Micromagnetic and atomistic and simulations of magnets

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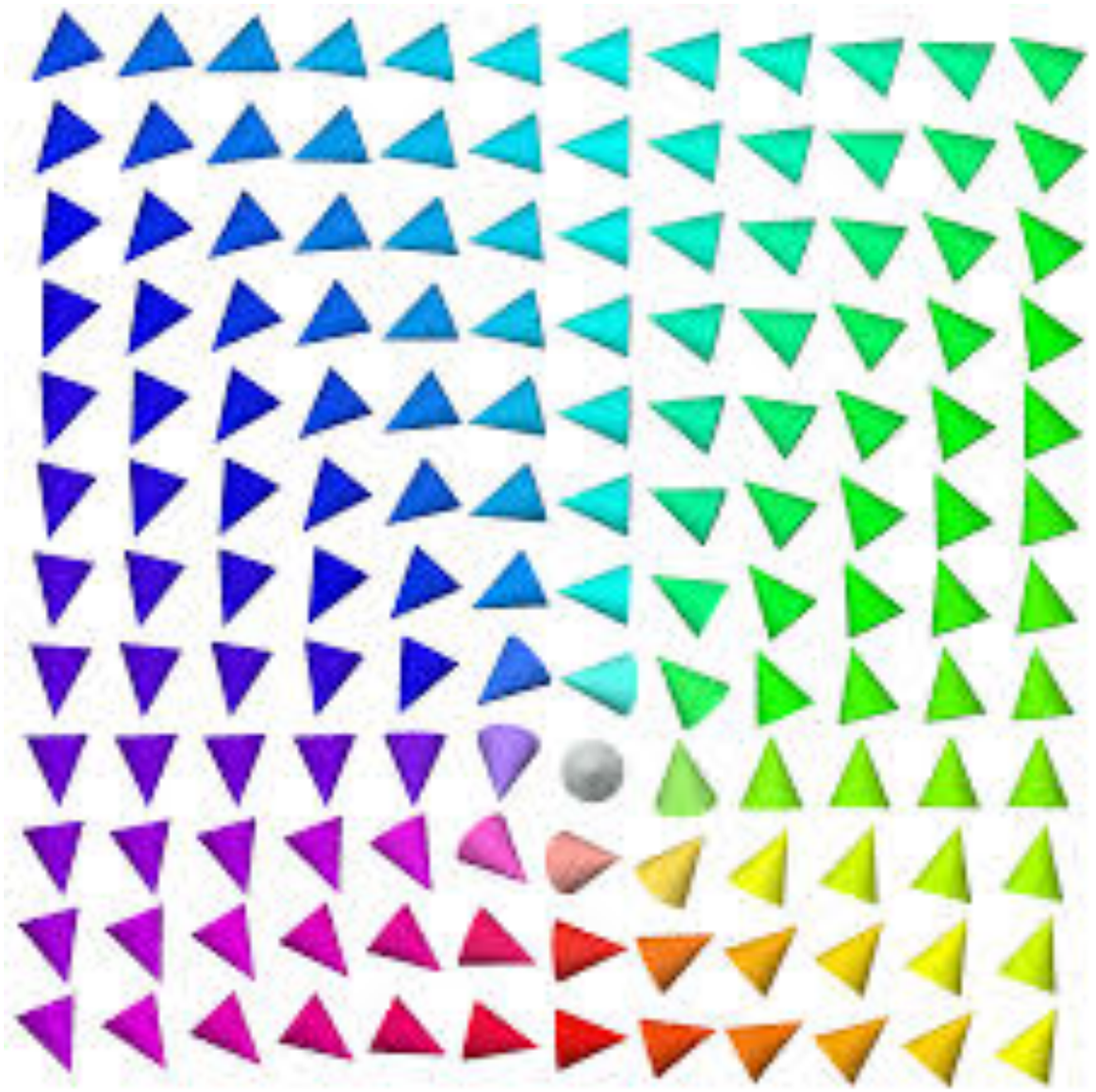
Overview

- Micromagnetics
  - Formulation and approximations
  - Energetic terms and magnetostatics Magnetisation dynamics
  - Foundations and approximations
- Atomistic spin models
  - Monte Carlo methods
  - Spin Dynamics
- Landau-Lifshitz-Bloch micromagnetics (this afternoon)

Micromagnetics

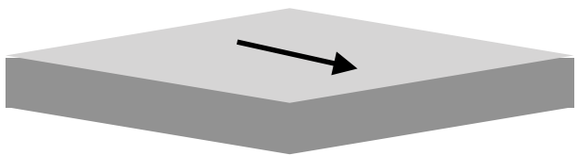


source: mumax

Why do we need magnetic simulations?

Demagnetization factors for different shapes

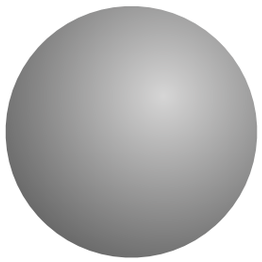
N = 0



Infinite thin film

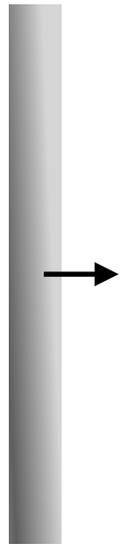
Infinitely long cylinder

N = 1/3

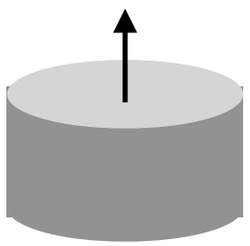


Sphere

N = 1/2

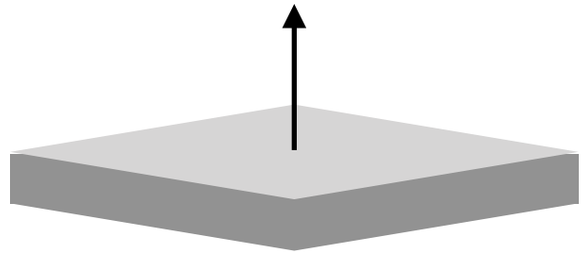


Infinitely long cylinder

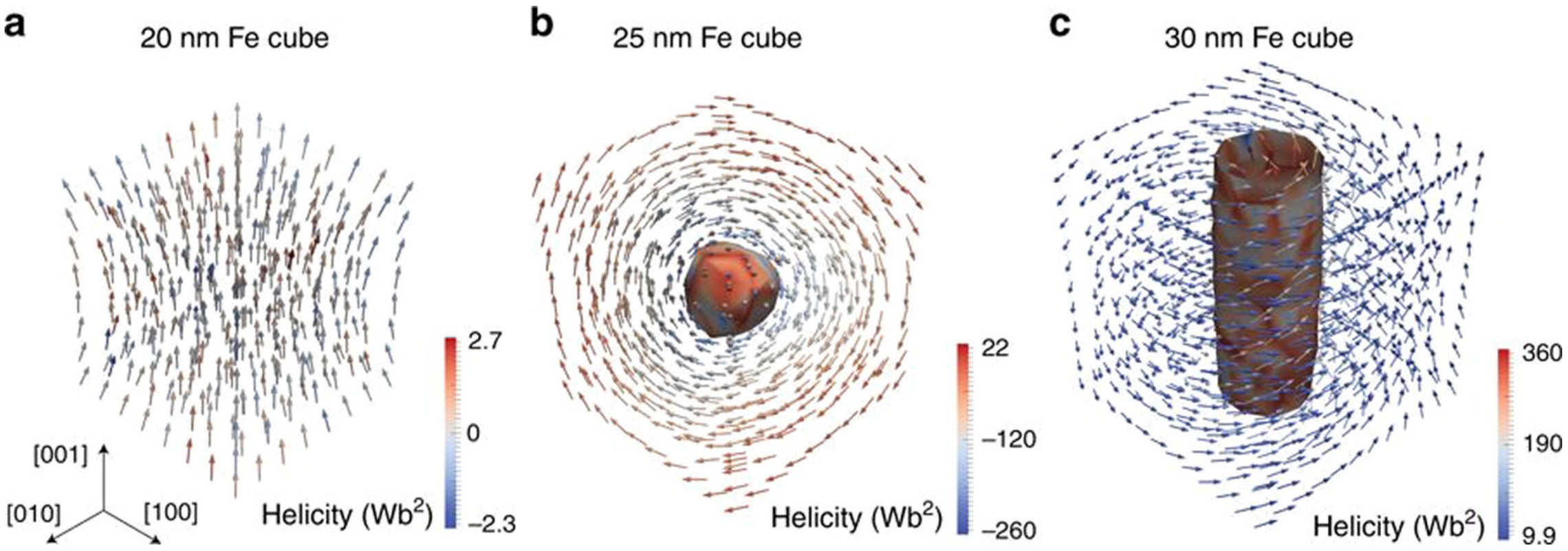


Short cylinder

N = 1



Why do we need magnetic simulations?



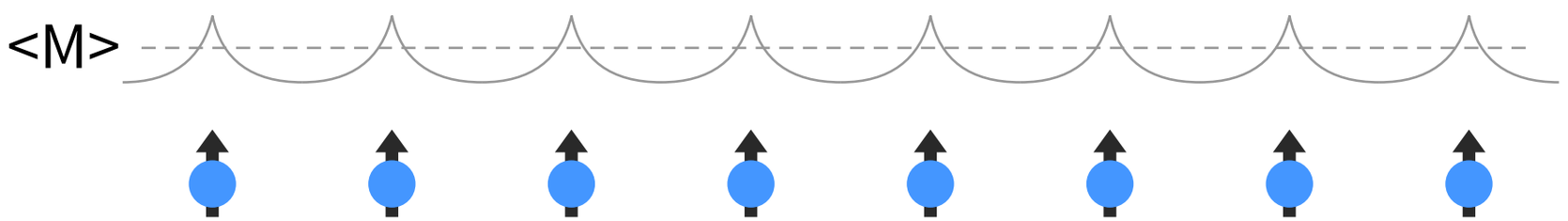
Jay Shah et al, Nature Communications 9 1173 (2018)

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)

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

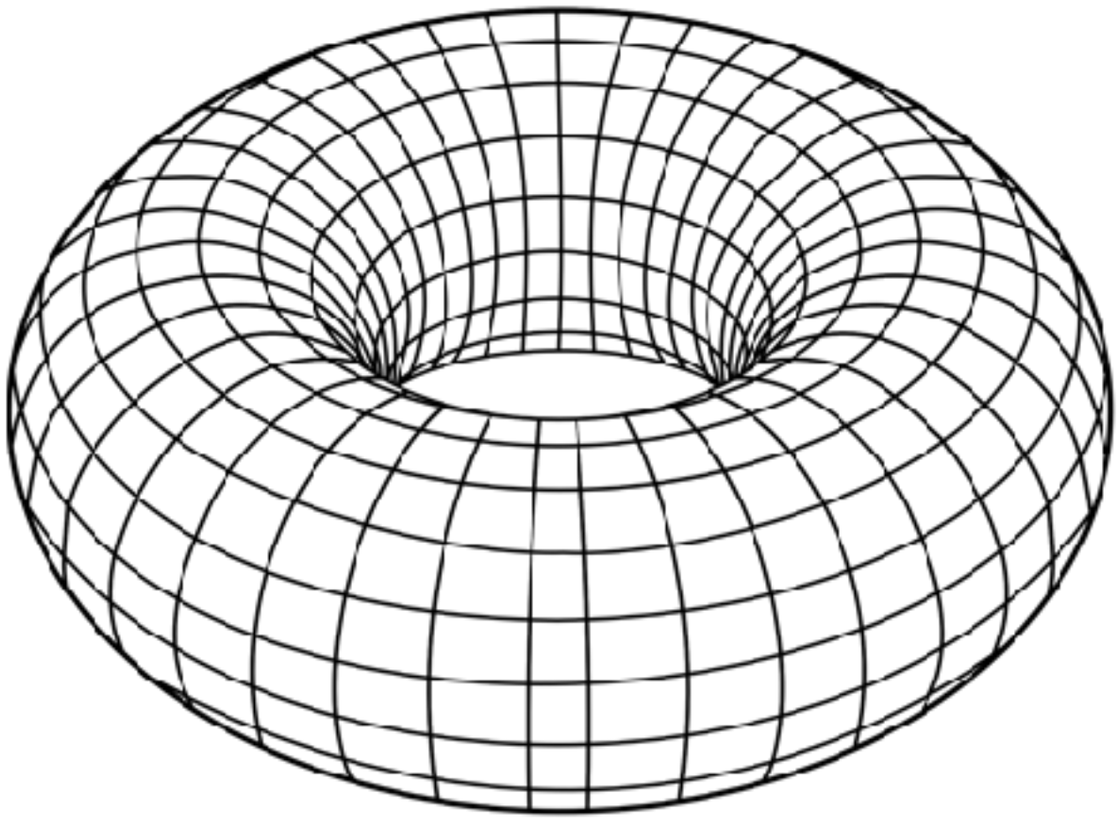
- Then consider a small volume of space (1 nm)^3 - (10 nm)^3 where the magnetization (and all atomic moments) are assumed to point along the same direction

Analytical micromagnetics

- An analytical branch of micromagnetics, treating magnetism on a small (micrometre) length scale

