Advanced micromagnetics and atomistic simulations of magnets

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ESM 2018

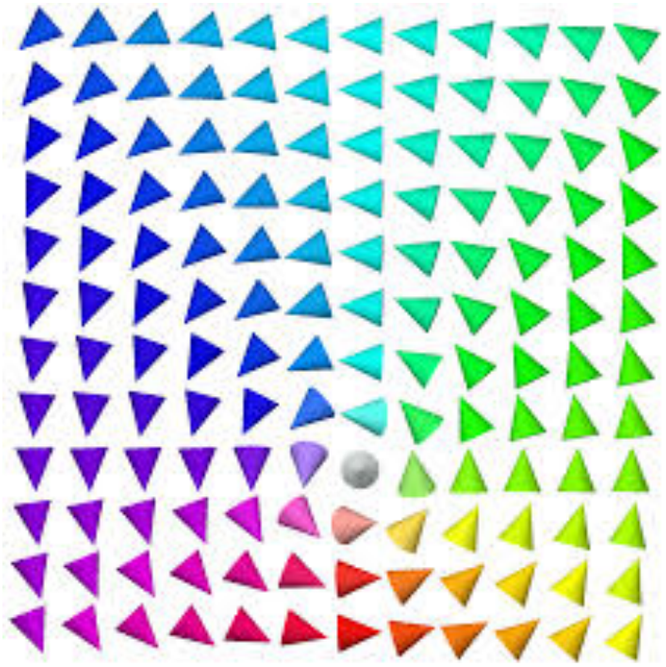
Overview

- Micromagnetics
  - Formulation and approximations
  - Energetic terms and magnetostatics
  - Magnetisation dynamics

- Atomistic spin models
  - Foundations and approximations
  - Monte Carlo methods
  - Spin Dynamics

- Landau-Lifshitz-Bloch micromagnetics (tomorrow)

Micromagnetics

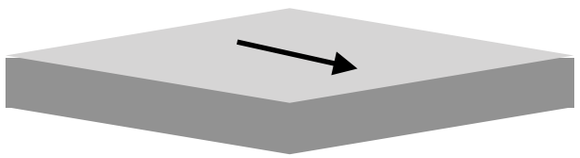


source: mumax

Why do we need magnetic simulations?

Demagnetization factors for different shapes

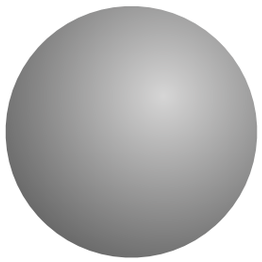
N = 0



Infinite thin film

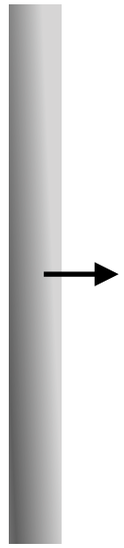
Infinitely long cylinder

N = 1/3

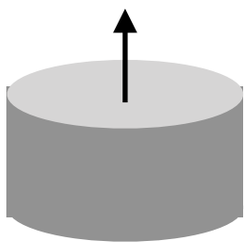


Sphere

N = 1/2

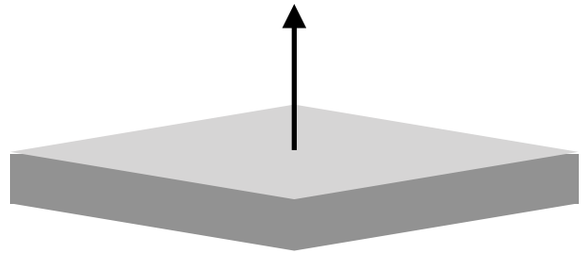


Infinitely long cylinder

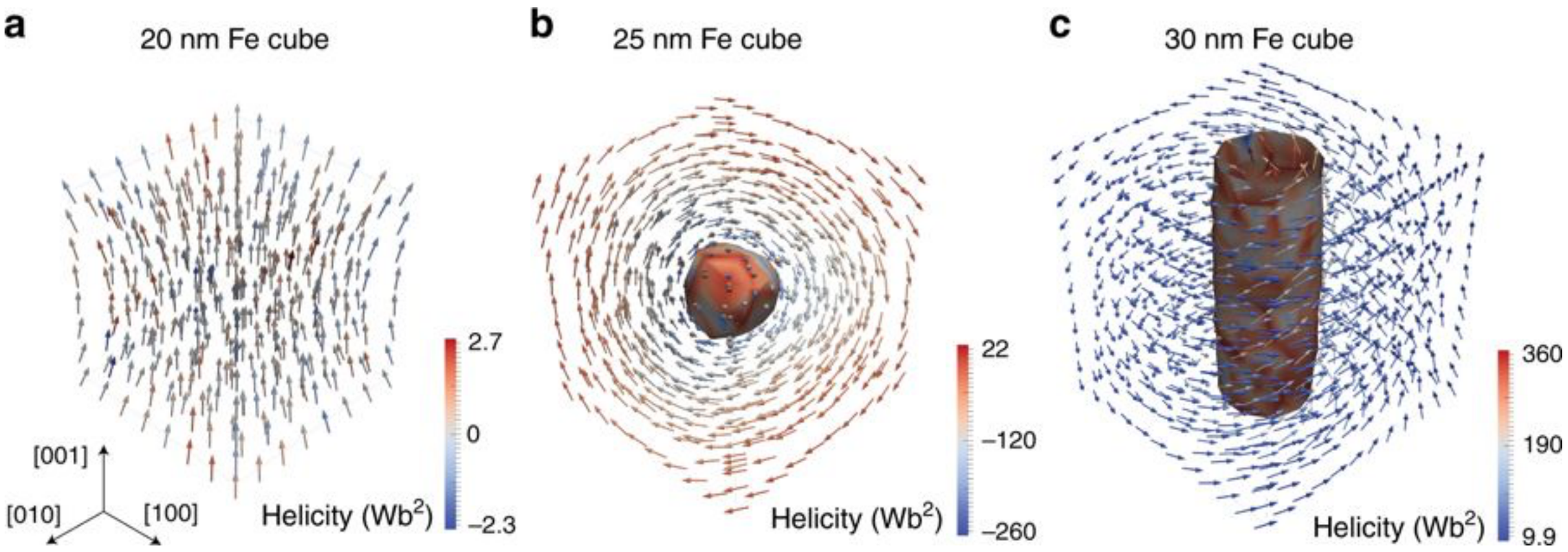


Short cylinder

N = 1



Why do we need magnetic simulations?



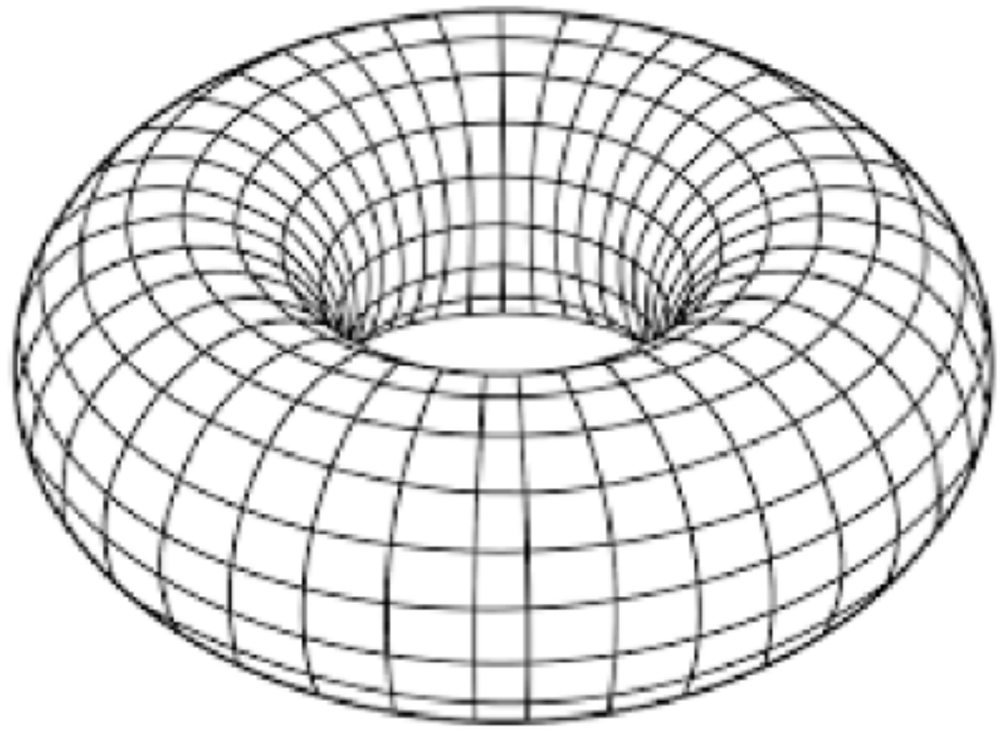
Jay Shah et al, Nature Communications 9 1173 (2018)

Why do we need magnetic simulations?

- Most magnetic problems are not solvable analytically
  - Complex shapes (cube or finite geometric shapes)
  - Complex structures (polygranular materials, multilayers, devices)
  - Magnetization dynamics
  - Thermal effects
  - Metastable phases (Skyrmions)

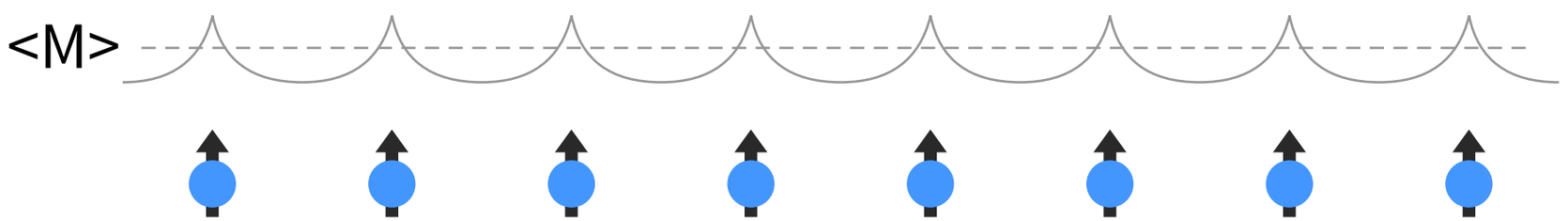
Analytical micromagnetics

- An analytical branch of micromagnetics, treating magnetism on a small (micrometre) length scale
- Mathematically messy but elegant
- When we talk about micromagnetics, we *usually* mean **numerical micromagnetics**



Numerical micromagnetics

- Treat magnetisation as a **continuum approximation**

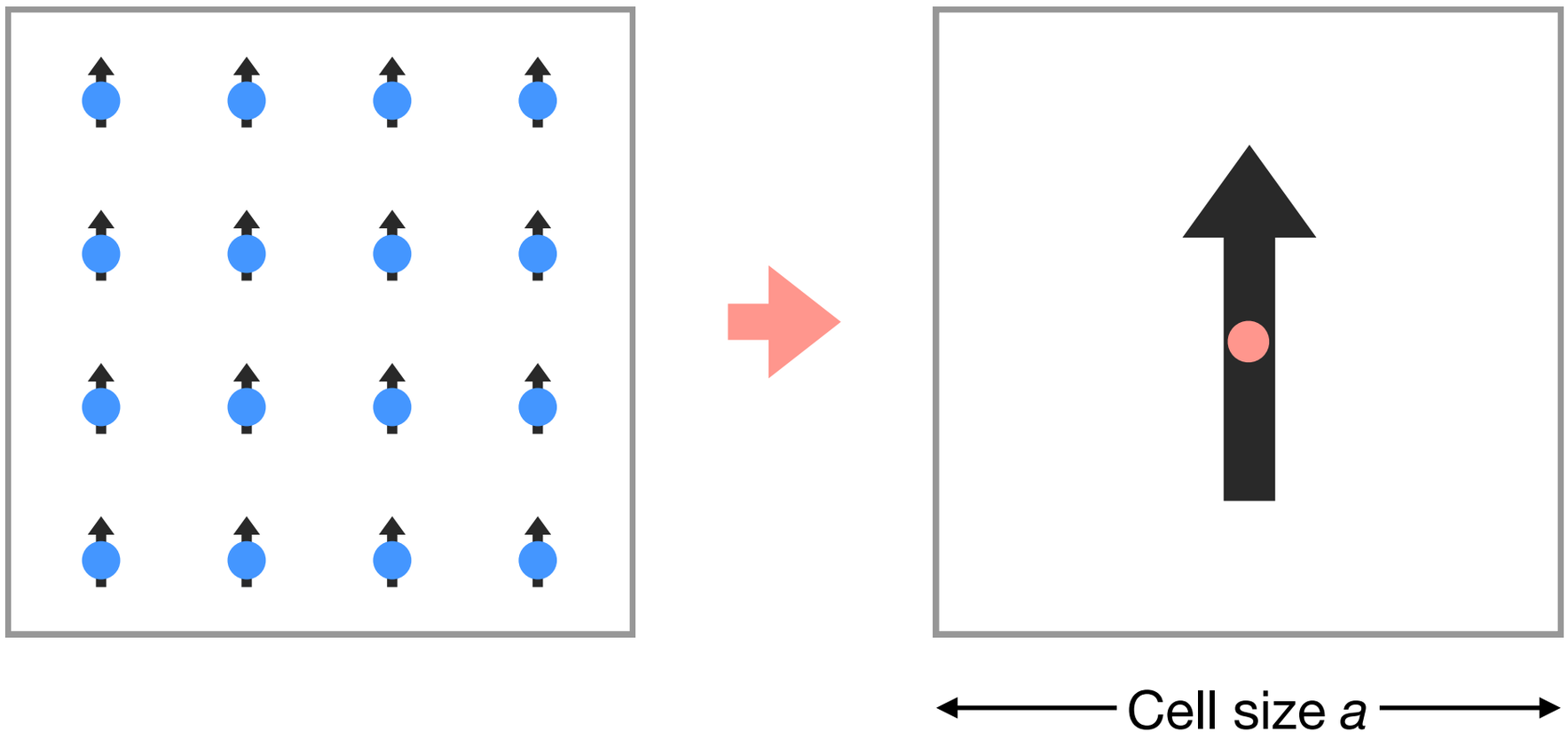


- Average over the local atomic moments to give an *average* moment density (magnetization) that is assumed to be continuous

- Then consider a small volume of space (1 nm)^3 - (10 nm)^3 where the magnetization (and all atomic moments) are assumed to point along the same direction

