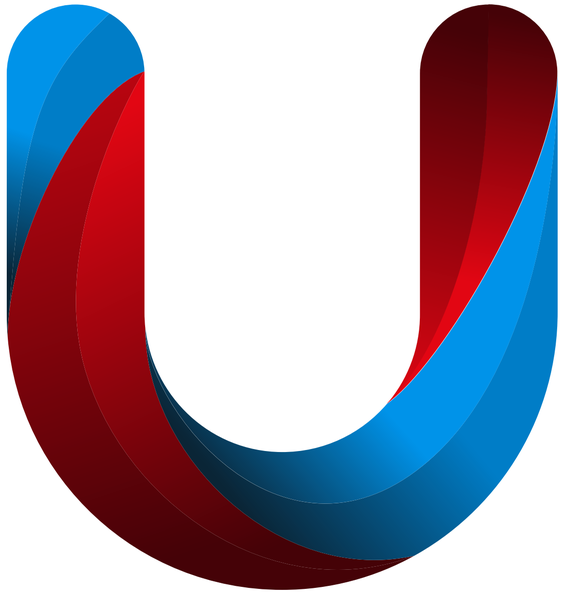
Samuel Holt[1], Swapneel Pathak[1,2], Martin Lang[1,2], Marijan Beg[3] and Hans Fangohr[1,2]

COMPUTATIONAL MICROMAGNETICS WITH



mag

Uber

https://tinyurl.com/solskymag22-ubermag

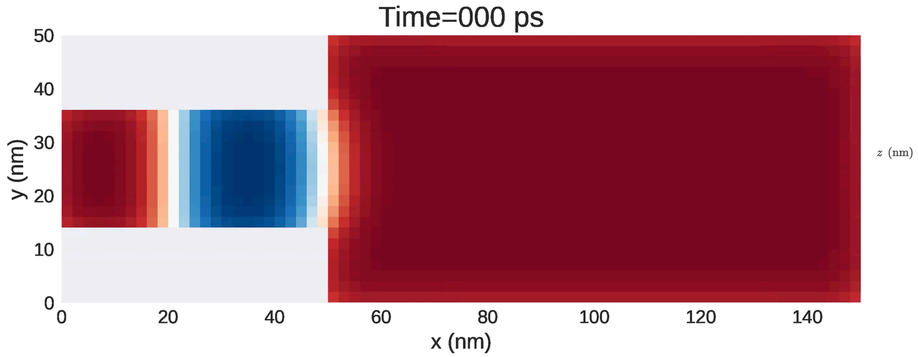
[1]University of Southampton, Southampton, United Kingdom
[2]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany
[3]Imperial College, London, United Kingdom

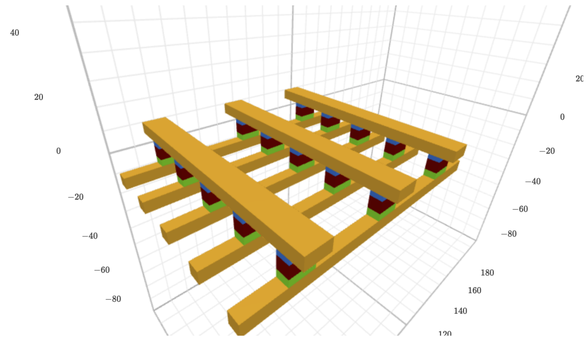
MOTIVATION: MICROMAGNETIC RESEARCH ENVIRONMENT UBERMAG

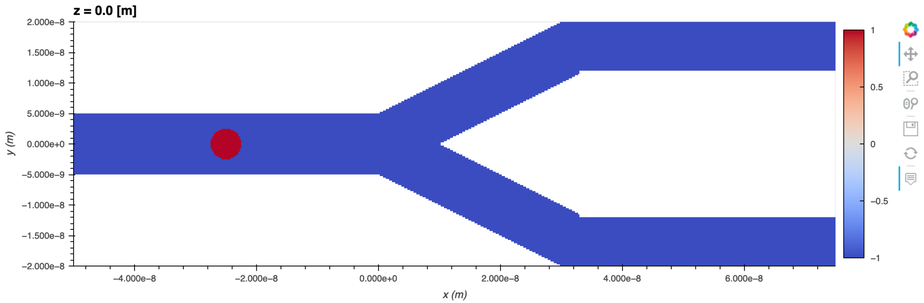
- Micromagnetic simulations are important
- Vision: simplify micromagnetic research
  - focus on the researchers and their time
  - make research *faster & more convenient*
  - and *more re-producible and re-usable*
  - build on existing micromagnetic simulators (OOMMF, mumax3)
    - Consider only finite difference micromagnetic solvers

