

VAMPIRE

PRACTICAL TUTORIAL

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VAMPIRE manual

<https://vampire.york.ac.uk/support/>

Resources for today

<https://www-users.york.ac.uk/~rfl500/resources/vampire/>



Setting up a simulation in Vampire

input file
(program control)

```
#-----  
# Creation attributes:  
#-----  
create:crystal-structure=fcc  
create:periodic-boundaries-x  
create:periodic-boundaries-y  
create:periodic-boundaries-z  
#-----  
# System Dimensions:  
#-----  
dimensions:unit-cell-size = 3.524 !A  
dimensions:system-size-x = 4.0 !nm  
dimensions:system-size-y = 4.0 !nm  
dimensions:system-size-z = 4.0 !nm  
...
```

material file
(material properties)

```
#-----  
# Number of Materials  
#-----  
material:num-materials=1  
#-----  
# Material 1 Nickel Generic  
#-----  
material[1]:material-name=Ni  
material[1]:damping-constant=0.01  
material[1]:exchange-matrix[1]=2.757e-21  
material[1]:atomic-spin-moment=0.606 !muB  
material[1]:uniaxial-anisotropy-constant=0.0  
material[1]:material-element=Ni
```

For information: getting and compiling vampire

- Need to get code from source repository

```
git clone https://github.com/richard-evans/vampire.git
```

- This creates a directory 'vampire'

```
cd vampire
```

- Checkout release version of the code

```
git checkout develop
```

- Compile

```
make serial
```

Running vampire

- Each simulation should be in a separate directory

```
mkdir vampire
cd vampire
mkdir curie
cd curie
```

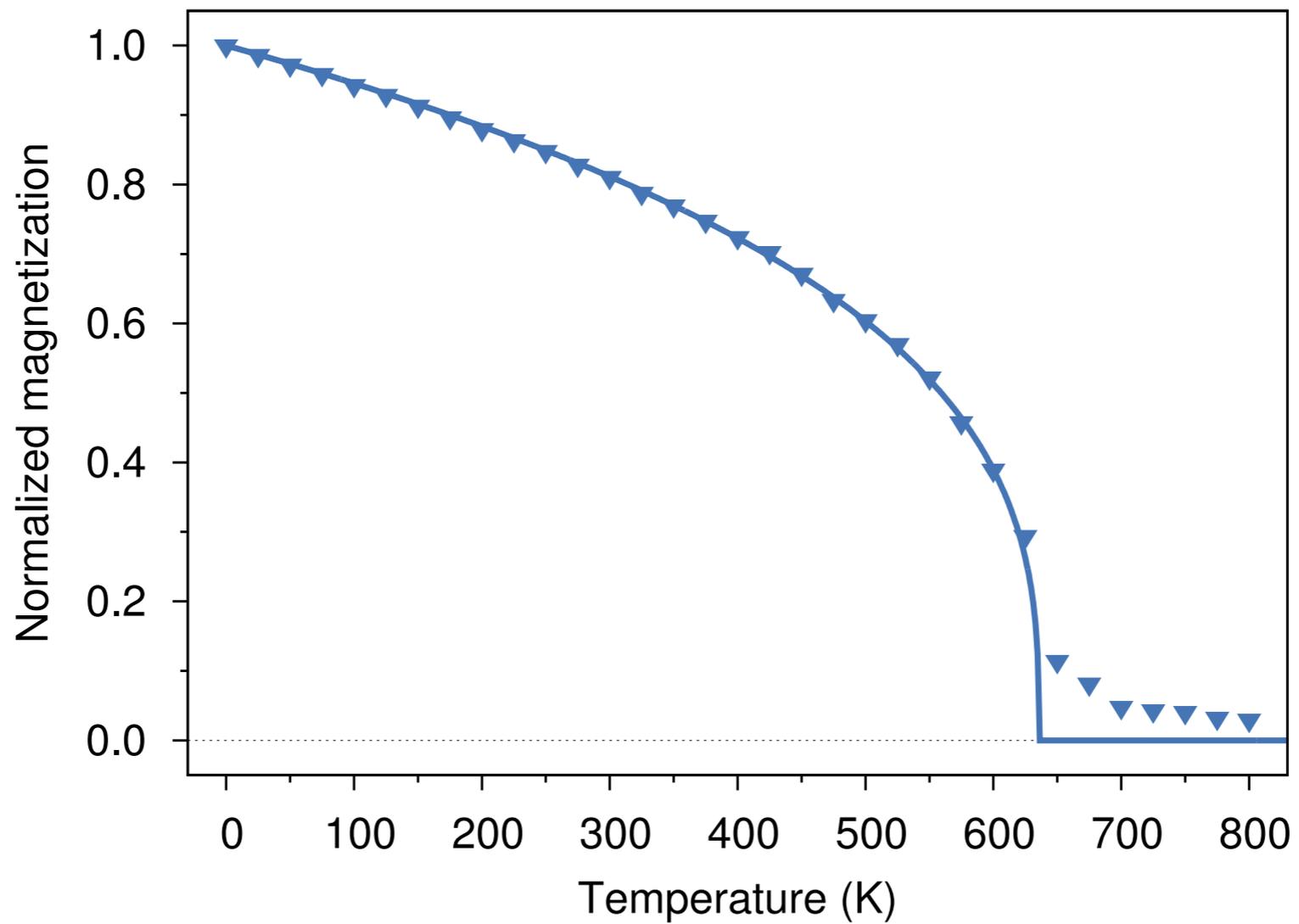
- Download the input files and executable

```
cp /v/courses/trilmax.public/Tutorial_3/curie/* .
```