The micromagnetic cell

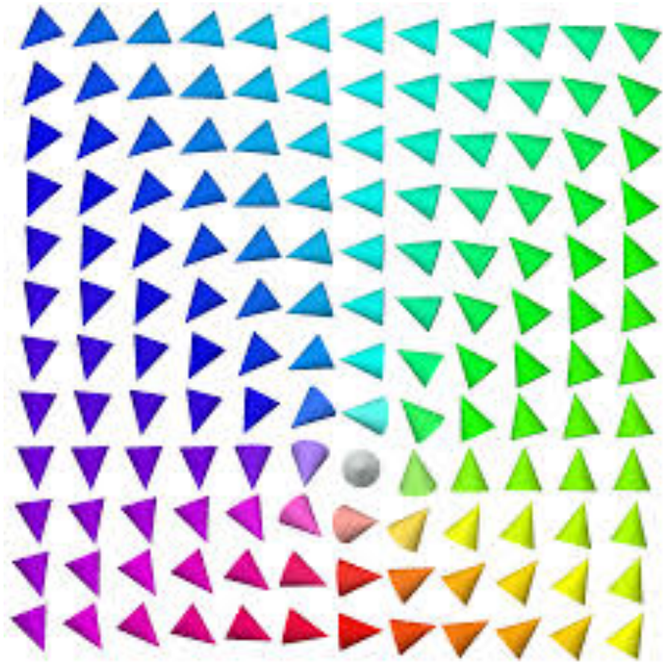
- This gives the fundamental unit of micromagnetics: the micromagnetic cell
- The magnetisation is resolved to a single point **magnetic moment**



- Generally a good approximation for simple magnets (local moment variations are weak) at low temperatures ($T < T_c/2$)

Micromagnetic problems

- A typical problem is then divided (discretised) into multiple micromagnetic cells



- Can now generally treat any micromagnetic problem by solving system of equations describing magnetic interactions

Micromagnetic energy terms

- Micromagnetics considers fundamental magnetic interactions
  - Magnetostatic interactions (zero current)
  - Exchange energy
  - Anisotropy energy
  - Zeeman energy

- Total energy is a summation over all micromagnetic cells

$$E_{\text{tot}} = E_{\text{demag}} + E_{\text{exchange}} + E_{\text{anisotropy}} + E_{\text{Zeeman}}$$

- Taking the derivative with respect to the local cell moment **m**, we can express this as a local magnetic field acting on the local moment

$$\mathbf{H}_{\text{eff}} = -\frac{1}{\mu_0 M_s} \frac{\mathrm{d}^2 E}{\mathrm{d}\mathbf{m}\mathrm{d}V}$$

Magnetostatics

- As each micromagnetic cell is a source of magnetic field, each one interacts with every other micromagnetic cell in the simulation via magnetic stray fields

- This is expressed as an integral over the volume magnetization of all other cells

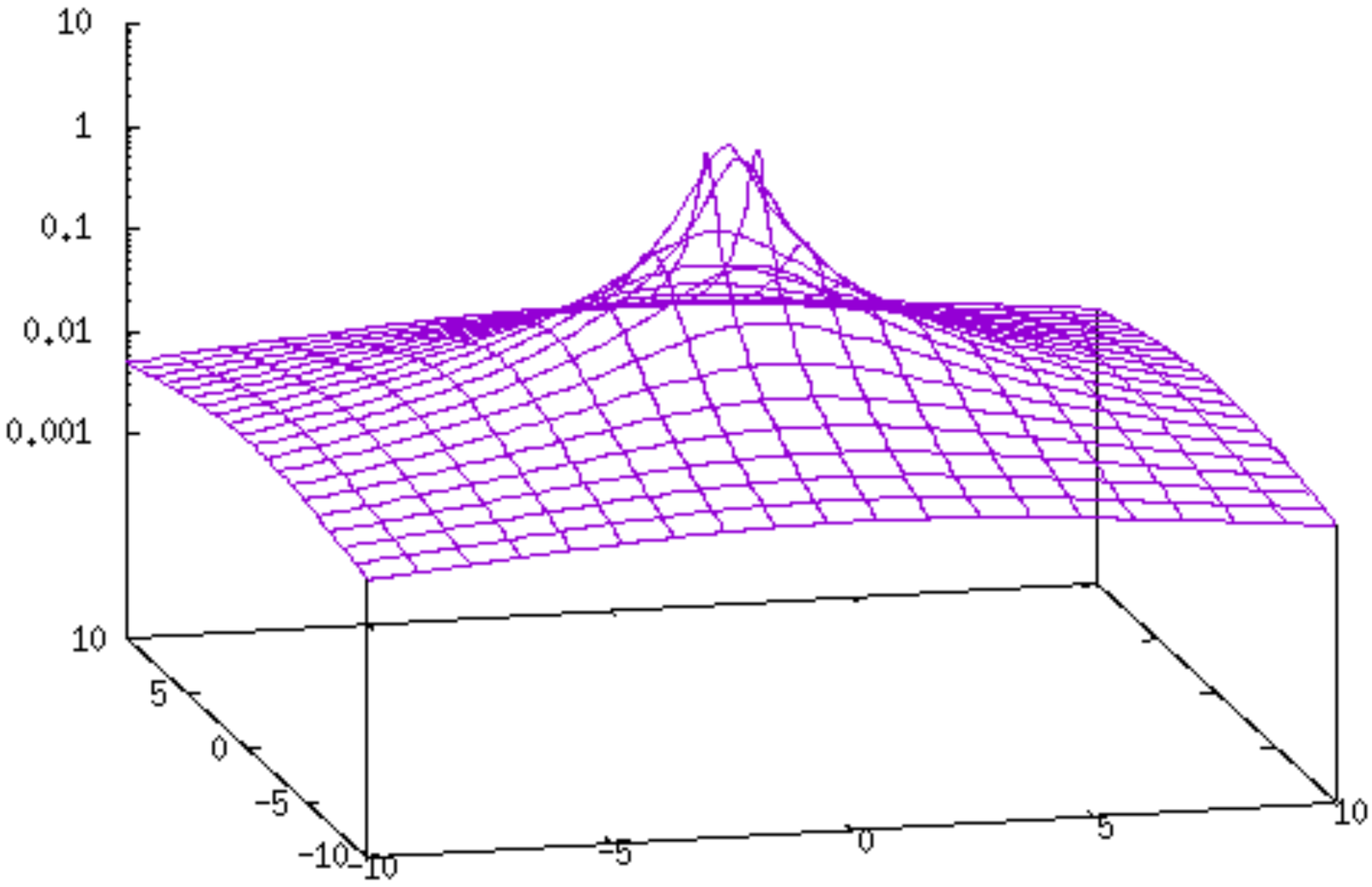
$$\mathbf{H}_\mathrm{d} = -\frac{1}{4\pi}\int_V \nabla \cdot \mathbf{M}\frac{\mathbf{r}}{r^3}\mathrm{d}V$$

- In implementation terms this is done by considering surface charges on cells and calculating the integral over the surface of the cell.

- The magnetostatic calculation is expensive since it scales with the square of the number of cells ($O \sim N^2$)

- Typically this is solved using a Fast Fourier Transform, which scales with $O \sim N \log N$

Fourier Transforms for interactions



- Given a regular cubic grid and some interaction that is **translationally invariant** the interactions can be calculated in Fourier space (useful for crystals)

$$\mathbf{F}(\mathbf{x}) = m(\mathbf{x})\, f(\mathbf{x}) \rightarrow DFT\,[\mathbf{F}(\mathbf{x})] = DFT\,[m(\mathbf{x})]\; DFT\,[f\,(\mathbf{x})]$$

Fast Fourier Transform

- DFT still an O(n^2) operation - not particularly helpful!
- But Fast Fourier Transform (FFT) has O(n log n) scaling
- Can reformulate the DFT as

$$F[n] = \sum_{k=0}^{N-1} f[k] W_N^{nk}$$

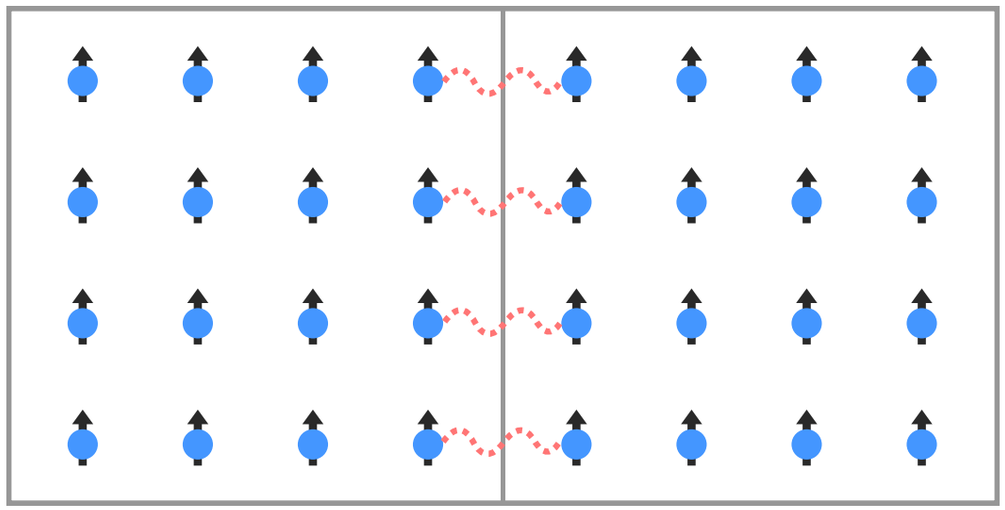
where W_N^{nk} is a periodic function that repeats for different combinations of n and k.

- Taking advantage of this symmetry through a Decimation in time method vastly reduces the number of operations that need to be performed (O(n $\log_2$ n)) (Cooley-Tukey algorithm and others)

http://jakevdp.github.io/blog/2013/08/28/understanding-the-fft/

Exchange interactions

- Continuum formulation of the Heisenberg exchange: neighbouring cells tend to prefer parallel alignment



- Effective exchange energy between cells from average of atomic exchange interactions J_{ij} over interaction length a (atomic spacing)

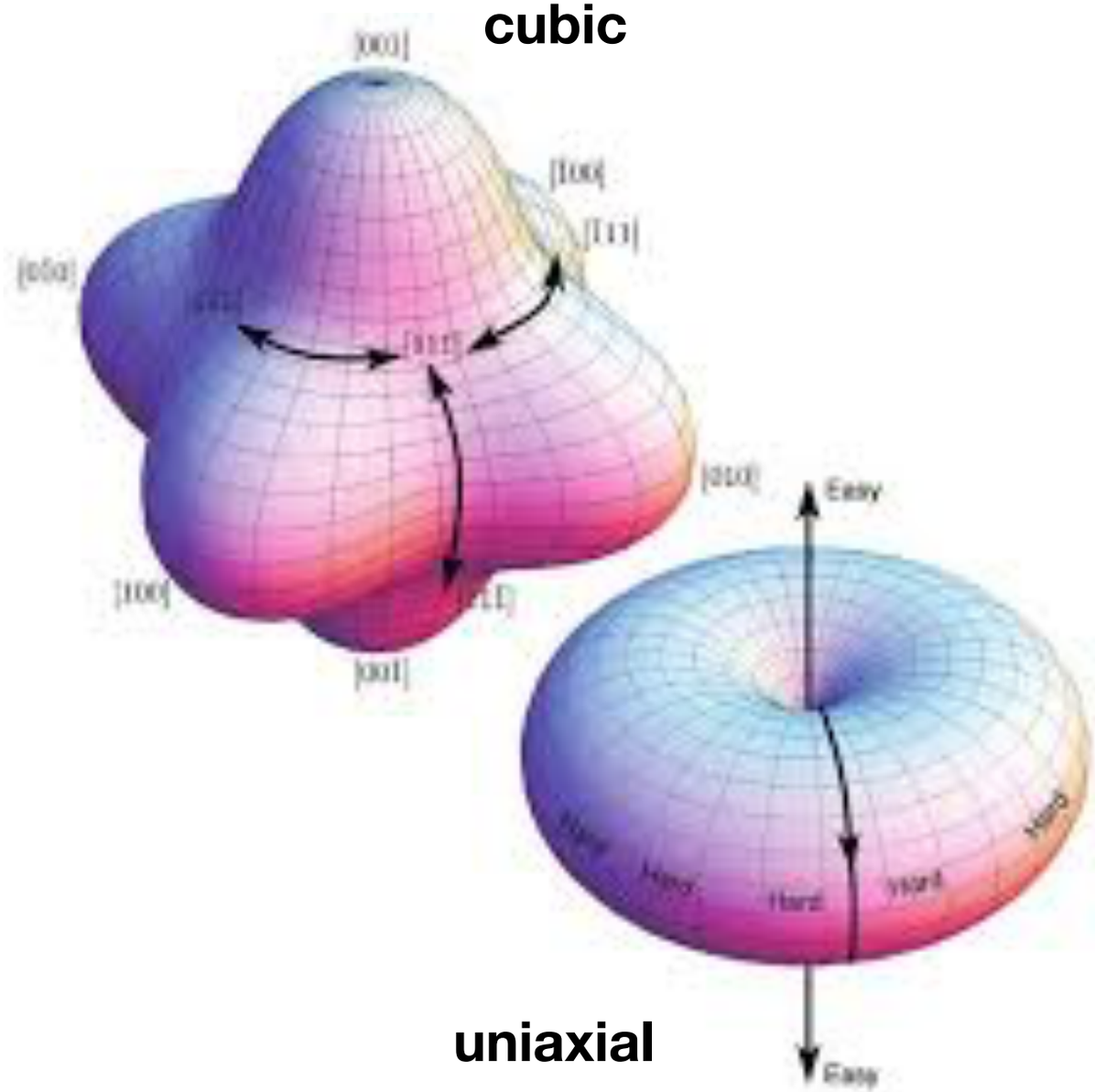
$$A = \frac{\sum_{ij} J_{ij}}{2a}$$

- Micromagnetic exchange field given by Laplacian

$$\mathbf{H}_{exch} = \frac{2A}{\mu_0 M_s} \nabla^2 \mathbf{m}$$

Magnetic anisotropy

- Preference for atomic magnetic moments to align with particular crystallographic directions (magnetocrystalline anisotropy)
- Purely quantum mechanical effect from spin-orbit coupling
- Gives a preference for magnetization to lie along particular spatial directions



