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# COMPUTATIONAL MICROMAGNETICS WITH



<https://tinyurl.com/solskymag22-ubermag>

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<sup>2</sup>Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

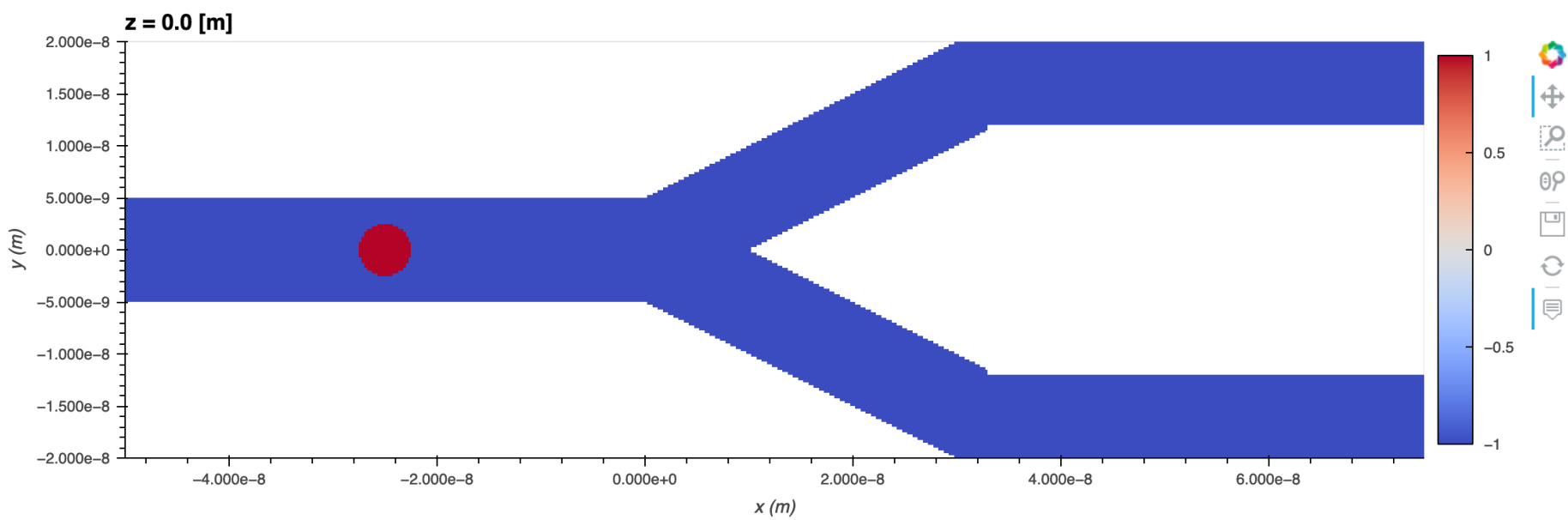
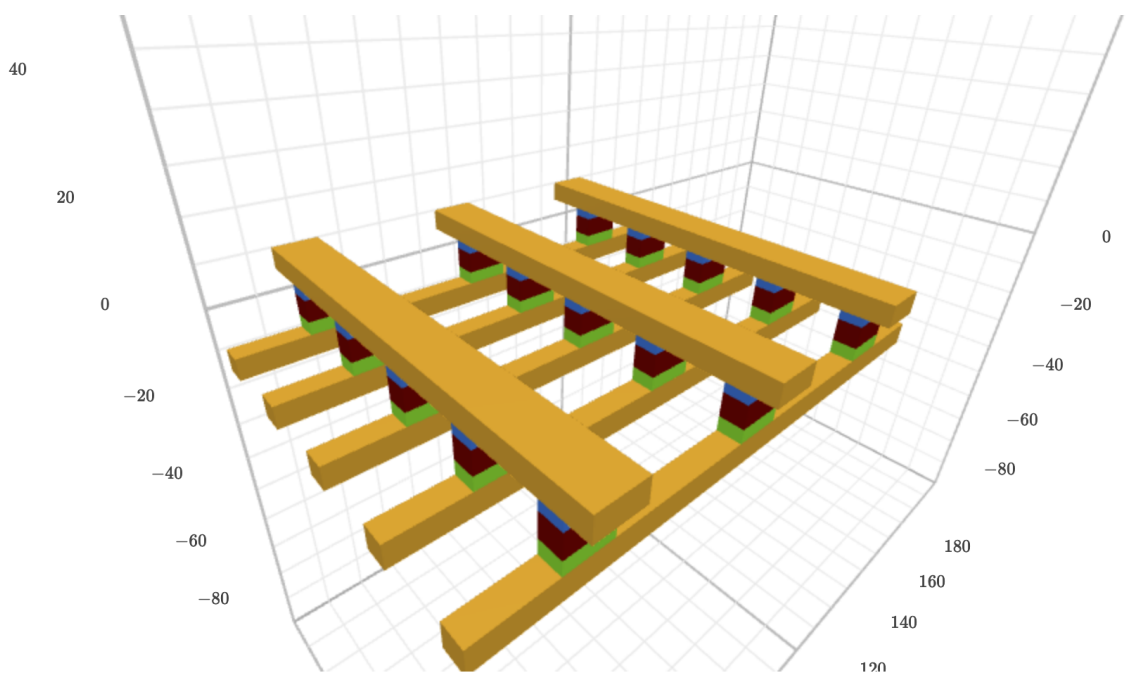
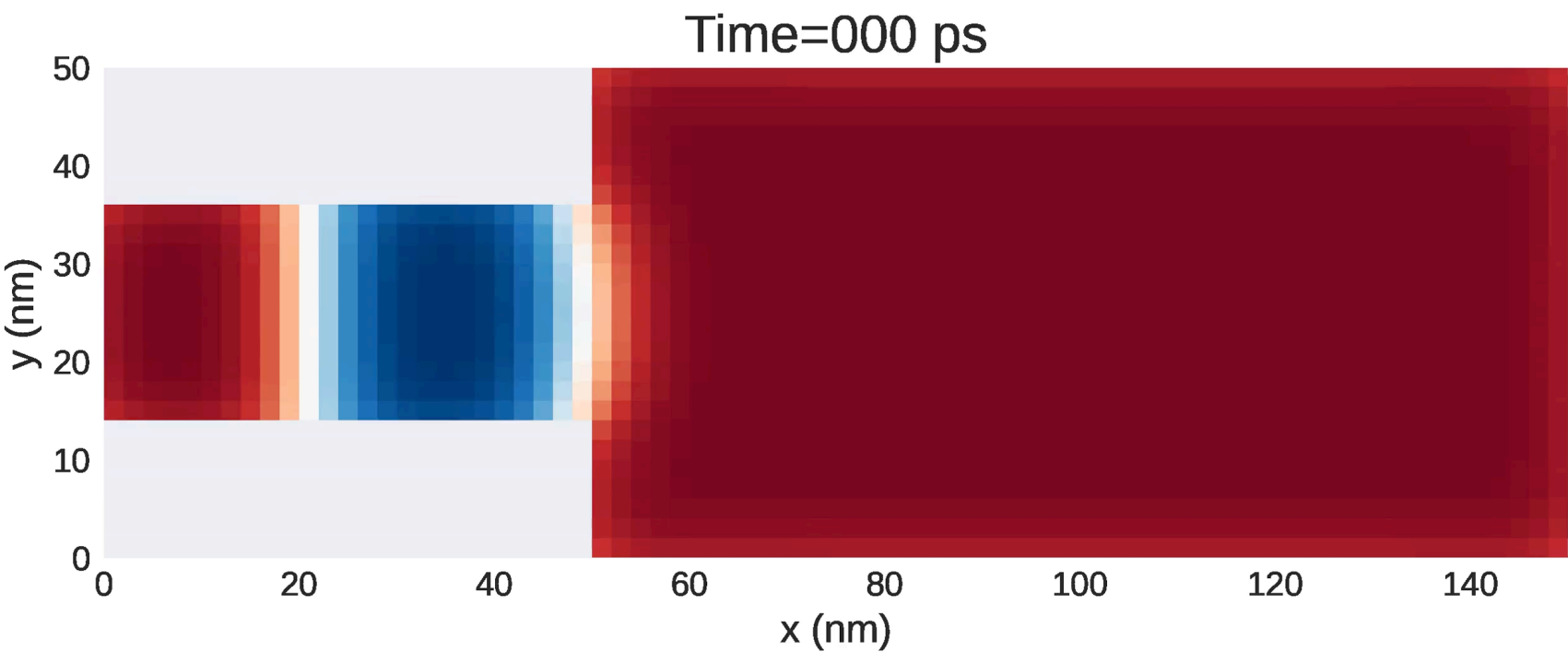
<sup>3</sup>Imperial College, London, United Kingdom

