CF-03 Python interface for OOMMF

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Overview – JOOMMF Project

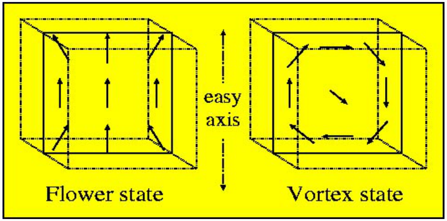
- Towards embedding OOMMF into the Jupyter Notebook ($\rightarrow$ J-OOMMF)
- Step 1: Drive OOMMF through Python interface
- Step 2: Develop data analysis tools
- Step 3: Interactive documentation, micromagnetic tutorial, reproducibility

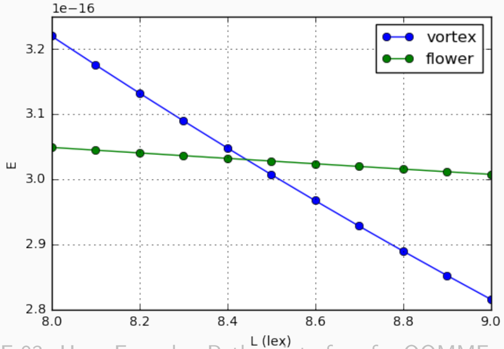
Status

Step 1 Prototype completed

- Python interface for OOMMF:
- "OOMMF Calculator" $\equiv$ OOMMFC

Standard Problem 3





Full problem specification:
`http://www.ctcms.nist.gov/~rdm/spec3.html`

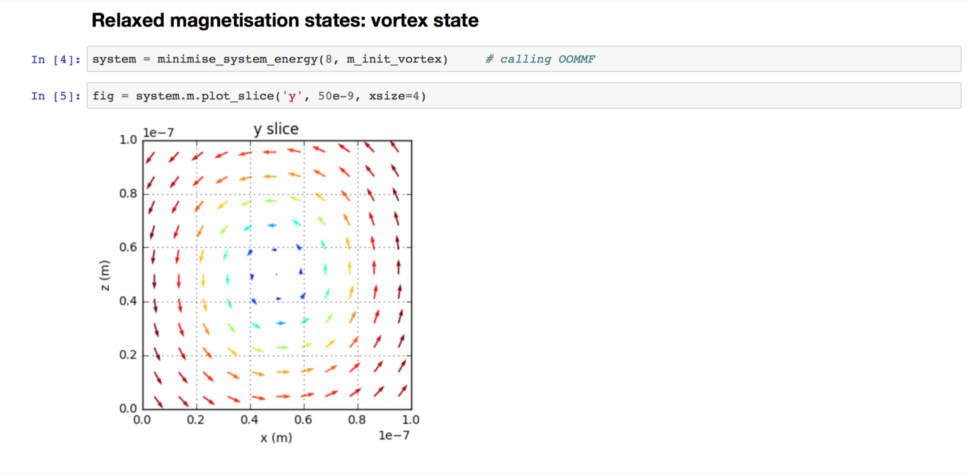
Live demonstration 1

```
In [1]: import oommfc as oc                # access to OOMMF Calculator

        import discretisedfield as df      # other setup to keep the next slides brief
        import numpy as np
        from math import sin, cos, pi, sqrt
        import matplotlib.pyplot as plt
        %matplotlib inline
```

Micromagnetic standard problem 3

```
In [2]: def m_init_flower(pos):
            """Given a pos vector pos = (x, y, z), return the magnetisation
            vector (mx, my, mz) for that position."""
            x, y, z = pos[0]/1e-9, pos[1]/1e-9, pos[2]/1e-9
            # flower pattern:
            mx = 0
            my = 2 * z - 1
            mz = -2 * y + 1
            norm_squared = mx**2 + my**2 + mz**2
            if norm_squared <= 0.05:
                return (1, 0, 0)
            else:
                return (mx, my, mz)

        def m_init_vortex(pos):
            """Given a pos vector pos = (x, y, z), return the magnetisation
            vector (mx, my, mz) for that position."""
            x, y, z = pos[0]/1e-9, pos[1]/1e-9, pos[2]/1e-9
            # vortex pattern
            mx = 0
            my = sin(pi/2 * (x-0.5))
            mz = cos(pi/2 * (x-0.5))

            return (mx, my, mz)
```