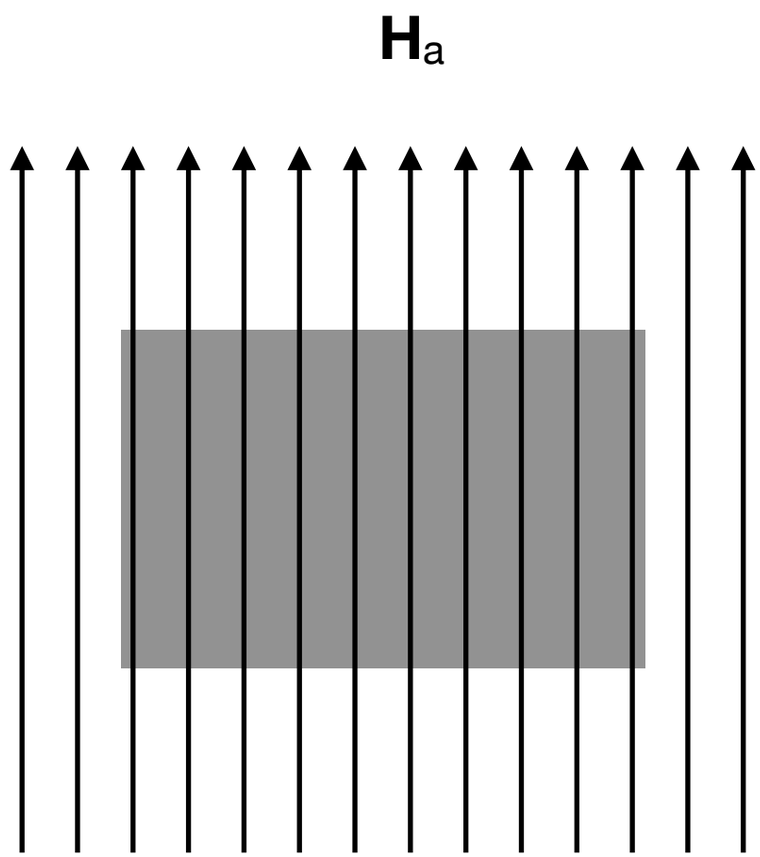
uniaxial

$$\mathbf{H}_{\text{anis}} = -\frac{1}{\mu_0 M_s}\frac{\partial F_{\text{anis}}}{\partial \mathbf{m}}$$

Applied magnetic field

- Coupling of the magnetic moment to external magnetic field

- Simple addition to the effective field +$\mathbf{H}_a$



Finite element micromagnetics

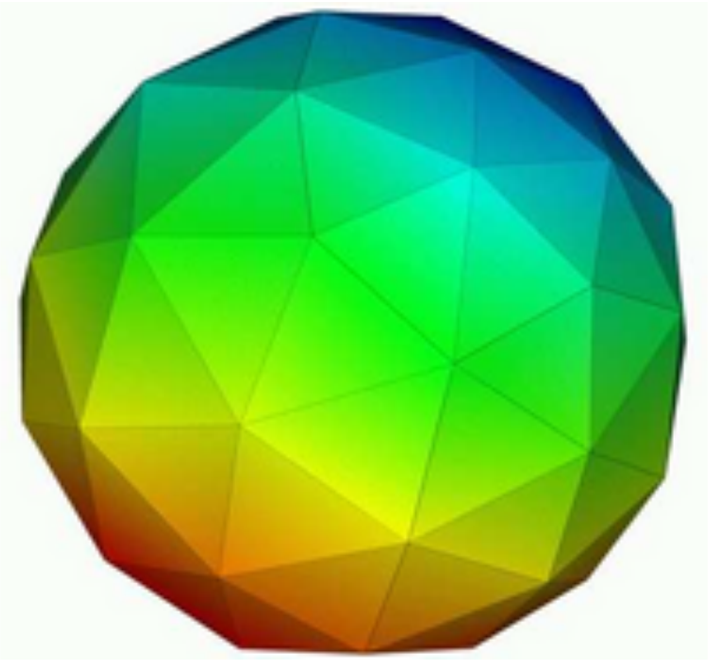
- The cubic discretisation described previously is known as **finite difference** micromagnetics, due to the derivative of the energy over a finite length

- An alternative formulation is **finite element** micromagnetics

- Space is discretised into tetrahedra - much better approximation for curved geometries and complex shapes

- Much more complicated to implement and set up numerically

- Dipole fields typically calculated with Boundary Element/Finite element (BE/FE) method

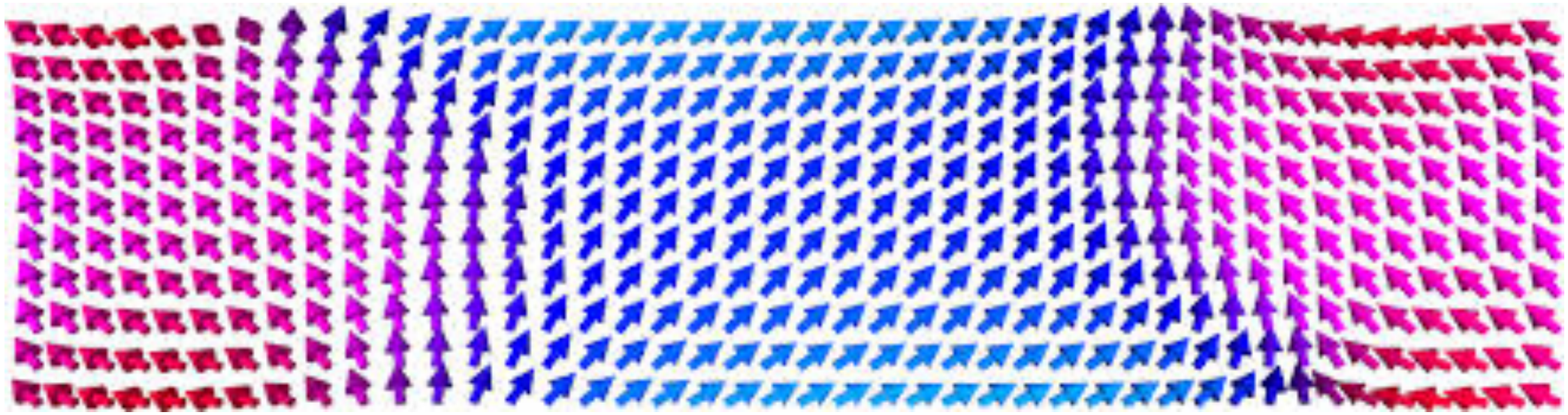


nmag

Josef Fidler and Thomas Schrefl 2000 J. Phys. D: Appl. Phys. 33 R135

Micromagnetic simulations

- Problem is defined in terms of set of interacting cells



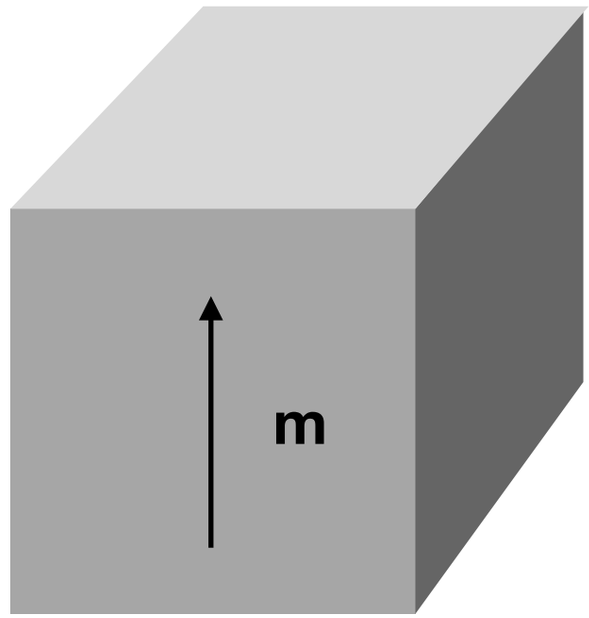
- Have defined a local field acting on each cell

$$\mathbf{H}_{\text{eff}} = \frac{2A}{\mu_0 M_s}\nabla^2\mathbf{m} - \frac{1}{\mu_0 M_s}\frac{\partial F_{\text{anis}}}{\partial \mathbf{m}} + \mathbf{H}_{\text{a}} + \mathbf{H}_{\text{d}}$$

- Final step is to actually evolve the magnetic configuration

Energy minimisation : conjugate gradient method

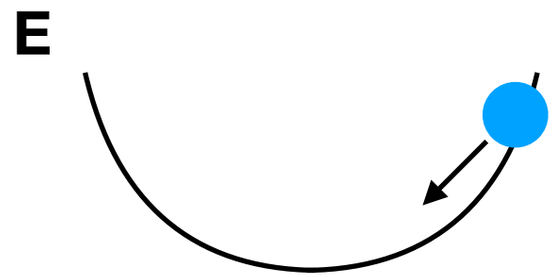
- Consider a uniformly magnetised cube



- Corners are a relatively high energy, as the magnetization is not perpendicular to the surface

- The magnetization would prefer to form a “flower” state to lower the total energy - this costs some exchange energy but gains a larger amount of magnetostatic energy.

- Conjugate gradient method considers the gradient of energy on each cell, and calculates the steepest trajectory. It then changes the magnetization direction along the steepest decent direction to reduce the energy in an iterative fashion



- After a number of steps the solution is converged (no further changes will reduce the energy), net torque

$$\mathbf{m} \times \mathbf{H}_{\text{eff}} = 0$$

Magnetisation dynamics

- Not all problems are limited to the ground-state magnetic configuration
- Many dynamic problems
  - Magnetic recording and sensing
  - Fast reversal dynamics
  - Microwave oscillators
  - Domain wall/Skyrmion dynamics
- Need an equation of motion to describe time evolution of the magnetization of each cell

Landau Lifshitz Gilbert equation

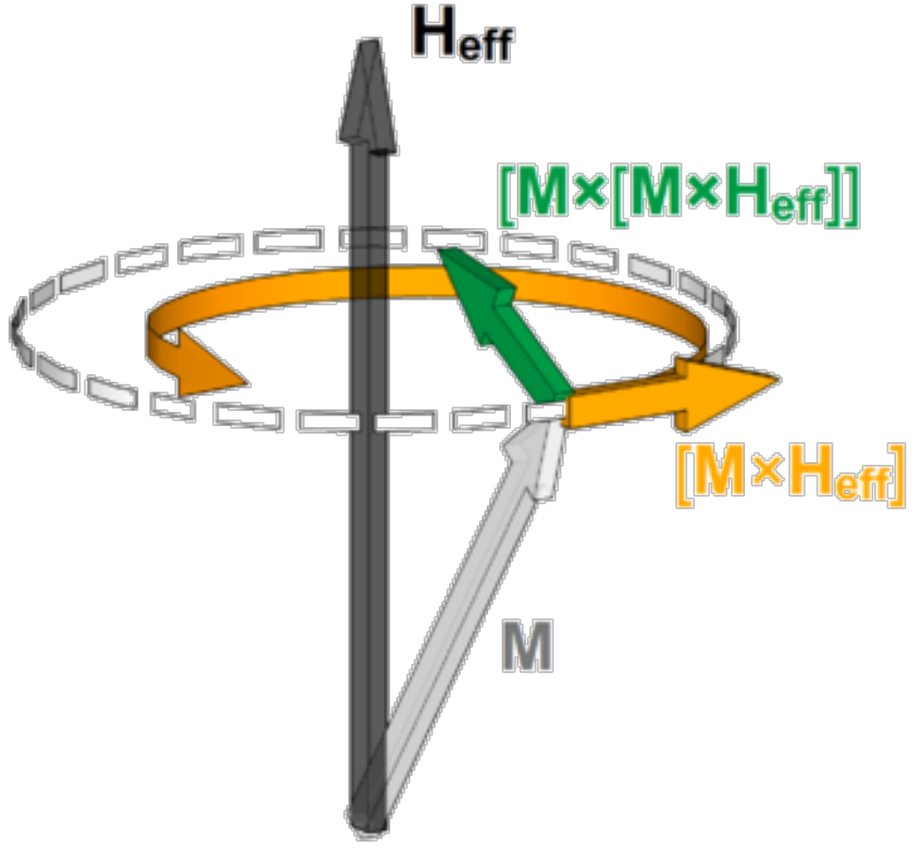
- Phenomenological equation of motion describing uniform magnetization dynamics

$$\frac{\partial \mathbf{M}(\mathbf{r},t)}{\partial t} = -\frac{\gamma}{1+\alpha^2}\mathbf{M}(\mathbf{r},t) \times \mathbf{H}_{eff}(\mathbf{r},t) - \frac{\alpha\gamma}{M_s(1+\alpha^2)}\mathbf{M}(\mathbf{r},t) \times (\mathbf{M}(\mathbf{r},t) \times \mathbf{H}_{eff}(\mathbf{r},t)).$$

- Consists of two terms - precession and relaxation

- Some quantum mechanical origins: Larmor precession

- Relaxation term is much more complex and hides a multitude of complex physical phenomena (dissipation of angular momentum)



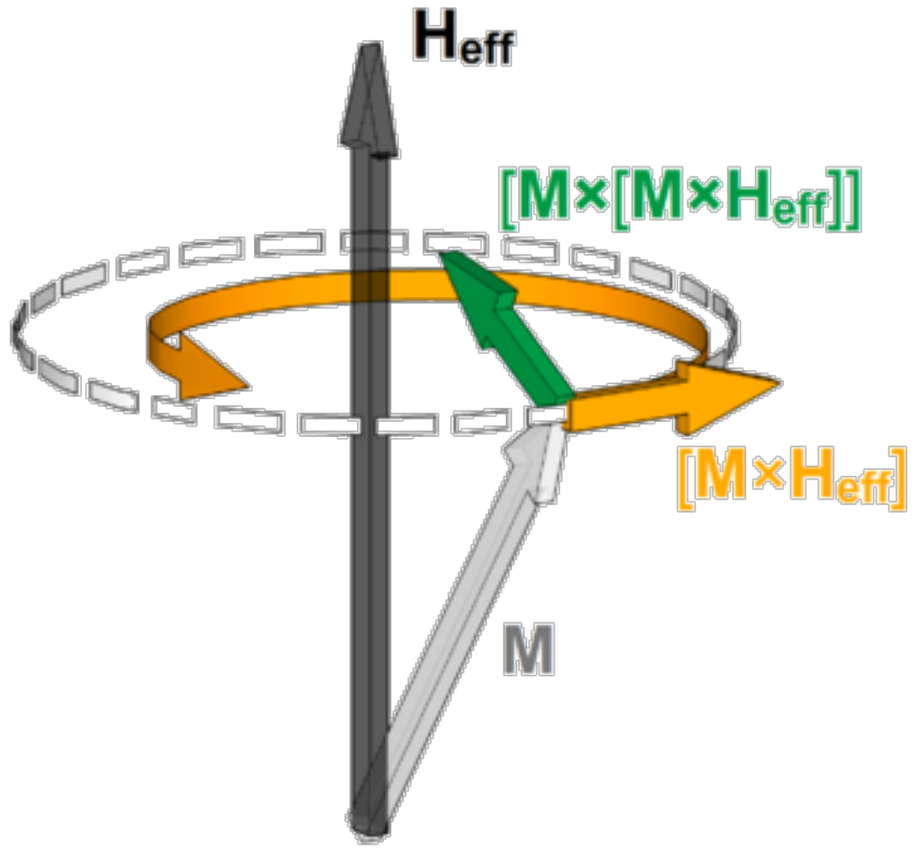
Numerical solution of the LLG equation

- Considering a small step in time, need to consider the evolution of the spin in the effective field