WHAT CAN BE DONE WITH UBERMAG? USAGE EXAMPLES

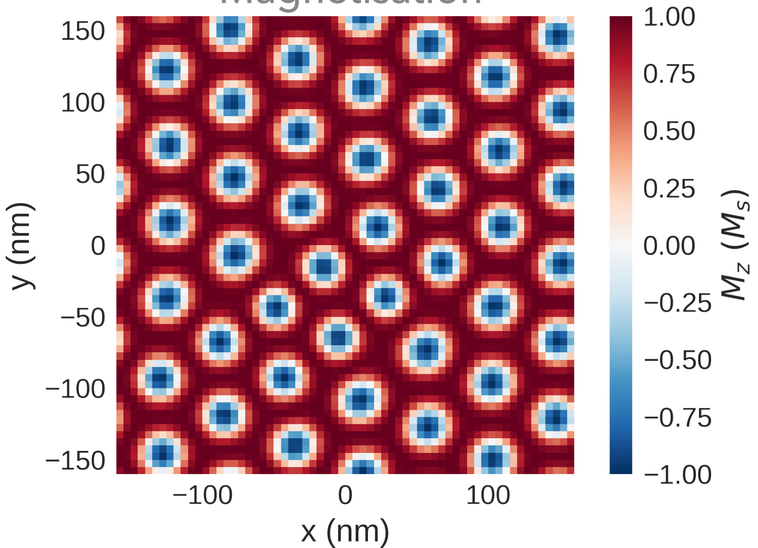
Domain wall skyrmion conversion



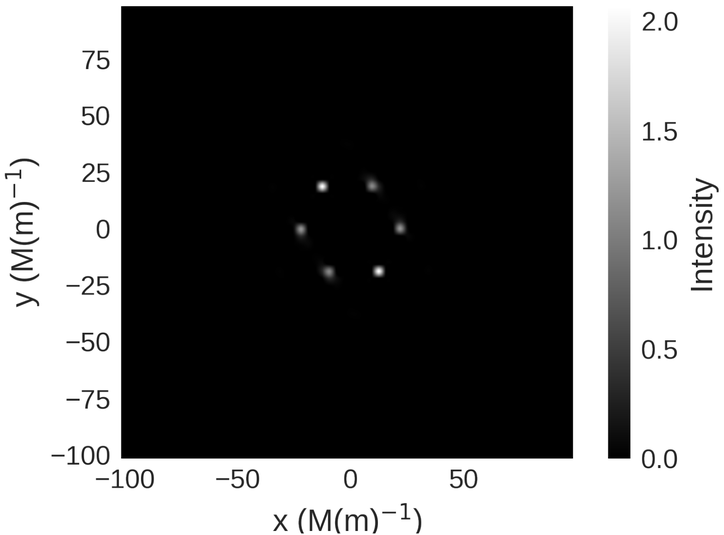




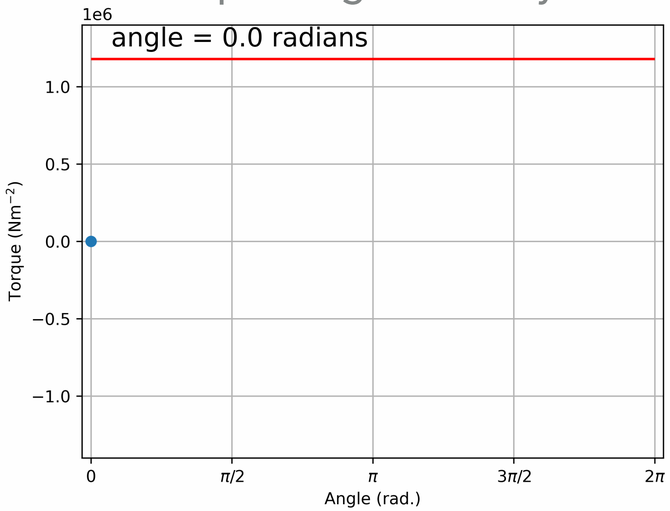
Magnetisation



SANS



Torque magnetometry

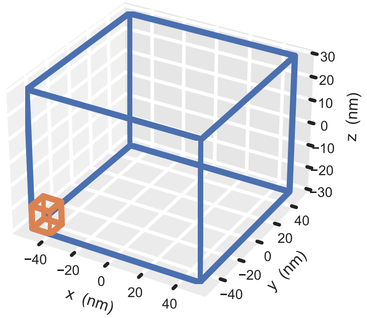


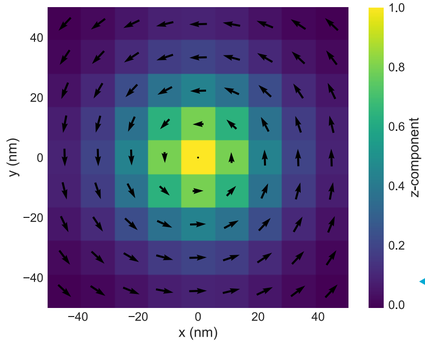
SEPARATION OF CONCERNS IN UBERMAG

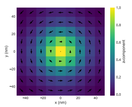
Researcher

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

```
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()
```