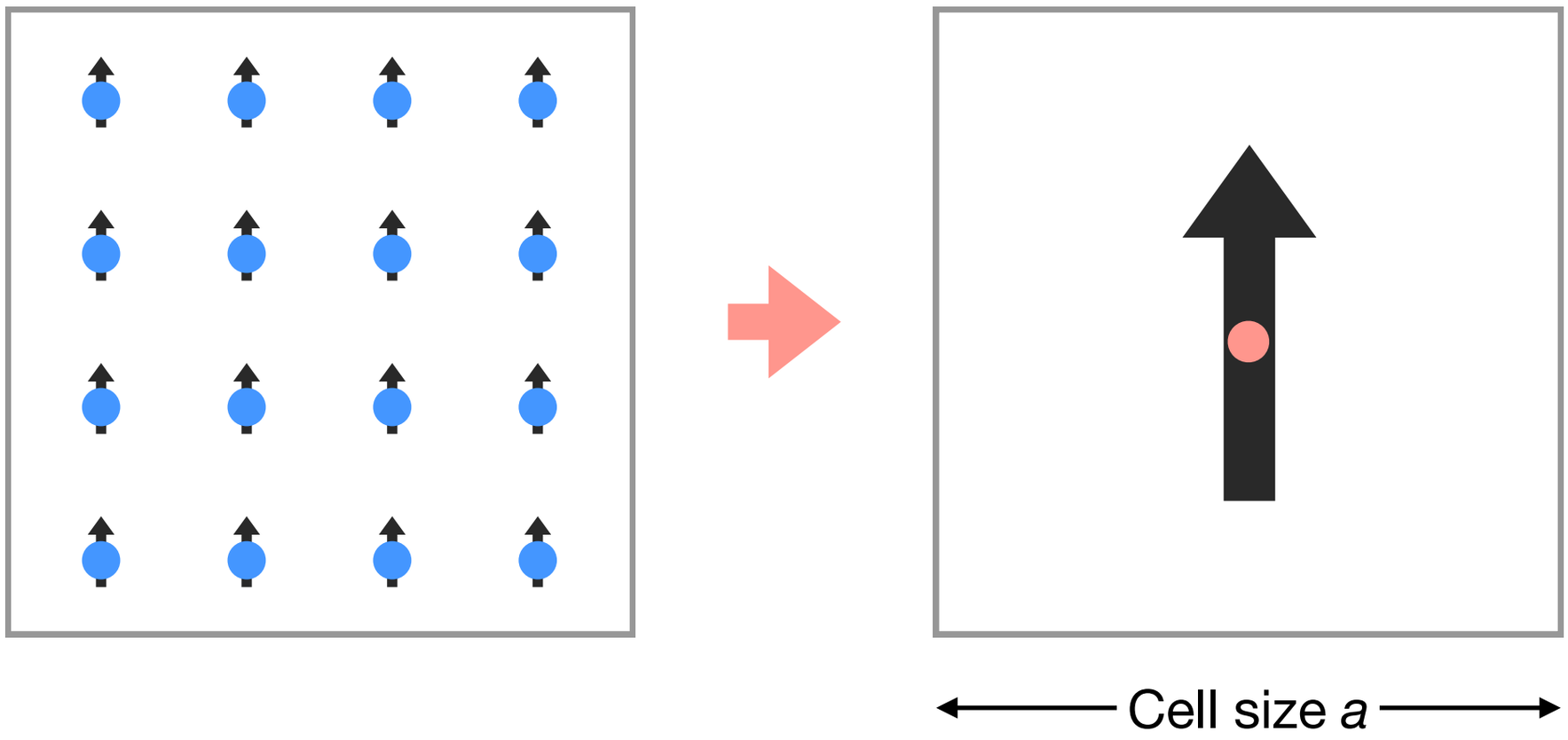
- Mathematically messy but elegant

- When we talk about micromagnetics, we *usually* mean **numerical micromagnetics**



The micromagnetic cell

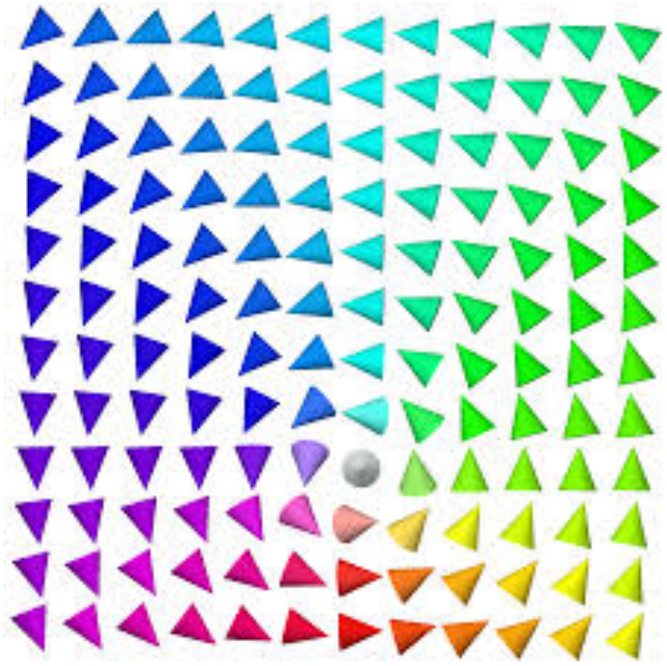
- This gives the fundamental unit of micromagnetics: the micromagnetic cell
- The magnetisation is resolved to a single point **magnetic moment**



- 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

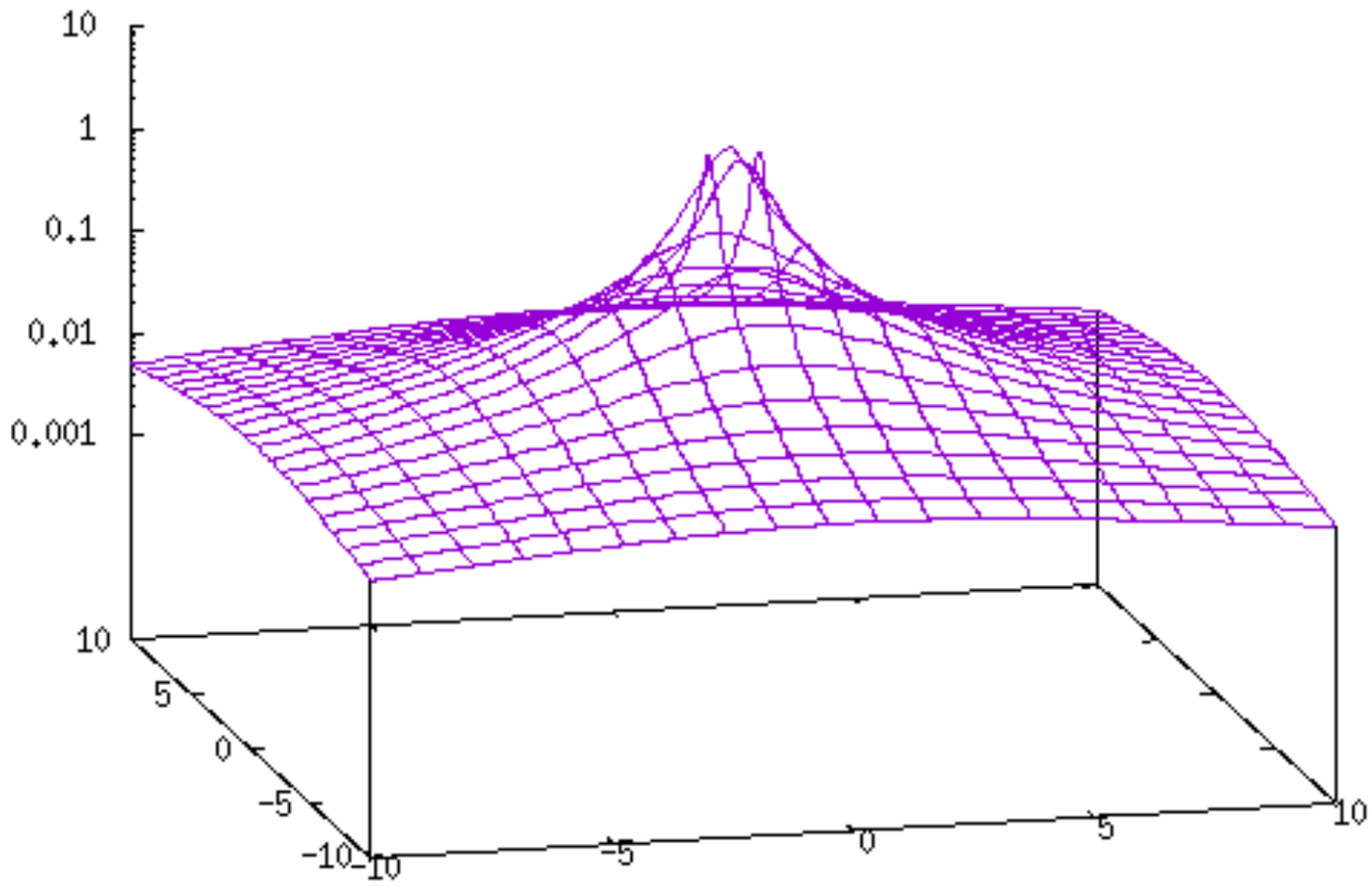
$$\mathbf{H}_\mathrm{d} = -\frac{1}{4\pi}\int_V \nabla\cdot\mathbf{M}\frac{\mathbf{r}}{r^3}\mathrm{d}V$$

- 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*) operation - not particularly helpful!
- But Fast Fourier Transform (FFT) has O(*N* log *N*) scaling
- Can reformulate the DFT as

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

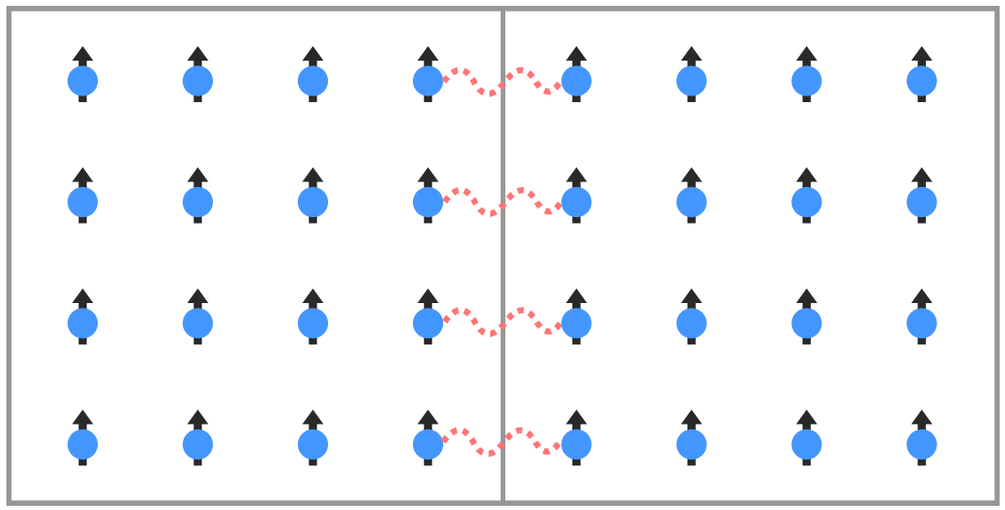
where W_{nk} is a periodic function that repeats for different combinations of *n* and *k*.

- 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)

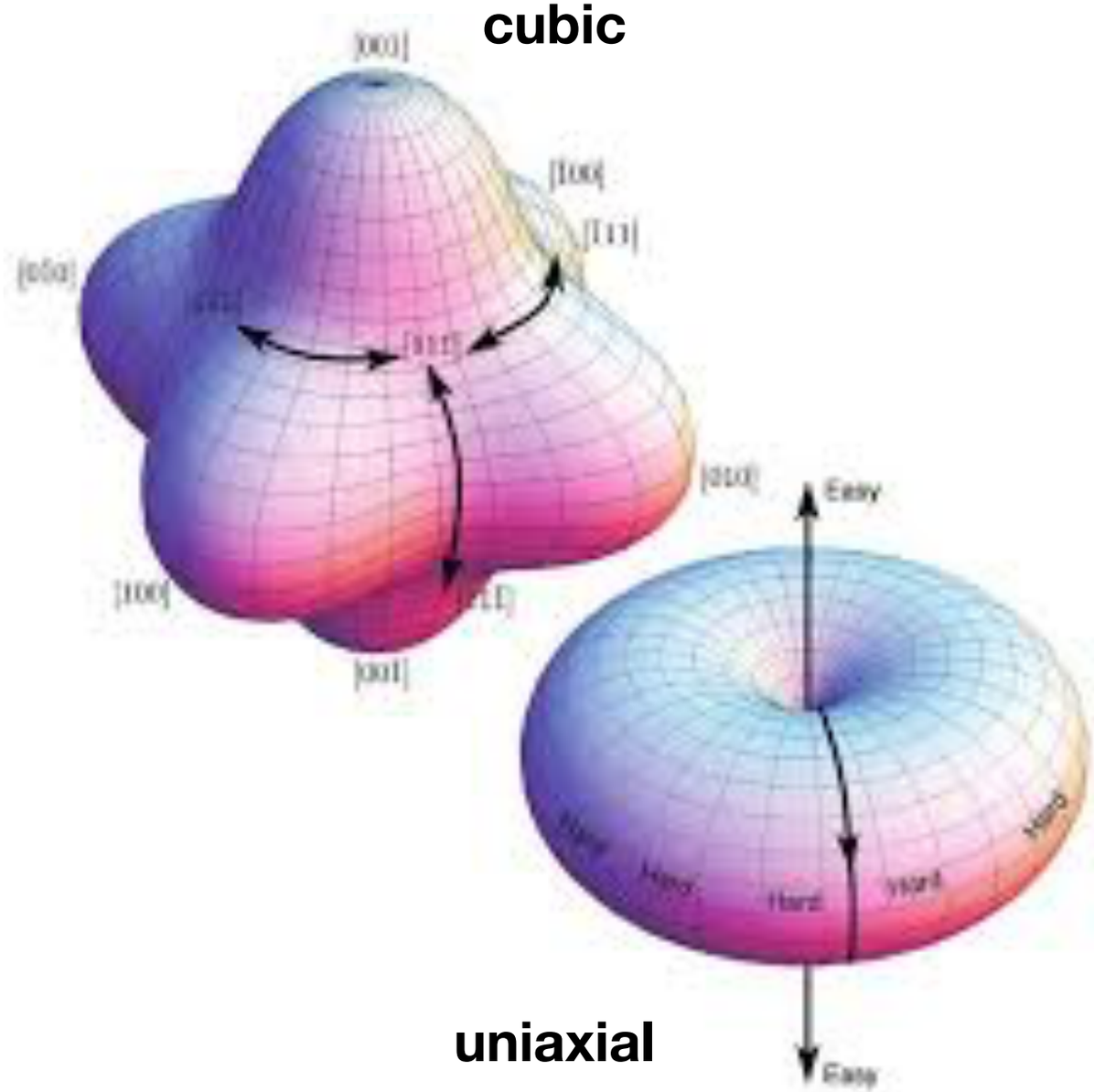
$$A = \frac{\sum_{ij} J_{ij}}{2a}$$

- 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

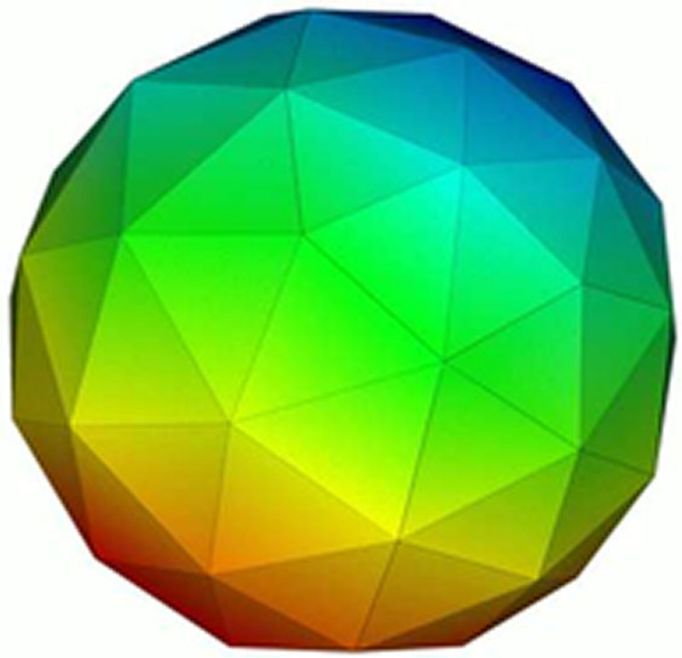
$$\mathbf{H}_{\text{anis}} = -\frac{1}{\mu_0 M_s}\frac{\partial F_{\text{anis}}}{\partial \mathbf{m}}$$