- A range of numerical integration schemes available (Euler, Heun, Runge-Kutta, semi-implicit)

- Time evolution is complex as the fields changes as spins move

- Higher order schemes typically best compromise of accuracy/speed as take into account intermediate changes of the local fields and moments



Stochastic LLG equation

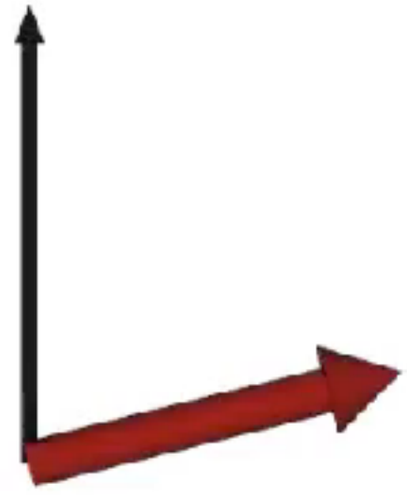
- As written, the LLG equation is strictly for zero temperature simulations

$$\mathbf{H}_{th} = \boldsymbol{\eta}(\mathbf{r},t)\sqrt{\frac{2\alpha k_B T}{\gamma \mu_0 M_s V \delta t}}$$

- Effective temperature dependent magnetic properties can be included, eg Ms(T), A(T), K(T)

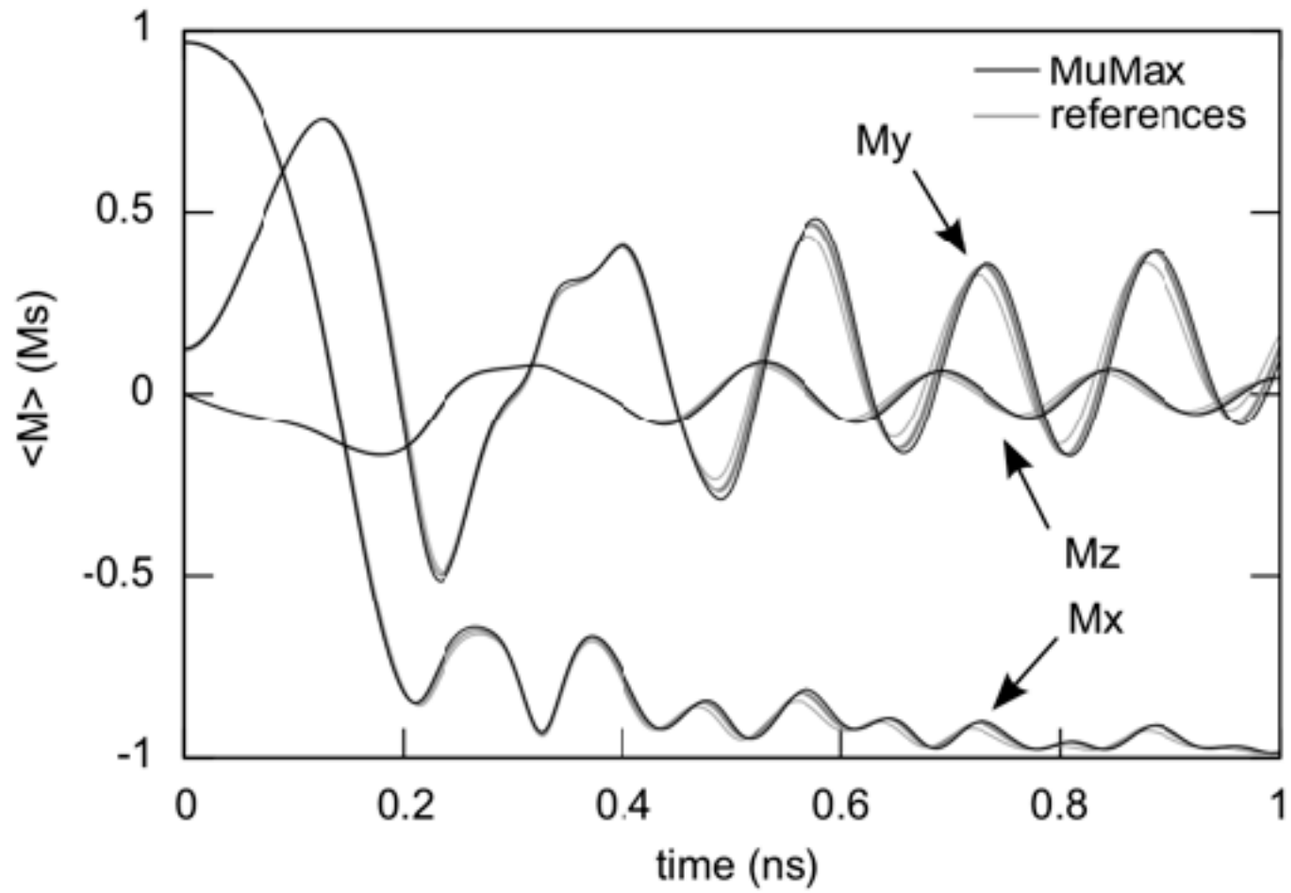
- Small cell size however means that there are thermal fluctuations of the magnetization at the nanoscale

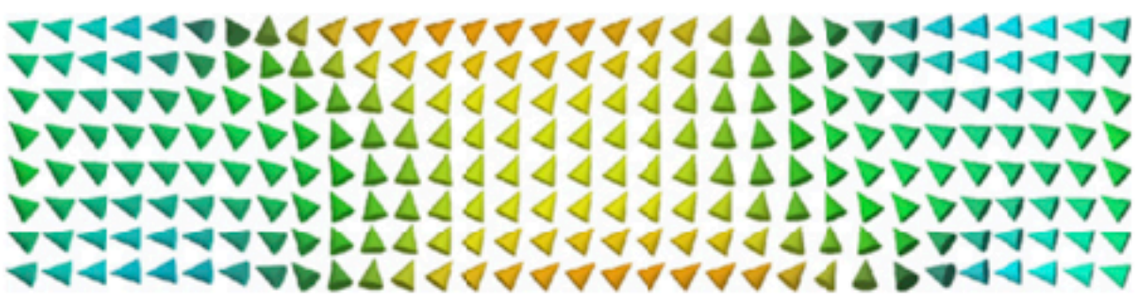
- Include a random ‘thermal’ field using a Langevin Dynamics formalism to simulate the effect of thermal fluctuations



Typical simulations I

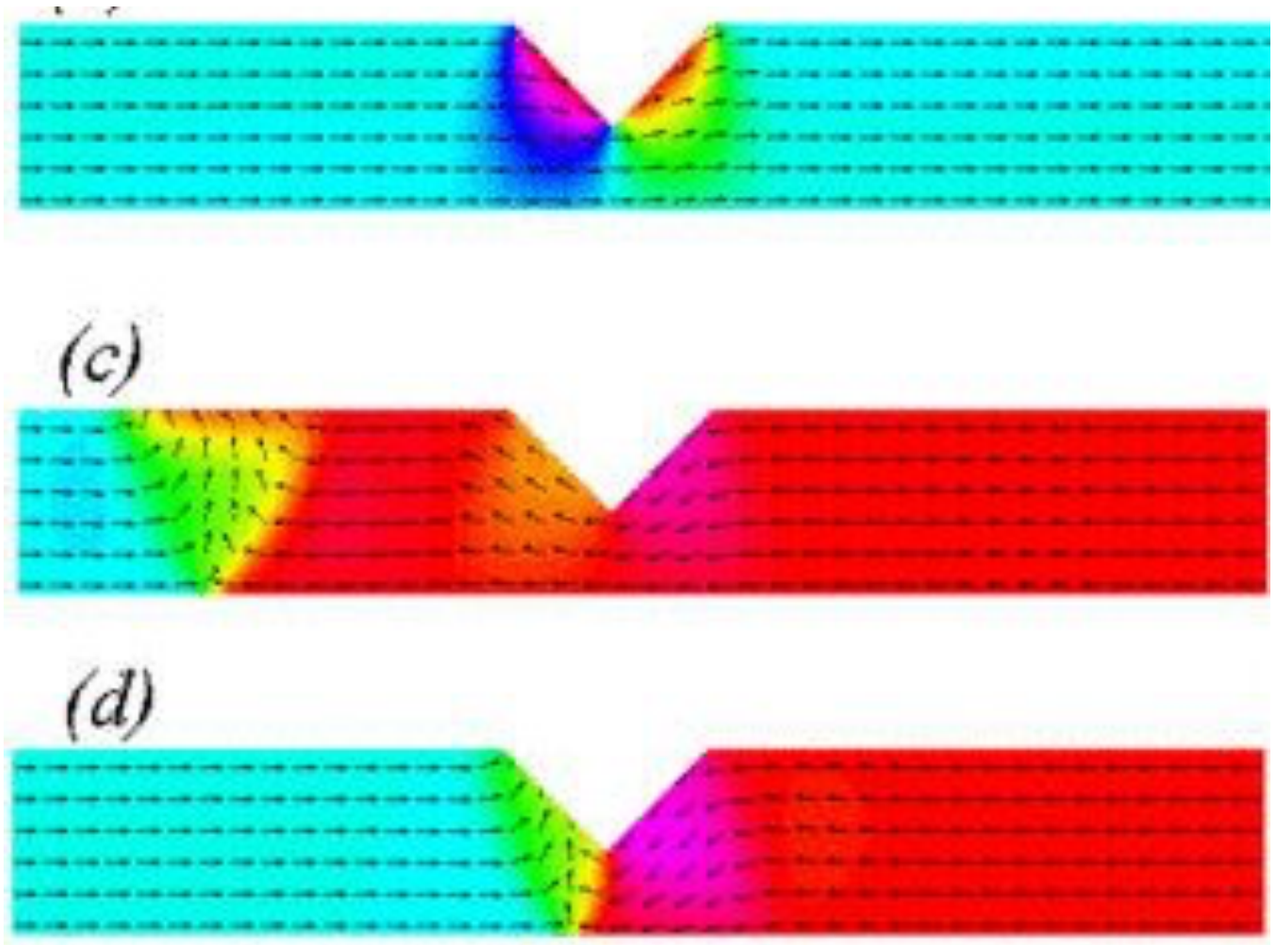
- Micromagnetic standard problems





Typical simulations II

- Domain wall dynamics



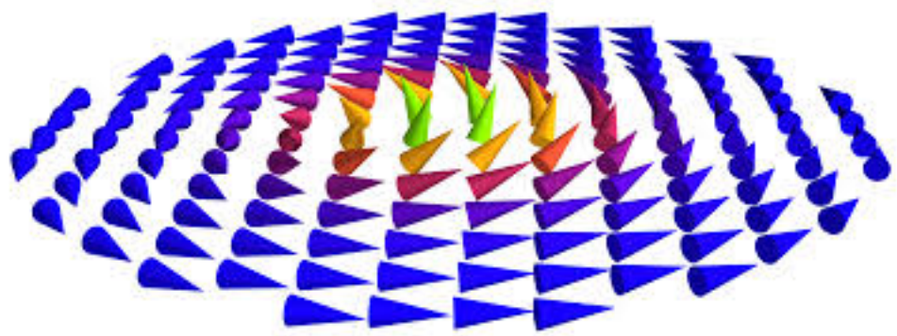
Codes for micromagnetics

- OOMMF - Object Oriented MicroMagnetic Framework - classic code with GUI

- muMAX - modern GPU code, much faster than OOMMF (~100x)

- MAGPAR - old finite element code, good but takes a week to find all the libraries to compile it

- nmag - finite difference/finite element code, development moved to a new code fidimag



- Several others available, some commercial

Atomistic spin models

Often we need to consider problems where continuum micromagnetics is a poor approximation

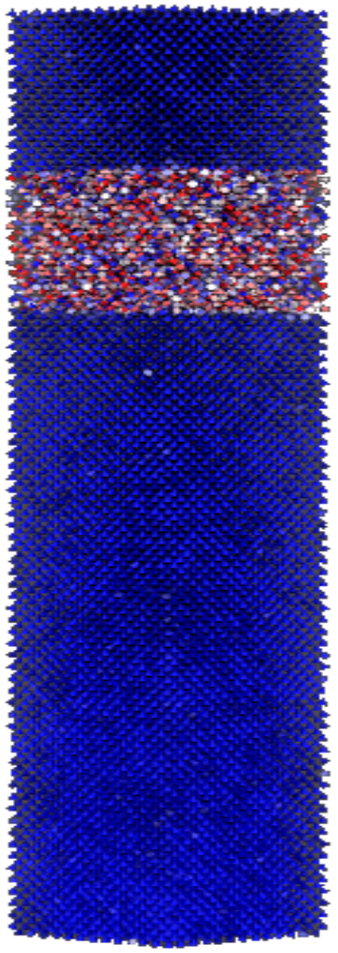
Multi-sublattice ferro, ferri and antiferromagnets

