Calculation of anisotropy energy and temperature dependence of anisotropy

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1st Advanced VAMPIRE Workshop

Constraint Monte Carlo algorithm

Constraint Monte Carlo (CMC) algorithm

1. Why Monte Carlo (MC) algorithms?
   - Determine macroscopic equilibrium quantities
2. Issue
   - Standard MC allows to determine magnetic properties at thermal equilibrium (magnetisation)
   - At thermal equilibrium magnetocrystalline energy (MAE) can’t be determined since magnetisation is parallel to easy axis
3. Solution
   - Investigate the system while in quasi-equilibrium condition

CMC

- CMC algorithm[1] allows to constrains the direction of the global magnetisation while it allows the single spins to vary

- This allows to calculate restoring torque acting on the magnetisation

- From the torque, MAE can be obtained

1. *Constrained Monte Carlo method and calculation of the temperature dependence of magnetic anisotropy*, P. Asselin, R. F. L. Evans, J. Barker, R. W. Chantrell, R. Yanes, O. Chubykalo-Fesenko, D. Hinzke, and U. Nowak, Phys. Rev. B 82, 054415 (2010)

CMC step

- In CMC trial move acts on 2 spins at time:
  1. (Assume constraint direction along +*z*-axis) Select 2 spins *i,j*
  2. Apply MC move to first spin $\hat{S}_i \rightarrow \hat{S}_i'$
  3. Move second spin $\hat{S}_j$ to compensate change of magnetisation in *xy*-components ($M_x = M_y = 0$):

$$\begin{cases} \hat{S}_{jx}' = \hat{S}_{ix} + \hat{S}_{jx} - \hat{S}_{ix}' \\ \hat{S}_{jy}' = \hat{S}_{iy} + \hat{S}_{jy} - \hat{S}_{iy}' \end{cases}$$

  4. Adjust z-component of new spin j

$$\begin{cases} \hat{S}_{jz}' = sign(\hat{S}_{jz})\sqrt{1 - \hat{S}_{jx}^2 - \hat{S}_{jy}^2} \\ 1 - \hat{S}_{jx}^2 - \hat{S}_{jy}^2 > 0 \end{cases}$$

CMC step

5. Calculate new magnetisation

$$\begin{cases} M_z' = M_z + \hat{S}_{iz}' + \hat{S}_{jz}' - \hat{S}_{iz} - \hat{S}_{jz} \\ M_z' > 0 \end{cases}$$

6. Calculate the change in energy

$$\begin{cases} \Delta E_i = E_i' - E_i \\ \Delta E_{ij} = \Delta E_i + \Delta E_j \end{cases}$$

7. Compute the acceptance probability of the moves

$$P = min\left\{1, \left(\frac{M_z'}{M_z}\right)^2 \frac{|\hat{S}_{jz}|}{|\hat{S}_{jz}'|} exp\left(-\Delta E_{ij}/k_B T\right)\right\}$$

Geometrical factor

Boltzmann probability density

Free energy

- In ensemble at constant temperature and volume, energy of the system given by Helmoltz free energy:

$$F = U - TS$$

- How can we obtain it?

  Calculating the restoring torque acting on the magnetisation of the system

Free energy

- For a reversible system, the variation of free energy is:

$$\Delta F = \int_a^b \delta W$$

- In a magnetic system the work *W* done on a system is equivalent to the torque *T* that acts on the whole system:

$$\begin{cases} \delta W = |T| d\vartheta \\ \vartheta = \text{angle formed by spin and net field acting on spins} \end{cases}$$

$$\Rightarrow \Delta F = -\int_a^b |T| d\vartheta$$

Torque

- Total torque acting on the system is given by

$$T = \sum_i T_i = \sum_i \hat{S}_i \times H_i = \sum_i \hat{S}_i \times \left(-\frac{\partial \mathcal{H}}{\partial \hat{S}_i} \right)$$

- The magnitude of the average of the total internal torque T is calculated from thermodynamic average of T:

$$|T| = \langle |T| \rangle$$

- Once the torque is calculated, the free energy can be computed

Uniaxial anisotropy

- Let's assume the material has a single axis along which the magnetic moments prefer to align → Uniaxial anisotropy

- Internal energy *U* is given by:

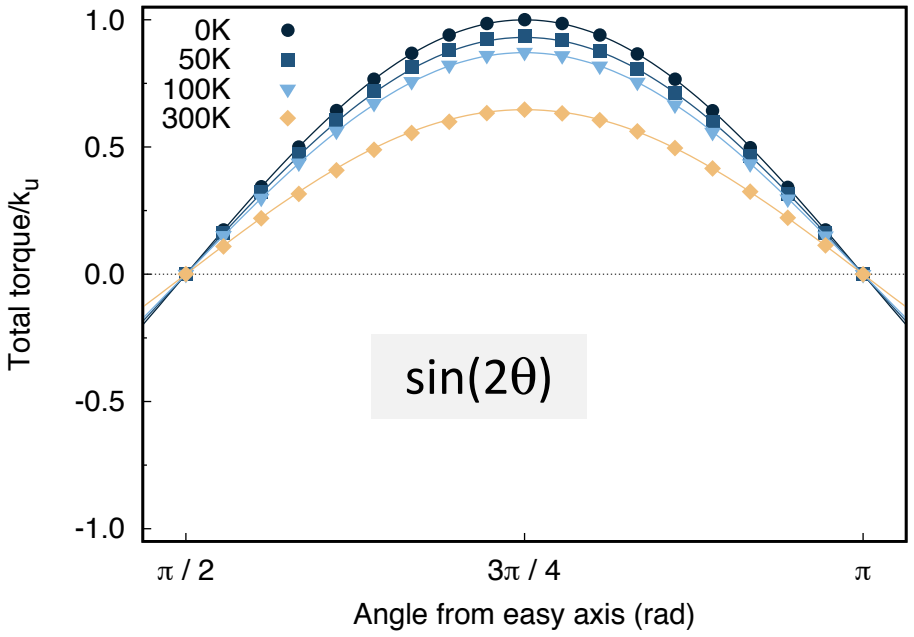
$$U = K_u \sin \vartheta^2$$

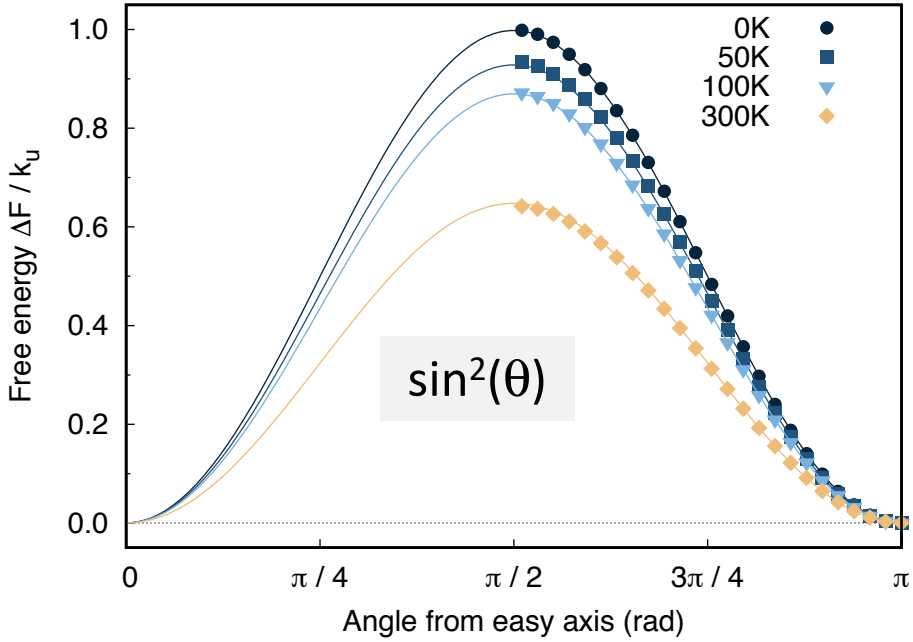
- At zero temperature

$$|T| = -\frac{\partial F}{\partial \vartheta} = -\frac{\partial U}{\partial \vartheta} = -K_u \sin 2\vartheta$$