- Now run the executable

```
~/vampire/vampire-serial
mpirun -np 8 ~/vampire/vampire-parallel
```

Practical: Curie temperature



Setting up a simulation in Vampire

input file
(program control)

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create:periodic-boundaries-x  
create:periodic-boundaries-y  
create:periodic-boundaries-z  
#-----  
# System Dimensions:  
#-----  
dimensions:unit-cell-size = 3.524 !A  
dimensions:system-size-x = 4.0 !nm  
dimensions:system-size-y = 4.0 !nm  
dimensions:system-size-z = 4.0 !nm  
...
```

material file
(material properties)

```
#-----  
# Number of Materials  
#-----  
material:num-materials=1  
#-----  
# Material 1 Nickel Generic  
#-----  
material[1]:material-name=Ni  
material[1]:damping-constant=0.01  
material[1]:exchange-matrix[1]=2.757e-21  
material[1]:atomic-spin-moment=0.606 !muB  
material[1]:uniaxial-anisotropy-constant=0.0  
material[1]:material-element=Ni
```

Spin Hamiltonian for Ni

$$\mathcal{H} = - \sum_{i < j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j - \sum_i k_u S_{i,z}^2$$

Ni.mat

```
#-----  
# Number of Materials  
#-----  
material:num-materials=1  
#-----  
# Material 1 Nickel Generic  
#-----  
material[1]:material-name=Ni  
material[1]:damping-constant=0.01  
material[1]:exchange-matrix[1]=2.757e-21  
material[1]:atomic-spin-moment=0.606 !muB  
material[1]:uniaxial-anisotropy-constant=5.47e-26  
material[1]:material-element=Ni
```

input

```
#-----  
# Creation attributes:  
#-----  
create:crystal-structure=fcc  
create:periodic-boundaries-x  
create:periodic-boundaries-y  
create:periodic-boundaries-z  
#-----  
# System Dimensions:  
#-----  
dimensions:unit-cell-size = 3.524 !A  
dimensions:system-size-x = 4.0 !nm  
dimensions:system-size-y = 4.0 !nm  
dimensions:system-size-z = 4.0 !nm  
#-----  
# Material Files:  
#-----  
material:file=Ni.mat  
#-----  
# Simulation attributes:  
#-----  
sim:temperature=300  
sim:minimum-temperature=0  
sim:maximum-temperature=800  
sim:temperature-increment=25  
sim:time-steps-increment=1  
sim:equilibration-time-steps=1000  
sim:loop-time-steps=1000
```

```
#-----  
# Program and integrator details  
#-----  
sim:program=curie-temperature  
sim:integrator=monte-carlo  
#-----  
# Data output  
#-----  
output:real-time  
output:temperature  
output:magnetisation  
output:magnetisation-length  
output:mean-magnetisation-length  
  
screen:temperature  
screen:mean-magnetisation-length
```

Running Vampire

```
rfle500@MacPro:~$ vampire
```

```
( _)
```

```
-----  
 \ \ / / _ ` | ' _ ` - \ | ' _ \ | | ' _ / _ \  
  \ v / ( _ | | | | | | | | _ ) | | | | | _ /  
   \_ / \_ , _ | | | | | | | | . _ / | | | | \_ _ |  
                                     | |  
                                     | |  
                                     | |
```

```
Version 3.0.3 Aug 4 2014 21:00:13
```

```
Licensed under the GNU Public License(v2). See licence file for details.
```

```
Lead Developer: Richard F L Evans <richard.evans@york.ac.uk>
```

```
Contributors: Weijia Fan, Phanwadee Chureemart, Joe Barker,  
              Thomas Ostler, Andreas Biternas, Roy W Chantrell
```