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



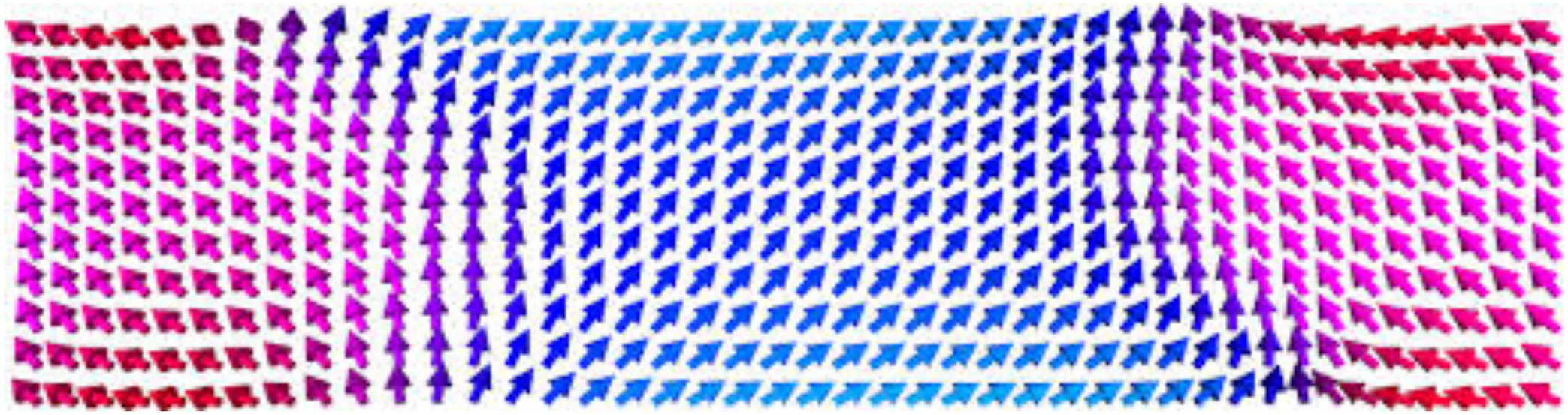
- Much more complicated to implement and set up numerically

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

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

Magnetisation dynamics

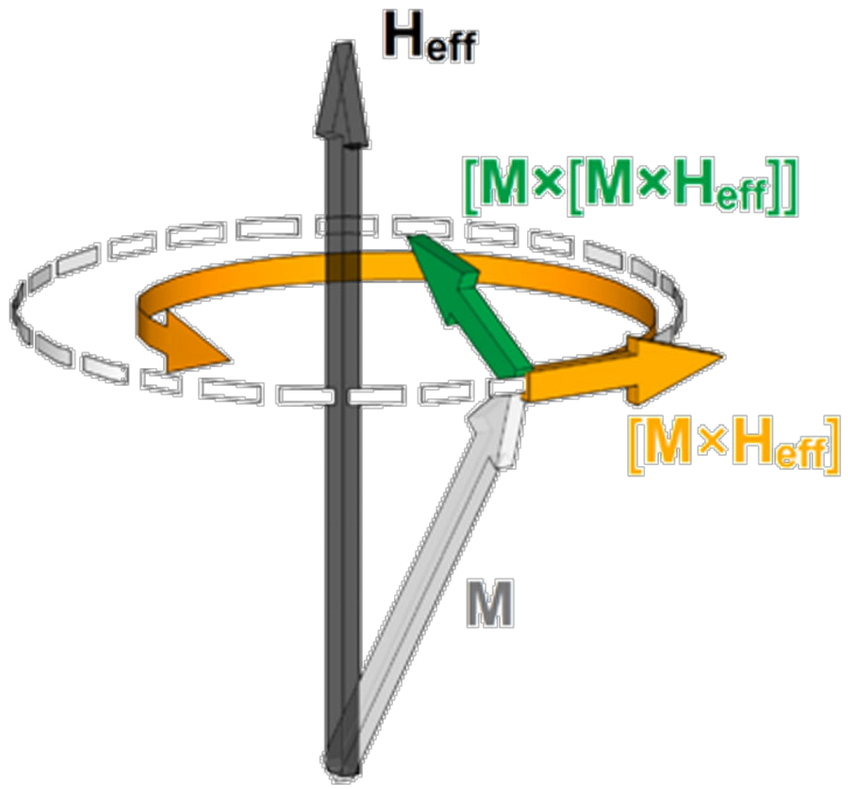
- Not all problems are limited to the ground-state magnetic configuration
- Many dynamic problems
  - Magnetic recording and sensing
  - Fast reversal dynamics
  - Microwave oscillators
  - Domain wall/Skyrmion dynamics
- Need an equation of motion to describe time evolution of the magnetization of each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

Landau Lifshitz Gilbert equation

- Phenomenological equation of motion describing uniform magnetization dynamics

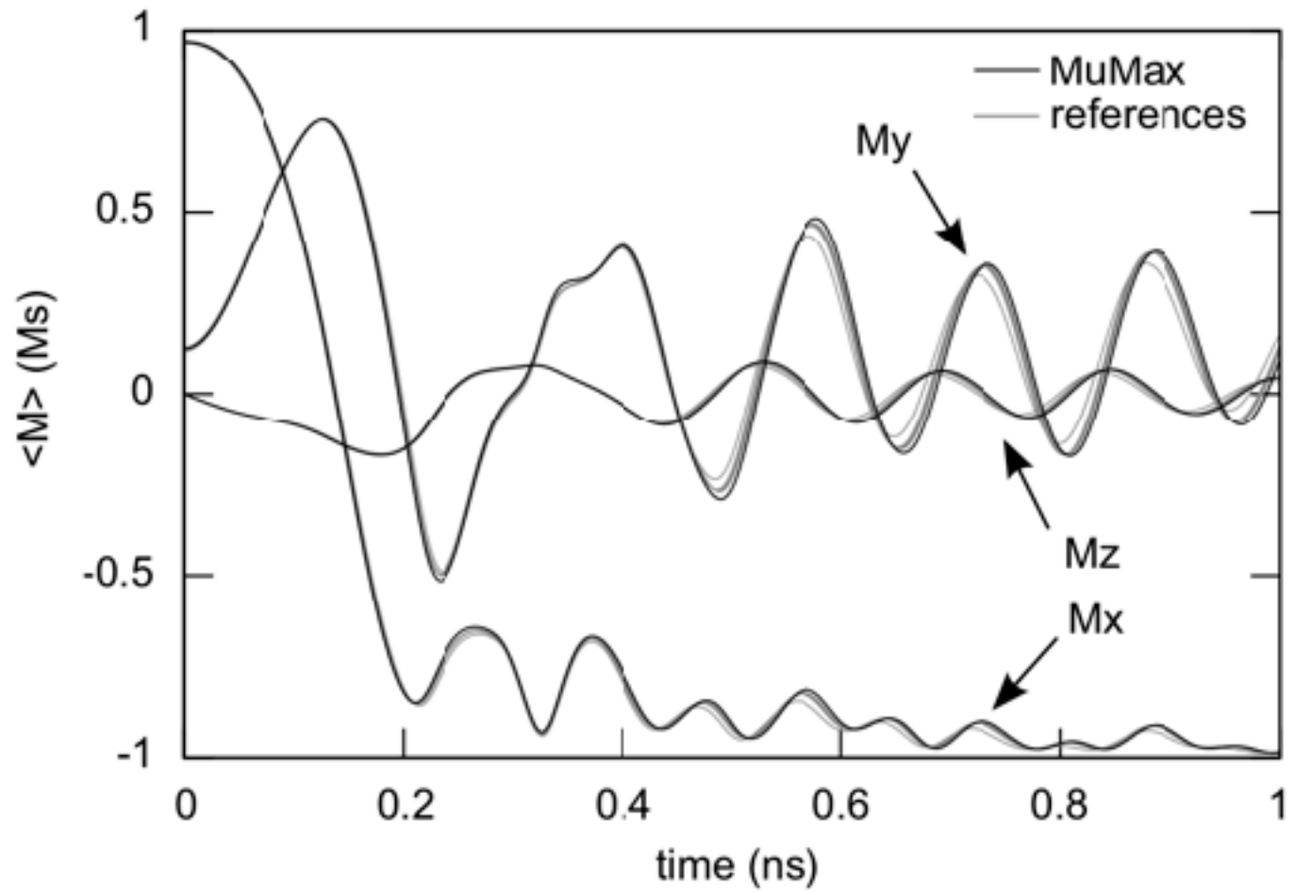
$$\frac{\partial \mathbf{M}(\mathbf{r},t)}{\partial t} = -\frac{\gamma}{1+\alpha^2}\mathbf{M}(\mathbf{r},t)\times\mathbf{H}_{eff}(\mathbf{r},t) - \frac{\alpha\gamma}{M_s(1+\alpha^2)}\mathbf{M}(\mathbf{r},t)\times(\mathbf{M}(\mathbf{r},t)\times\mathbf{H}_{eff}(\mathbf{r},t)).$$

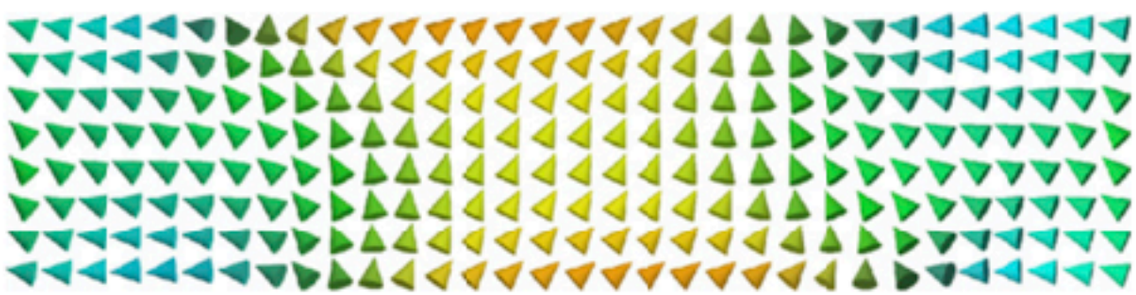
- Consists of two terms - precession and relaxation
- Some quantum mechanical origins: L'armour precession
- Relaxation term is much more complex and hides a multitude of complex physical phenomena (dissipation of angular momentum)