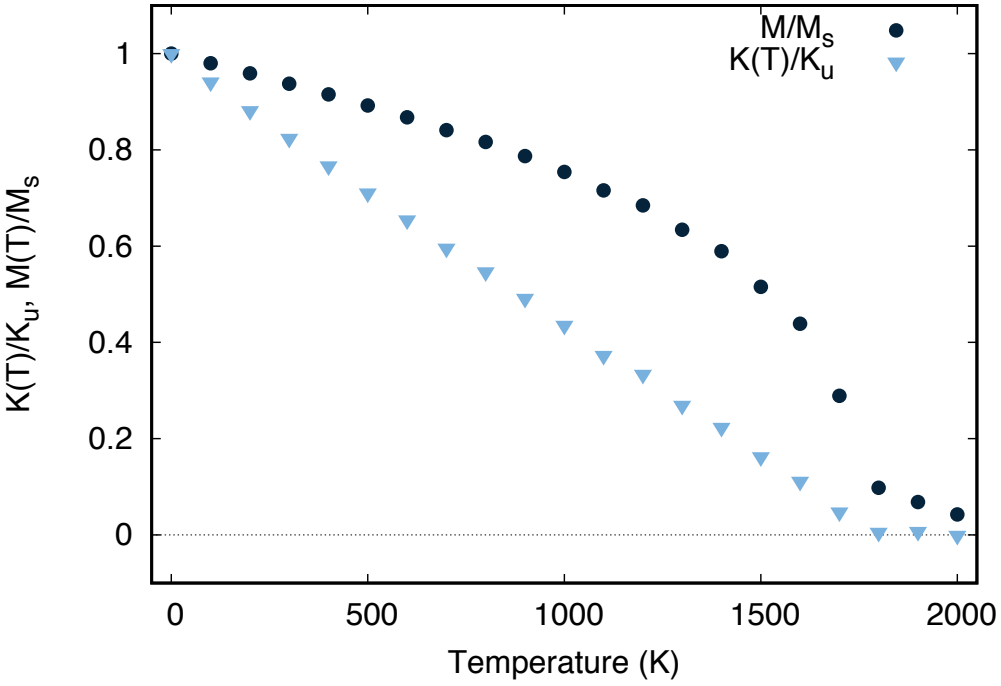
- $\sin 2\vartheta$ holds at all temperatures, while $K_u \rightarrow K_u(\mathrm{T})$

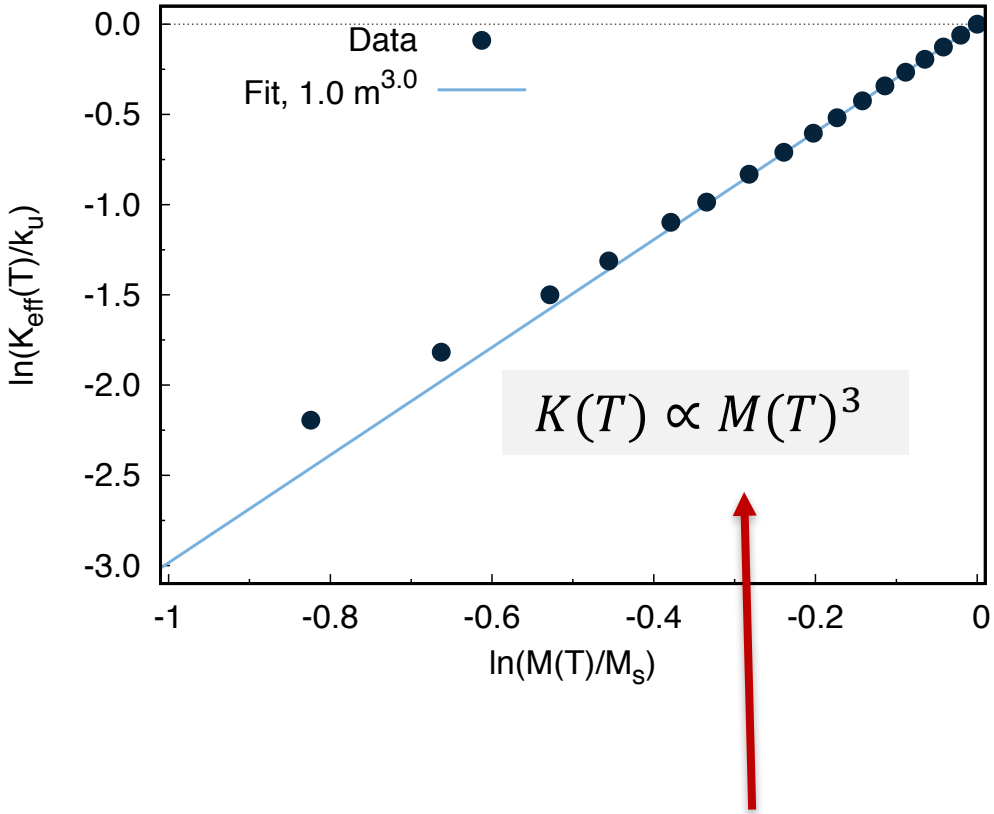
Uniaxial anisotropy: Torque & free energy





Uniaxial anisotropy: Temperature scaling





$$K(T) \propto M(T)^3$$

In agreement with Callen-Callen theory[2]

2. *H. B. Callen and E. Callen, J. Phys. Chem. Solids 27, 1271 (1966).*

Hands on

Main parameters for CMC simulations

```
sim:constraint-angle-theta-minimum  = 0.0
sim:constraint-angle-theta-maximum  = 0.0
sim:constraint-angle-theta-increment= 10.0

sim:constraint-angle-phi-minimum  = 0.0
sim:constraint-angle-phi-maximum  = 90.0
sim:constraint-angle-phi-increment= 15.0

sim:integrator = constrained-monte-carlo
sim:program    = cmc-anisotropy

output:constraint-theta
output:constraint-phi
output:mean-magnetisation-length
output:mean-total-torque
```

Plotting data with gnuplot

In bash we can sort the data in a file based on specific keys (-k):

```
>sort -k 1g -k 3g output
```

Enter in gnuplot:

```
> Gnuplot
```

#column ($) 3 is the azimuthal angle phi, column 6 is y-component of torque
##In gnuplot we can have conditional statements with the following syntax:

```
($1==0   ?$3:0/0):($6)
```

#Once in gnuplot, type the following commands where

```
> plot ‘<sort -k 1g -k 3g output’  u($1==0?$3:0/0):($6)  w l
```

