

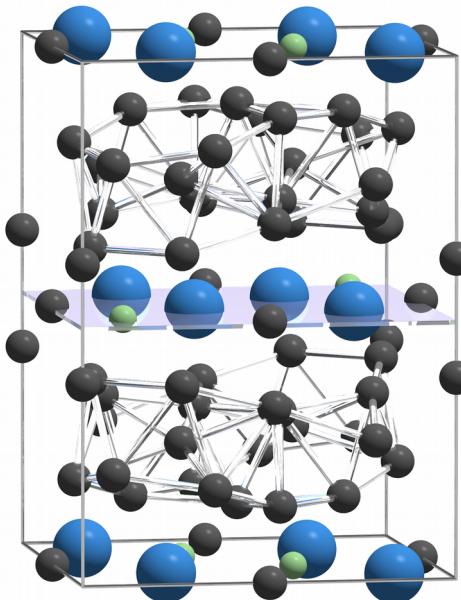
# **Customised unit cell files (\*.ucf)**

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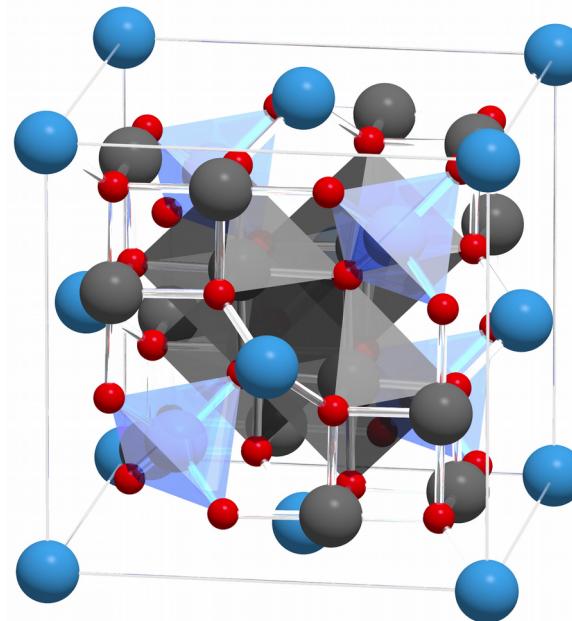
VAMPIRE workshop – 25<sup>th</sup> of July 2019

# Why using customised unit cell files?

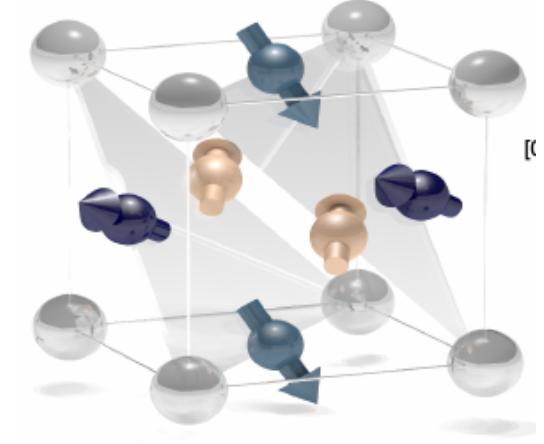
## 1. Complex crystal structures



NdFeB unit cell  
(Image from Richard Evans)



Magnetite  
(Image from Daniel Meilak)

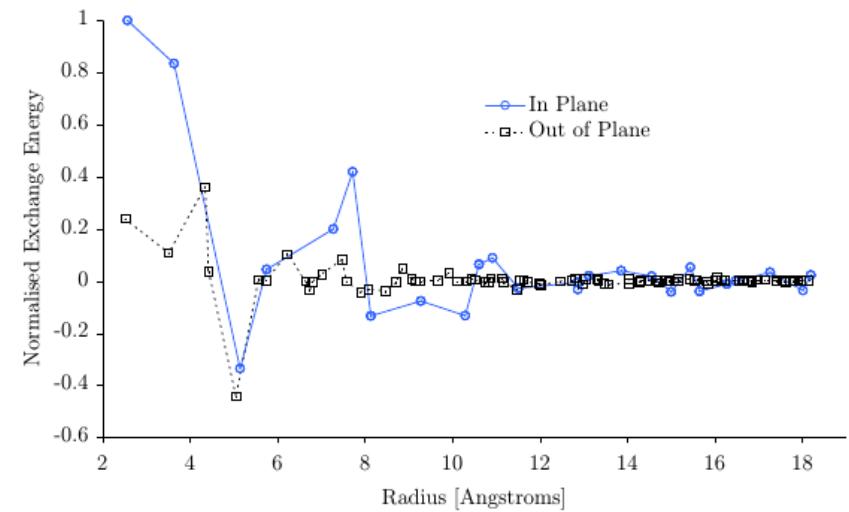
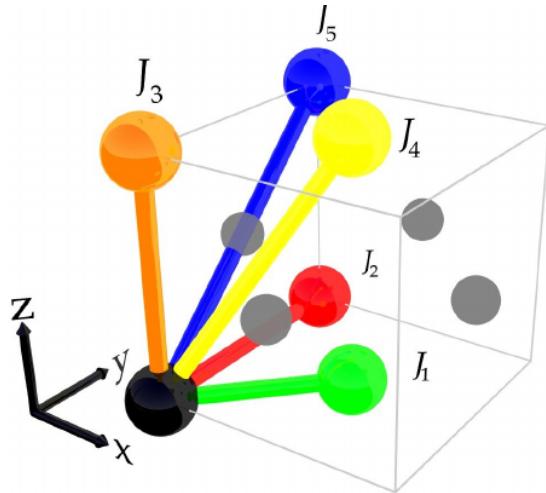


IrMn3  
(Image from Sarah Jenkins))

[1] Westmoreland, S. C., et al. "Multiscale model approaches to the design of advanced permanent magnets." Scripta Materialia 148 (2018): 56-62.

# Why using customised unit cell files?

## 2. Long-range interactions;

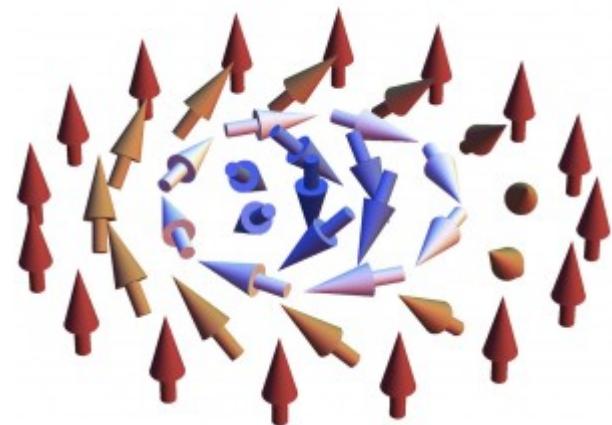


Exemple of FePt interactions;  
(extracted from R.Evans)

# Why using customised unit cell files?

## 3. Full exchange tensor

$$\mathcal{J}_{ij} = \begin{bmatrix} J_{xx} & D_{ij}^z & -D_{ij}^y \\ -D_{ij}^z & J_{yy} & D_{ij}^x \\ D_{ij}^y & -D_{ij}^x & J_{zz} \end{bmatrix}$$



# Why using customised unit cell files?

## 4. Multi-scale modelling

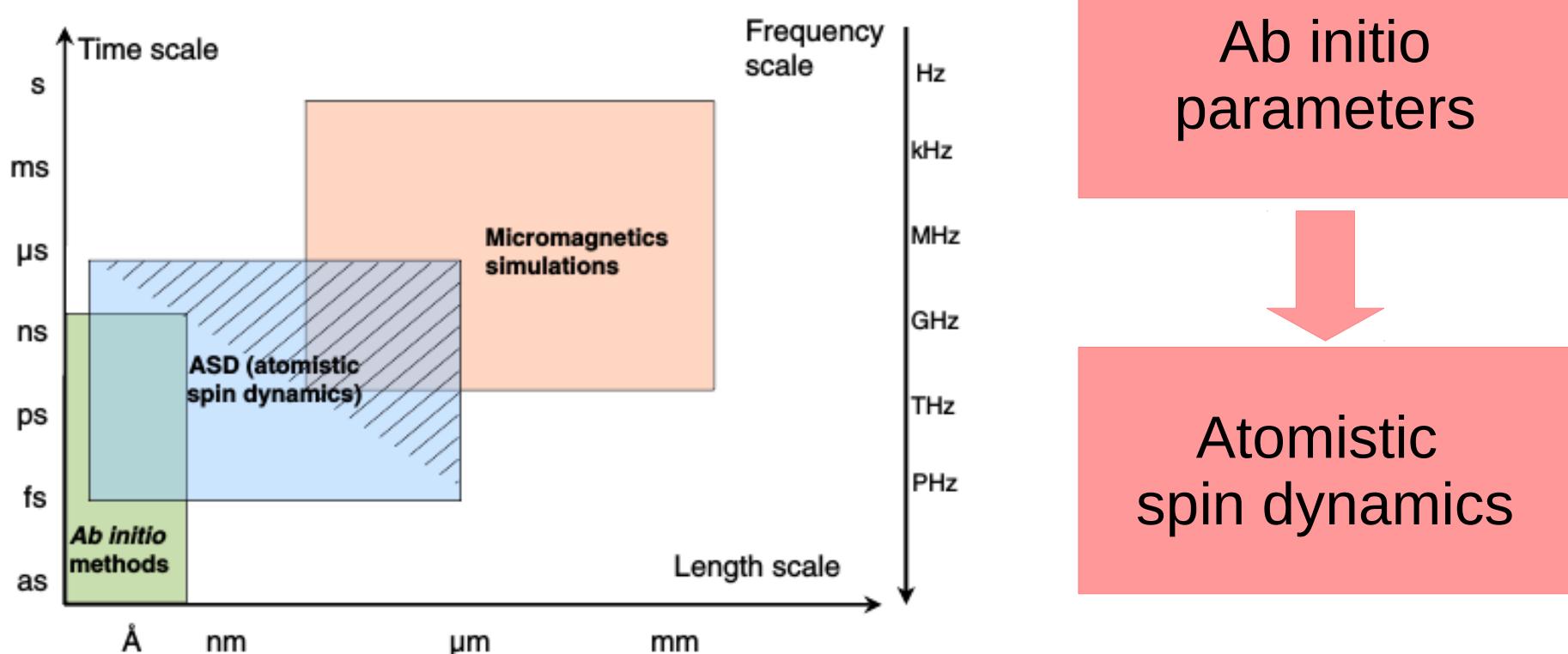
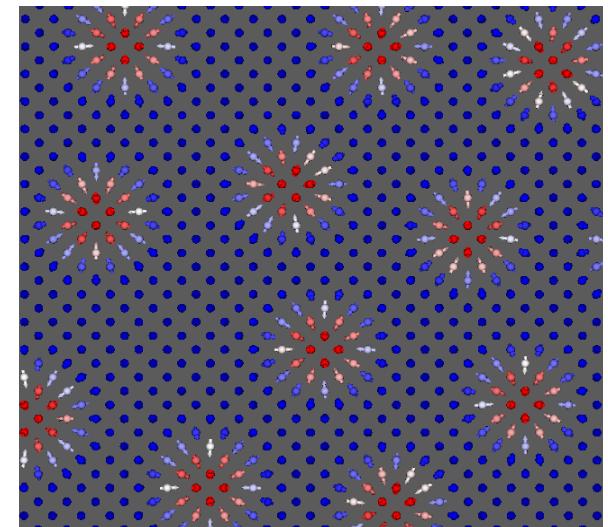
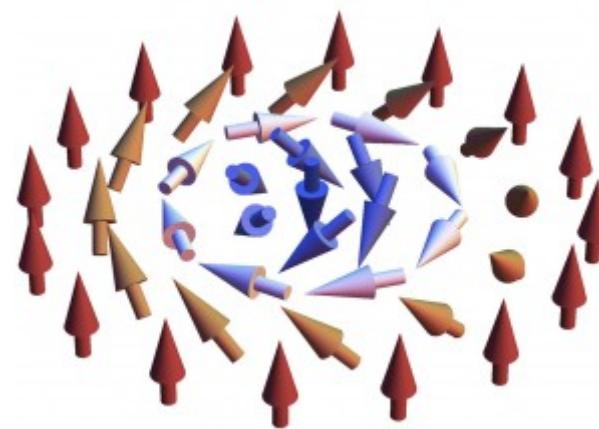
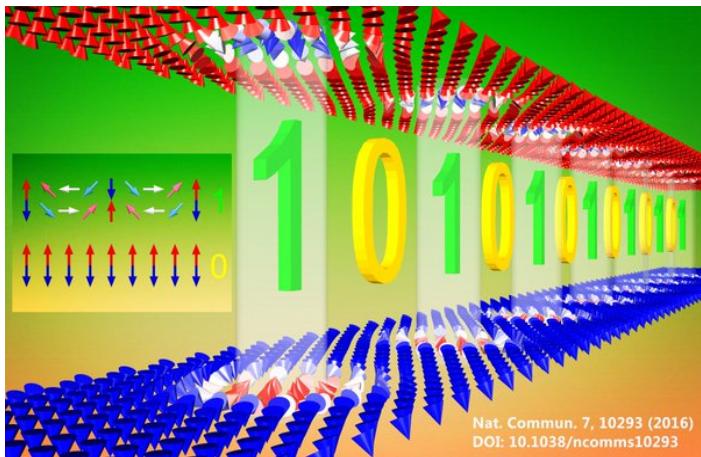


Figure extracted from: Etz, Corina, et al. "Atomistic spin dynamics and surface magnons." Journal of Physics: Condensed Matter 27.24 (2015): 243202.