Typical simulations I

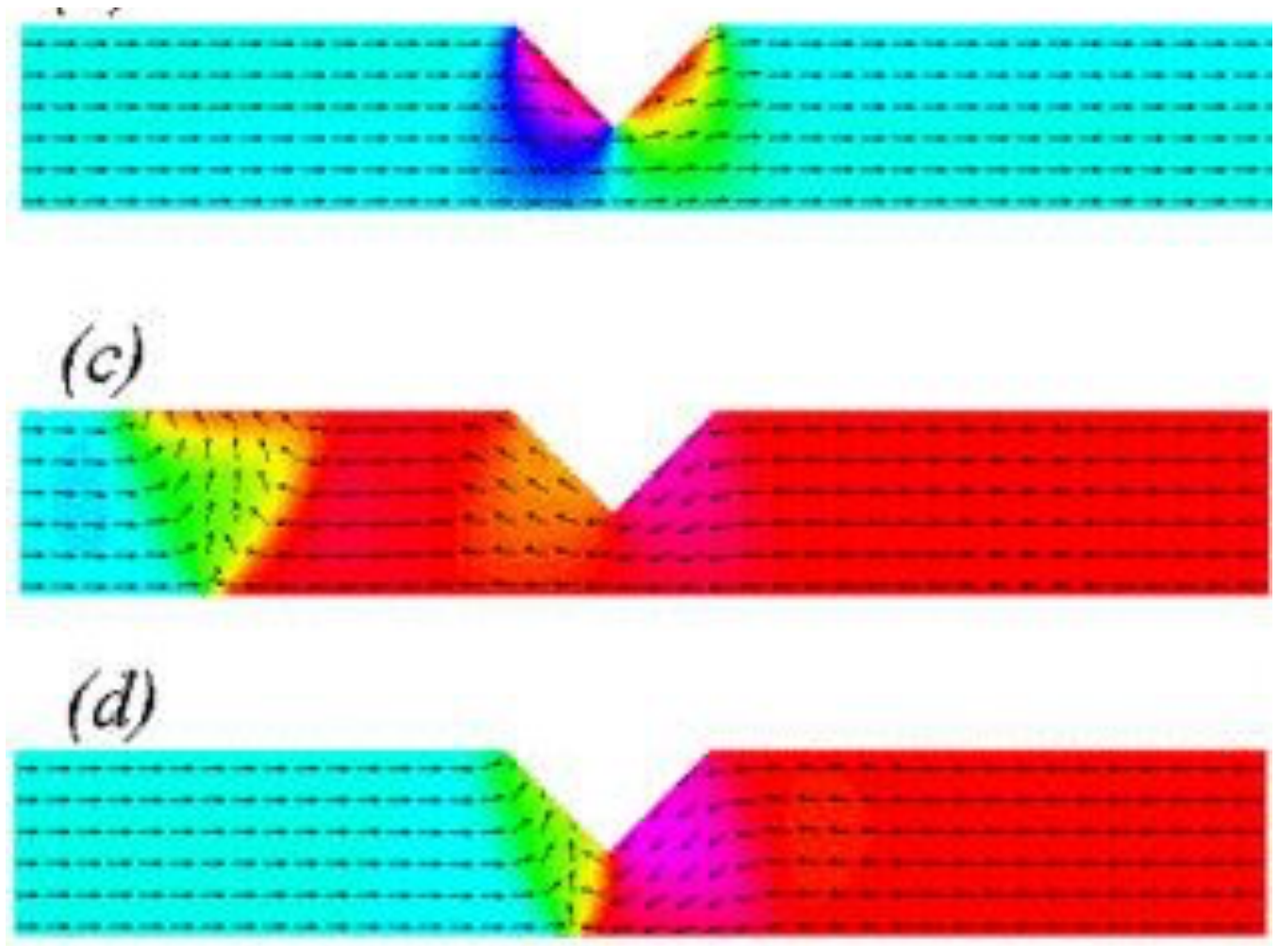
- Micromagnetic standard problems





Typical simulations II

- Domain wall dynamics



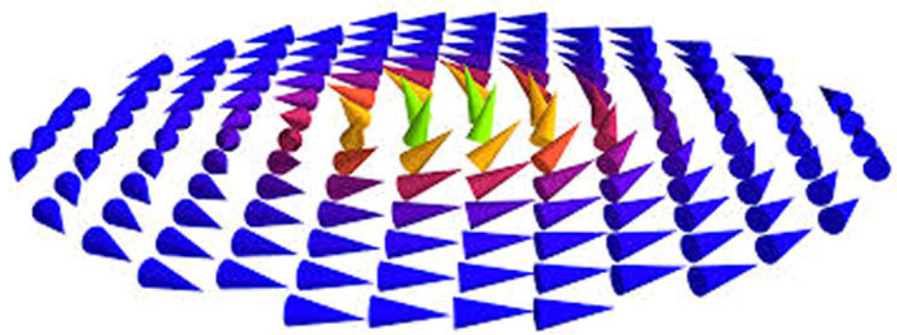
Codes for micromagnetics

- 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

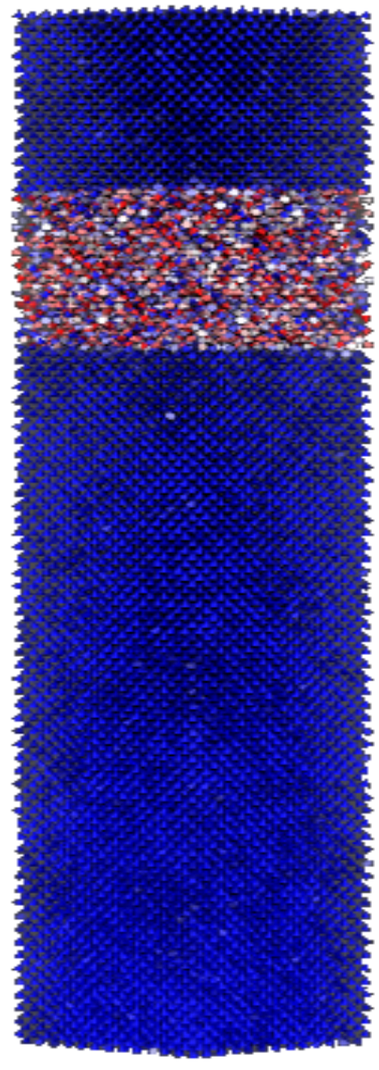


- Several others available, some commercial

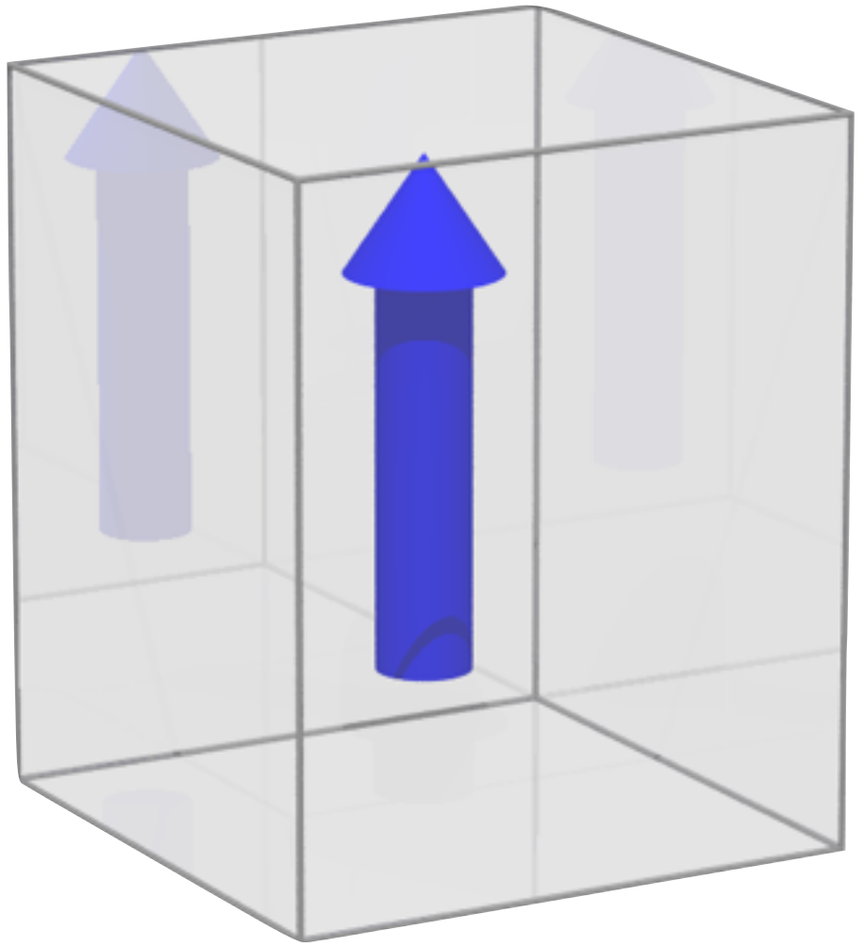
Atomistic spin models

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

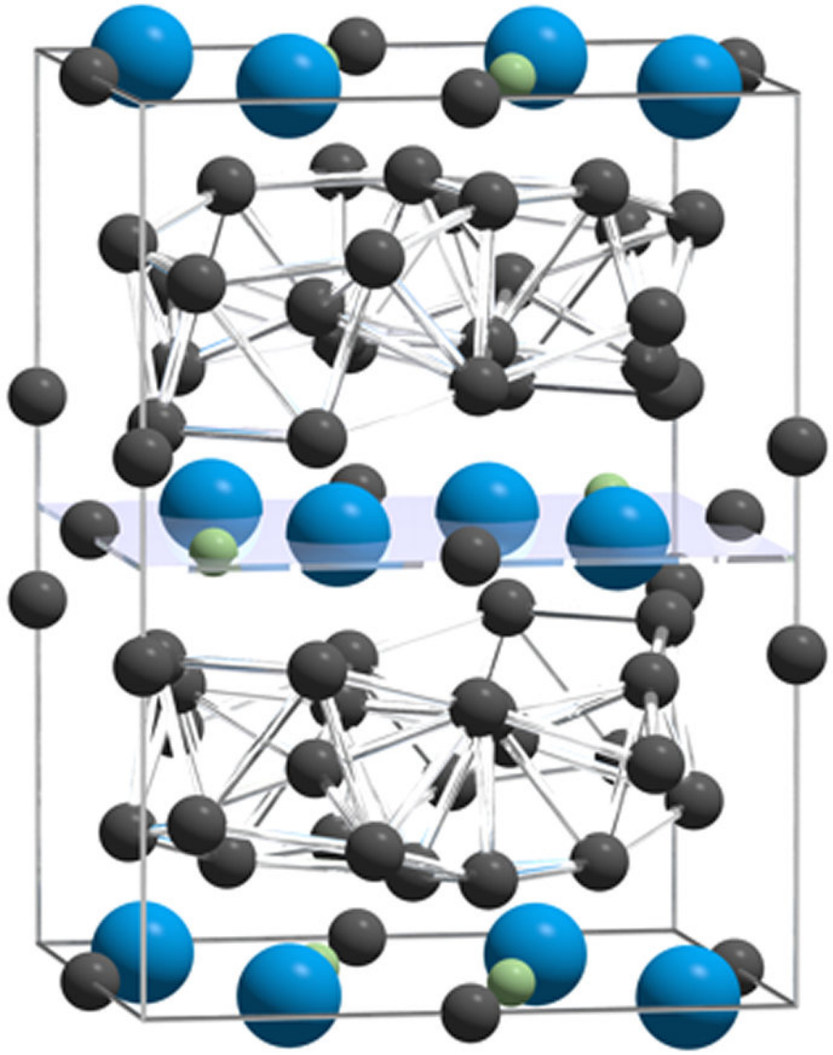
- Multi-sublattice ferro, ferri and antiferromagnets
- Realistic particles with surface effects
- Elevated temperatures near Tc
- Magnetic interfaces
- Crystal defects and disorder



Example: $Nd_2Fe_{14}B$ permanent magnets

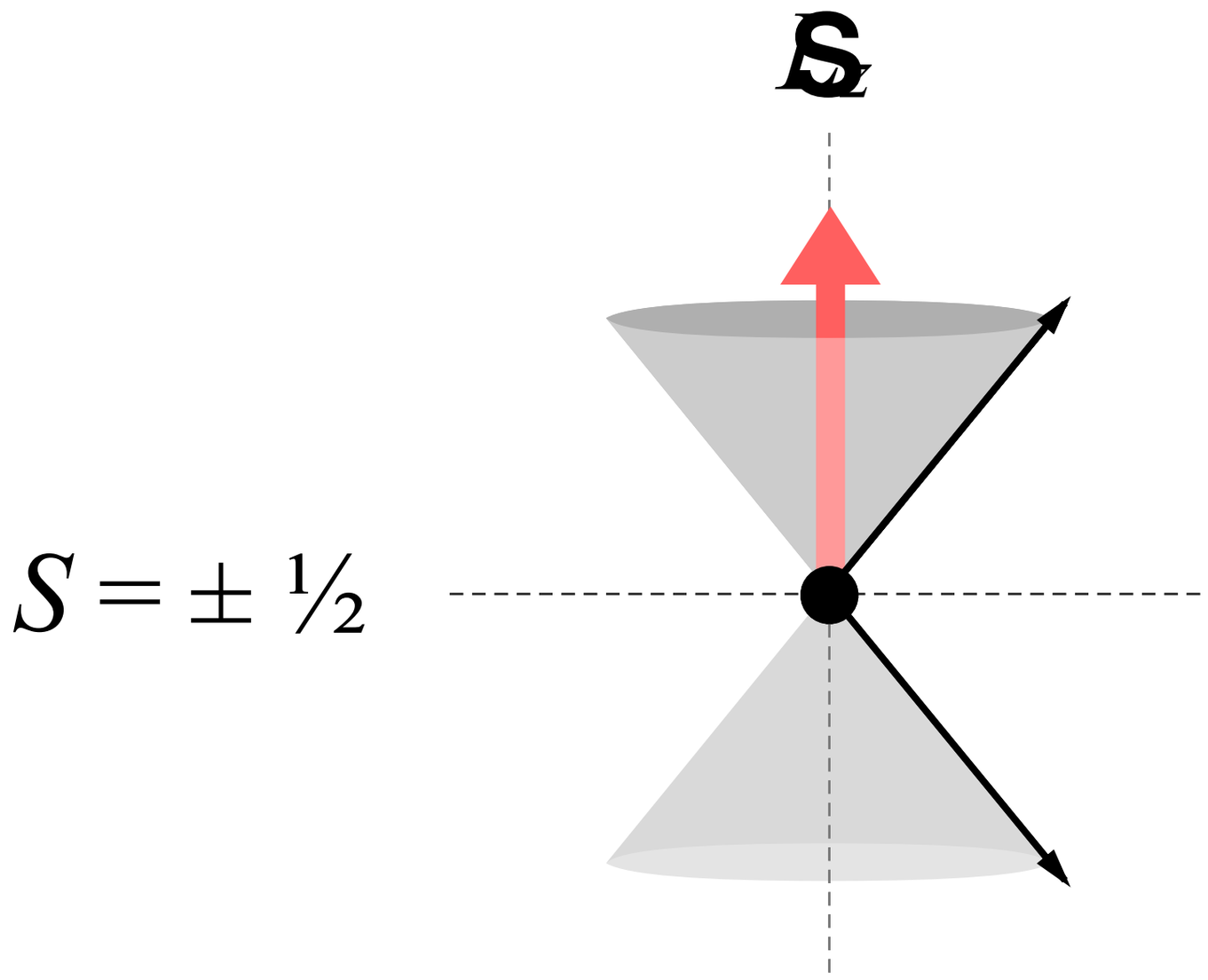


Micromagnetics



Atomistic

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



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

Classical spin Hamiltonian: The Heisenberg model

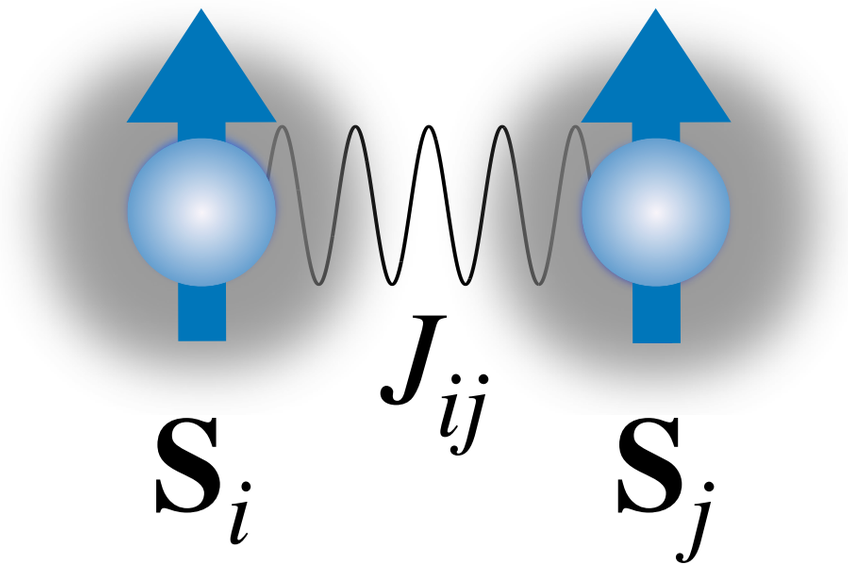
We can write a generalised spin Hamiltonian for a magnetic system as

$$\mathscr{H} = \mathscr{H}_{\text{exc}} + \mathscr{H}_{\text{ani}} + \mathscr{H}_{\text{app}}$$

consisting of the Heisenberg exchange energy, anisotropy and applied field terms.