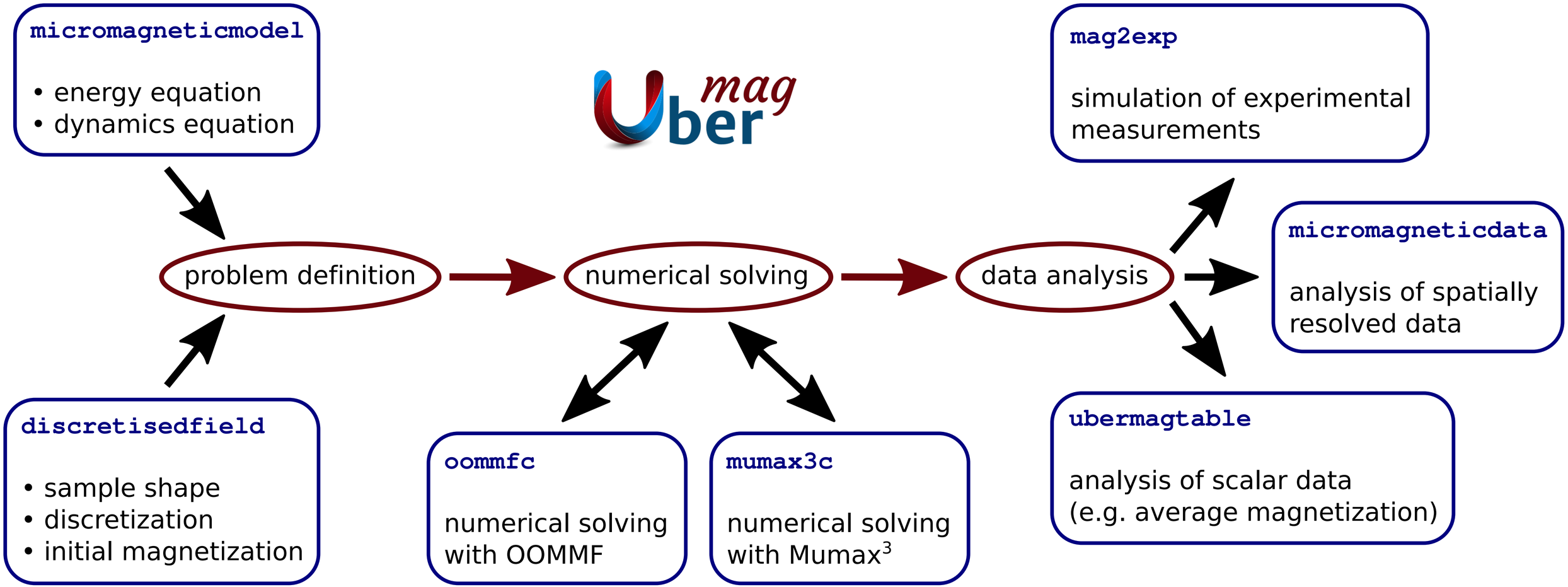




Automated backend

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

WHAT IS UBERMAG – WORKFLOW CHART



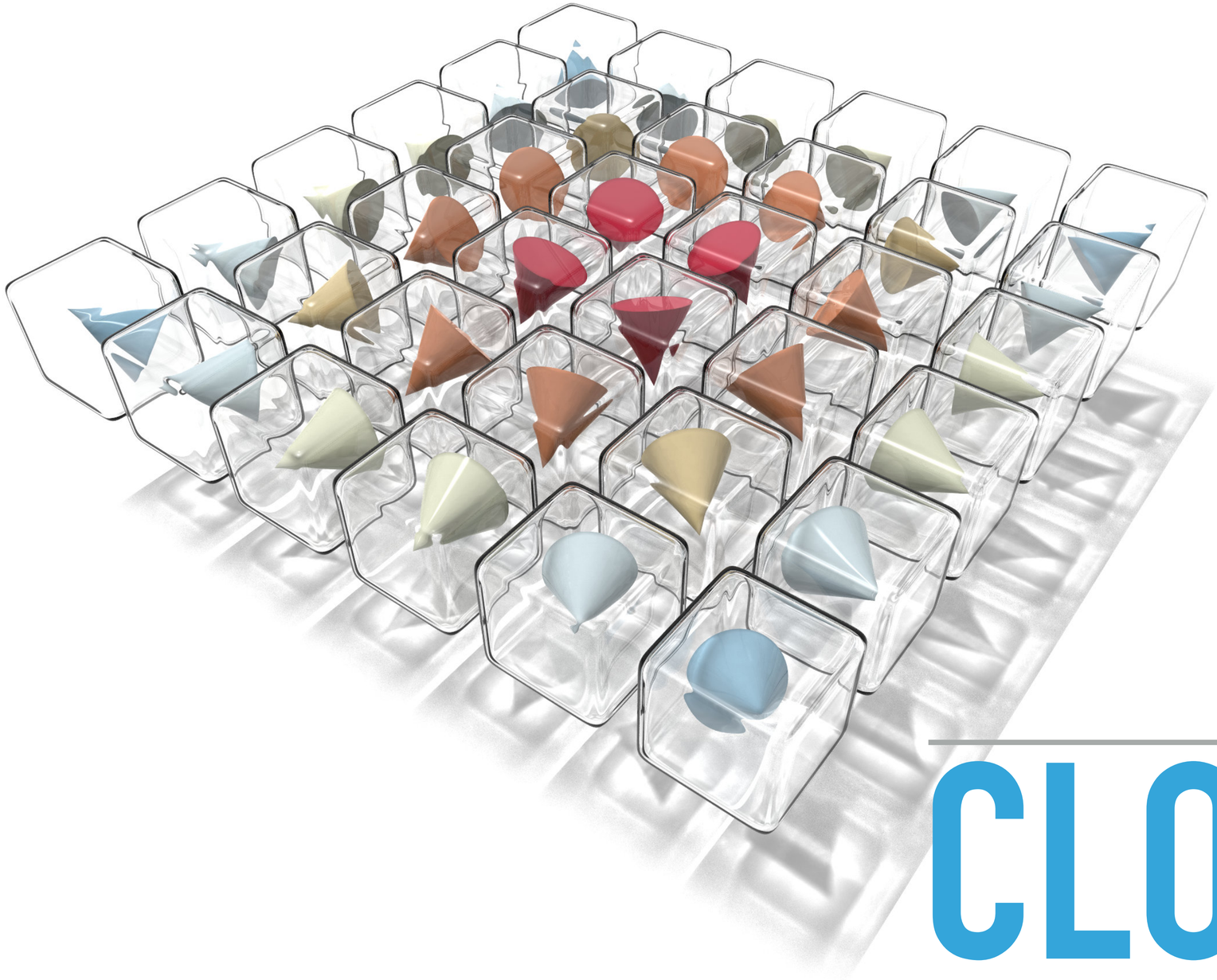
THIS WORKSHOP — MANY CONCEPTS AND LITTLE TIME

- Rapid tour involving
  - Ubermag concepts
  - Jupyter Notebook (executable document hosted in browser)
  - Python (a programming language)
  - Computational micromagnetics and experimental magnetism
- Can only provide an introduction and overview
- But: questions are welcome any time – let's make this interactive!

