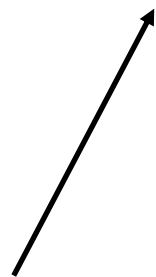


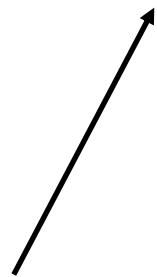
# Dipole Fields

# The Spin Hamiltonian

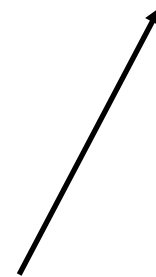
$$\mathcal{H} = \mathcal{H}_{exc} + \mathcal{H}_{ani} + \mathcal{H}_{app} + \mathcal{H}_{dip}$$



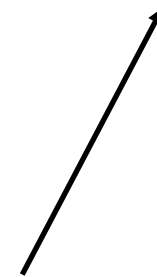
Exchange



Anisotropy

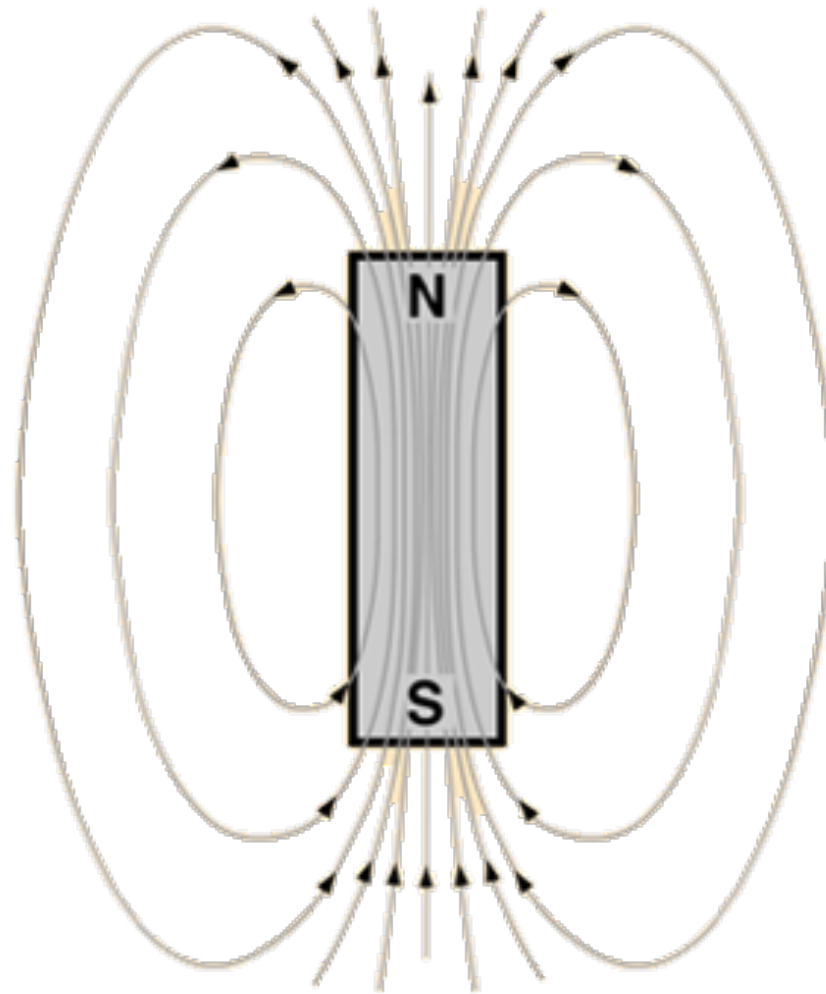


Applied field



Dipole

# The Dipole field



# The demagnetising field

$$\mathbf{H} = -\mathbf{N} \cdot \mathbf{m}$$

↓                      ↓                      ↓  
Vector                      Tensor                      Vector

$$\mathbf{H}_{\text{demag}}^{\text{mc},p} = \frac{\mu_0}{4\pi} \left( \sum_{p \neq q} \frac{3(\mathbf{m}_{\text{mc}}^q \cdot \hat{\mathbf{r}})\hat{\mathbf{r}} - \mathbf{m}_{\text{mc}}^q}{r^3} \right) - \frac{\mu_0}{3} \frac{\mathbf{m}_{\text{mc}}^p}{V_{\text{mc}}^p}$$

$$\mathbf{H}_{\text{demag}}^{\text{mc},p} = \frac{\mu_0}{4\pi} \left( \sum_{p \neq q} \mathbf{M}_{pq} \cdot \mathbf{m}_{\text{mc}}^q \right) - \frac{\mu_0}{3} \frac{\mathbf{m}_{\text{mc}}^p}{V_{\text{mc}}^p}.$$