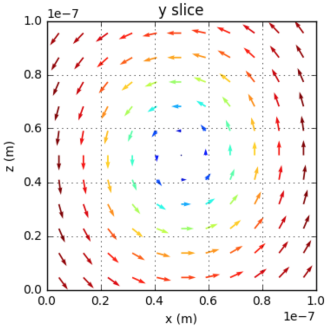
Live demonstration 2



Relaxed magnetisation states: vortex state

```
In [4]: system = minimise_system_energy(8, m_init_vortex)      # calling OOMMF
```

```
In [5]: fig = system.m.plot_slice('y', 50e-9, xsize=4)
```

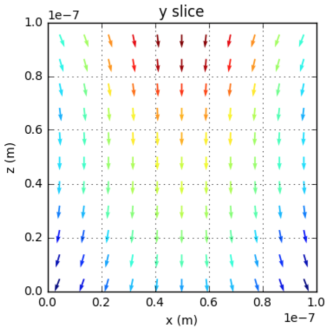


Live demonstration 3

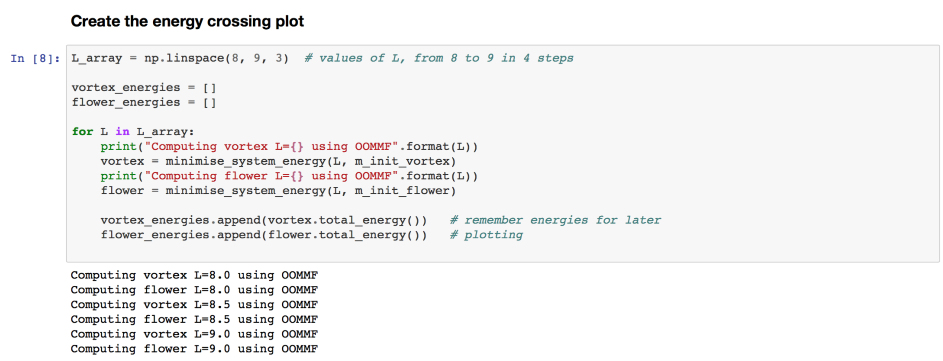
Flower state:

```
In [6]: system = minimise_system_energy(8, m_init_flower)
```

```
In [7]: fig = system.m.plot_slice('y', 50e-9, xsize=4)
```



Live demonstration 4



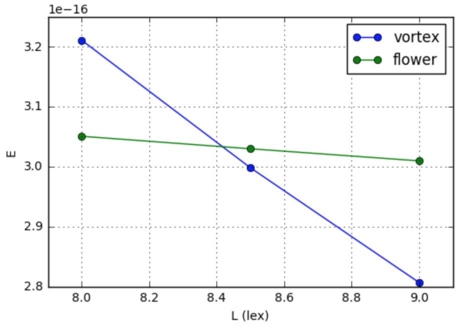
Create the energy crossing plot

In [8]:
```
L_array = np.linspace(8, 9, 3)  # values of L, from 8 to 9 in 4 steps

vortex_energies = []
flower_energies = []

for L in L_array:
    print("Computing vortex L={} using OOMMF".format(L))
    vortex = minimise_system_energy(L, m_init_vortex)
    print("Computing flower L={} using OOMMF".format(L))
    flower = minimise_system_energy(L, m_init_flower)

    vortex_energies.append(vortex.total_energy())   # remember energies for later
    flower_energies.append(flower.total_energy())   # plotting
```