WORKSHOP MATERIALS — SLIDES, EXAMPLES, POINTERS

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

- Outline today
  - Welcome (Hans Fangohr)
  - Small Ubermag example from scratch: vortex (Martin Lang)
  - Application examples Ubermag (Sam Holt)
  - Closing (Hans Fangohr)



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 phy
solve them using `Ubermag`. If you are new to `ubermag` you
started which will give a gentle introduction into all the p
try to be concise and only cover one use case. For a mor
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

- Modular design of Ubermag
  - Can use components independently; for example `mag2exp`

[1] Marijan Beg et al, AIP Advances 7, 056025, https://doi.org/10.1063/1.4977225 (2017)

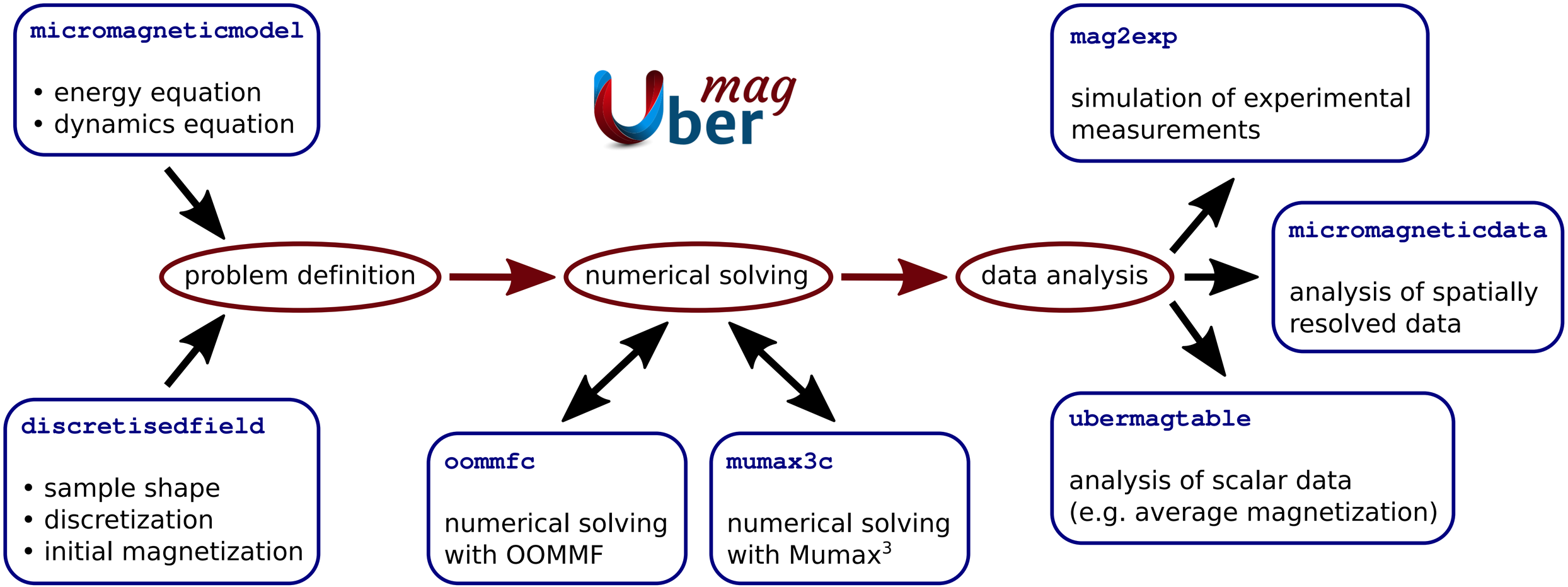
DISCUSSION UBERMAG DESIGN

- 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.

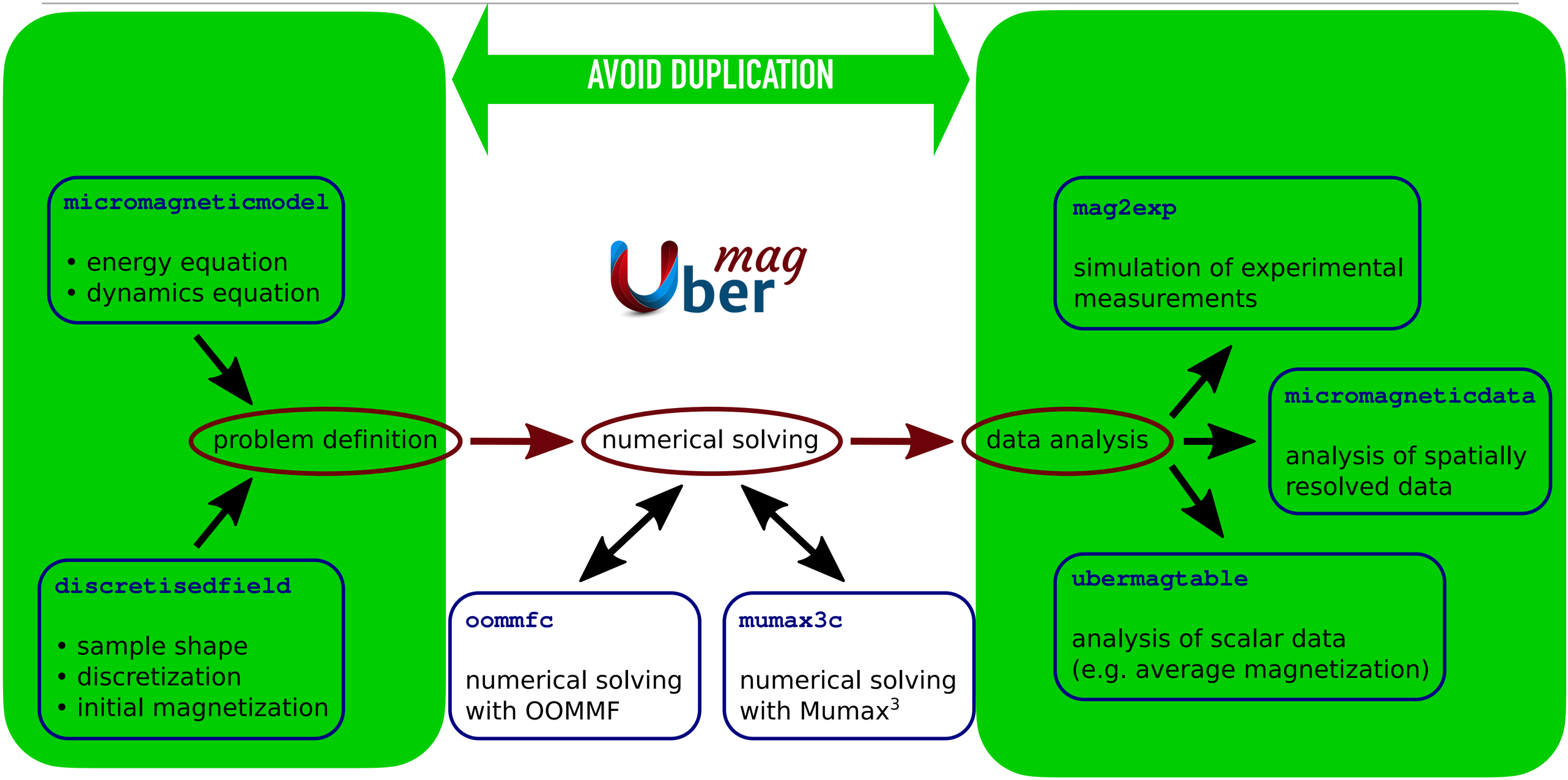
[2] Marijan Beg etal. Ubermag: IEEE TransMag, vol. 58, no. 2, pp. 1-5, Art no. 7300205, https://doi.org/10.1109/TMAG.2021.3078896 (2022)

