

Micromagnetics and atomic spin dynamics

European School of Magnetism 2026

Anders Bergman, Dept. of Physics and Astronomy

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Outline

Introducing relevant simulation techniques

Introduction

Spin models

Micromagnetics

**Atomistic Spin
Dynamics**

Motivation

Topics from this school

Exchange interactions &
magnetic ordering

Spin waves & magnonics

Domains & domain walls

Magnetization reversal
processes

Motivation

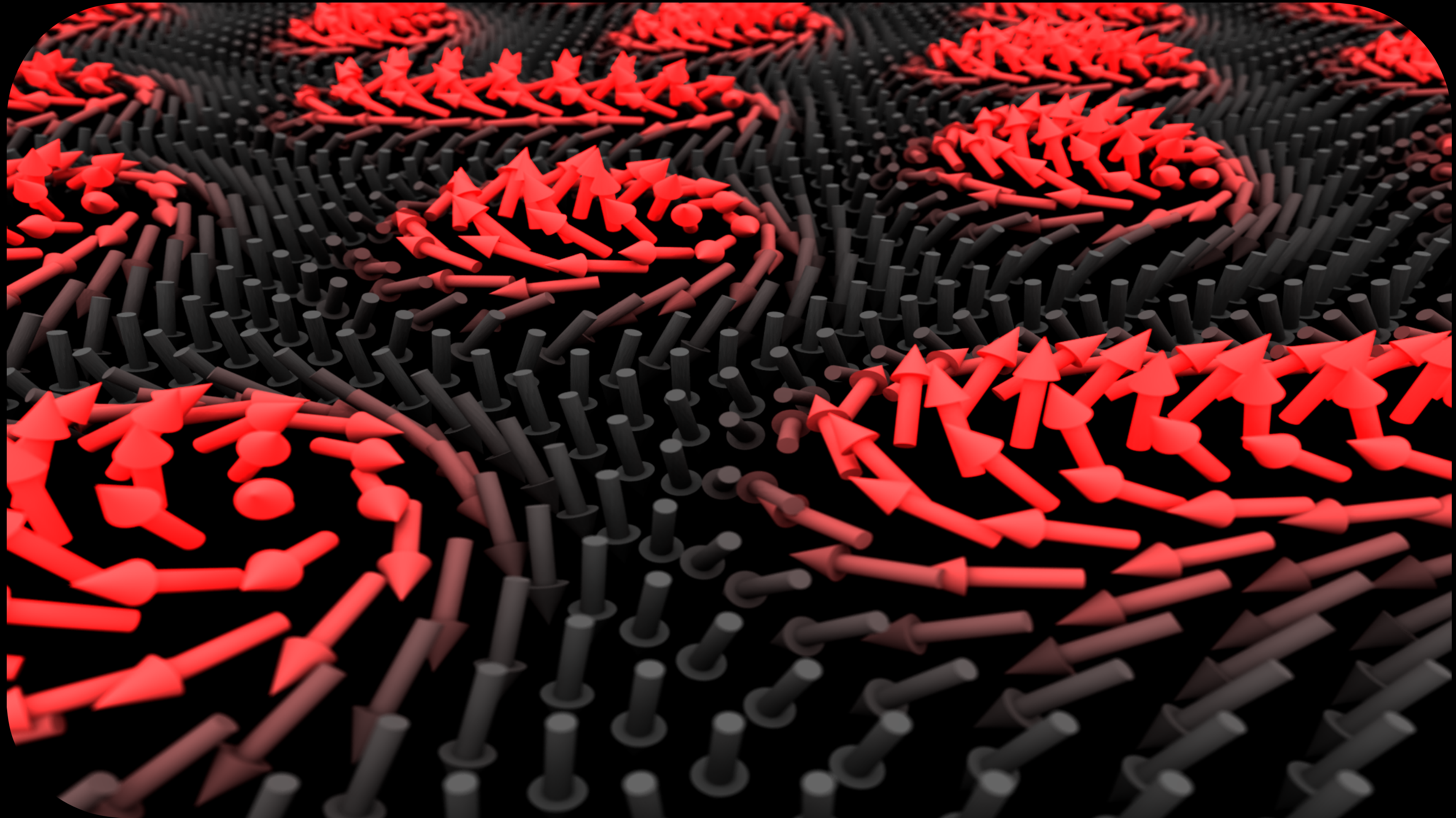
Topics from this school

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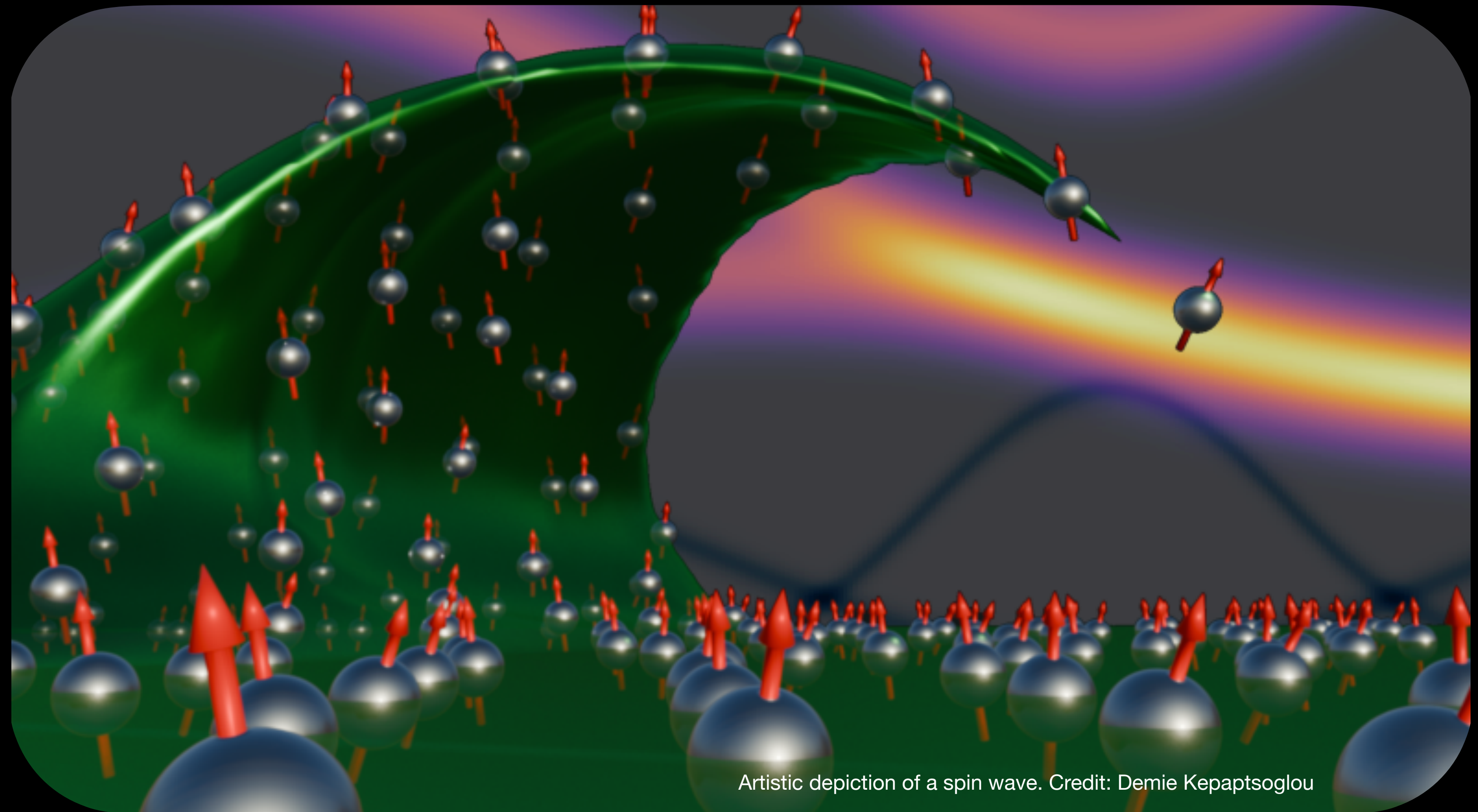
Topics from this school

Exchange interactions &
magnetic ordering

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processes



Artistic depiction of a spin wave. Credit: Demie Kepaptsoglou

Motivation

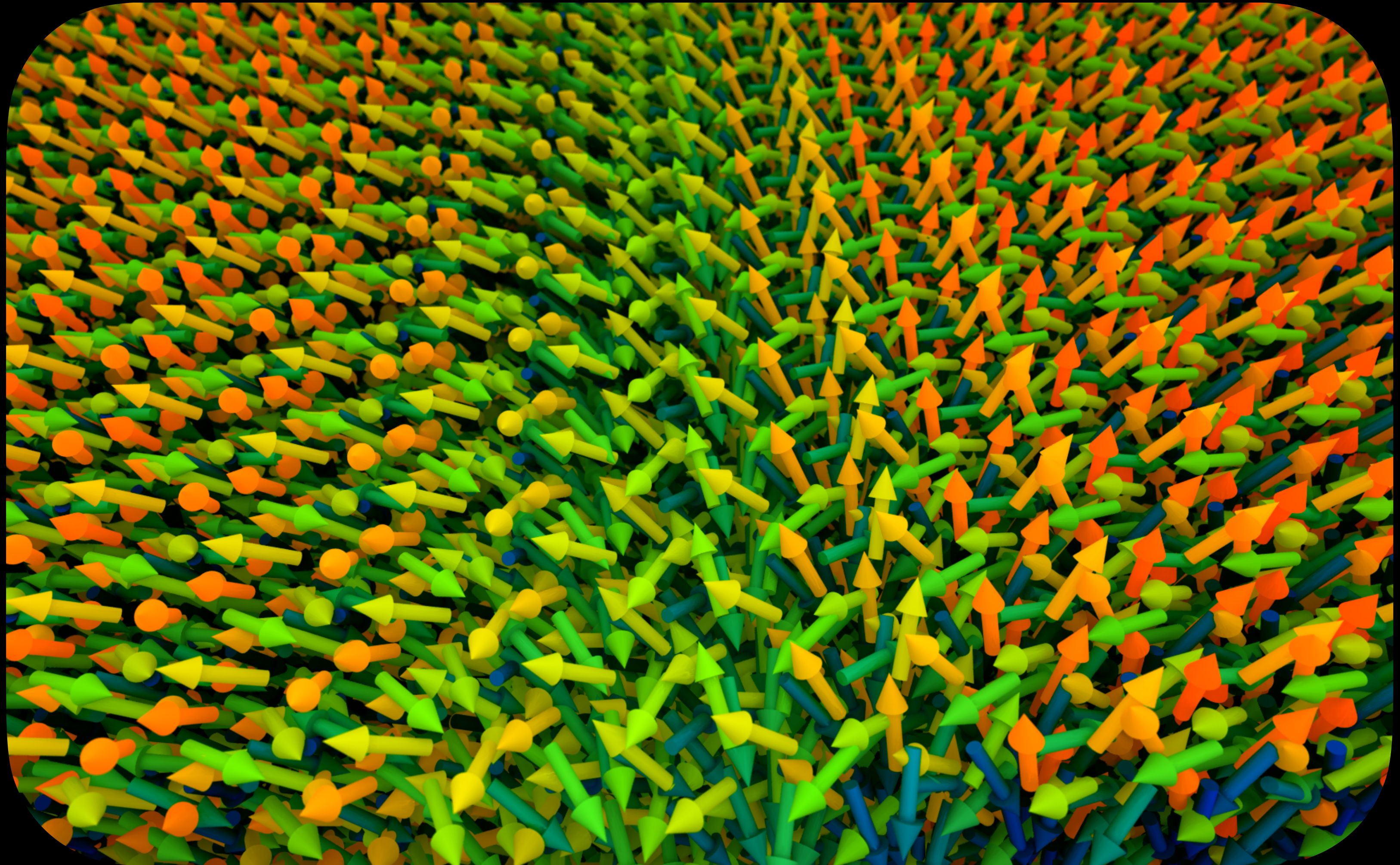
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processes



Motivation

Topics from this school

Exchange interactions &
magnetic ordering

Spin waves & magnonics

Domains & domain walls

**Magnetization reversal
processes**



Scales of magnetism

Time-scales across orders of magnitude

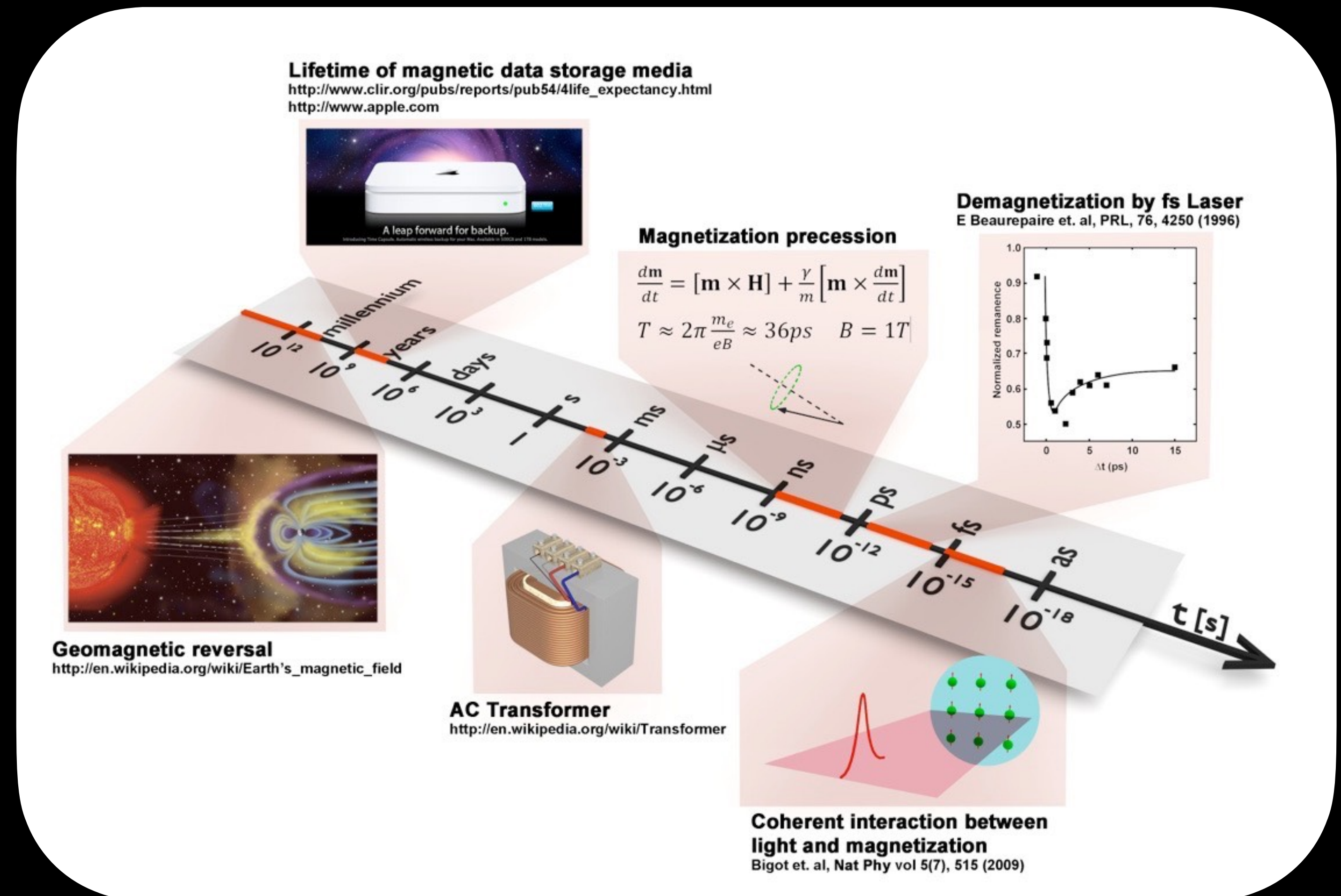
Electronic processes: sub-ps

Localized moments: ps / THz

Domains / Dipole magnons: ns / GHz

Magnetic storage: years

Geomagnetic reversal: millenia



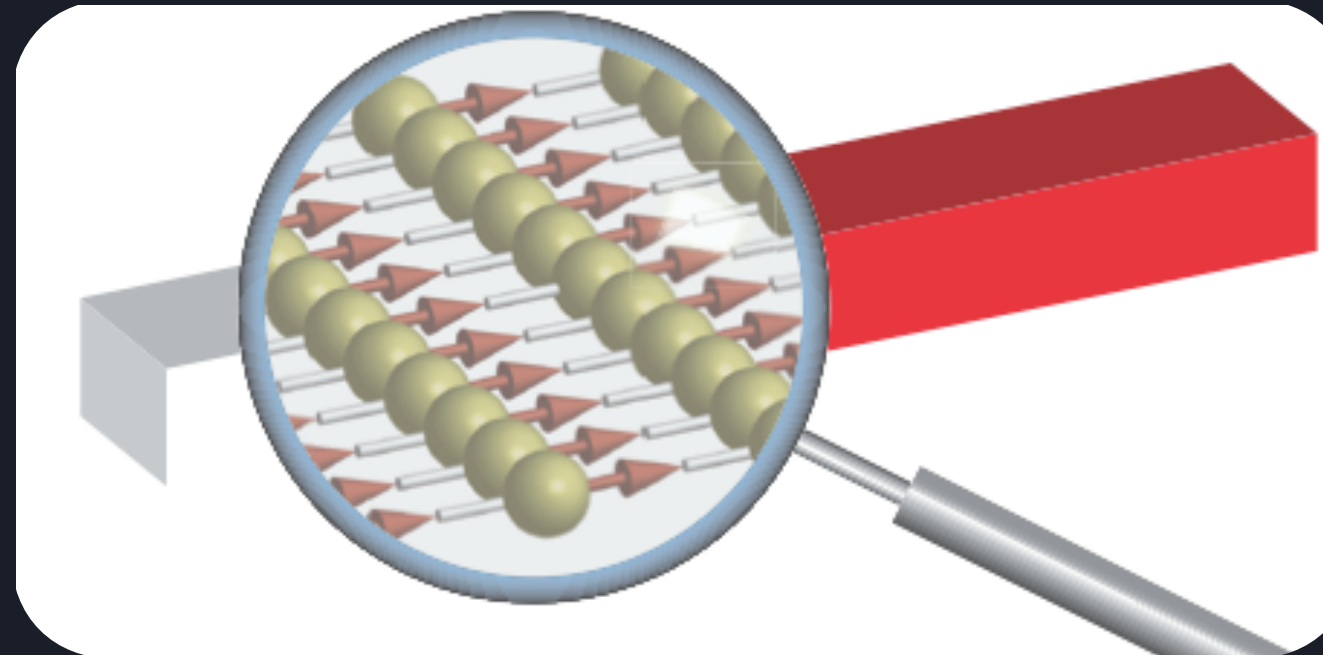
Scales of magnetism

From continuum to discrete and back again

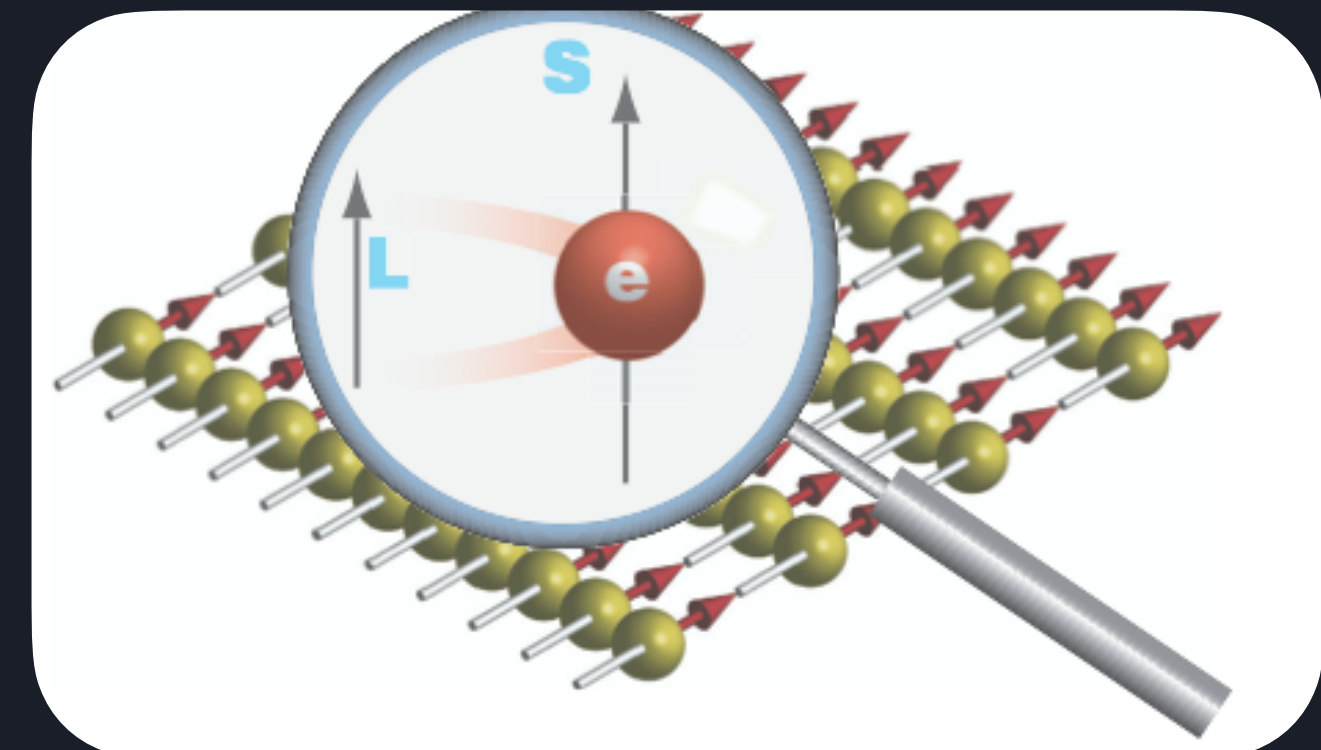
"Device scale"



