



# A multiscale approach to magnetisation dynamics



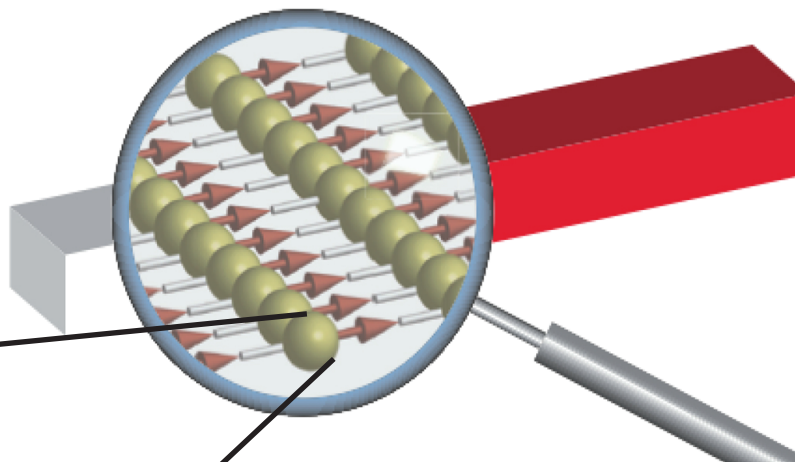