# Magnetic Skyrmions



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

# Outline

- Overview on magnetic skyrmions;
- Exchange tensor and Dzyaloshinskii-Moryia interaction (DMI);
- Hands on: create your own unit cell file;
- Hands on: Skyrmion generation using unit cell file and in-built DMI interaction;
- Beyond Heisenberg model: Higher order exchange interactions;

# Dzyaloshinskii-Moryia interaction (DMI)

- Originally suggested by Dzyaloshinskii (1957) in an attempt to describe the weak ferromagnetism in  $\alpha\text{-Fe}_2\text{O}_3$  and was derived later on by Moriya (1960);
- Dzyaloshinskii-Moriya interaction (DMI) originates from the antisymmetric part of exchange interaction under the consideration of a strong spin-orbit coupling (SOC) and inversion symmetry.

# Dzyaloshinskii-Moryia interaction (DMI)

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

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

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

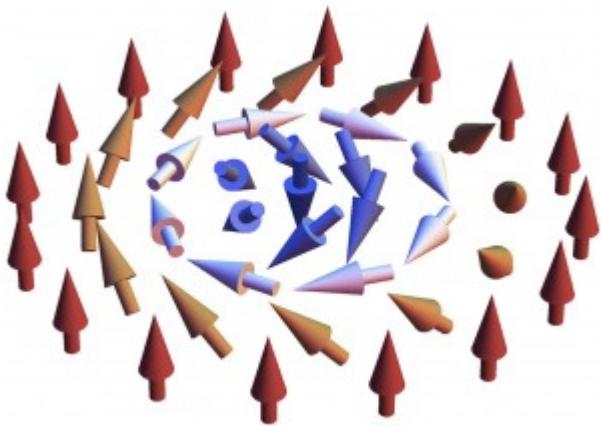
$$J_{ij} = \frac{1}{3} Tr(\mathcal{J}_{ij}), \quad \mathcal{J}_{ij}^S = \frac{\mathcal{J}_{ij} + \mathcal{J}_{ij}^t}{2} - J_{ij} \mathbf{I}, \quad \mathcal{J}_{ij}^A = \frac{\mathcal{J}_{ij} - \mathcal{J}_{ij}^t}{2}, \quad (4)$$

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

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

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

# Simple cubic lattice

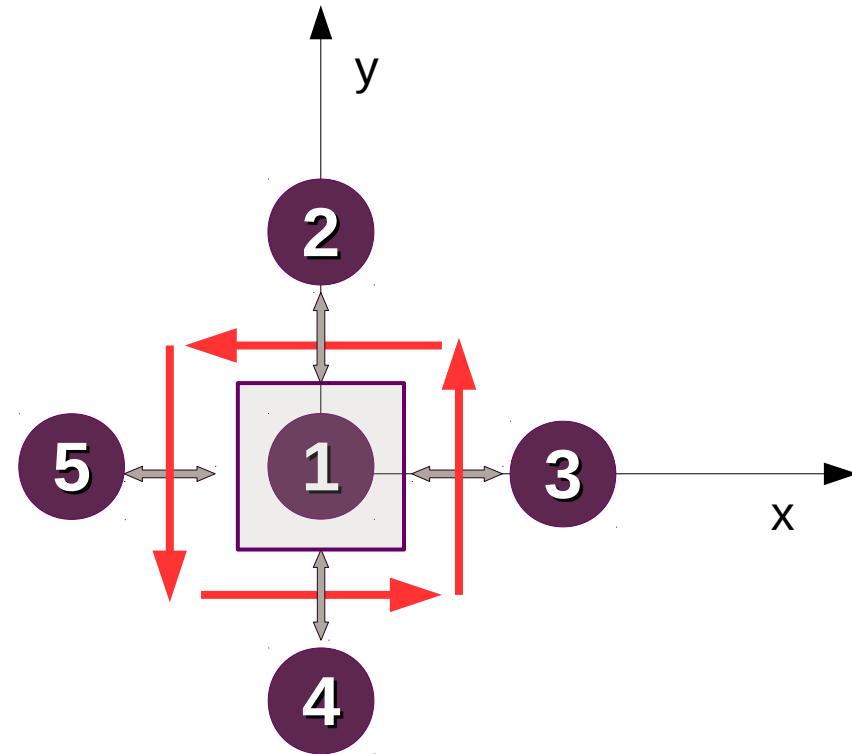


**1-5**  
D=(0,-1,0)

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

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

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



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

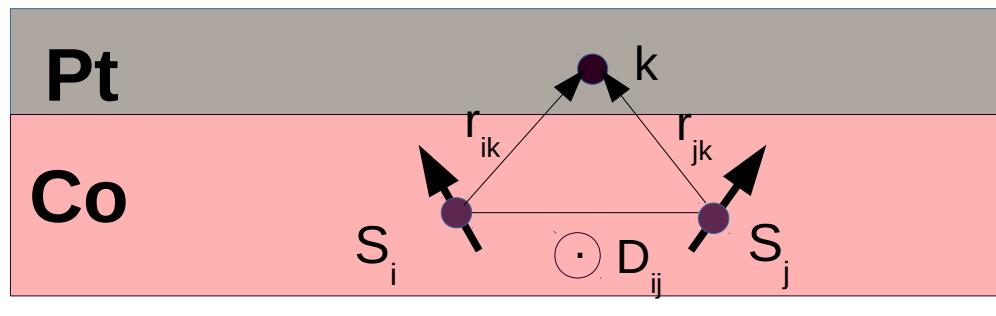
→ DMI unit vector  
↔ Link

# Dzyaloshinskii-Moryia interaction in VAMPIRE

**Method 1** - DMI is included by the user in the exchange tensor in the unit-cell file:

$$\mathcal{J}_{ij}^A = \begin{bmatrix} 0 & D_{ij}^z & -D_{ij}^y \\ -D_{ij}^z & 0 & D_{ij}^x \\ D_{ij}^y & -D_{ij}^x & 0 \end{bmatrix}$$

**Method 2** – in built DMI



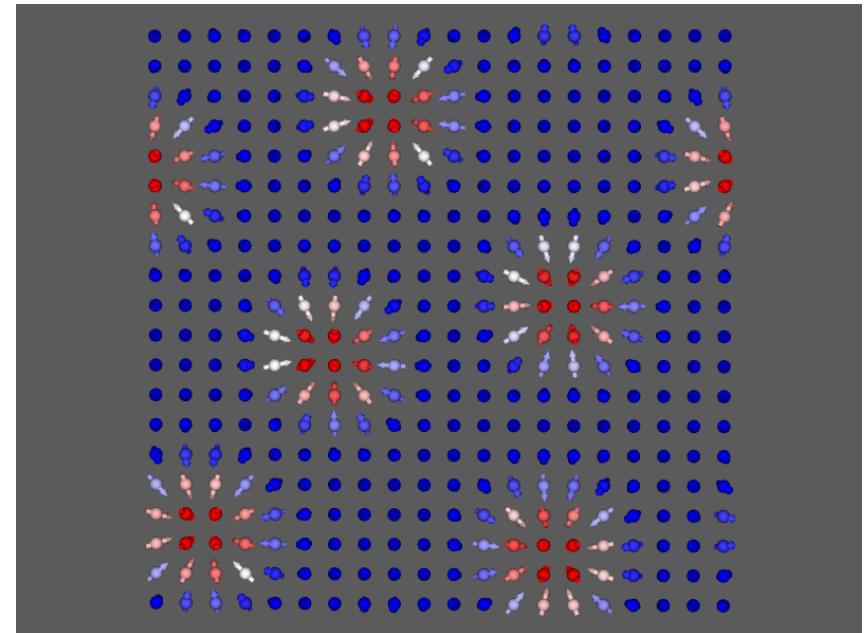
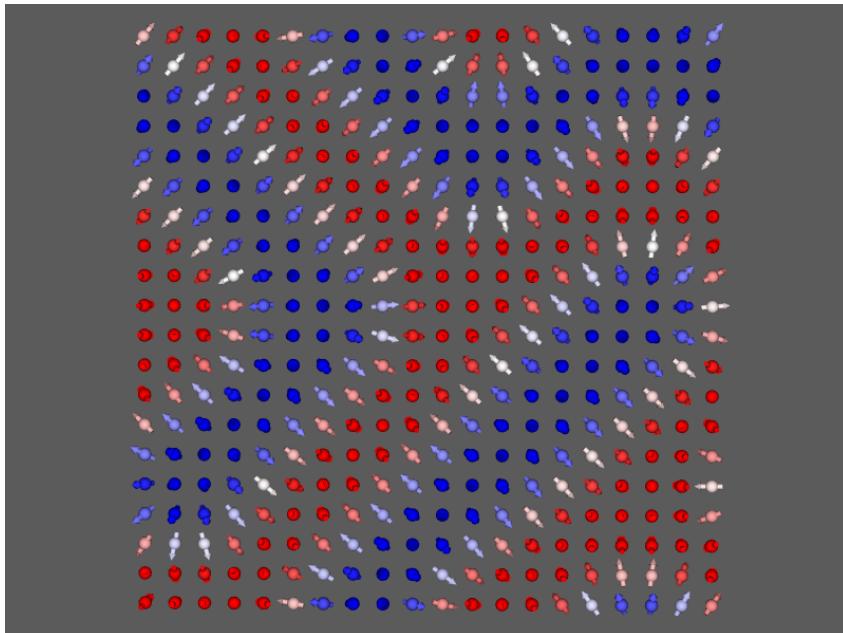
$$(r_{ik}, r_{jk}) < r_c$$

$$\mathbf{D}_{ij} = \mathbf{r}_{ik} \times \mathbf{r}_{jk}$$

$$E_{DMI} = \mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j)$$

# Ground-state

- Zero Field Cooling  
(stripe domains)
- Field Cooling  
(4T-skyrmions)

