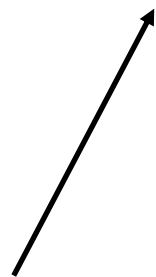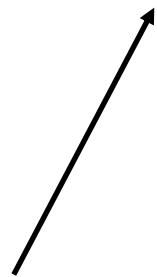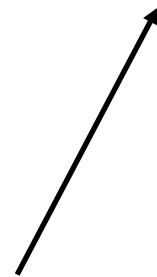# Dipole Fields

The Spin Hamiltonian

$$\mathcal{H} = \mathcal{H}_{exc} + \mathcal{H}_{ani} + \mathcal{H}_{app} + \mathcal{H}_{dip}$$
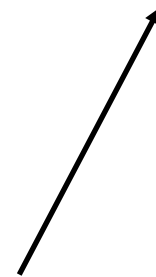
Exchange   Anisotropy   Applied field   Dipole
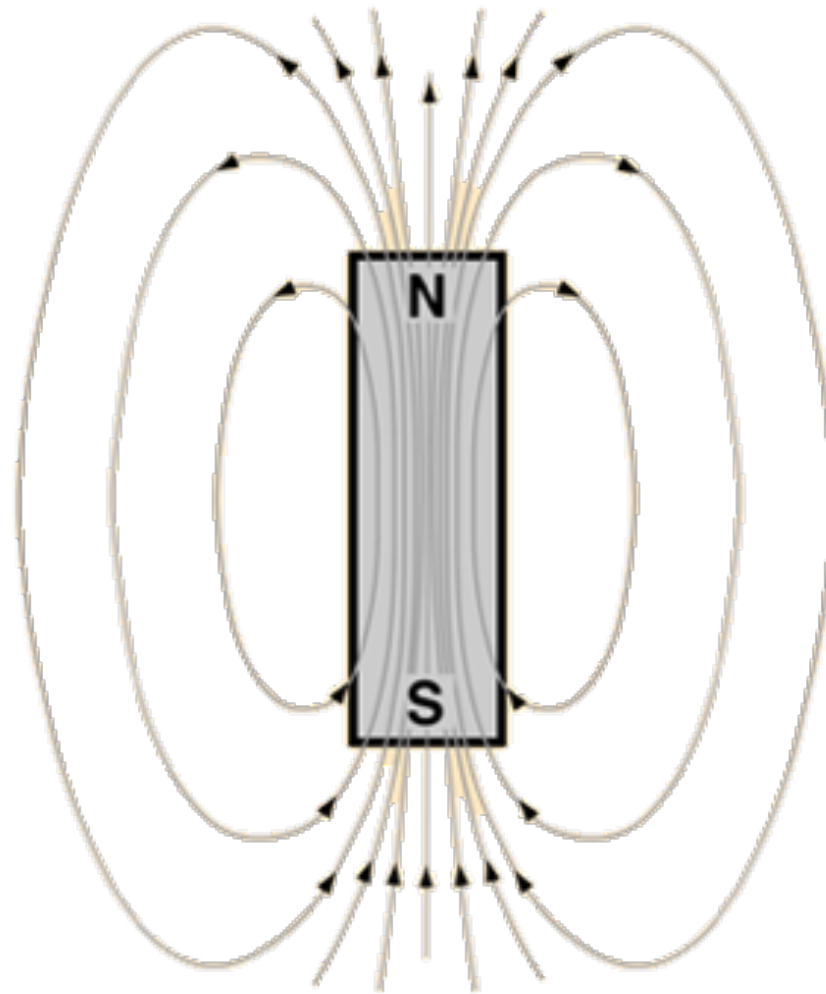
The Dipole field