```
Compiled with: GNU C++ Compiler
```

```
Compiler Flags:
```

```
=====  
Mon Aug 4 21:56:21 2014  
=====
```

```
Initialising system variables
```

```
Creating system
```

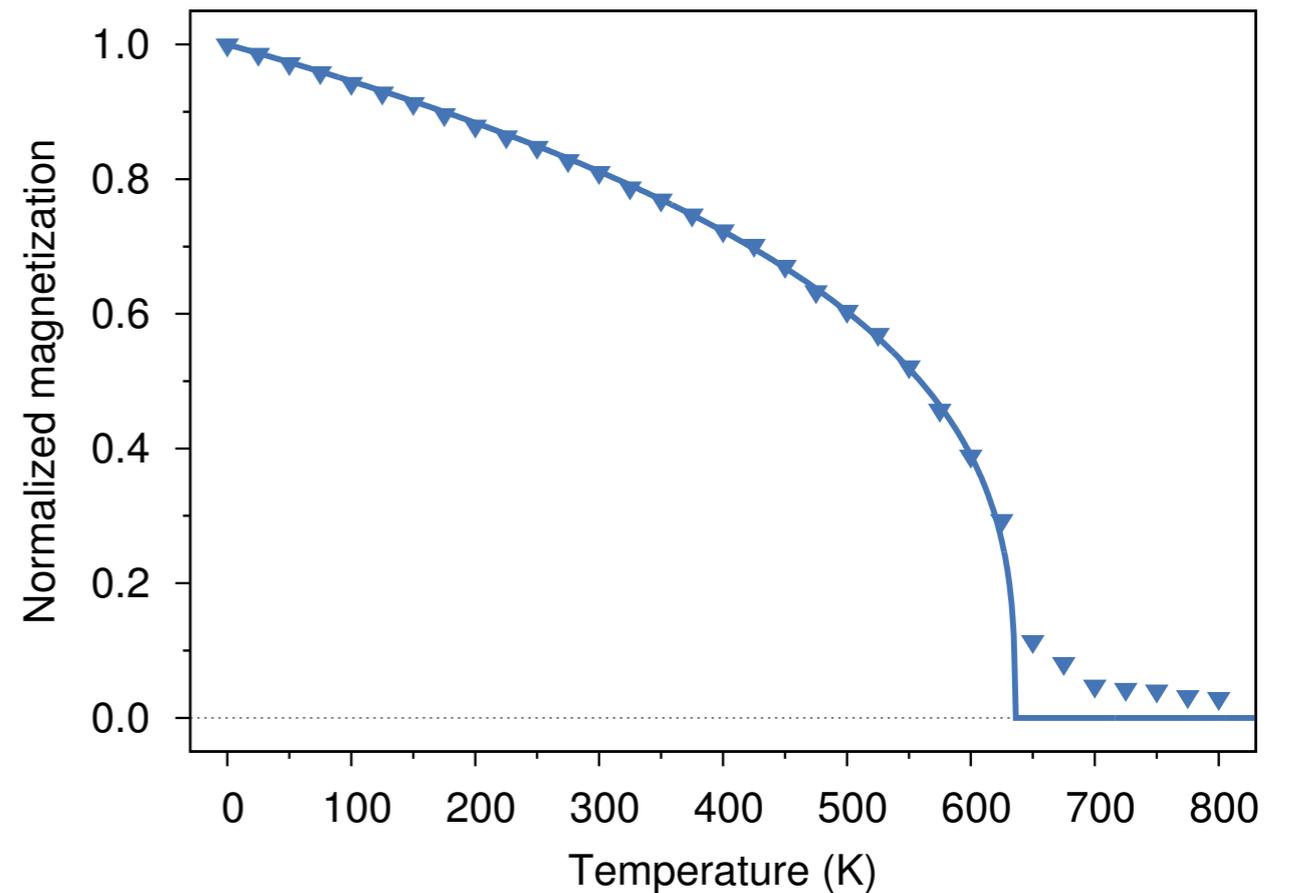
Curie temperature calculation

Calculate phase transition in Ni

Essential temperature dependent property of a magnetic material

$$\mathcal{H} = - \sum_{i < j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

$$J_{ij} = \frac{3k_B T_c}{\gamma z}$$

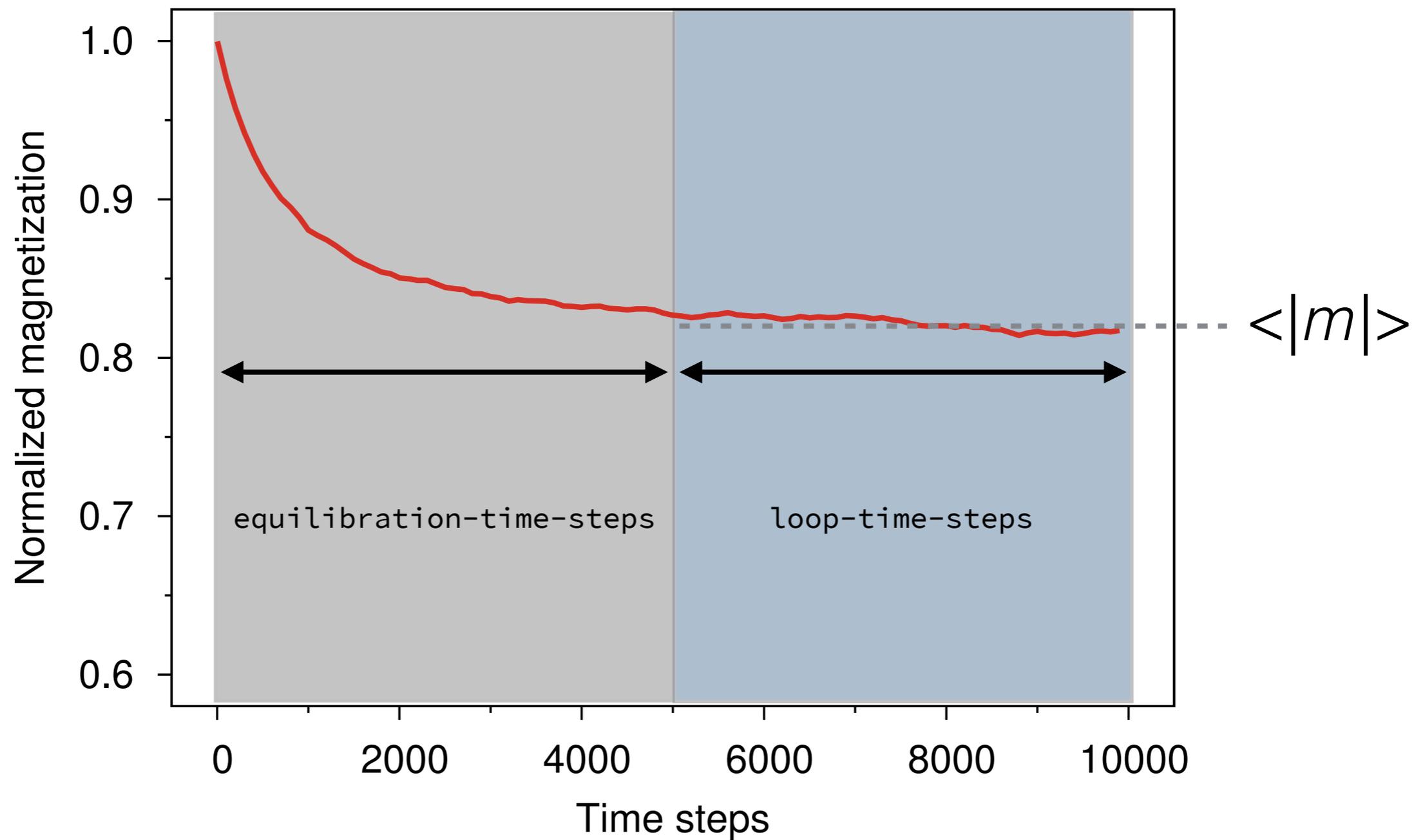


input

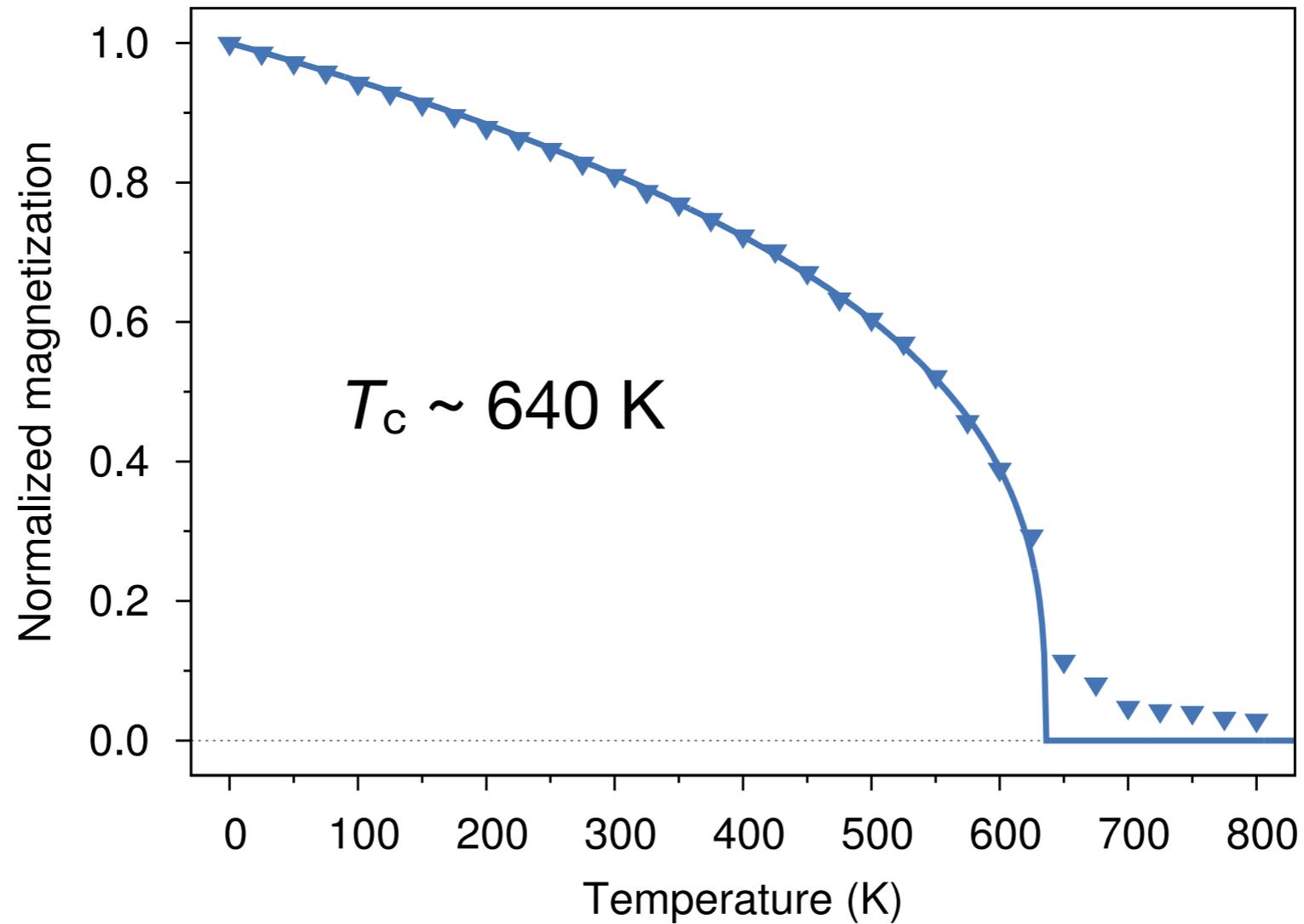
```
#-----  
# Creation attributes:  
#-----  
create:crystal-structure=fcc  
create:periodic-boundaries-x  
create:periodic-boundaries-y  
create:periodic-boundaries-z  
#-----  
# System Dimensions:  
#-----  
dimensions:unit-cell-size = 3.524 !A  
dimensions:system-size-x = 4.0 !nm  
dimensions:system-size-y = 4.0 !nm  
dimensions:system-size-z = 4.0 !nm  
#-----  
# Material Files:  
#-----  
material:file=Ni.mat  
#-----  
# Simulation attributes:  
#-----  
sim:temperature=300  
sim:minimum-temperature=0  
sim:maximum-temperature=800  
sim:temperature-increment=25  
sim:time-steps-increment=1  
sim:equilibration-time-steps=1000  
sim:loop-time-steps=1000
```