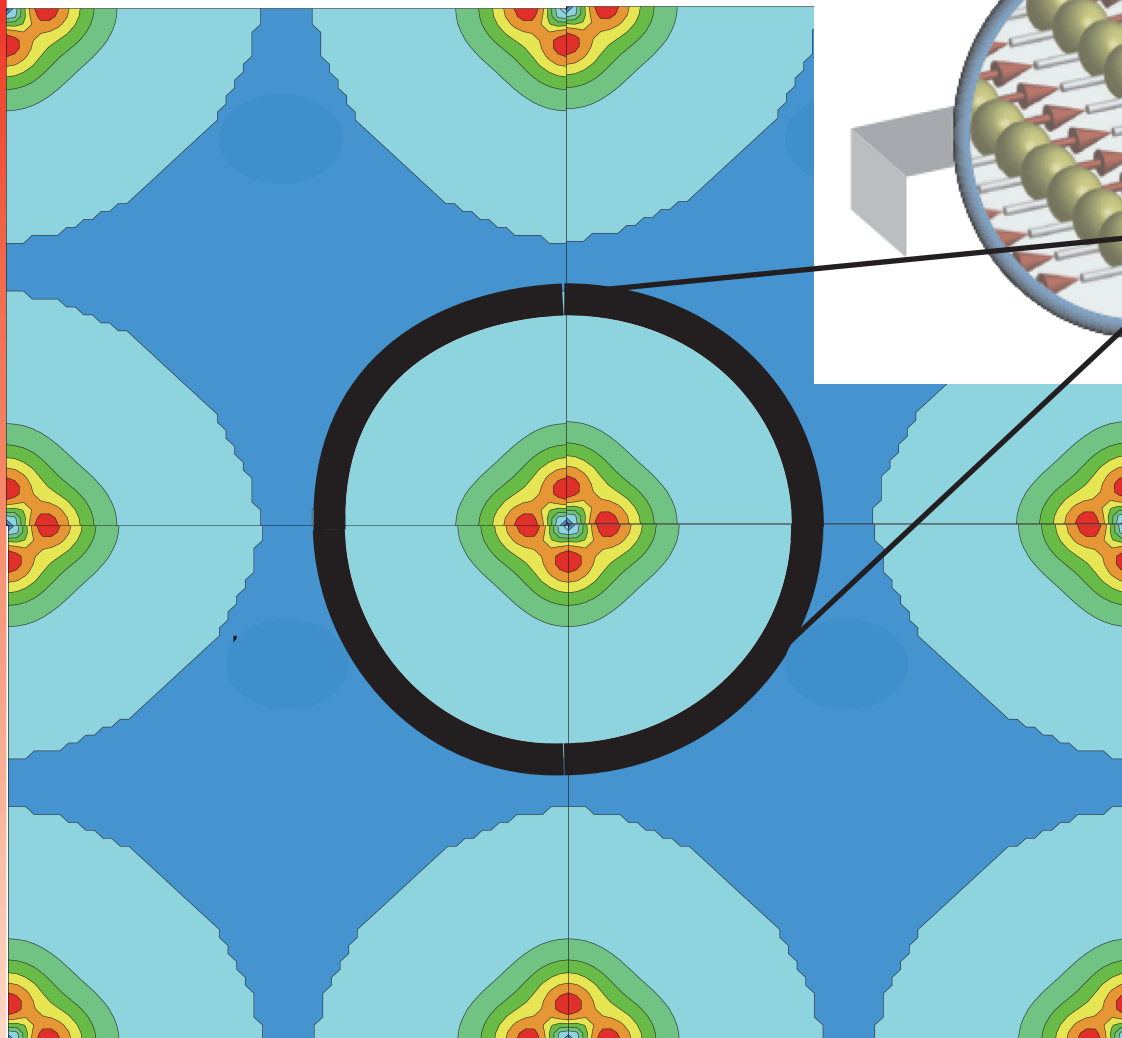
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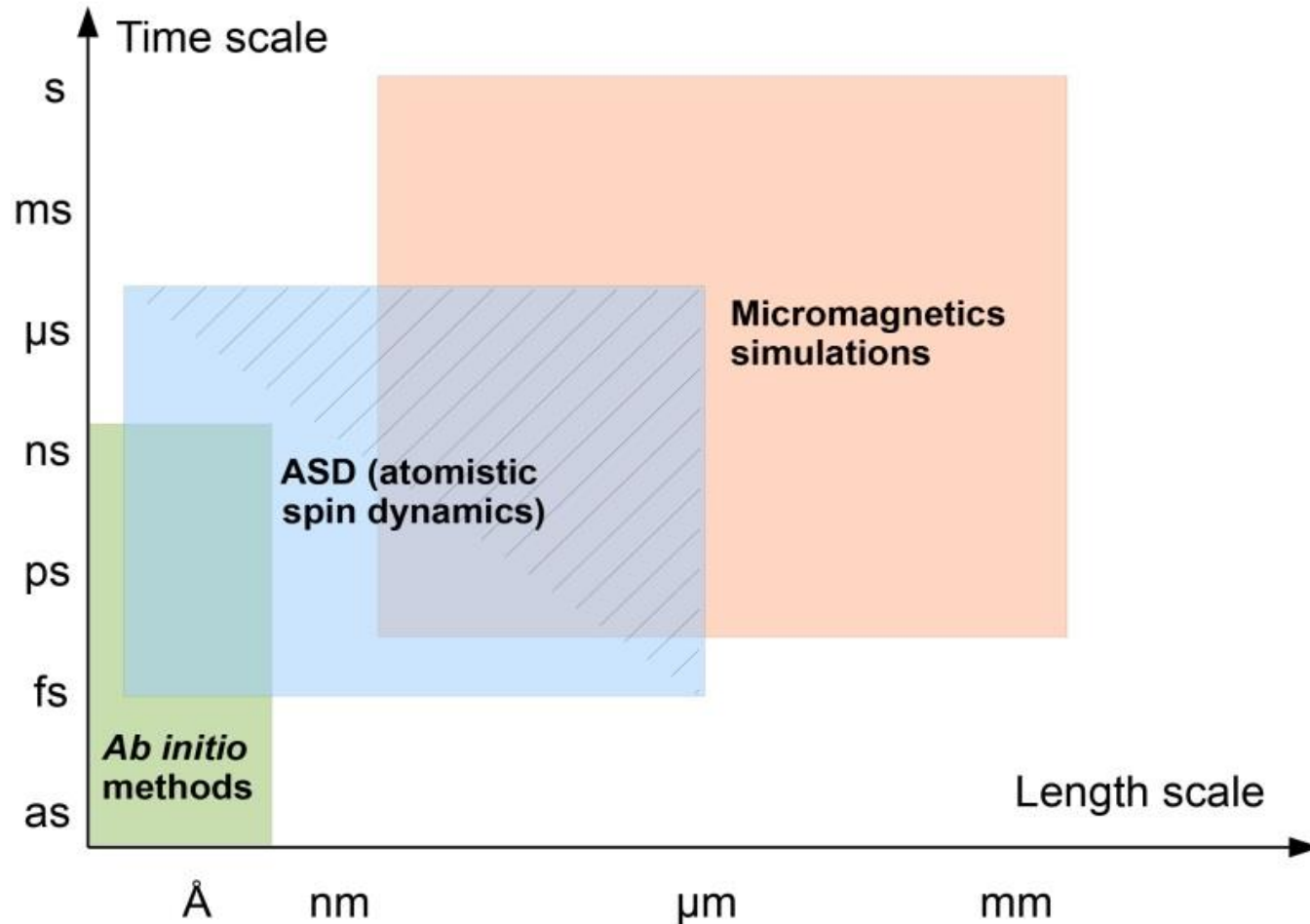