The self interaction term

The term due to the other dipoles

$$\mathbf{M}_{pq} = \begin{bmatrix} (3r_x r_x - 1)/r_{pq}^3 - 1/3 & 3r_x r_y & 3r_x r_z \\ 3r_x r_y & (3r_y r_y - 1)/r_{pq}^3 - 1/3 & 3r_y r_z \\ 3r_x r_z & 3r_y r_z & (3r_z r_z - 1)/r_{pq}^3 - 1/3 \end{bmatrix}$$

# Problems?

- The dipole fields are proportional to  $r^3$ .
- Whereas in general the exchange dies off exponentially.
- The dipole fields are far longer range. Cant be cut off, still significant a couple of hundred nm away.
- Calculations of dipole fields are very computationally expensive.

# Dipole field calculations

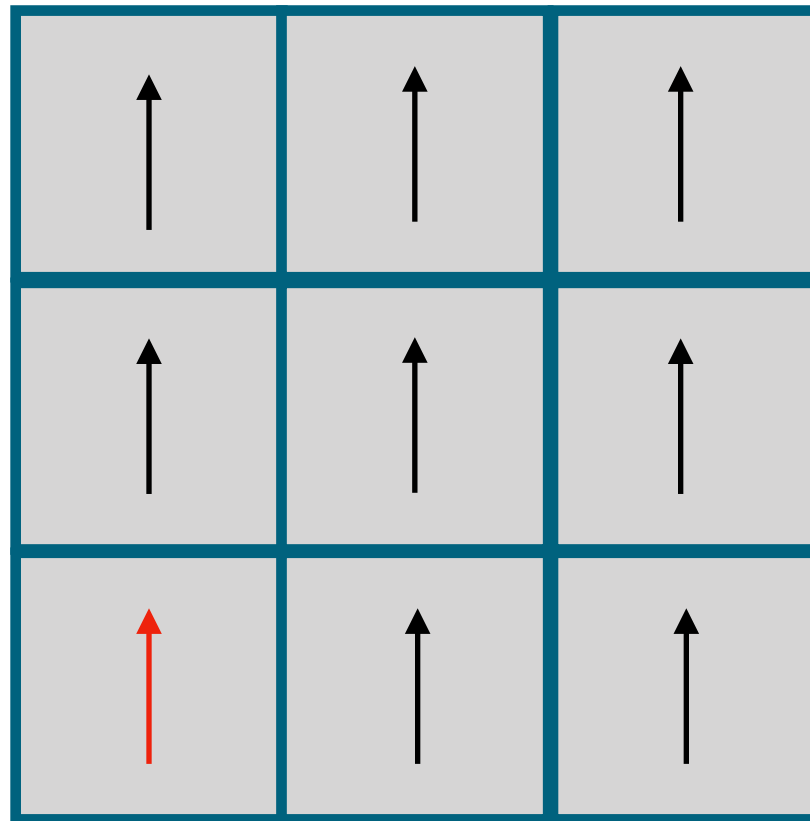
- **Atomistic** - slow but accurate.
- **Macrocell** - fast but inaccurate.
- **Tensor** - fast and more accurate.
- **Hierarchical** - even faster and more accurate.
- **FFT**- maybe even faster but slightly inaccurate.

# Atomistic

- Calculated between every atom in the system - scales as  $N(N-1)$ . Where  $N$  = number of atoms.
- Very slow! Impossible for systems larger than a couple of nm.
- Very accurate calculation - good for complex magnetic structures such as domain walls, AFM's