```
#-----  
# Program and integrator details  
#-----  
sim:program=curie-temperature  
sim:integrator=monte-carlo  
#-----  
# Data output  
#-----  
output:real-time  
output:temperature  
output:magnetisation  
output:magnetisation-length  
output:mean-magnetisation-length
```

Curie temperature calculation



Curie temperature calculation



$$m(T) = \left[1 - \left(\frac{T}{T_c} \right) \right]^\beta$$

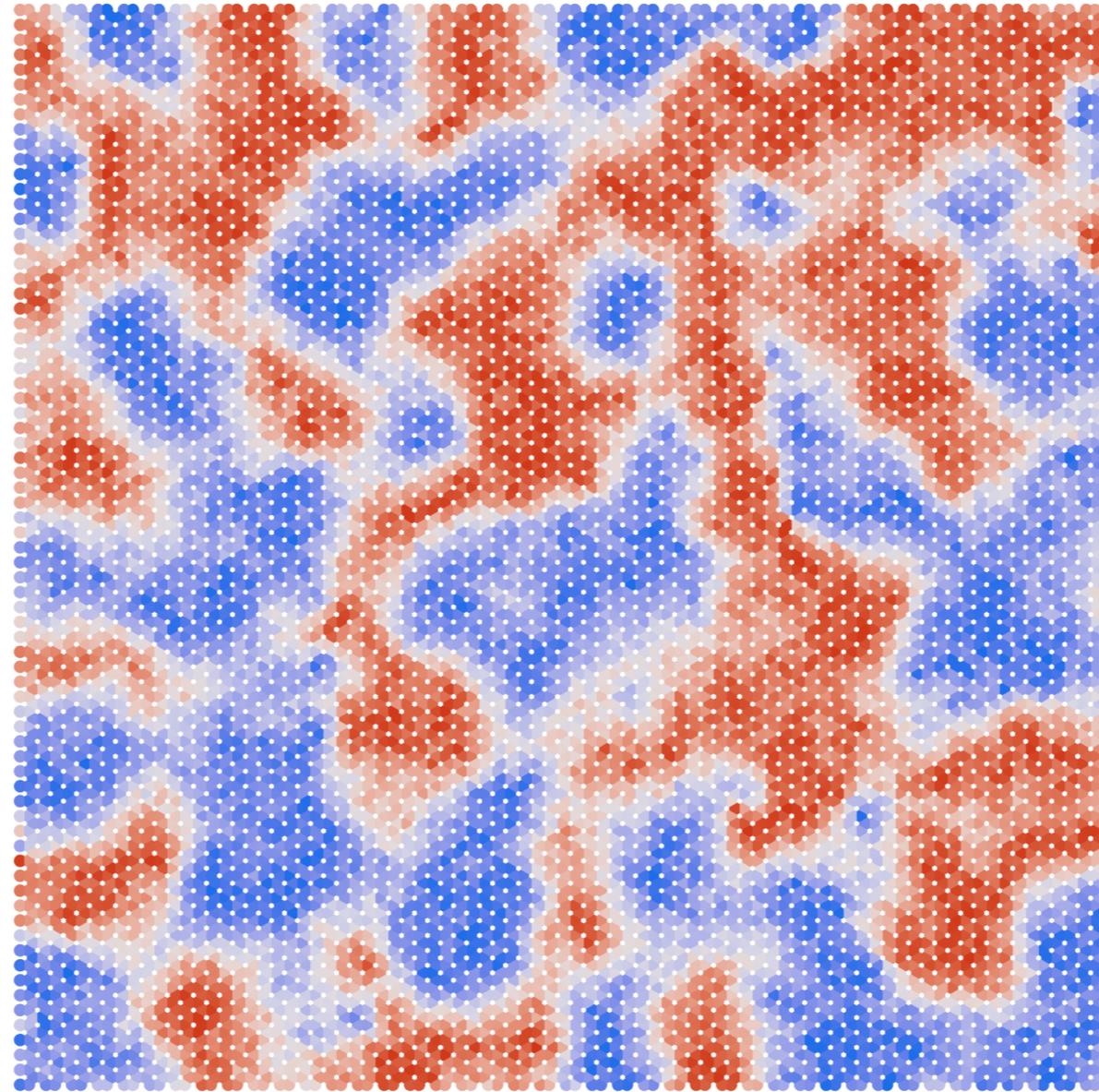
Plotting data with python