Atomistic scale



Electronic scale



Scales of magnetism

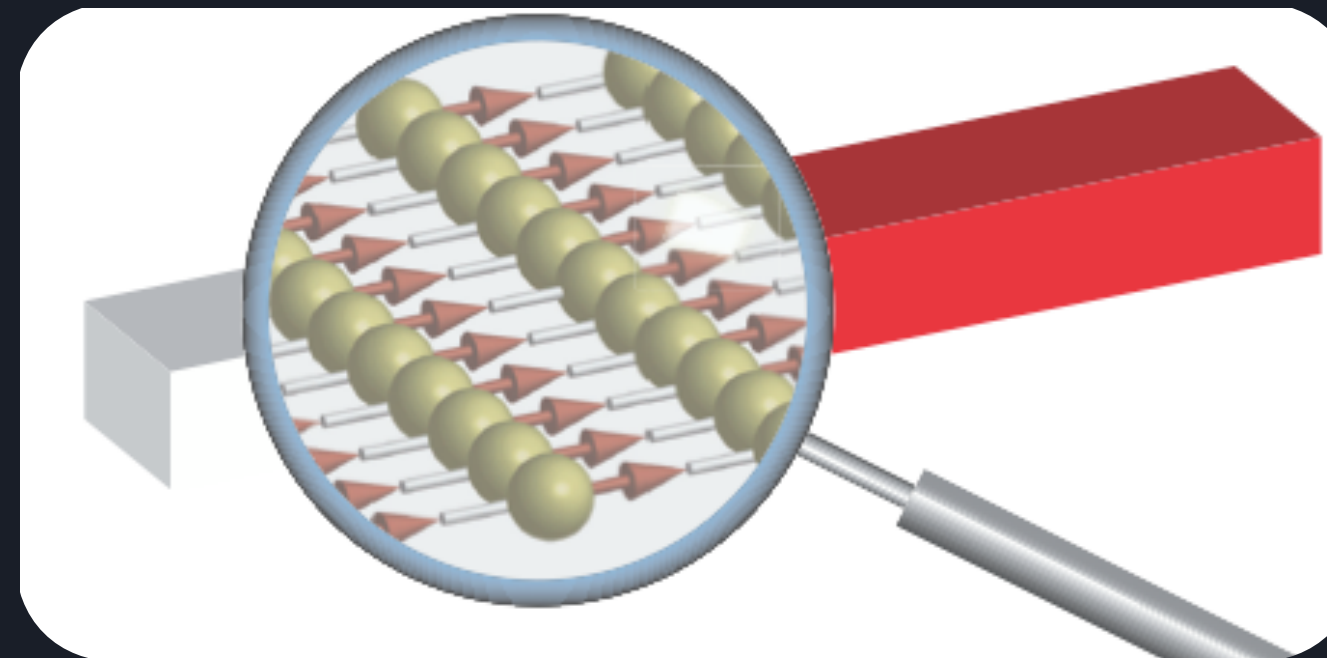
From continuum to discrete and back again

"Device scale"



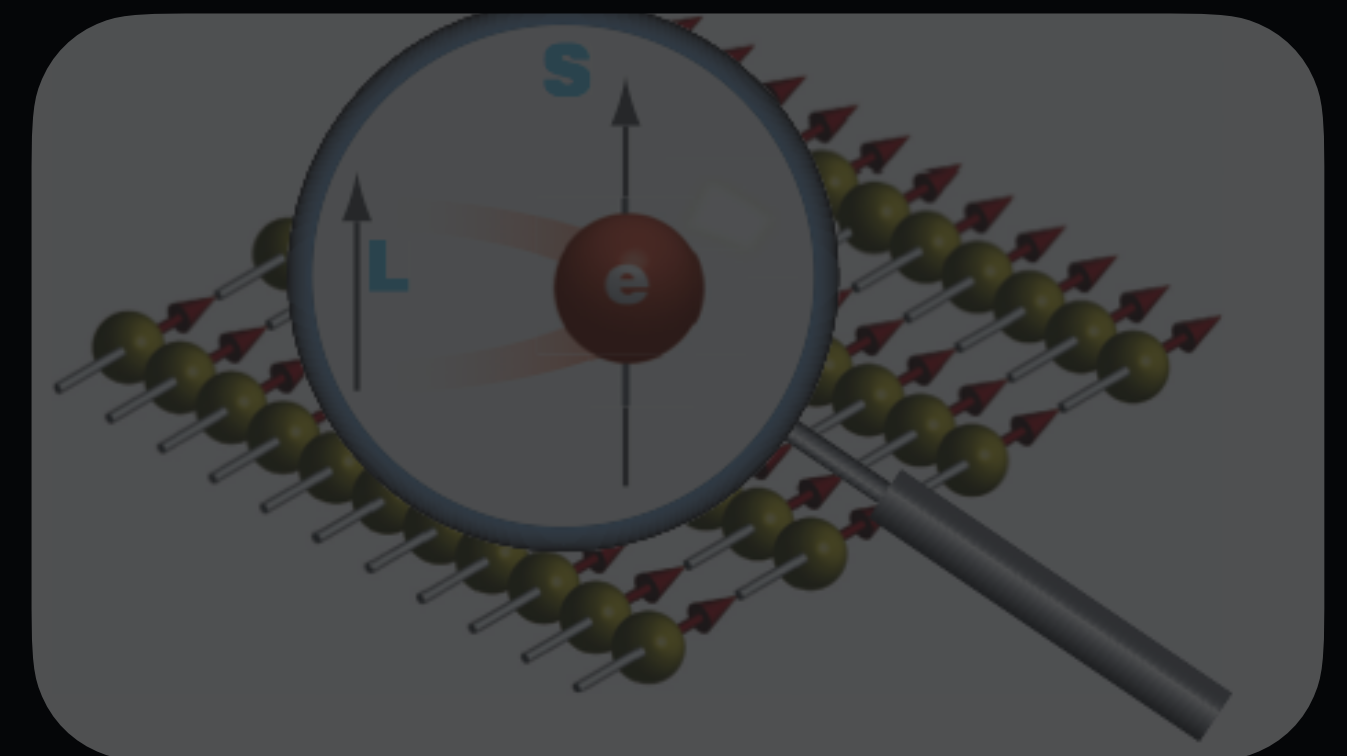
Micromagnetics

Atomistic scale



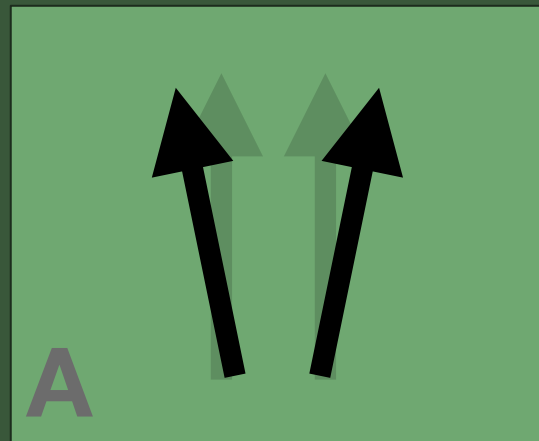
Atomistic Spin Dynamics

Electronic scale



Spin models

Energy cost from a reference state



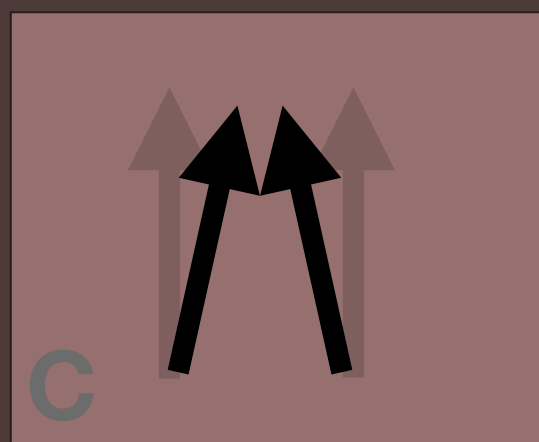
Exchange energy:
The cost of changing the angle between magnetic moments.

Heisenberg exchange interaction ($E_A = E_C$)



Anisotropy energy:
The cost in energy related to rotating the magnetization

Magnetocrystalline anisotropy: Microscopic origin (spin-orbit coupling)
Shape anisotropy: Magnetostatic origin (dipole-dipole interactions)



Antisymmetric exchange:
Direction of angle matters ($E_A \neq E_C$)

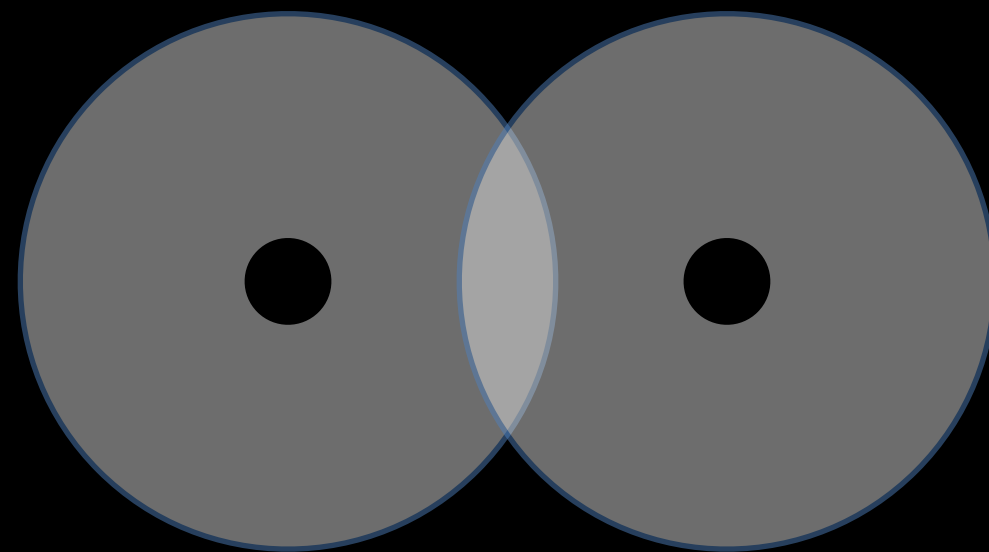
Dzyaloshinskii-Moriya interaction (SOC + lack of inversion symmetry)

Spin models

More on exchange interactions

Direct exchange

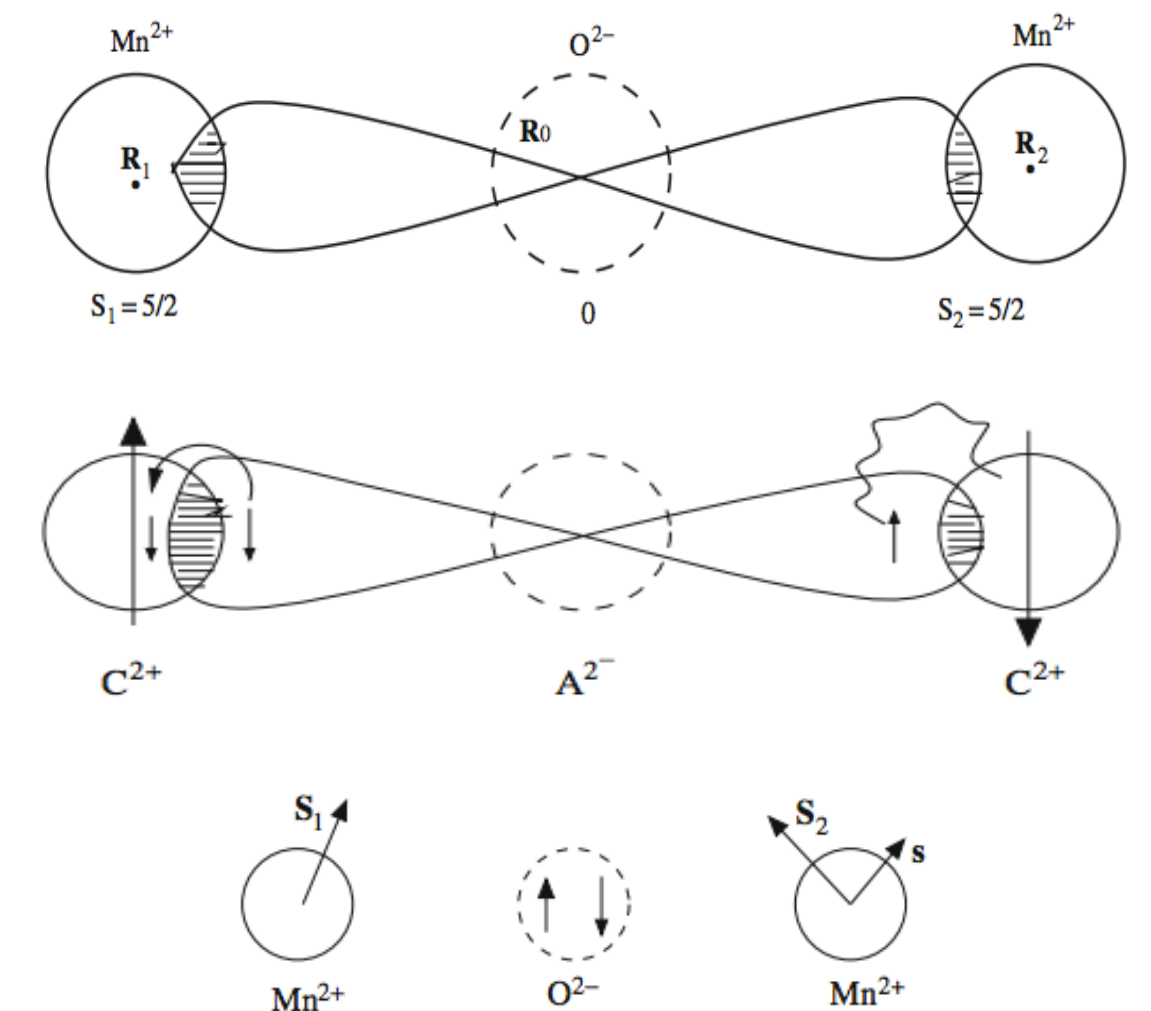
Overlapping wave-functions.
Strong but short-ranged



Super-exchange and double-exchange

Typically insulating systems
Mediated through non-magnetic ions
Antiferromagnetic

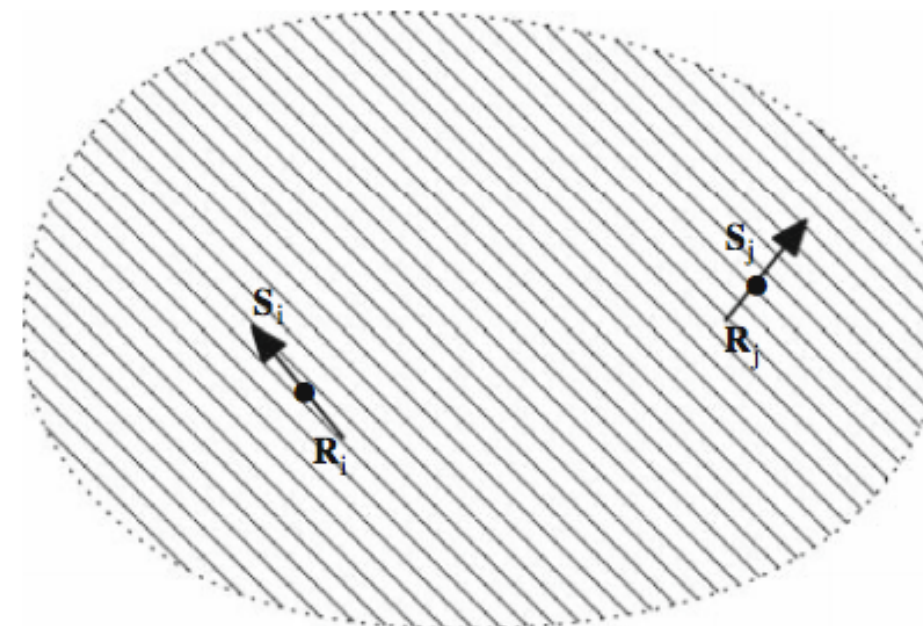
Super: Kanamori-Goodenough



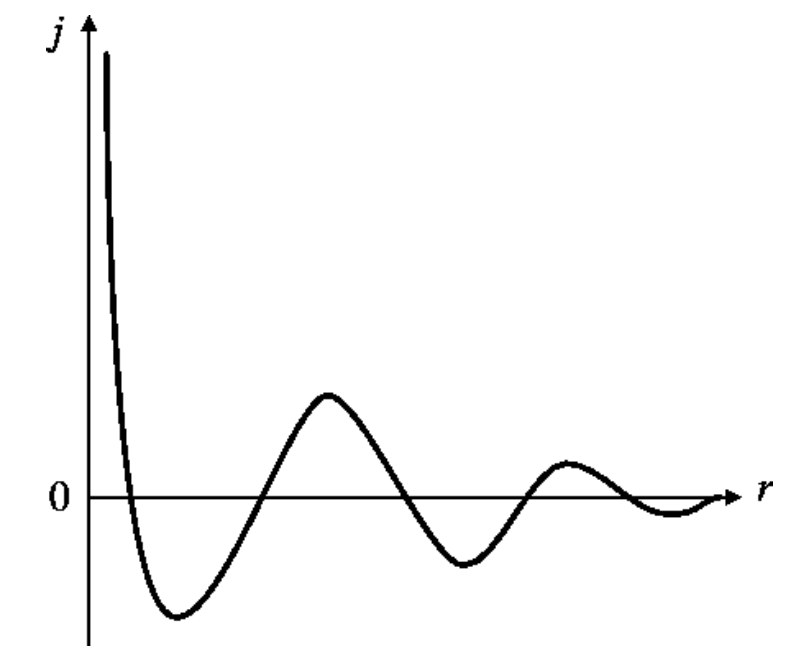
RKKY exchange

Localized electrons interact through
conduction electrons

Long ranged
Oscillatory

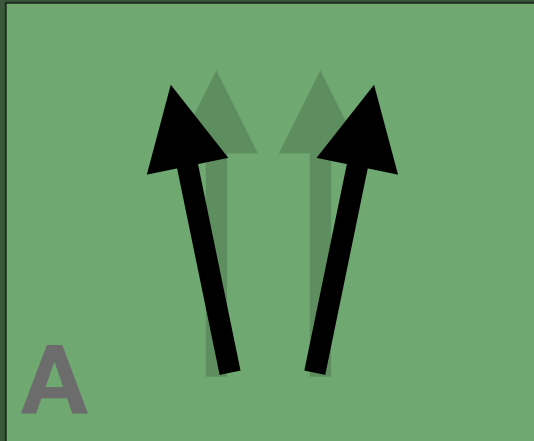


$$J^{RKKY} \propto \frac{\cos 2k_F R}{R^3}$$



Spin models

Energy cost from a reference state



Exchange energy:

The cost of changing the angle between magnetic moments.

Heisenberg exchange interaction ($E_A = E_C$)

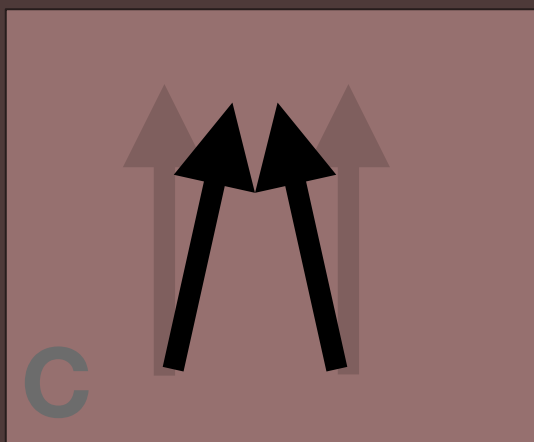


Anisotropy energy:

The cost in energy related to rotating the magnetization

Magnetocrystalline anisotropy: Microscopic origin (spin-orbit coupling)

Shape anisotropy: Magnetostatic origin (dipole-dipole interactions)



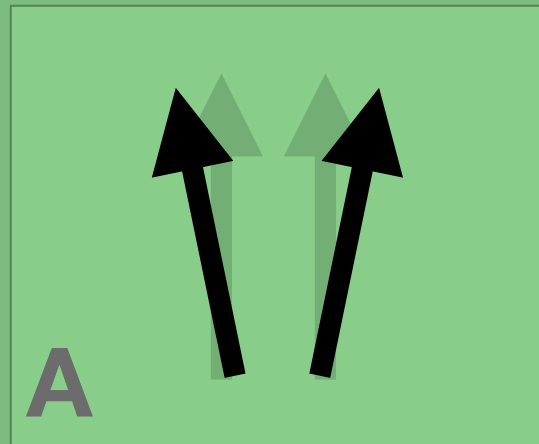
Antisymmetric exchange:

Direction of angle matters ($E_A \neq E_C$)

Dzyaloshinskii-Moriya interaction (SOC + lack of inversion symmetry)

Spin models

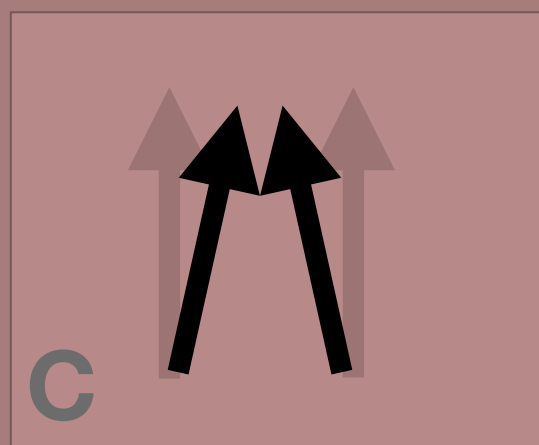
Terms of the Hamiltonian



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



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



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

Spin models

The zoo of interactions

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

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

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

$$\mathcal{H}_{dd} = -\frac{1}{2} \sum_{i \neq j} Q_{ij}^{\mu\nu} m_i^\mu m_j^\nu$$

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

Higher order terms,

Multi-spin interactions,

Spin-lattice couplings...