# Bare macrocell approach



# Bare macrocell approach

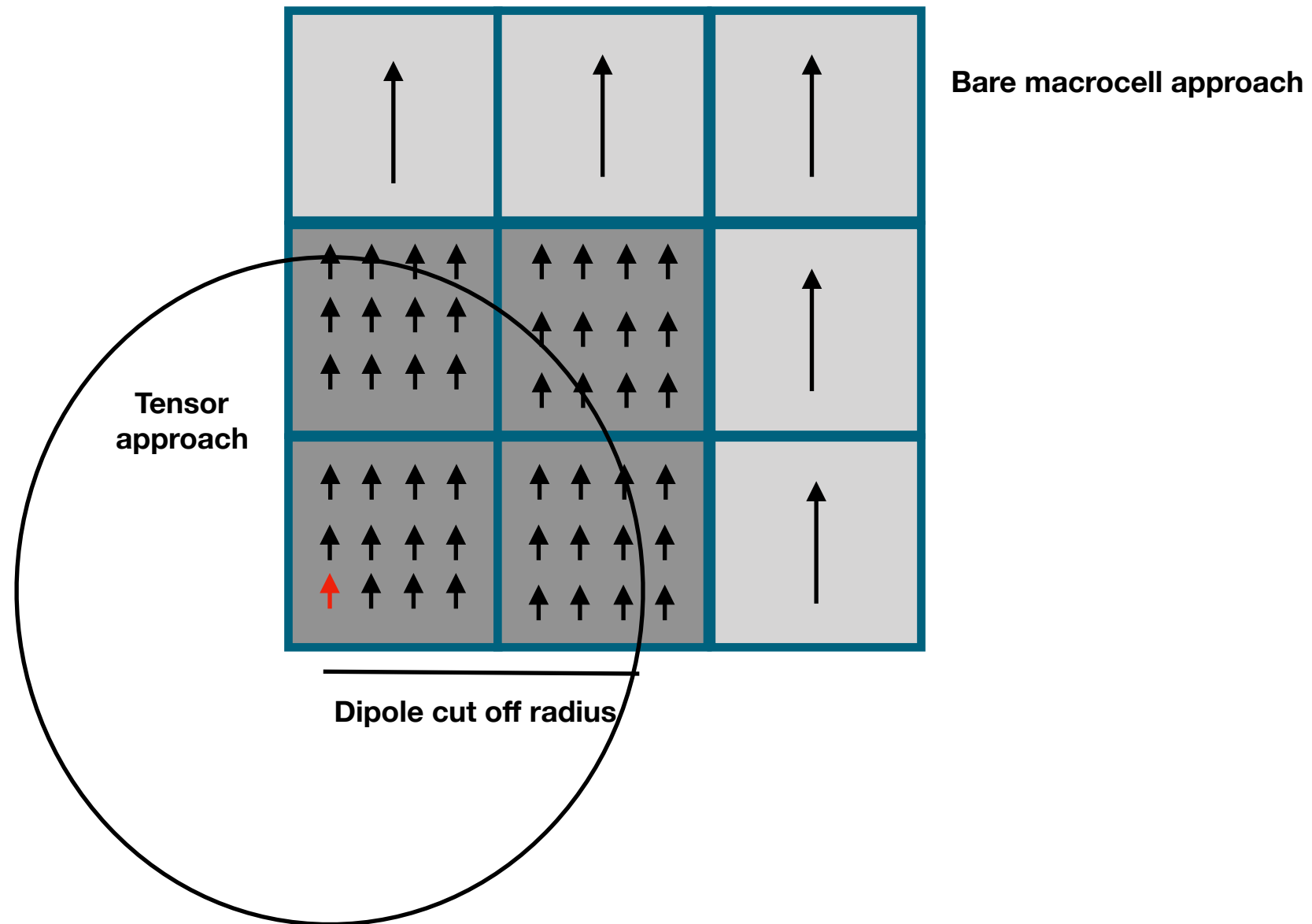
- The system is divided into cubic macro-cells
- Each cell is supposed to have uniform magnetisation
- The dipolar interaction is calculated between macro-cells considering for each one a pairwise summation.
- A self-demagnetisation term is added, to include the internal field of the macro-cell.

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

# Bare macrocell approach

- Often the magnetisation inside a block is not fully aligned.
- Still scales  $N(N-1)$  - here  $N$  is the number of macrocells.  
This can be slow.
-

# Inter-intra dipole approach



# 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)

$$\begin{aligned}
 \mathbf{B}^{\text{dip}} &= \mathbf{B}_q^{\text{dip}} + \mathbf{B}_p^{\text{dip}} + \mathbf{B}_p^{\text{self}} \\
 &= \underbrace{\mathbf{D}_{qp}^{\text{inter}} \vec{m}_p}_{\text{INTER}} + \underbrace{\mathbf{D}_{pp}^{\text{intra}} \vec{m}_p + \frac{8\pi}{3} \vec{m}_p / V_p}_{\text{INTRA}}
 \end{aligned}$$

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

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

Interaction between moments inside cell p (atomistic)

# Inter-intra dipole approach

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  $\sim 2$  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.

# Hands on

- Create a thin film of permalloy.
- This is an alloy of Ni and Iron.  $\sim 20\text{nm} \times 20\text{nm} \times 1\text{nm}$

(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



- Run a time-series to see what the magnetisation does over time if started in a random configuration.

