# Generating skyrmions using VAMPIRE (application to customised .ucf)

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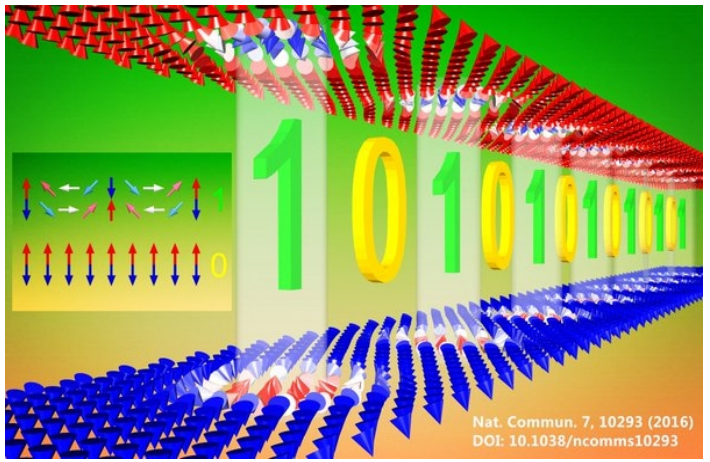
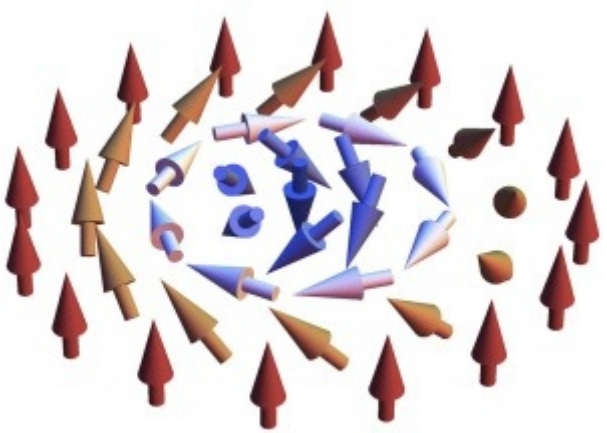
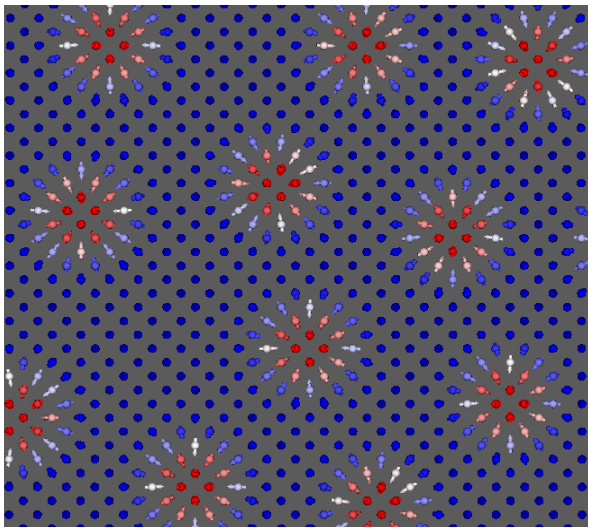
# Magnetic Skyrmions





- Skyrmions -chiral nanoscale bubles;
  -high tolerance to material defects as they are topologically protected;
  -propagation under spin-polarized currents;

# Outline

- How to create your own unit cell file;
- Exchange tensor and  Dzyaloshinskii-Moryia interaction (DMI);
- Skyrmion generation;

# Dzyaloshinskii-Moryia interaction (DMI)

$$\mathscr{H}_{exch} = -\frac{1}{2}\sum_{i\neq j} \mathbf{S}_i^{\alpha}\, \mathscr{J}_{ij}^{\alpha\beta}\, \mathbf{S}_j^{\beta}\,, \quad \alpha,\beta = x,y,z \qquad (1)$$

$$\mathscr{H}_{DM} = \mathbf{D}_{ij}\cdot(\mathbf{S}_i \times \mathbf{S}_j) \qquad (2)$$

$$\mathscr{J}_{ij} = J_{ij}\mathbf{I} + \mathscr{J}_{ij}^{S} + \mathscr{J}_{ij}^{A} \qquad (3)$$