# Atomistic description



# Multiscale simulations





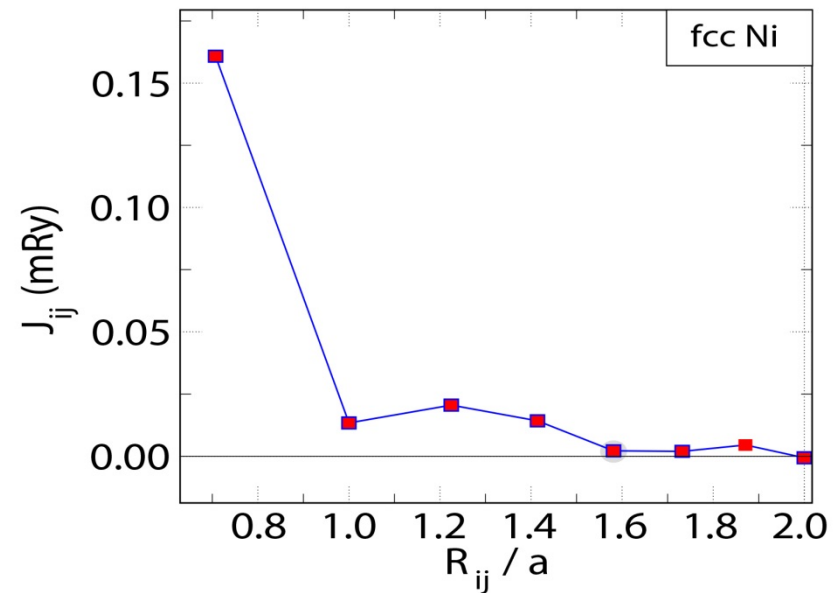
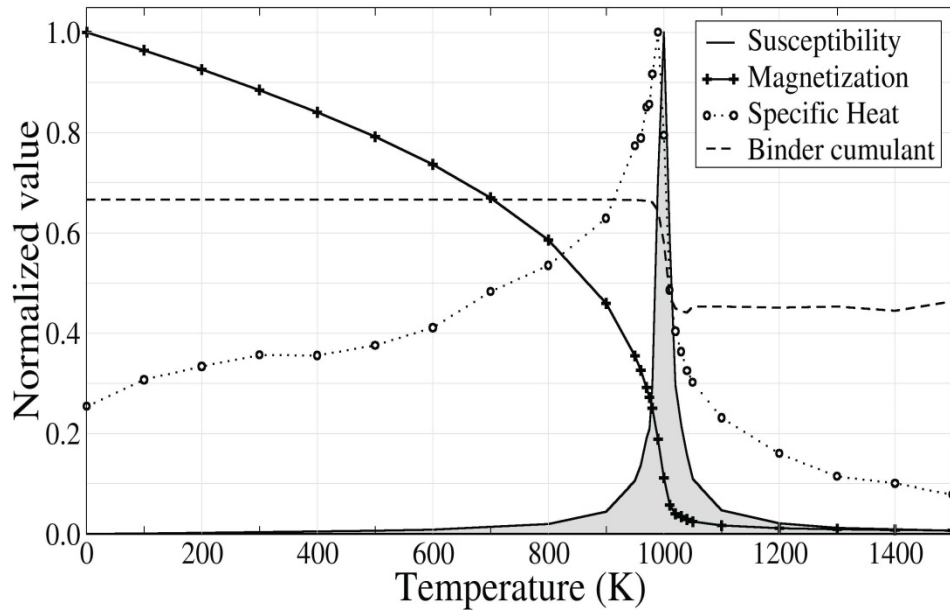
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# Heisenberg spin Hamiltonian

