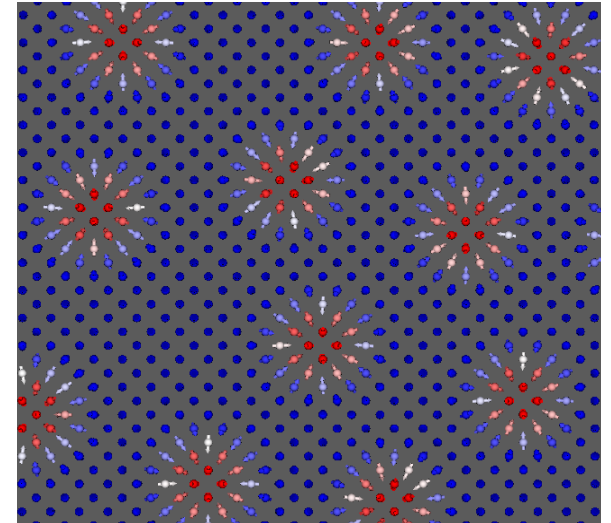
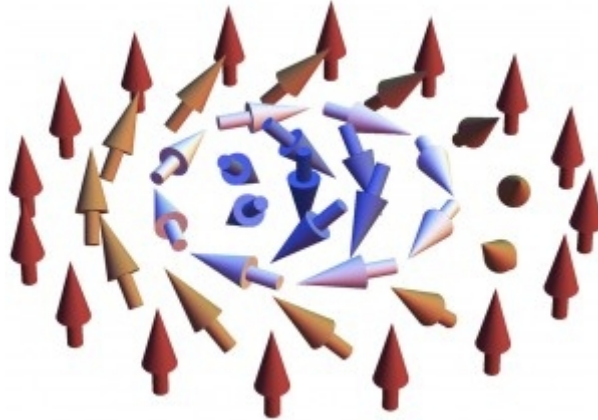
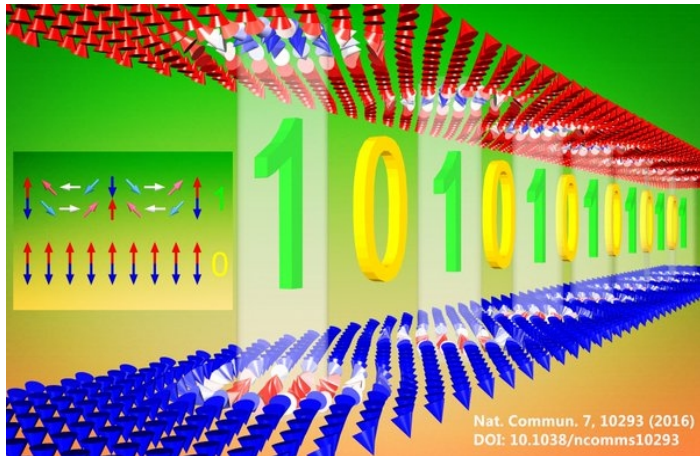


**Generating skyrmions using
VAMPIRE
(application to customised .ucf)**

Mara Strungaru

Magnetic Skyrmions



- Skyrmions -chiral nanoscale bubbles;
 - 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)