FILE to plot

COLUMNS to plot

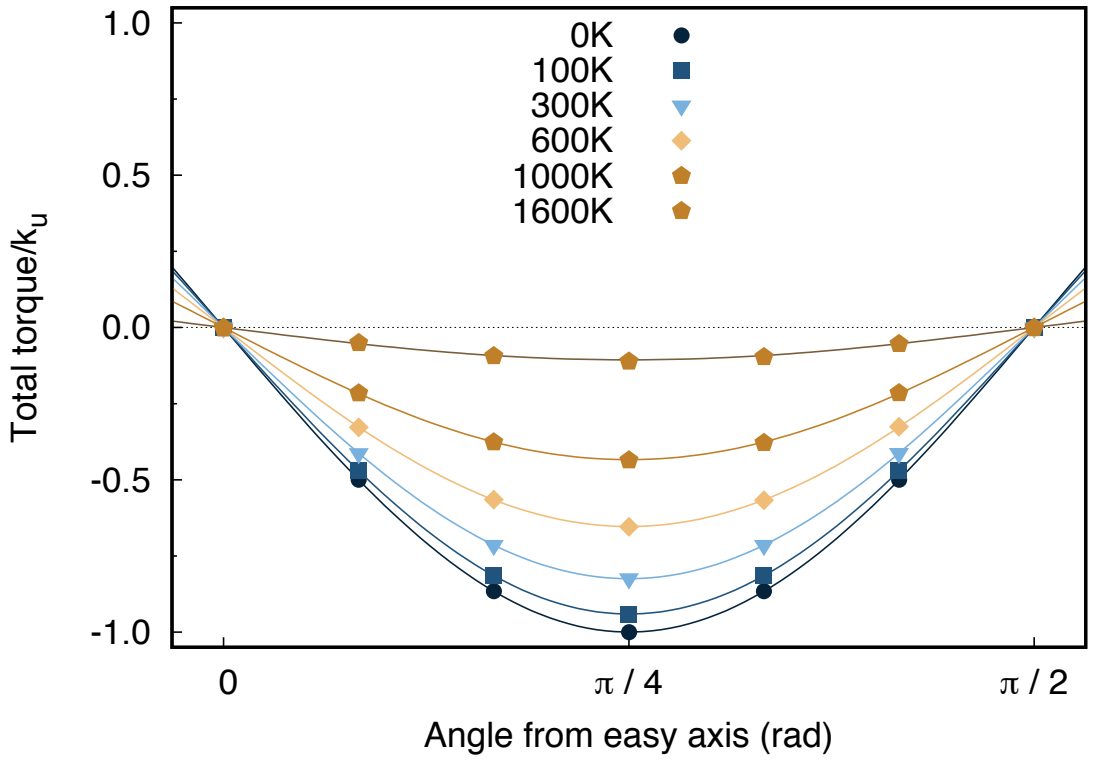
PLOT with lines

Practice on CMC

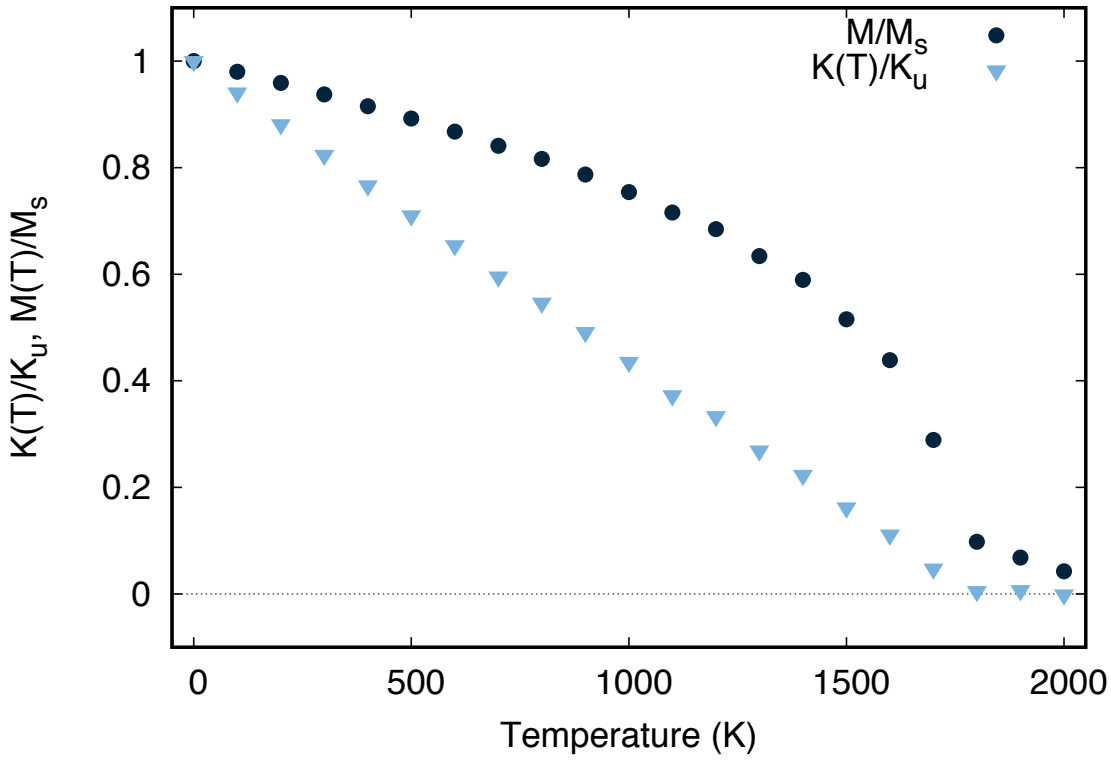
1.1 Uniaxial anisotropy

1. Create the input files for bulk uniaxial bcc Co (Suggestion: for material parameters use those in Co.mat in vampire folder)
2. Calculate torque acting on magnetisation as function of angle between constrained direction of the magnetisation and easy axis for different temperatures.
3. Calculate energy barrier and temperature dependence of anisotropy.

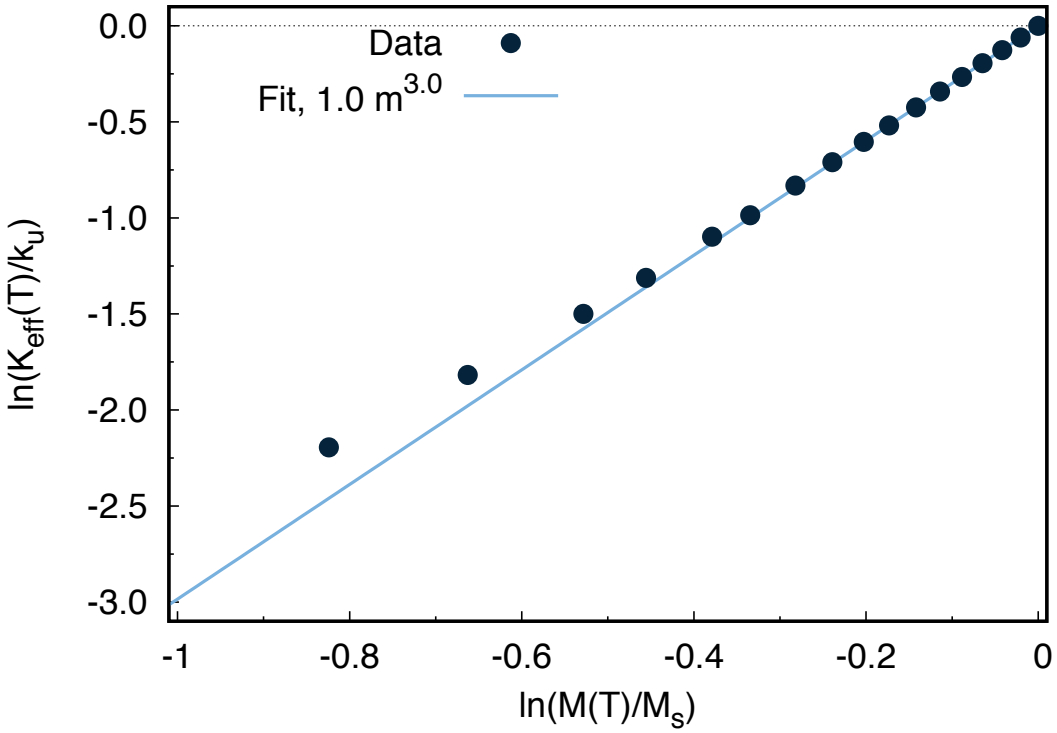
Torque


1.0
0.5
0.0
-0.5
-1.0
Total torque/k_u
0K
100K
300K
600K
1000K
1600K
0
π / 4
π / 2
Angle from easy axis (rad)