Heisenberg exchange

As for the Ising model, the exchange energy is now expressed between two interacting spins by the dot product of their spin directions and summing over all pairs



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

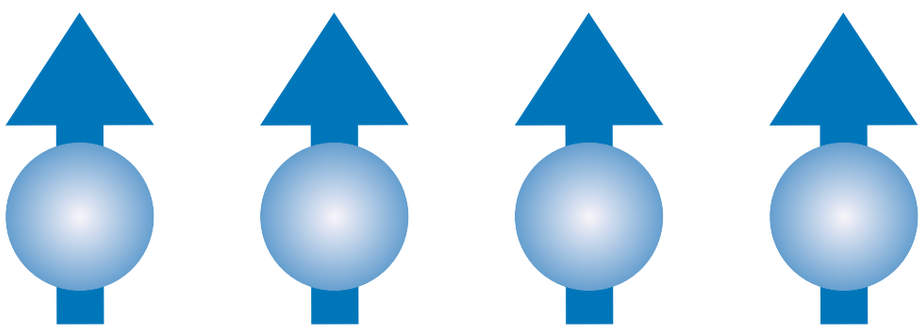
where J_{ij} is the isotropic exchange energy and $\mathbf{S}_{i,j}$ are unit **vectors** describing the directions of spins i and j respectively.

Heisenberg exchange: sign effects

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

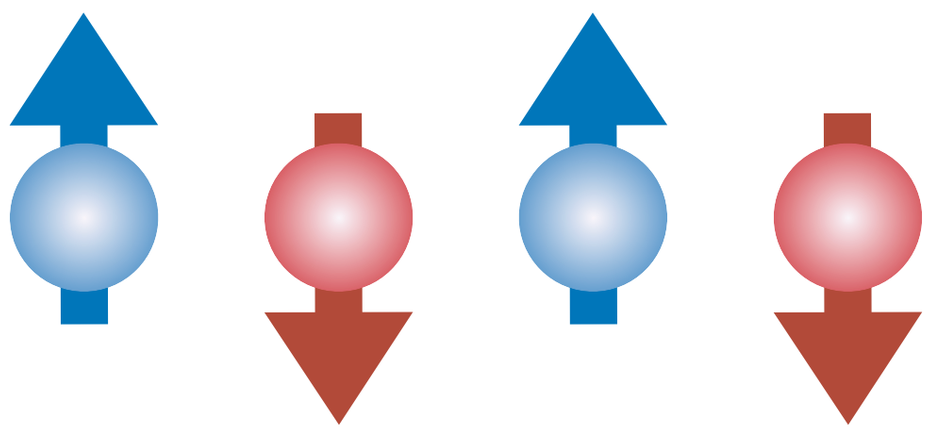
For the exchange interactions it is important to note the significance of the sign of the exchange constant.

$J_{ij} > 0$



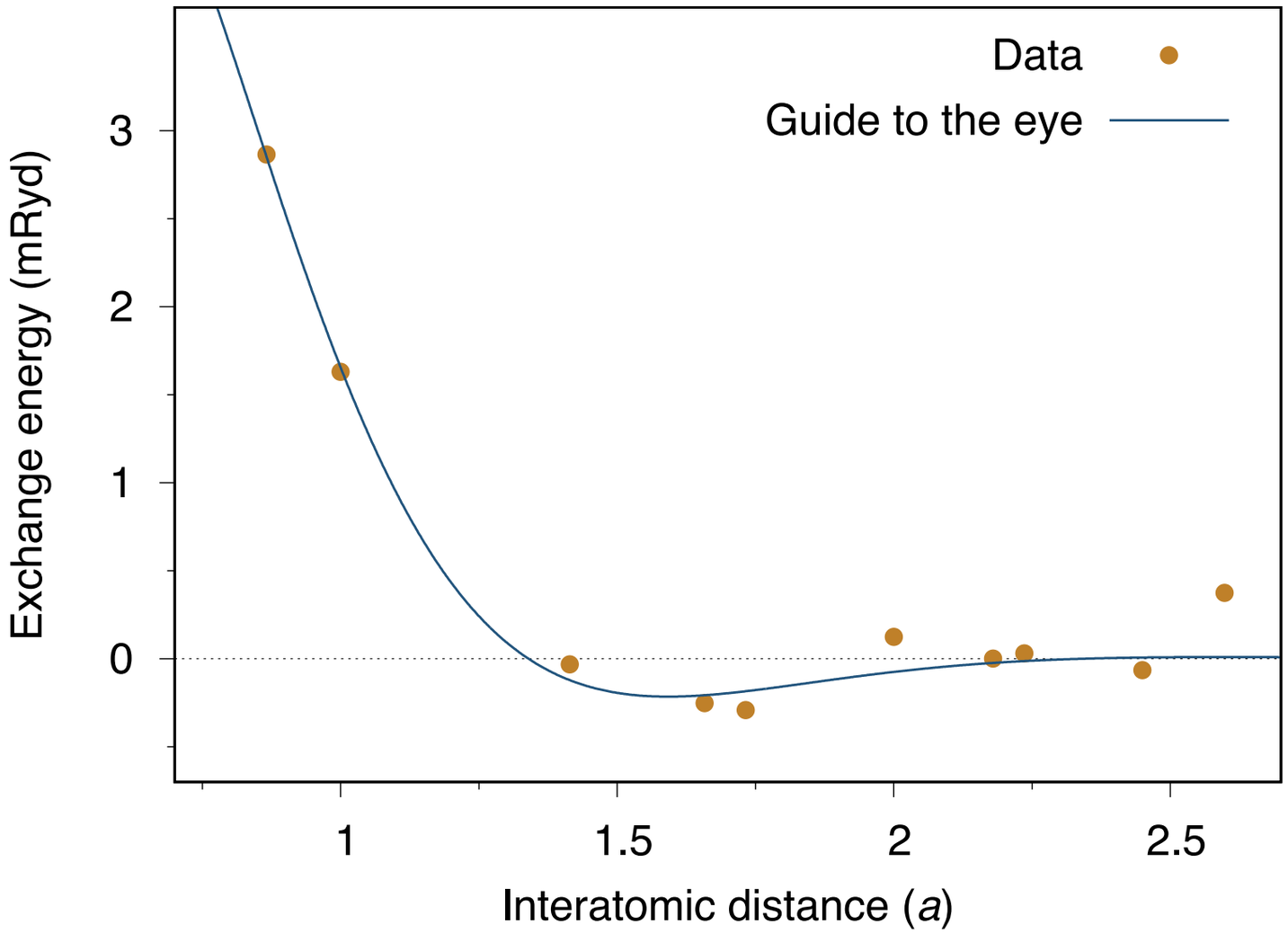
Ferromagnetism

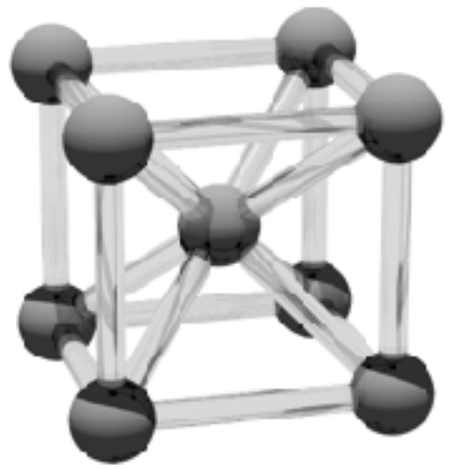
$J_{ij} < 0$



Antiferromagnetism

Heisenberg exchange: distance dependence





BCC Fe

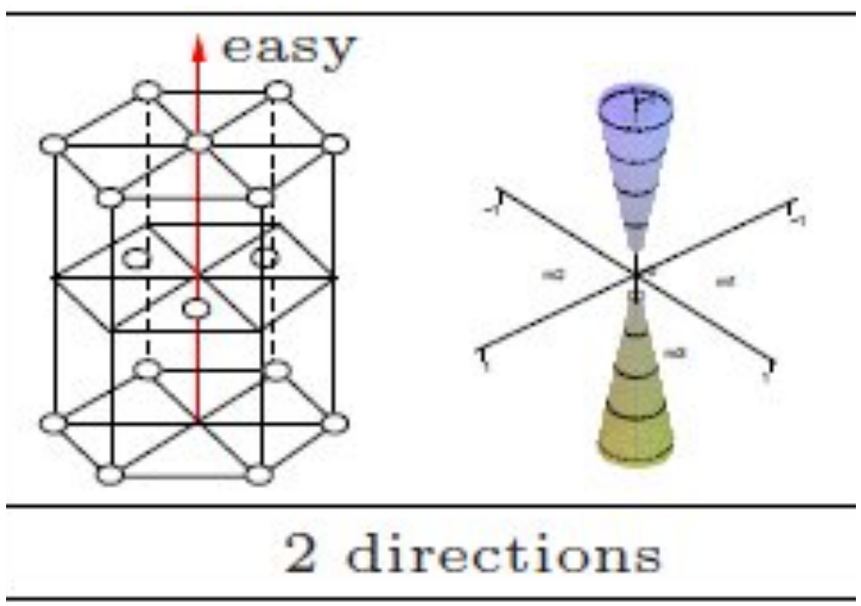
Due to the strong distance dependence of the exchange interaction, it is often truncated to include nearest neighbours only. This significantly reduces the computational effort while being a good approximation for many materials of interest.

Classical spin Hamiltonian: Uniaxial anisotropy

Magnetic anisotropy gives a preference for spins to point along particular crystal directions

The simplest form is uniaxial anisotropy, where the spins prefer to line along a single axis $\mathbf{e}$, where the energy is given by

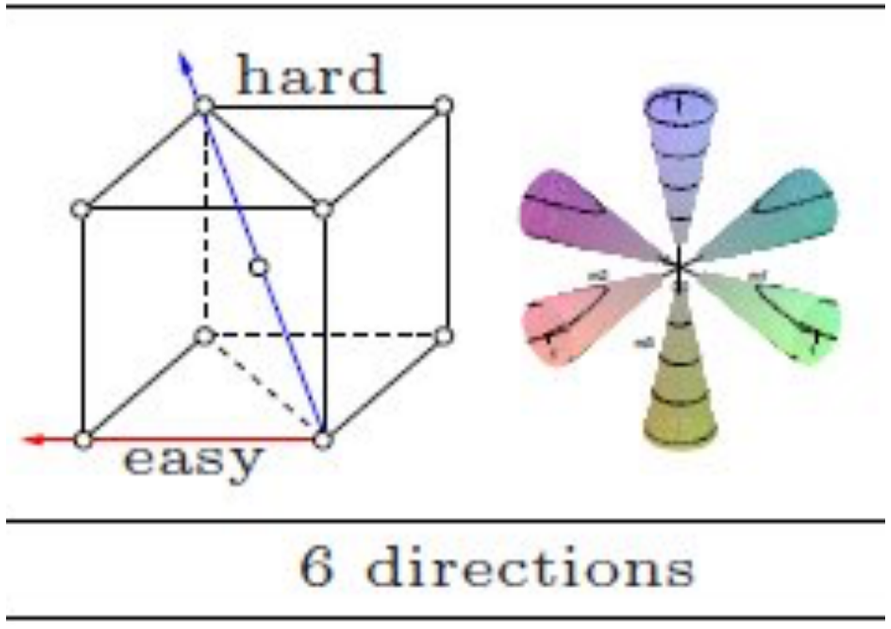
$$\mathscr{H}_{\text{ani}}^{\text{cub}} = -k_{\text{u}} \sum_i \left(\mathbf{S}_i \cdot \mathbf{e}_i\right)^2 = k_{\text{u}} \sum_i \sin^2\theta + \text{const}$$



Classical spin Hamiltonian: Cubic anisotropy

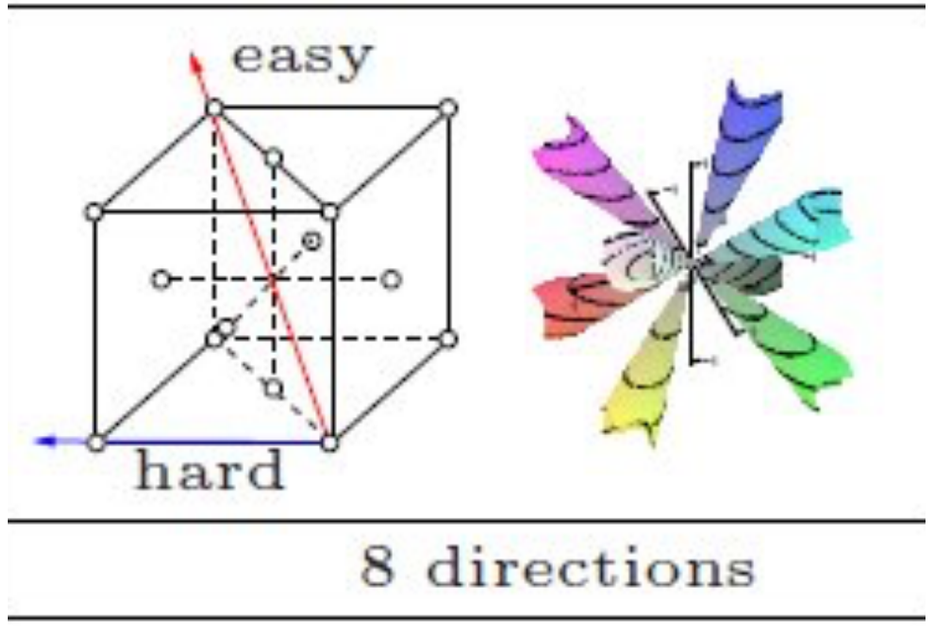
Most cubic crystals have cubic anisotropy where the spin prefers to align along particular crystal directions where the energy is given by

$$\mathscr{H}_{\text{ani}}^{\text{cub}} = \frac{k_{\text{c}}}{2} \sum_i S_x^4 + S_y^4 + S_z^4$$