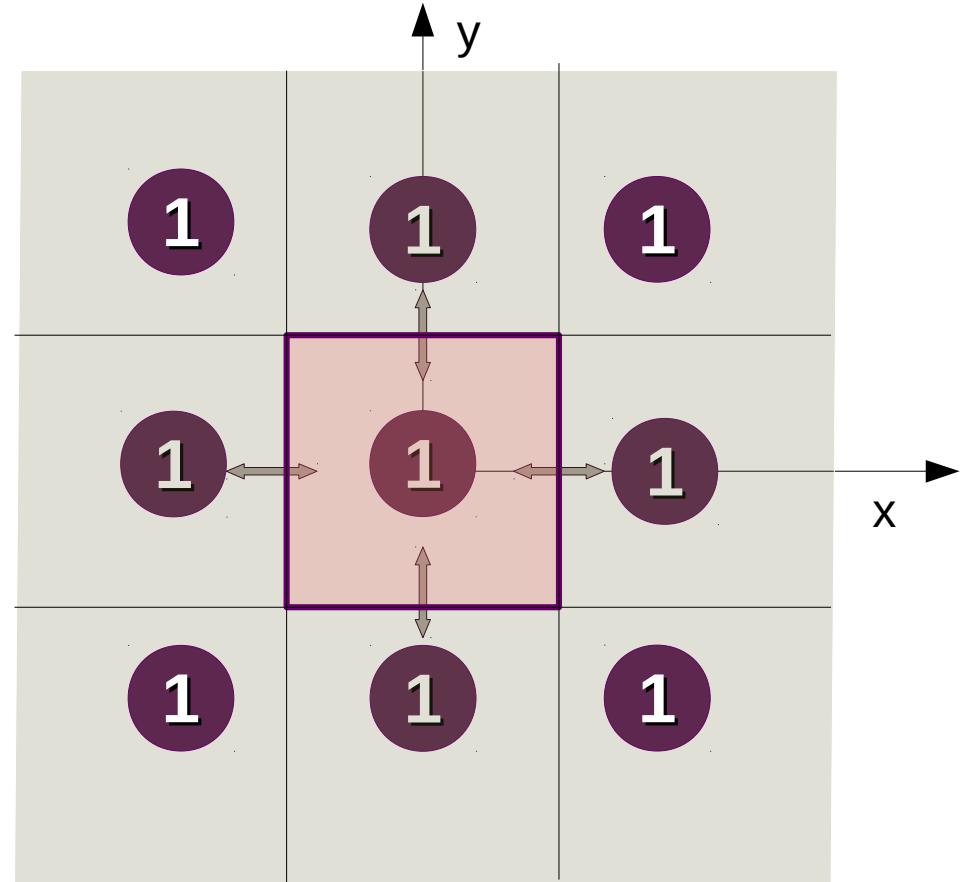


# Create your own unit cell file

## 1) Create system

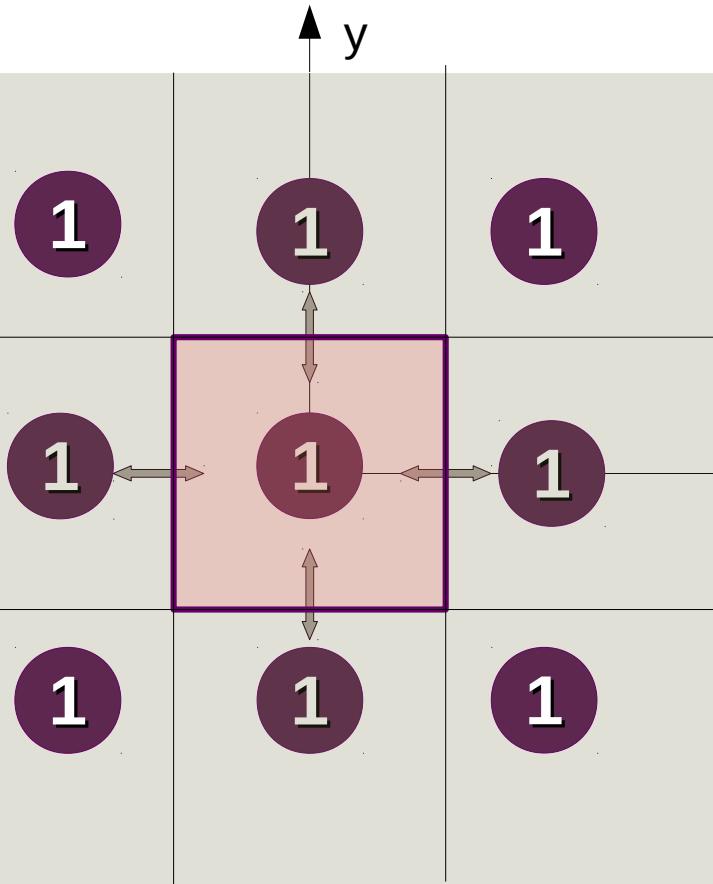
- Start from a unit cell of 1 atom.
- Replicate the system to create the super-cell for PBC.
- Calculate nearest neighbours.
- Write the code as generally as possible.

## 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

Relative distance

Exchange type:

Isotropic

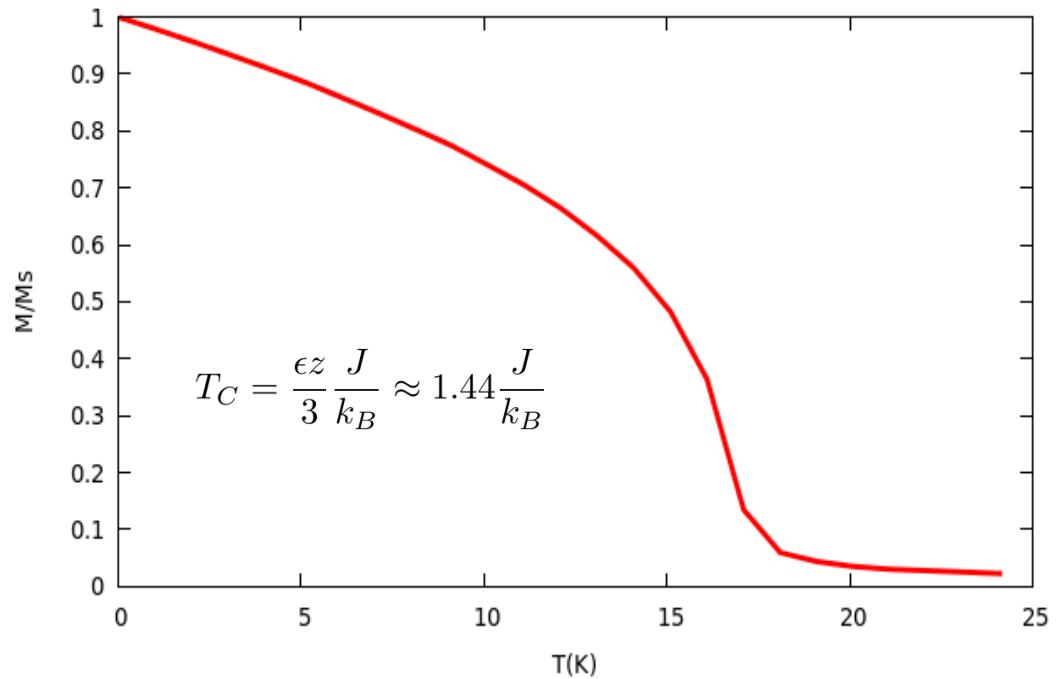
Vectorial

Tensorial

Exchange values (J/link)

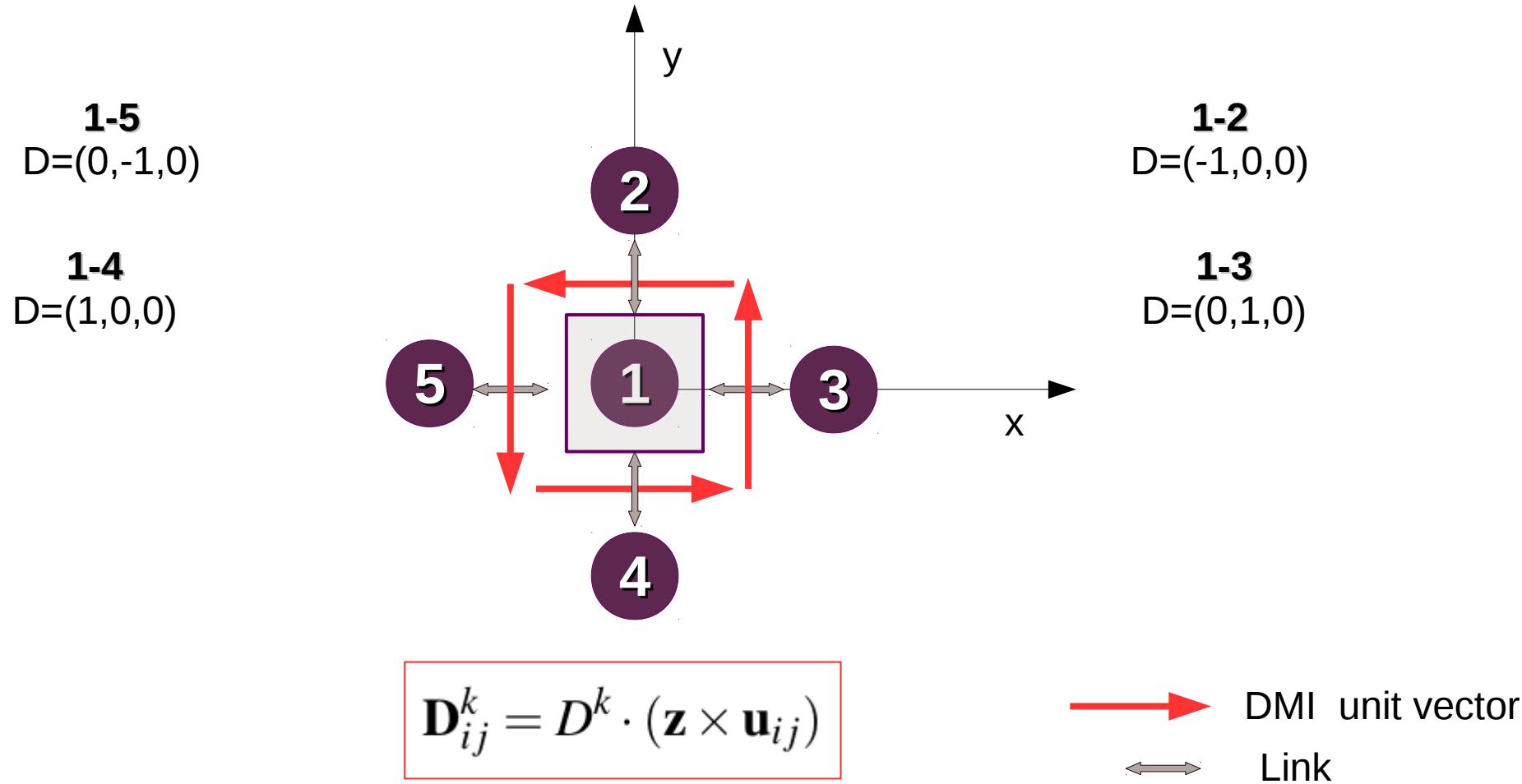
# Generating skyrmions; Setting isotropic exchange;

- Git checkout develop
- Make -B serial -j 8
- Set up a simple cubic system;
- Set small Tc for faster simulations;
- Check magnetisation versus temperature;



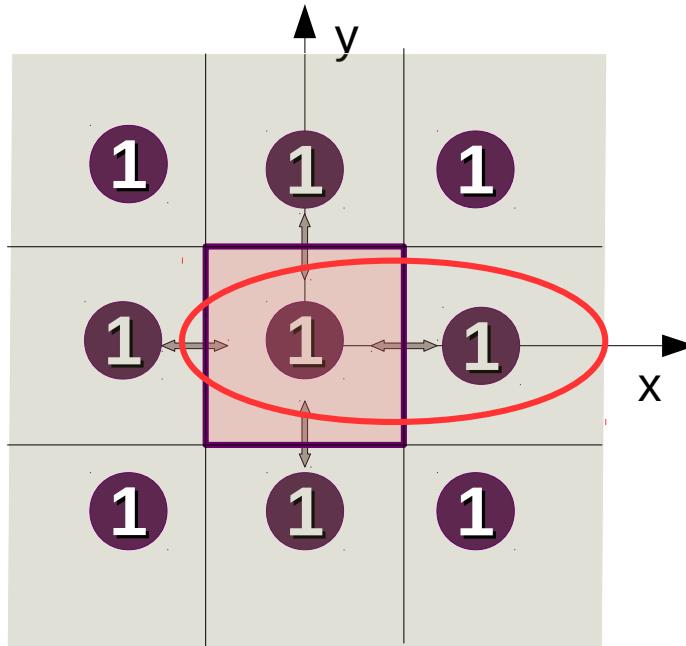
**$J = 1.6 \times 10^{-22} \text{ J/link}, T_c = 16.7 \text{ K}$**

# Simple cubic lattice



# Add DMI

Add DMI interaction in \*.ucf file based on the symmetry of the unit cell you are using;

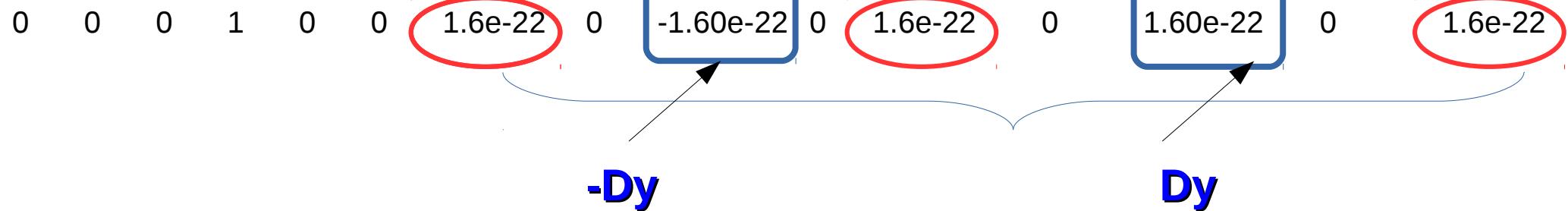


$$\mathbf{D}_{ij}^k = D^k \cdot (\mathbf{z} \times \mathbf{u}_{ij})$$

$$\mathbf{D} = (0, 1, 0)$$

$$\mathcal{J}_{ij} = \begin{bmatrix} J_{xx} & D_{ij}^z & -D_{ij}^y \\ -D_{ij}^z & J_{yy} & D_{ij}^x \\ D_{ij}^y & -D_{ij}^x & J_{zz} \end{bmatrix}$$

The interaction should look like:



# System creation (input)

```
#-----
# Creation attributes:
#-----
#create:crystal-structure=sc
create:periodic-boundaries-x
create:periodic-boundaries-y
#create:periodic-boundaries-z

#-----
# System Dimensions:
#-----
#dimensions:unit-cell-size=1 Å
dimensions:system-size-x = 2!nm
dimensions:system-size-y = 2!nm
dimensions:system-size-z = 0.1!nm
```

**20 x 20 x 1 atoms**

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

# 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
```

**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:

1 1 1

#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 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-22	0	1.6e-22	0	-1.60e-22	0	1.6e-22
3	0	0	0	-1	0	1.6e-22	0	0	1.6e-22	1.60e-22	0	0	-1.60e-22	1.6e-22

# Plotting and animation

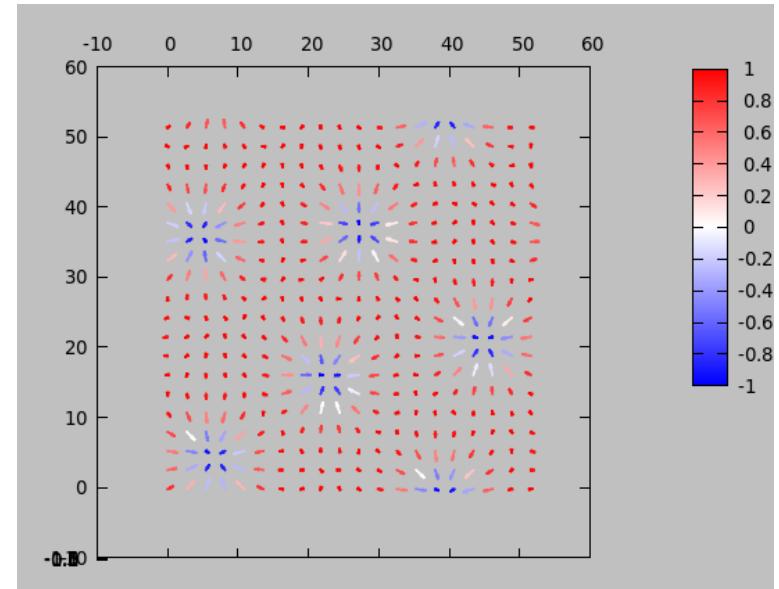
## Gnuplot alternative

- 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
```

Or run sh visualise.sh

```
convert -delay 10 -loop 0 *.png animation.gif
```



# Povray

```
./vdc  
povray spins
```

In: spins.pov

Set\_Camera\_Sky(<1, 0, 0>)

```
#declare sscale0=2.0;           Spin size  
#declare rscale0=1.2;          Atom size  
#declare cscale0=3.54;
```

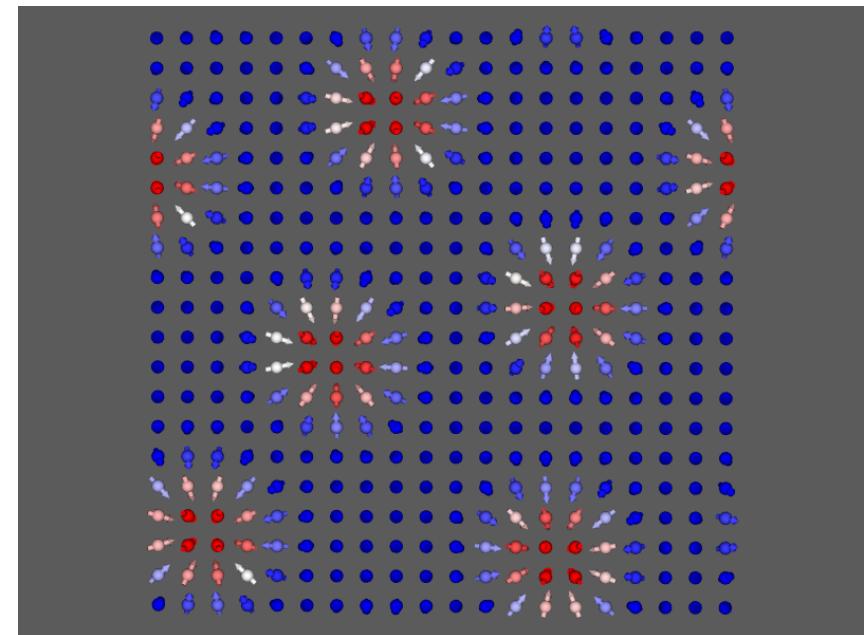
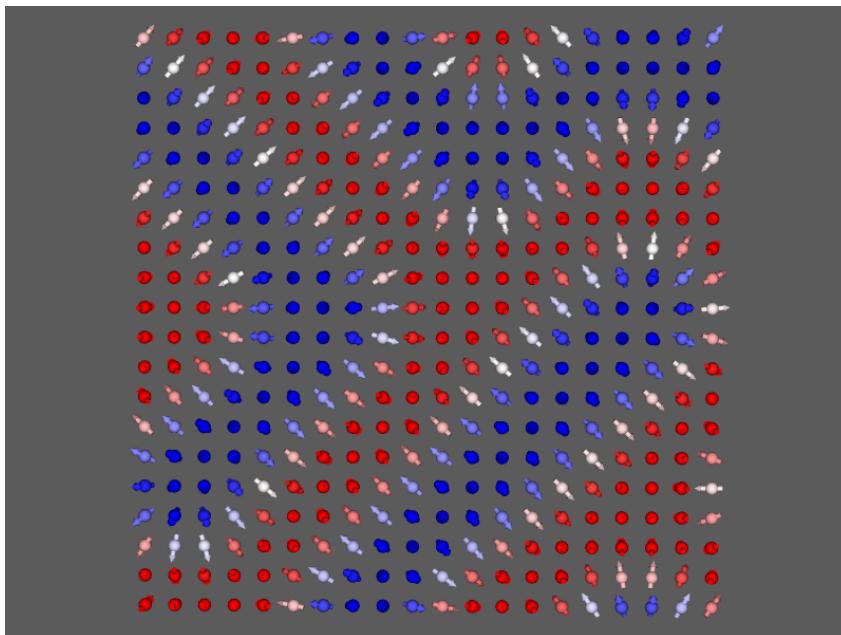
# Plot script

Check for visualise.sh

```
1 #!/bin/bash
2 run_folder=$PWD
3 rm -r Plots
4 mkdir Plots
5 for i in `seq 20 1 30`
6 do
7
8 paste atoms-coords.data spins-000000$i.data > plot.data
9
10 cat <<EOF >plot.gnu
11 set terminal pngcairo size 1200,600 font "Helvetica,14" background rgb 'gray'
12 set output 'out_config.png'
13 set view 0,0
14 set size square
15 set cbrange [-1:1]
16 set xrange [-1:21]
17 set yrange [-1:21]
18 set palette defined (-1 "blue", 0 "white", 1 "red")
19 set xlabel "x";set ylabel "y"; set zlabel "z"
20 set multiplot layout 1,2 title 'Frame $i'
21 sp "plot.data" u 3:4:5:(\$6):(\$7):(\$8):8 w vectors palette lw 1.5 t 'M', '' u 3:4:5:8 w points palette pt 7 ps 1 t 'Mz'
22 set view 90,0
23 sp "plot.data" u 3:4:5:(\$6):(\$7):(\$8):8 w vectors palette lw 1.5 t 'M', '' u 3:4:5:8 w points palette pt 7 ps 1 t 'Mz'
24
25 unset multiplot
26 EOF
27
28 gnuplot plot.gnu
29 mv out_config.png Plots/config_$i'.png'
30
31
32
33 done
```

# Answer

- Zero Field Cooling  
(stripe domains)
- Field Cooling  
(4T-skyrmions)

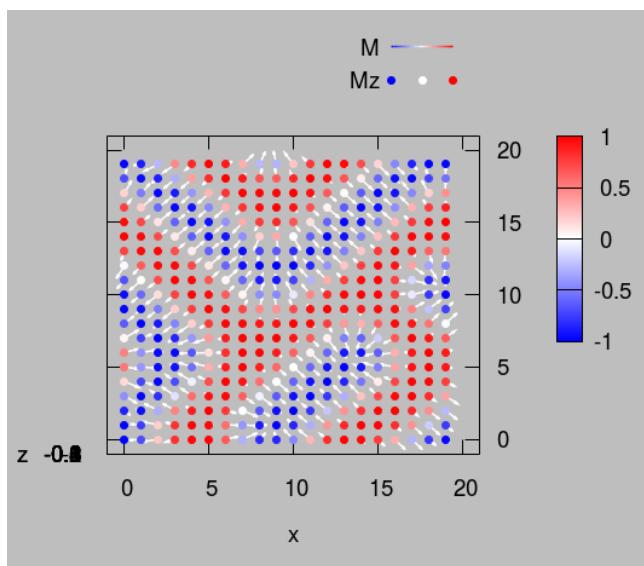


# Try different values of:

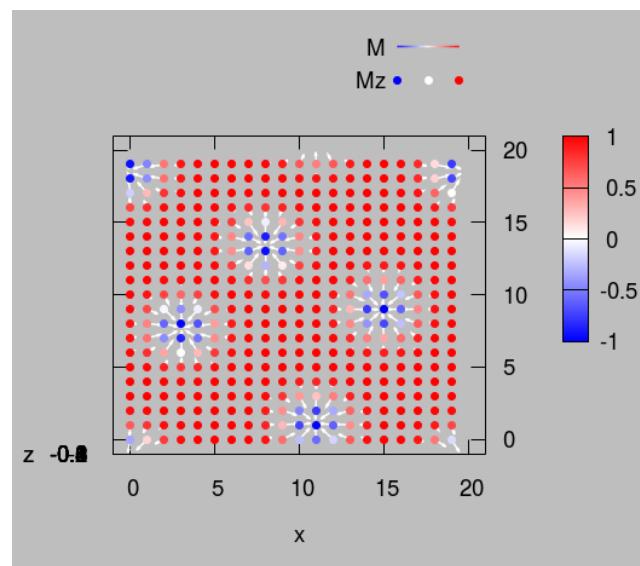
- Increase size of the system!
- Cooling times; 100 ps; 500 ps etc.
- Applied field;
- Ratio between exchange and DMI;
- Anisotropy constants;
- Different temperatures;