Spin models

The effective Hamiltonian

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

Model limitations:

- Magnetic moments with fixed length
- Constant interaction strengths

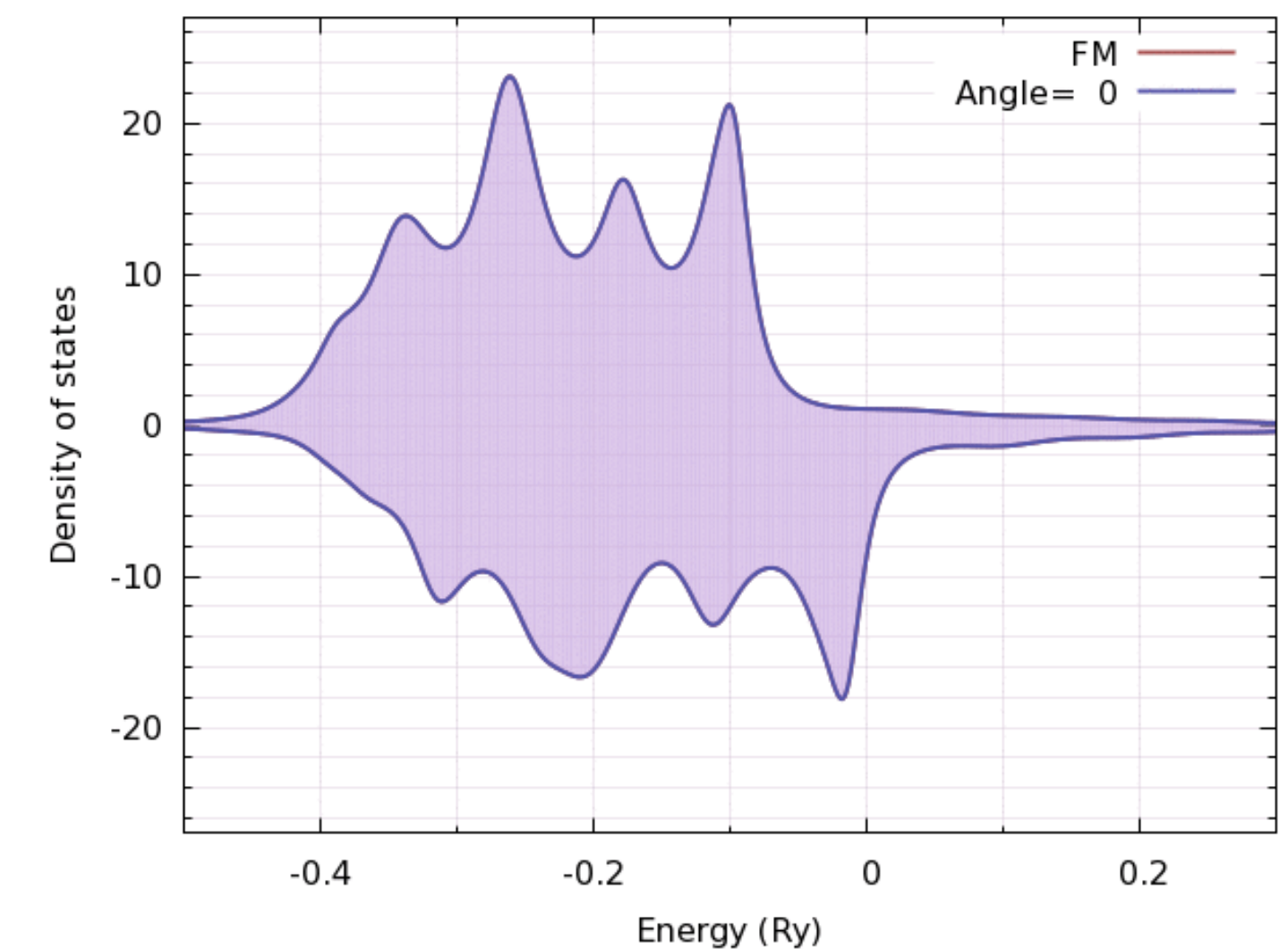
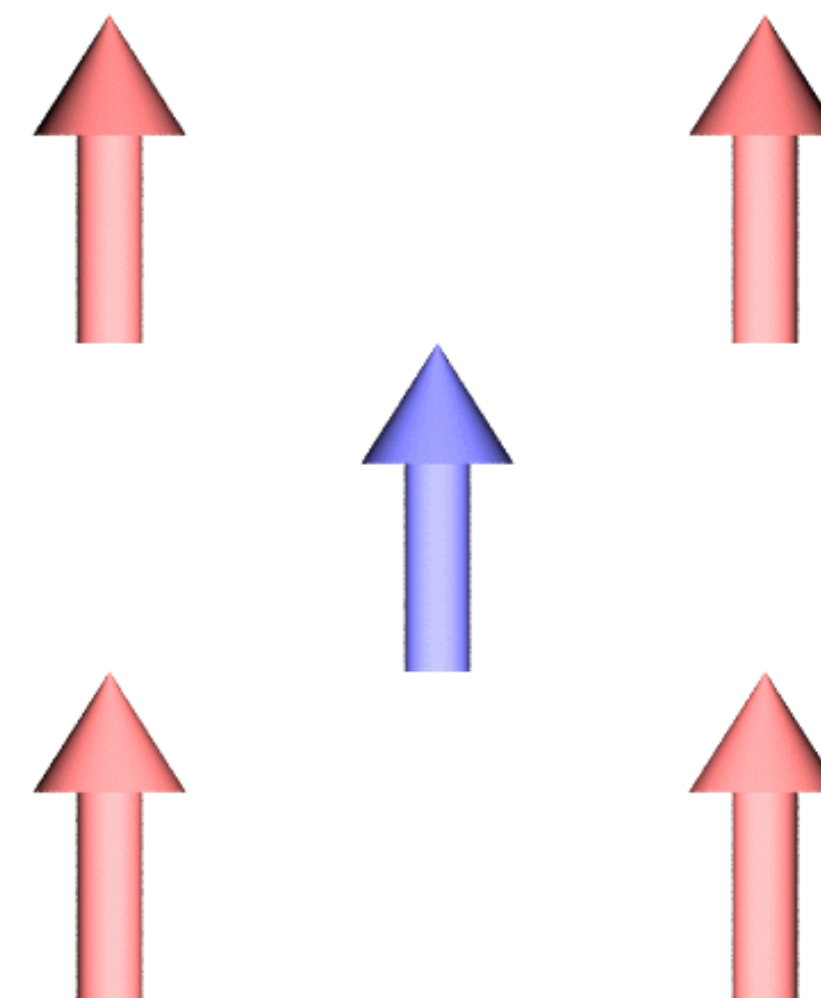
Real materials:

- Magnetic moments can vary
- Configurational dependent interactions

The Heisenberg Hamiltonian

With added terms depending on system

Warning: Beware of conventions!



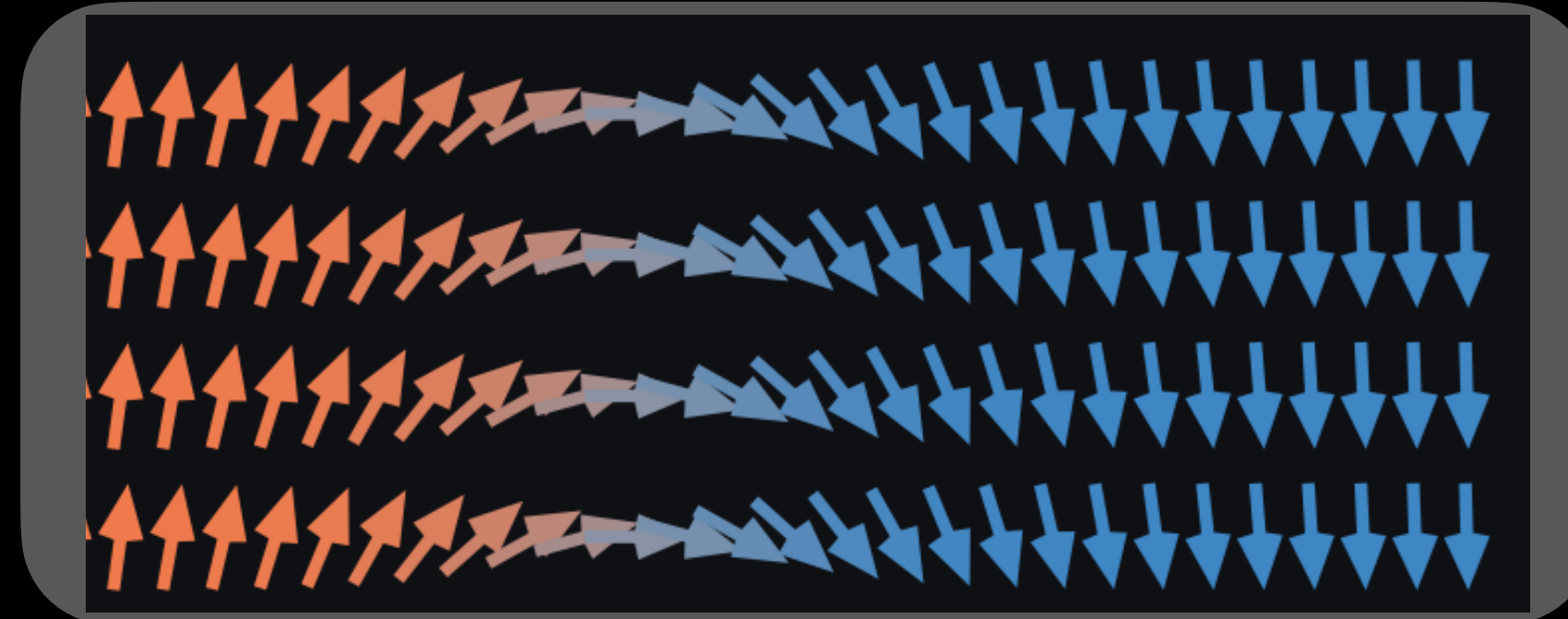
Micromagnetism

The magnetisation density



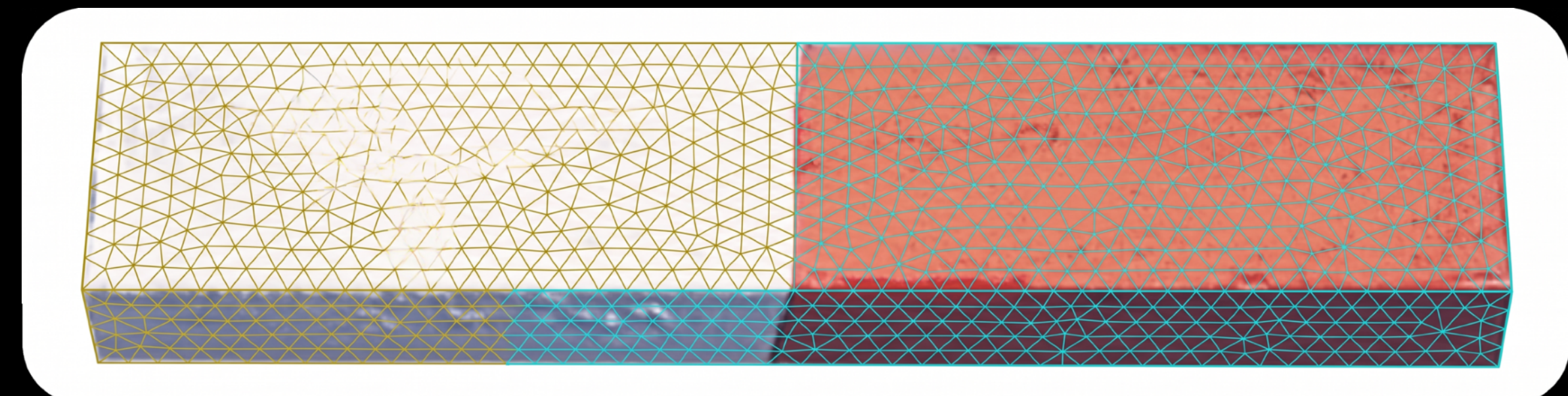
A μm^3 cube of Fe contains $\sim 10^{11}$ atoms:
Too costly for an atomistic method

Domain wall width of Fe:
 ~ 60 nm



Smooth, continuous
magnetisation density

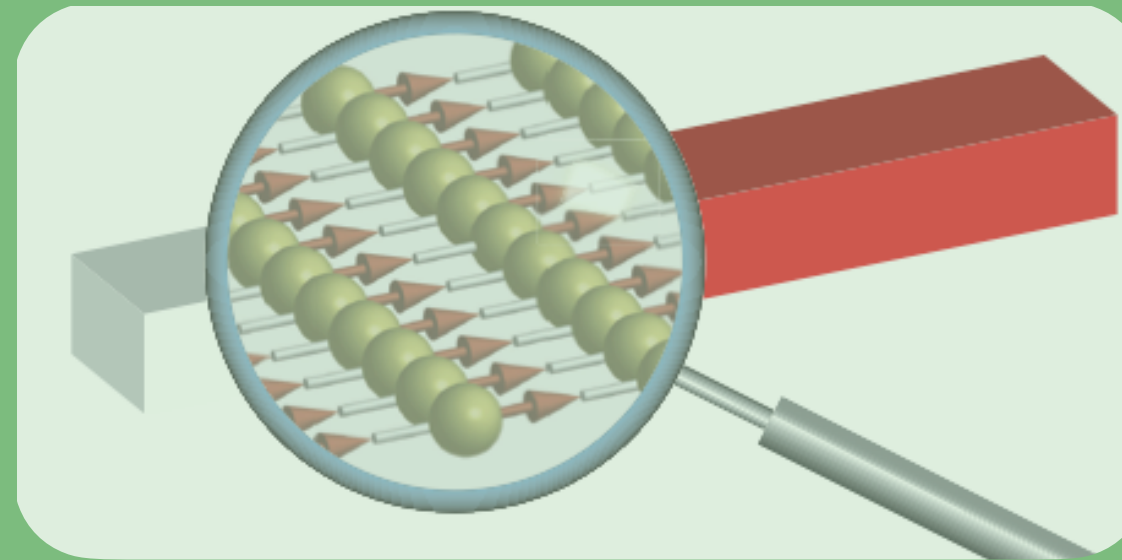
Consider the energetics and dynamics of
the magnetisation density instead



Micromagnetism

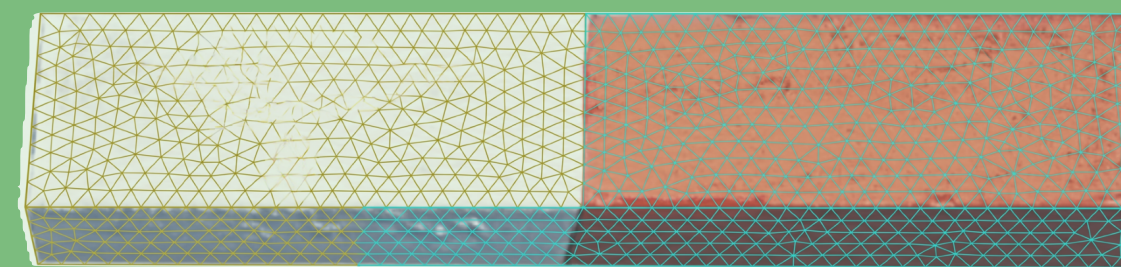
Energy from moments to density

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



$$\mathbf{e}_i \cdot \mathbf{e}_j = 1 - \frac{1}{2} |\mathbf{e}_i - \mathbf{e}_j|^2 \quad \mathbf{e}_j \approx \mathbf{e}_i + (\mathbf{r}_{ij} \cdot \nabla) \mathbf{m}$$

$$E_{ex} = \int_V A (\nabla \mathbf{m})^2 dV$$



A
is the
micromagnetic
exchange stiffness

$$A \propto \frac{1}{V_c} \sum_j J_{0j} r_{0j}^2$$

Unit: energy/length

Fe: ~20 pJ/m
Co: ~30 pJ/m
Py: ~10 pJ/m

Micromagnetism

Other contributions

$$E[\mathbf{m}] = \int_V \left\{ A(\nabla \mathbf{m})^2 + \varepsilon_{\text{ani}} + \varepsilon_{\text{DMI}} - \mu_0 M_s \mathbf{m} \cdot \mathbf{H}_{\text{ext}} - \frac{\mu_0}{2} M_s \mathbf{m} \cdot \mathbf{H}_d \right\} dV$$

Magnetocrystalline anisotropy

Uniaxial:

$$\varepsilon_{\text{ani}}^{\text{uni}} = -K_u (\mathbf{m} \cdot \hat{\mathbf{u}})^2$$

Cubic:

$$\varepsilon_{\text{ani}}^{\text{cub}} = K_1 (m_x^2 m_y^2 + m_y^2 m_z^2 + m_z^2 m_x^2) + K_2 m_x^2 m_y^2 m_z^2$$

Dzyaloshinskii-Moriya interactions

Bulk-like:

$$\varepsilon_{\text{DMI}}^{\text{bulk}} = D \mathbf{m} \cdot (\nabla \times \mathbf{m})$$

Interfacial:

$$\varepsilon_{\text{DMI}}^{\text{int}} = D [m_z (\nabla \cdot \mathbf{m}) - (\mathbf{m} \cdot \nabla) m_z]$$

Magnetostatic (dipole) interactions

$$\nabla \times \mathbf{H}_d = 0 \Rightarrow \mathbf{H}_d = -\nabla U, \quad \nabla^2 U = \nabla \cdot \mathbf{M}$$

Bulk and surface contributions to U

$$U(\mathbf{r}) = \frac{1}{4\pi} \left[\int_V \frac{\rho_m}{|\mathbf{r} - \mathbf{r}'|} dV' + \oint_S \frac{\sigma_m}{|\mathbf{r} - \mathbf{r}'|} dS' \right]$$

Weak but long-ranged!

Micromagnetism

From energy to dynamics, via fields

$$H_{\text{eff}}(r) = - \frac{1}{\mu_0 M_s} \frac{\delta E}{\delta m(r)}$$

$$\frac{2A}{\mu_0 M_s} \nabla^2 \mathbf{m}$$

$$-\frac{2D}{\mu_0 M_s} (\nabla \times \mathbf{m})$$

$$\frac{2K_u}{\mu_0 M_s} (\mathbf{m} \cdot \hat{\mathbf{u}}) \hat{\mathbf{u}}$$

$$-\frac{2D}{\mu_0 M_s} [(\nabla \cdot \mathbf{m}) \hat{\mathbf{z}} - \nabla m_z]$$

$$\mathbf{H}_{\text{ext}}$$

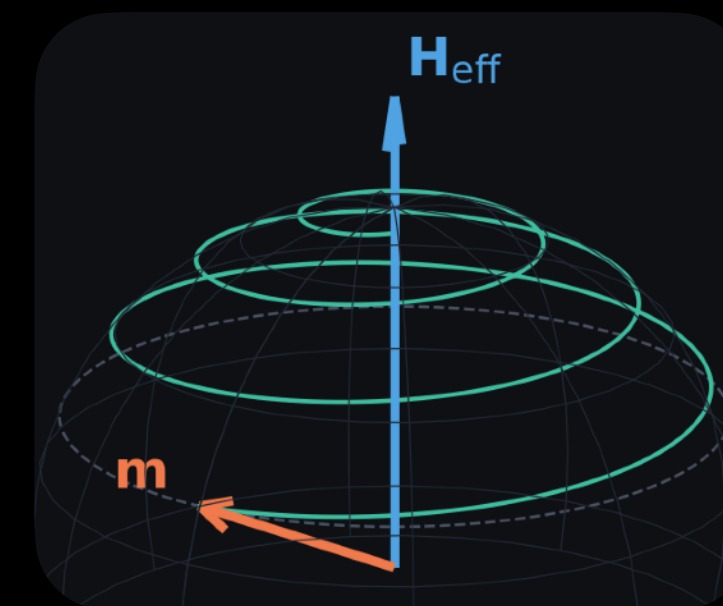
$$\mathbf{H}_d$$

Conservative dynamics:

$$\frac{d\mathbf{m}}{dt} = -\gamma_0 \mathbf{m} \times \mathbf{H}_{\text{eff}}$$

With added dissipation: Landau-Lifshitz equation

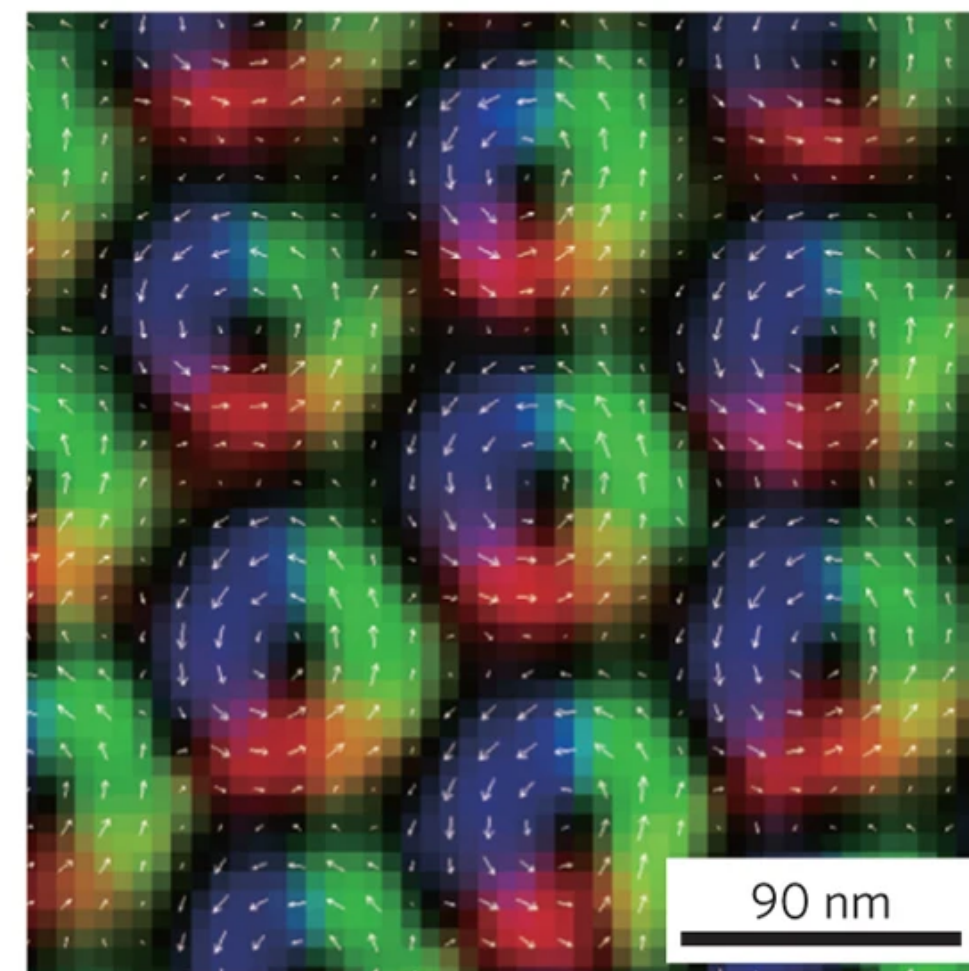
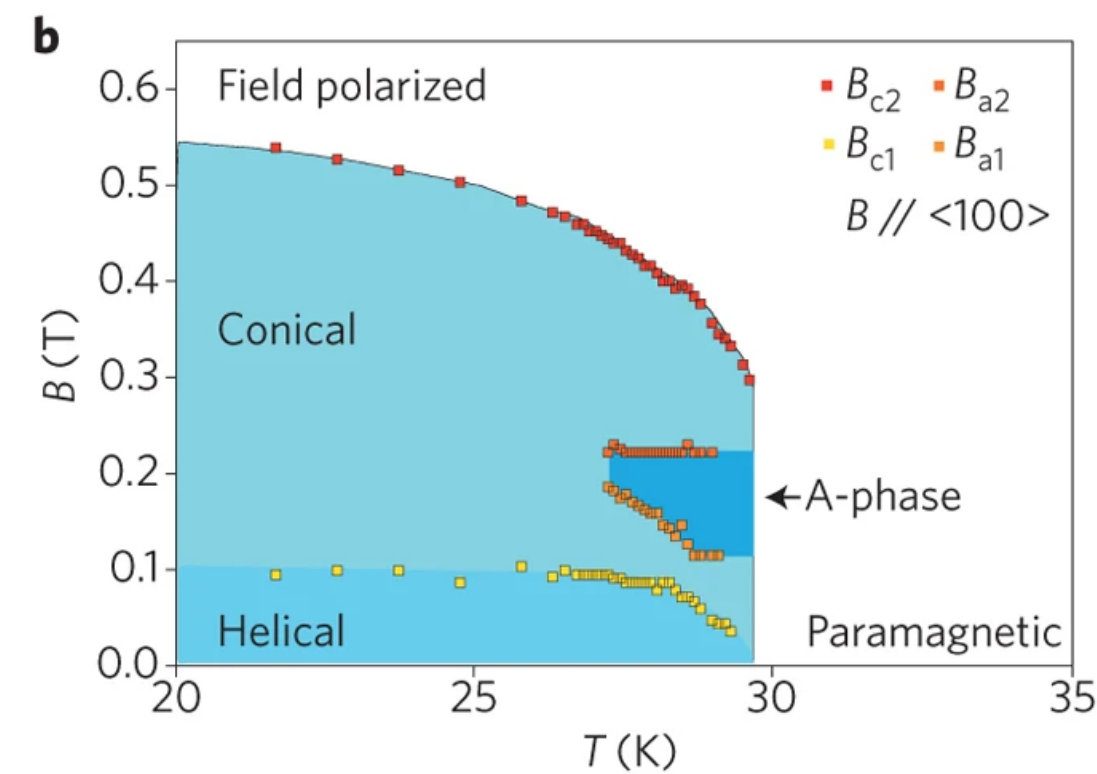
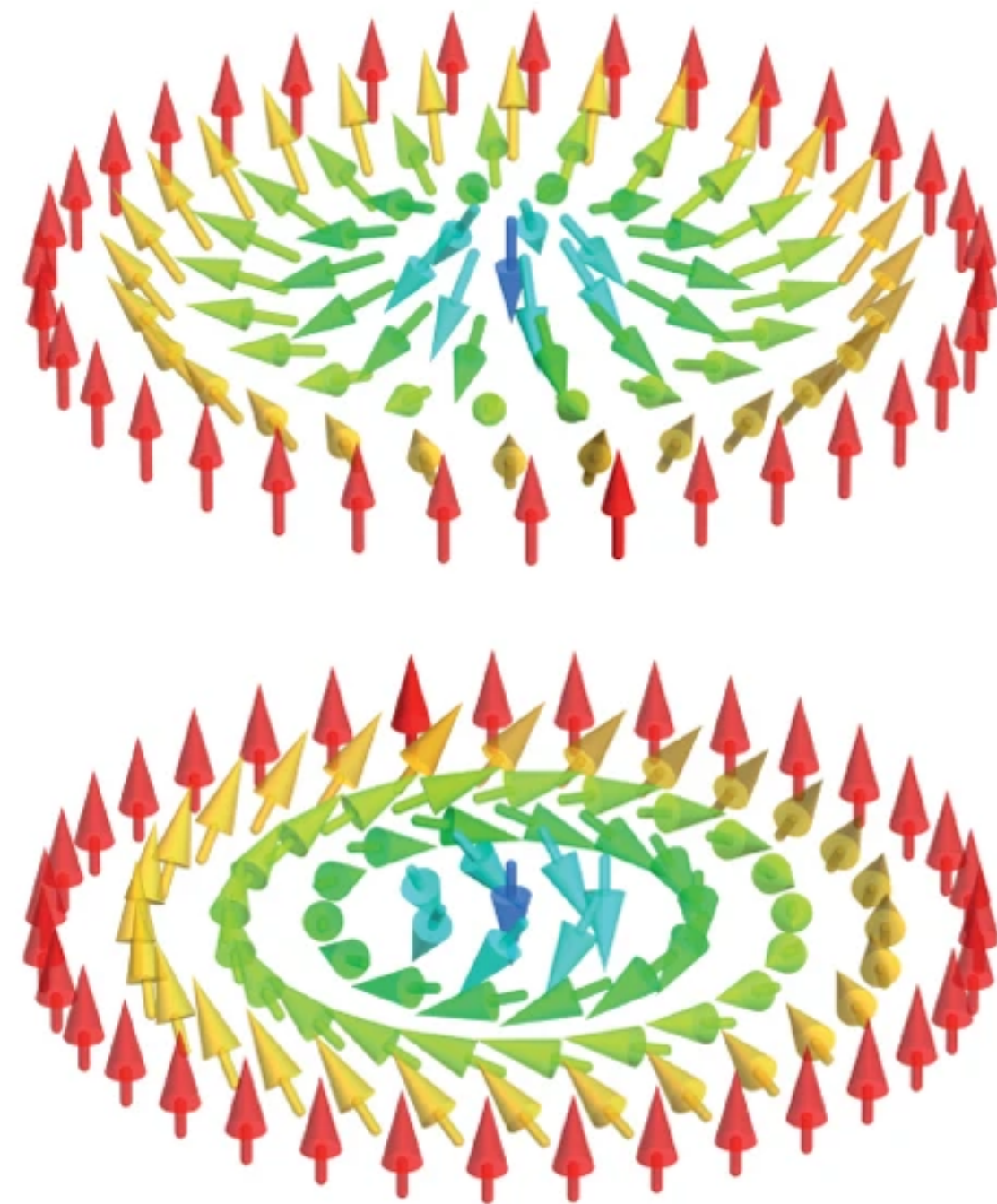
$$\frac{\partial \mathbf{m}}{\partial t} = -\frac{\gamma_0}{1 + \alpha^2} [\mathbf{m} \times \mathbf{H}_{\text{eff}} + \alpha \mathbf{m} \times (\mathbf{m} \times \mathbf{H}_{\text{eff}})]$$



Micromagnetism

Case study I: Skyrmions and current driven dynamics

Skyrmions



S. Mühlbauer et al. Science **323** 915 (2009) X.Z. Yu et al. Nature **465** 901 (2010))

Current driven dynamics

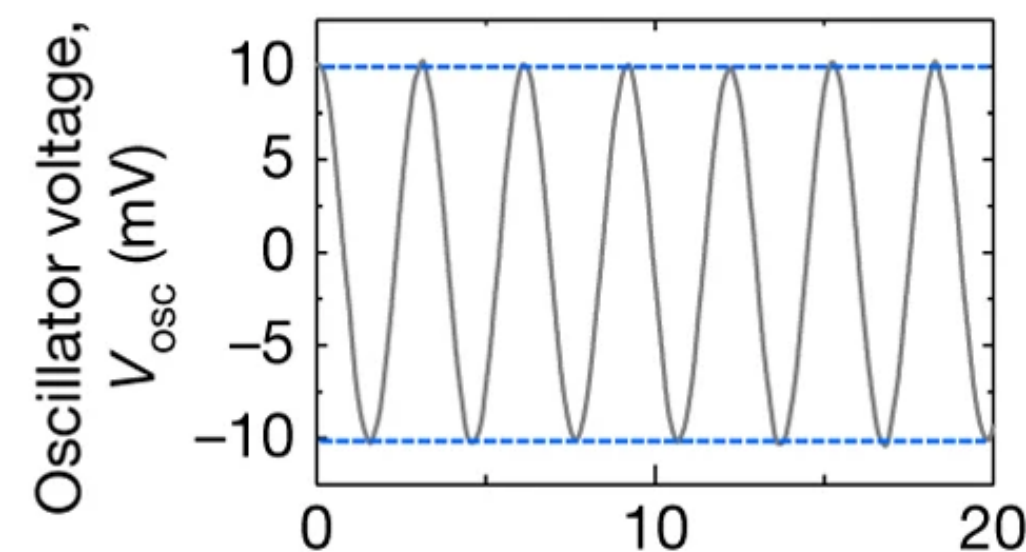
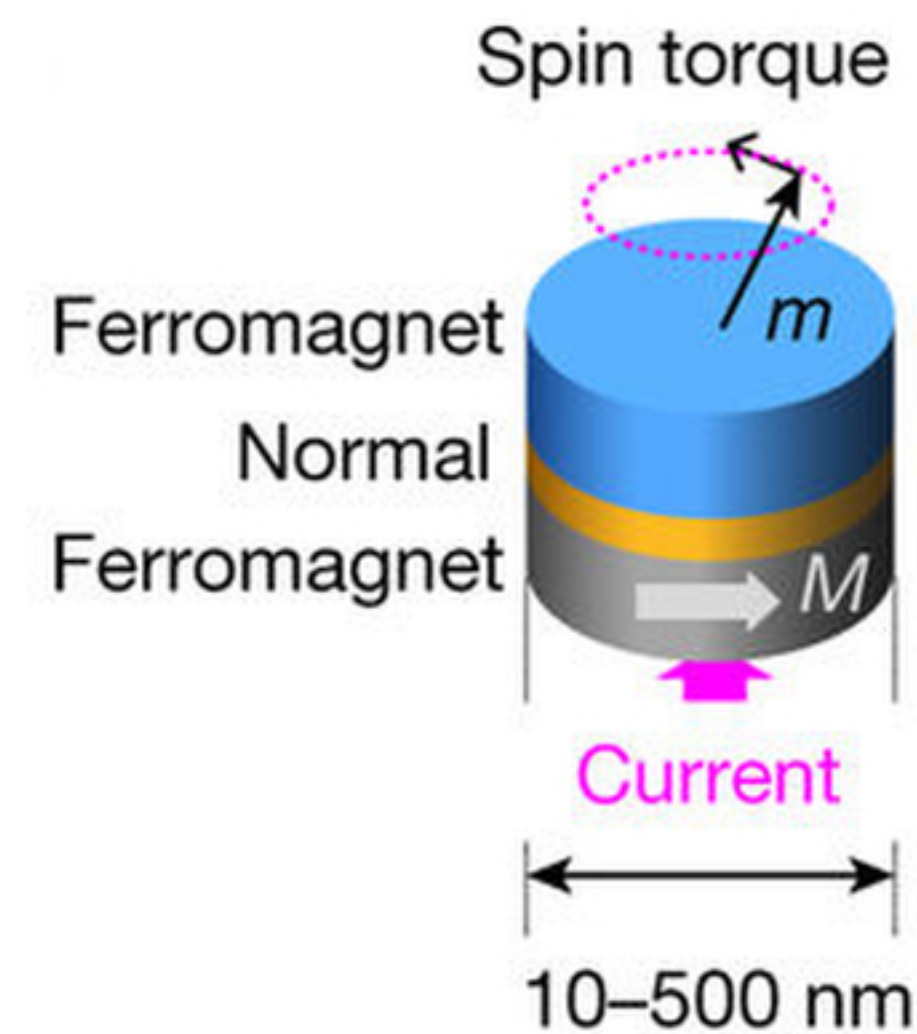


A. Fert et al. Nature Nano. **8** 152 (2013)

Micromagnetism

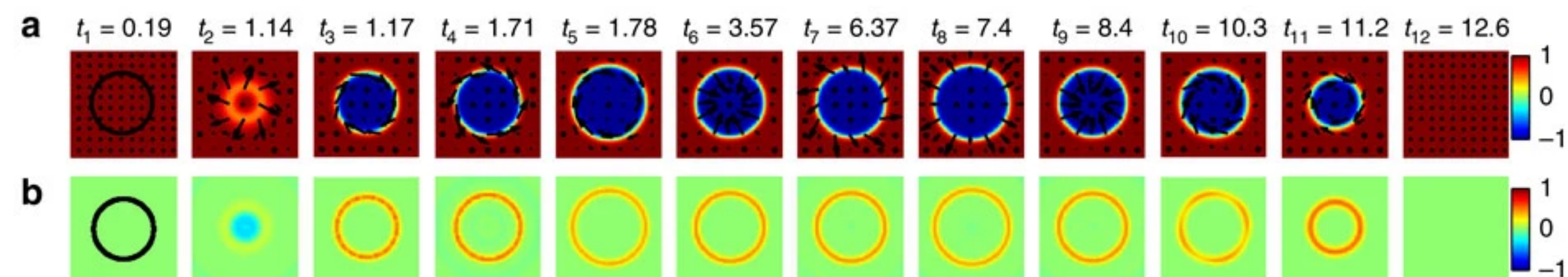
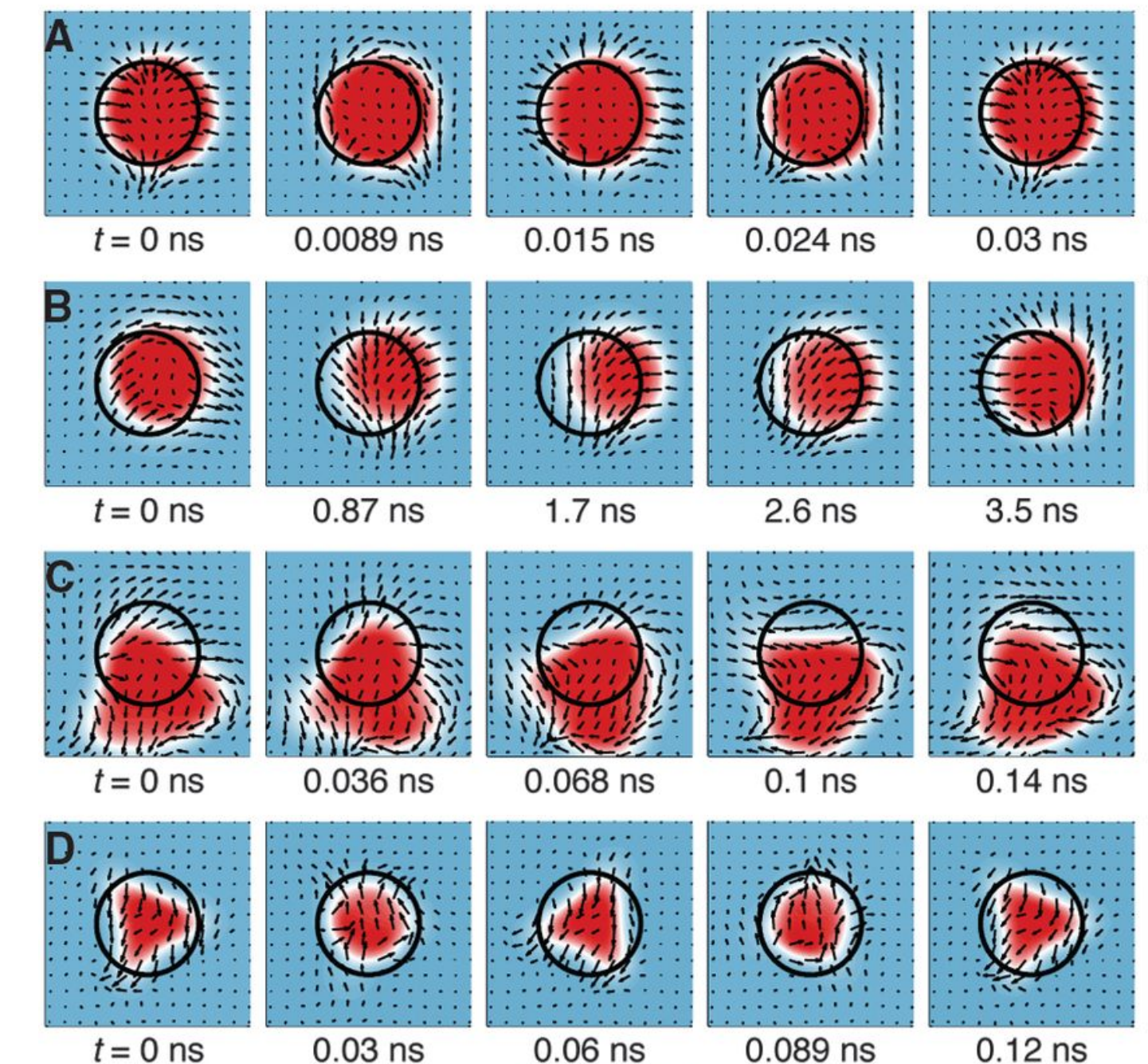
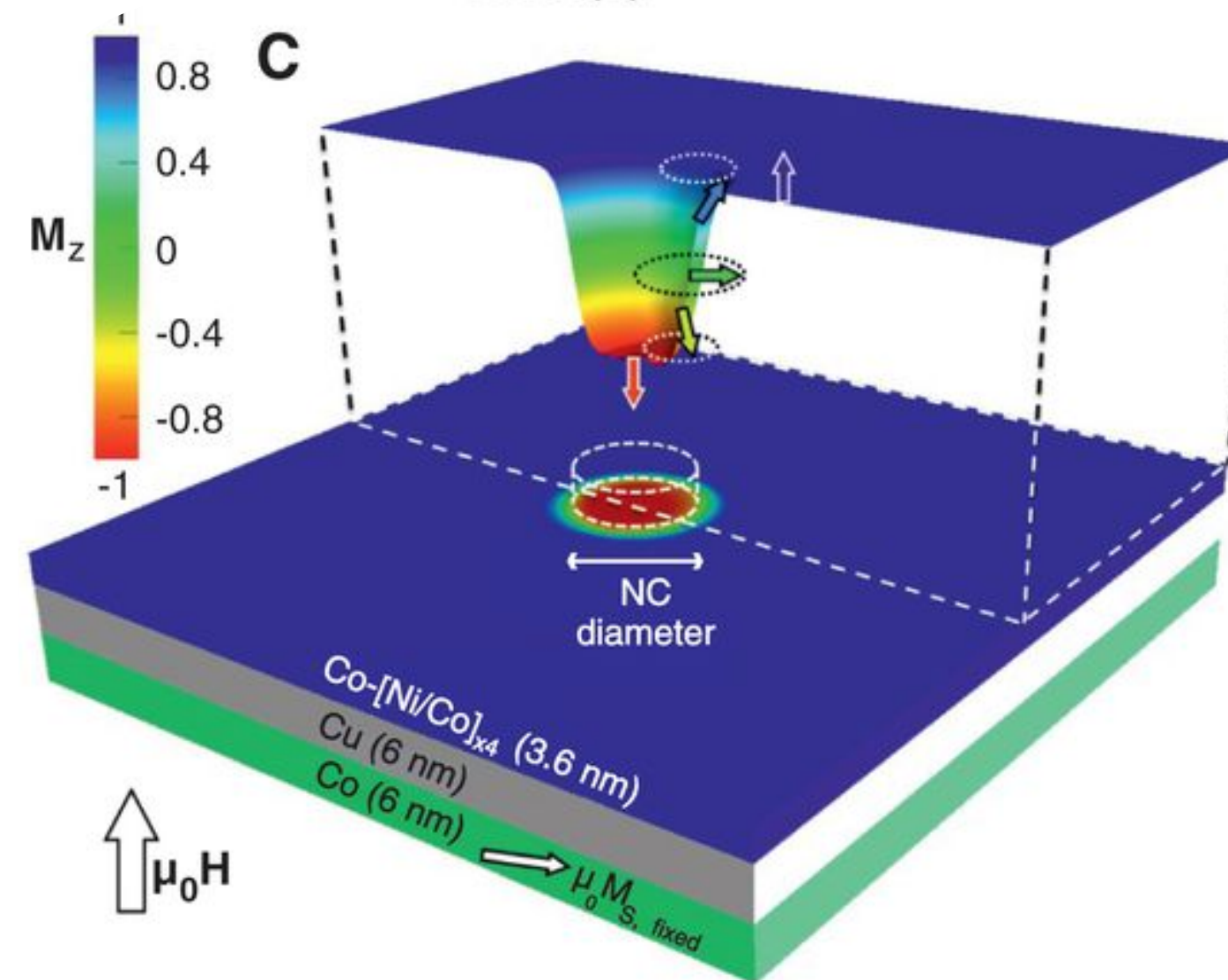
Case study II: Spin Torque–Generated Solitons

