oommf`)
  - Spack (`spack install oommf`)