$$J_{ij} = \frac{1}{3}Tr(\mathscr{J}_{ij}),\ \mathscr{J}_{ij}^{S} = \frac{\mathscr{J}_{ij} + \mathscr{J}_{ij}^{t}}{2} - J_{ij}\mathbf{I},\ \mathscr{J}_{ij}^{A} = \frac{\mathscr{J}_{ij} - \mathscr{J}_{ij}^{t}}{2}, \qquad (4)$$

$$D_{ij}^{x} = \frac{\mathscr{J}_{ij}^{yz} - \mathscr{J}_{ij}^{zy}}{2},\ D_{ij}^{y} = \frac{\mathscr{J}_{ij}^{zx} - \mathscr{J}_{ij}^{xz}}{2},\ D_{ij}^{z} = \frac{\mathscr{J}_{ij}^{xy} - \mathscr{J}_{ij}^{yx}}{2} \qquad (5)$$

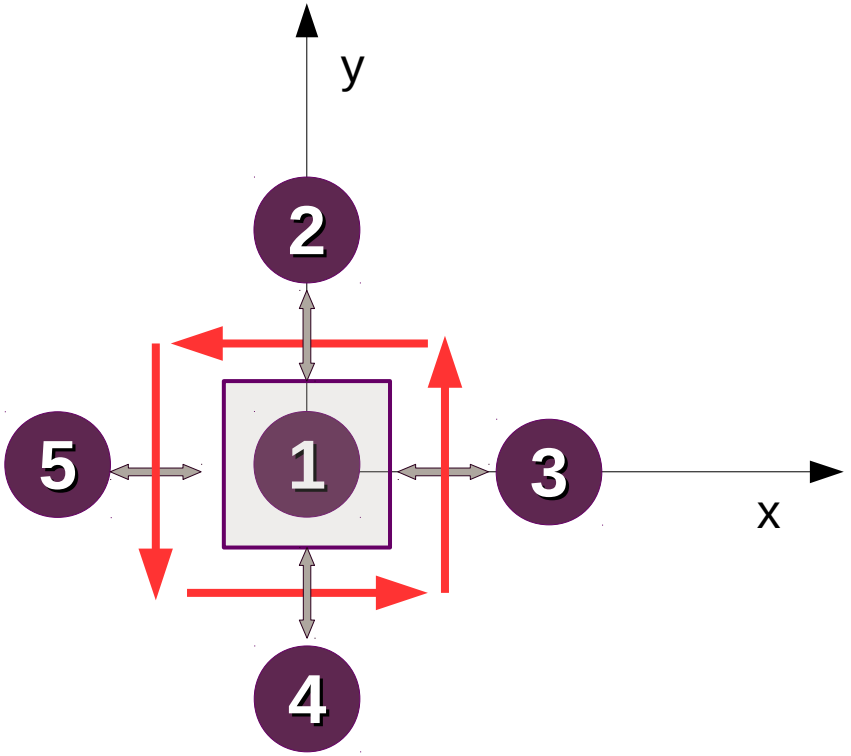
$$\mathscr{J}_{\mathbf{ij}}^{\mathbf{A}} = \begin{bmatrix} 0 & D_{ij}^{z} & -D_{ij}^{y} \\ -D_{ij}^{z} & 0 & D_{ij}^{x} \\ D_{ij}^{y} & -D_{ij}^{x} & 0 \end{bmatrix} \qquad (6)$$