# Different fields

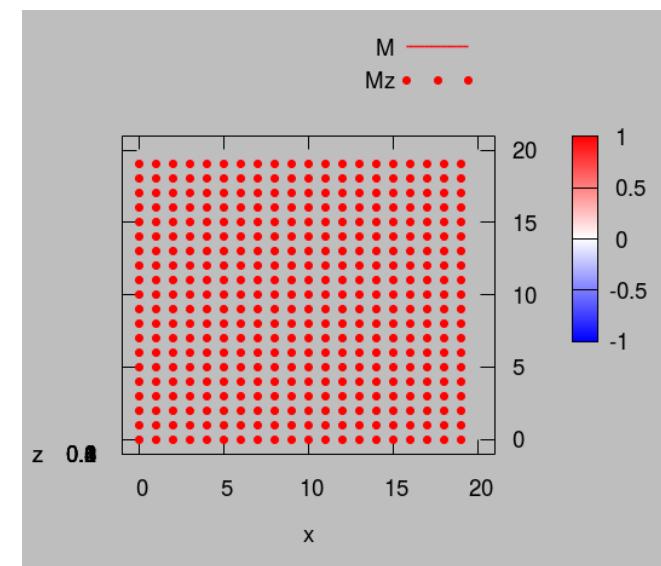
B=1T



B=5T

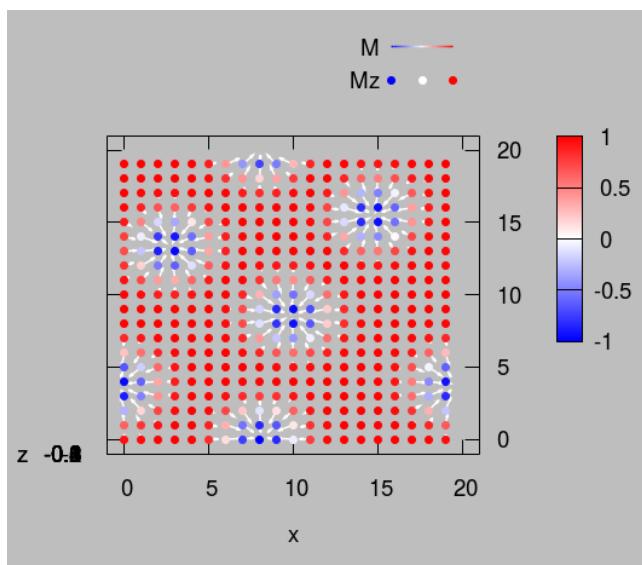


B=10T

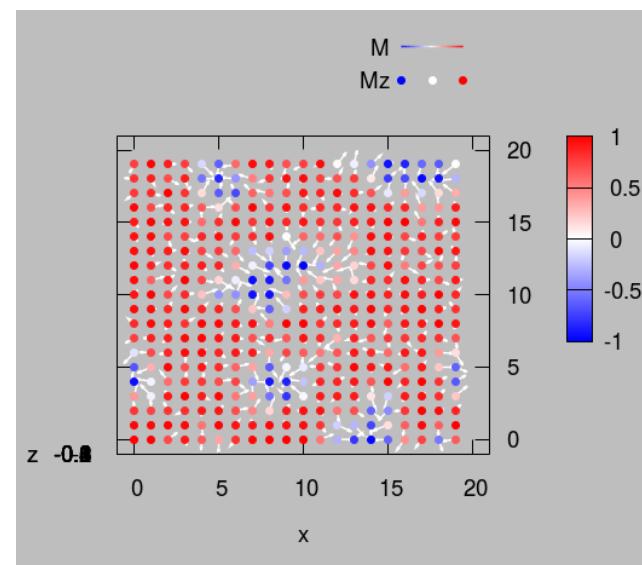


# Different temperatures

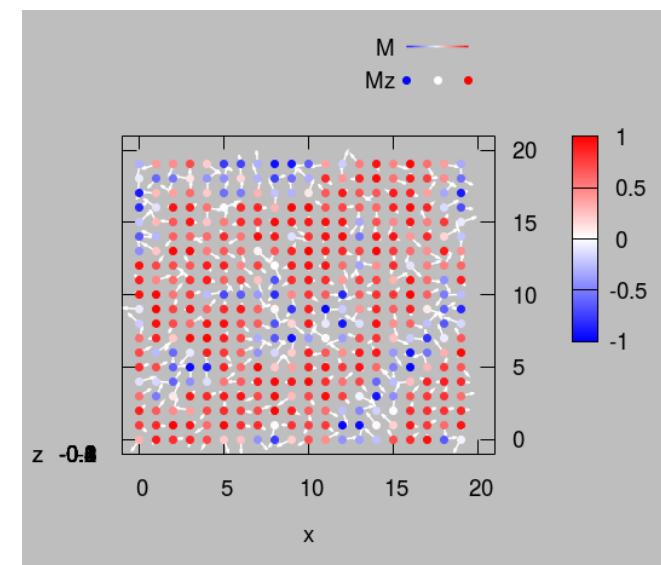
T=0K



T=5K

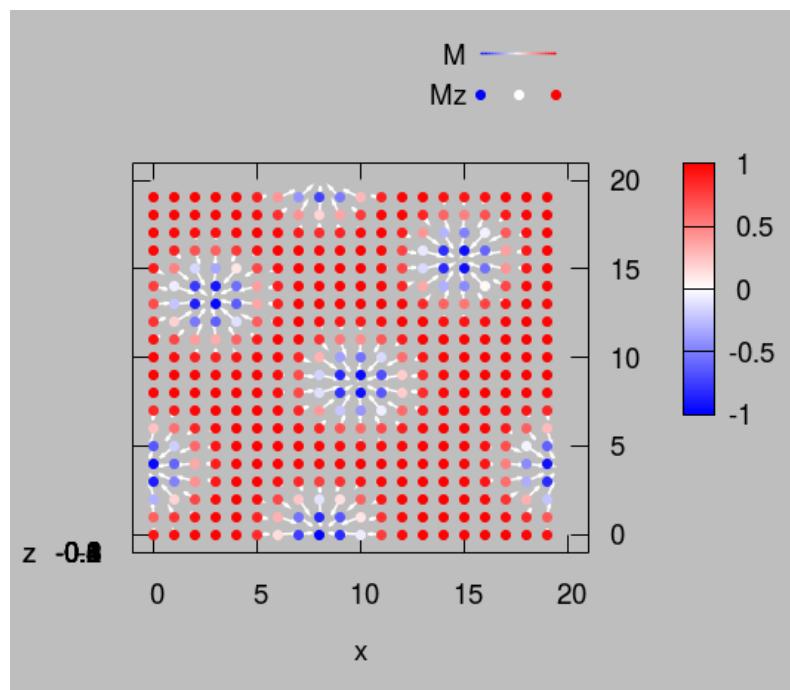


T=10K

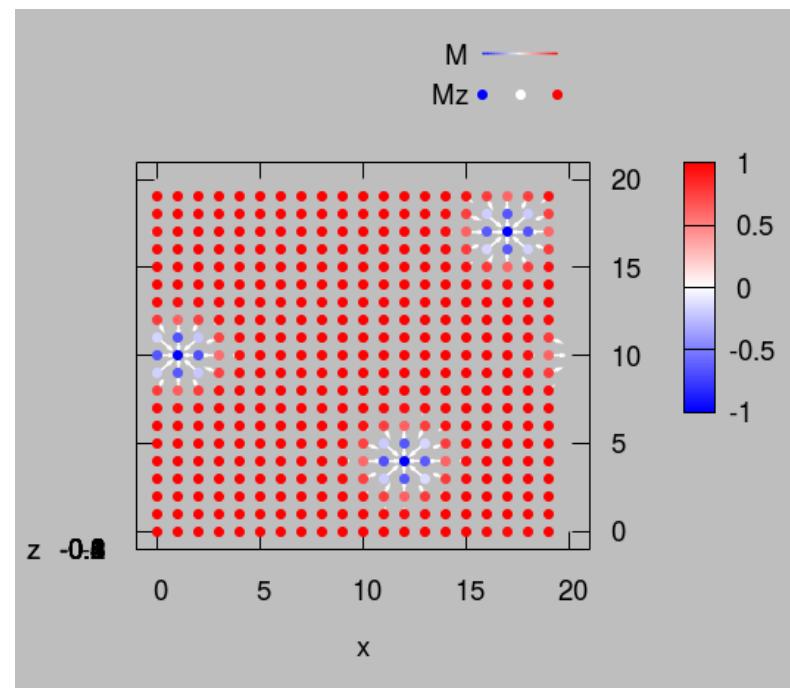


# Different anisotropies

$K=5e-23$



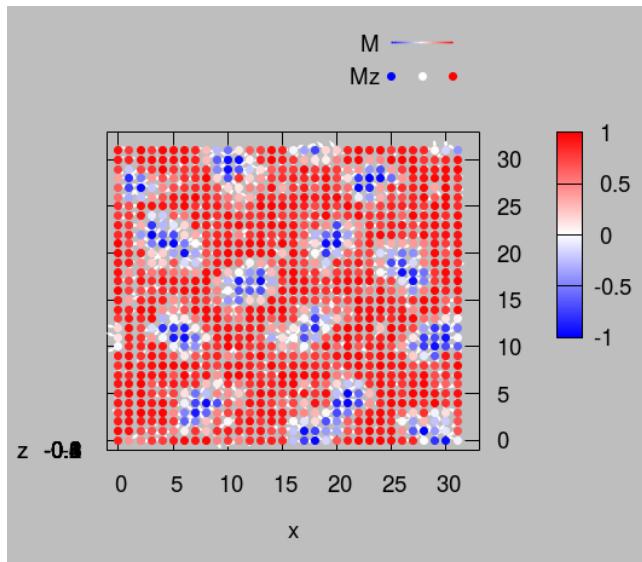
$K=10e-23$



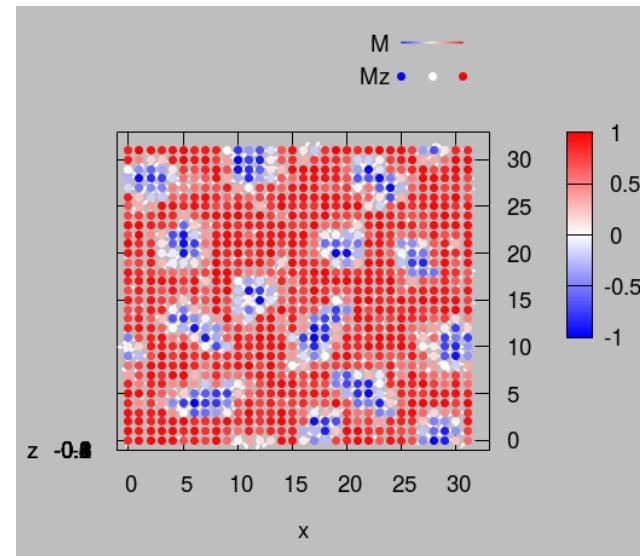
# Different skyrmion interactions

T=5K

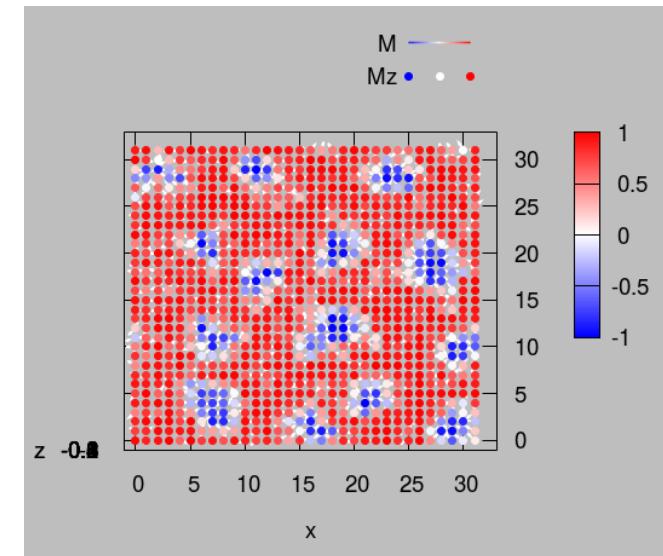
Frame 66

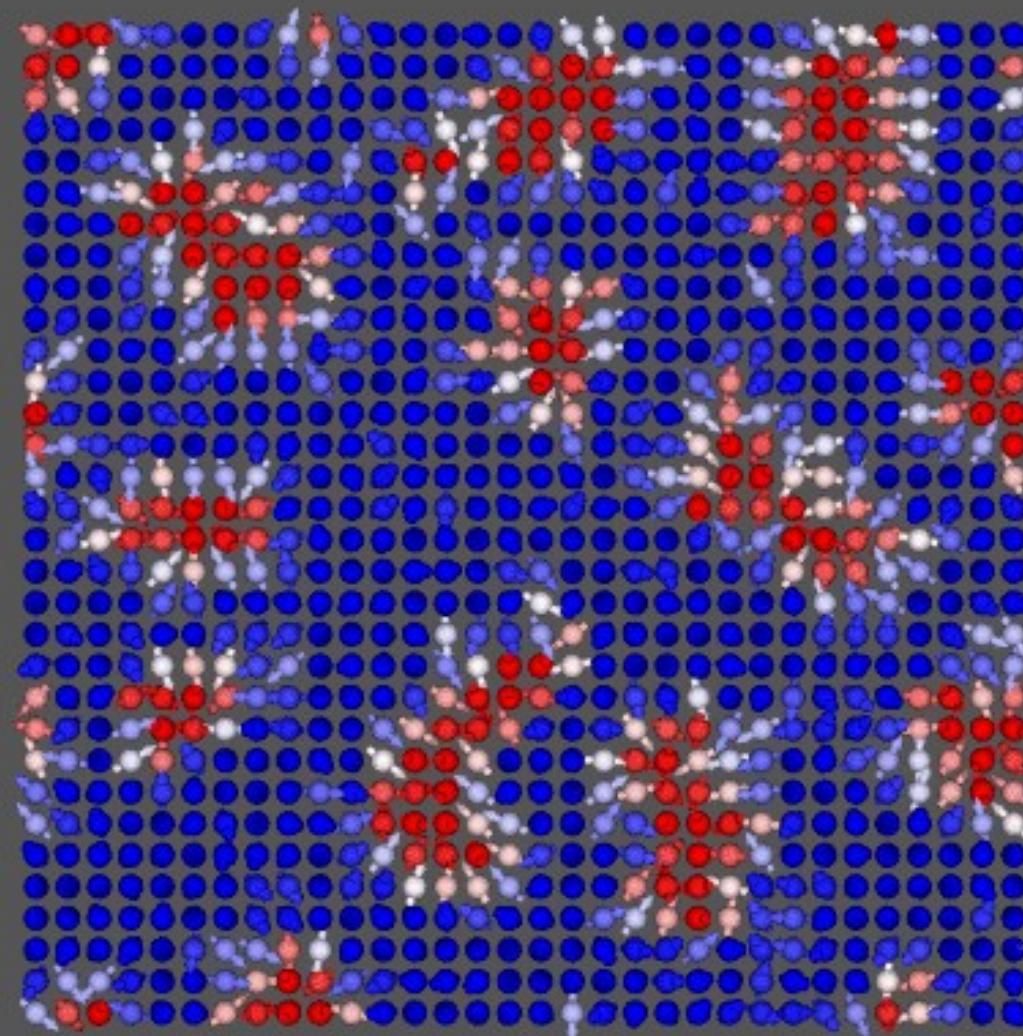


Frame 67

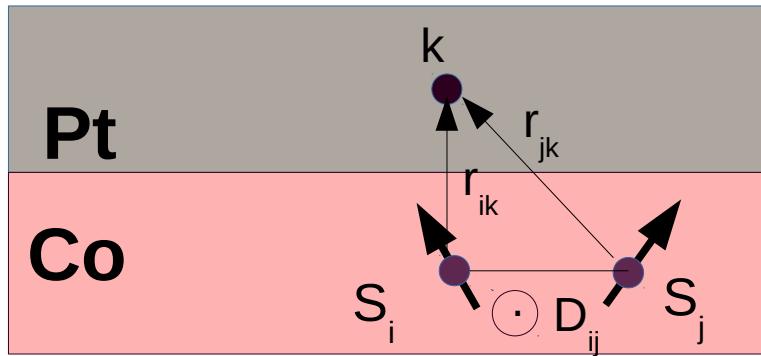


Frame 68





# Method 2: In-built DMI



$$(r_{ik}, r_{jk}) < r_c$$

$(r_{ik}, r_{jk})$  are then renormalised

$$\mathbf{D}_{ij} = \mathbf{r}_{ik} \times \mathbf{r}_{jk}$$

$$E_{DMI} = \mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j)$$

# Method 2: In-built DMI

## input

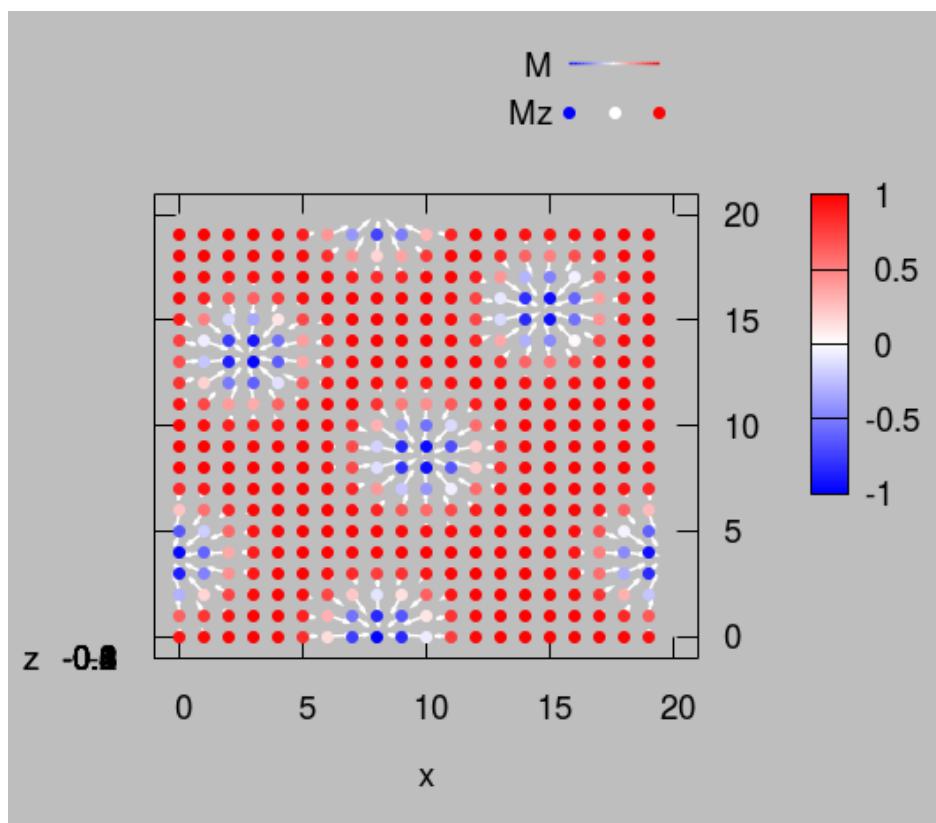
```
# Creation attributes:  
#-----  
create:crystal-structure=sc  
  
create:periodic-boundaries-x  
create:periodic-boundaries-y  
#-----  
# System Dimensions:  
#-----  
dimensions:unit-cell-size = 1 !A  