$$H_{spin} = - \sum_{\langle ij \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

$$H_{spin} = -J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

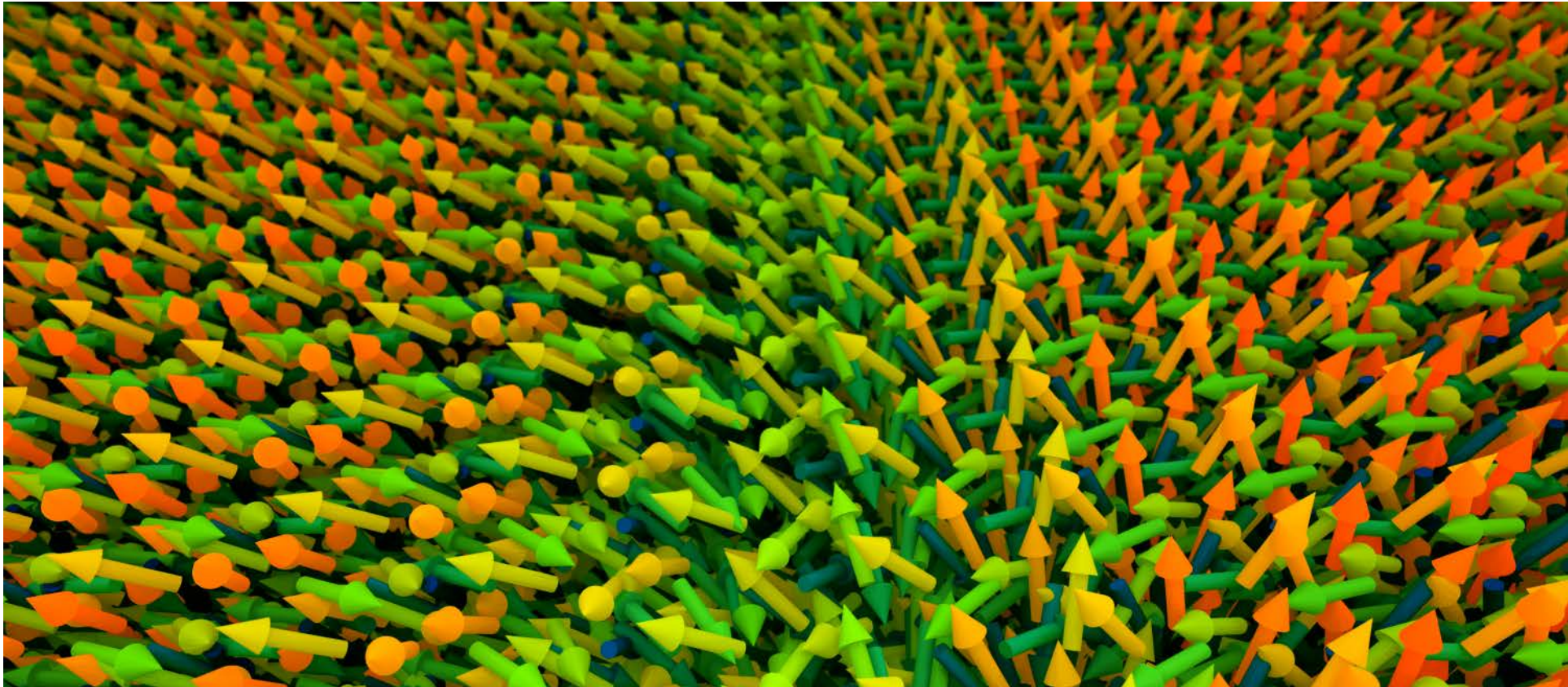
M vs T for bcc Fe





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# Magnetization dynamics on the atomic scale

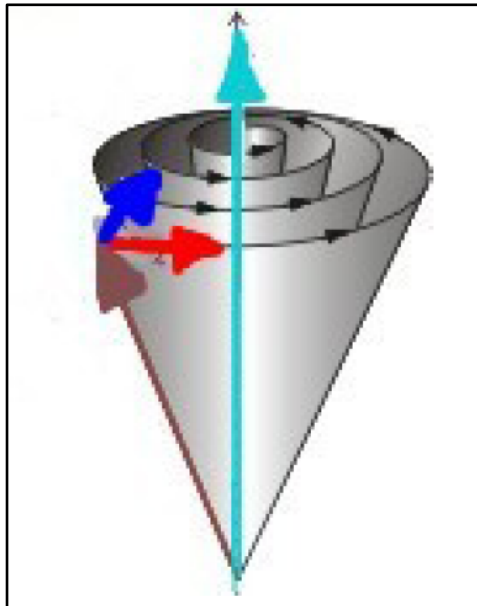




# Atomistic Landau-Lifshitz equation

$$\frac{d\mathbf{m}_i}{dt} = -\gamma \mathbf{m}_i \times \mathbf{B}_i - \gamma \frac{\alpha}{m_i} [\mathbf{m}_i \times [\mathbf{m}_i \times \mathbf{B}_i]]$$

Precession                  Damping



$$\frac{\partial \mathbf{m}_i}{\partial t} = -\gamma \mathbf{m}_i \times \mathbf{B}_i - \gamma \frac{\alpha}{m} [\mathbf{m}_i \times [\mathbf{m}_i \times \mathbf{B}_i]]$$