Realistic particles with surface effects

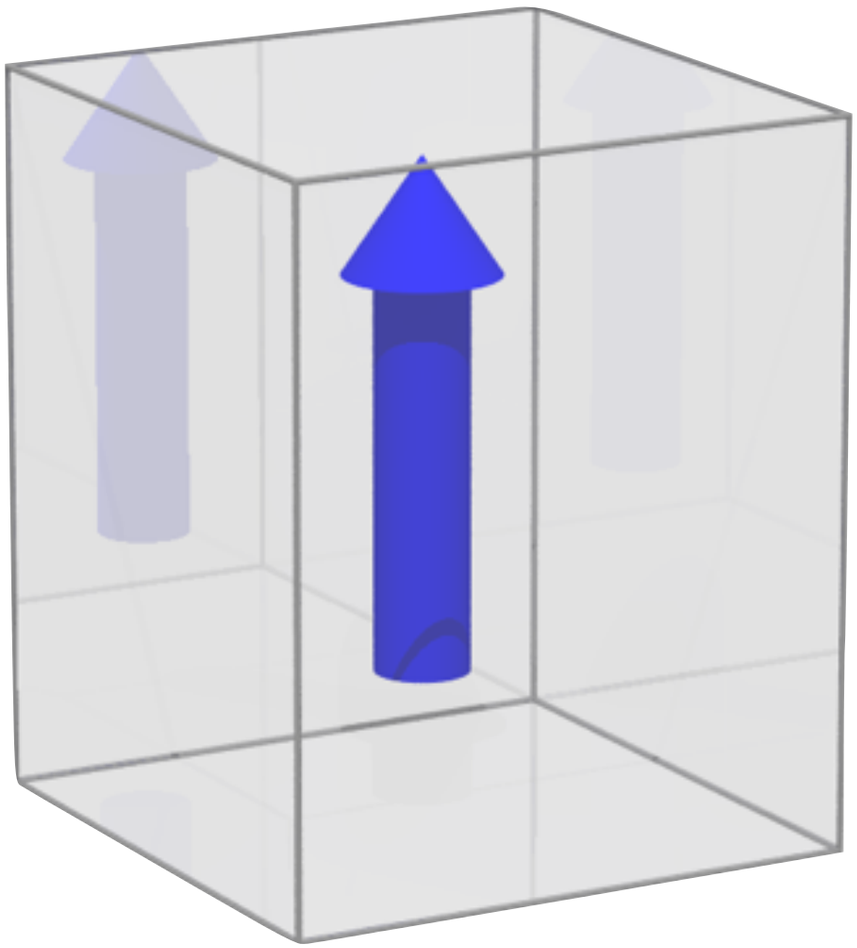
Elevated temperatures near T_c

Magnetic interfaces

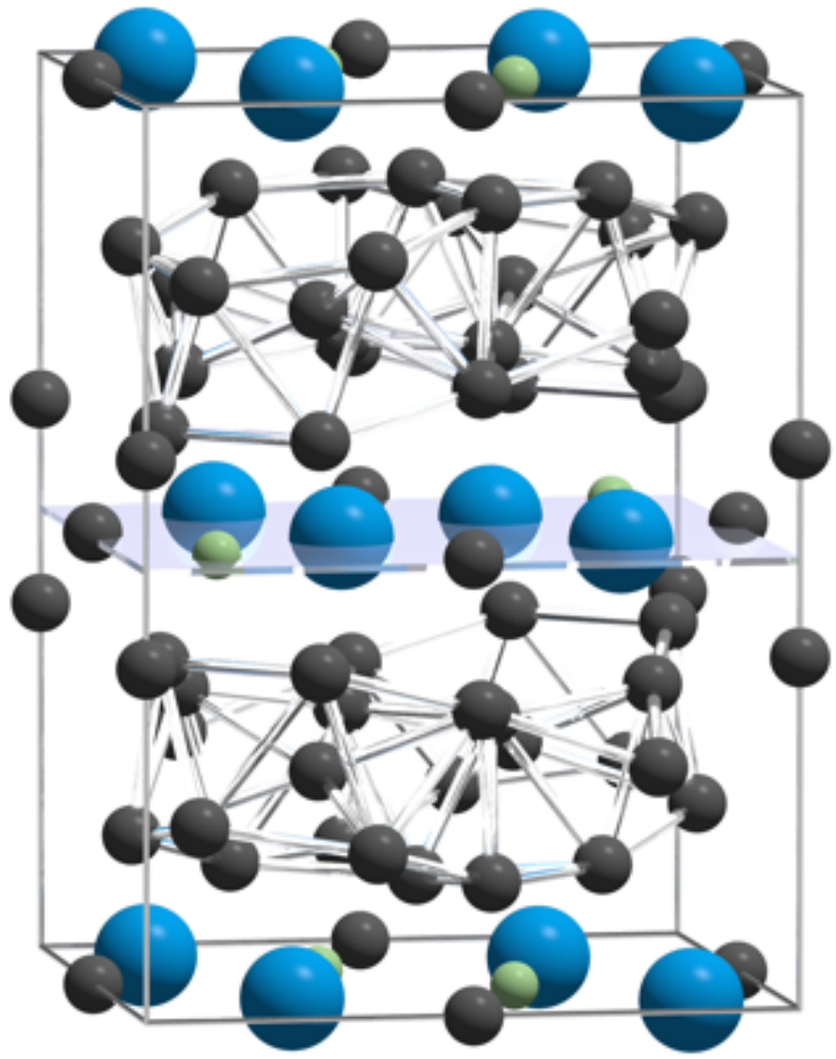
Crystal defects and disorder



Example: $Nd_2Fe_{14}B$ permanent magnets

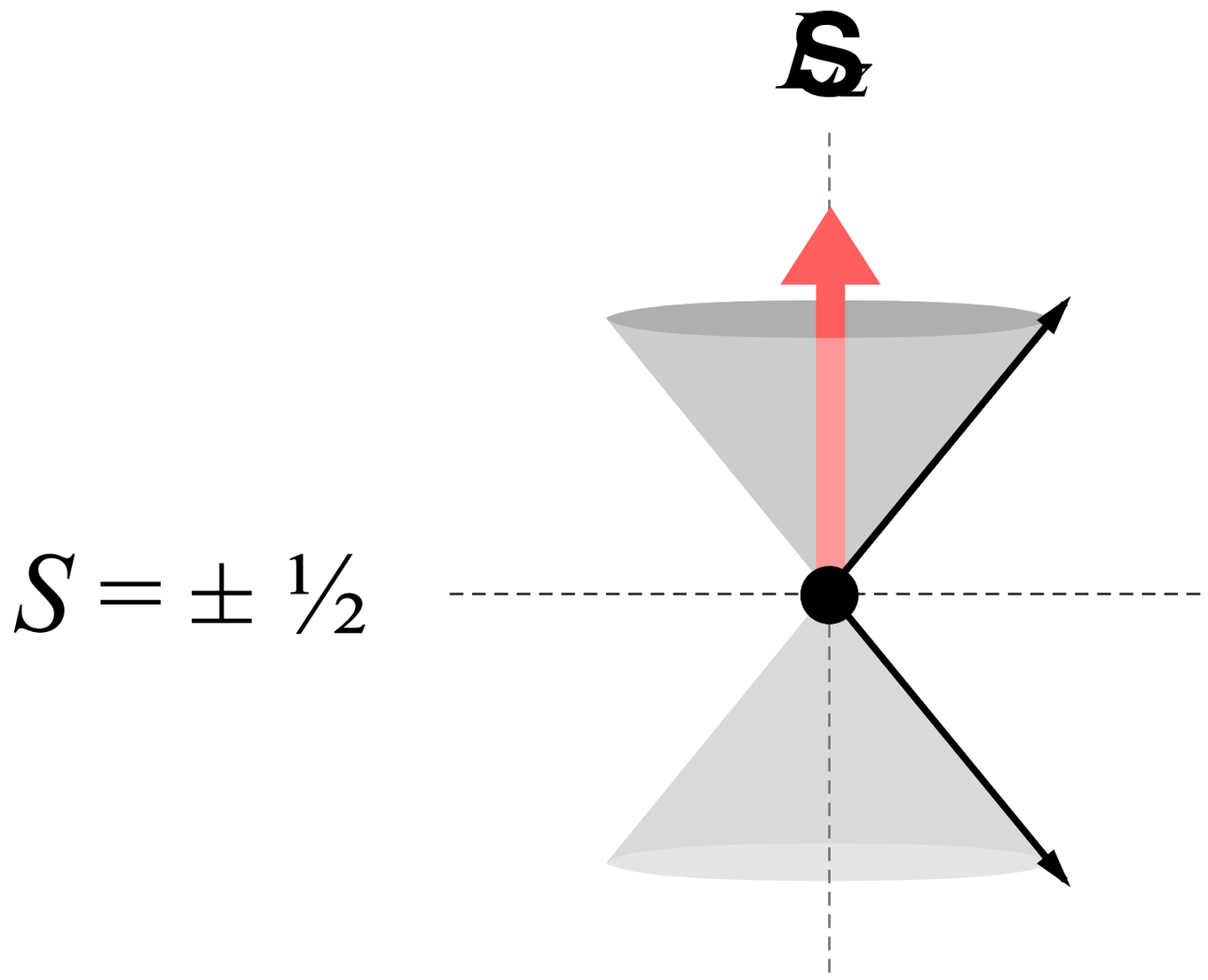


Micromagnetics



Atomistic

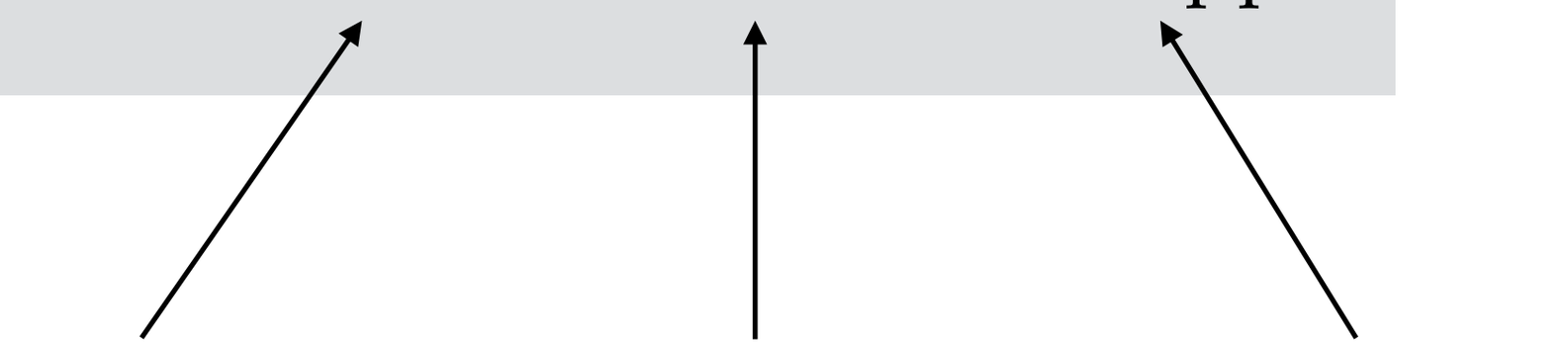
The atomistic model treats each atom as possessing a localized magnetic ‘spin’



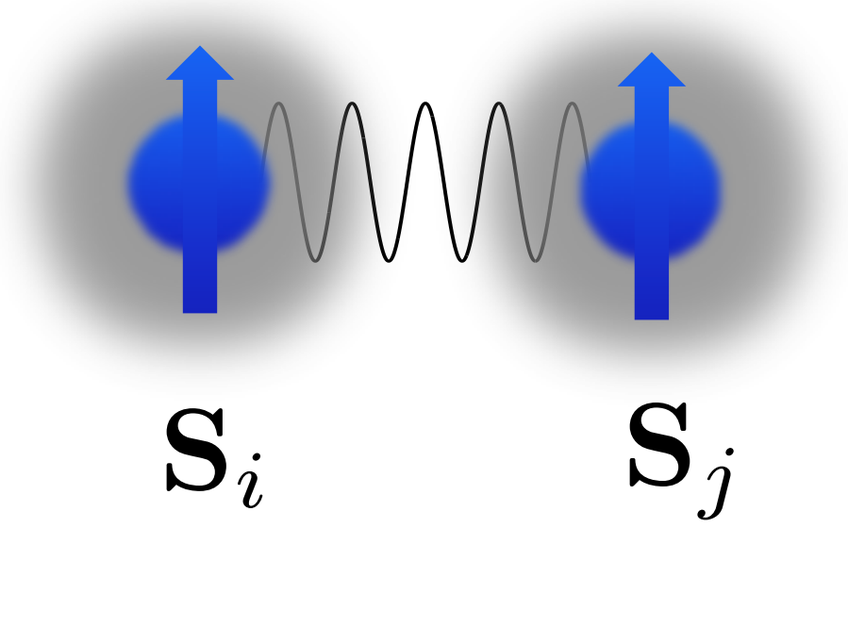
$|\mathbf{S}| = \mu_B$

The ‘spin’ Hamiltonian

$$\mathcal{H} = \mathcal{H}_{\mathrm{exc}} + \mathcal{H}_{\mathrm{ani}} + \mathcal{H}_{\mathrm{app}}$$



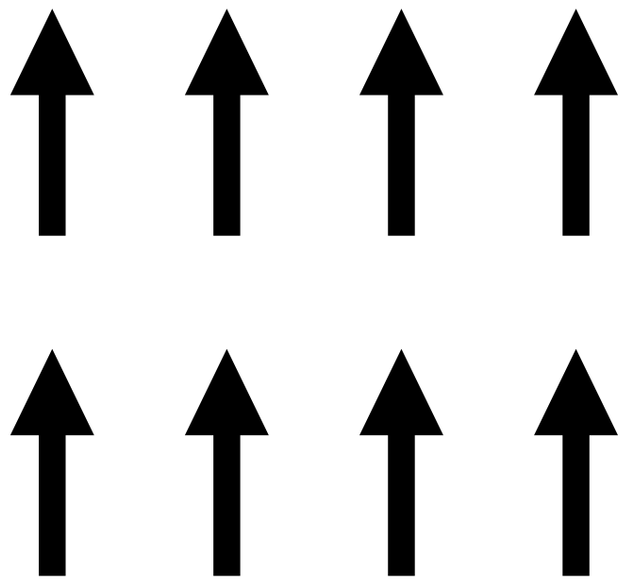
Foundation of the atomistic model is Heisenberg exchange