# MOTIVATION: MICROMAGNETIC RESEARCH ENVIRONMENT UBERMAG

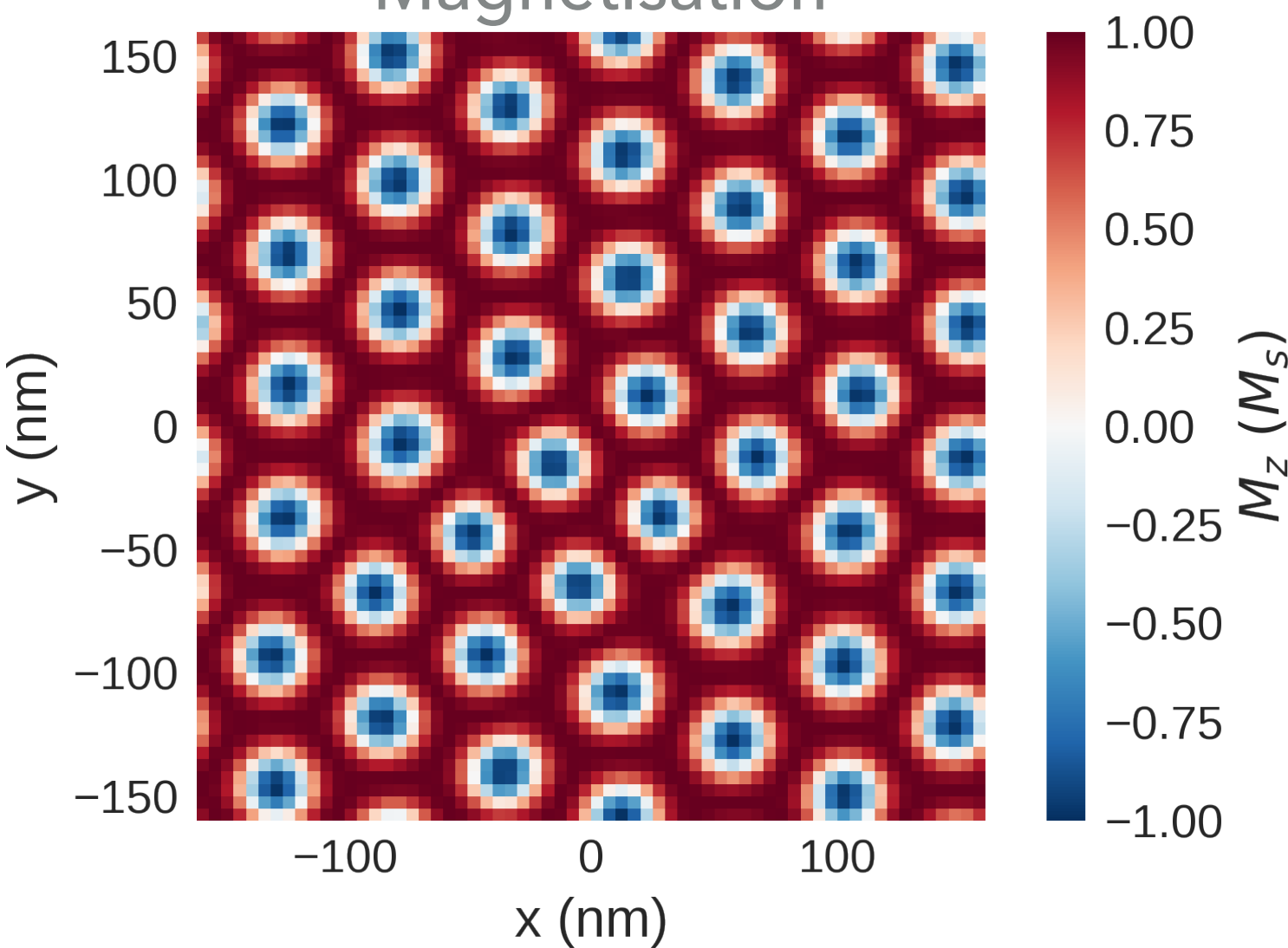
- ▶ Micromagnetic simulations are important
- ▶ Vision: simplify micromagnetic research
  - ▶ Focus on the researchers and their time
  - ▶ Make research *faster & more convenient*
  - ▶ and *more re-producible and re-usable*
- ▶ Build on existing micromagnetic simulators (OOMMF, mumax3)