```
import matplotlib.pyplot as plt  
import numpy as np
```

```
T, m = np.loadtxt("output", unpack=True)
```

```
plt.plot(T,m)
```

Magnetic textures in 2D materials



Spin textures input file

```
#-----  
# Simplified input for spin texture  
# calculation  
#-----  
material:file = vampire.mat  
#-----  
# Creation attributes:  
#-----  
create:crystal-structure = honeycomb  
  
dimensions:unit-cell-size = 12.0  
dimensions:system-size-x = 50 !nm  
dimensions:system-size-y = 50 !nm  
dimensions:system-size-z = 0.1 !nm
```

```
#-----  
# Simulation attributes:  
#-----  
sim:equilibration-temperature = 5.0  
sim:temperature = 5.0  
sim:total-time-steps = 10000  
sim:equilibration-time-steps = 10000  
sim:time-steps-increment = 10  
sim:time-step = 1 !fs  
#-----  
# Program and integrator details  
#-----  
sim:program = time-series  
sim:integrator = llg-heun  
#-----  
# Data output  
#-----  
output:real-time  
output:material-magnetisation  
  
config:atoms  
config:atoms-output-rate = 1000
```

Spin textures material file

```
#-----  
material:num-materials = 1  
#-----  
# Material 1  
#-----  
material[1]:material-name = Cr  
material[1]:material-element = Cr  
material[1]:unit-cell-category = 1  
material[1]:atomic-spin-moment = 3.707 ! muB  
material[1]:initial-spin-direction = random  
material[1]:damping-constant = 0.1  
material[1]:uniaxial-anisotropy-constant = 4.7996290630874307e-23  
material[1]:uniaxial-anisotropy-direction = 0,0,1  
material[1]:exchange-matrix[1] = 1.0e-21
```

Visualisation with POV-Ray

```
make vdc
```

```
~/vampire/util/vdc/vdc --povray
```

```
povray -W800 -H600 +A0.3 +KFI20 +KFF20 spins.pov
```

In spins.pov, change the parameters to:

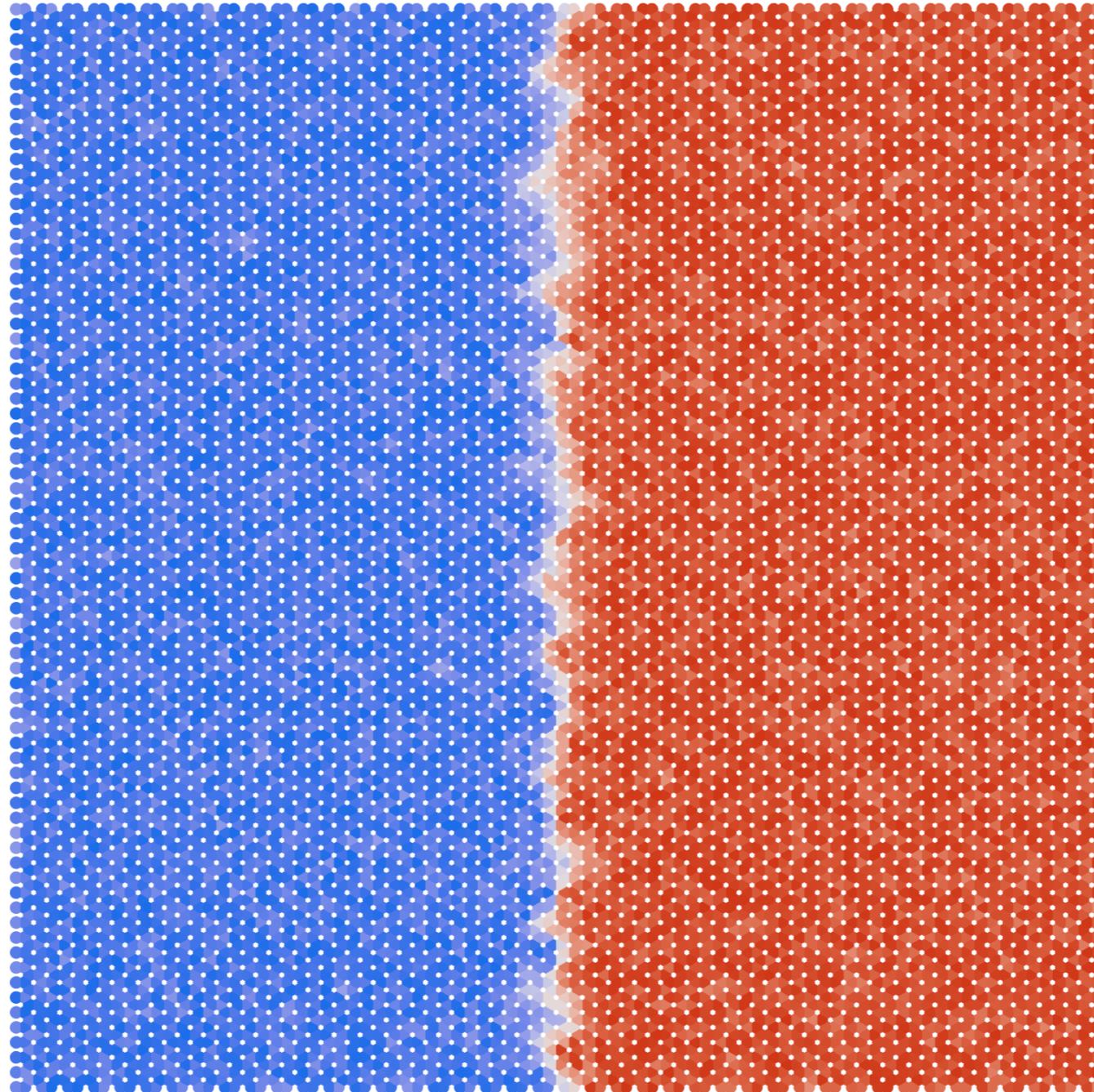
```
Set_Camera_Sky(<0,1,0>)
```