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

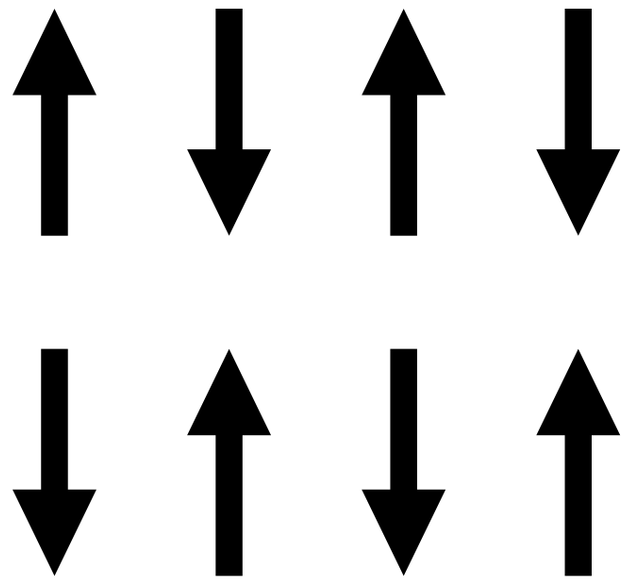
Natural discrete limit of magnetization

Exchange interaction determines type of magnetic ordering



$J_{ij} > 0$

Ferromagnet



$J_{ij} < 0$

Anti-ferromagnet

Exchange energy defines the Curie / Néel temperature of the material

$$J_{ij} = \frac{3k_B T_\mathrm{c}}{\epsilon z}$$

Mean field approximation with correction factor for spin waves

D. A. Garanin, Physical Review B **53**, 11593 (1996)

Exchange tensor

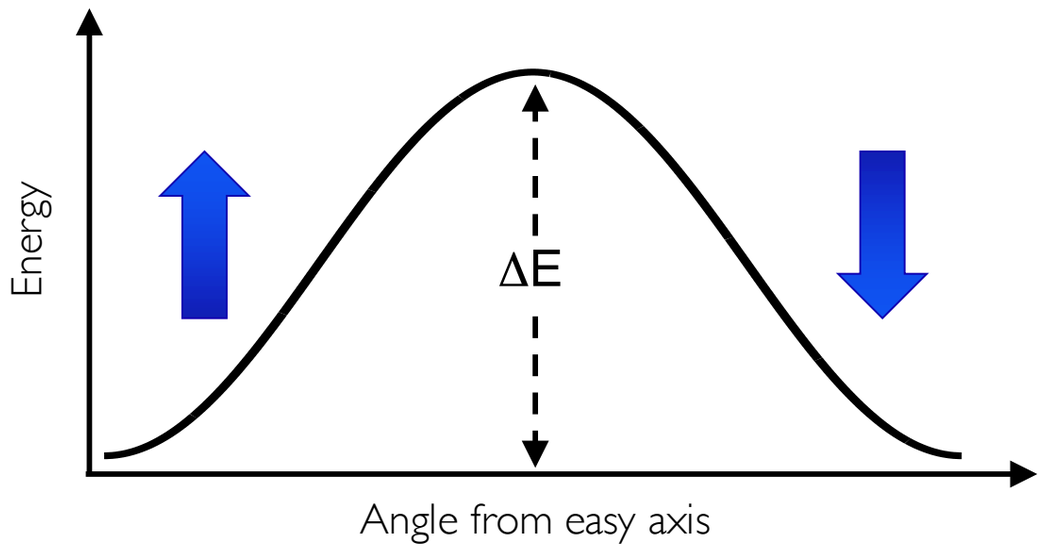
- Can express the exchange interaction as a tensor, where the exchange energy is orientation dependent

$$\mathcal{H}_{\mathrm{exc}}^{\mathrm{M}} = -\sum_{i<j} \left[S_x^i S_y^i S_z^i\right] \begin{bmatrix} J_{xx} & J_{xy} & J_{xz} \\ J_{yx} & J_{yy} & J_{yz} \\ J_{zx} & J_{zy} & J_{zz} \end{bmatrix} \begin{bmatrix} S_x^j \\ S_y^j \\ S_z^j \end{bmatrix}$$

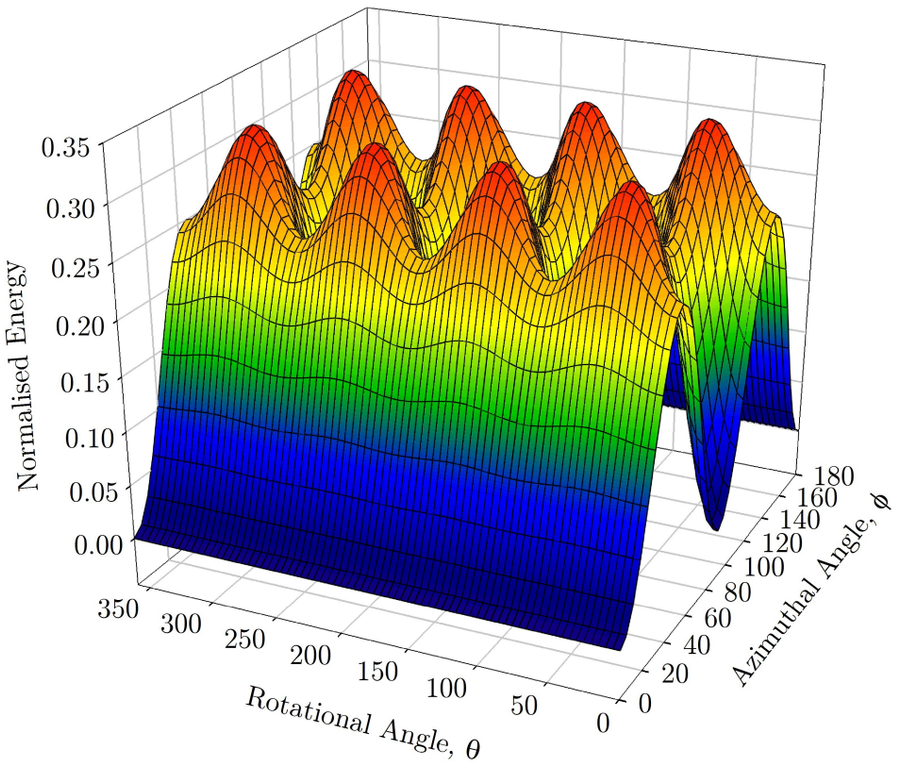
- Encapsulates isotropic exchange, mediated 2-ion anisotropy and Dzyaloshinskii-Moriya interaction into a compact form

Magnetic anisotropy energy

Uniaxial



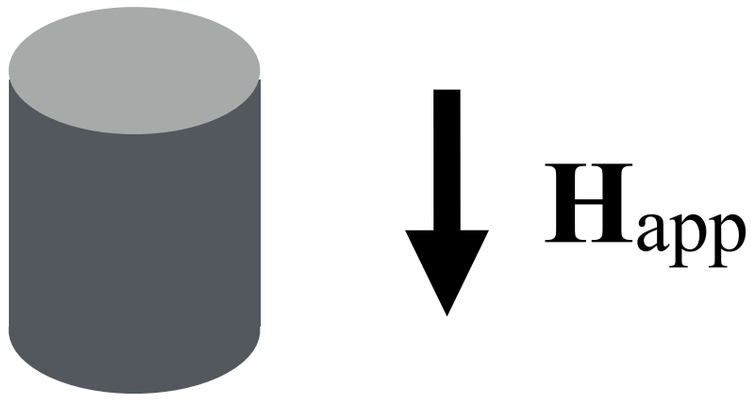
Cubic



$$\mathcal{H}_{\text{ani}}^{\text{uni}} = -k_{\text{u}} \sum_i \left(\mathbf{S}_i \cdot \boldsymbol{e}\right)^2$$

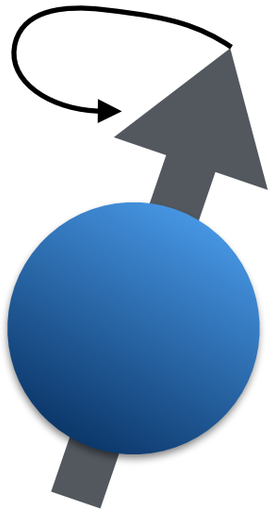
$$\mathcal{H}_{\text{ani}}^{\text{cub}} = \frac{k_{\text{c}}}{2} \sum_i \left(S_x^4 + S_y^4 + S_z^4\right)$$

Externally applied fields



$$\mathcal{H}_{\text{app}} = -\sum_i \mu_{\text{s}} \mathbf{S}_i \cdot \mathbf{H}_{\text{app}}$$

Integration methods



Ising model

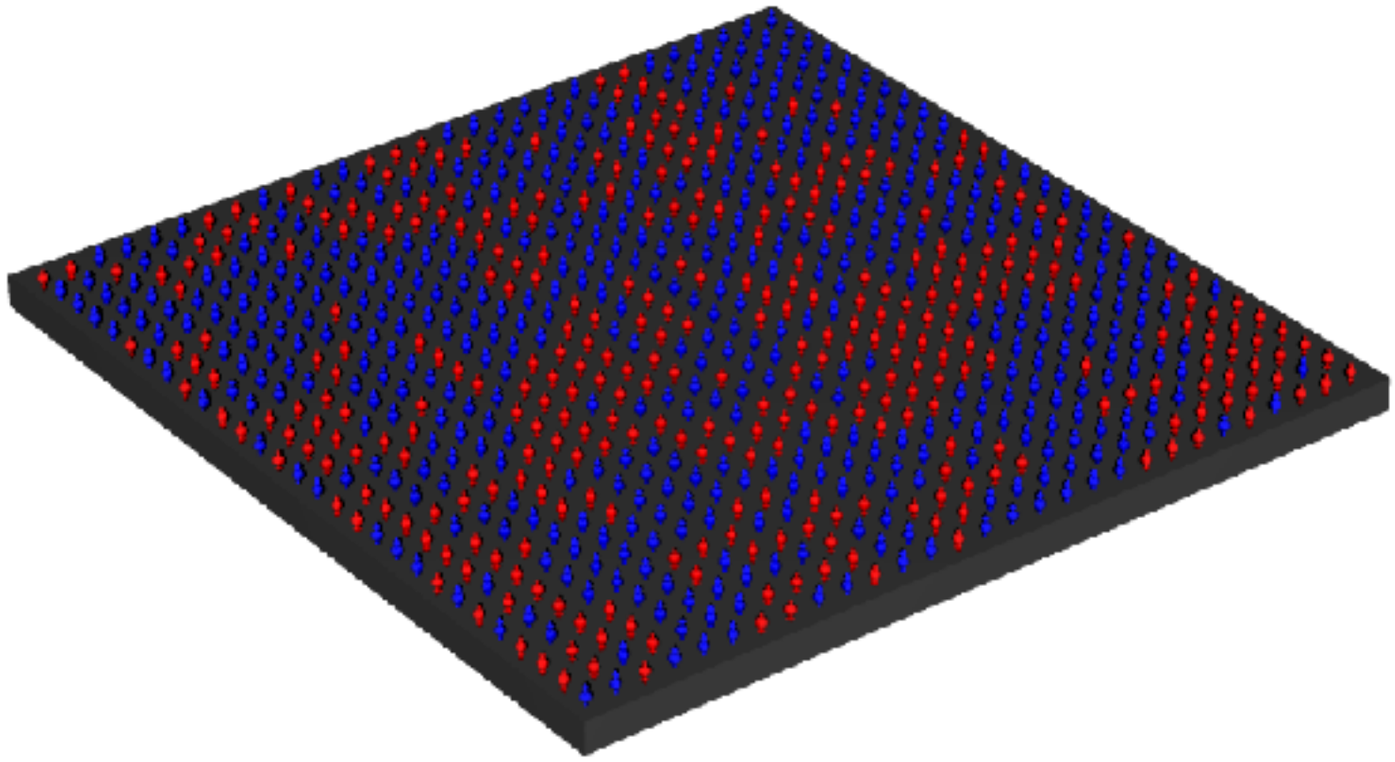
Beitrag zur Theorie des Ferromagnetismus [1]).

Von **Ernst Ising** in Hamburg.

(Eingegangen am 9. Dezember 1924.)

Es wird im wesentlichen das thermische Verhalten eines linearen, aus Elementarmagneten bestehenden Körpers untersucht, wobei im Gegensatz zur Weissschen Theorie des Ferromagnetismus kein molekulares Feld, sondern nur eine (nicht magnetische) Wechselwirkung benachbarter Elementarmagnete angenommen wird. Es wird gezeigt, daß ein solches Modell noch keine ferromagnetischen Eigenschaften besitzt und diese Aussage auch auf das dreidimensionale Modell ausgedehnt.

1. Annahmen. Die Erklärung, die P. Weiss [2]) für den Ferromagnetismus gegeben hat, ist zwar formal befriedigend, doch läßt sie besonders die Frage nach einer physikalischen Erklärung der Hypothese des molekularen Feldes offen. Nach dieser Theorie wirkt auf jeden

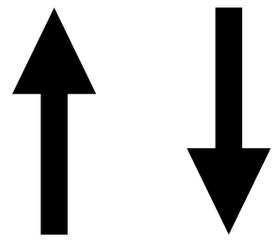


Simplest model of spin-1/2 ferromagnet phase transition

“Toy model”

Ising model

Two allowable states, up, down

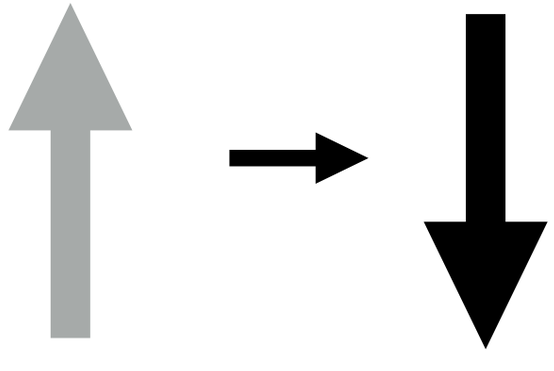


Energy barrier between states defined by exchange energy

$$\mathcal{H}_{\text{exc}} = -\sum_{i \neq j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