6 directions

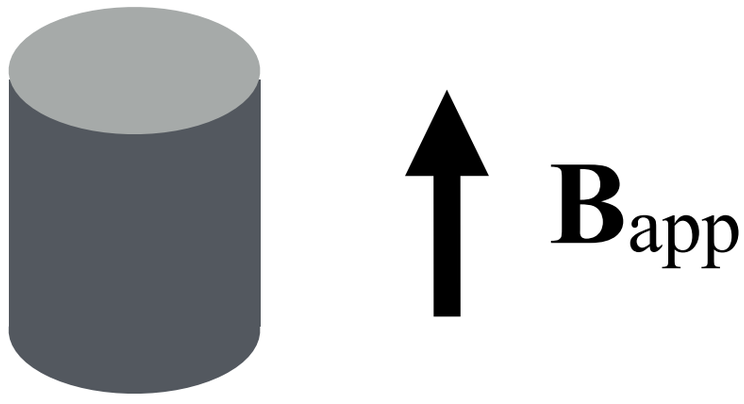
$k_{\text{c}} > 0$



8 directions

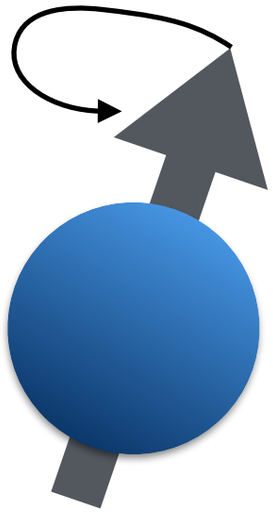
$k_{\text{c}} < 0$

Externally applied fields



$$\mathscr{H}_{\text{app}} = -\sum_i \mu_i \mathbf{S}_i \cdot \mathbf{B}_{\text{app}}$$

Integration methods



Monte Carlo methods for classical spin models

Monte Carlo methods for classical spin models

In classical spin models we can evolve the system thermodynamically using Monte Carlo Metropolis, computing the energy difference from the initial $\mathbf{S}_i$ and trial $\mathbf{S}_i'$ states

$$\Delta E = E\left(\mathbf{S}_i'\right) - E\left(\mathbf{S}_i\right)$$

where the move is then accepted with probability

$$P = \exp\left(-\frac{\Delta E}{k_{\mathrm{B}} T}\right)$$

The Monte Carlo algorithm needs to ensure detailed balance and ergodicity (all states are accessible), which can be achieved by the appropriate choice of trial move.

Random move

The most obvious choice of trial move is to pick a random direction in 3D space for the spin. These needs to be done in a way which does not bias any particular direction.

Picking three uniform random numbers along x,y,z and normalising introduces a bias into the number of vectors generated along the cube edges

Sampling with a Normal distribution $\Gamma_{x,y,z}$ in the same way ensures a uniform distribution on a random sphere.

$$\Gamma_\alpha = \mathbb{R} \in \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{\alpha-\mu}{\sigma}^2\right)}$$

$$\alpha = x, y, z$$

Although correct, the random method has the disadvantage that most trial moves will be rejected at low temperatures, and so this is not a very efficient algorithm.

$$\mathbf{S}' = \frac{\mathbf{\Gamma}}{|\mathbf{\Gamma}|} = \frac{\mathbf{\Gamma}}{\sqrt{\Gamma_x^2 + \Gamma_y^2 + \Gamma_z^2}}$$

Gaussian random move

At low temperatures, spin moves near the current direction are likely to be favourable

We can modify the new spin position to be close by adding a small shift to the existing spin direction using the same method as random sampling and normalising the resulting spin length

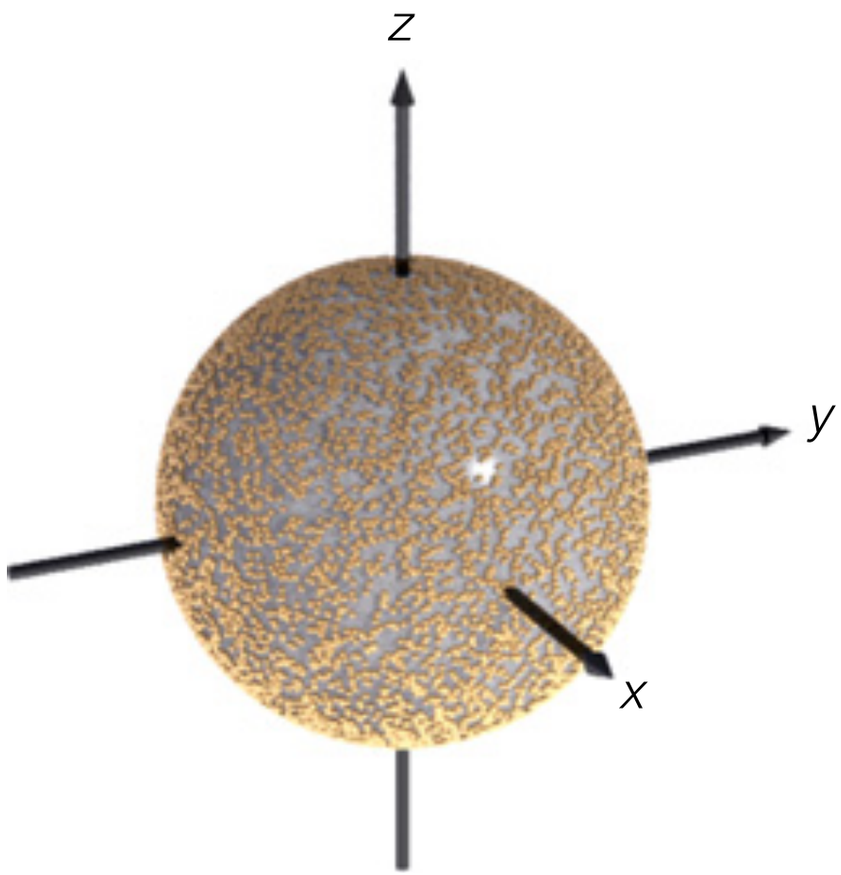
$$\mathbf{S}_i' = \frac{\mathbf{S}_i + \sigma_G \mathbf{\Gamma}}{|\mathbf{S}_i + \sigma_G \mathbf{\Gamma}|}$$

†Hinzke D and Nowak U *Comput. Phys. Commun.* 121 334 (1999)

Sampling

A plot of the sampling for uniform and Gaussian moves shows the distributed trial moves with respect to the starting spin direction along z

a



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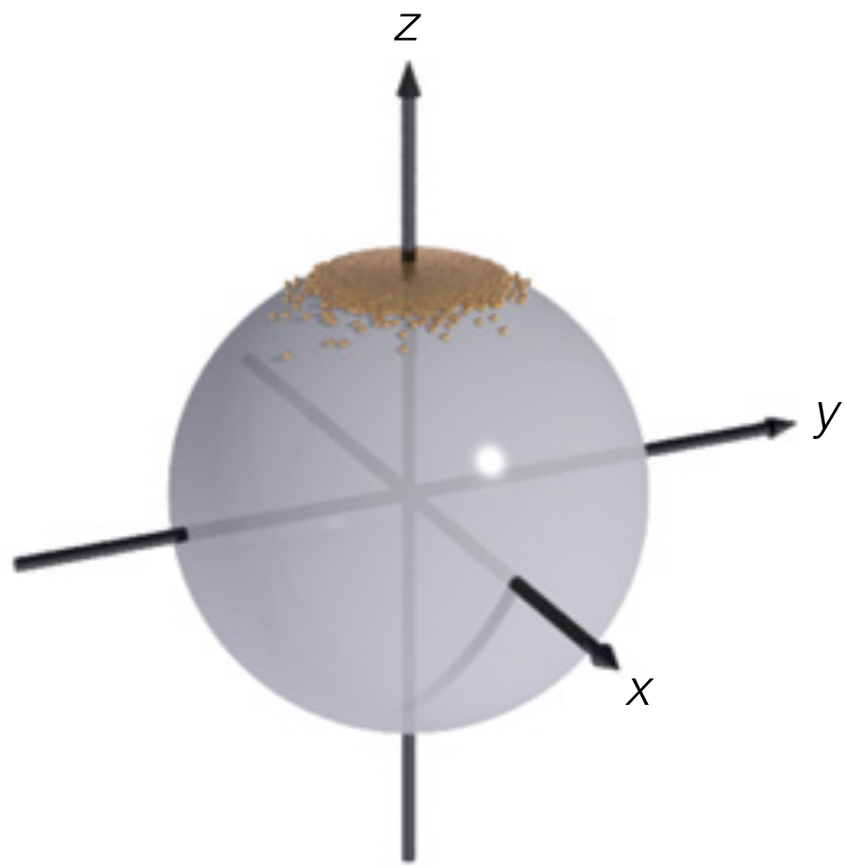


Adaptive moves

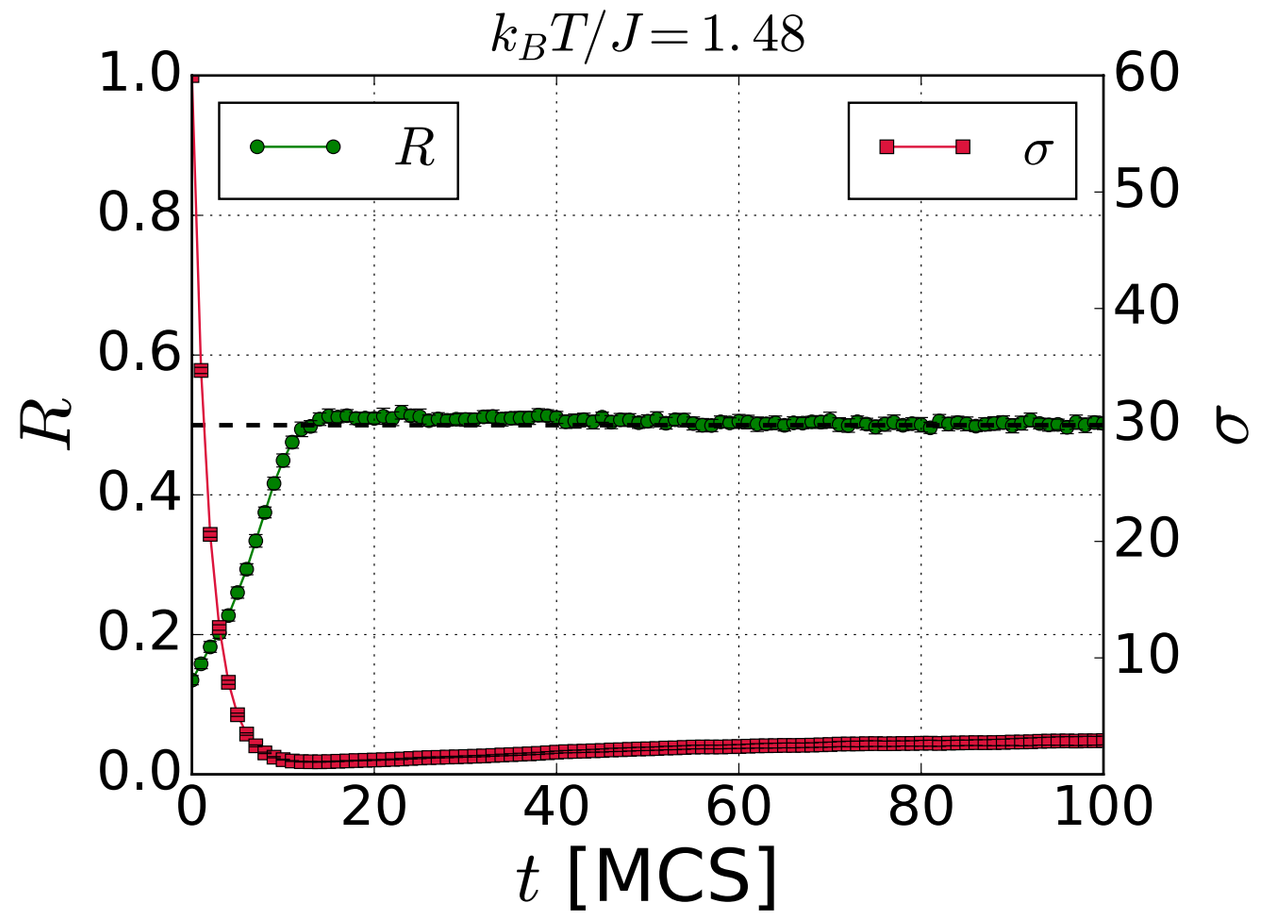
While efficient at moderate temperatures, the Hinzke-Nowak method suffers from poor acceptance at low temperatures

One possible solution is an adaptive algorithm, based on a modified Gaussian move, that aims to maintain an acceptance rate of 0.5