Prec

Energy dissipation

The e

$$\frac{dE}{dt} = \frac{dE}{d\mathbf{m}} \cdot \frac{d\mathbf{m}}{dt} = \mathbf{B} \cdot \frac{d\mathbf{m}}{dt}$$

$$\mathbf{B} \cdot \frac{d\mathbf{m}}{dt} \propto 0 + \alpha$$

$$\frac{dE}{dt} \longleftrightarrow \alpha$$



# Calculated interaction terms

$$\mathbf{B}_i = - \frac{dH}{dm_i}$$

$$\mathcal{H}_{iex} = -\frac{1}{2} \sum_{i \neq j} J_{ij} \mathbf{m}_i \cdot \mathbf{m}_j$$

Heisenberg exchange

$$\mathcal{H}_{DM} = -\frac{1}{2} \sum_{i \neq j} \mathbf{D}_{ij} \cdot \mathbf{m}_i \times \mathbf{m}_j$$

Dzyaloshinskii-Moriya exchange

$$\mathcal{H}_{ani} = K \sum_i (\mathbf{m}_i \cdot \mathbf{e}_{ani})^2$$

Uniaxial anisotropy

$$\mathcal{H}_{ext} = -\mathbf{B}_{ext} \cdot \sum_i \mathbf{m}_i$$

Applied magnetic field