```
background { color White } // background colour
```

```
#declare ssize = 0.01;
```

```
#declare rsize = 8.2;
```

Magnetic domain walls



Domain wall input file

```
#-----  
# Simplified input for domain wall  
# calculation  
#-----  
material:file = vampire.mat  
#-----  
# Creation attributes:  
#-----  
create:crystal-structure = honeycomb  
  
dimensions:unit-cell-size = 12.0  
dimensions:system-size-x = 50 !nm  
dimensions:system-size-y = 50 !nm  
dimensions:system-size-z = 0.1 !nm  
  
create:select-material-by-geometry
```

```
#-----  
# Simulation attributes:  
#-----  
sim:equilibration-temperature = 5.0  
sim:temperature = 5.0  
sim:total-time-steps = 10000  
sim:equilibration-time-steps = 10000  
sim:time-steps-increment = 1  
sim:time-step = 0.1 !fs  
#-----  
# Program and integrator details  
#-----  
sim:program = time-series  
sim:integrator = llg-heun  
#-----  
# Data output  
#-----  
output:real-time  
output:material-magnetisation  
  
config:atoms  
config:atoms-output-rate = 1000
```

```
material:num-materials = 2
#-----
# Material 1
material[1]:material-name = Cr
material[1]:unit-cell-category = 1
material[1]:atomic-spin-moment = 3.707 ! muB
material[1]:initial-spin-direction = 0, 0, 1
material[1]:damping-constant = 0.1
material[1]:uniaxial-anisotropy-constant = 4.799e-23
material[1]:uniaxial-anisotropy-direction = 0,0,1
material[1]:geometry-file = geo1.txt
material[1]:exchange-matrix[1] = 1.0e-21
material[1]:exchange-matrix[2] = 1.0e-21
#-----
# Material 2
material[2]:material-name = Cr
material[2]:material-element = Fe
material[2]:unit-cell-category = 1
material[2]:atomic-spin-moment = 3.707 ! muB
material[2]:initial-spin-direction = 0, 0, -1
material[2]:damping-constant = 0.1
material[2]:uniaxial-anisotropy-constant = 4.800755450776671e-23
material[2]:uniaxial-anisotropy-direction = 0,0,1
material[2]:geometry-file = geo2.txt
material[2]:exchange-matrix[1] = 1.0e-21
material[2]:exchange-matrix[2] = 1.0e-21
#-----
```

Domain wall material file

Domain wall geometry files

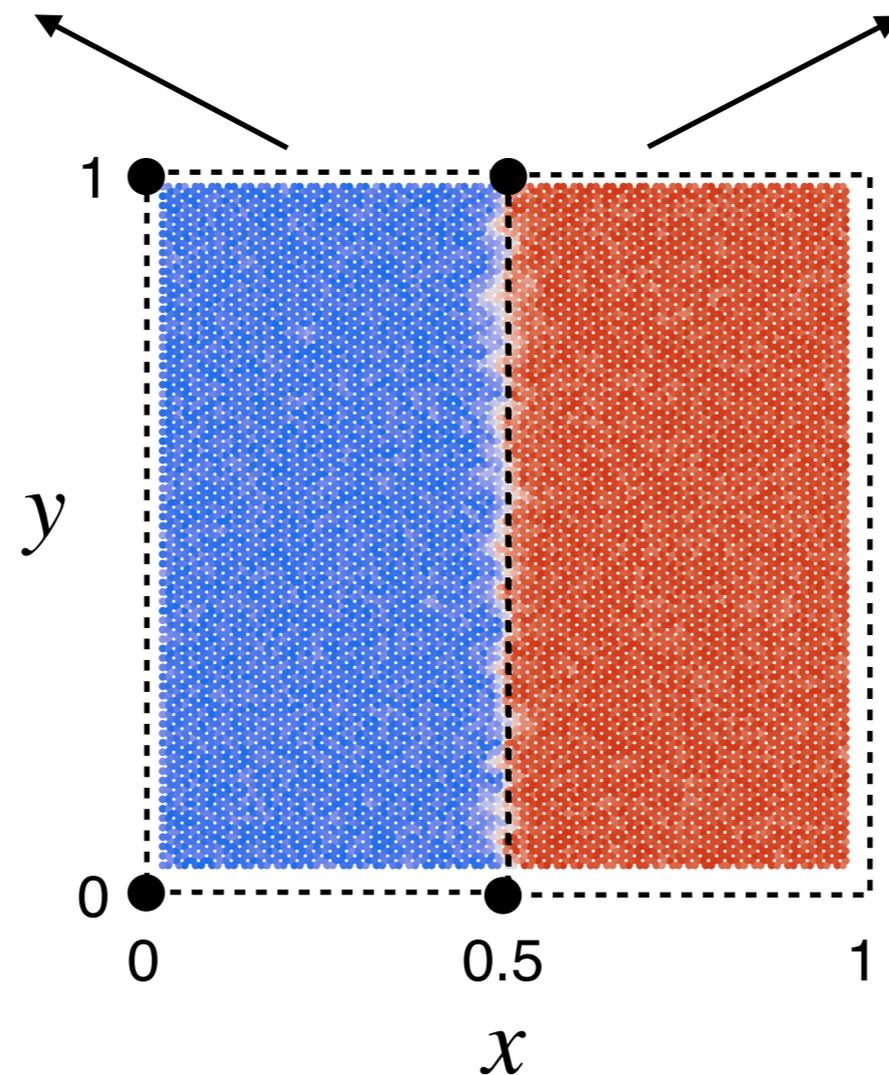
sim:applied-field-strength = 1.0 !T

geo1.txt