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

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

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

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

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

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

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

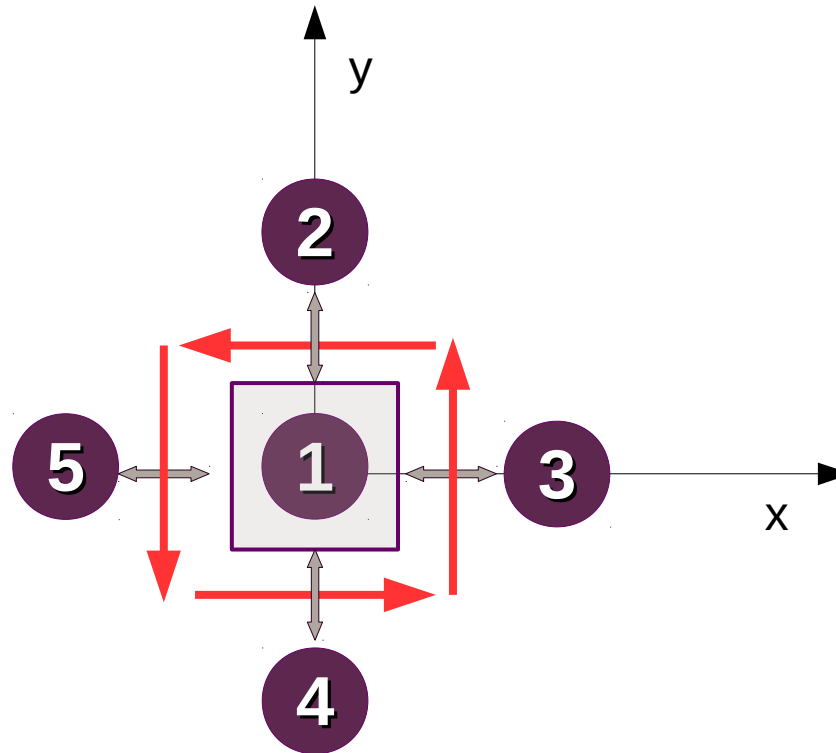
Simple cubic lattice

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

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

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

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

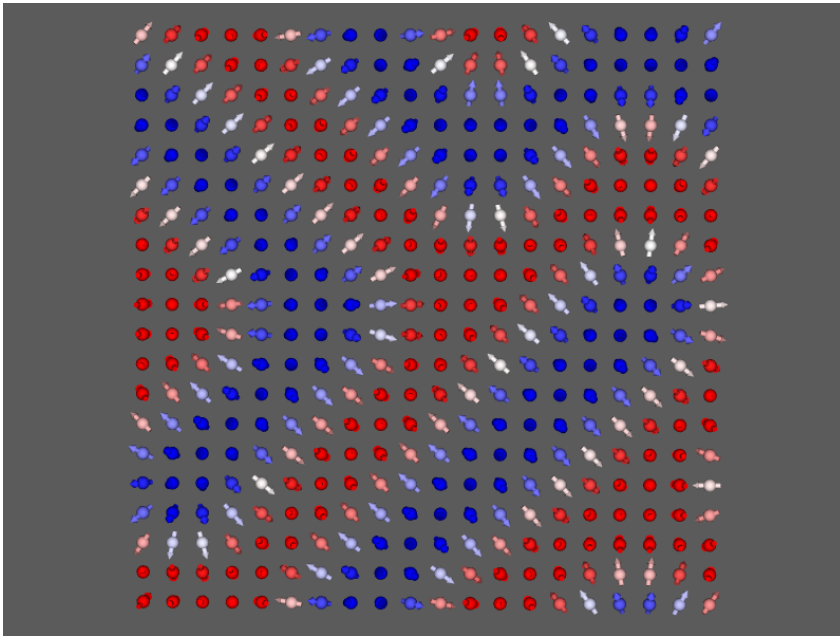


$$\mathbf{D}_{ij}^k = D^k \cdot (\mathbf{z} \times \mathbf{u}_{ij})$$

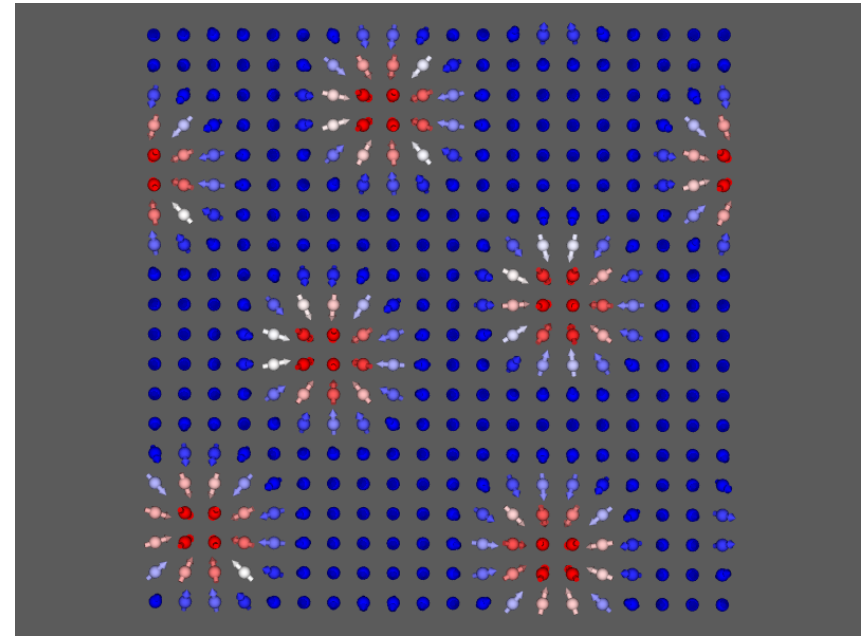


Ground-state

- Zero Field Cooling
(stripe domains)