Temperature scaling



Scaling of anisotropy vs magnetisation



Practice on CMC

1.2 Cubic anisotropy

1. Create the input files for bulk cubic bcc Fe. The following parameters can be used:

   (a) Nearest-neighbours exchange constant $J_{ij} = 7.05e-21$ J/link

   (b) Cubic anisotropy energy constant $k_c = 5.65e-25$ J/atom

   (c) Magnetic moment $\mu_s = 2.2\mu_B$

   (d) Lattice constant $a_0 = 2.86$ Ang

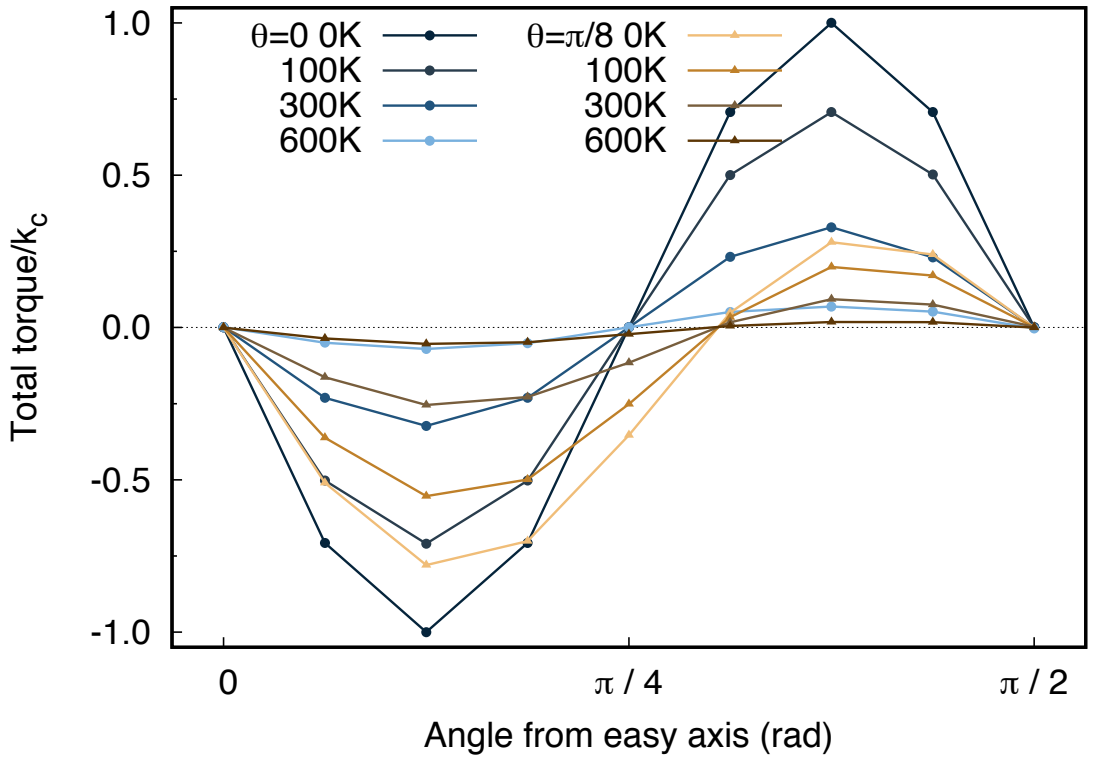
2. Calculate torque for different temperatures.

3. Calculate energy barrier and temperature dependence of energy barrier.

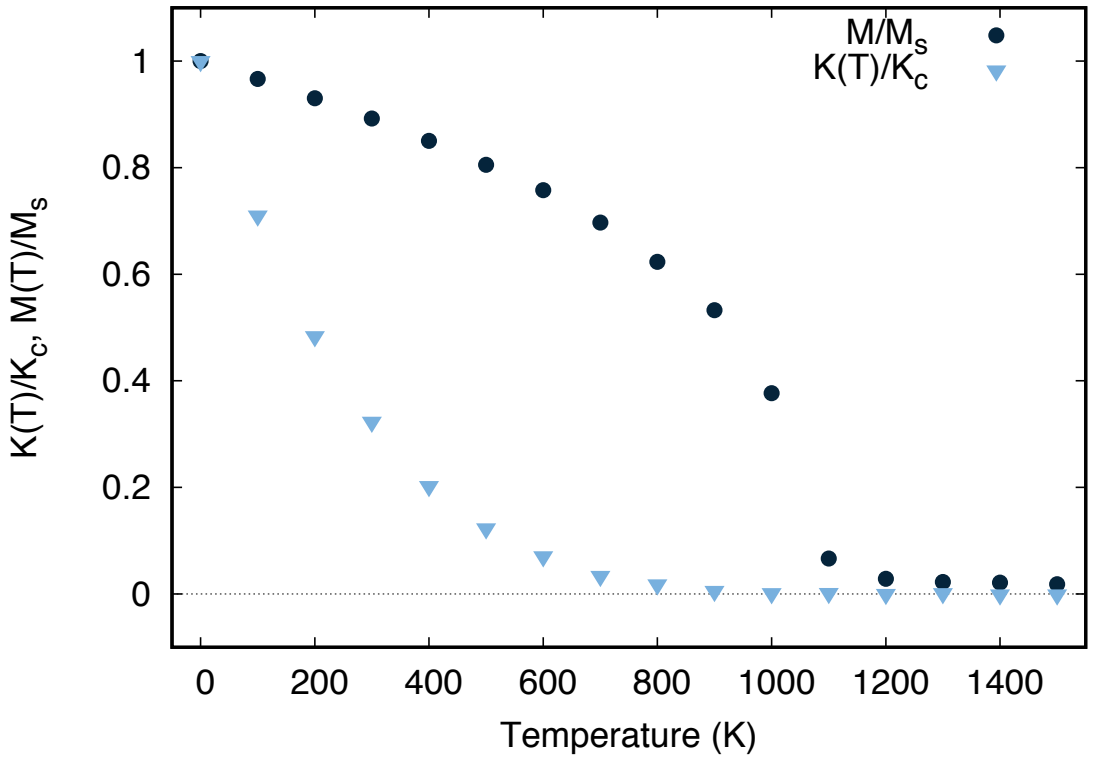
4. Compare the result with uniaxial case and obtain scaling of magnetisation and anisotropy for both cases.

Torque

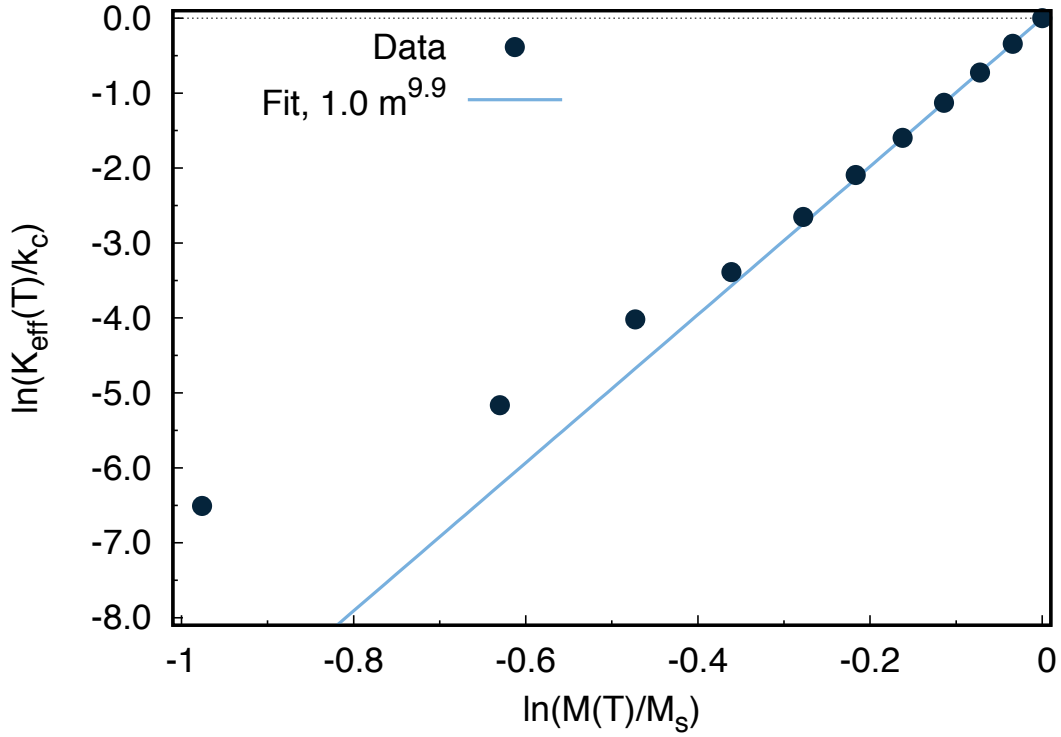
Torque depends on both rotational (θ) and azimuthal (ϕ) angle