```
4  
0.0 0.0  
0.5 0.0  
0.5 1.0  
0.0 1.0
```

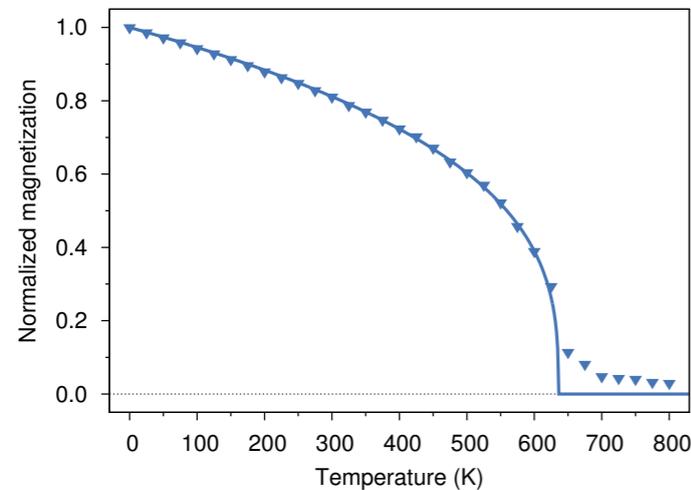
geo2.txt

```
4  
0.5 0.0  
1.0 0.0  
1.0 1.0  
0.5 1.0
```



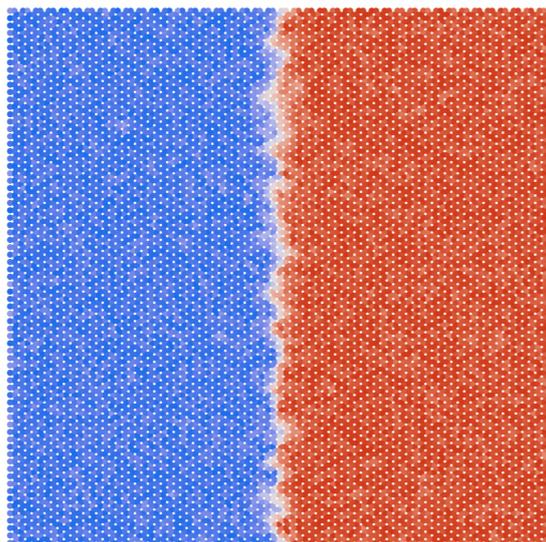
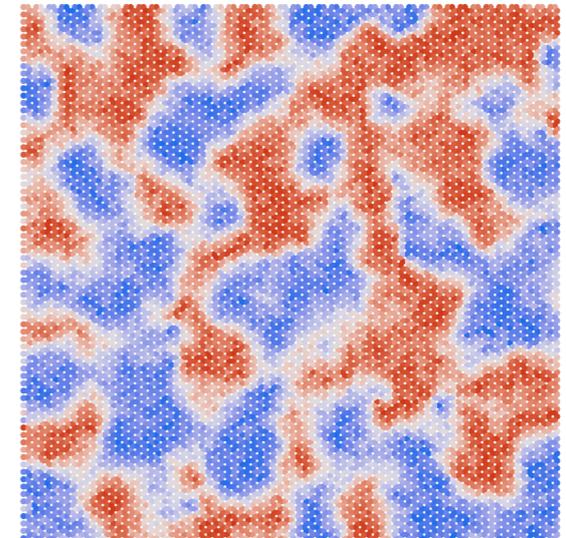
Summary

You have now completed some basic simulations:



Curie Temperature

2D textures



Domain walls