# WHAT CAN BE DONE WITH UBERMAG? USAGE EXAMPLES

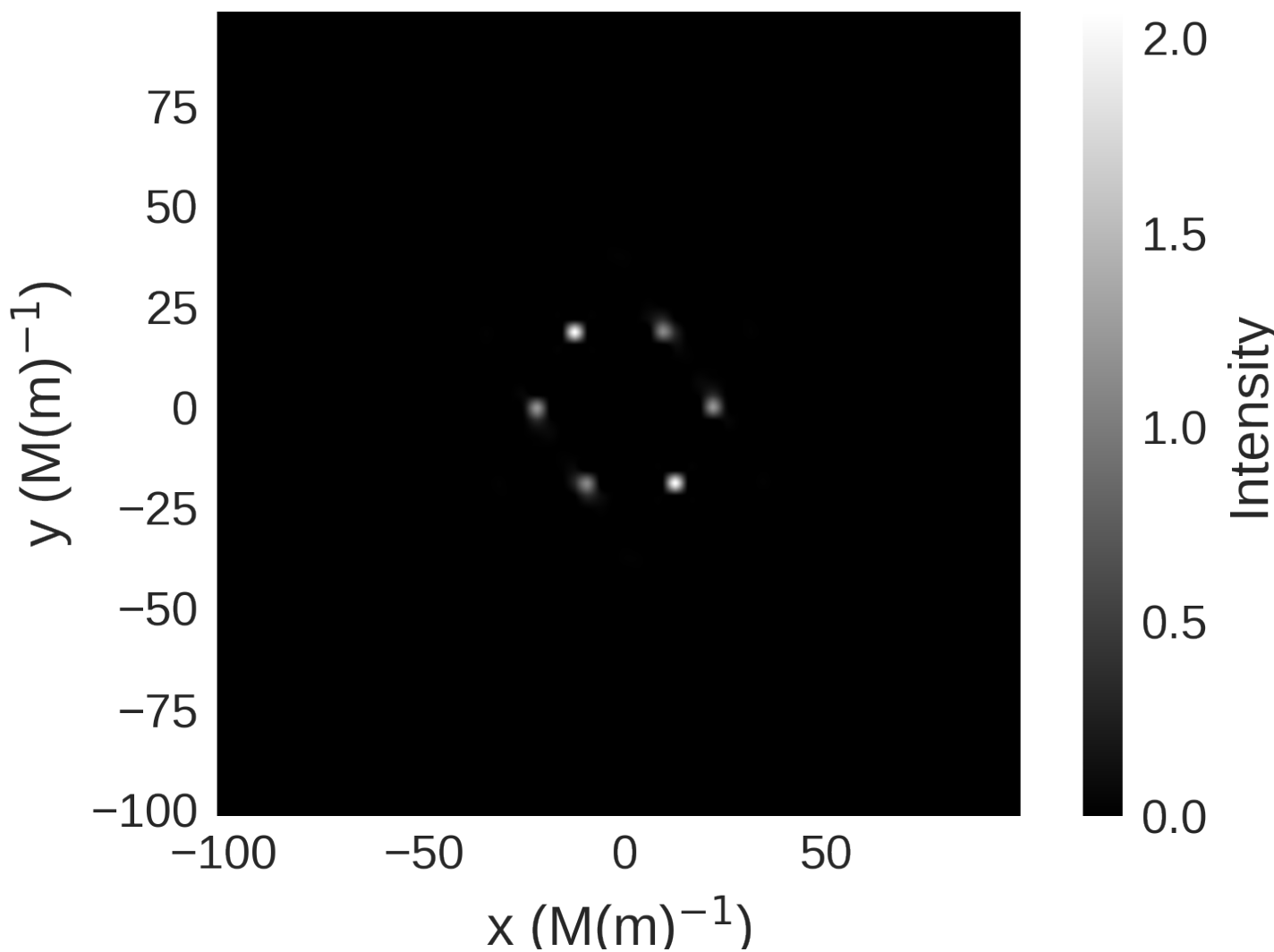
Domain wall skyrmion conversion



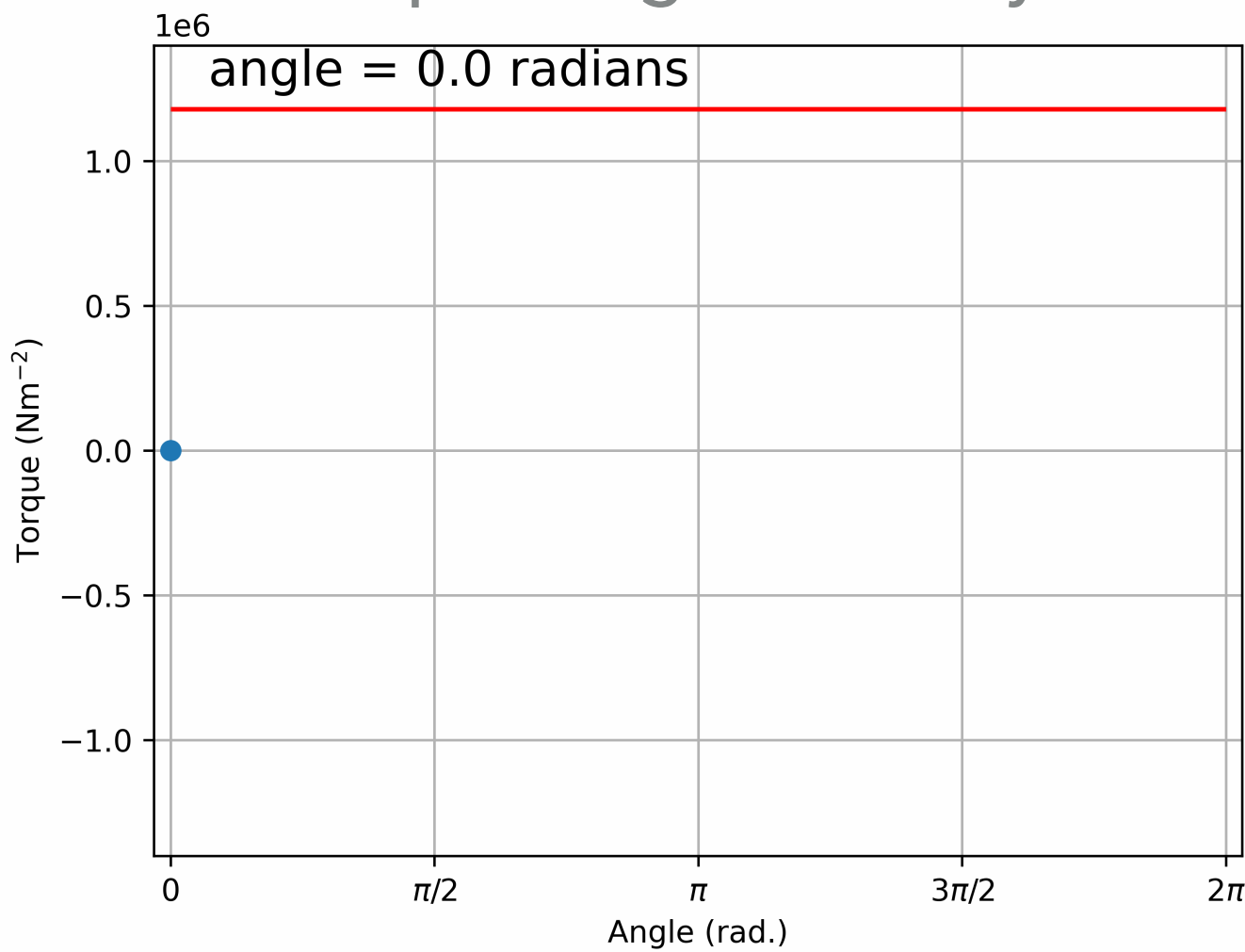