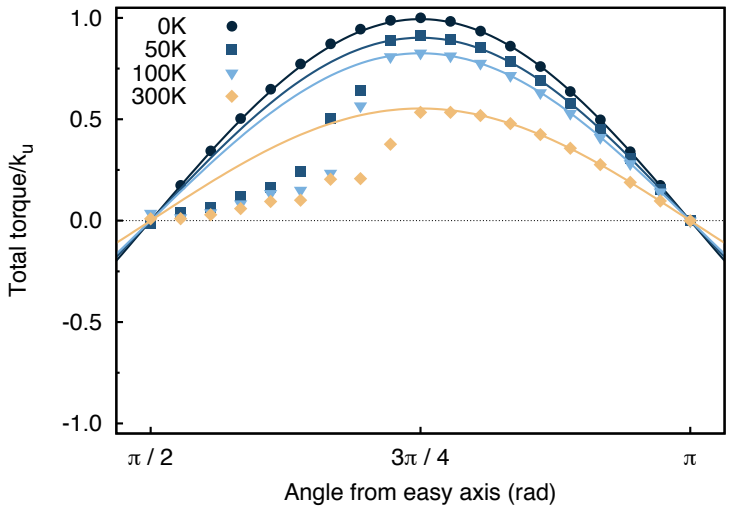
Temperature scaling

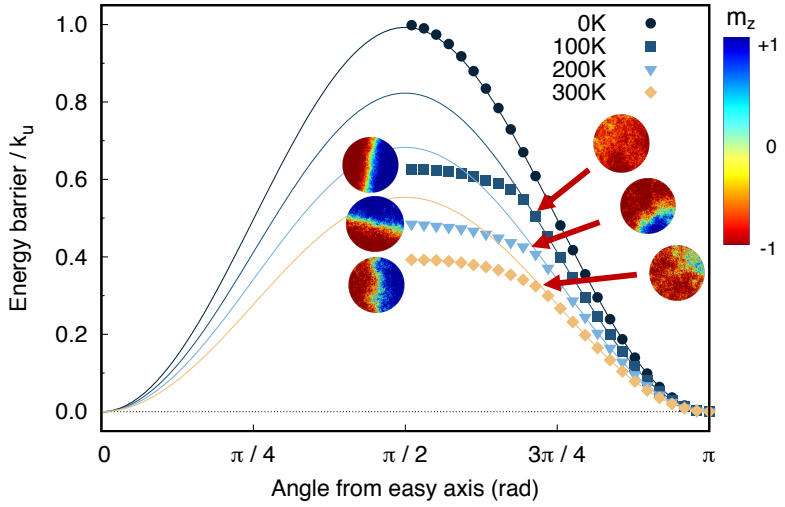


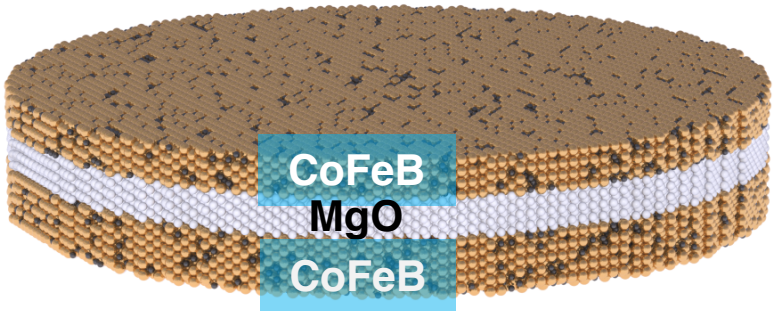
Scaling of anisotropy vs magnetisation

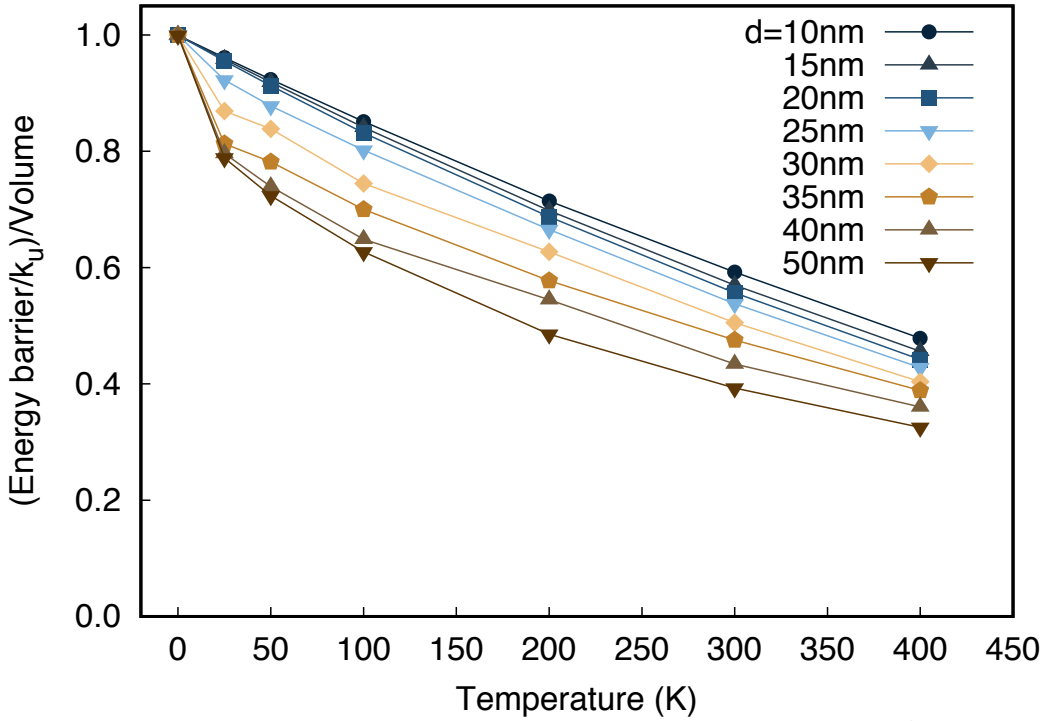


More complex systems

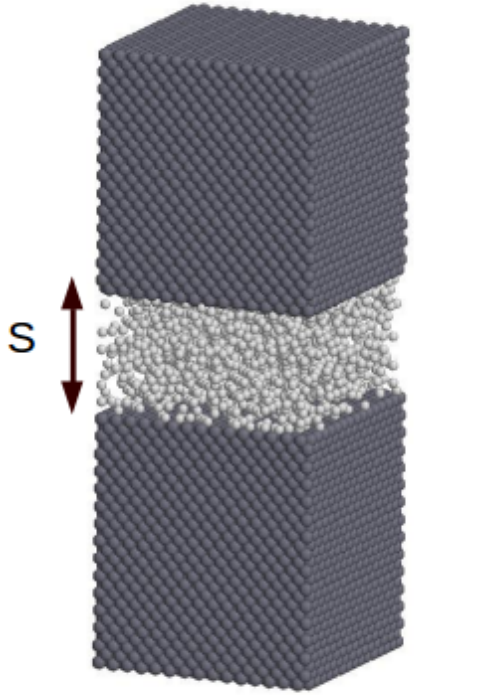


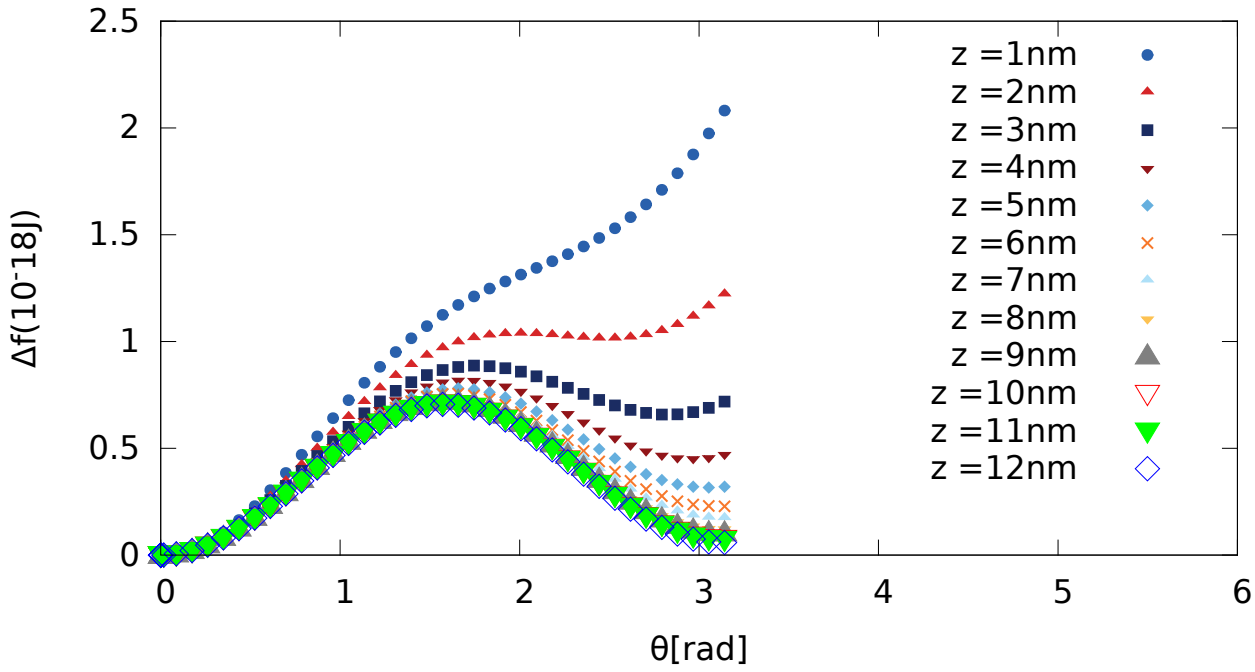






More complex systems





Images and data kindly from
Razvan Ababei

Practice on CMC

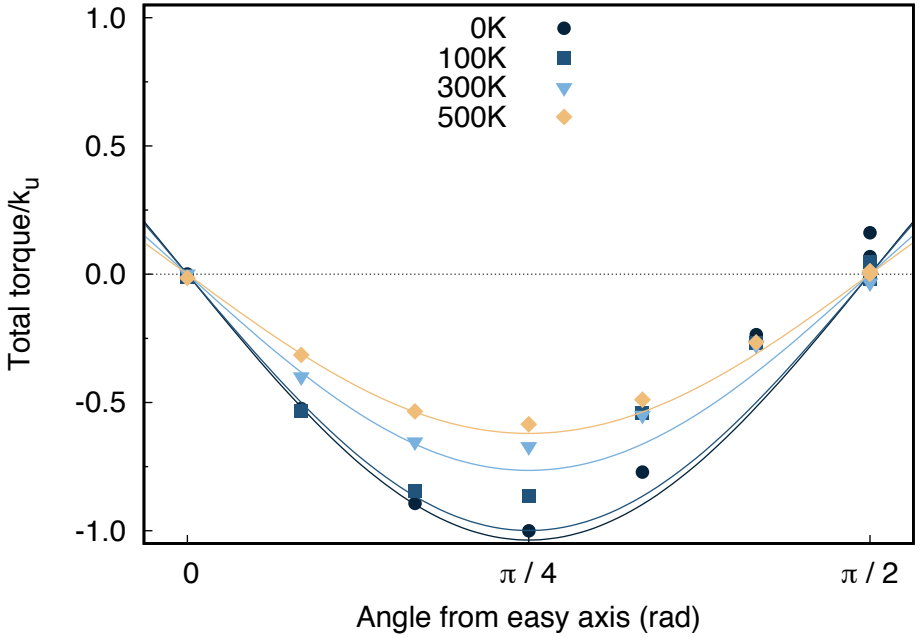
1.3 Constraining a single material

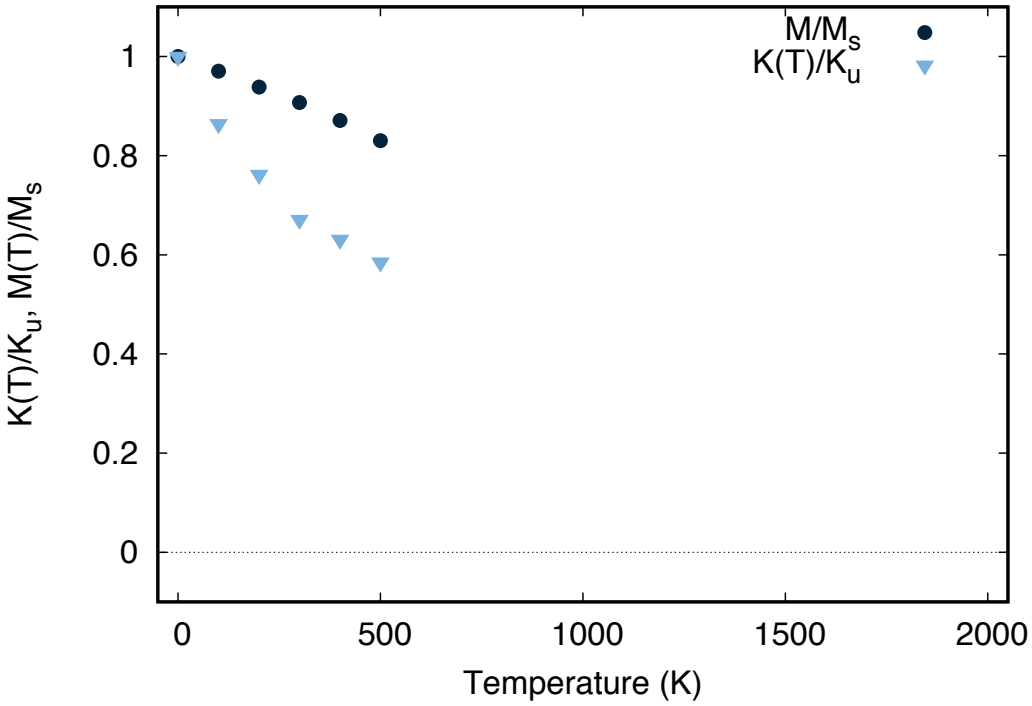
1. Create a bi-layer structure of cubic Fe and uniaxial Co
2. Calculate torque for different temperatures when constraining
   (a) cubic Fe only;
   (b) uniaxial Co only.