Monte Carlo algorithm

1. Pick a new trial state (or move)



2. Evaluate energy before (E_1) and after (E_2) spin flip

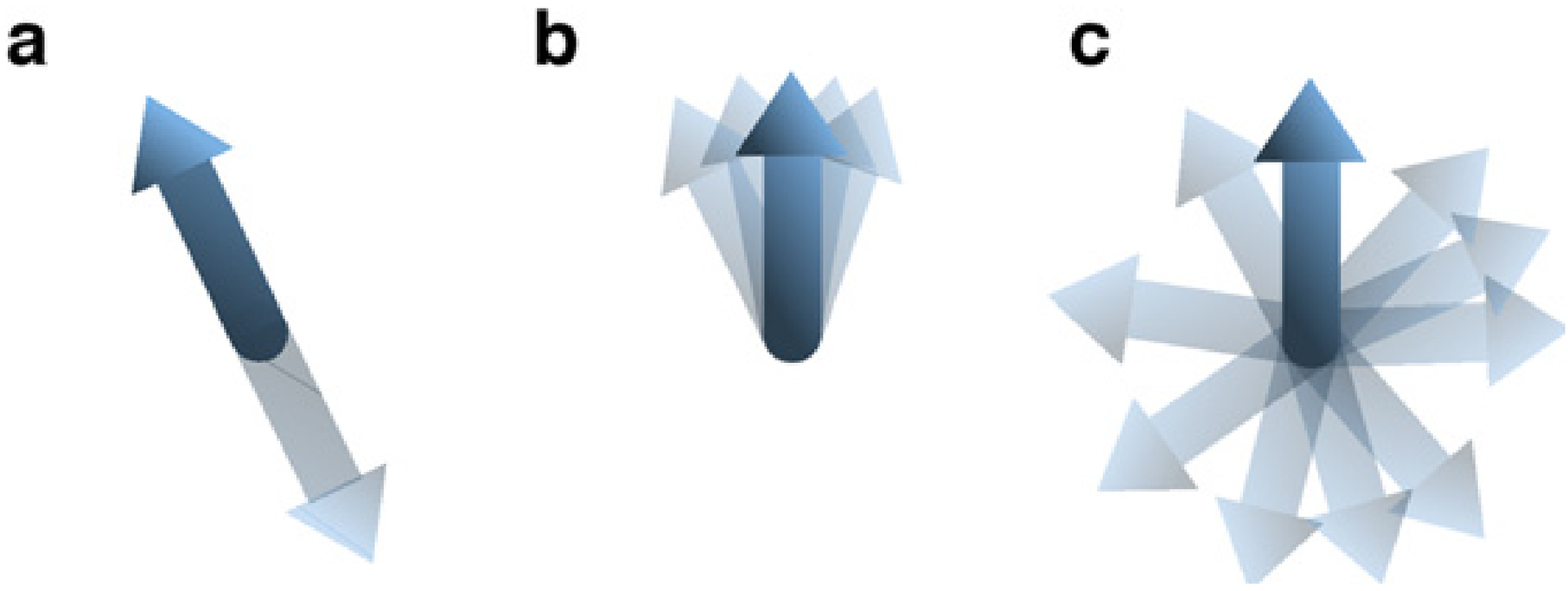
3. Evaluate energy difference between states

$$\Delta E = (E_2 - E_1)$$

4. Accept move with probability

$$\exp(-\Delta E/k_B T)$$

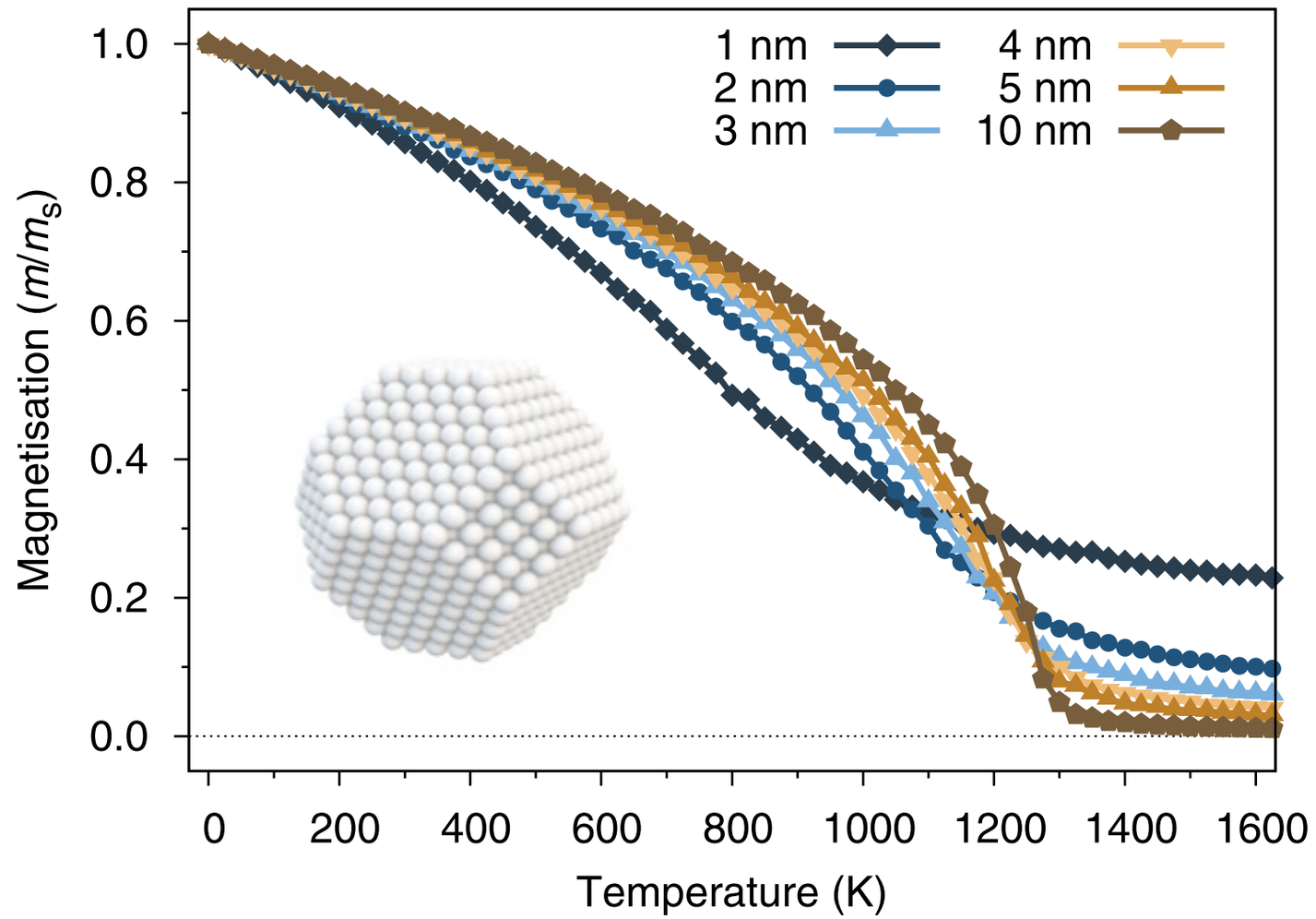
Extension to 3D Heisenberg model straightforward



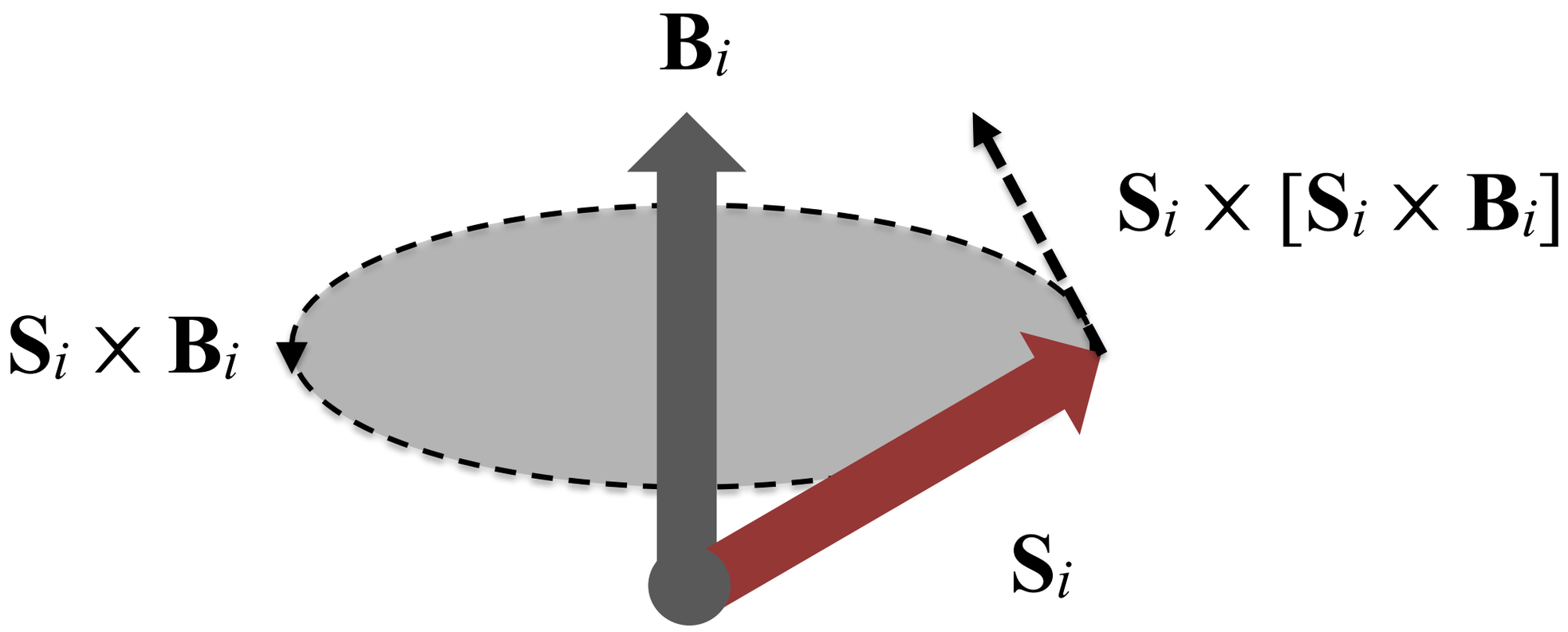
Use a combination of different trial moves

Temperature dependent magnetization for different particle sizes

- Calculate m(T) curves for different particle sizes of Co
- Includes the effect of missing exchange bonds on the particle surface
- Curie temperature and criticality depends on size



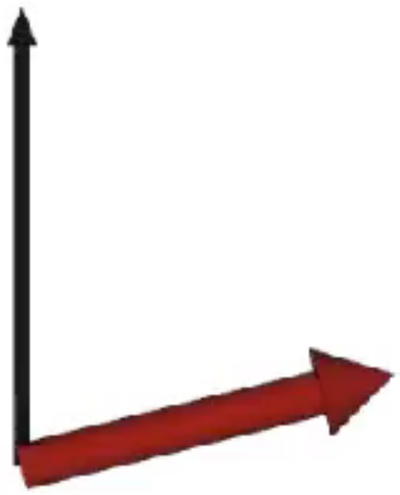
Spin dynamics



$$\frac{\partial \mathbf{S}_i}{\partial t} = -\frac{\gamma_i}{(1+\lambda_i^2)}[\mathbf{S}_i \times \mathbf{B}_i + \lambda_i \mathbf{S}_i \times (\mathbf{S}_i \times \mathbf{B}_i)]$$

Stochastic Landau-Lifshitz-Gilbert equation

$$\mathbf{B}_i = \zeta_i(t) - \frac{1}{\mu_i}\frac{\partial \mathscr{H}}{\partial \mathbf{S}_i}$$



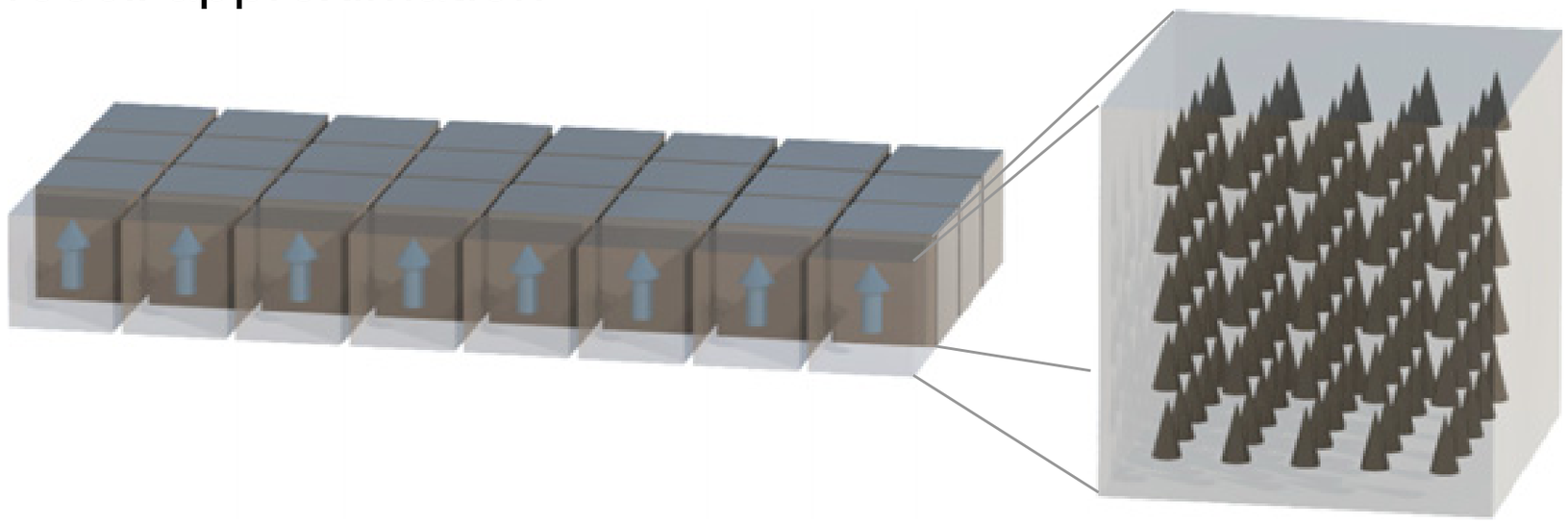
$$\zeta_i = \langle \zeta_i^a(t)\zeta_j^b(t)\rangle = 2\delta_{ij}\delta_{ab}(t-t')\frac{\lambda_i k_B T}{\mu_i \gamma_i}$$

$$\langle \zeta_i^a(t)\rangle = 0$$

Magnetostatics in atomistic spin models

- Magnetostatics a weak effect at short distances, particularly at the atomic scale