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

KEY IDEAS


micromagneticmodel
• energy equation
• dynamics equation
Ubermag
problem definition
numerical solving
data analysis
discretisedfield
• sample shape
• discretization
• initial magnetization
oommfc
numerical solving with OOMMF
mumax3c
numerical solving with Mumax3
mag2exp
simulation of experimental measurements
micromagneticdata
analysis of spatially resolved data
ubermagtable
analysis of scalar data (e.g. average magnetization)

KEY IDEAS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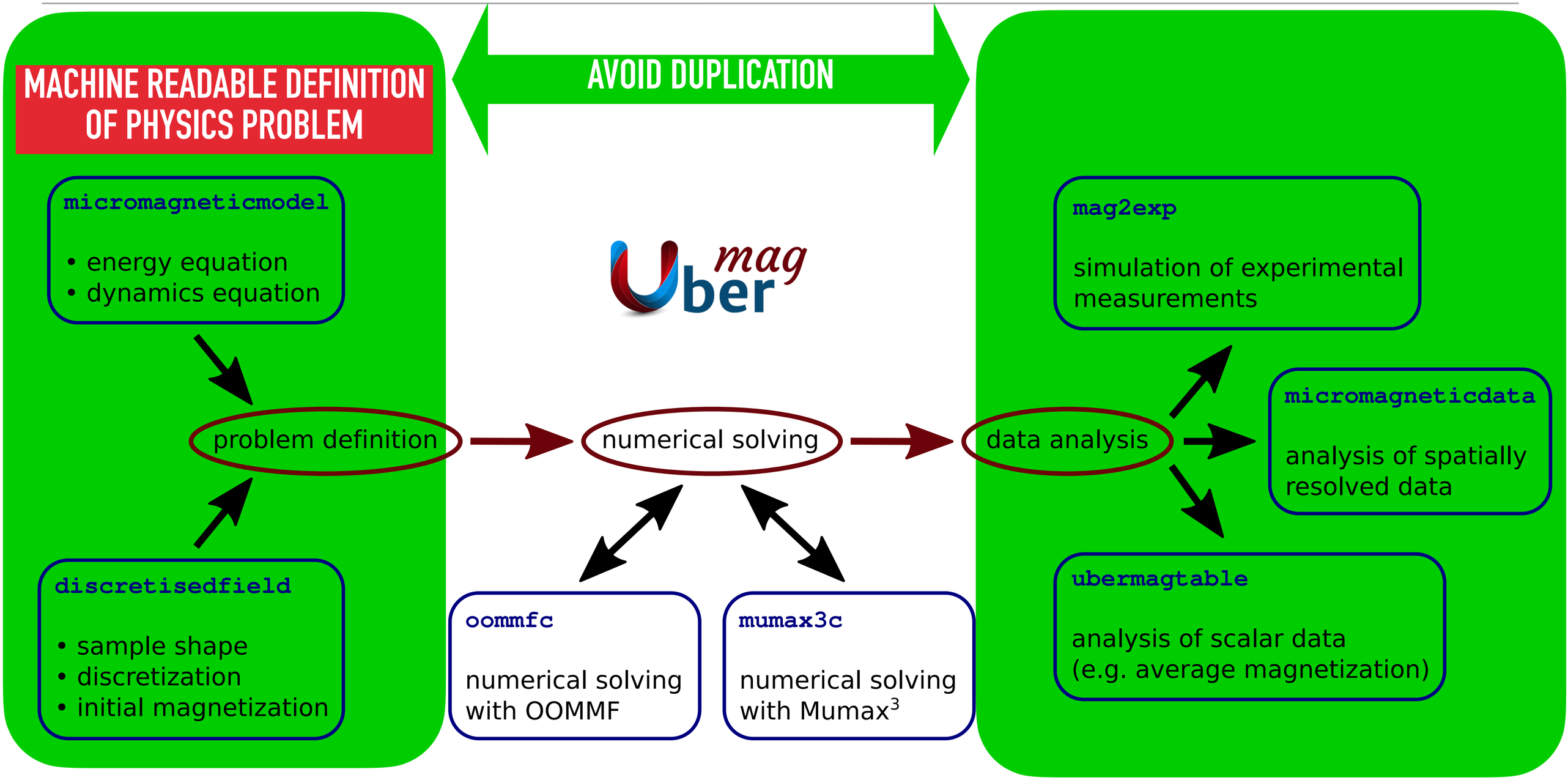
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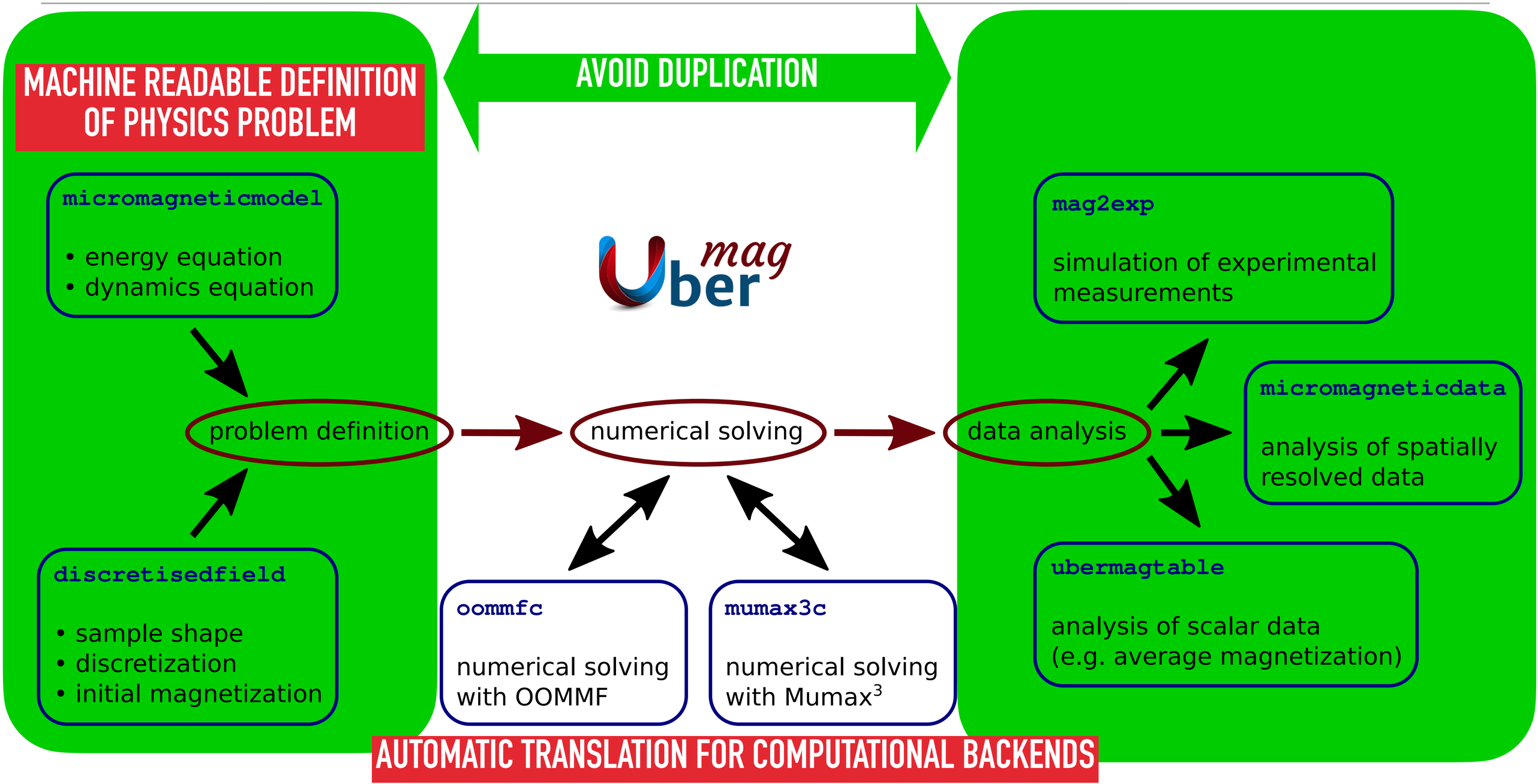