The demagnetising field

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

Vector   Vector

Tensor

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

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

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^2. 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
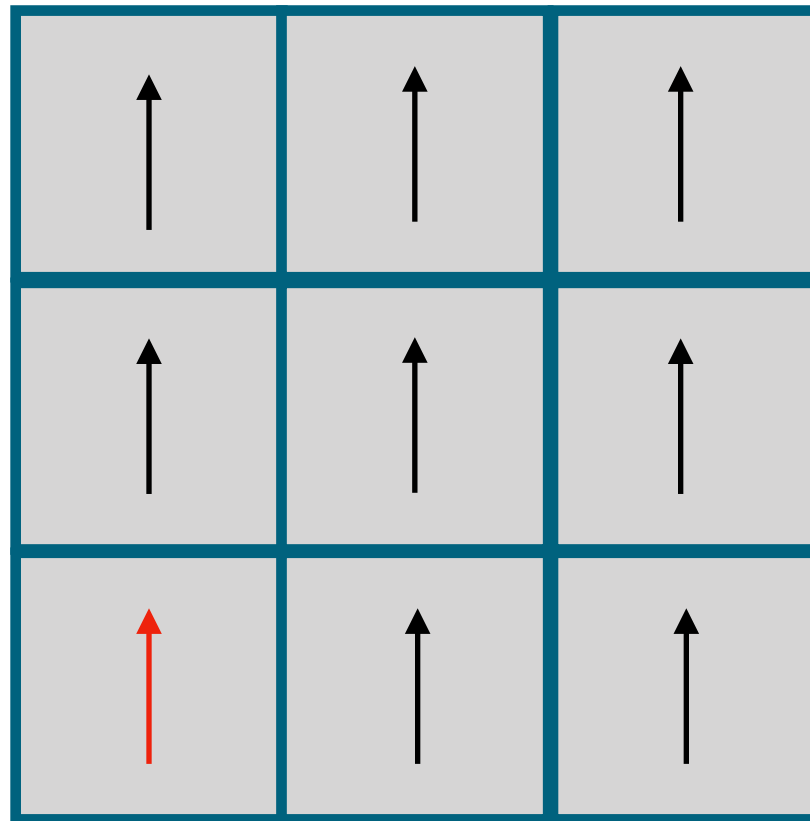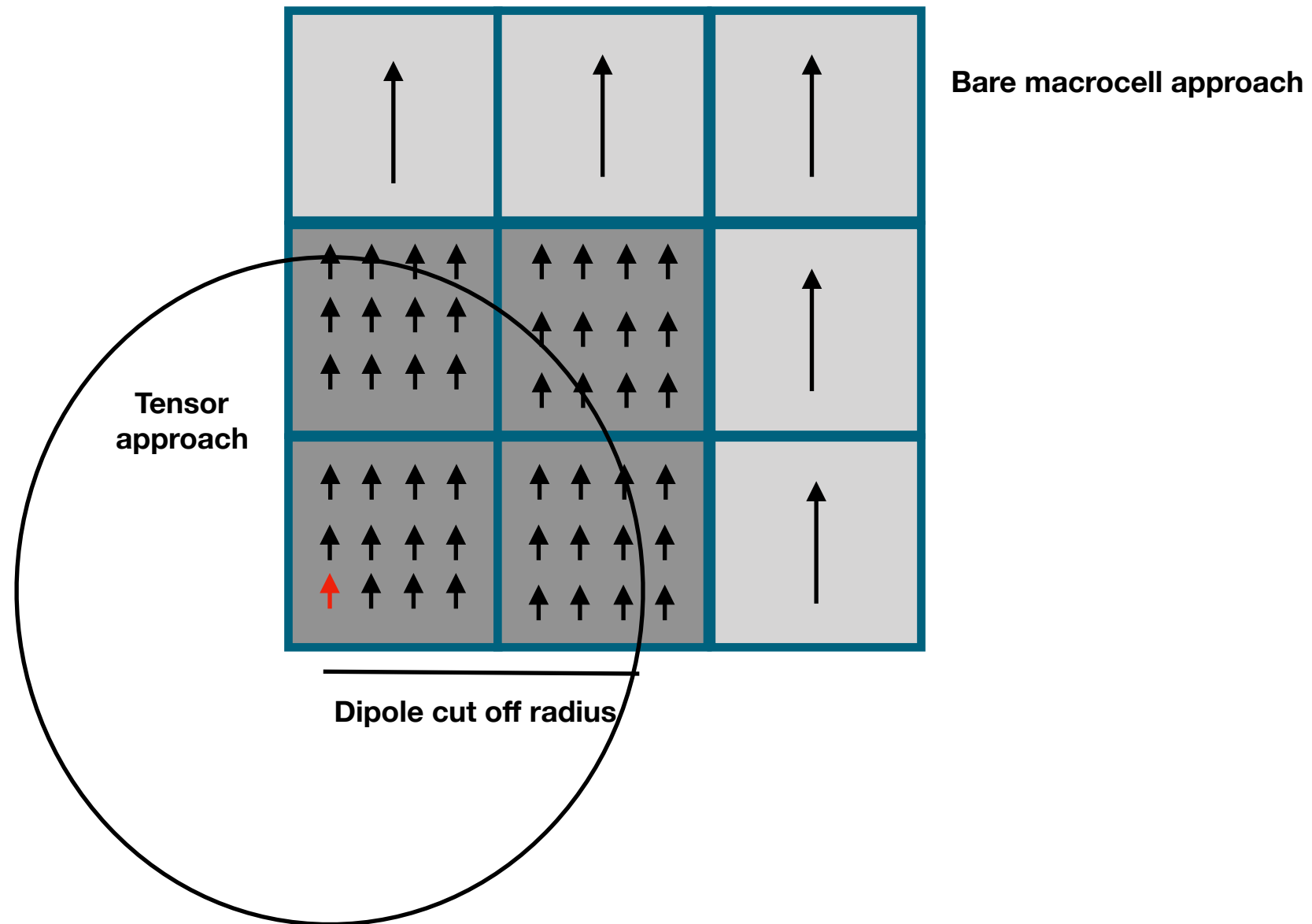
Bare macrocell approach

- 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.