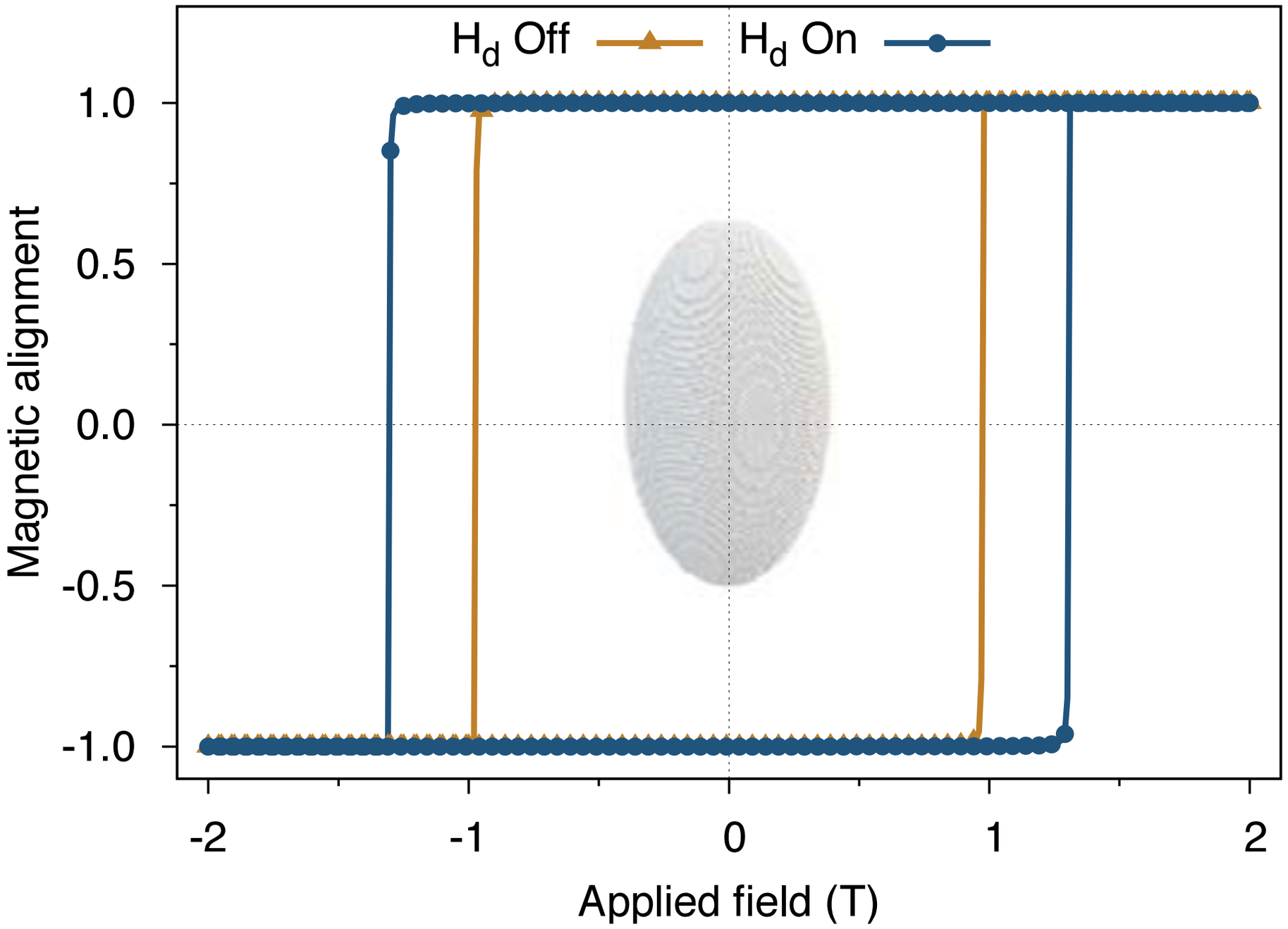
- We therefore use a micromagnetic approach to the demagnetizing field: macrocell approximation



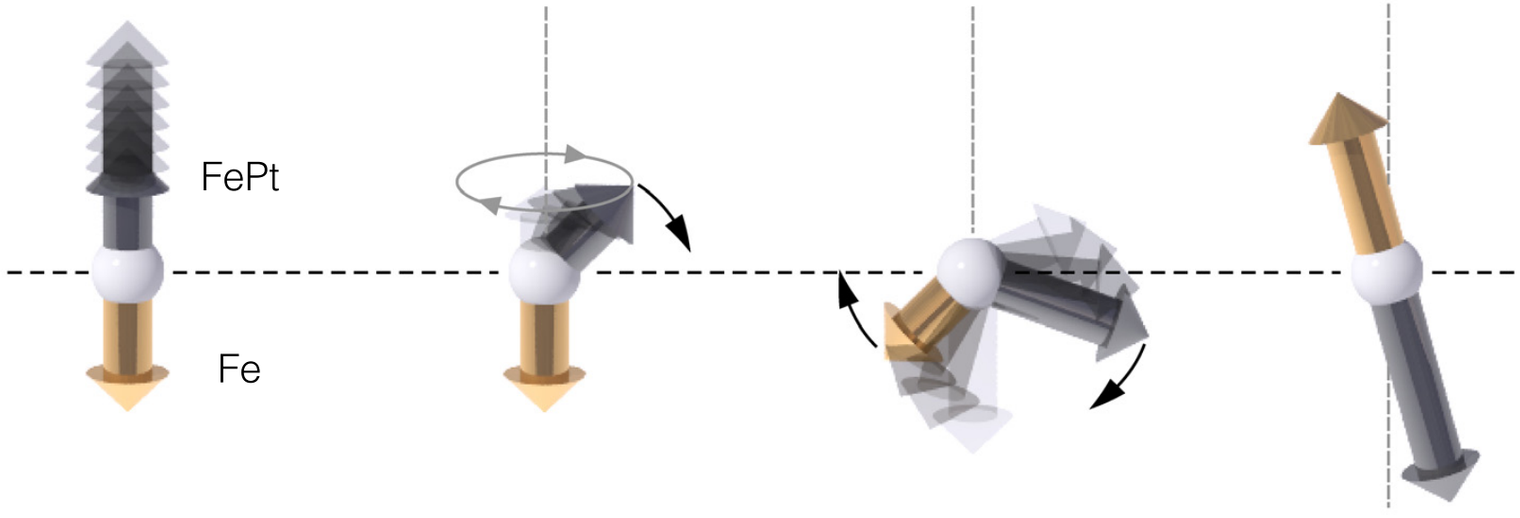
- Local moments are summed into a cell and the continuum approximation applied

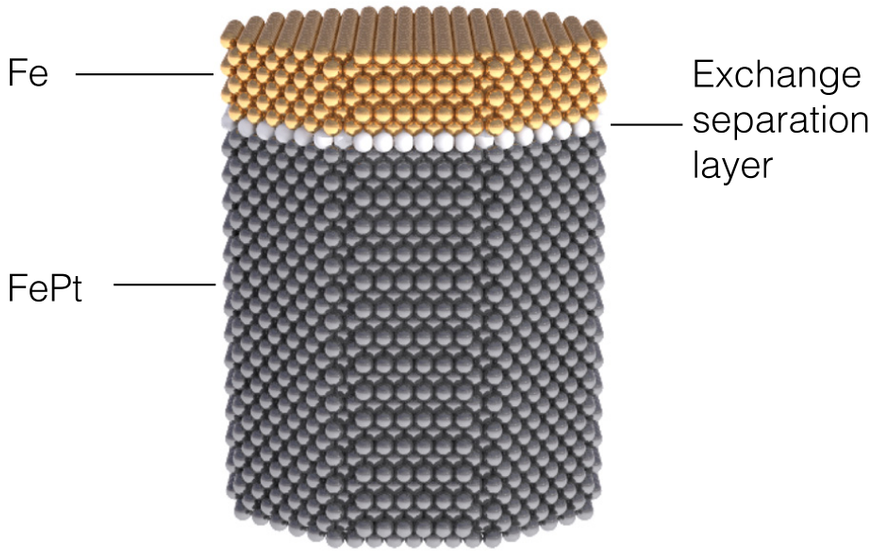
- Interaction between cells encapsulated in a **dipole tensor**, built from atomistic dipole-dipole interactions, dipole field at large ranges

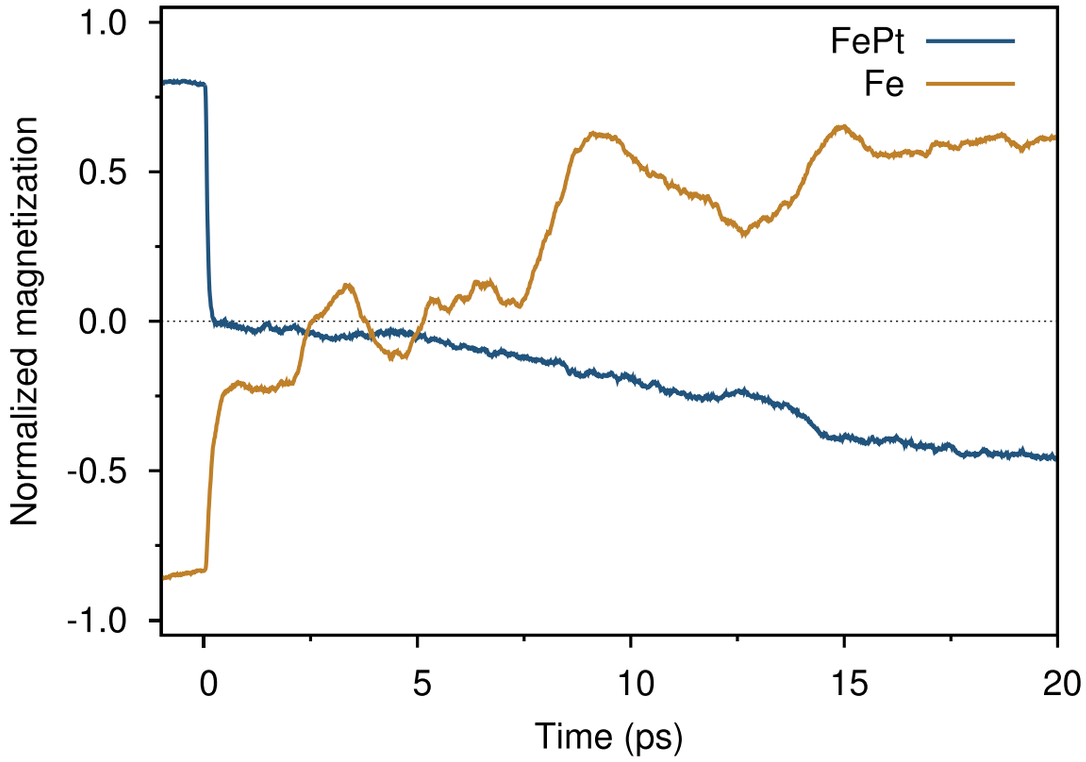
Typical simulations: hysteresis simulations



Typical simulations: ultrafast spin dynamics







R F L Evans et al, Appl. Phys. Lett. (2014)

VAMPIRE

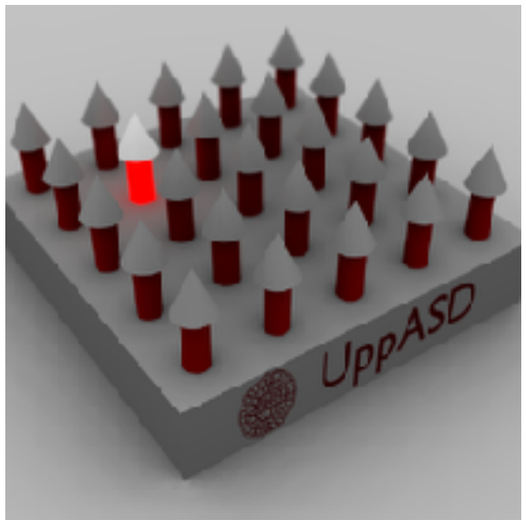
vampire.york.ac.uk

Review article

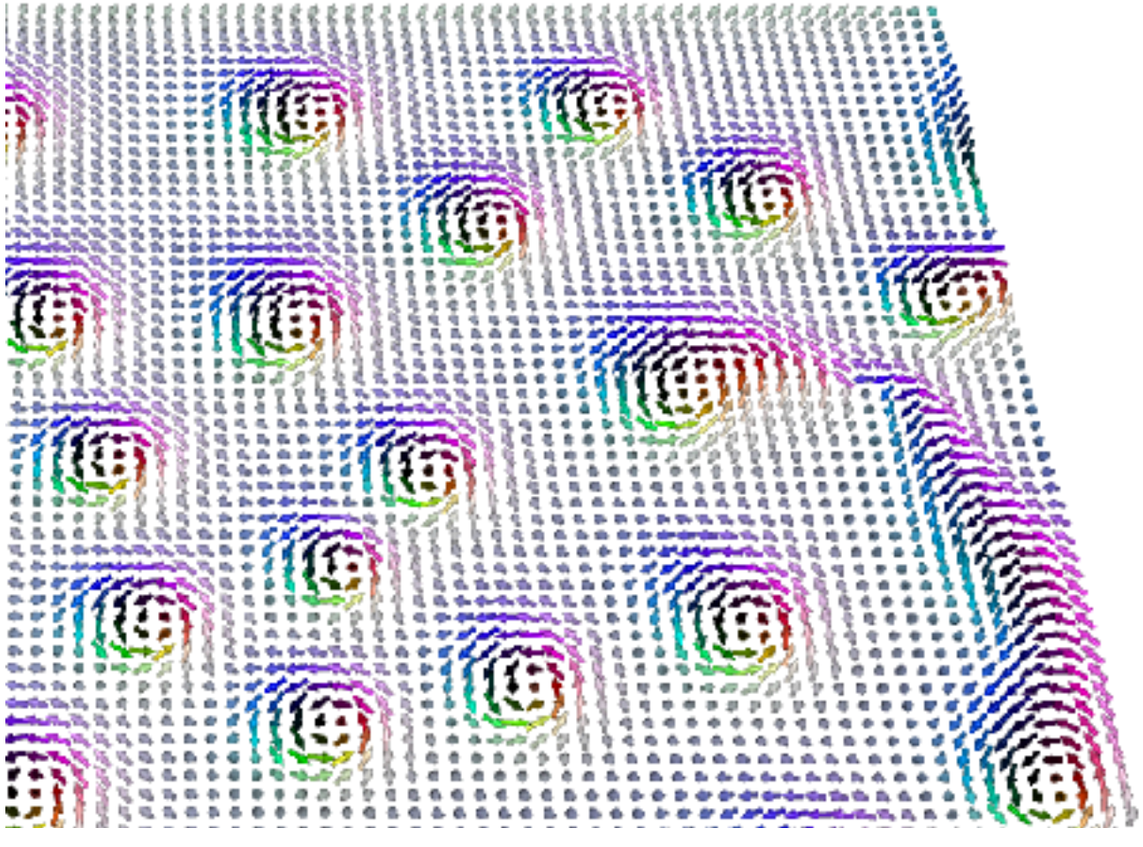
R F L Evans *et al*, J. Phys.: Condens. Matter 26 (2014) 103202

Other codes for atomistic simulations

- UppASD - good for linking to first principles simulations, spin wave spectra etc



- SPIRIT - online interactive tool https://spirit-code.github.io



Summary

- Covered the essential elements of micromagnetic simulations and their formulation
- Introduced atomistic spin models, their fundamentals