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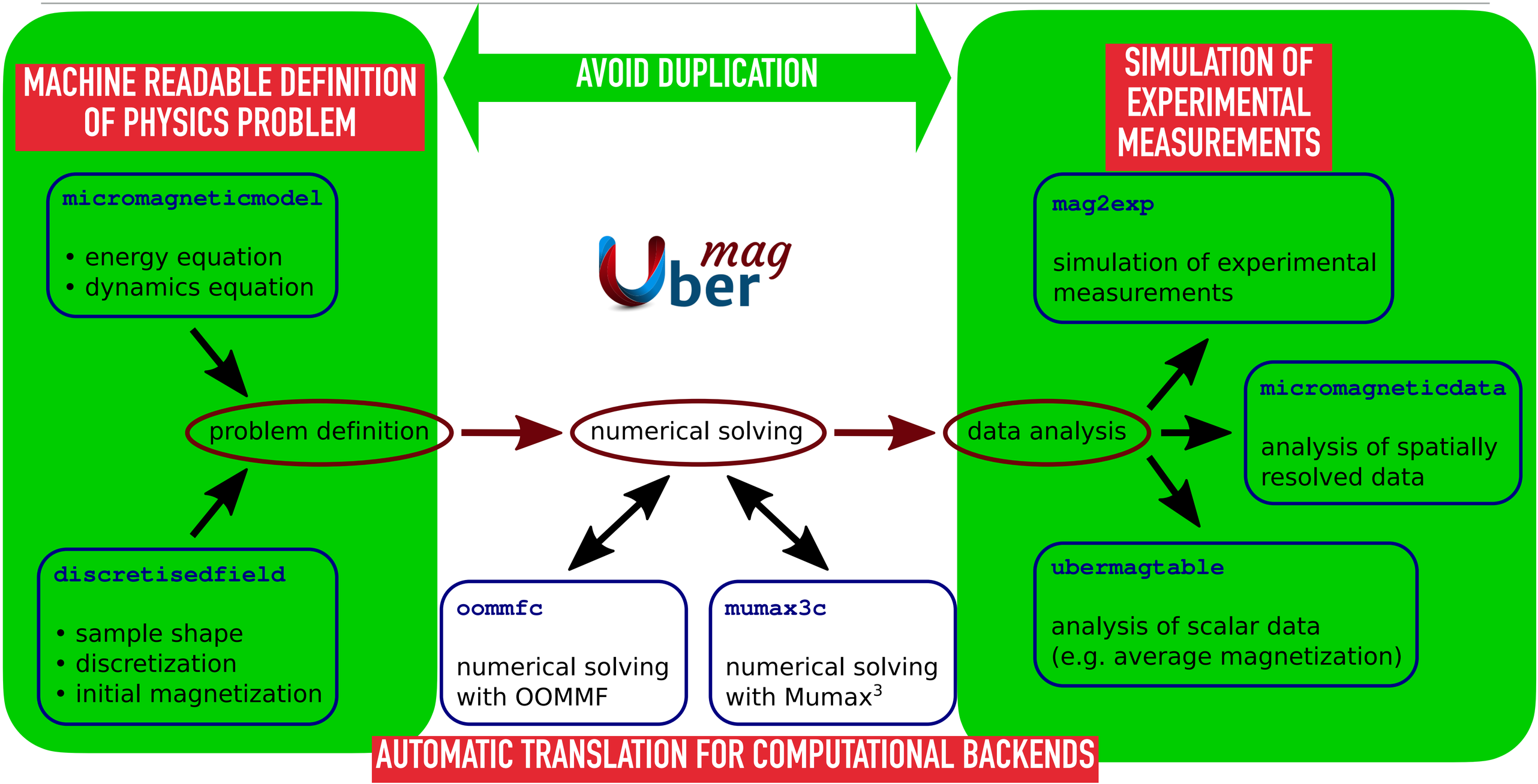
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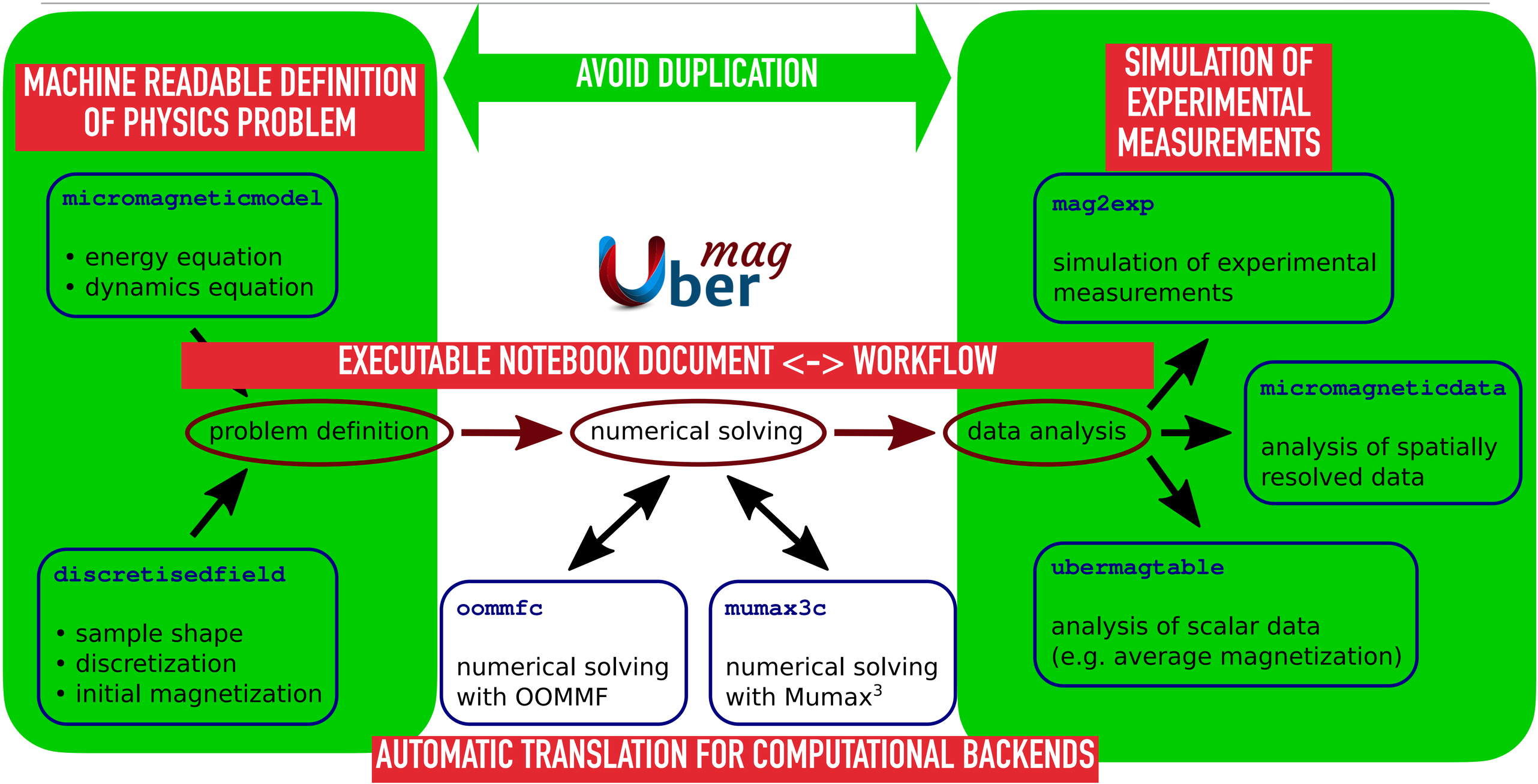
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AUTOMATIC TRANSLATION FOR COMPUTATIONAL BACKENDS