$$\mathbf{D}_{ij}^{k} = D^{k}\cdot(\mathbf{z}\times\mathbf{u}_{ij})$$

# Simple cubic lattice

**1-5**
D=(0,-1,0)

**1-4**
D=(1,0,0)




**1-2**
D=(-1,0,0)

**1-3**
D=(0,1,0)

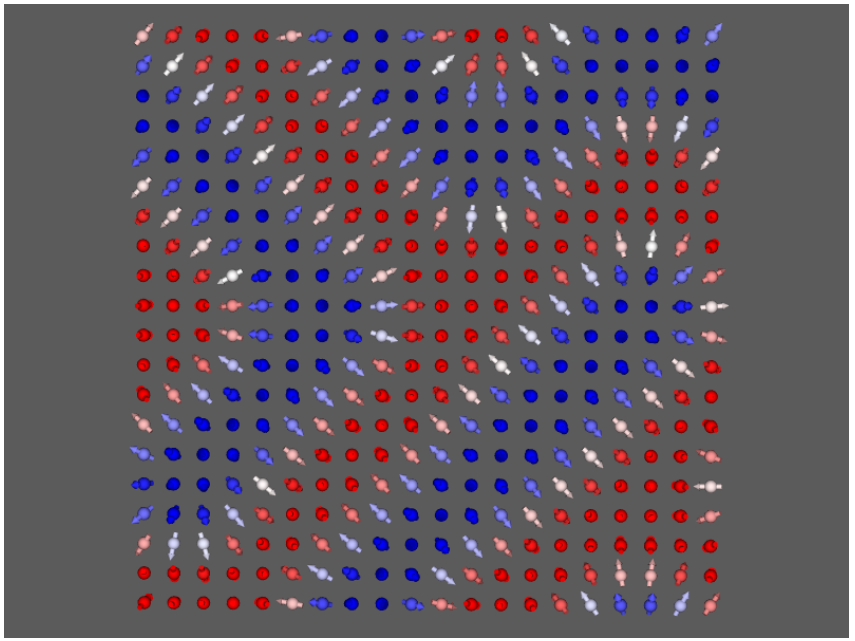
$$\mathbf{D}_{ij}^{k} = D^{k} \cdot (\mathbf{z} \times \mathbf{u}_{ij})$$

DMI unit vector

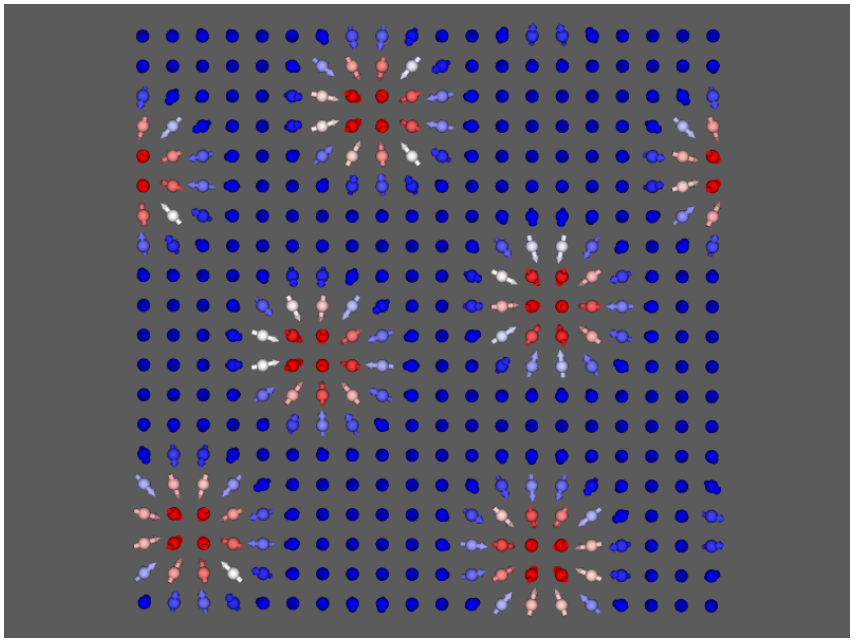
Link

# Ground-state

- Zero Field Cooling (stripe domains)



- Field Cooling (4T-skyrmions)