Magnetisation



SANS

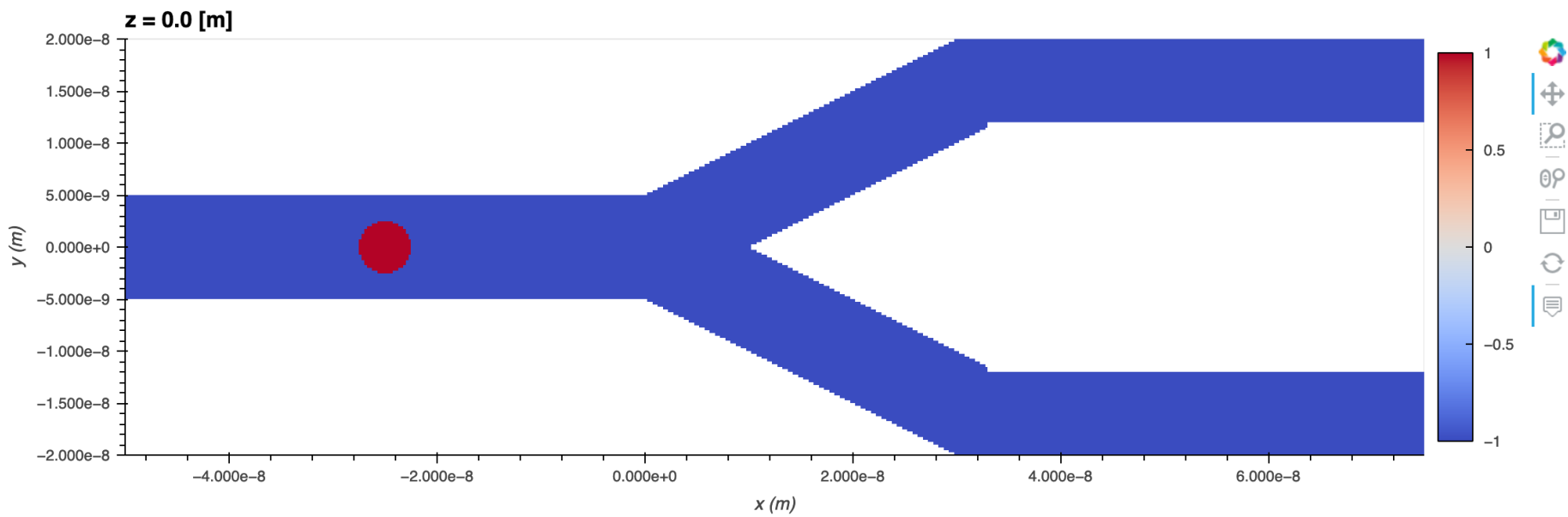
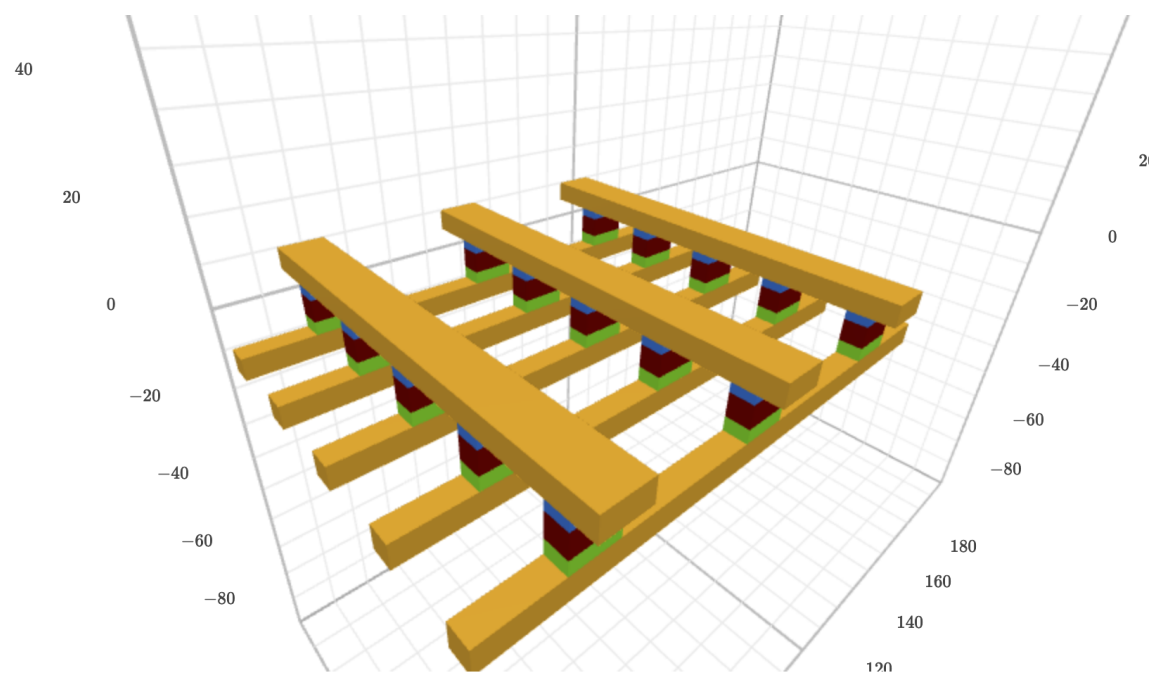
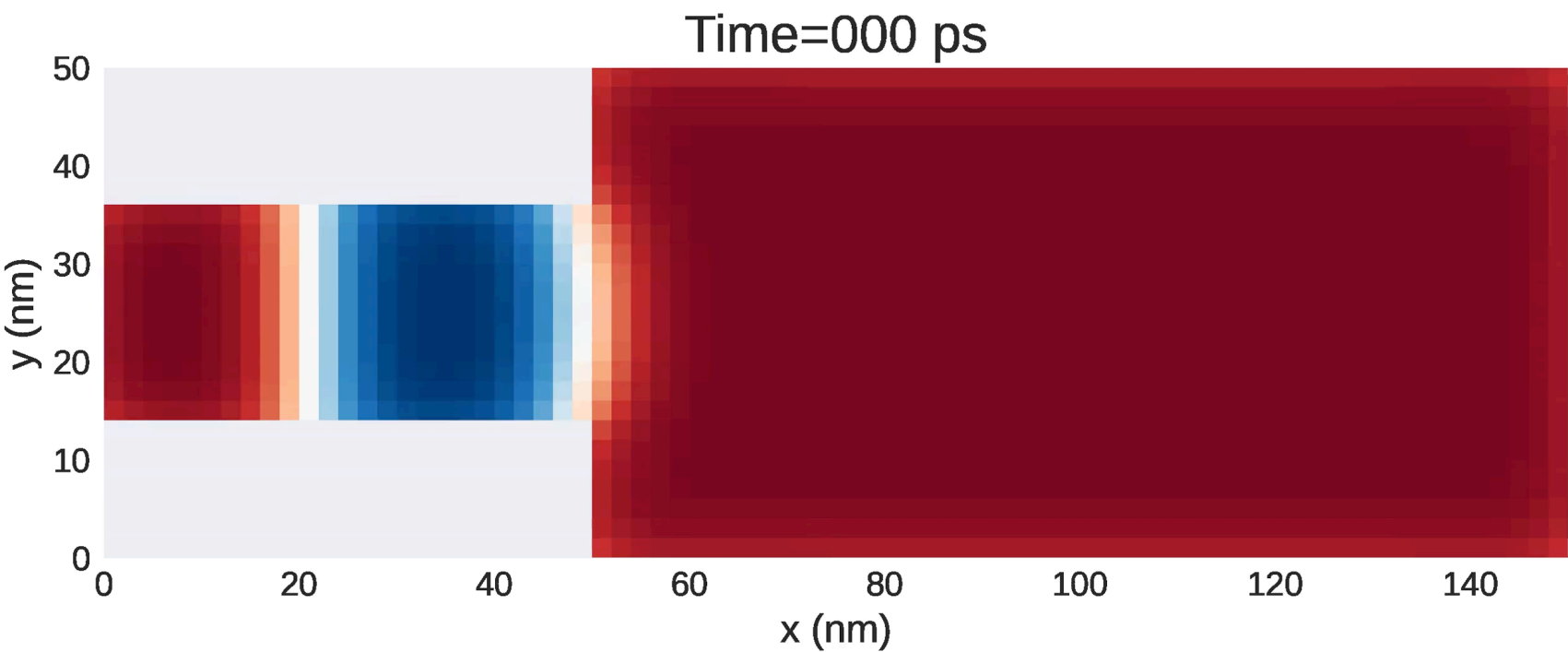