- Field Cooling
(4T-skyrmions)

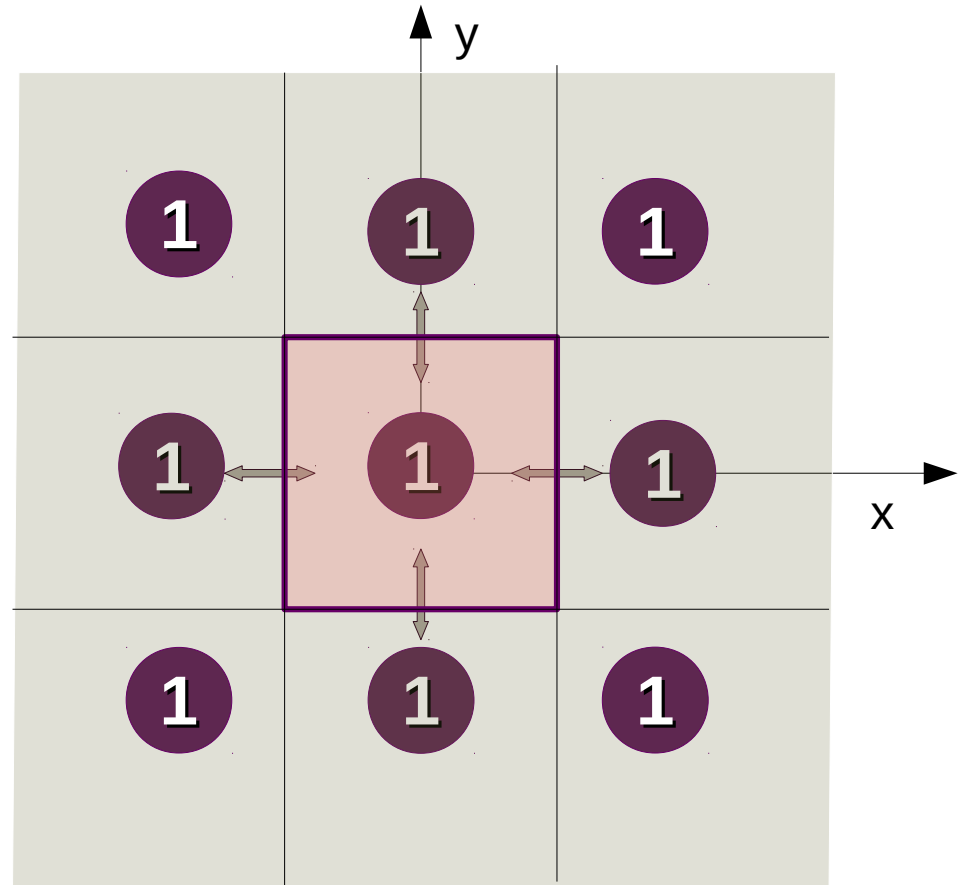


Steps to follow

1) Create system

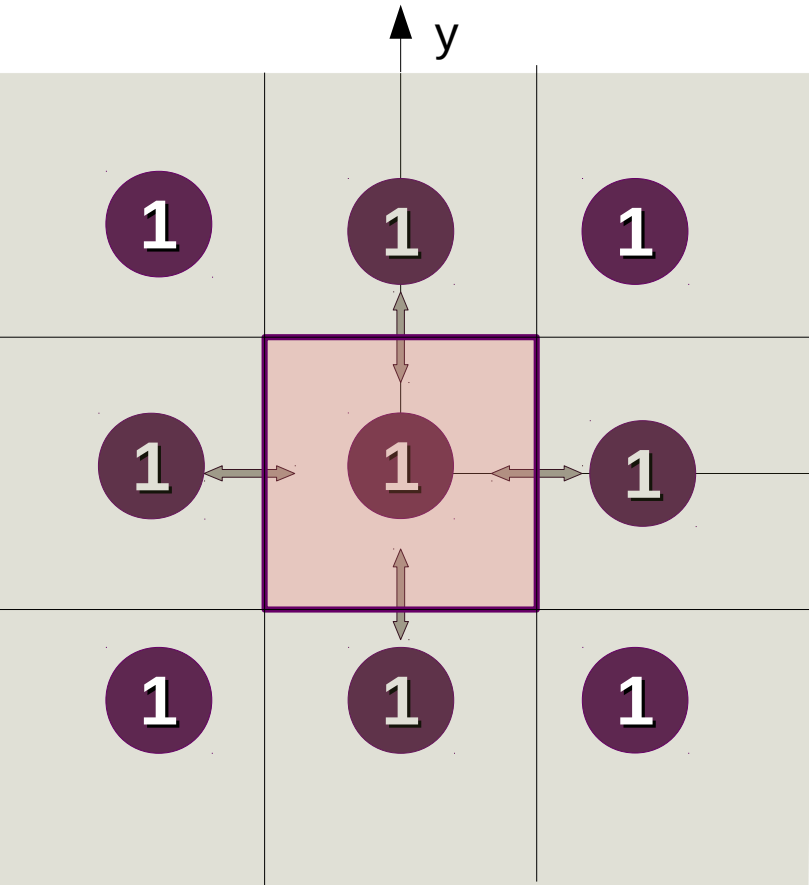
- Start from a unit cell of 1 atom.
- Replicate the system to create the super-cell for PBC.
- Calculate nearest neighbours.
- Write the code as generally as possible.

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

n	exctype	id	i	j	dx	dy	dz	Jij
0	...	0	0	0	1	0	0	11.2e-21
1	...	1	0	0	-1	0	0	11.2e-21
2	...	2	0	0	0	1	0	11.2e-21
3	...	3	0	0	0	-1	0	11.2e-21
4	...	4	0	0	0	0	1	11.2e-21
5	...	5	0	0	0	0	-1	11.2e-21

Exchange type:

Isotropic
Vectorial
Tensorial

Exchange values (J/link)

Relative distance

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
```

```
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
```

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

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

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
```