Change the simulation to a time series

```
Sim:program=time-series
```

Set the simulation parameters

```
sim:temperature = 0.0  
sim:time-steps-increment = 1000  
sim:total-time-steps = 1000000  
sim:time-step = 1 !fs
```

Set the starting spin directions to be random

```
material[1]:initial-spin-direction = random
```

# Dipole calculations for an elongated cylinder!

- Again run a time series for permalloy. But now instead of a plane run an elongated sphere.
- What should happen to the magnetisation?

```
dimensions:system-size-x = 2 !nm  
dimensions:system-size-y = 2 !nm  
dimensions:system-size-z = 8 !nm
```

```
create:cylinder  
dimensions:particle-size = 4 !nm  
dimensions:particle-shape-factor-x = 0.5  
dimensions:particle-shape-factor-y = 0.5  
dimensions:particle-shape-factor-z = 2
```

# Now add in the dipole fields!

Include a cell size for the macrocell sections

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

Choose your dipole parameters

```
dipole:solver=tensor/macrocell
```

```
dipole:field-update-rate=100
```

```
dipole:cutoff-radius=2 - this is in cell sizes
```

**Task: Compare the different  
dipole solvers**

# Future dipole field calculations

$$\mathbf{H} = -\mathbf{N} \cdot \mathbf{m}$$

$$\mathcal{F}(H) = -\mathcal{F}(N)\mathcal{F}(m)$$

$$H = -\mathcal{F}_{inv}(\mathcal{F}(N)\mathcal{F}(m))$$

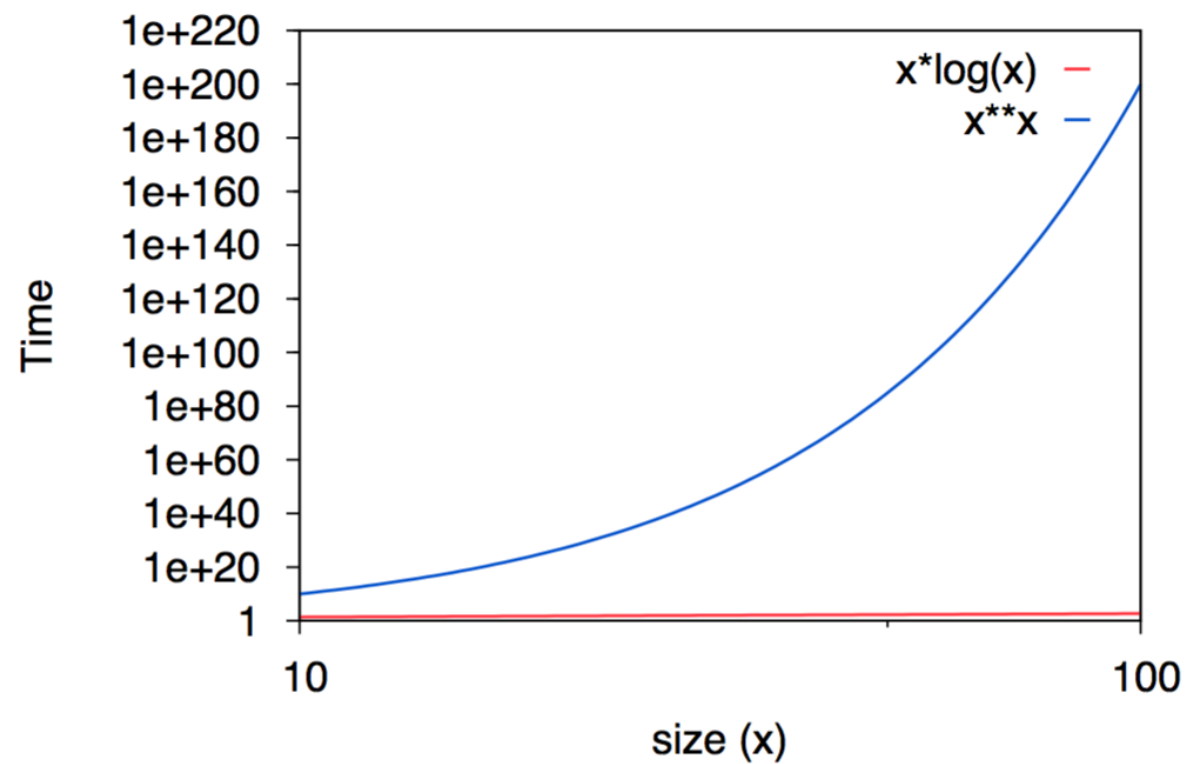


Only needs to be calculated once.

- Assumes the crystal structure is spatially invariant.
- This is true because we split the system into cubic cells.

# FFT

Old	$N^N$
FFT	$N \log(N)$



- Predicted speed increase

# Hierarchical