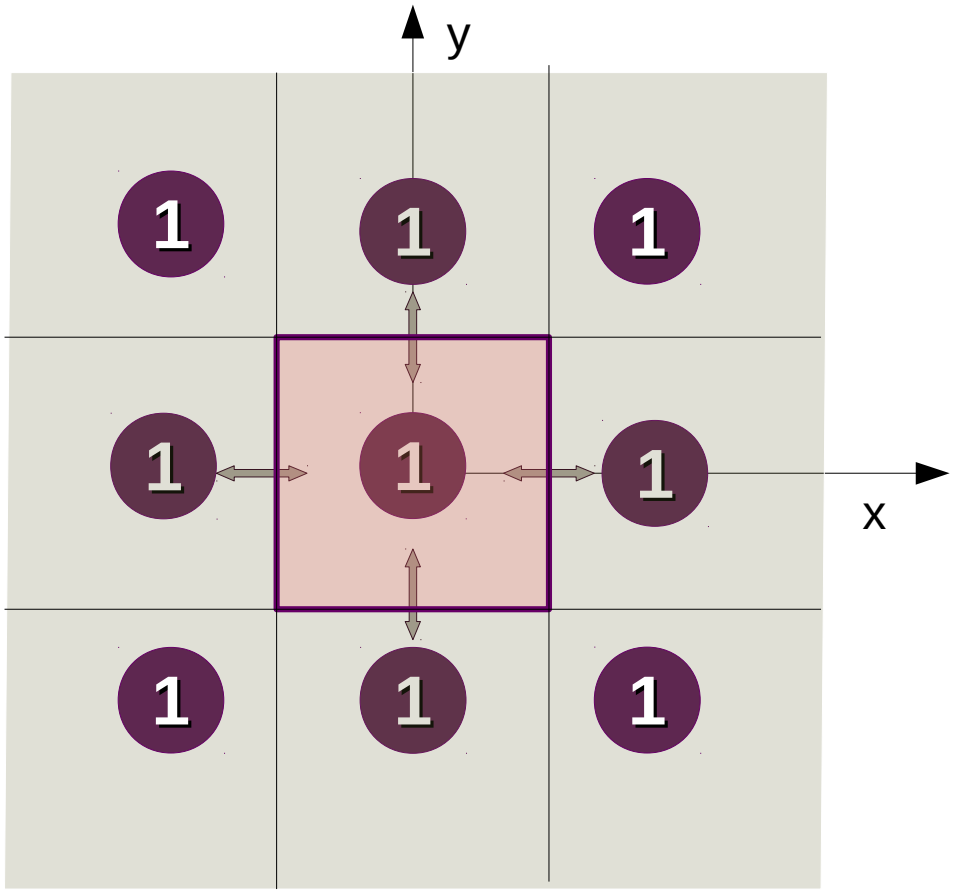


# Steps to follow

1) Create system

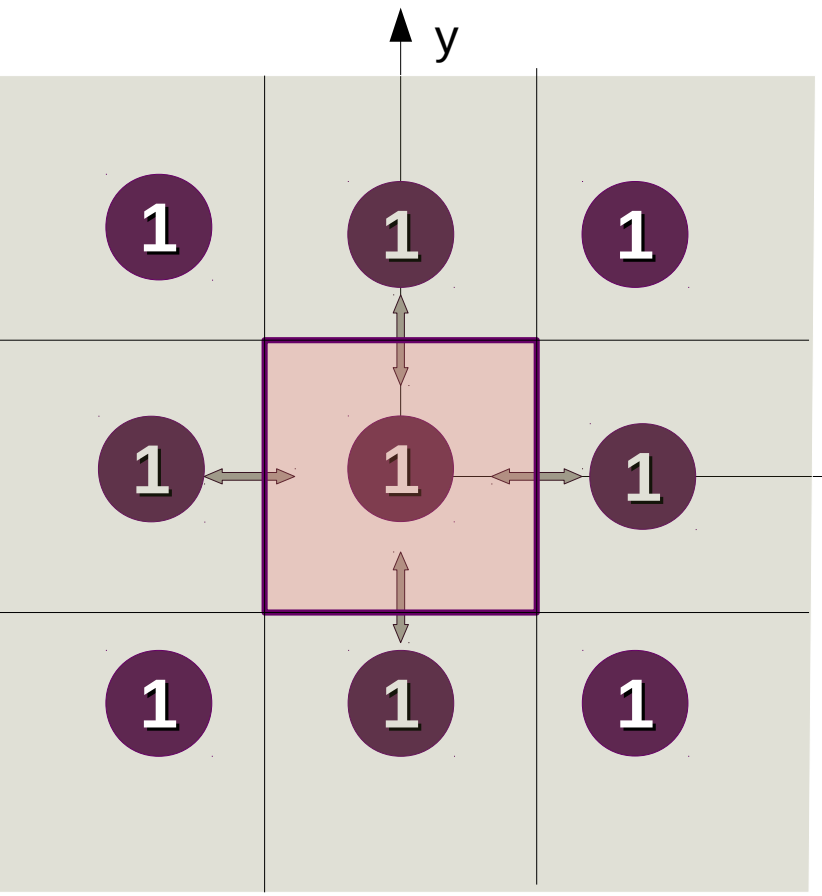
- Start from a unit cell of 1 atom.
- Replicate the system to create the super-cell for PBC.
- Calculate nearest neighbours.
- Write the code as generally as possible.