Spin torque oscillator



Y. Zhou et al. Nature **547** 428 (2017)

Magnetic solitons

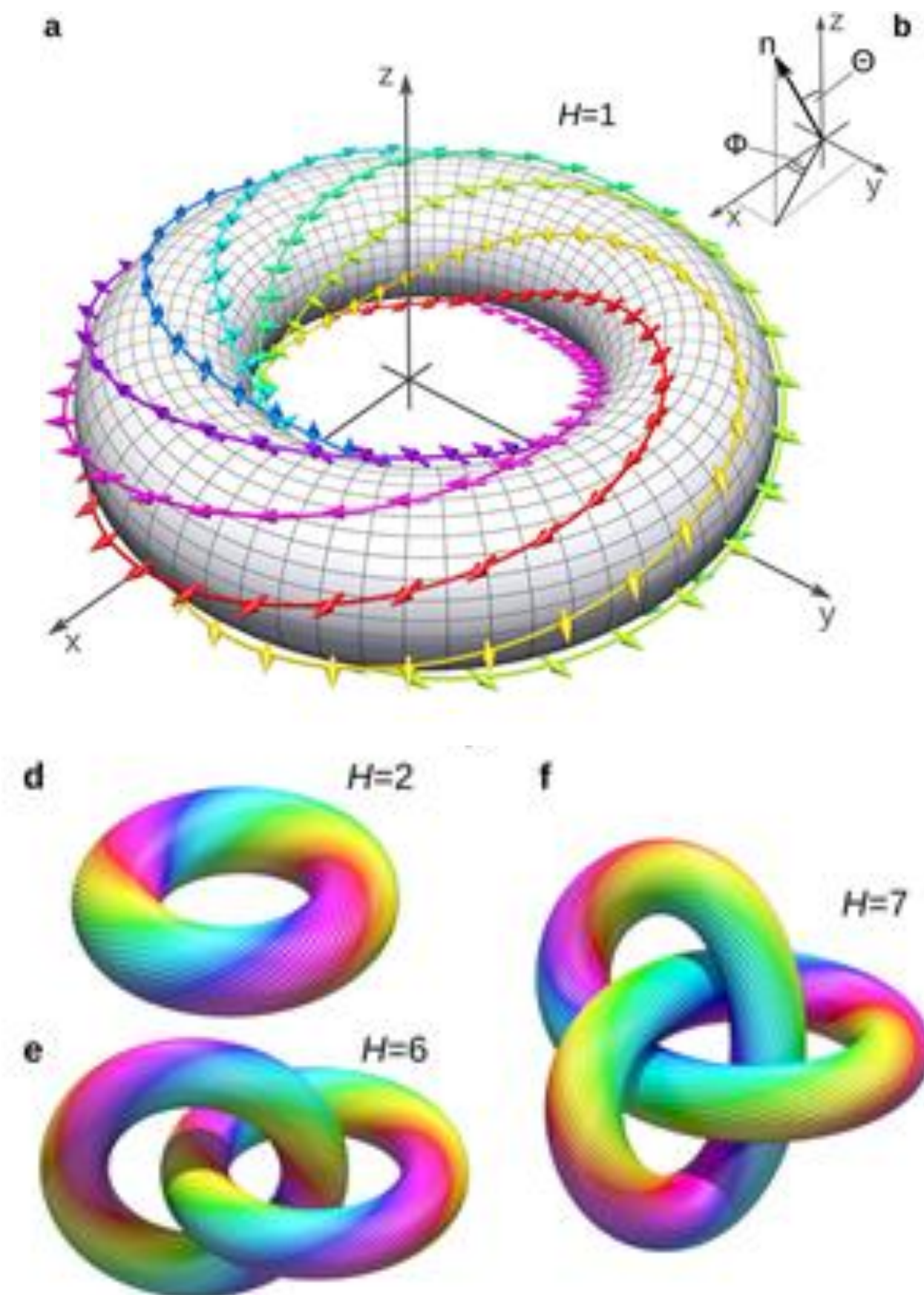


S. M. Mohseni et al. Science **338** 6125 (2015)

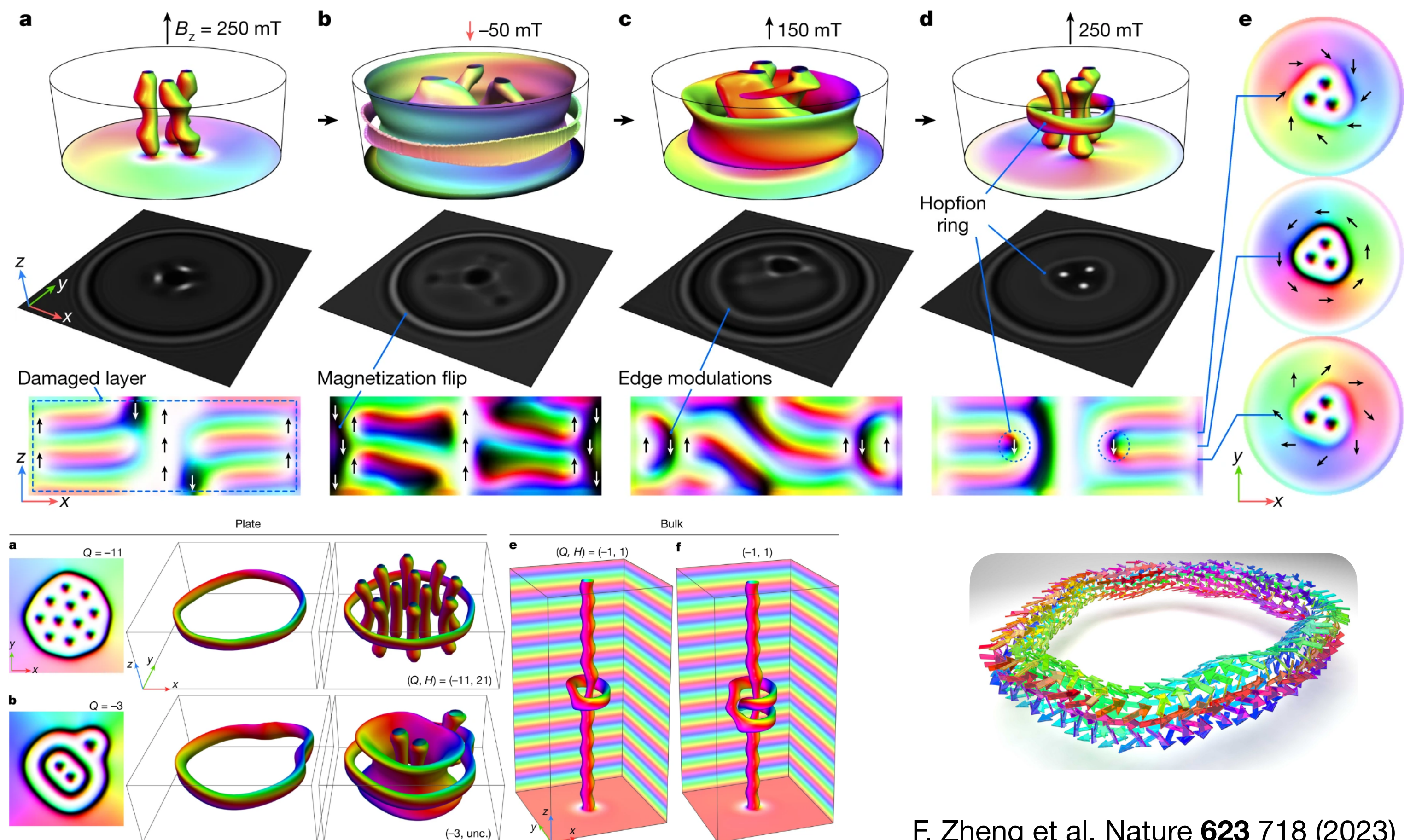
Y. Zhou et al. Nat. Comm. **6** 8193 (2015)

Case study II: Magnetic hopfions

Hopfions

F. N. Rybakov et al. APL Mater. **10** 111113 (2022)

Simulations of hopfions in FeGe

F. Zheng et al. Nature **623** 718 (2023)

Atomistic Spin Dynamics

Back to the Heisenberg Hamiltonian

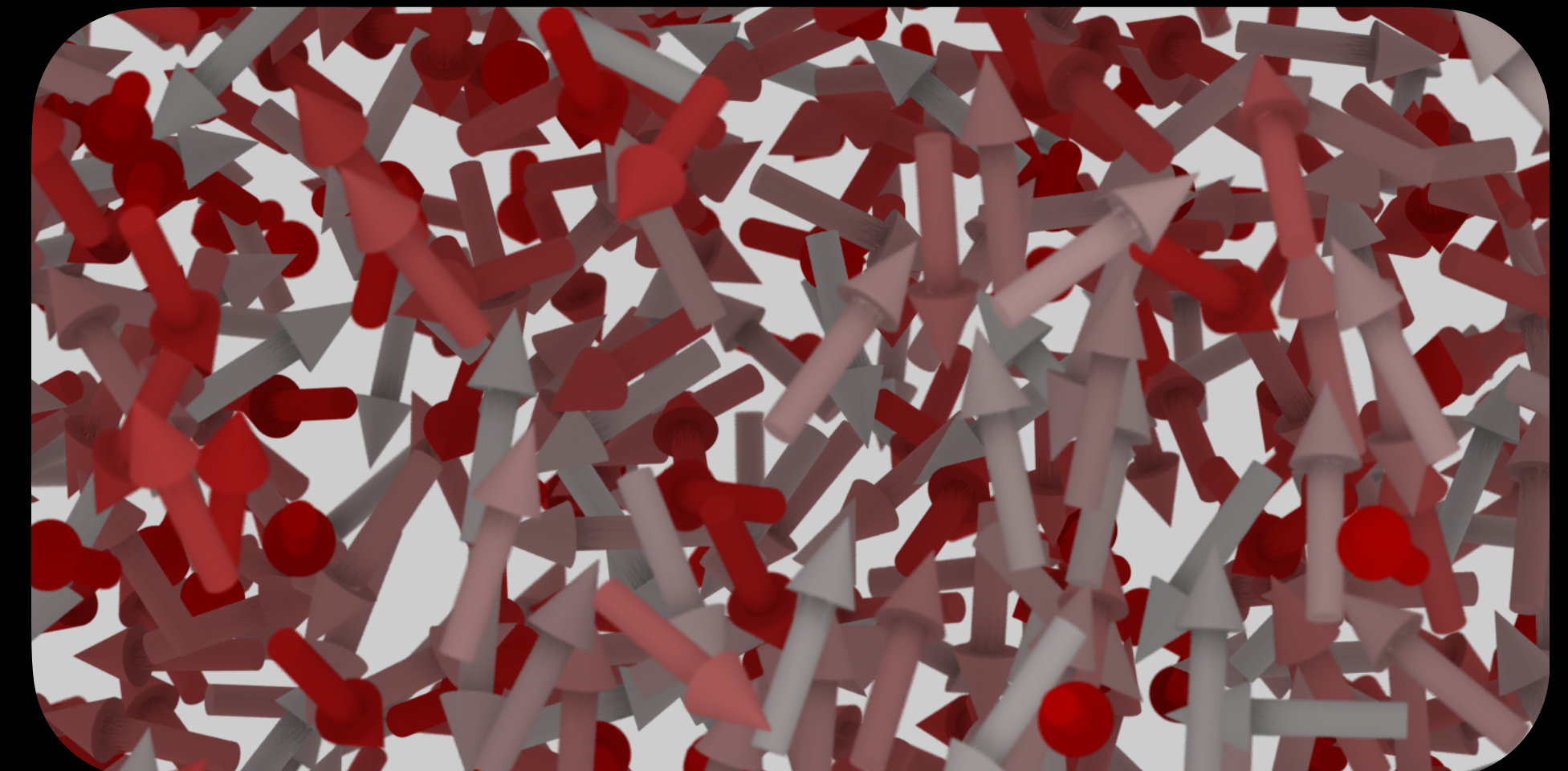
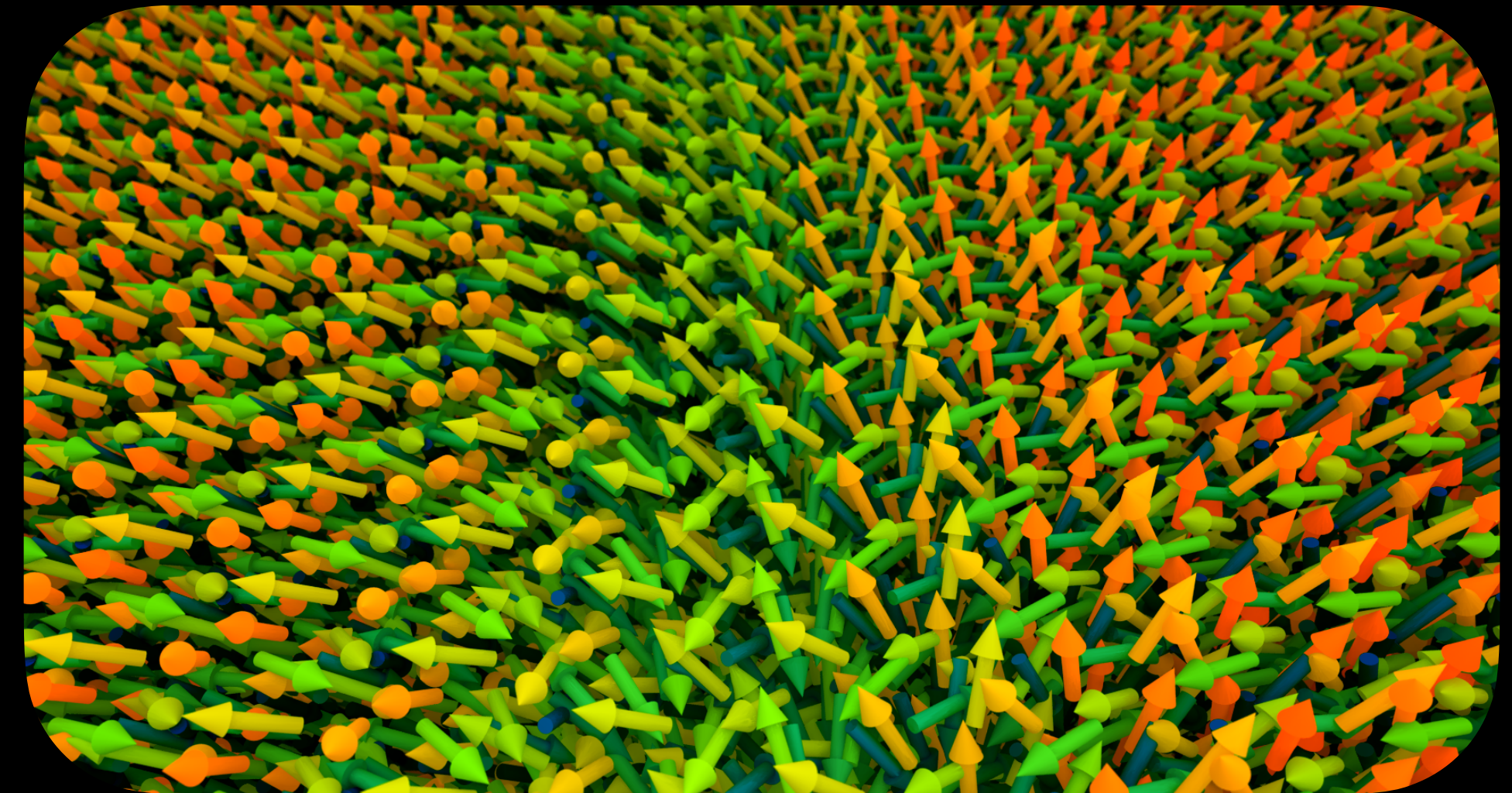
$$\mathcal{H} = -\frac{1}{2} \sum_{i \neq j} J_{ij} \mathbf{m}_i \cdot \mathbf{m}_j + \dots$$

Effective magnetic field:

$$\mathbf{B}_i = -\frac{\partial \mathcal{H}}{\partial \mathbf{m}_i}$$

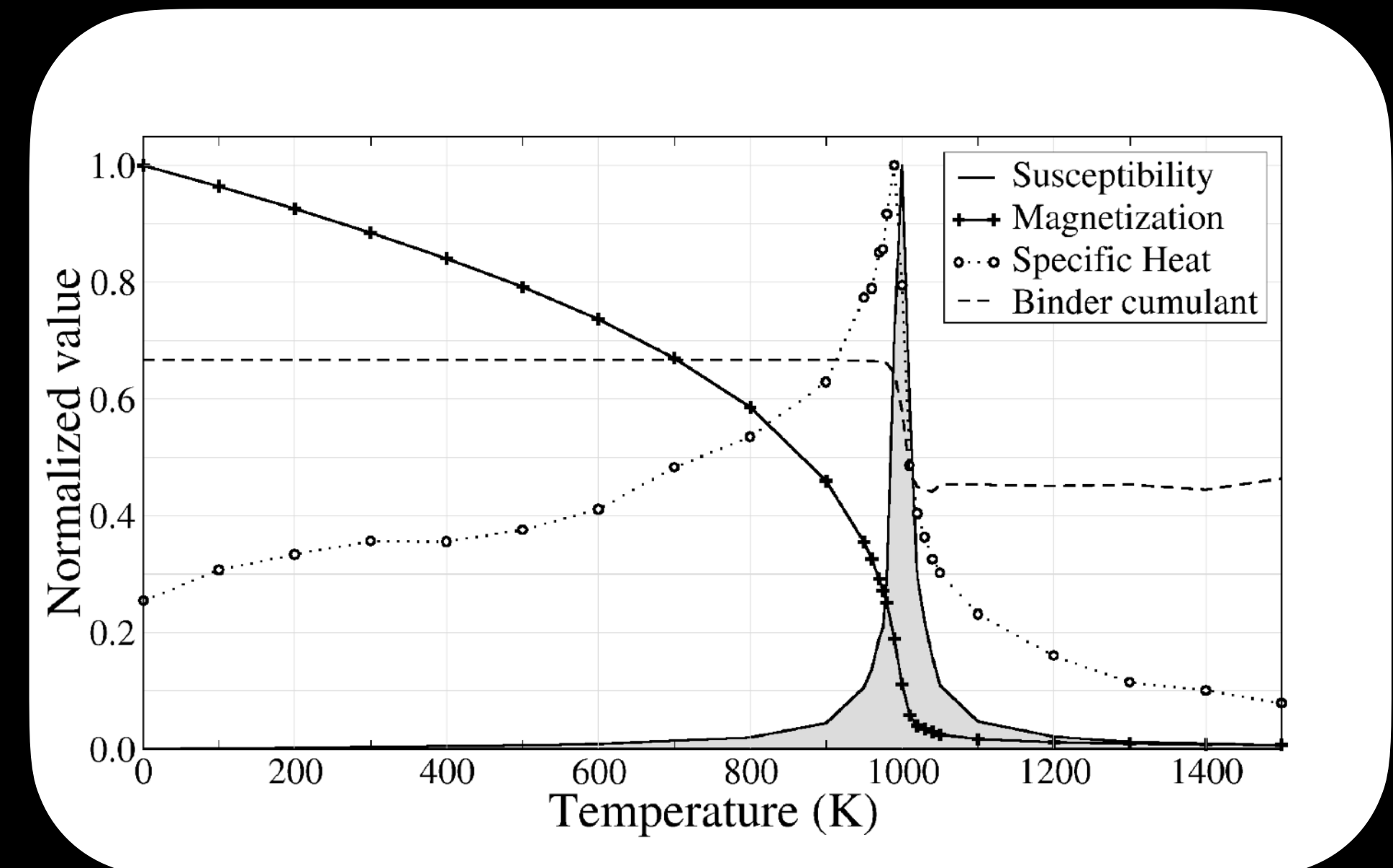
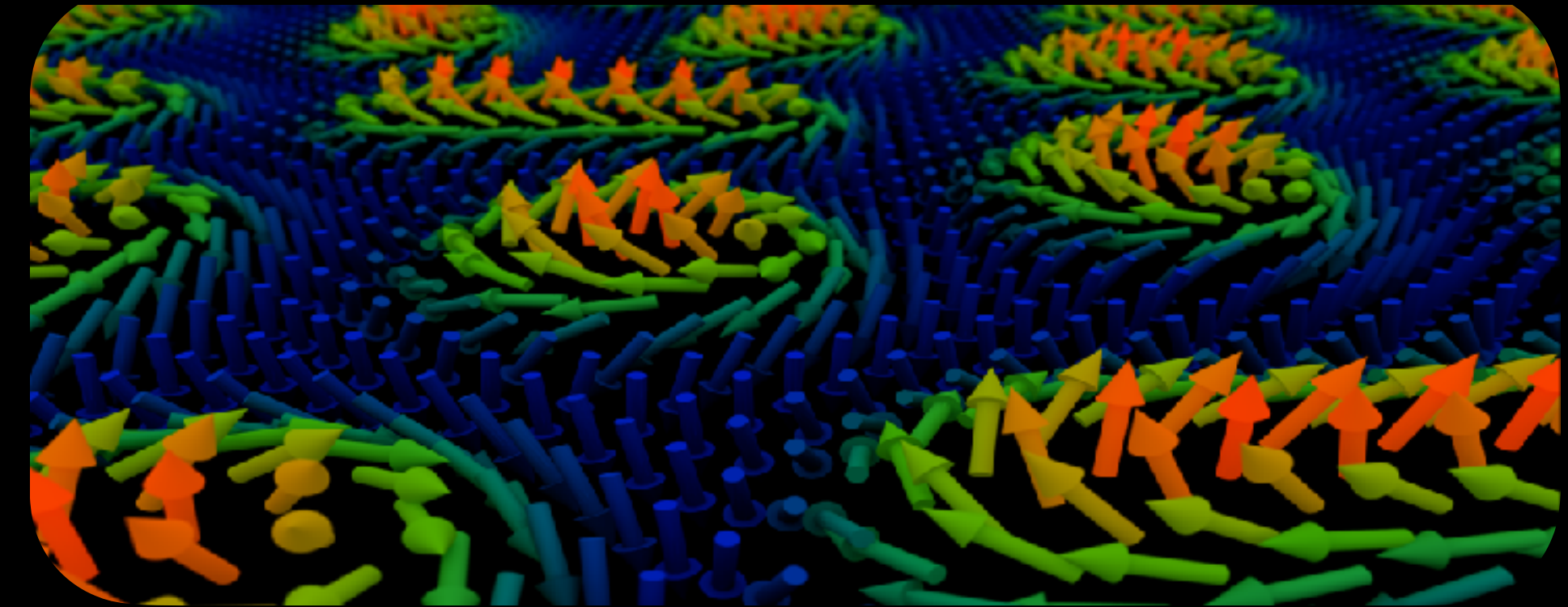
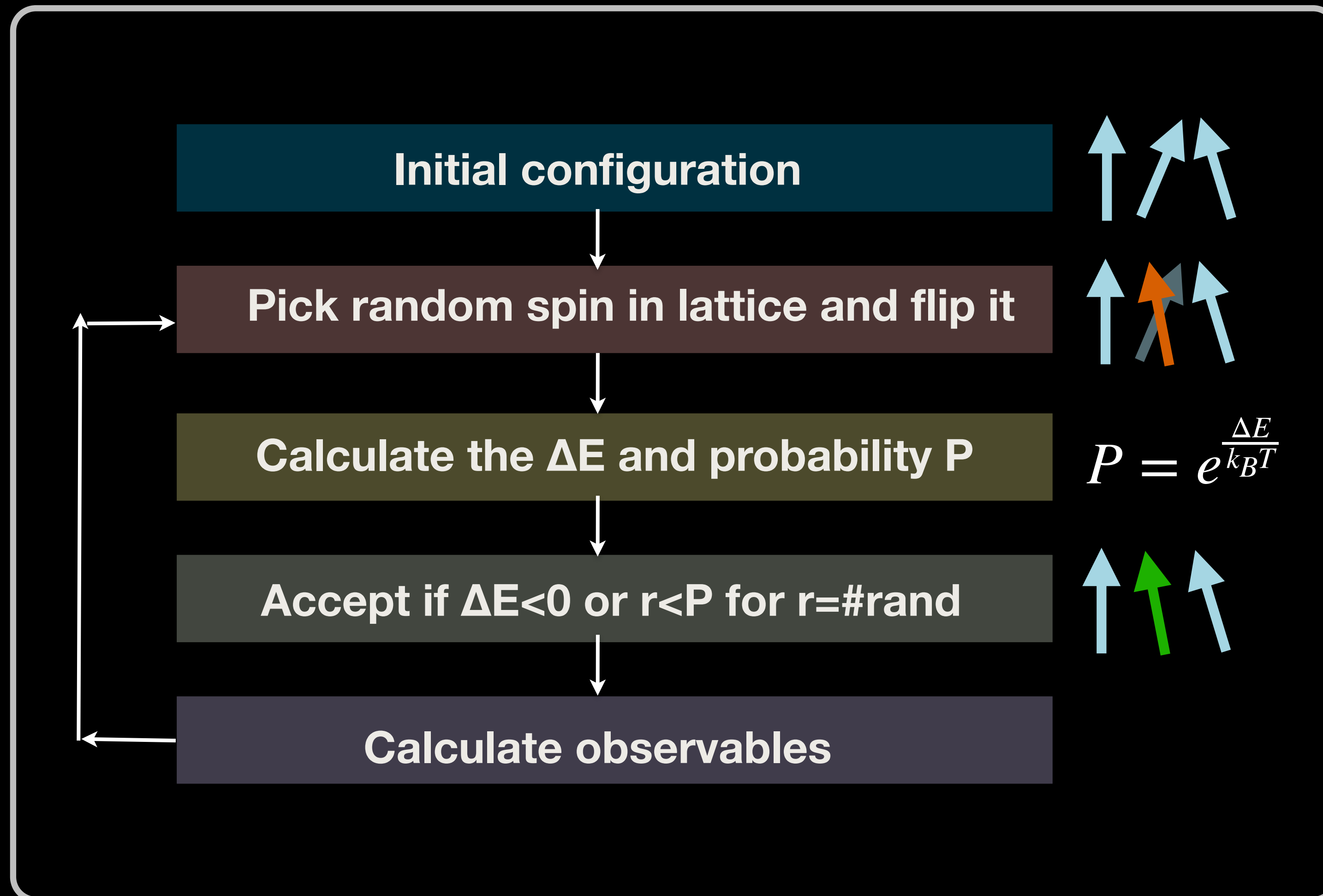
Landau-Lifshitz-Gilbert
EOM:

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



Monte Carlo methods

Ground states and thermodynamics



Monte Carlo methods

Real-life minimisation example

Ising Hamiltonian

$$H = - \sum_{\langle i,j \rangle} J \sigma_i \sigma_j \quad J = +1$$

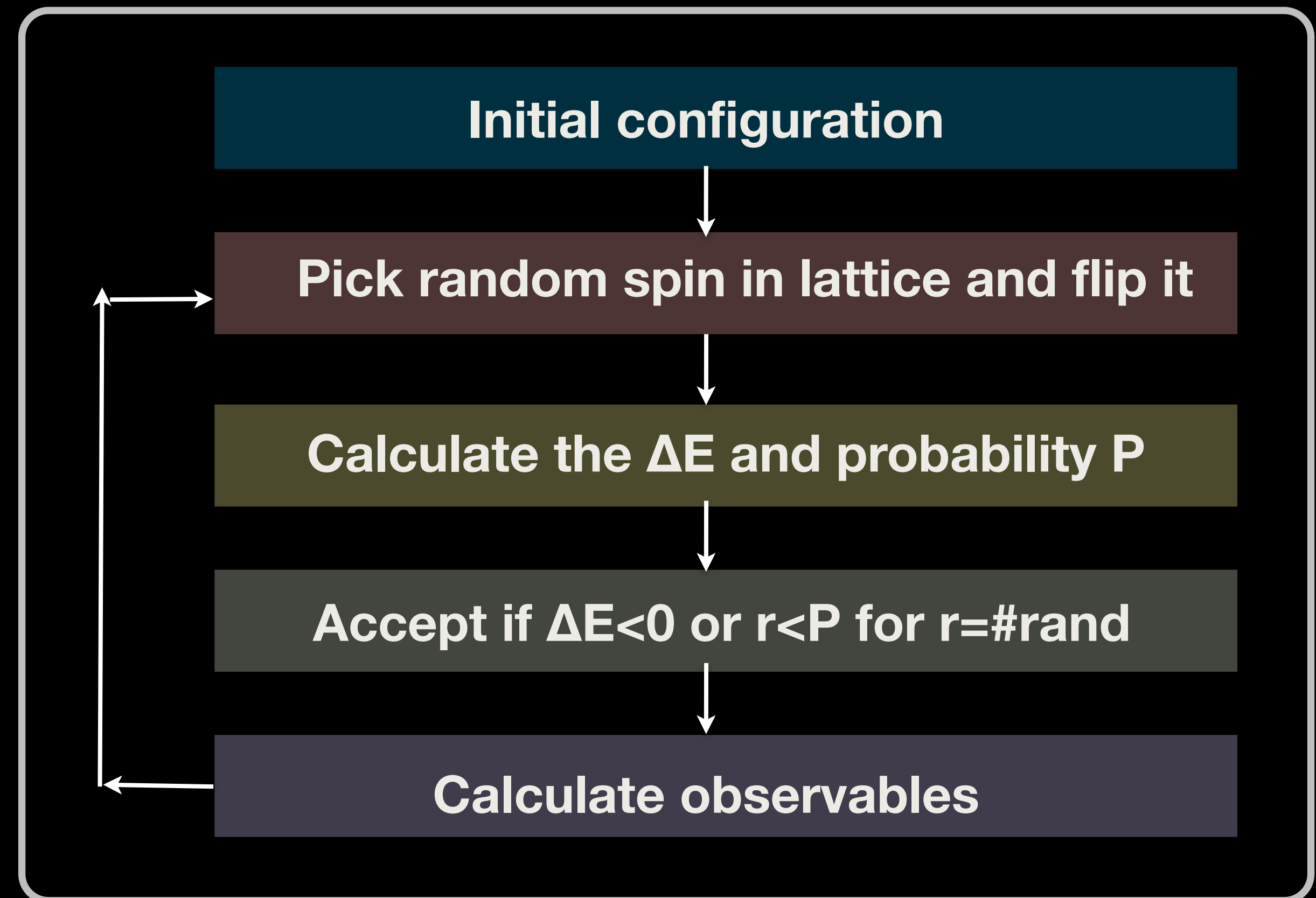
$$\sigma = -1 = \downarrow$$



$$\sigma = +1 = \uparrow$$



$\langle i,j \rangle$ = your nearest neighbours



Atomistic Spin Dynamics

Back to the Heisenberg Hamiltonian again..

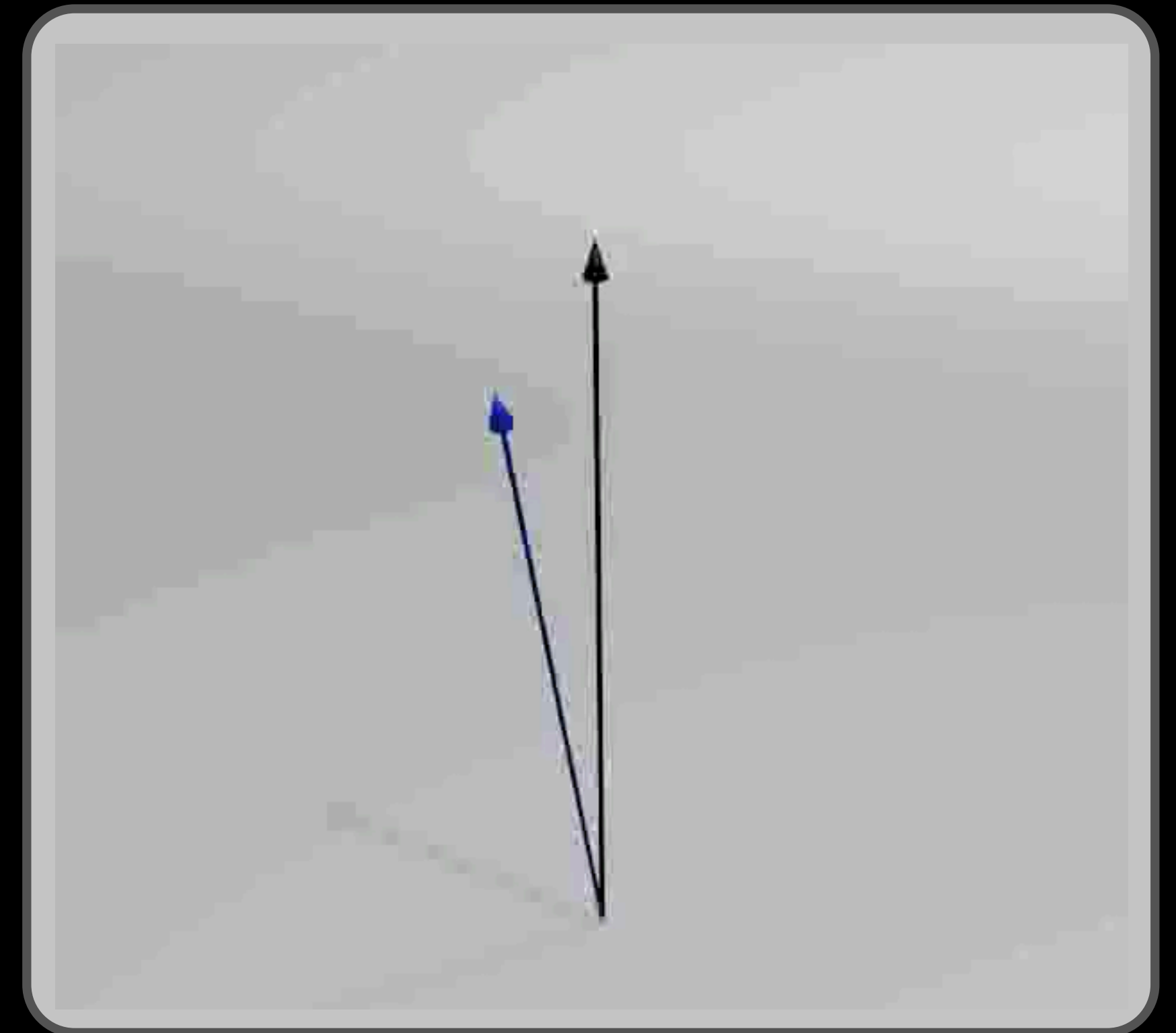
$$\mathcal{H} = -\frac{1}{2} \sum_{i \neq j} J_{ij} \mathbf{m}_i \cdot \mathbf{m}_j + \dots$$

Effective magnetic field:

Landau-Lifshitz-Gilbert
EOM:

$$\mathbf{B}_i = -\frac{\partial \mathcal{H}}{\partial \mathbf{m}_i}$$

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



Dissipation rate:
Gilbert damping α

Atomistic Spin Dynamics

Temperature and Stochastic ODE

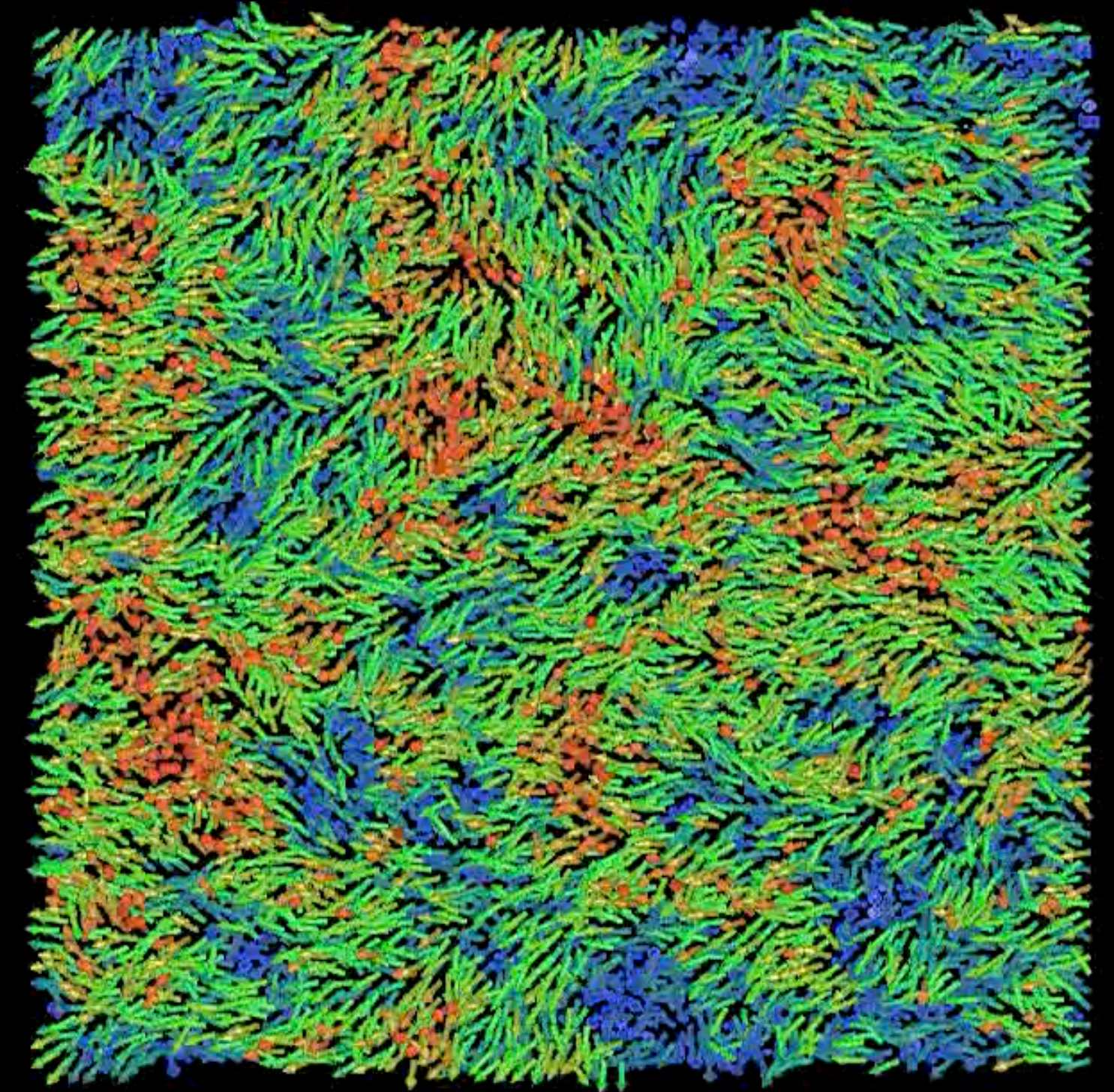
Langevin dynamics: Fluctuating field

$$\langle b_{i,\mu}^{fl}(t) \rangle = 0, \langle b_{i,\mu}^{fl}(t) b_{j,\nu}^{fl}(t') \rangle = 2\tilde{D} \delta_{\mu\nu} \delta_{ij} \delta(t - t')$$