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

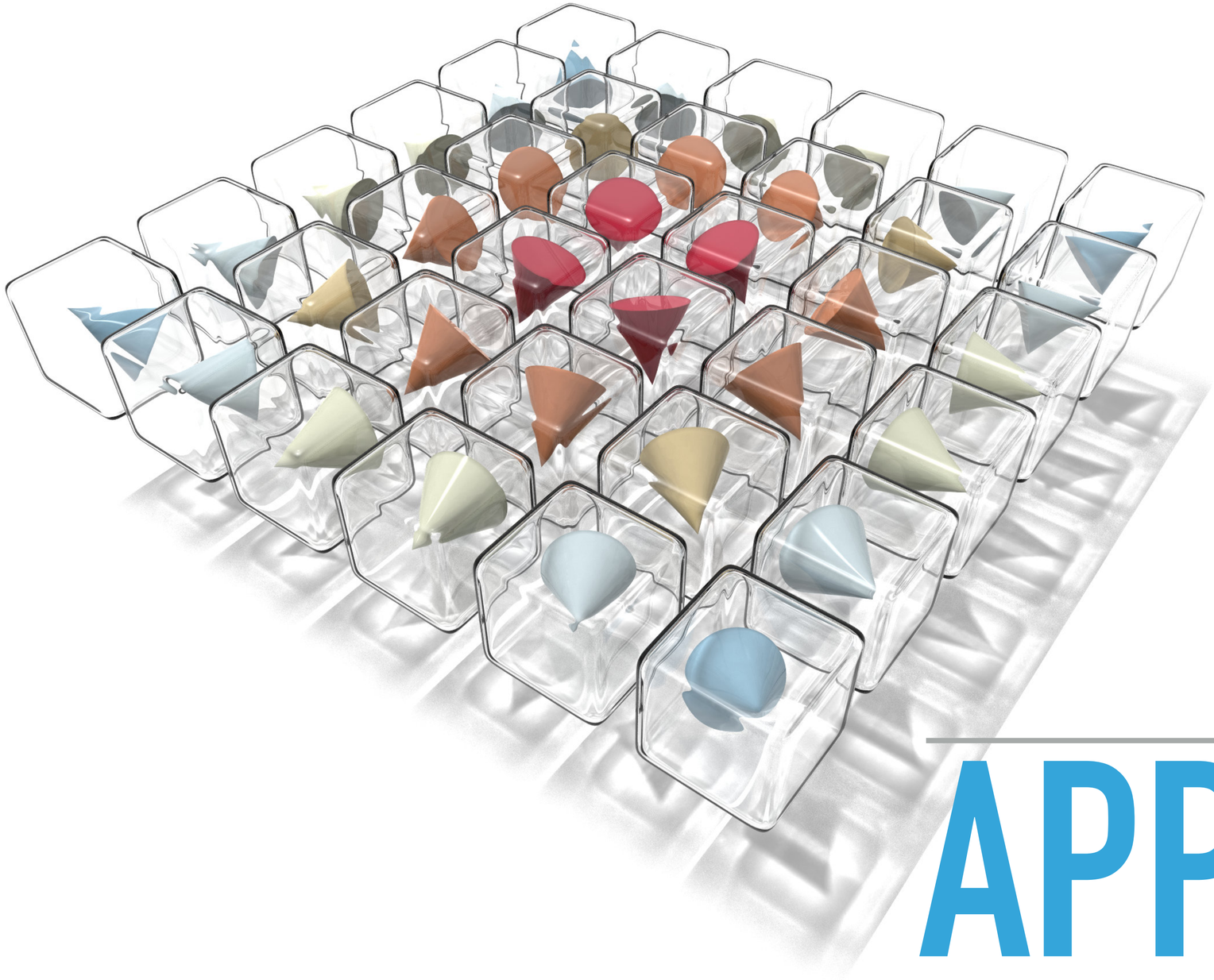
  Get in touch for exploration of options (hans.fangohr@mpsd.mpg.de)

ACKNOWLEDGEMENTS

- Ryan A. Pepper, Thomas Kluyver, James Loudon, Thomas Hicken, David Cortés Ortuño, Jeroen Mulkers, Jonathan Leliaert
- Financial support
  - EPSRC Programme grant on Skyrmionics (EP/N032128/1)
  - Horizon 2020 European Research Infrastructure OpenDreamKit project (Project ID 676541).
  - Fonds Wetenschappelijk Onderzoek (FWO-Vlaanderen) Project No. G098917N

Workshop materials: https://tinyurl.com/solskymag22-ubermag

Contact: hans.fangohr@mpsd.mpg.de



APPENDIX

RELEVANT REFERENCES

- 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, etal, *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)