dimensions:system-size-x = 2 !nm  
dimensions:system-size-y = 2 !nm  
dimensions:system-size-z = 0.2 !nm  
  
#-----  
# Material Files:  
#-----  
material:file=sc.mat  
  
exchange:dmi-cutoff-range = 1.42 !A
```

## Material file

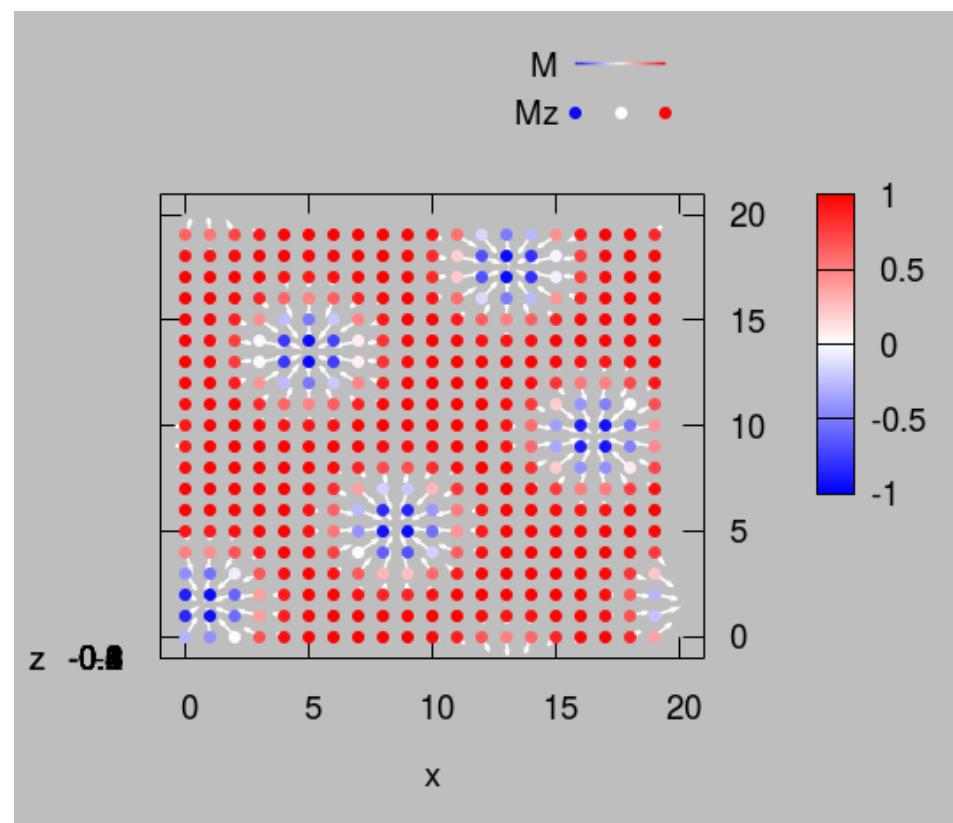
```
material:num-materials = 2  
#-----  
# Material 1 Cobalt Generic  
#-----  
material[1]:material-name=Co  
material[1]:damping-constant=1.0  
material[1]:exchange-matrix[1]=1.6e-22  
material[1]:atomic-spin-moment=1.72 !muB  
material[1]:uniaxial-anisotropy-constant=5e-23  
material[1]:minimum-height=0.0  
material[1]:maximum-height=0.5  
material[1]:dmi-constant[2] = 2.26274169979695e-22  
material[1]:initial-spin-direction = random  
  
#-----  
# Material 2 Platinum Generic  
#-----  
material[2]:material-name=Pt  
material[2]:material-element=Fe  
material[2]:minimum-height=0.5  
material[2]:maximum-height=1.0  
material[2]:non-magnetic = keep
```

# Comparison

Tensorial DMI

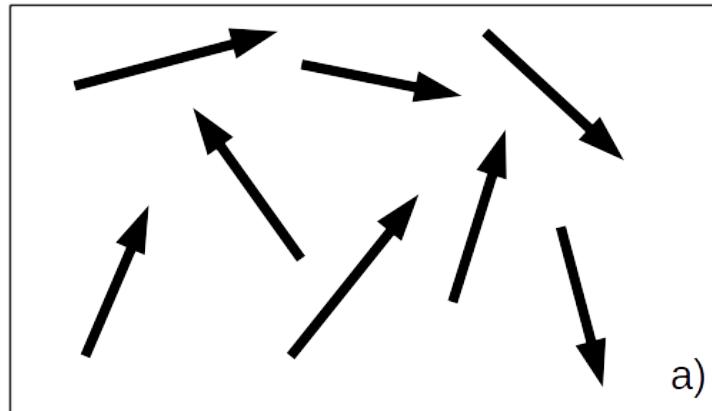


In built DMI

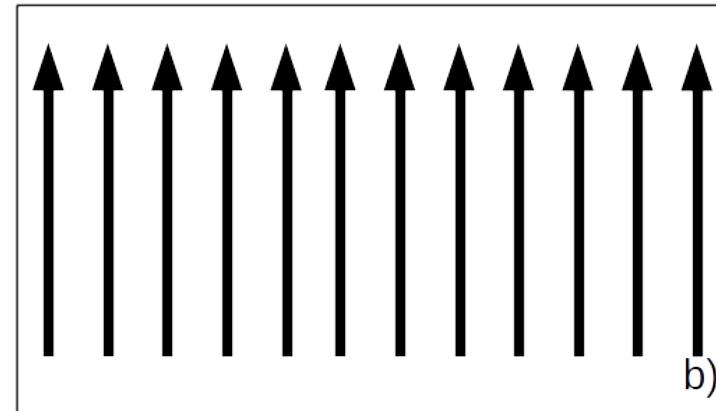


# Complex crystall structures Part 2: Higher-order exchange & Metamagnets

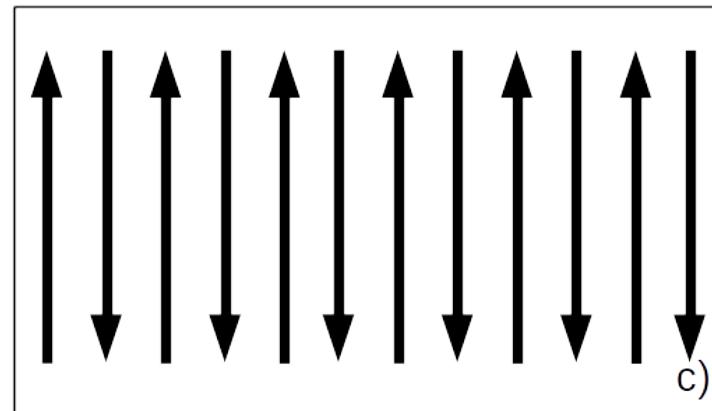
# What is a metamagnet?