i.e. white noise

Magnitude of fluctuations

$$D = \frac{\alpha}{(1 + \alpha^2)} \frac{\eta}{\mu_B m} \quad \eta = k_B T$$

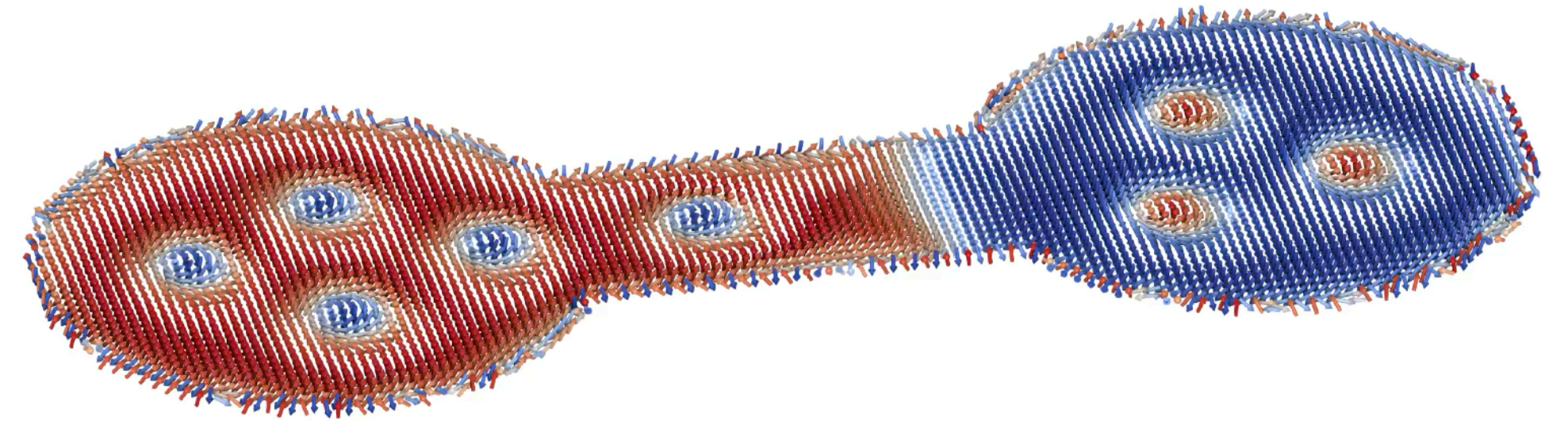
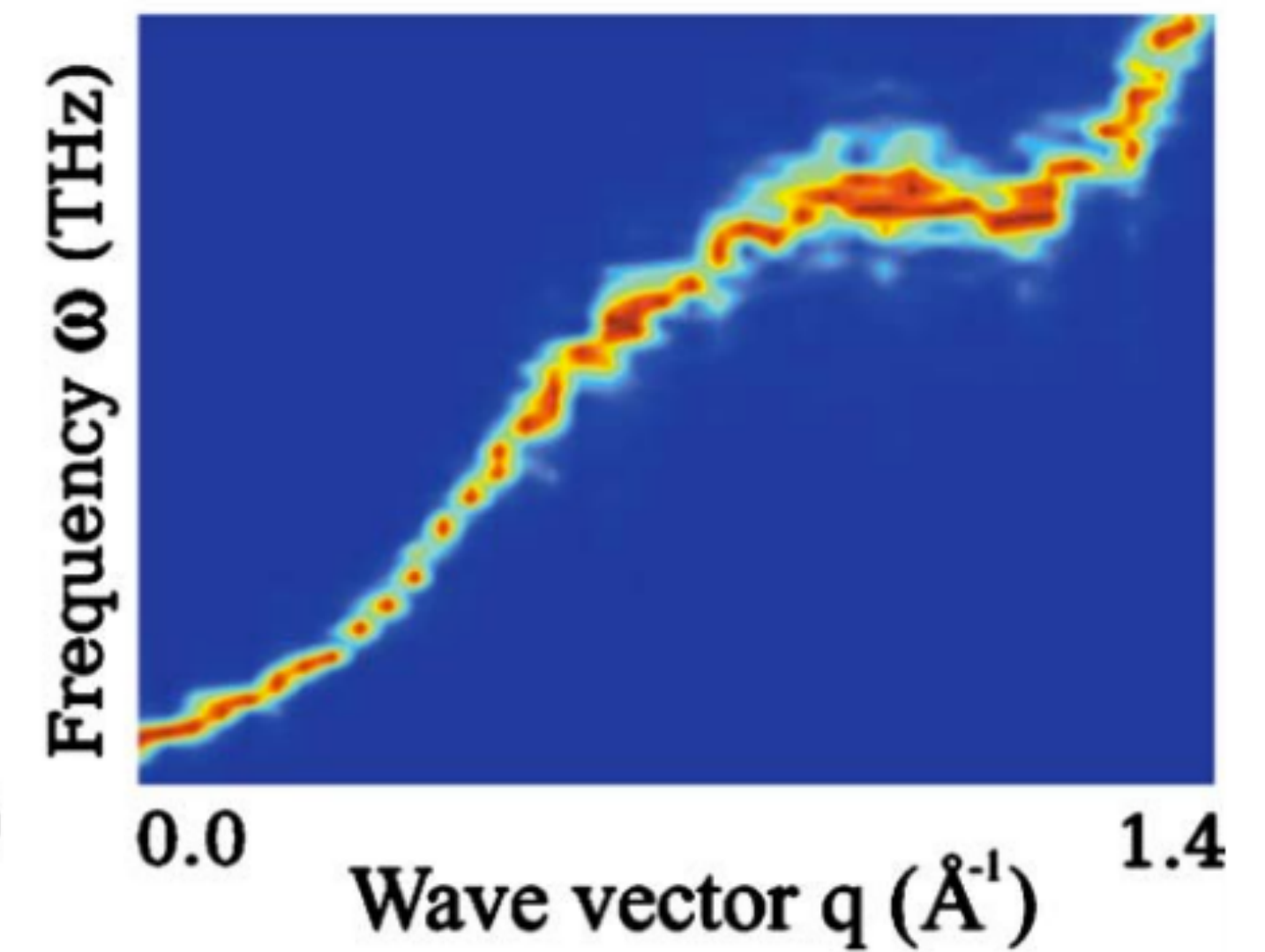
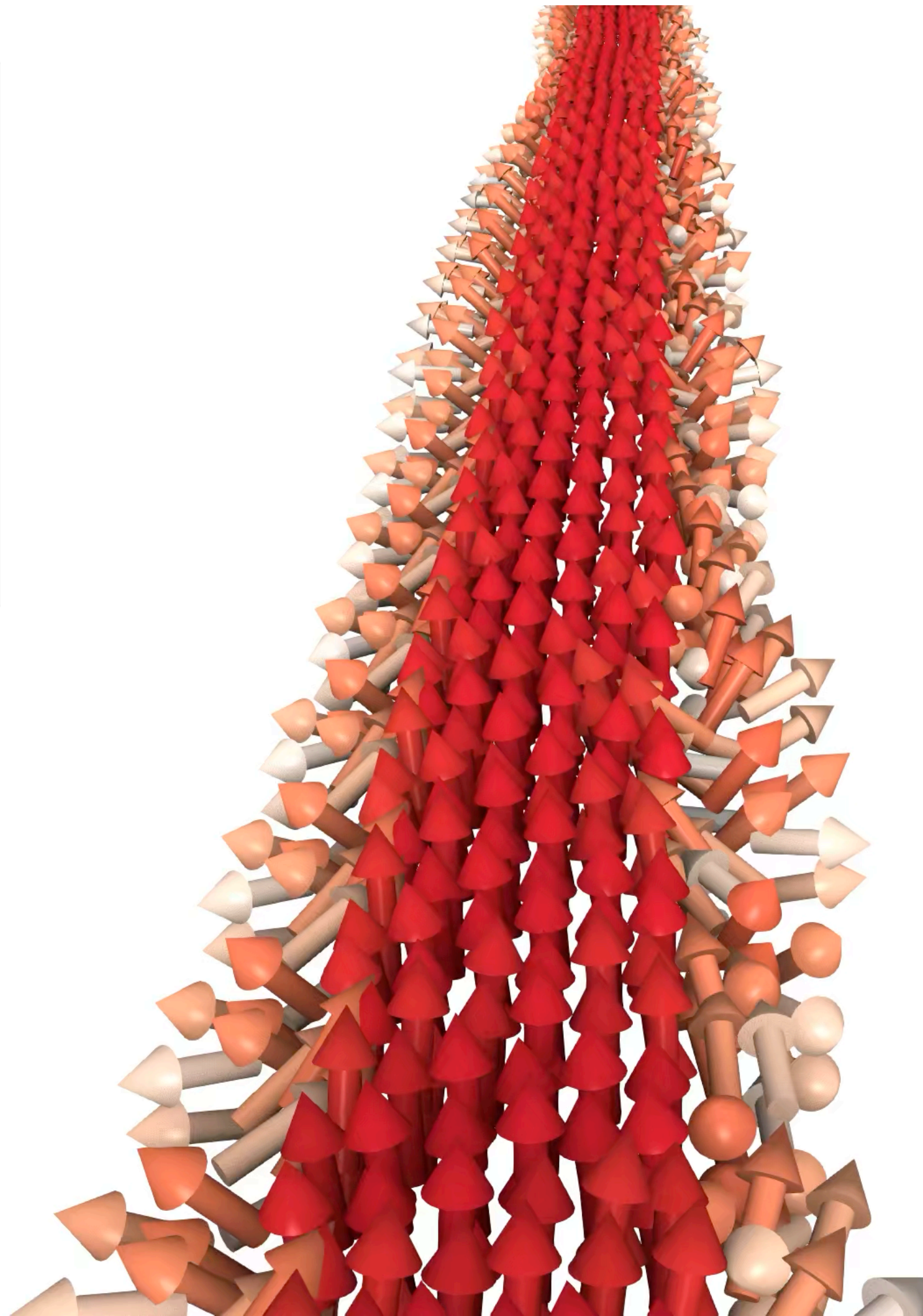
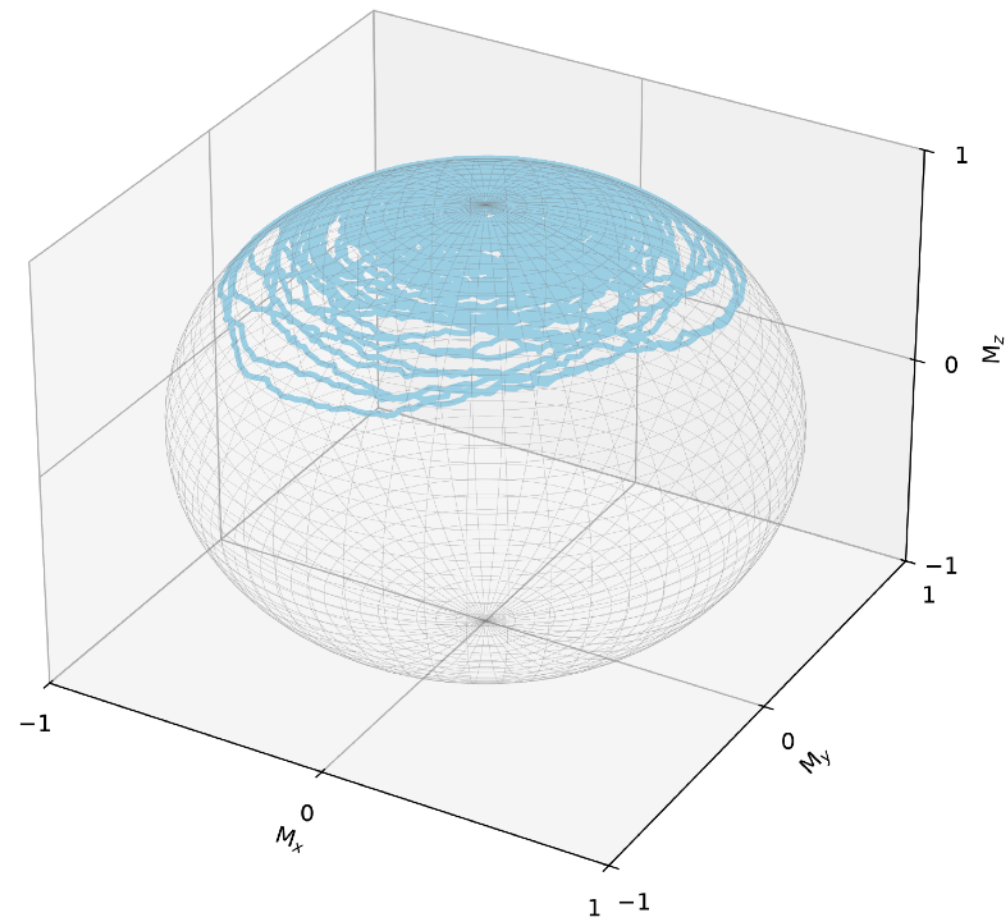
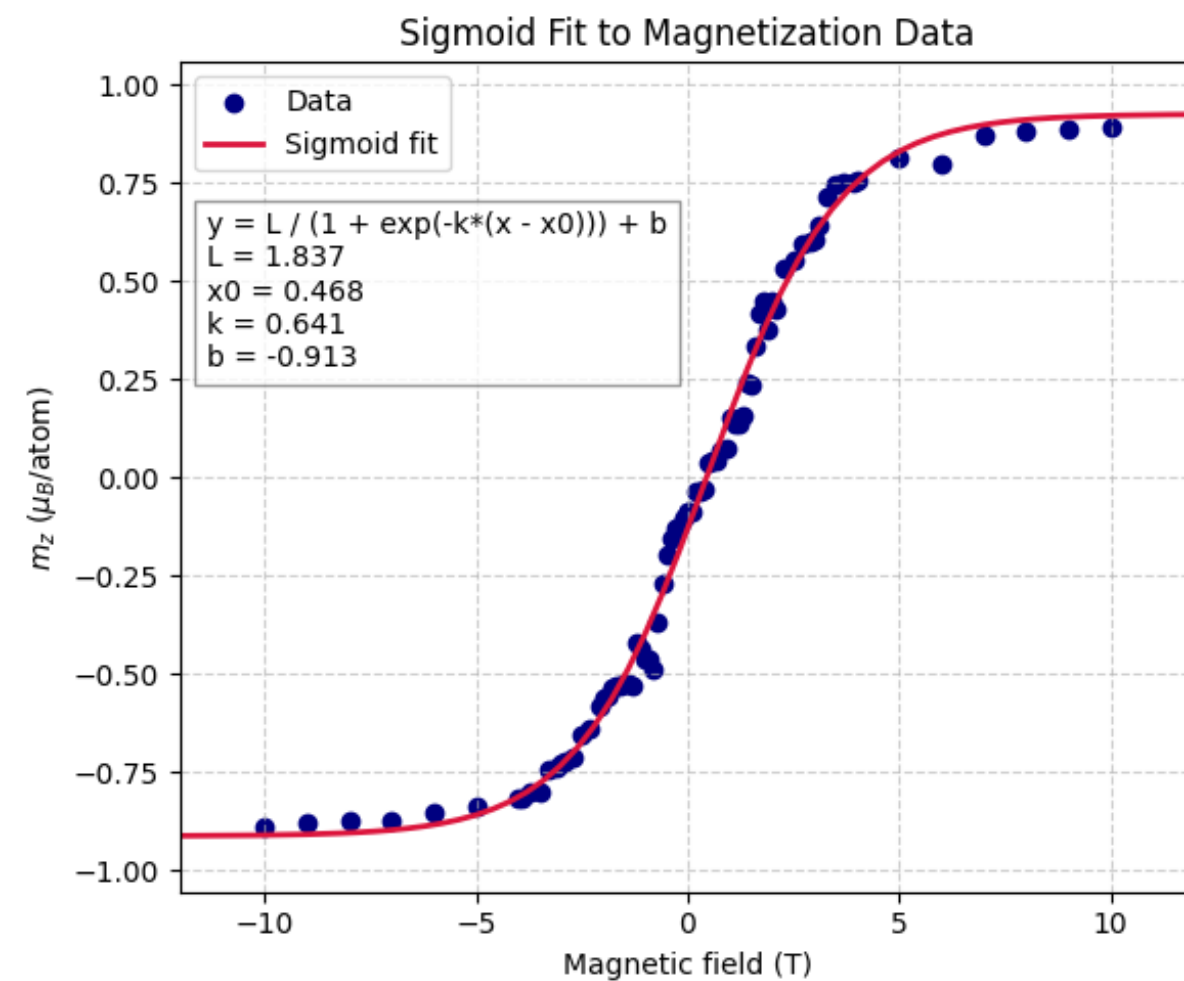


Stochastic Landau-Lifshitz equation on Gilbert form

$$\frac{d\mathbf{m}_i}{dt} = -\gamma \mathbf{m}_i \times (\mathbf{B}_i + b_i(T)) - \alpha \frac{\gamma}{m_i} \mathbf{m}_i \times (\mathbf{m}_i \times (\mathbf{B}_i + b_i(T)))$$

Atomistic Spin Dynamics

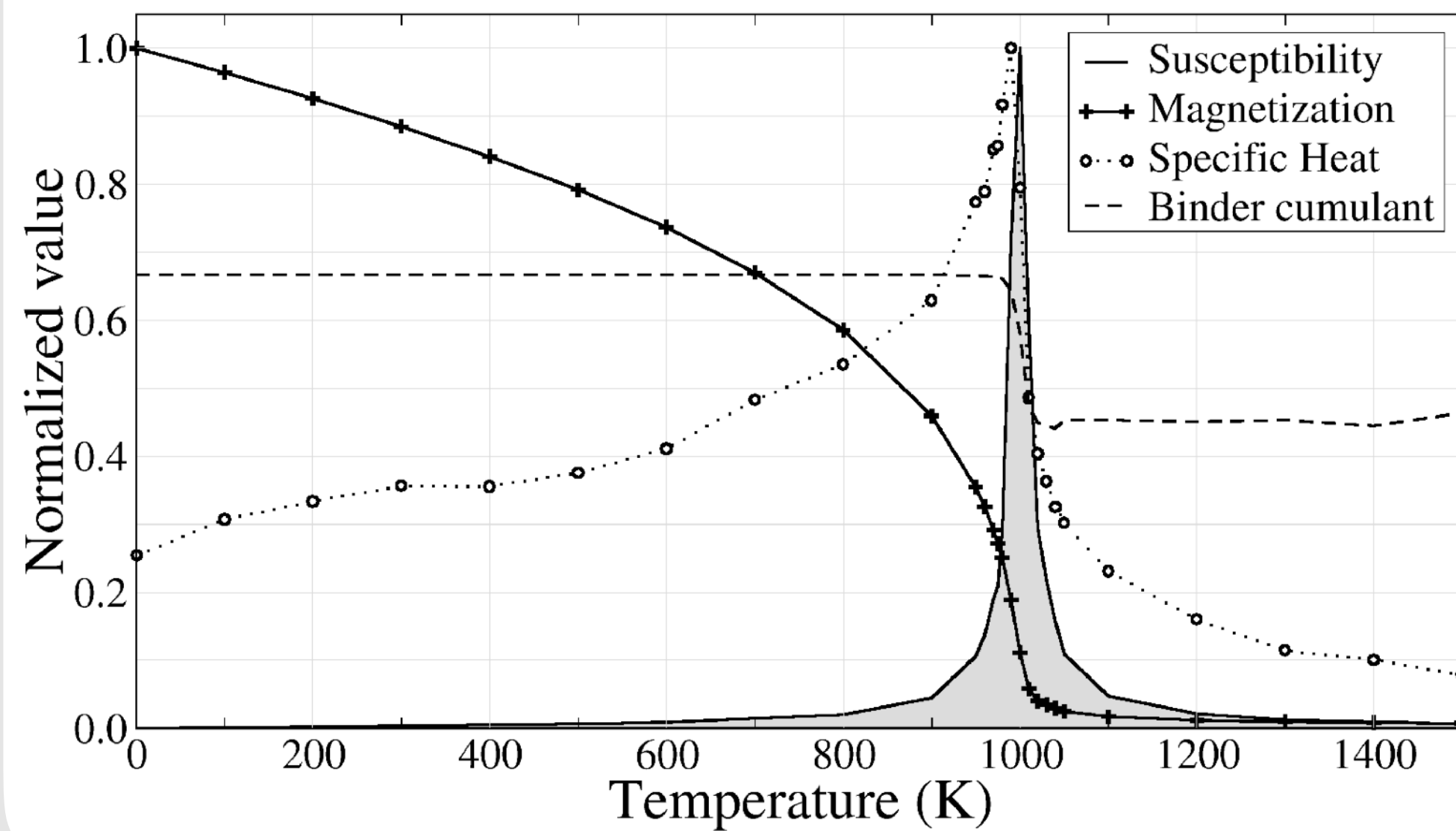
Some examples of dynamic measurables



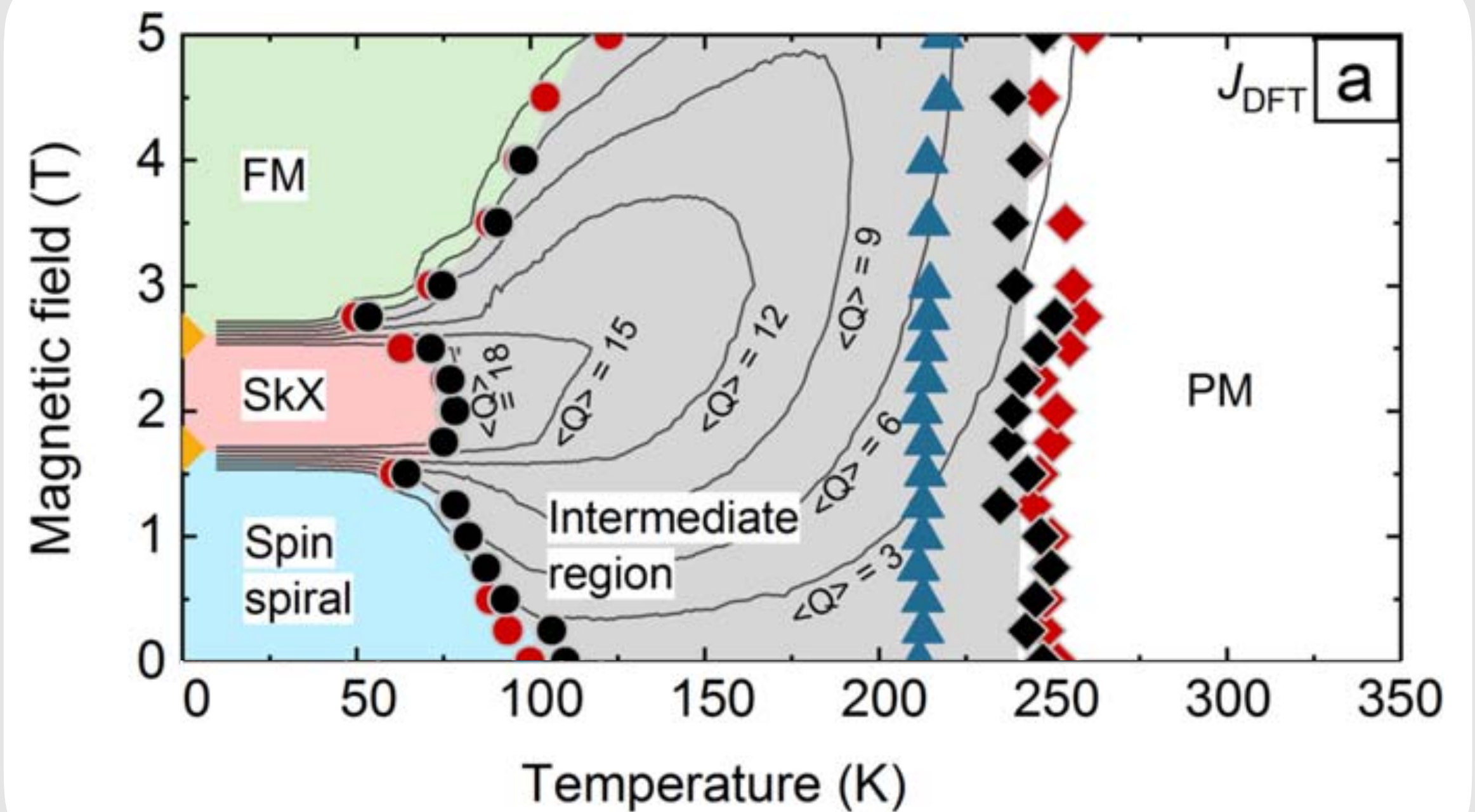
Atomistic Spin Dynamics (or Monte Carlo)

Phase diagrams

Thermodynamic measurables
bcc Fe:

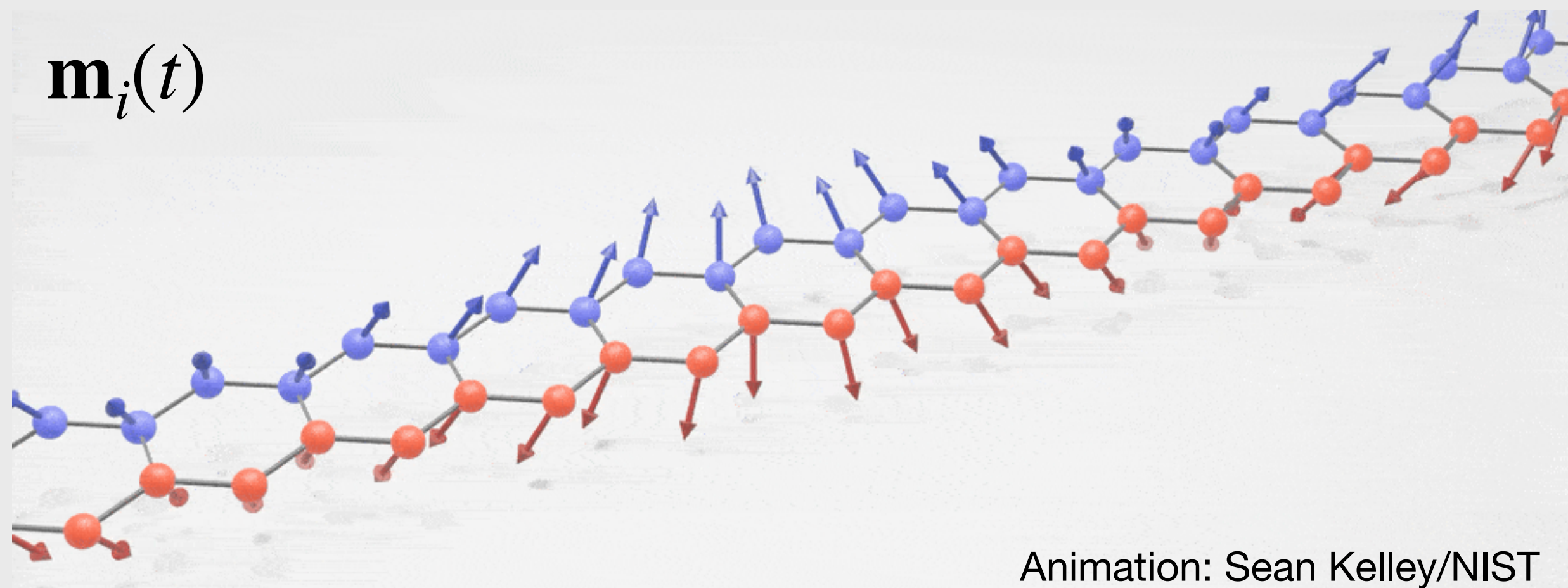


Magnetic state stability
Pd/Fe/Ir(111)