3. Obtain energy barrier and temperature dependence of anisotropy. How do they compare with the single material case?

Main parameters for CMC simulations

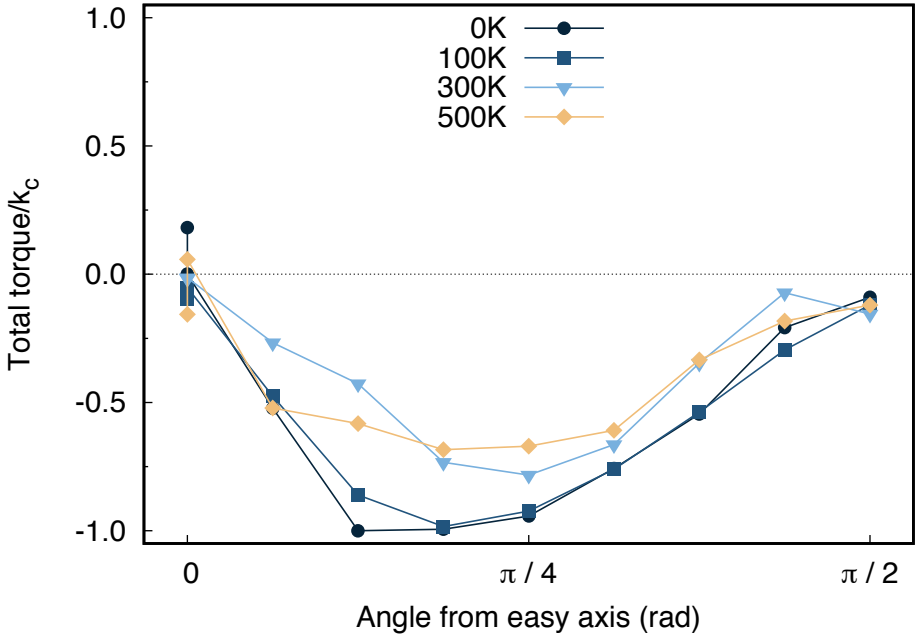
```
material[1]:constrained=true  #false for other material

material[1]:constraint-angle-theta-minimum=0.0
material[1]:constraint-angle-theta-maximum=0.0
material[1]:constraint-angle-theta-increment=10.0

material[1]:constraint-angle-phi-minimum=0.0
material[1]:constraint-angle-phi-maximum=90.0
material[1]:constraint-angle-phi-increment=15.0

#-----------------------------------------
#-----------------------------------------
sim:integrator   = hybrid-constrained-monte-carlo
sim:program = hybrid-cmc

output:material-constraint-theta
output:material-constraint-phi
```