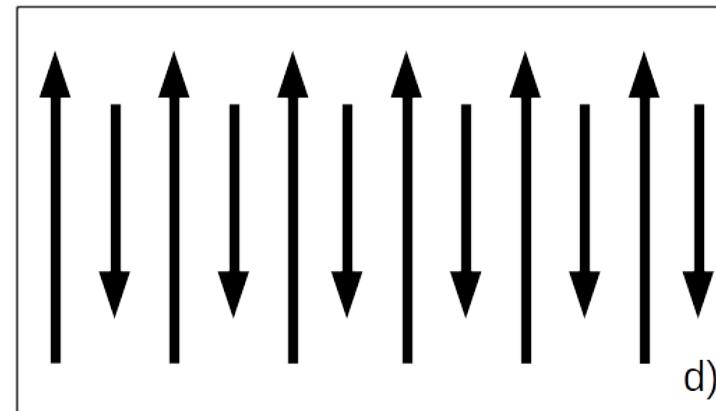
a)



b)



c)

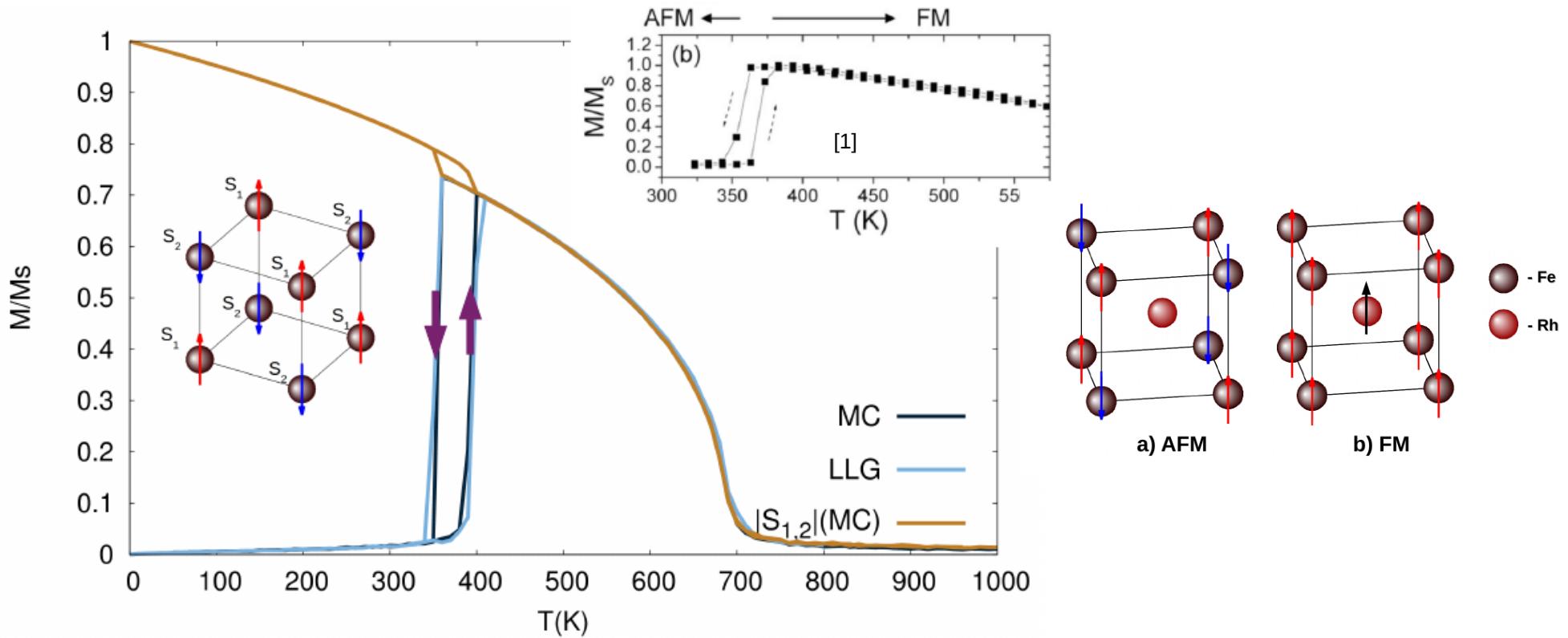


d)

a) Paramagnet (**PM**); b) Ferromagnet (**FM**); c) Antiferromagnet (**AFM**); d) Ferrimagnet ;

A **metamagnet** refers in general to a class of materials in which a small change in an external parameter (field, temperature, pressure) leads towards a large change in the magnetisation.

# FeRh metamagnet



Thermal hysteresis associated with the coexistence of both AFM and FM during the first-order phase transition. The system simulated is of  $32 \times 32 \times 32$  atoms with periodic boundary conditions and temperature resolution of 10K. The absolute value of the magnetisation of the two sub-lattices ( $S_{1,2} = S_1 = |S_2|$ ) is plotted during heating and cooling, the same value of thermal hysteresis being observed (gold curve). (Inset) Measurement of thermal hysteresis for a 100-nm-thick FeRh film, extracted from [1] G.Ju et al.

# Beyond Heisenberg model; Higher-order exchange interactions;

- Pointed out by Herring in 1966.
- Can be derived from the Hubbard model, the first non-trivial term being given by the four-spin exchange (M. Takahashi, Journal of Physics C: Solid State Physics 10, 1289 (1977)). 4-spin interaction or ring-exchange arises from for consecutive hops of electrons from one spin configuration to the spin flipped one.

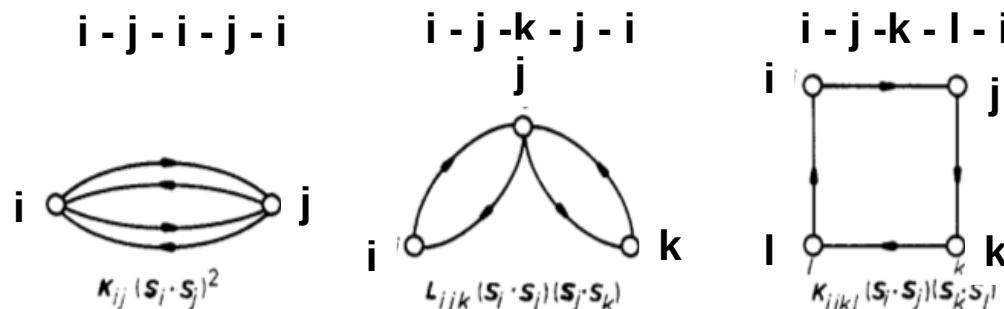


Figure 1. Schematic representation of the various types of four-spin interaction

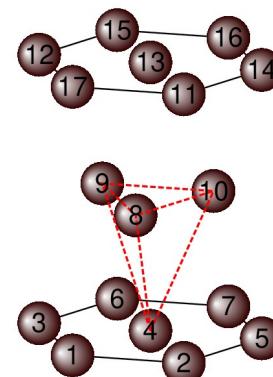
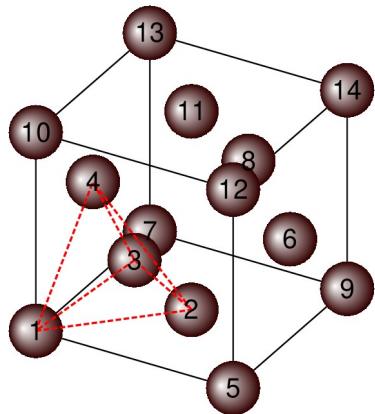
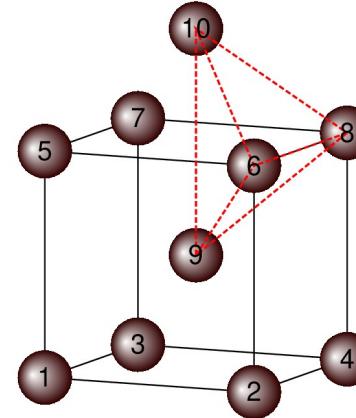
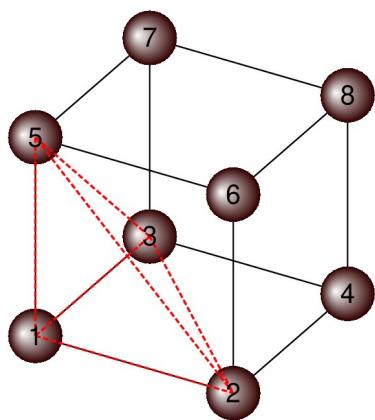
Adler, Oitma, 1978

$$\mathcal{H} = -\frac{1}{2} \sum_{i,j} J_{ij} (\mathbf{S}_i \cdot \mathbf{S}_j) - \frac{1}{3} \sum_{i,j,k,l} D_{ijkl} (\mathbf{S}_i \cdot \mathbf{S}_j)(\mathbf{S}_k \cdot \mathbf{S}_l) - k_u \sum_i (\mathbf{S}_i \cdot \mathbf{e})^2$$

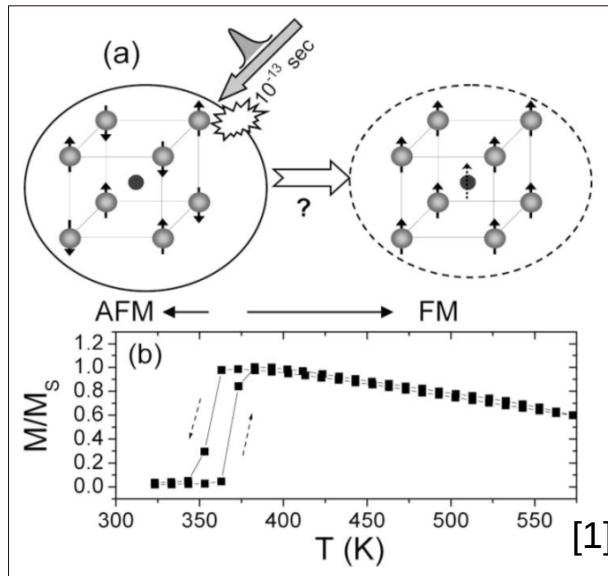
**! They scale with the magnetic moment to the 4th-order !**

- 2015- J. Barker and R. Chantrell managed to model the metamagnetic transition via the four-spin exchange. They suggest that the heat during the magnetic transition drives the structural changes.

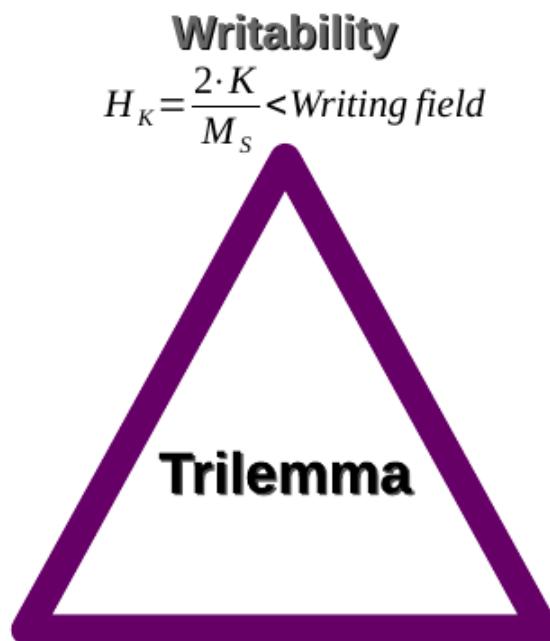
# Four-spin quartets for different crystal structures



# Motivation



[1] Ju, Ganping et al. Ultrafast generation of ferromagnetic order via a laser-induced phase transformation in FeRh thin films, Physical Review Letters (2004)

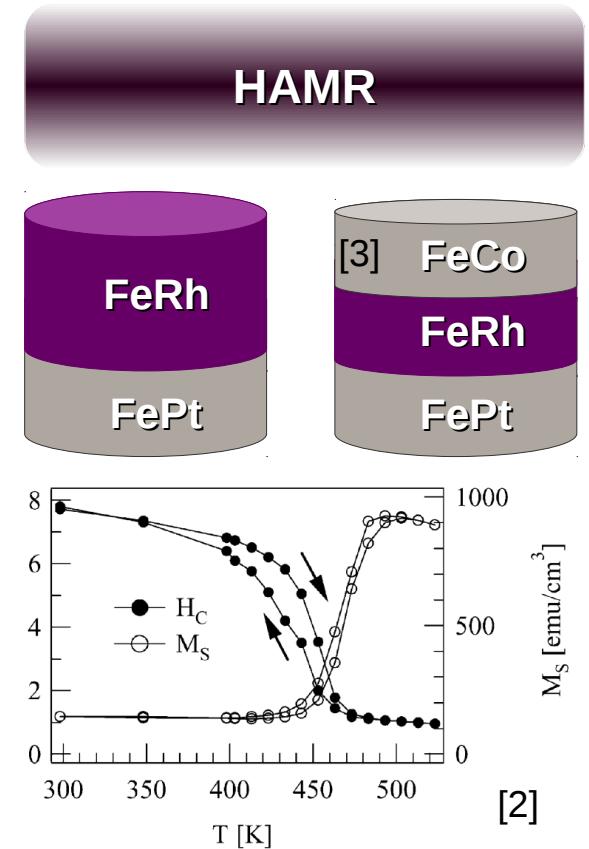


**SNR (Signal to noise ratio)**

$$SNR \approx \sqrt{N}$$

**Thermal stability**

$$\Delta E = K \cdot V \left(1 - \frac{H}{H_K}\right)^n$$



[2] J.U.Thiele et al. Magnetic and Structural Properties of FePt–FeRh Exchange Spring Films for Thermally Assisted Magnetic Recording Media, IEEE TRANSACTIONS ON MAGNETICS, VOL. 40, NO. 4, JULY 2004

[3] T. J. Zhou et al. The concept and fabrication of exchange switchable trilayer of FePt/FeRh/FeCo with reduced switching field, JOURNAL OF APPLIED PHYSICS 111, 07C116 (2012)