Atomistic Spin Dynamics

Magnons

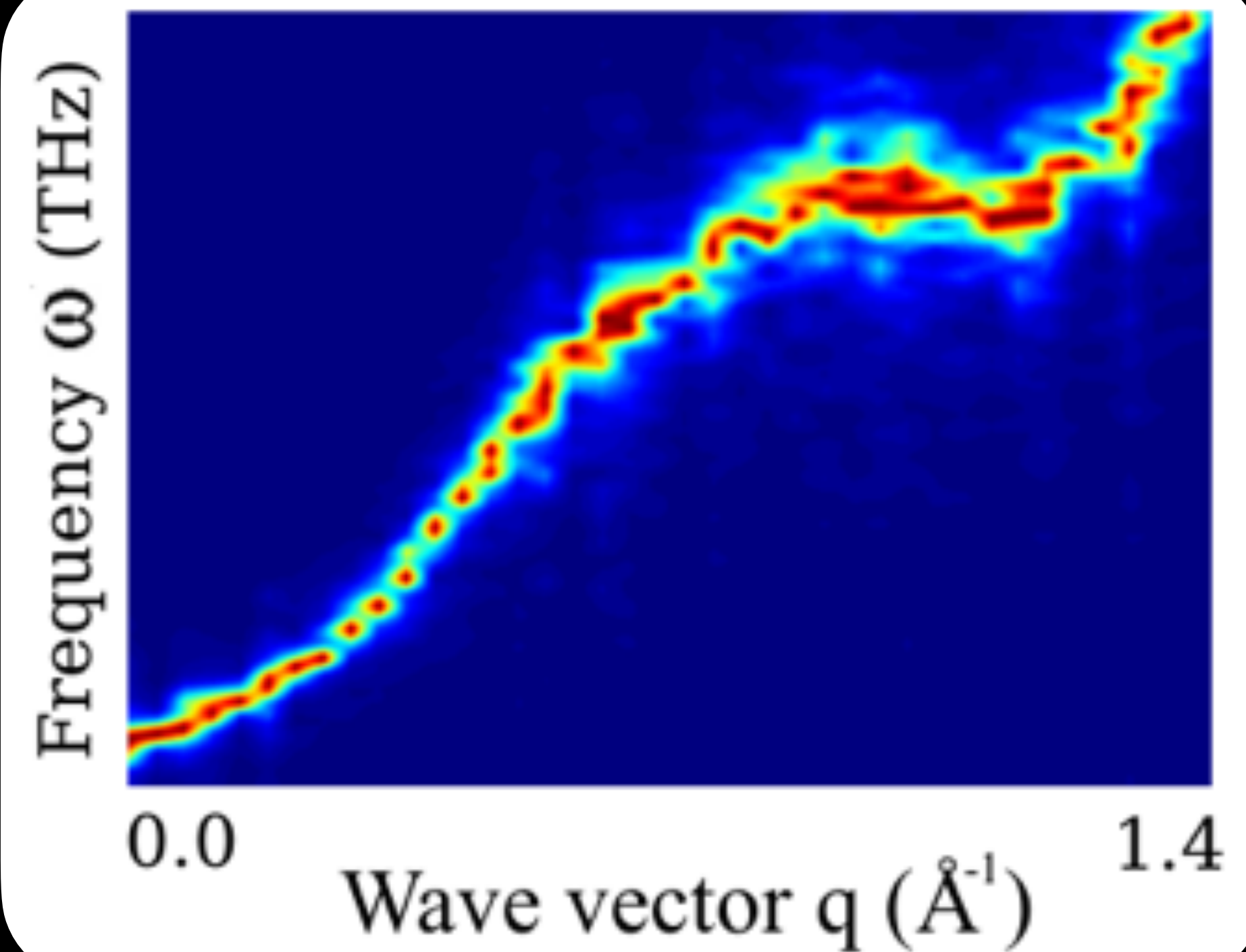


Spatial and temporal correlations

$$C^k(\mathbf{r} - \mathbf{r}', t) = \langle m_{\mathbf{r}}^k(t) m_{\mathbf{r}'}^k(0) \rangle - \langle m_{\mathbf{r}}^k(t) \rangle \langle m_{\mathbf{r}'}^k(0) \rangle$$

Fourier transform -> Dynamic structure factor

$$S^k(\mathbf{q}, \omega) = \frac{1}{\sqrt{2\pi N}} \sum_{\mathbf{r}, \mathbf{r}'} e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')} \int_{-\infty}^{\infty} e^{i\omega t} C^k(\mathbf{r} - \mathbf{r}', t) dt$$



Compare with scattering experiments

Alternative: Linear spin-wave theory

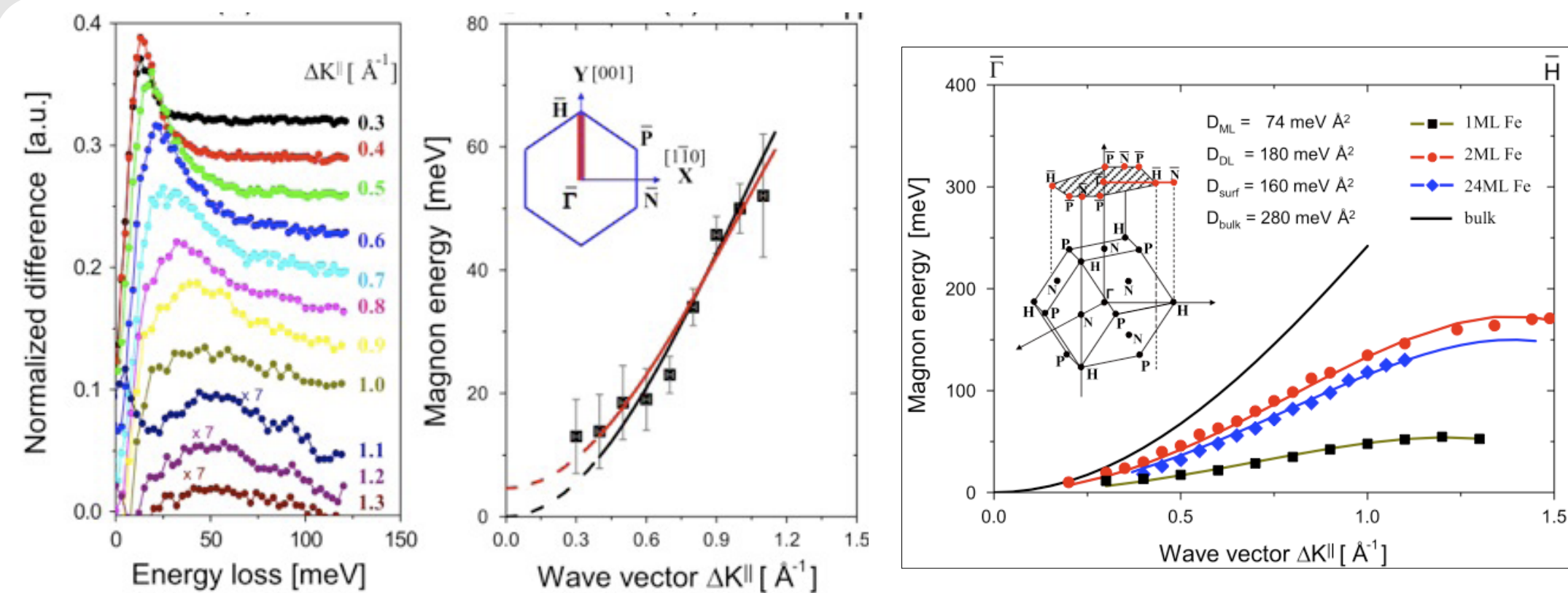
Atomistic Spin Dynamics

Showcase I: Magnon softening in Fe/W(110)

Spin-polarized electron energy loss spectroscopy (SPEELS)

1 Fe ML on W(110)

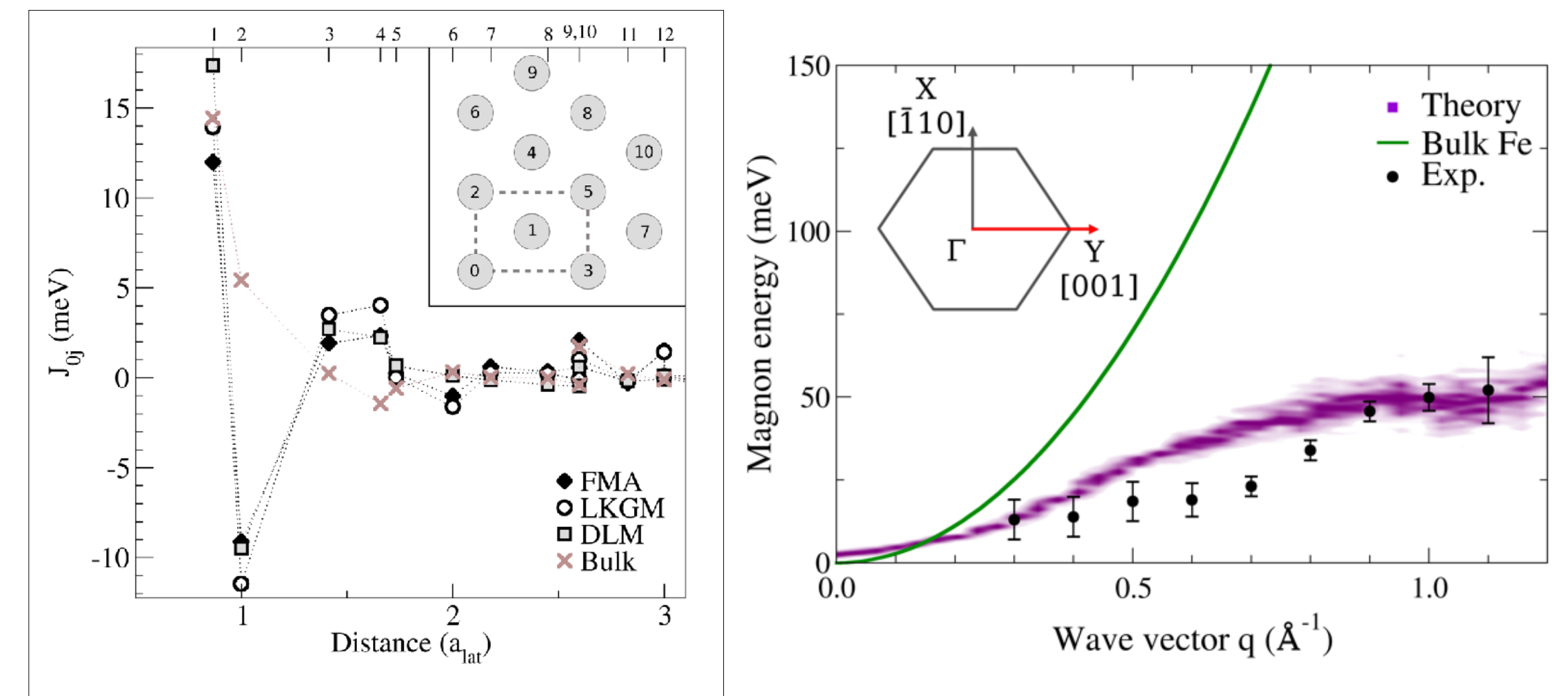
First ever spin wave monolayer measurement



Significant softening compared to bulk Fe
Why? Unclear

J. Prokop et al. PRL **102** 177206 (2009)

Density functional theory
+
Atomistic spin dynamics



Softening captured.
Why: Antiferromagnetic next-nearest neighbours

A. Bergman et al PRB **81** 144416 (2010)

Atomistic Spin Dynamics

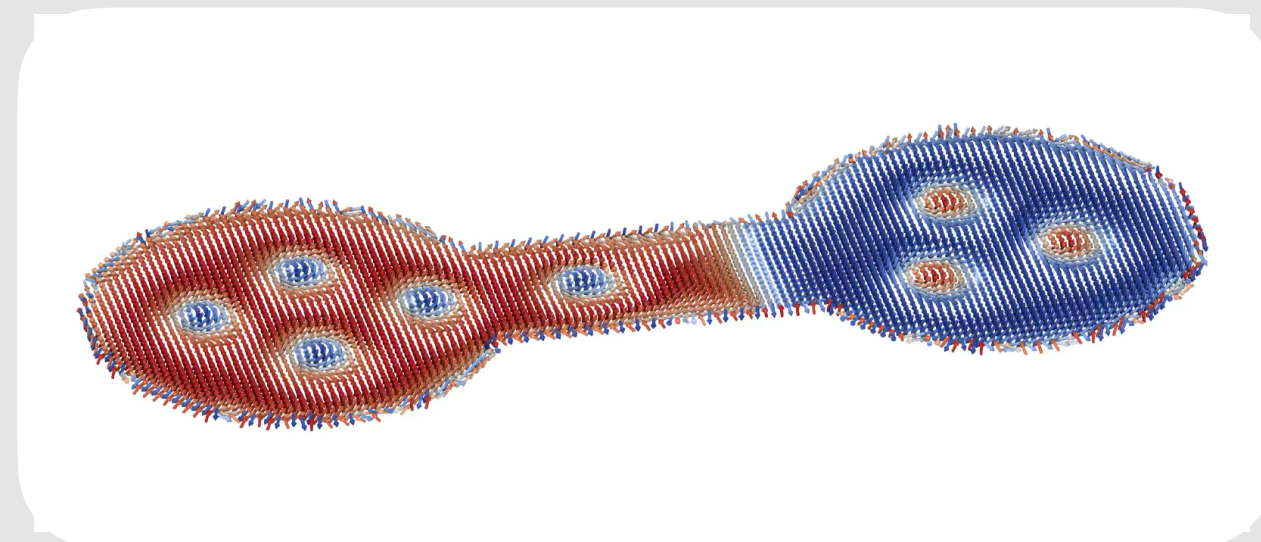
Showcase III: Spin-orbit assisted switching

Current driven dynamics:
Spin transfer torques (STT)
Spin orbit torques (SOT)

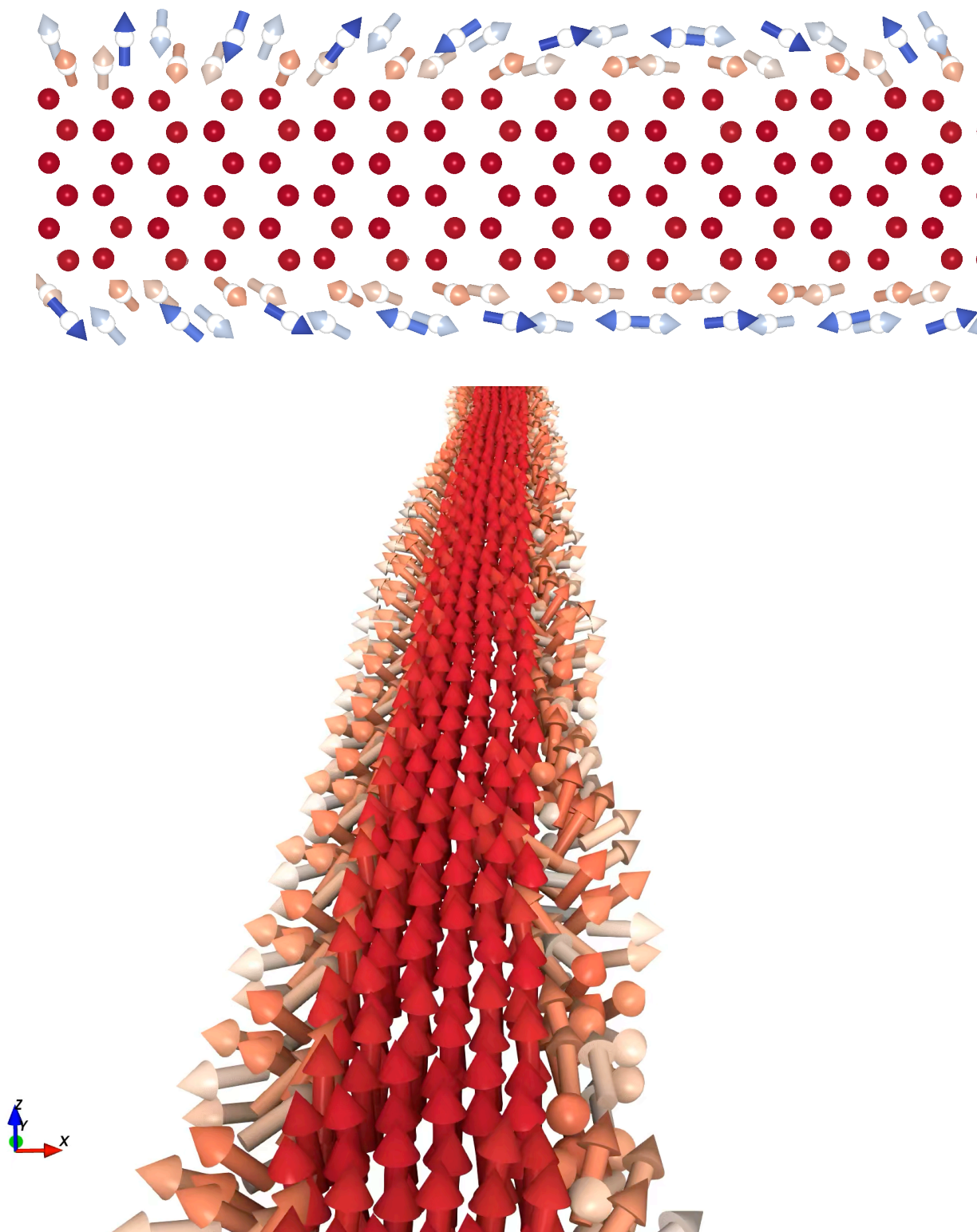
$$\mathbf{B}_{\text{SOT}} = B_{\text{PT}}^{\text{SOT}} (\boldsymbol{\sigma} - \alpha_G \mathbf{m} \times \boldsymbol{\sigma}) + B_{\text{RT}}^{\text{SOT}} (\mathbf{m} \times \boldsymbol{\sigma} + \alpha_G \boldsymbol{\sigma})$$

$$\mathbf{B}_{\text{PT}}^{\text{SHE}} = \beta_{\text{SOT}} \frac{\hbar j_e \theta_{\text{SH}}}{2eM_{\text{sd}}} = \beta_{\text{SOT}} \mathbf{B}_{\text{RT}}^{\text{SHE}}$$

Can also act on magnetization gradients



Example: Fe₃GeTe₂ nano-flakes



Summary and conclusion

Versatile tools for many different applications

Micromagnetic simulations

Magnetization density

Micrometer scale

Minimisation

Domain walls

Dipole-driven dynamics

GHz regime

Selected reference

"Magnetism and Magnetic Materials"
by J.M.D. Coey

Selection of codes

mumax3



oommf



Atomistic Spin Dynamics

Localised moments

First-principles exchange interactions

Thermodynamics

Phase diagrams

Correlations

Exchange magnons and spin waves

Selected reference

"Atomistic Spin Dynamics -
Foundations and Applications"
by O. Eriksson et al.

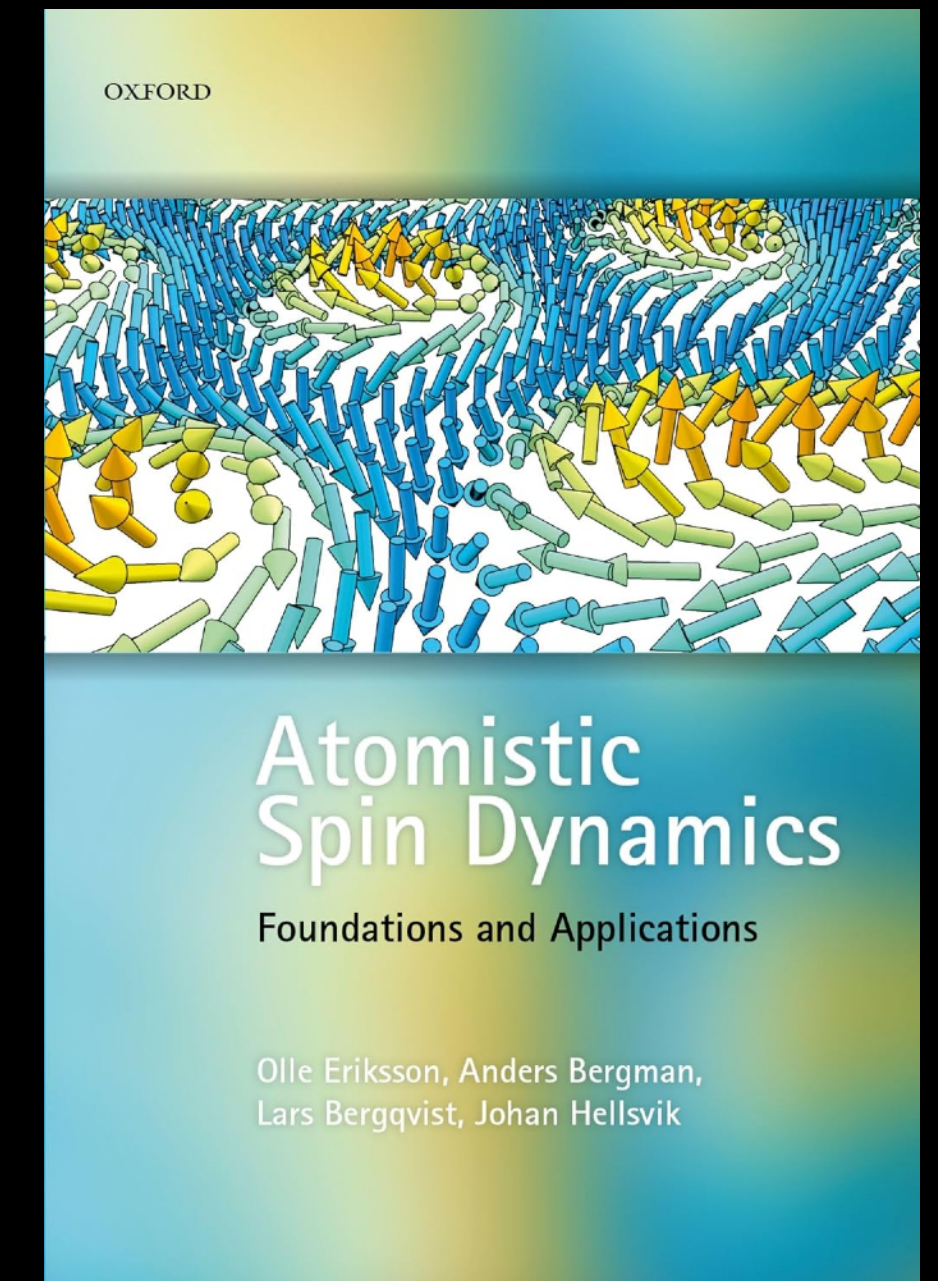
Selection of codes

Spirit

Spilady

Vampire

UppASD



<https://tinyurl.com/uppasd-book>

Thank you!