2) Calculate DMI vectors



# Unit cell file .ucf

Simple cubic.ucf




```
# Unit cell size:
3.54 3.54 3.54
# Unit cell vectors:
1.0 0.0 0.0
0.0 1.0 0.0
0.0 0.0 1.0
# Atoms num, id cx cy cz mat lc hc
1
0 0.5 0.5 0.5 0 0 0
# Interactions n exctype, id i j dx dy dz Jij
6
....
0   0   0    1  0  0   11.2e-21
1   0   0   -1  0  0   11.2e-21
2   0   0    0  1  0   11.2e-21
3   0   0    0 -1  0   11.2e-21
4   0   0    0  0  1   11.2e-21
5   0   0    0  0 -1   11.2e-21
i   j
```

Exchange type:

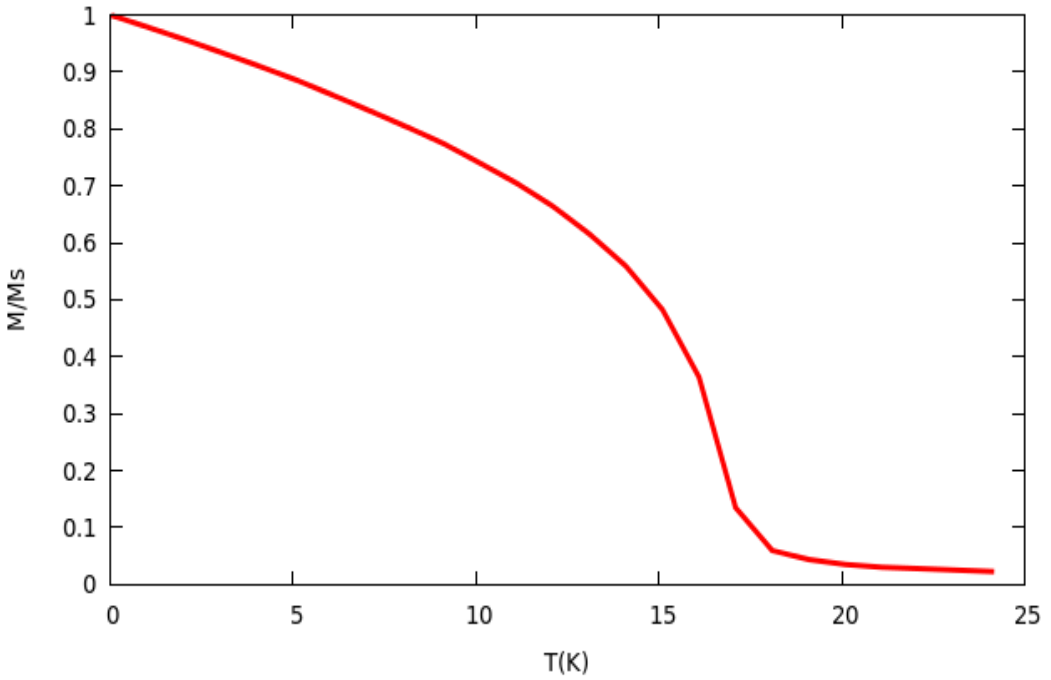
Isotropic
Vectorial
Tensorial

Exchange values (J/link)

Relative distance

# Parameters

- Small Tc for faster simulations;
- Check the critical temperature before the addition of DMI;
- Add a DMI equal in strength with the exchange;




The interaction should look like:

***J* =1.6e-22 J/link**

0 0 0 1 0 0 1.6e-22 0 -1.60e-22 0 1.6e-22 0 1.60e-22 0 1.6e-22

**-Dy** **Dy**

# Field-cooling simulation (input)

```
material:file=Co.mat
material:unit-cell-file = "file.ucf"
#----------------------------------------
# Simulation attributes:
#----------------------------------------
sim:total-time-steps=3000000
sim:equilibration-temperature=30
sim:equilibration-time-steps = 10000
sim:time-steps-increment = 1
sim:time-step=1e-16
```

```
#----------------------------------------
# Program and integrator details
#----------------------------------------

sim:program=field-cool
sim:integrator=llg-heun
```

```
sim:minimum-temperature=0
sim:maximum-temperature=30.0
sim:applied-field-strength=0.0
sim:cooling-time=100!ps
sim:cooling-function = gaussian  !or linear
```

# Field-cooling simulation (input)

```
material:file=Co.mat
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```

```
#----------------------------------------
# Program and integrator details
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sim:program=field-cool
sim:integrator=llg-heun
```

**Set the xyz dimensions in order to have just 1 layer!**

```
sim:minimum-temperature=0
sim:maximum-temperature=30.0
sim:applied-field-strength=0.0
sim:cooling-time=100!ps
sim:cooling-function = gaussian  !or linear
```

# Output (input)