300 points



```
config:atoms
```

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

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 00 10 0 1.6e-22 0 -1.60e-22 0 1.6e-22 0 1.60e-22 0 1.6e-22

1 00 01 0 1.6e-22 0 0 0 1.6e-22 -1.60e-22 0 1.60e-22 1.6e-22

2 00 -10 0 1.6e-22 0 1.60e-22 0 1.6e-22 0 -1.60e-22 0 1.6e-22

3 00 0-10 1.6e-22 0 0 0 1.6e-22 1.60e-22 0 -1.60e-22 1.6e-22

Field-cooling simulation (input)

```
material:file=Co.mat
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#-----
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sim:equilibration-time-steps = 10000
sim:time-steps-increment = 1
sim:time-step=1e-16
```

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

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

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

Plotting and animation

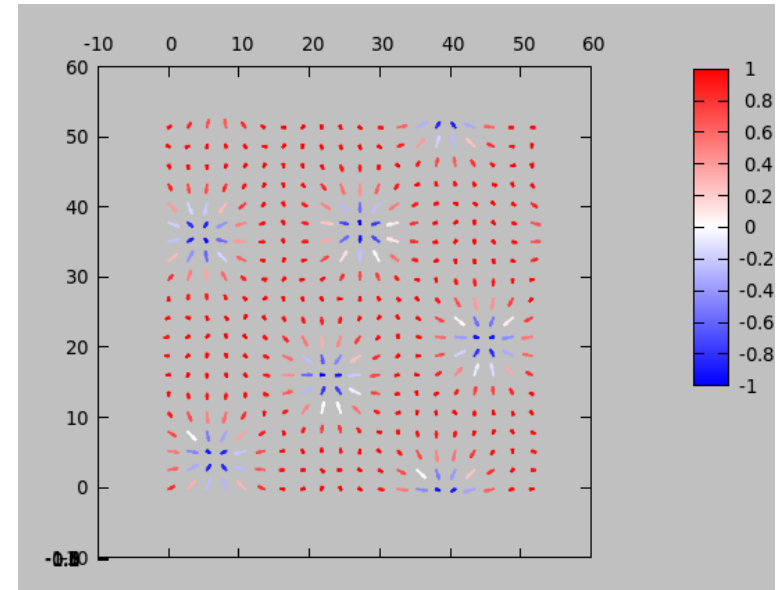
Gnuplot alternative

- 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;