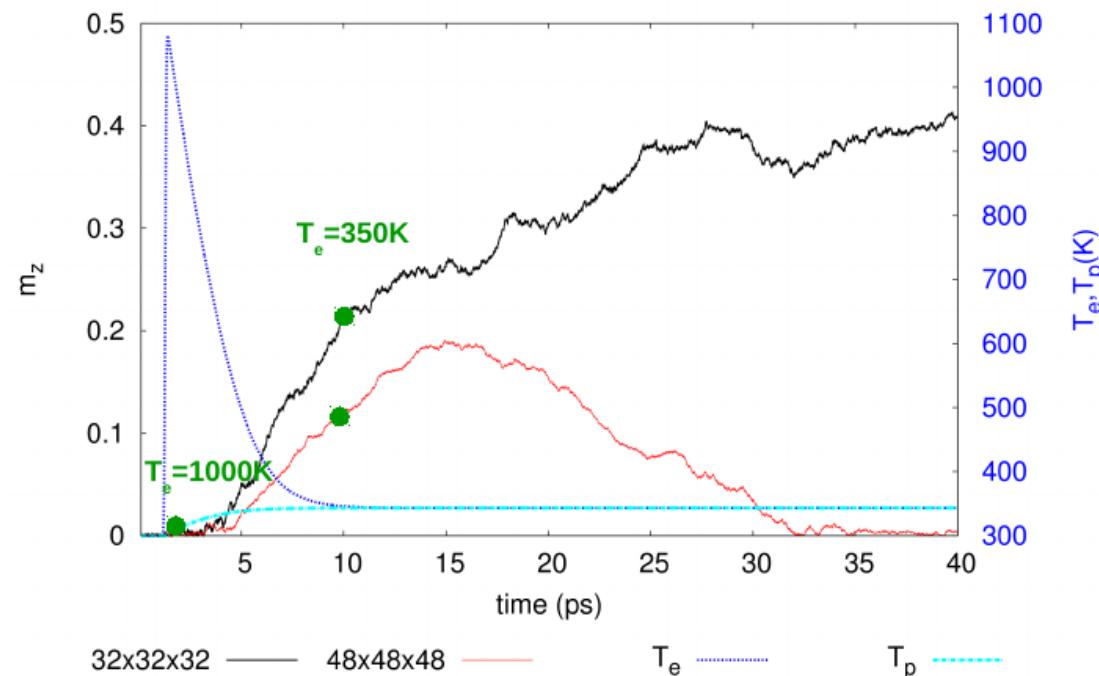
# Ultrafast generation of FM ordering in FeRh

Two temperature model:

$$C_{e0}T_e \frac{dT_e}{dt} = -G_{ep}(T_e - T_p) + P(t)$$

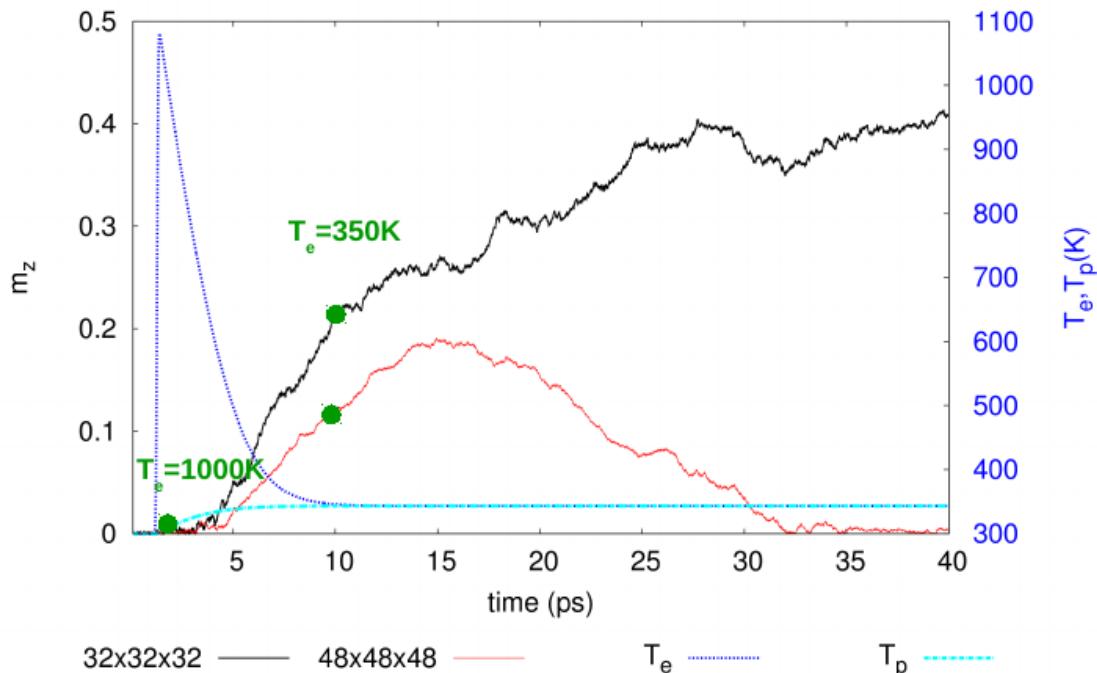
$$C_p \frac{dT_p}{dt} = -G_{ep}(T_e - T_p)$$

Quantity	Symbol	Value	Units
Electron-heat capacity constant	$C_{e0}$	$3.5 \times 10^{-3}$	$Jmol^{-1}K^{-2}$
Phonon specific heat capacity	$C_p$	$4.54 \times 10^1$	$Jmol^{-1}K^{-1}$
Electron-phonon thermalization time	$\tau_{ep}$	$1 \times 10^{-12}$	s
Electron-phonon coupling factor	$G_{ep}$	$1.05 \times 10^{12}$	$Jmol^{-1}K^{-1}s^{-1}$
Thermal bath coupling constant	$\alpha$	0.1	

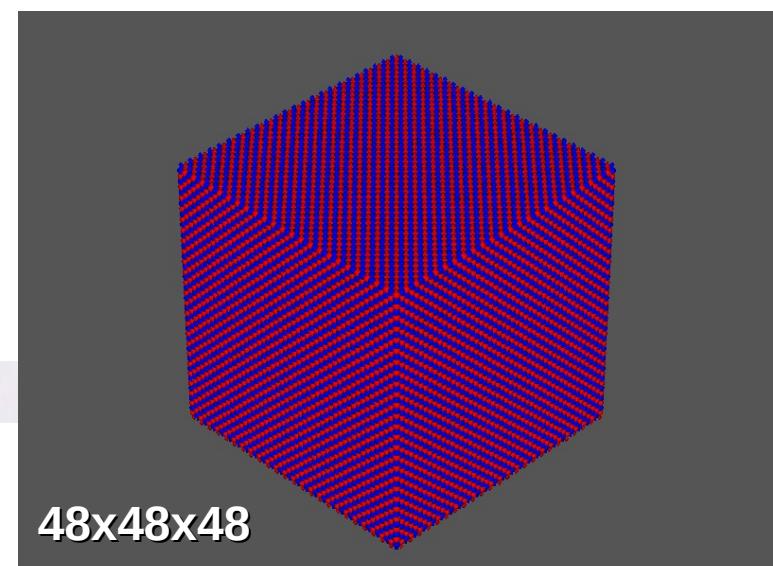
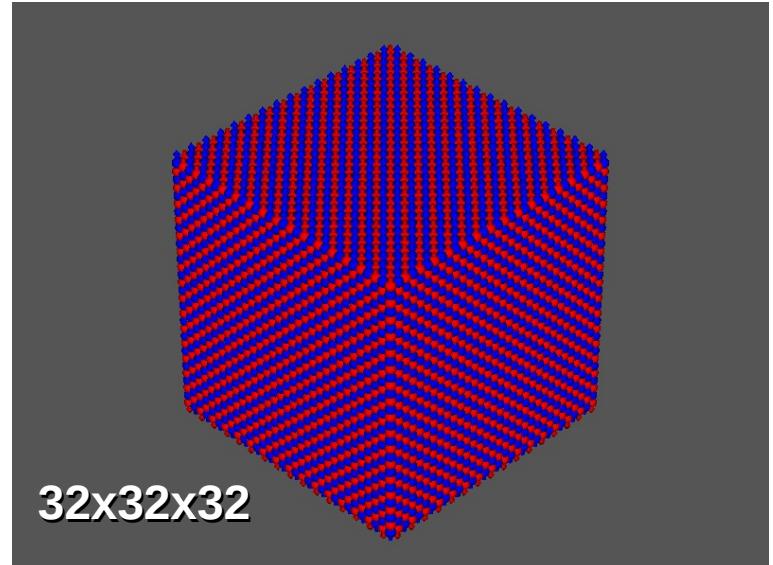


Ultrafast formation of ferromagnetic ordering in FeRh obtained by applying a 100fs laser pulse. The z component of the reduced magnetisation is plotted for the 32x32x32 and 48x48x48 atoms system with periodic boundary conditions.

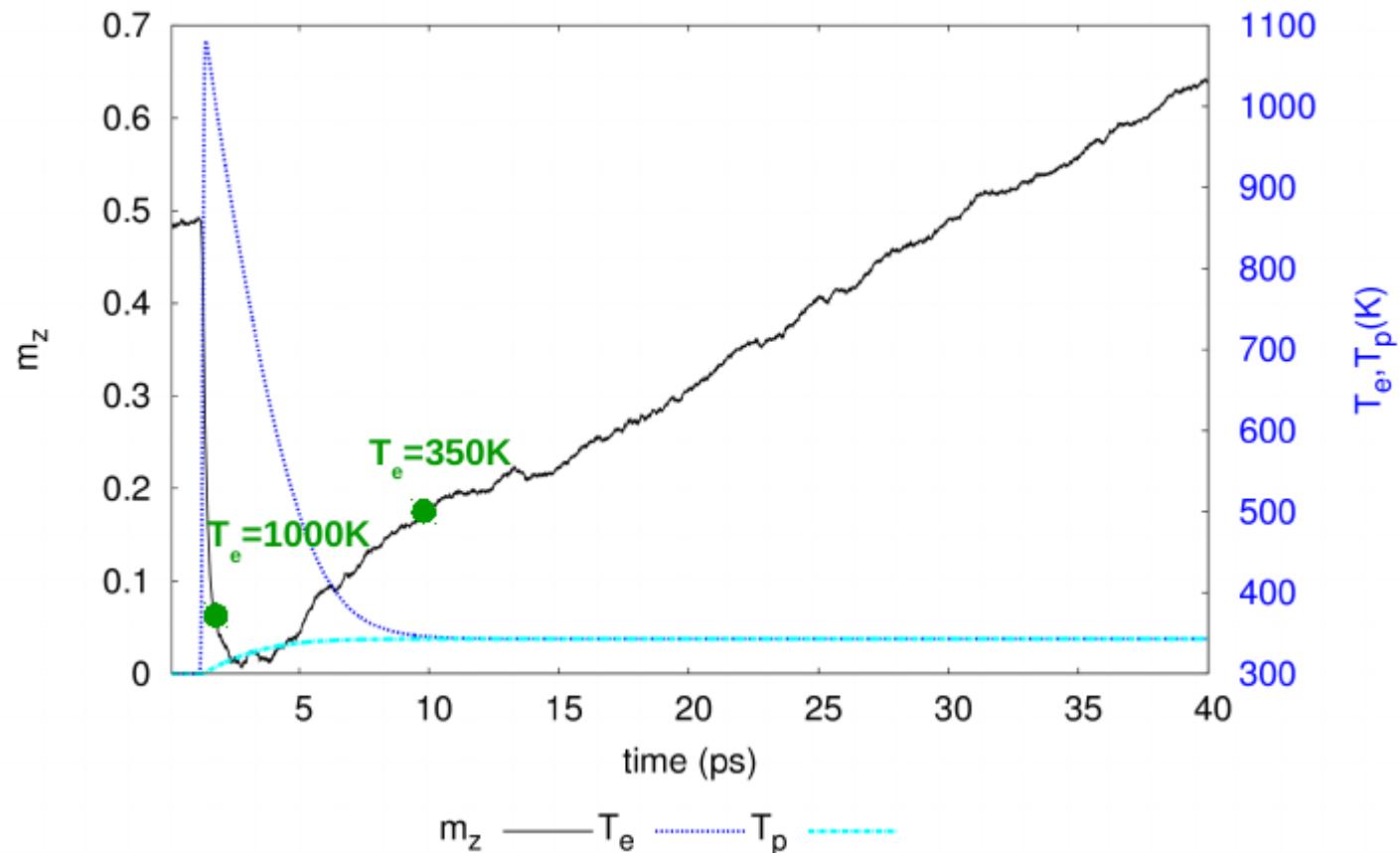
# Mixed phases during heating



Ultrafast formation of ferromagnetic ordering in FeRh obtained by applying a 100fs laser pulse. The z component of the reduced magnetisation is plotted for the  $32 \times 32 \times 32$  and  $48 \times 48 \times 48$  atoms system with periodic boundary conditions.



# Ultrafast generation of FM ordering in FePt/FeRh



Ultrafast formation of ferromagnetic ordering in FePt/FeRh thin film system after applying an 100fs laser pulse. The system is periodic in xy direction (48x48) and consists of 16 layers of FeRh and 11 layers of FePt.

# Ultrafast generation of FM ordering in FePt/FeRh