```
#----------------------------------------
# data output
#----------------------------------------
output:output-rate = 10000
output:real-time
output:temperature
output:mean-magnetisation-length
output:magnetisation-length
output:magnetisation
output:mean-susceptibility

config:atoms
config:atoms-output-rate=100000
```

300 points

30 data files with the spins configurations

# Co.mat

```
#==========================================
# Sample vampire material file V3+
#==========================================

#------------------------------------------
# Number of Materials
#------------------------------------------
material:num-materials=1
#------------------------------------------
# Material 1 Cobalt Generic
#------------------------------------------
material[1]:material-name=Co
material[1]:damping-constant=1.0
material[1]:initial-spin-direction=random
material[1]:atomic-spin-moment=1.72 !muB
material[1]:uniaxial-anisotropy-constant=5e-23
```

# .ucf answer

```
#Unit cell size:
2.715     2.715     2.715
#Unit cell vectors:
1     0     0
0     1     0
0     0     1
# Atoms num_atoms, num_materials;id cx cy cz mat cat hcat:
1
0     0     0     0     0     1     0
# Interactions n exctype;  IID i j dx dy dz Jxx Jxy Jxz Jyx Jyy Jyz Jzx Jzy Jzz:
4     tensorial
0     0 0   1 0  0    1.6e-22  0     -1.60e-22      0     1.6e-22     0          1.60e-22        0          1.6e-22
1     0 0   0 1  0    1.6e-22  0     0              0     1.6e-22     -1.60e-22  0               1.60e-22    1.6e-22
2     0 0  -1 0  0    1.6e-22  0     1.60e-220      1.6e-22     0          -1.60e-22       0          1.6e-22
3     0 0   0 -1 0    1.6e-22  0     0              0     1.6e-22     1.60e-22   0               -1.60e-22   1.6e-22
```

# Field-cooling simulation (input)

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sim:minimum-temperature=0
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sim:applied-field-strength=0.0
sim:cooling-time=100!ps
sim:cooling-function = gaussian
```

```
#----------------------------------------
# Program and integrator details
#----------------------------------------
```

```
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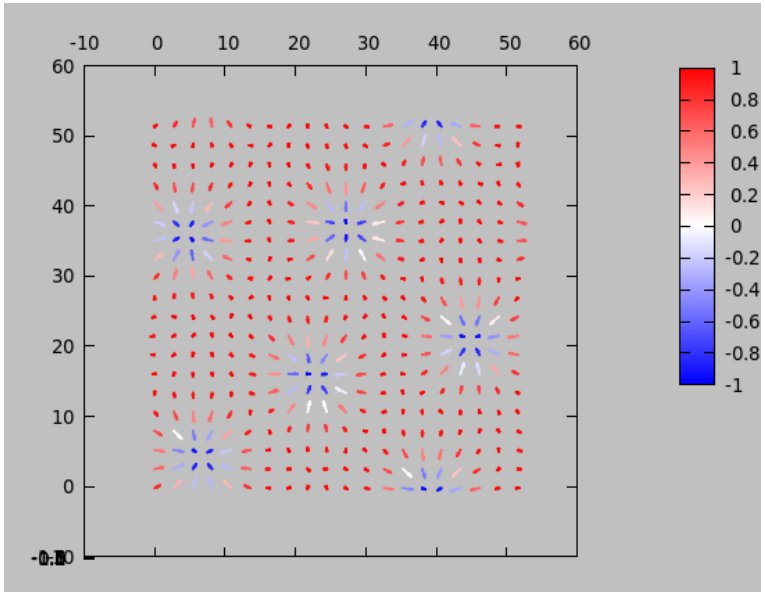
sim:integrator=llg-heun
```

# Plotting and animation

## **Gnuplot** alternative




- paste atoms-coords.data spins-00000030.data >> atoms_30.dat

```
gnuplot> set view 0,0
gnuplot> set palette defined (-1 "blue", 0 "white", 1 "red")
gnuplot> set xlabel "x";set ylabel "y"; set zlabel "z"
gnuplot> sp "atoms_30.dat" u 3:4:5:($6):($7):($8):8 w vectors palette lw 1.5 t ""
gnuplot> sp "atoms_30.dat" u 3:4:5:8 w p palette pt 7
```

## **povray**

```
Set_Camera_Sky(<1,0,0>) in spins.pov
povray spins
convert -delay 10 -loop 0 *.png animation.gif
```

# Try different values of:

- Increase size of the system!
- Cooling times; 100 ps; 500 ps etc.
- Applied field;
- Ratio between exchange and DMI;
- Anisotropy constants;