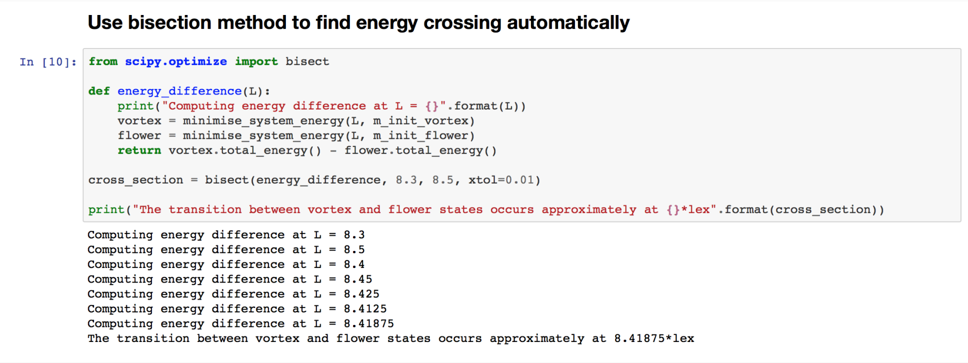
```
Computing vortex L=8.0 using OOMMF
Computing flower L=8.0 using OOMMF
Computing vortex L=8.5 using OOMMF
Computing flower L=8.5 using OOMMF
Computing vortex L=9.0 using OOMMF
Computing flower L=9.0 using OOMMF
```

Live demonstration 5

In [9]:
```
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([7.9, 9.1])
plt.grid()
plt.legend();
```



Live demonstration 6



Use bisection method to find energy crossing automatically

In [10]:
```
from scipy.optimize import bisect

def energy_difference(L):
    print("Computing energy difference at L = {}".format(L))
    vortex = minimise_system_energy(L, m_init_vortex)
    flower = minimise_system_energy(L, m_init_flower)
    return vortex.total_energy() - flower.total_energy()

cross_section = bisect(energy_difference, 8.3, 8.5, xtol=0.01)

print("The transition between vortex and flower states occurs approximately at {}*lex".format(cross_section))
```

```
Computing energy difference at L = 8.3
Computing energy difference at L = 8.5
Computing energy difference at L = 8.4
Computing energy difference at L = 8.45
Computing energy difference at L = 8.425
Computing energy difference at L = 8.4125
Computing energy difference at L = 8.41875
The transition between vortex and flower states occurs approximately at 8.41875*lex
```

Benefits

Present

- OOMMF simulation study in single (Python) file
- Multiple simulation runs within the same script
- Exploit existing libraries and tools (root finding)

Future

- Embedding interactive simulation data analysis, and visualisation
- Reproducibility
- Interactive documenation
- ...

How does the interface to OOMMF work?

Via MIF files

1. write MIF file
2. execute OOMMF
3. read output files

Why ?

- most robust approach
- see `https://arxiv.org/abs/1609.07432` for details

How to install?

1. Need OOMMF natively installed
   (and set variable `OOMMFTCL` to point to `oommf.tcl` file)
   or
   Docker (`http://docker.com`)
2. Need Python (Suggest Anaconda distribution)
3. Install oommfc via

   ```
   $> pip install oommfc
   ```

Is it ready to use?

Software ready to use?

- Yes(-ish)
- interface may change, although we try to avoid it
- beta users and questions welcome

Installation and support workshop for OOMMFC

- Wednesday 17:00 - 19:00 (today)
- Thursday 17:00 - 19:00 (tomorrow)

Outside "Galerie 4" on Level 2, drop-in anytime

Summary

Python interface for OOMMF (OOMMF Calculator)

- part of JOOMMF Project
- invite the community to engage
  - with ideas, questions and bug reports
  - subscribe to `joommf-news` mailing list
  - come to workshop tonight/tomorrow
- http://joommf.github.io

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