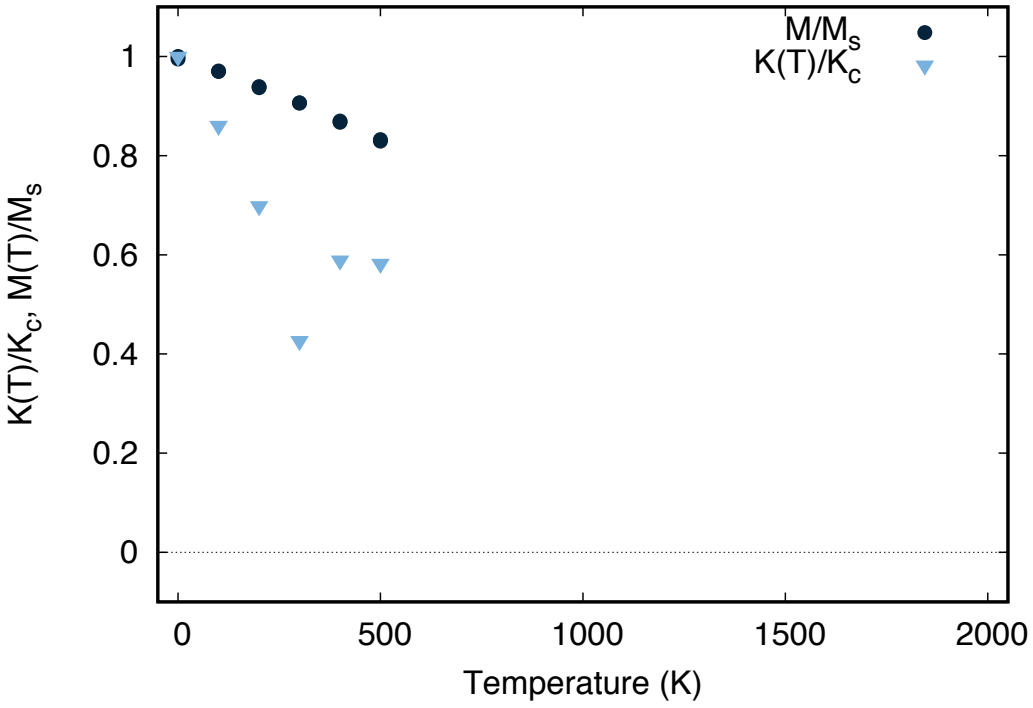
Constraining only uniaxial material





Constraining only uniaxial material





Practice on CMC

1.4 Finite system size effect

1. Calculate torque and anisotropy at different temperatures for a thin film 2 nm thick composed as:

   (a) 30% uniaxial out-of-plane anisotropy with $k_u = 1.0e-23$ J/atom

   (b) 70% cubic in-plane anisotropy with $k_c = 5.5e-25$ J/atom

   with exchange coupling:

   (a) $J_{ij}^{uni-uni} = 1.5e-20$ J/link

   (b) $J_{ij}^{uni-cub} = 1.5e-20$ J/link

   (c) $J_{ij}^{cub-cub} = 7.5e-21$ J/link

2. Perform the same simulations varying the total thickness of the film, but keeping constant the number of layers characterised by uniaxial anisotropy.

Dipole fields

Dipole energy

For N interacting dipoles (macro-cells), the total dipole-dipole energy is given by:

$$E_{\mathrm{dip}} = -\frac{1}{2}\sum_{q\neq p}^{N} \vec{m}_q \frac{\mu_0}{4\pi} \mathrm{D}_{qp} \vec{m}_p$$

Where D_{qp} is the dipolar matrix and $\vec{m}_{p,q}$ are the moments of the dipoles p,q. In terms of magnetic induction E_{dip} can be written as:

$$E_{\mathrm{dip}} = -\frac{1}{2}\sum_{q\neq p}^{N} \vec{m}_q \mathrm{B}_q^{\mathrm{dip}}$$

where $\mathrm{B}_q{}^{\mathrm{dip}}$ is the dipolar field experienced by moment q.

Bare macro-cell approach

- The system is divided into cubic macro-cells
- Each cell is supposed to have uniform magnetisation
- The dipolar interaction is calculated between macro-cells considering for each one a pairwise summation.
- A self-demagnetisation term is added, to include the internal field of the macro-cell.

$$\mathrm{H}_q^{\mathrm{dip}} = \frac{\mu_0}{4\pi} \sum_{q \neq p} \frac{3\left(\mu_p \cdot \hat{r}_{qp}\right)\hat{r}_{qp} - \mu_p}{\left|r_{qp}\right|^3} - \frac{\mu_0}{3}\frac{\mu_q}{V_q}$$

Inter-intra dipole approach

We can write the dipolar matrix as summation of the contribution from interaction with other cells (inter) and internal to the macrocell (intra) [G. J. Bowden *et al,* J.Phys.:Condens. Matter,28(2016),066001]:

$$\mathrm{B}^{\mathrm{dip}} = \mathrm{B}_q^{\mathrm{dip}} + \mathrm{B}_p^{\mathrm{dip}} + \mathrm{B}_p^{\mathrm{self}}$$

$$= \underbrace{\mathrm{D}_{qp}^{\mathrm{inter}}\vec{m}_p}_{\text{INTER}} + \underbrace{\mathrm{D}_{pp}^{\mathrm{intra}}\vec{m}_p + \frac{8\pi}{3}\vec{m}_p/V_p}_{\text{INTRA}}$$

$$\mathrm{D}_{qp}^{\mathrm{inter}} + \mathrm{D}_{pp}^{\mathrm{intra}} = \sum_{q_j}^{n_q}\sum_{p_i}^{n_p} \mathrm{D}_{qj,pi}^{\mathrm{inter}} + \sum_{p_i \neq p_j}^{n_p}\sum_{p_i}^{n_p} \mathrm{D}_{pjpi}^{\mathrm{intra}} = \mathbf{D}_{qp}$$

Interaction between the spins in cell p and spins in cell q (atomistic)

Interaction between moments inside cell p (atomistic)

Inter-intra dipole approach

- $\mathrm{B}_p^{\mathrm{self}} = \frac{8\pi}{3}\vec{m}_p$ represent the Maxwellian internal field of a dipole.

- $\vec{m}_p$ is the macro-moment of the cell p and V_p is the volume of the same cell.

- D_{qp}^{inter} , D_{pp}^{intra} do not correspond to real dipole-dipole matrices, but their sum D_{qp} does.

- D_{qp}^{inter} , D_{pp}^{intra} are casted in terms of usual dipolar matrix

Dipolar matrixes

The dipolar matrix for the interaction between different macro-cells, is given by:

$$\mathbf{D}_{qj,pi}^{\text{inter}} = \frac{1}{r_{piqj}^3}\begin{bmatrix} (3x_{piqj}^2 - 1) & 3x_{piqj}y_{piqj} & 3x_{piqj}z_{piqj} \\ 3y_{piqj}x_{piqj} & (3y_{piqj}^2 - 1) & 3y_{piqj}z_{piqj} \\ 3z_{piqj}x_{piqj} & 3z_{piqj}y_{piqj} & (3z_{piqj}^2 - 1) \end{bmatrix}$$

Same in case of internal term (replace $qj \rightarrow pj$) for $\mathbf{D}_{pi,pj}^{\text{intra}}$.

Warning: Assumption is that moments in the macro-cell are all aligned along the same direction, i.e. parallel to each other.