The Gaussian width is dynamically adapted according to

$$f = \frac{0.5}{1 - R}$$

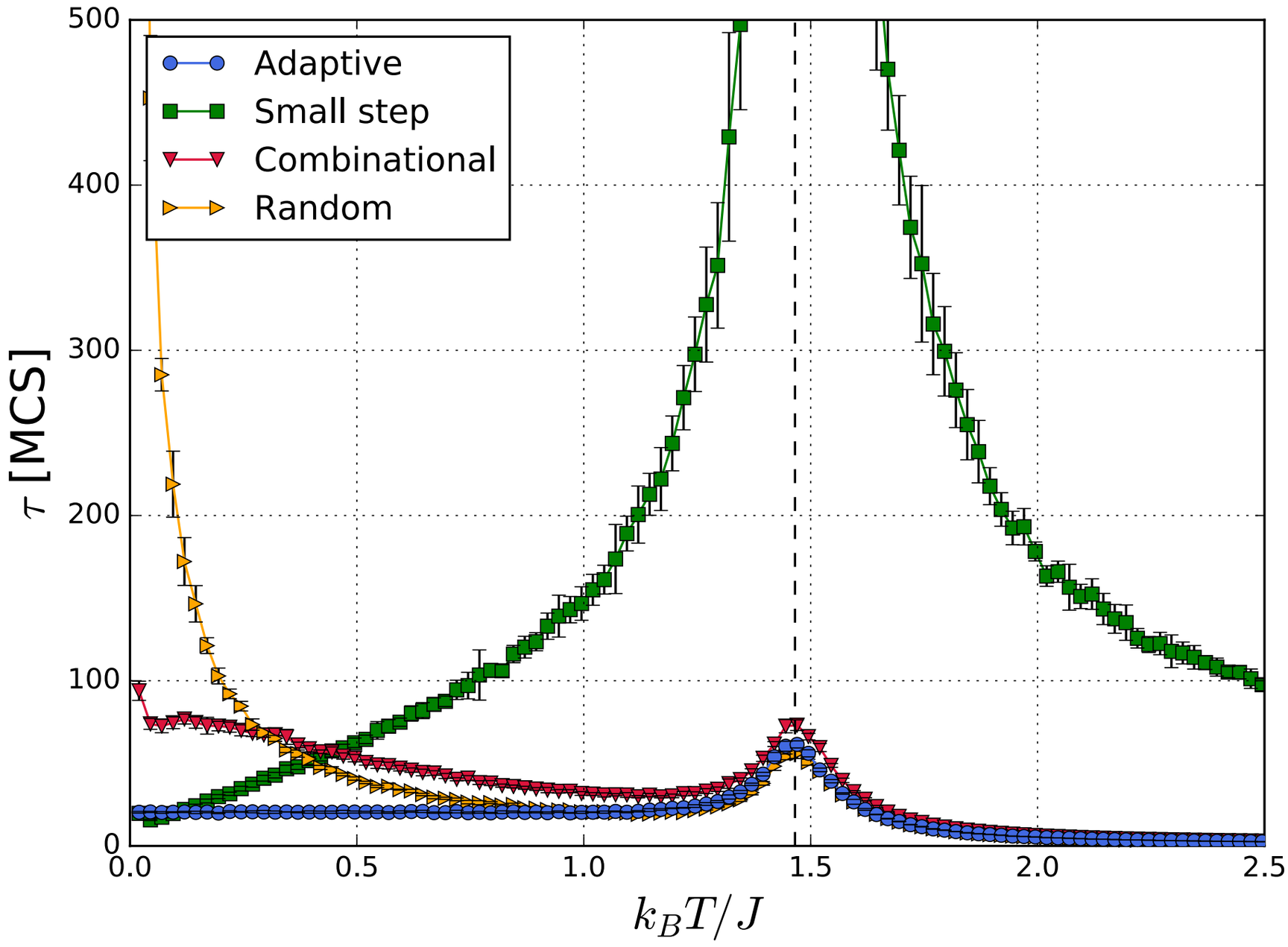
Where R is the acceptance rate and f is a multiplying factor applied to the width σ. If R=0.5, then the multiplying factor is 1 to maintain the same acceptance rate



J D Alzate-Cardona *et al J. Phys.: Condens. Matter* **31** 095802 (2019)

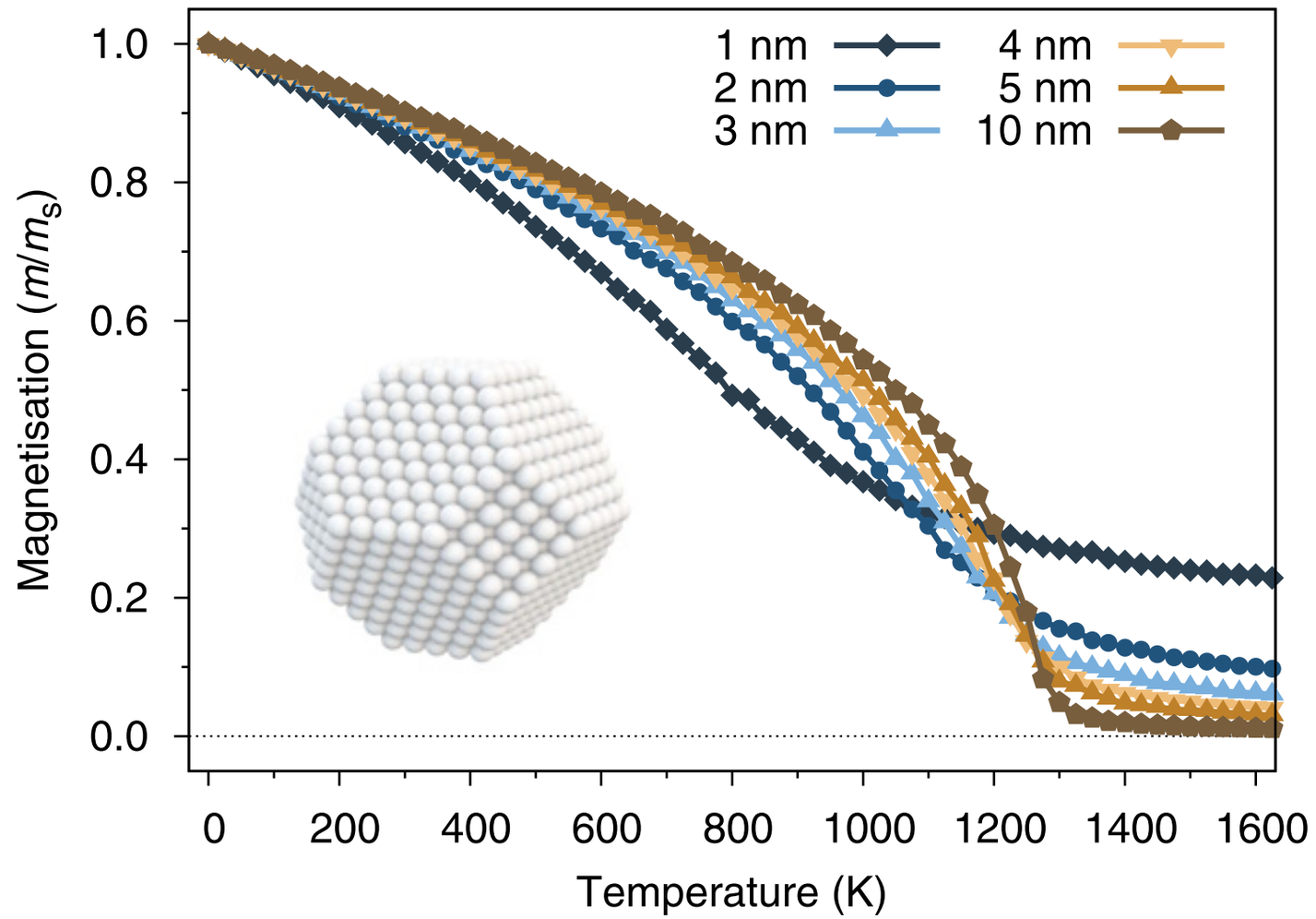
Comparison of algorithms

Compute the time for each algorithm to reach thermal equilibrium magnetization as a function of temperature



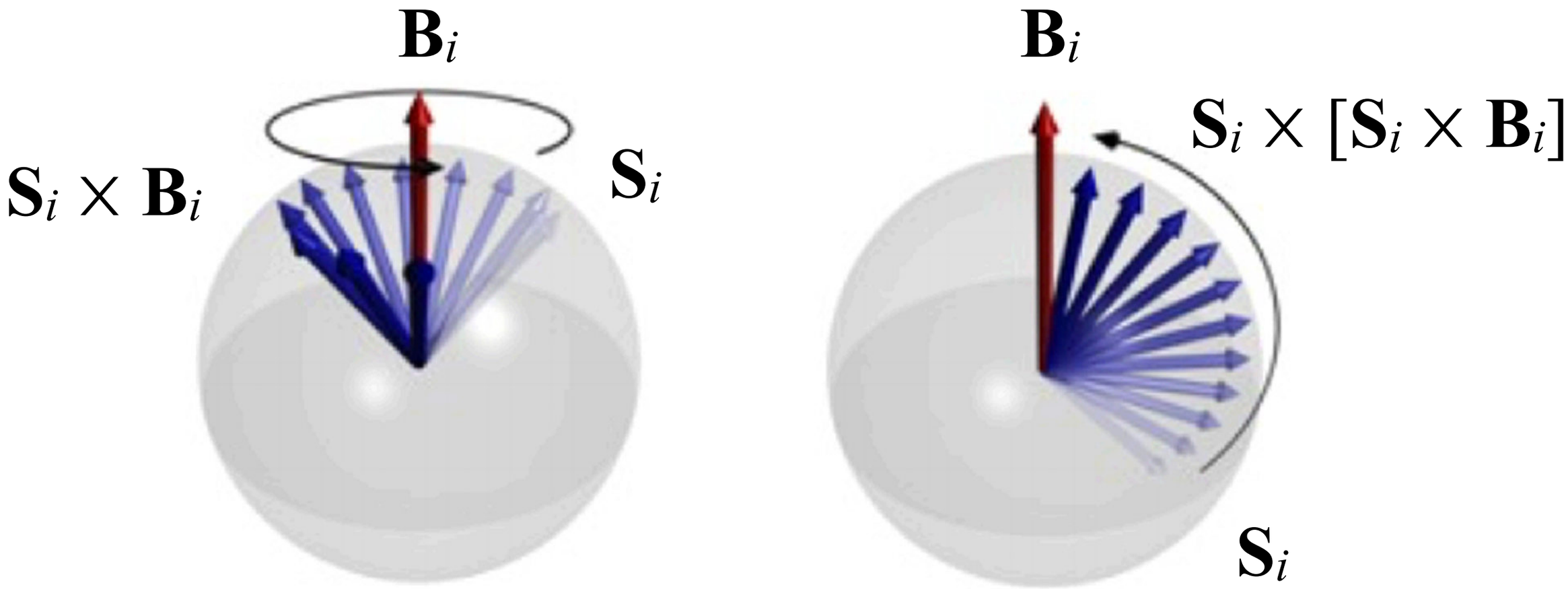
Temperature dependent magnetization for different particle sizes

- 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



Atomistic spin dynamics

Landau Lifshitz Gilbert (LLG) equation



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

Magnetic field (equivalent to the force)

As with molecular dynamics, the magnetic field presses the forces on the local magnetic moments, and comes from the negative derivative of the spin Hamiltonian with respect to the local spin moment $\mathbf{S}_i$

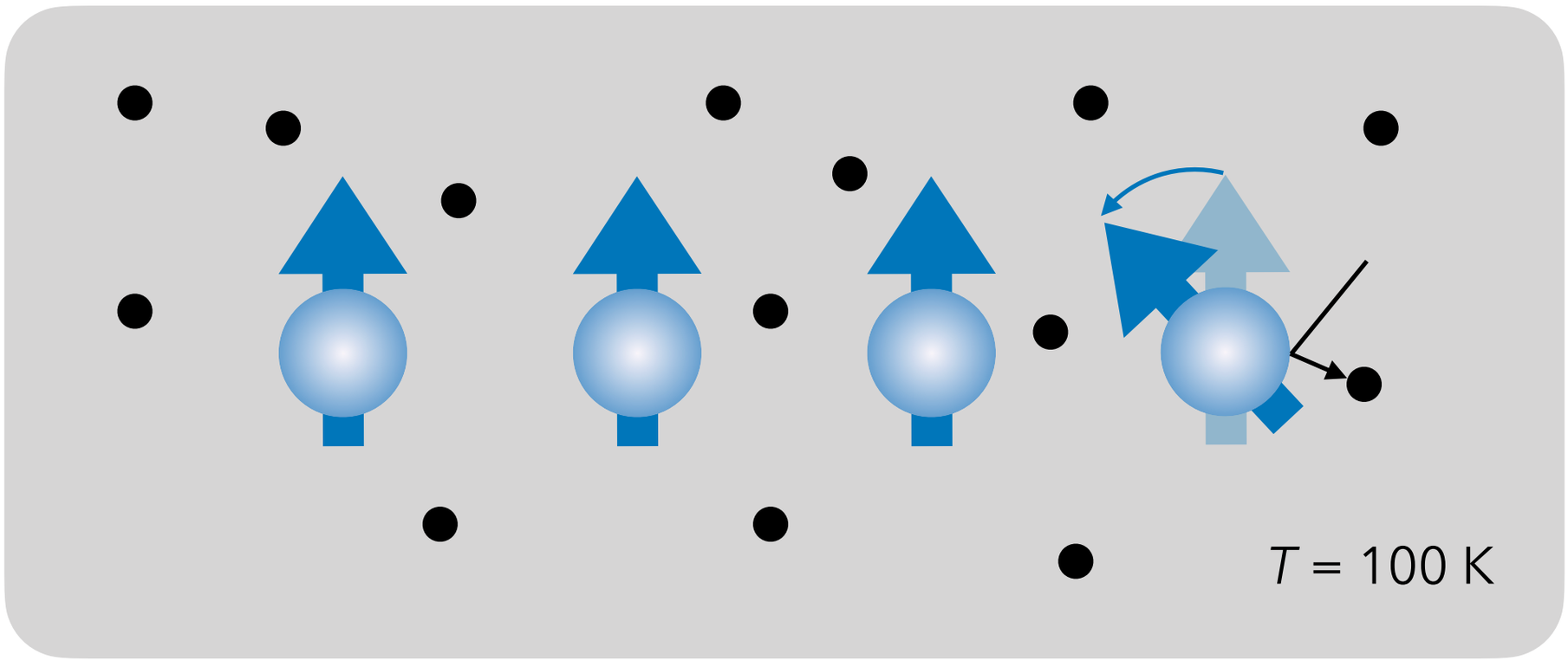
$$\mathbf{B}_i = -\frac{1}{\mu_i}\frac{\partial \mathscr{H}}{\partial \mathbf{S}_i}$$

Here the magnetic spin moment μ_i acts in a similar manner to the mass in a molecular dynamics simulation - the larger the moment the slower the dynamics

