Calculation of anisotropy energy and temperature dependence of anisotropy

A. Meo, R. W. Chantrell, R. F. L. Evans

Department of Physics, University of York, York, YO10 5DD, UK

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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

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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 \((M_x = M_y = 0)\):
     \[
     \begin{align*}
     \hat{S}_{jx}' &= \hat{S}_{ix} + \hat{S}_{jx} - \hat{S}_{ix}' \\
     \hat{S}_{jy}' &= \hat{S}_{iy} + \hat{S}_{jy} - \hat{S}_{iy}'
     \end{align*}
     \]
  4. Adjust z-component of new spin j
     \[
     \begin{align*}
     \hat{S}_{jz}' &= \text{sign}(\hat{S}_{jz}) \sqrt{1 - \hat{S}_{jx}^2 - \hat{S}_{jy}^2} \\
     1 - \hat{S}_{jx}^2 - \hat{S}_{jy}^2 &> 0
     \end{align*}
     \]
CMC step

5. Calculate new magnetisation

\[
\begin{aligned}
M'_z &= M_z + \hat{S}'_{iz} + \hat{S}'_{jz} - \hat{S}_{iz} - \hat{S}_{jz} \\
M'_z &> 0
\end{aligned}
\]

6. Calculate the change in energy

\[
\begin{aligned}
\Delta E_i &= E'_i - E_i \\
\Delta E_{ij} &= \Delta E_i + \Delta E_j
\end{aligned}
\]

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:

\[
\delta W = |T|d\vartheta
\]

\( \vartheta = \) angle formed by spin and net field acting on spins

\[\Rightarrow \Delta F = - \int_{a}^{b} |T|d\vartheta \]
Torque

• Total torque acting on the system is given by

\[ T = \sum_{i} T_i = \sum_{i} \hat{S}_i \times H_i = \sum_{i} \hat{S}_i \times \left( -\frac{\partial H}{\partial \hat{S}_i} \right) \]

• 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:

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

• At zero temperature

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

• $\sin 2\theta$ holds at all temperatures, while $K_u \rightarrow K_u(T)$
Uniaxial anisotropy: Torque & free energy

![Total torque graph](image1)

- Total torque graph shows the torque as a function of the angle from the easy axis (rad) for different temperatures: 0K, 50K, 100K, and 300K.

![Free energy graph](image2)

- Free energy graph illustrates the free energy change ($\Delta F$) as a function of the angle from the easy axis (rad) at the same temperatures.

- The equations used in the graphs are:
  - Total torque: $\sin(2\theta)$
  - Free energy change: $\sin^2(\theta)$
Uniaxial anisotropy: Temperature scaling

\[ K(T)/K_u \propto M(T)/M_s \]

In agreement with Callen-Callen theory\(^2\)

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
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

Angle from easy axis (rad)

Total torque $k_u$
Temperature scaling

![Graph showing the relationship between temperature (K) and the normalized quantities K(T)/K_u and M(T)/M_s.](image)
Scaling of anisotropy vs magnetisation

$$\ln\left(\frac{K_{\text{eff}}(T)}{k_u}\right)$$ vs $$\ln\left(\frac{M(T)}{M_s}\right)$$

Data

Fit, 1.0 m³
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 ($\theta$) and azimuthal ($\phi$) angle
Temperature scaling

$\frac{K(T)}{K_c}$, $\frac{M(T)}{M_s}$

Temperature (K)
Scaling of anisotropy vs magnetisation

\[
\ln\left(\frac{K_{\text{eff}}(T)}{k_c}\right) \quad \text{vs} \quad \ln\left(\frac{M(T)}{M_s}\right)
\]

Data

Fit, 1.0 m^{9.9}
More complex systems

The diagrams illustrate the variation of total torque with temperature and the energy barrier for different system sizes. The graphs show the dependency on the angle from the easy axis for various temperatures (0K, 50K, 100K, 300K) and system thicknesses (d=10nm, 15nm, 20nm, 25nm, 30nm, 35nm, 40nm, 50nm). The CoFeB/MgO system is depicted in the diagrams, with the magnetic state represented by the color map and the torque curves indicating the orientation of the easy axis.
More complex systems

\[ \Delta f(10^{-18}) \]

Images and data kindly from Razvan Ababei
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

![Graph showing the relation between angle from easy axis (rad) and total torque/k_u.](image)

![Graph showing the relation between temperature (K) and K(T)/K_u, M(T)/M_s.](image)
Constraining only uniaxial material

![Graph showing angular and torque relationship](image)

- Total torque $K/k_c$ vs. angle from easy axis (rad)
- Temperature $T$ vs. $K(T)/K_c$, $M(T)/M_s$
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:

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

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 $E_{\text{dip}}$ can be written as:

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

where $B_{q}^{\text{dip}}$ 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.

\[ H_{q}^{\text{dip}} = \frac{\mu_{0}}{4\pi} \sum_{q \neq p} \frac{3(\mu_{p} \cdot \hat{r}_{qp})\hat{r}_{qp} - \mu_{p}}{|r_{qp}|^{3}} - \frac{\mu_{0} \mu_{q}}{3 V_{q}} \]
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]:

$$B^{\text{dip}} = B_q^{\text{dip}} + B_p^{\text{dip}} + B_p^{\text{self}}$$

$$= D^{\text{inter}} q p \vec{m}_p + D^{\text{intra}} p p \vec{m}_p + \frac{8\pi}{3} \vec{m}_p / V_p$$

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

Interaction between moments inside cell p (atomistic)
Inter-intra dipole approach

- $B_p^{\text{self}} = \frac{8\pi}{3} \vec{m}_p$ 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.

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

- $D_{qq}^{\text{inter}}, D_{pp}^{\text{intra}}$ are casted in terms of usual dipolar matrix
Dipolar matrixes

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

\[
D_{qj,pi}^{\text{inter}} = \frac{1}{r_{piqj}^3} \begin{bmatrix}
(3x_{piqj}^2 - 1) & 3x_{piqj}y_{piqj} & 3x_{piqj}z_{piqj} \\
3y_{piqj}x_{piqj} & (3y_{piqj}^2 - 1) & 3y_{piqj}z_{piqj} \\
3z_{piqj}x_{piqj} & 3z_{piqj}y_{piqj} & (3z_{piqj}^2 - 1)
\end{bmatrix}
\]

Same in case of internal term (replace \(qj\rightarrowpj\)) for \(D_{pi,pj}^{\text{intra}}\).

**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 $D^{\text{intra}}$ 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 = $k_0 = c/a$

$$D = \frac{1}{k_0^2 - 1} \left( \frac{k_o}{\sqrt{k_o^2 - 1}} \text{arcosh} \ k_o - 1 \right)$$

$$D = \frac{1}{1 - k_0^2} \left( 1 - \frac{k_o}{\sqrt{1 - k_o^2}} \text{arccos} \ k_o \right)$$
Hands on
Main parameters

cells: macro-cell-size = 10.1 Å

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

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

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

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

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

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

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

   (h) $a_0 = 3.55 \text{ Ang}$

   (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 configurations

• 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 configurations: How to compile it

```bash
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 your time!