Torque magnetometry

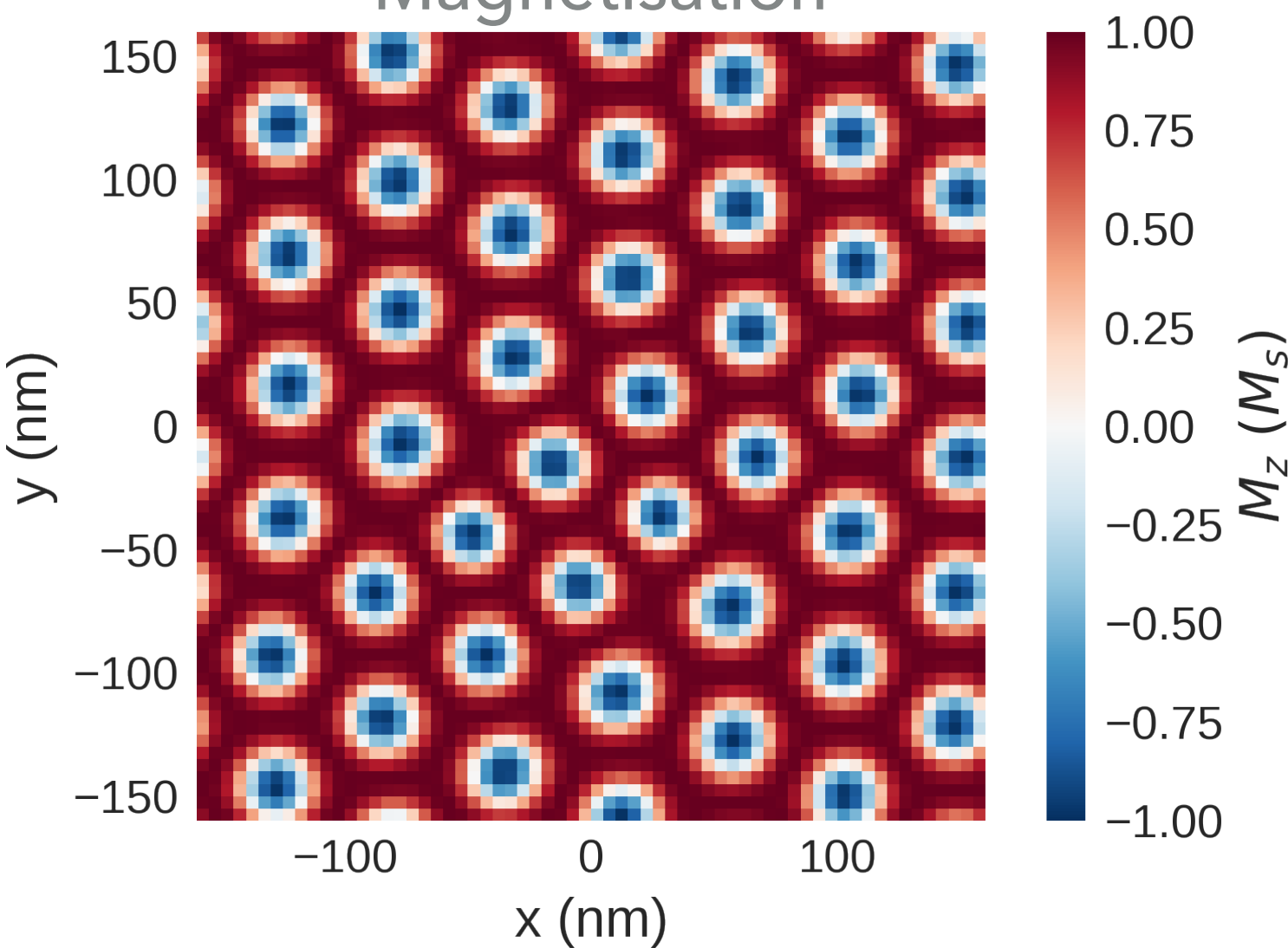


# WHAT CAN BE DONE WITH UBERMAG? USAGE EXAMPLES

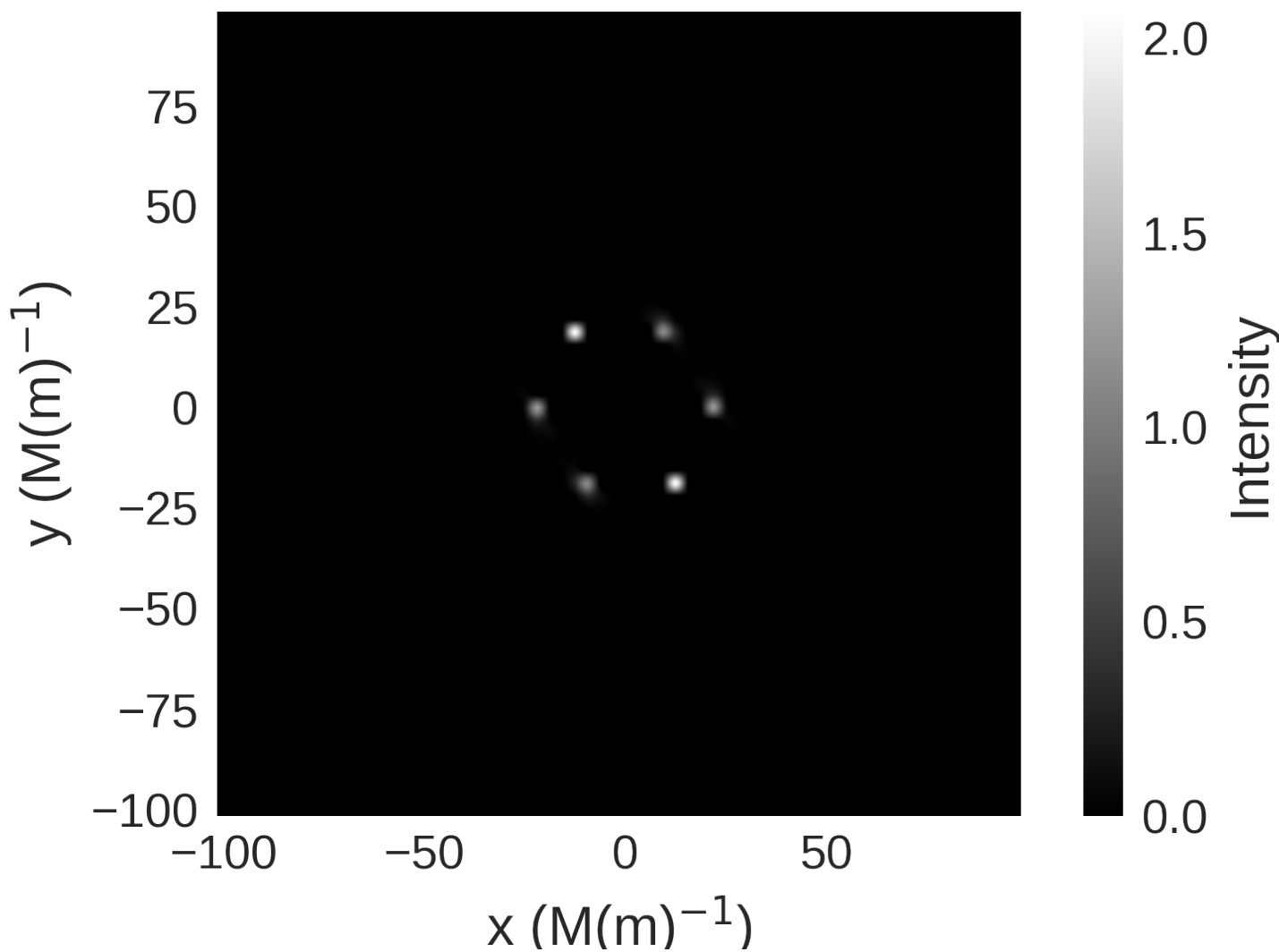
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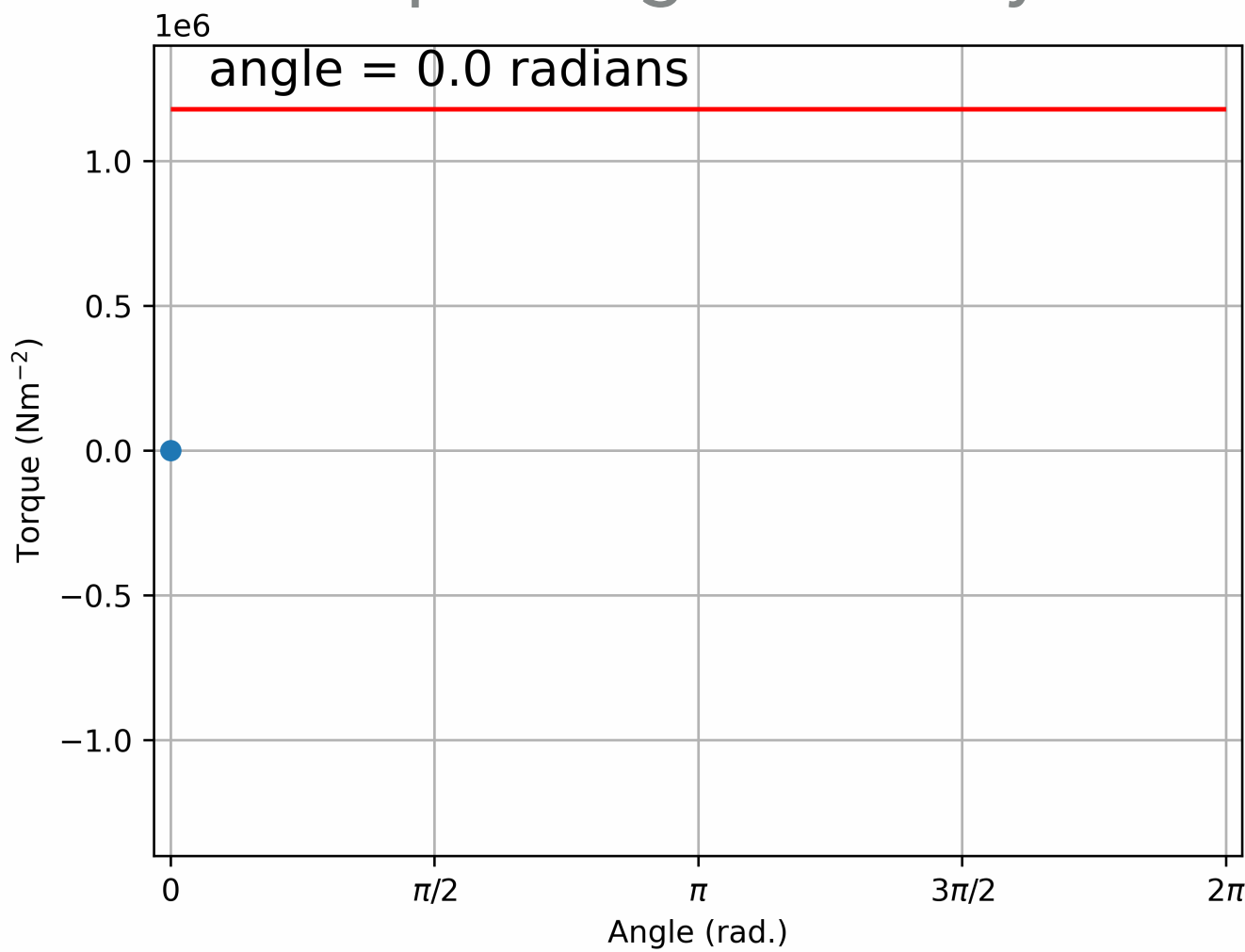
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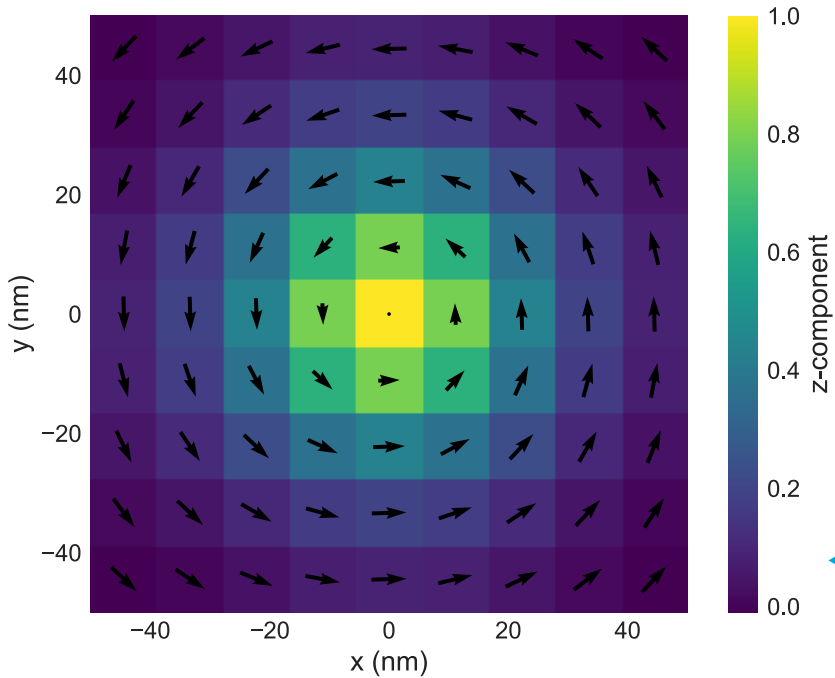
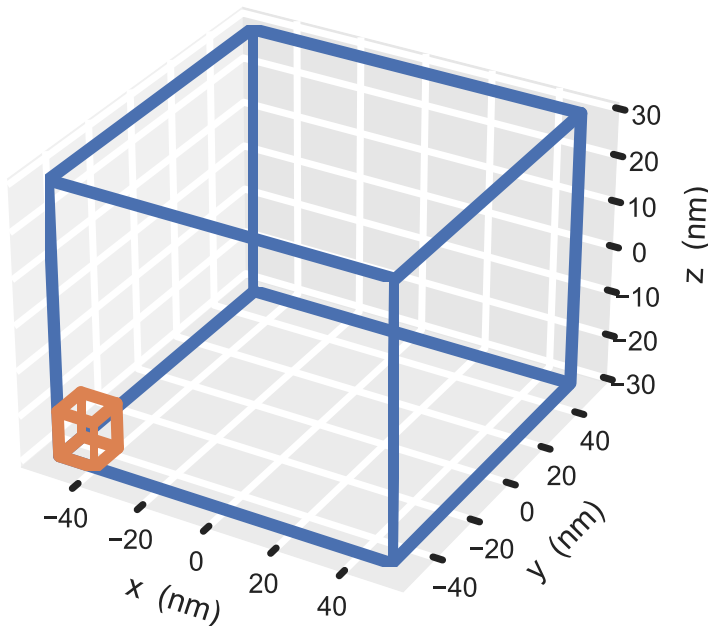


# SEPARATION OF CONCERNS IN UBERMAG



Researcher

$$E = \int_V \left[ -A \mathbf{m} \cdot \nabla^2 \mathbf{m} - \mu_0 M_s \mathbf{m} \cdot \mathbf{H} + w_d \right] dV$$



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]:

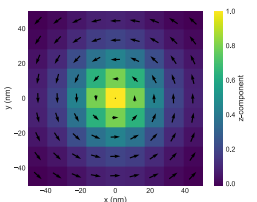
```
mesh = df.Mesh(p1=(-50e-9, -50e-9, -30e-9),
               p2=(50e-9, 50e-9, 30e-9),
               cell=(10e-9, 10e-9, 10e-9))
system.m = df.Field(mesh, dim=3, norm=4e5,
                   value=vortex_fun)
```

In [3]:

```
md.drive(system)
```

In [4]:

```
system.m.orientation.plane('z').mpl()
```



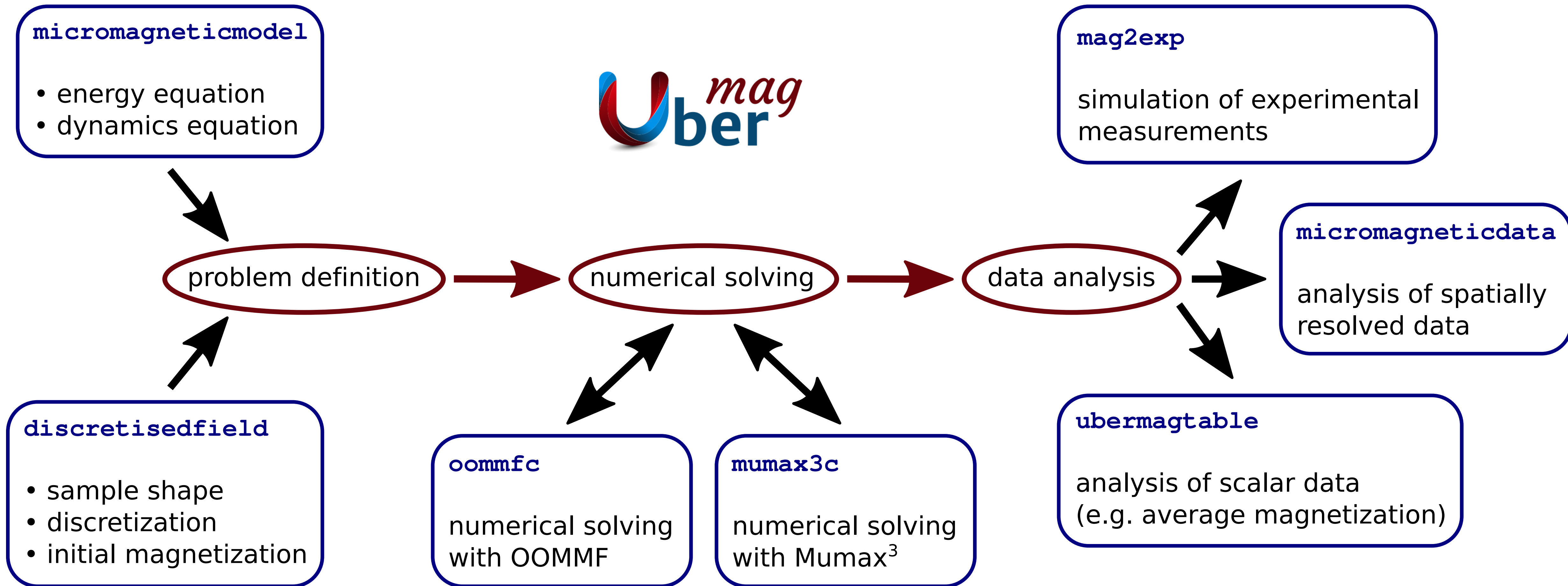
Automated  
backend

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





# WHAT IS UBERMAG – WORKFLOW CHART



# THIS WORKSHOP — MANY CONCEPTS AND LITTLE TIME

- ▶ Rapid tour involving
  - ▶ Ubermag concepts
  - ▶ Jupyter Notebook – executable document hosted in browser
  - ▶ Python – a programming language
  - ▶ Computational micromagnetics and experimental magnetism techniques
- ▶ Can only provide an introduction & show what is possible

## WORKSHOP MATERIALS

- ▶ <https://tinyurl.com/solskymag22-ubermag>
- ▶ Repository on Github  
full URL: <https://github.com/ubermag/workshop/blob/2022-06-29/README.md>
- ▶ Mailing list – future training materials will be announced
- ▶ Slides and notebooks to follow available after workshop

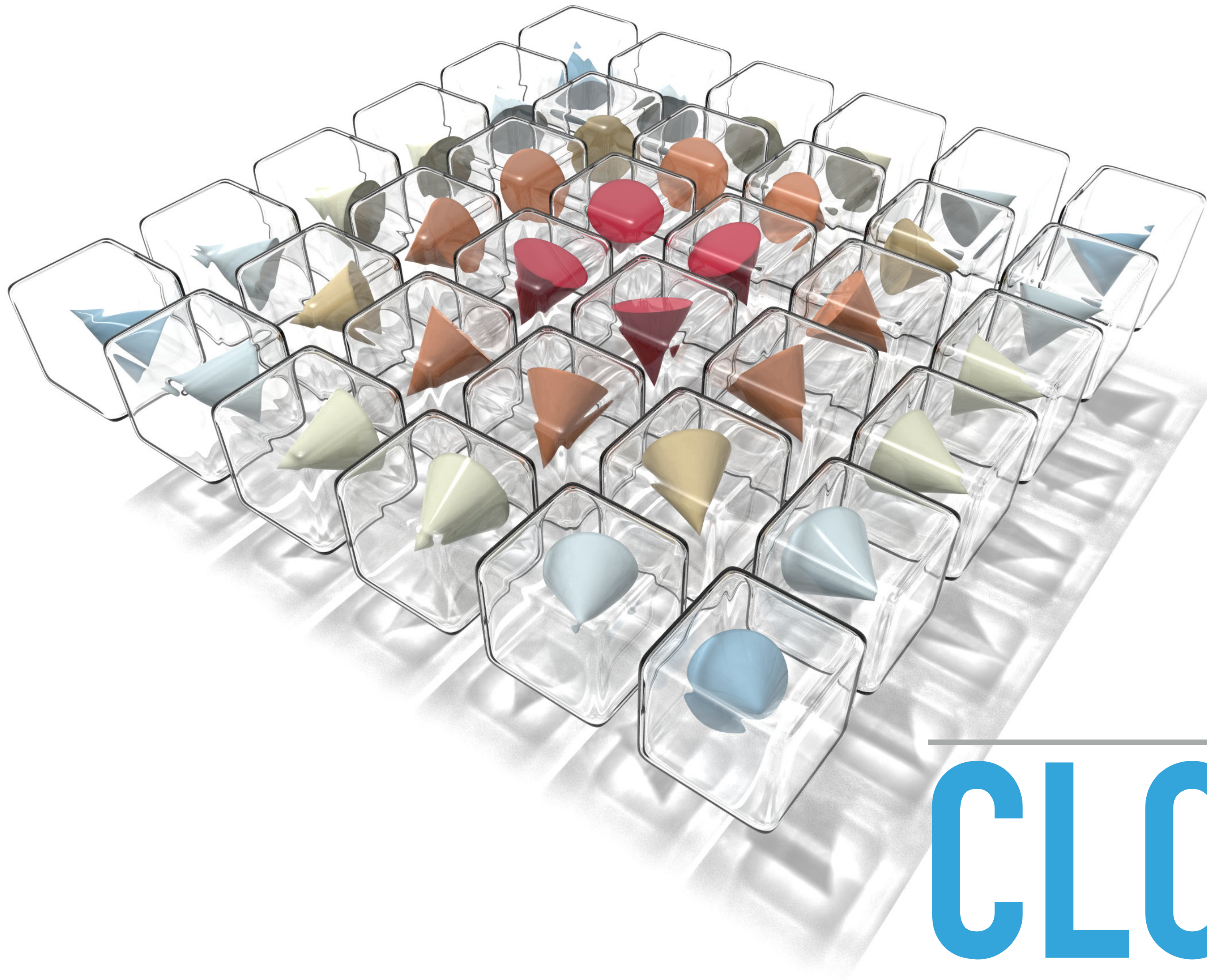




# OUTLINE

- ▶ Welcome (Hans Fangohr)
- ▶ Small Ubermag example from scratch: vortex (Martin Lang)
- ▶ Application examples Ubermag (Sam Holt)
- ▶ Closing (Hans Fangohr)
  
- ▶ Optional: Informal discussions





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**CLOSING**



# SURVIVED UBERMAG WORKSHOP – FURTHER RESOURCES

- ▶ Ubermag home page (<https://ubermag.github.io/>) provides
  - ▶ [Getting started tutorials](#)
  - ▶ [Variety of examples](#) (see list at the right)
  - ▶ [Github Help issues](#)
  - ▶ [Mailing list "ubermag-users"](#)
  - ▶ Ubermag team at this meeting

Workshop materials:

<https://tinyurl.com/solskymag22-ubermag>

## Examples

The notebooks show in this section are all tailored to physics problems and solve them using **Ubermag**. If you are new to **ubermag** you should start with [started](#) which will give a gentle introduction into all the possibilities. We try to be concise and only cover one use case. For a more detailed overview of features please refer to the [Package documentation](#) and

[Standard problem 3](#)

[Standard problem 4](#)

[Standard problem 5](#)

[FMR standard problem](#)

[Deriving energy values](#)

[Calculating a stray field using an airbox method](#)

[Skyrmion in a disk](#)

[Field operations 2](#)

[Simulation at finite temperature](#)

[Fixed subregions](#)

[Hysteresis simulations](#)

[Multiple energy terms of the same class](#)

[Negative exchange energy constant](#)

[Periodic boundary conditions](#)

[RKKY energy term](#)

[Sine-hysteresis](#)

[Both spatially and time varying field](#)

[Spatially varying parameters 1](#)

[Spatially varying parameters 2](#)

[Time-varying field](#)

[Time-dependent fields and currents](#)

# DISCUSSION UBERMAG DESIGN

- ▶ Ubermag is embedded [1] in Python programming language
  - ▶ Full power of Python language available
  - ▶ Access to growing set of data analysis libraries
  - ▶ Needs Python skills to fully exploit, but collections of recipes are available
- ▶ Modular design of Ubermag
  - ▶ Can use components independently; for example `mag2exp`

# DISCUSSION UBERMAG DESIGN

- ▶ Ubermag is embedded in Jupyter notebook [2]:  
Mixing simulation and analysis commands with output and annotation:
  - ▶ Supports better reproducibility and re-usability [3]
  - ▶ Zero-install tutorials / demos / reproducible publications using “Binder”  
([Example: vortex](#)). Need only web browser locally.

[2] Marijan Beg et al. Ubermag: IEEE TransMag, vol. 58, no. 2, pp. 1-5, Art no. 7300205, <https://doi.org/10.1109/TMAG.2021.3078896> (2022)

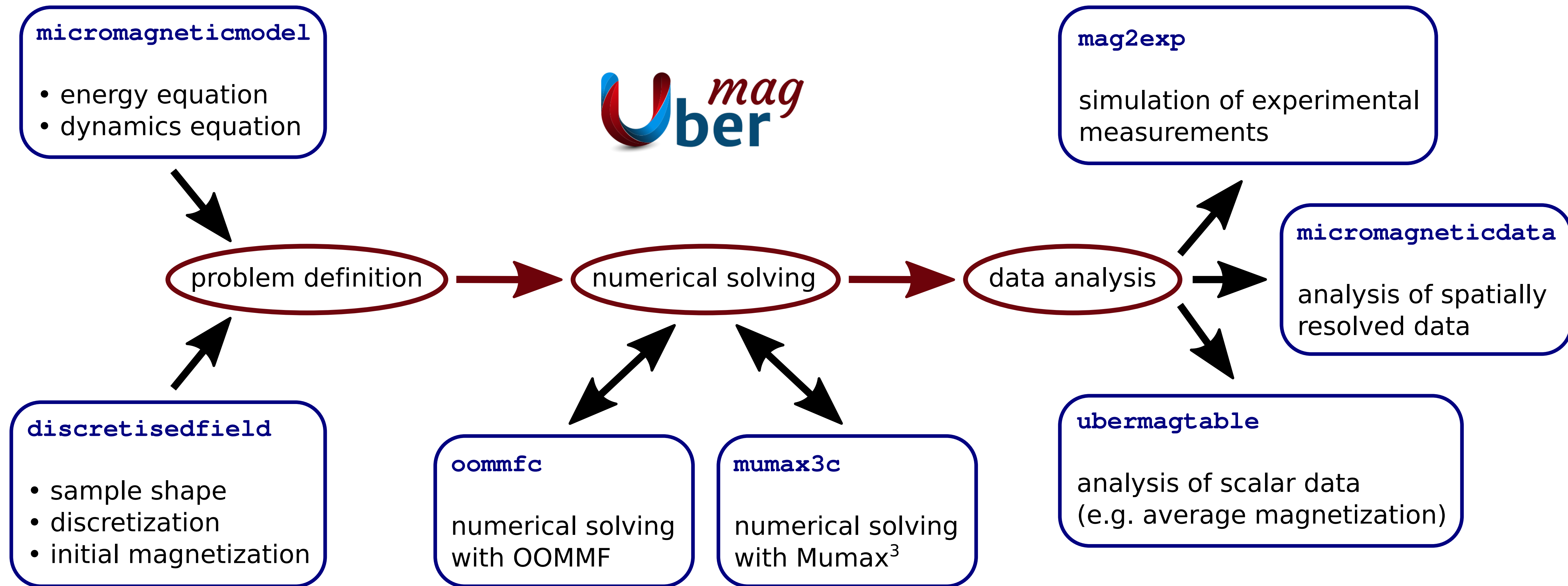
[3] Marijan Beg et al, Computing in Science & Engineering 23, 36-46, <https://doi.org/10.1109/MCSE.2021.3052101> (2021)

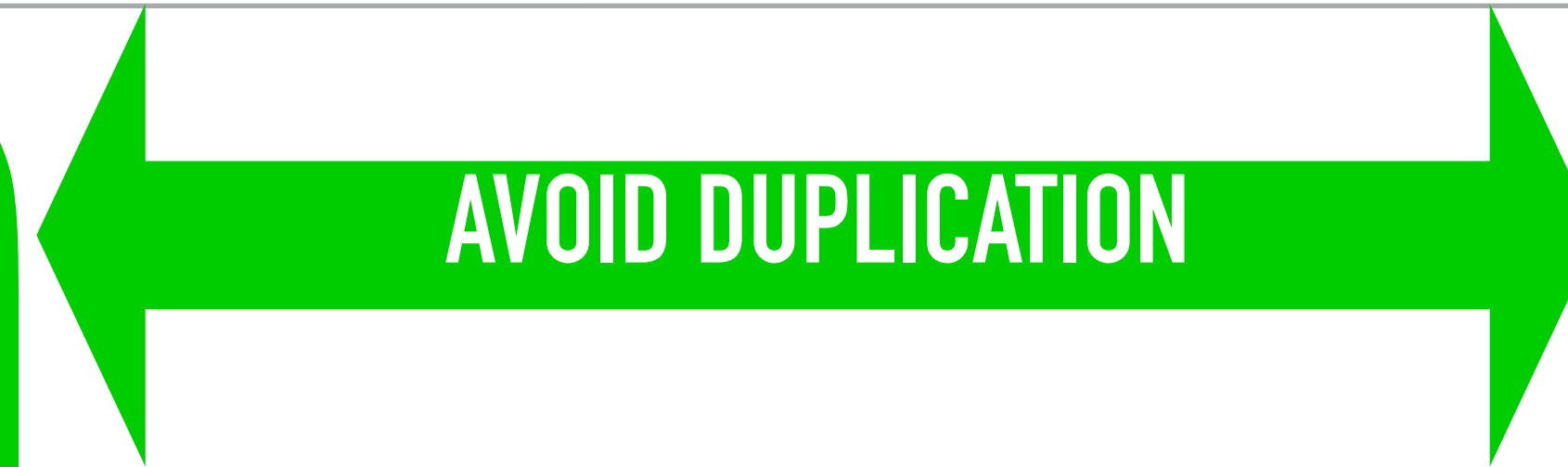
# GET INVOLVED?

- ▶ Opportunities for joint work, for example:
  - ▶ Tailor Ubermag for your research problem
  - ▶ Integrate your simulation engine into Ubermag framework
  - ▶ Make your research more reproducible &
  - ▶ Contribute to open source tools used by the community

Get in touch for exploration of options ([hans.fangohr@mpsd.mpg.de](mailto:hans.fangohr@mpsd.mpg.de))







**micromagneticmodel**

- energy equation
- dynamics equation

problem definition

**discretisedfield**

- sample shape
- discretization
- initial magnetization

numerical solving

**oommfc**

numerical solving  
with OOMMF

**mumax3c**

numerical solving  
with Mumax<sup>3</sup>

data analysis

**mag2exp**

simulation of experimental  
measurements

**micromagneticdata**

analysis of spatially  
resolved data

**ubermagtable**

analysis of scalar data  
(e.g. average magnetization)