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

Bare macrocell approach

- Often the magnetisation inside a block is not fully aligned.

- Still scales N^2 - here N is the number of macrocells. This can be slow.

-

Inter-intra dipole approach

Bare macrocell approach

Tensor
approach

Dipole cut off radius

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)

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

$$= D_{qp}^{inter}\vec{m}_p + D_{pp}^{intra}\vec{m}_p + \frac{8\pi}{3}\vec{m}_p/V_p$$

INTER   INTRA

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

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:

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

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

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.

Hands on

- Create a thin film of permalloy.

- This is an alloy of Ni and Iron. ~ 20nm*20nm*1nm

(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

- 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]:intial-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

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

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

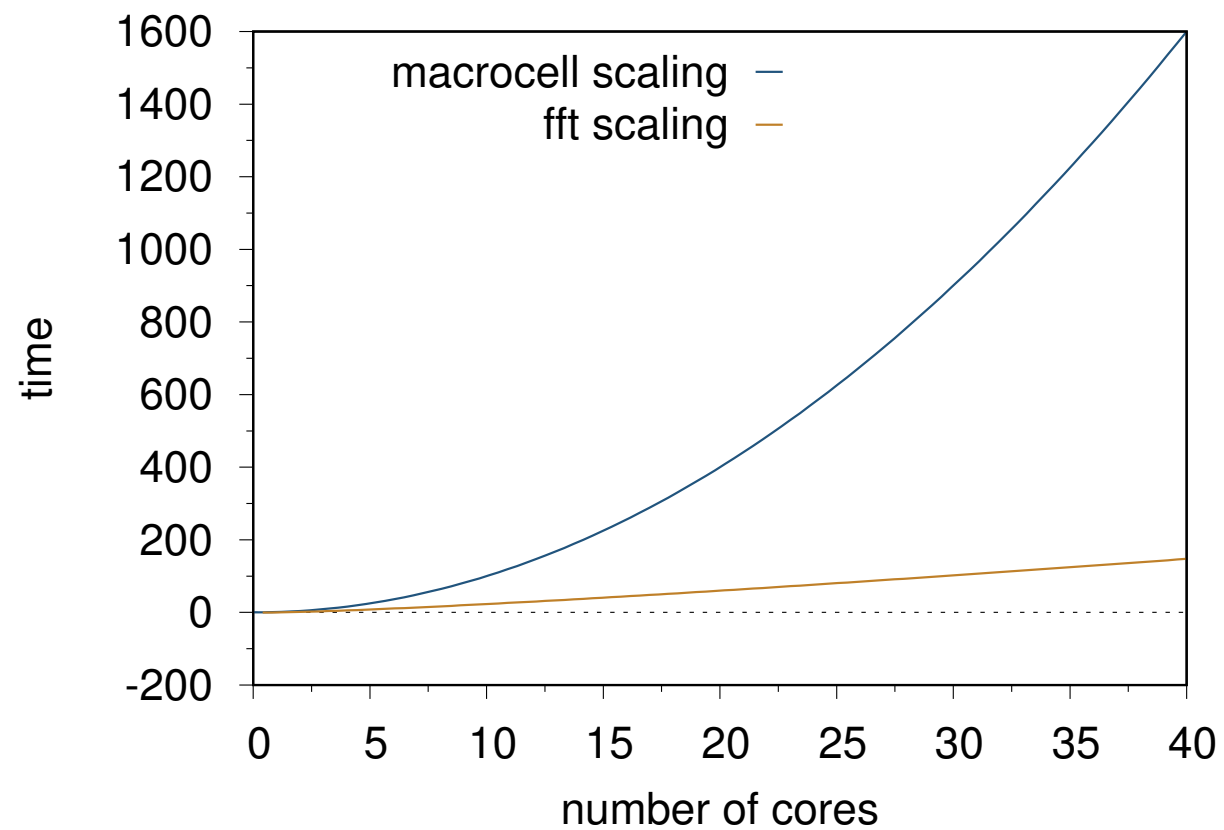$$H = -\mathcal{F}_{inv}(\mathcal{F}(N)\mathcal{F}(m))$$

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

Macrocell.   N^2

FFT $Nlog(N)$

- Predicted speed increase

Hierarchical