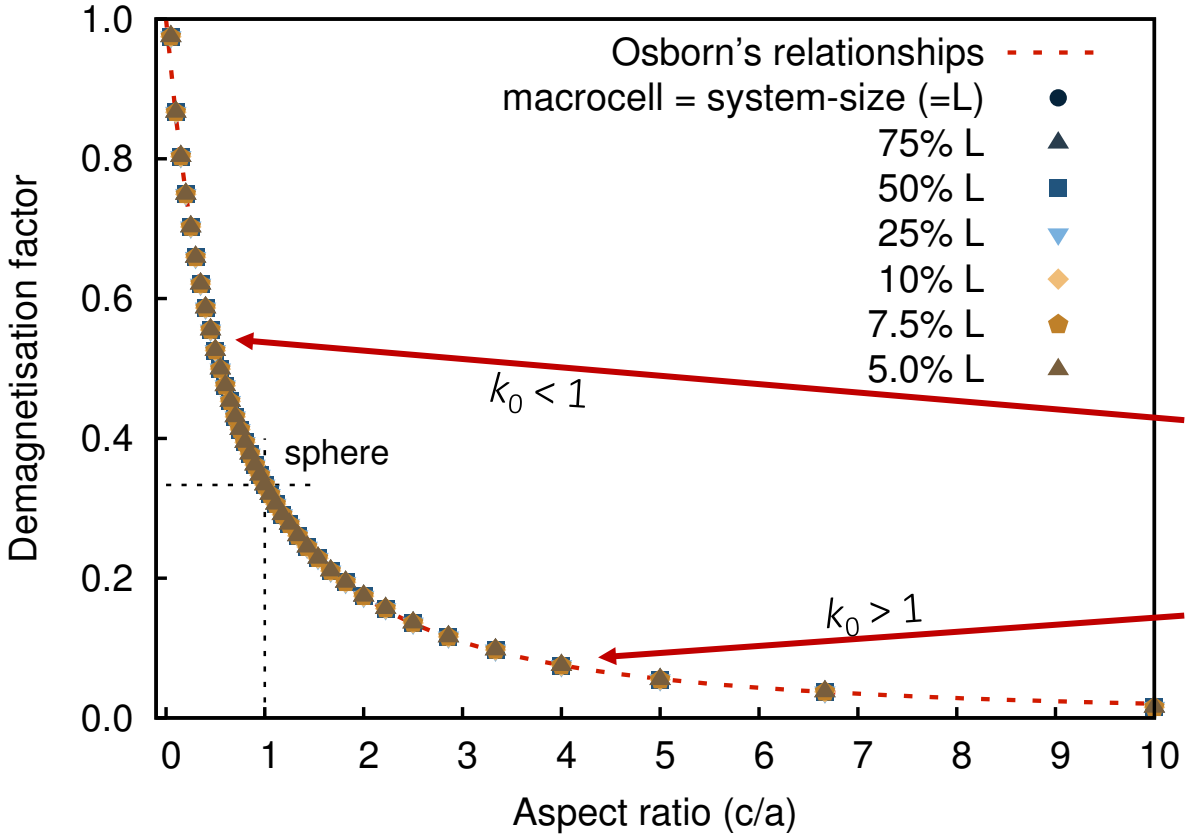
Notes on the approach

- This approach works independently of the shape of the macro-cell.

- After ~ 2 macro-cells, contribution of intra term D^{intra} becomes negligible and a bare macro-cell method could be used.

- Since it requires parallel moments, the size of the macro-cell should be less than the domain-wall width.

Test: Demagnetisation factor of ellipsoid



Osborn's relationship:

Aspect ratio = k_0 = c/a

$$D = \frac{1}{\kappa_o^2 - 1}\left(\frac{\kappa_o}{\sqrt{\kappa_o^2 - 1}}\operatorname{arcosh}\,\kappa_o - 1\right)$$

$$D = \frac{1}{1 - \kappa_o^2}\left(1 - \frac{\kappa_o}{\sqrt{1 - \kappa_o^2}}\arccos\,\kappa_o\right)$$

Hands on

Main parameters

```
cells:macro-cell-size=10.1 !A


dipole:solver=tensor
dipole:field-update-rate=100
dipole:cutoff-radius=2
```

Practice on Dipole fields

1. Create thin film 10 nm wide and 1 nm thick with parameters of permalloy:

   (a) $J_{ij}^{Ni-Ni} = 3.78e-23$ J/link

   (b) $J_{ij}^{Fe-Fe} = 3.78e-23$ J/link

   (c) $J_{ij}^{Fe-Ni} = 3.78e-23$ J/link

   (d) $k_u^{Ni} = 3.355e-26$ J/atom

   (e) $k_u^{Fe} = 3.355e-26$ J/atom

   (f) $\mu_s^{Ni} = 0.62\,\mu_B$

   (g) $\mu_s^{Fe} = 30\,\mu_B$

   (h) $a_0 = 3.55$ Ang

   (i) Lattice structure = FCC

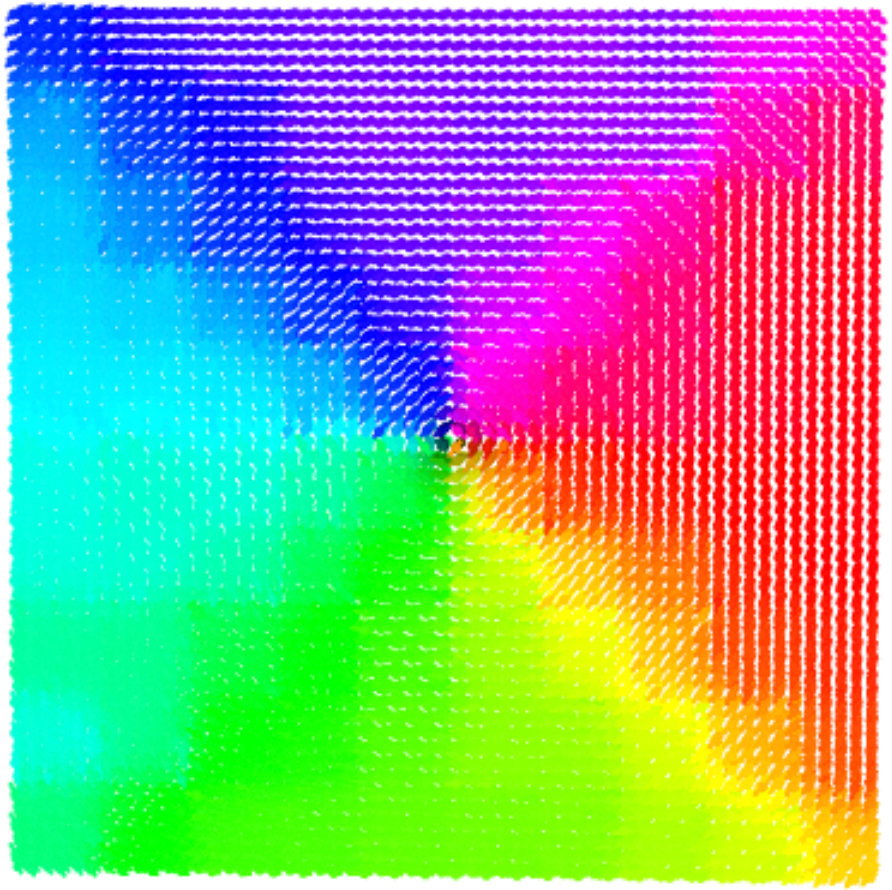
   (j) macro-cell size = 10Ang

Practice on Dipole fields

2. Perform time evolution of the magnetisation starting from random spin configuration with and without magnetostatic: do the results differ?

3. Vary the system dimensions/magnetic moment/macro-cell size.

Practice on Dipole fields – final snapshot



Povray – visualising spin cofigurations

- Download Povray from github repository:
  https://github.com/POV-Ray/povray/tree/3.7-stable

- To install look at “README.md” in “unix” directory:

Povray – visualising spin cofigurations: How to compile it

```
git clone https://github.com/POV-Ray/povray.git
```

```
cd unix/
```

```
./prebuild.sh
```

```
cd ../
```

```
./configure COMPILED_BY="your name <email@address>"
```

```
make
```

```
make install
```

Povray – Running povray

```
> /path/to/vdc/vdc
```

```
> povray spins   # generate all snapshots
```

```
 # or you can do
```

```
> povray +KFI0 –KFF0 spins.pov
```

```
# You can add some option as size of the image
```

```
> povray –W800 –H600 spins
```

```
# You can add some option as antialiasing
```

```
> povray +A0.3  spins
```

Thank you for you time!