Langevin Dynamics for spin models

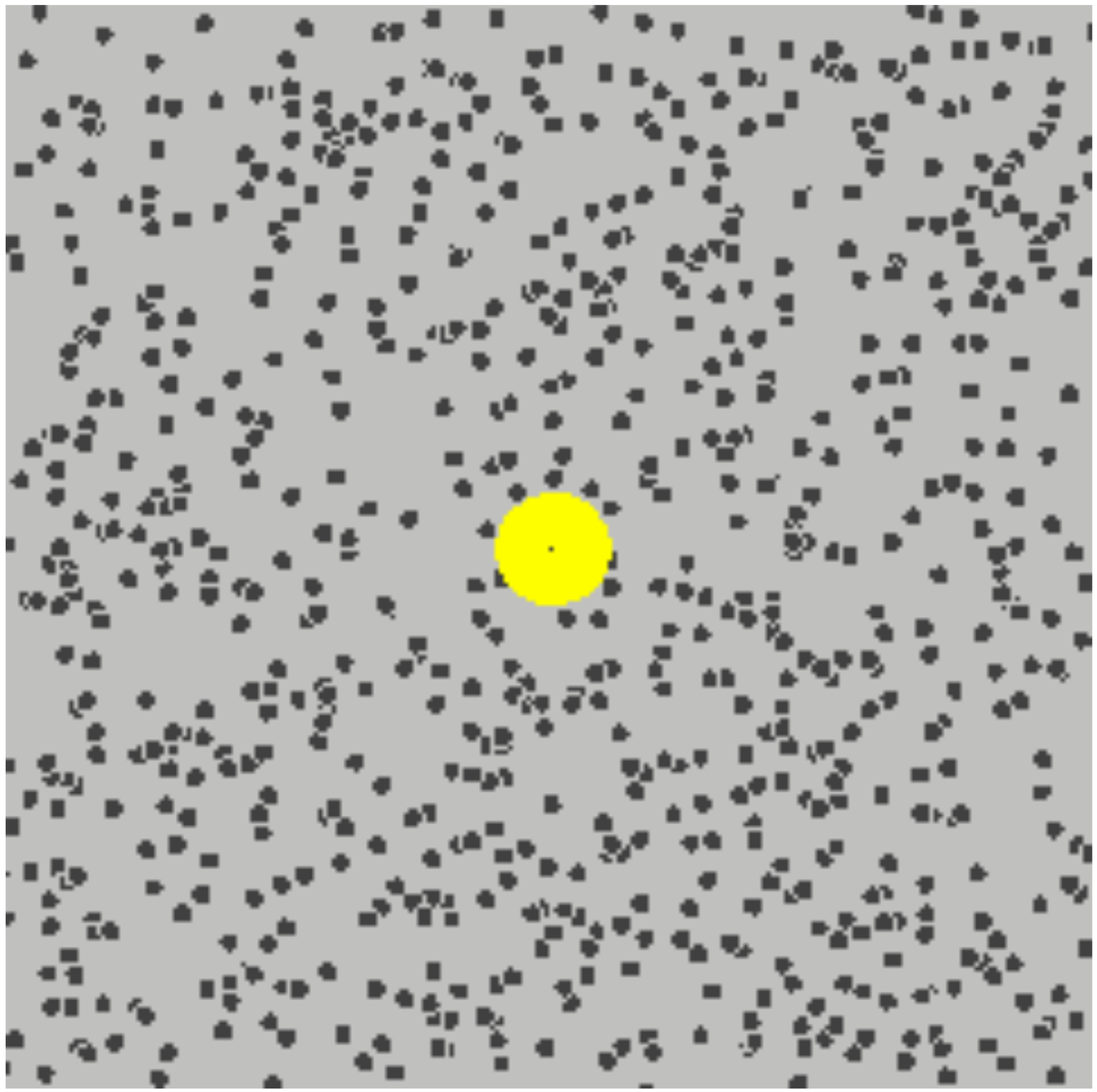
So far the dynamics of the spins in the LLG equation are deterministic

Need a way to simulate the effects of thermal fluctuations of the spins: a heat bath



Langevin thermostat

The Langevin thermostat assumes the spins are embedded in a medium of particles (photons, electrons, phonons) which emulate Brownian motion



Langevin Dynamics

The LLG equation is dissipative - it removes energy from the system via the second relaxation term

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

We can add “fluctuations” to represent the effects of the heat bath

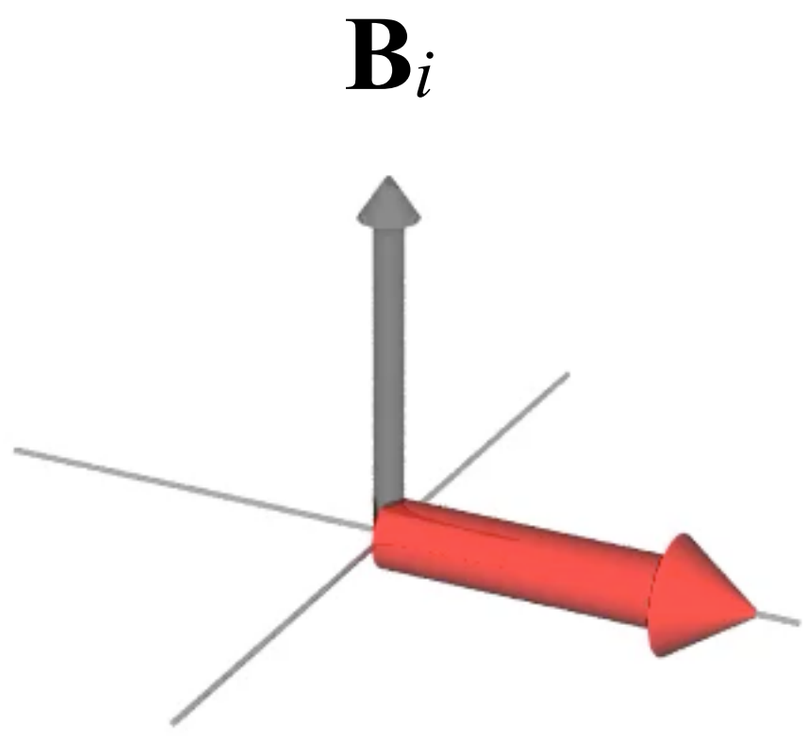
The fluctuation and dissipation terms must balance in thermal equilibrium and can be formally proven by solving the Fokker-Plank equation using the fluctuation-dissipation theorem (balance of terms)

Stochastic Landau-Lifshitz-Gilbert equation

Thermal effects are modelled with Langevin Dynamics, where the system is embedded in a heat bath and random thermal motions arise from collisions with microscopic particles (electrons) in the bath

Effective field

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



Statistical properties of the noise

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

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

No spatial correlation δ_{ij}

No time correlation δ_{ab}

Mean fluctuation over time is zero

VAMPIRE

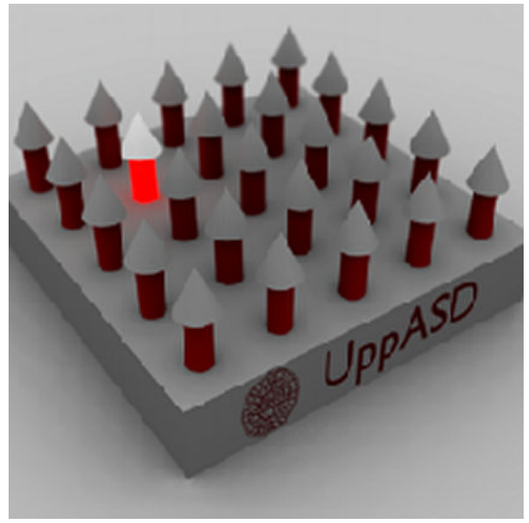
vampire.york.ac.uk

Review article

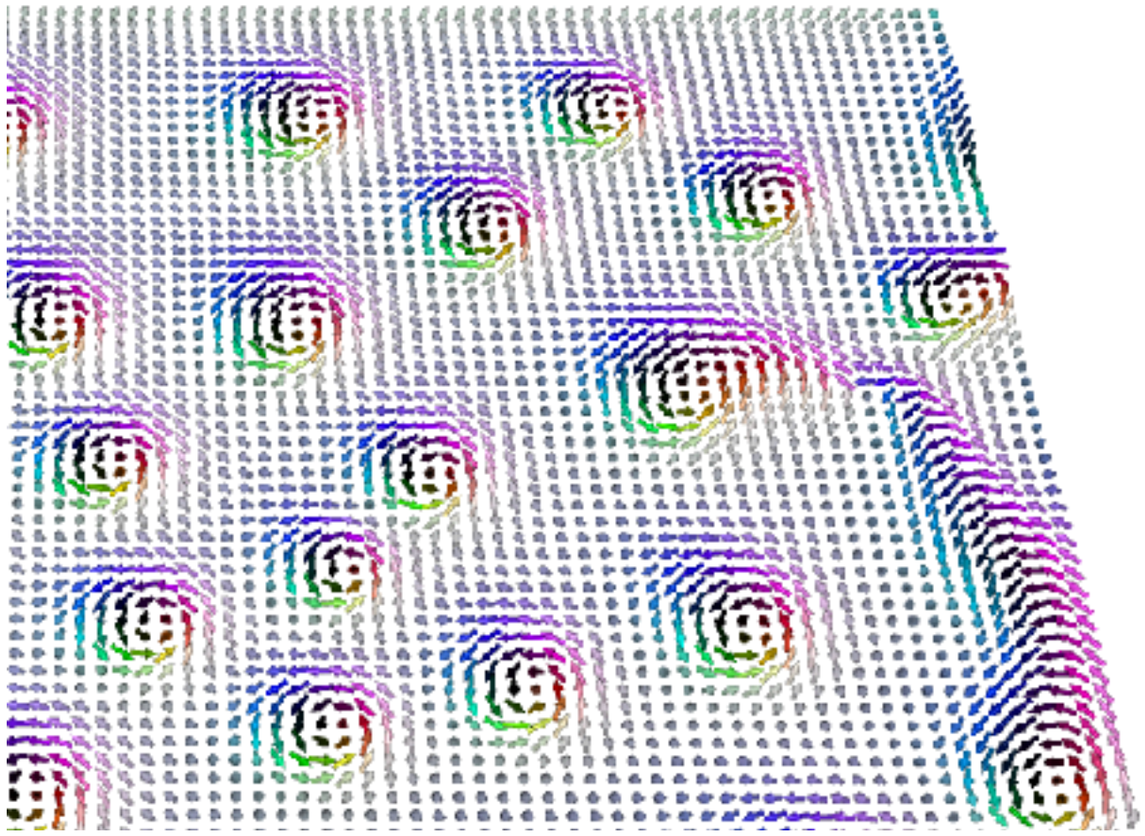
R F L Evans *et al*, J. Phys.: Condens. Matter 26 (2014) 103202

Other codes for atomistic simulations

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

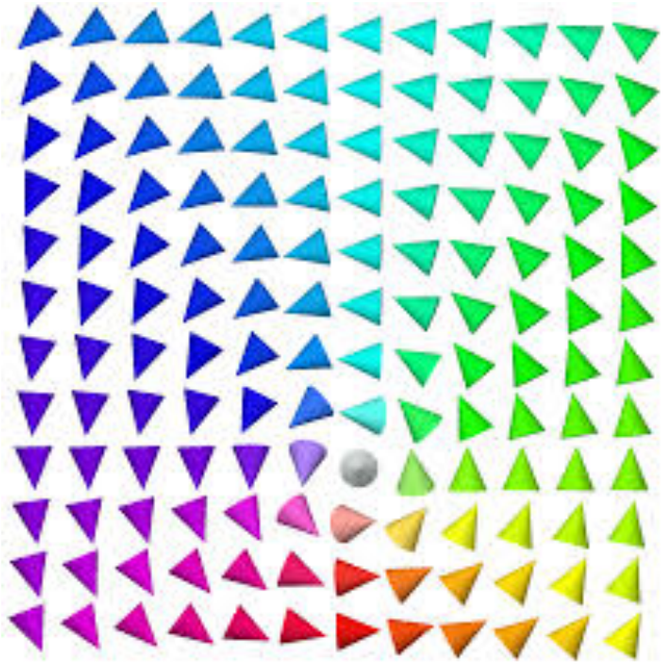


- SPIRIT - online interactive tool https://spirit-code.github.io



Summary

- Covered the essential elements of micromagnetic simulations and their formulation

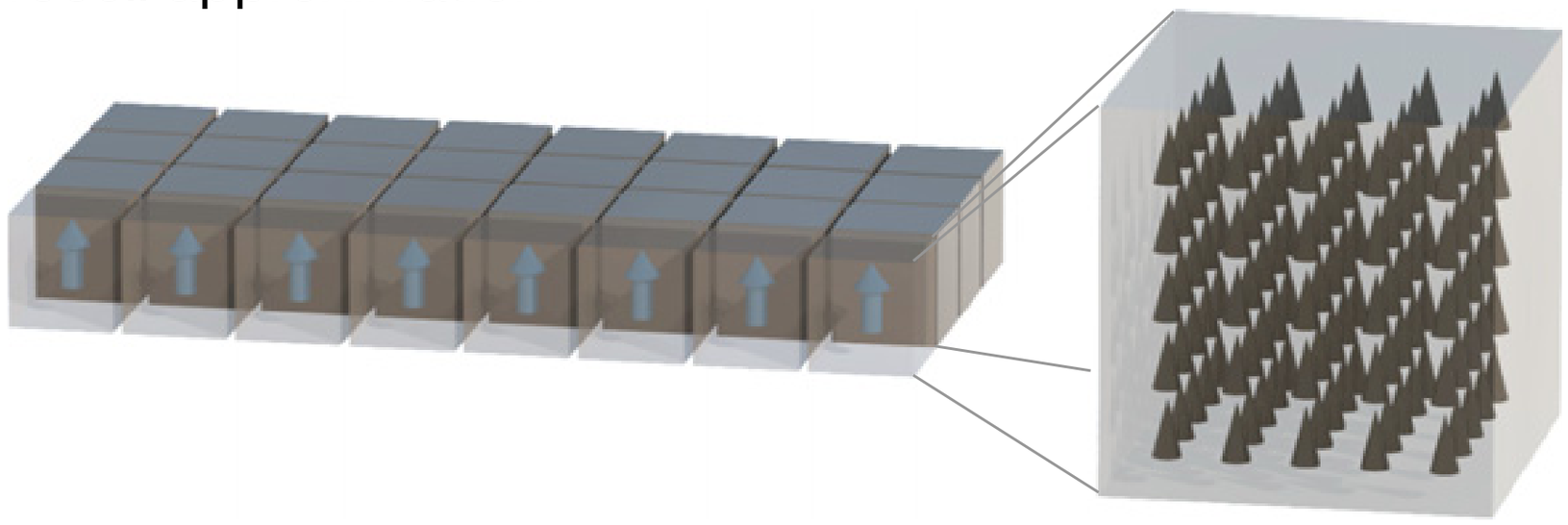


- Introduced atomistic spin models, their fundamentals

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