**MACHINE READABLE DISCRETION  
OF PHYSICS PROBLEM**

AVOID DUPLICATION

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## KEY IDEAS

MACHINE READABLE DISCRETION  
OF PHYSICS PROBLEM

AVOID DUPLICATION

SIMULATION OF  
EXPERIMENTAL  
MEASUREMENTS`micromagneticmodel`

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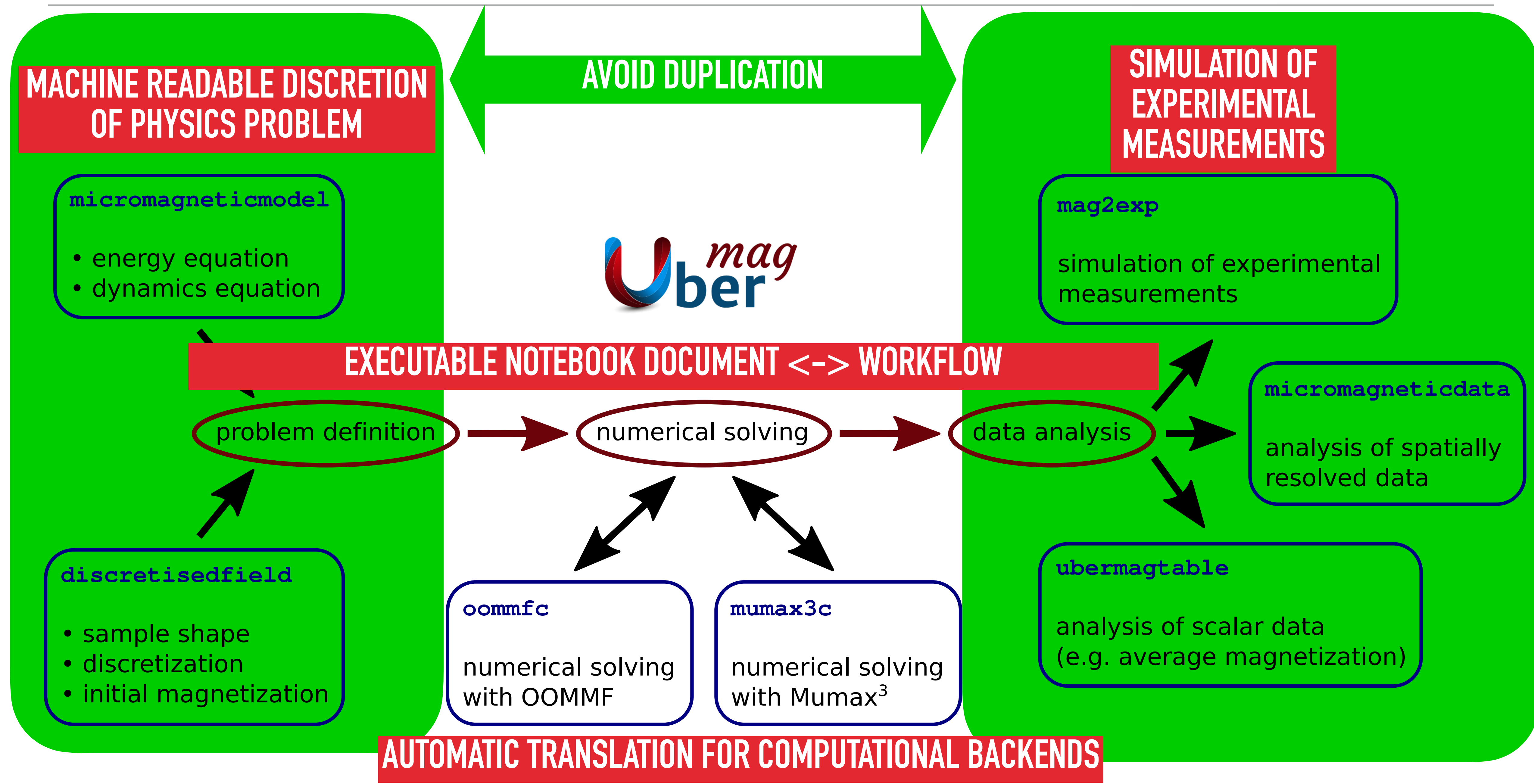
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AUTOMATIC TRANSLATION FOR COMPUTATIONAL BACKENDS

## KEY IDEAS



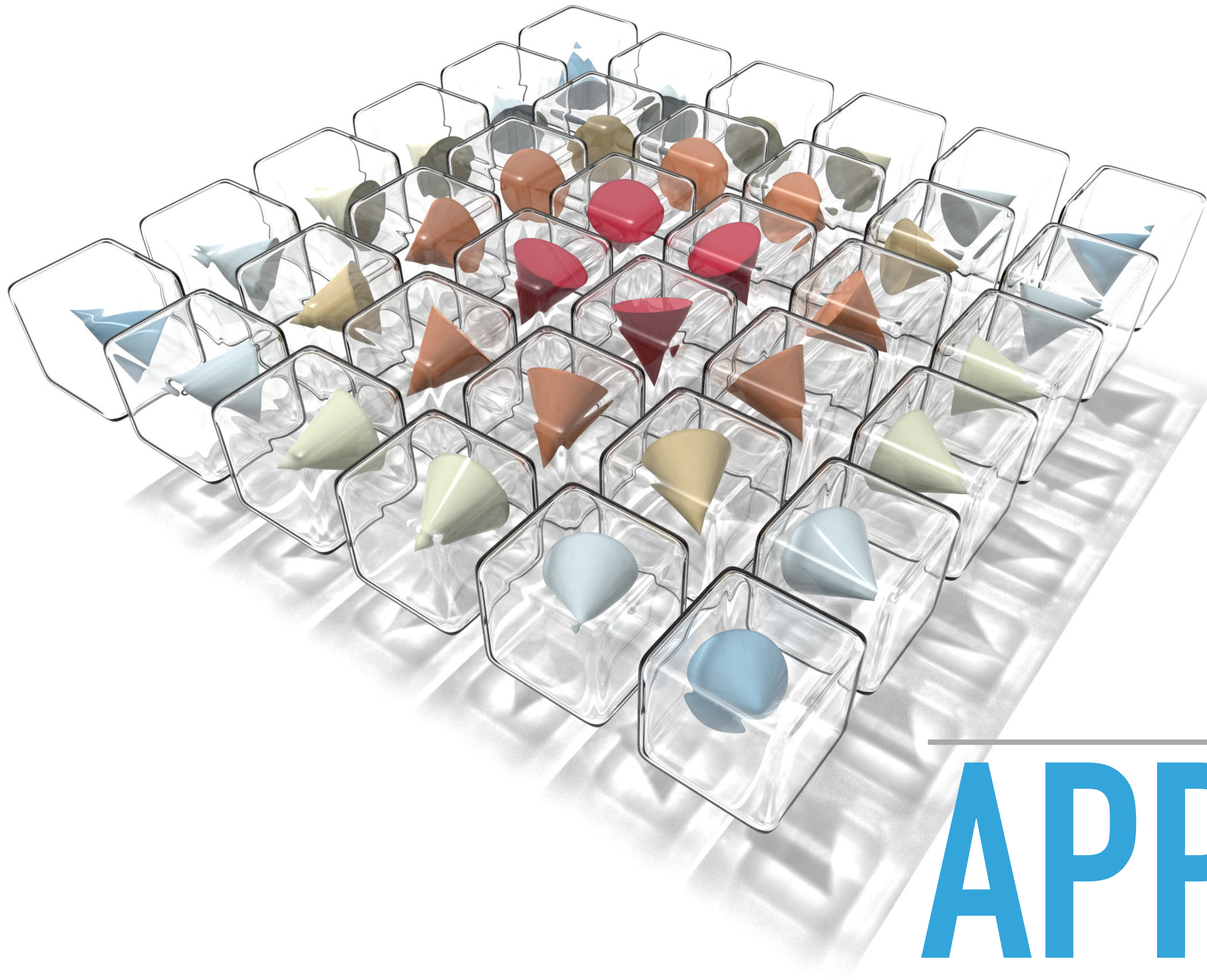


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- ▶ Financial support
  - ▶ EPSRC Programme grant on Skymionics (EP/N032128/1)
  - ▶ Horizon 2020 European Research Infrastructure OpenDreamKit project (Project ID 676541).
  - ▶ Fonds Wetenschappelijk Onderzoek (FWO-Vlaanderen) Project No. G098917N







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# APPENDIX



# RELEVANT REFERENCES

- ▶ Official Ubermag references:
  - ▶ 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, <https://doi.org/10.1063/1.4977225> (2017)
  - ▶ Marijan Beg, Martin Lang and Hans Fangohr, *Ubermag: Toward More Effective Micromagnetic Workflows*, IEEE Transactions on Magnetics, vol. 58, no. 2, pp. 1-5, Feb. 2022, Art no. 7300205, <https://doi.org/10.1109/TMAG.2021.3078896> (2022)
- ▶ Publications relating to Jupyter Notebooks for science:
  - ▶ Hans Fangohr, Marijan Beg, et al, *Data exploration and analysis with Jupyter notebooks*, Proceedings of the 17th International Conference on Accelerator and Large Experimental Physics Control Systems ICALEPCS2019, TUCPR02, <https://jacow.org/icalepcs2019/papers/tucpr02.pdf> (2020)
  - ▶ Marijan Beg, Juliette Belin, Thomas Kluyver, Alexander Konovalov, Min Ragan-Kelley, Nicolas Thiery, Hans Fangohr *Using Jupyter for reproducible scientific workflows*, Computing in Science & Engineering 23, 36-46, <https://doi.org/10.1109/MCSE.2021.3052101> (2021)