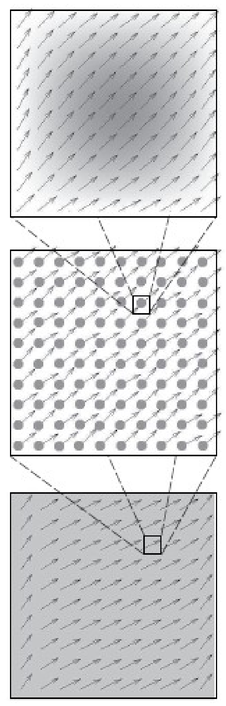
Johan Hellsvik, Björn Skubic, Lars Nordström, Olle Eriksson

Department of Physics and Materials Science
Uppsala University, Sweden

DYNAMICS OF DILUTED MAGNETIC SEMICONDUCTORS FROM ATOMISTIC SPIN DYNAMICS SIMULATIONS

Different length scales in magnetization dynamics

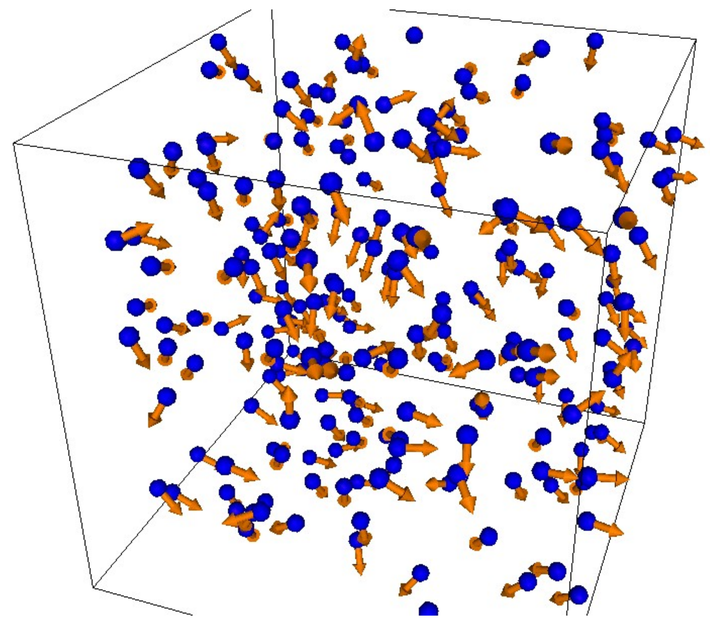
Time dependent Spin-polarized Density Functional Theory (TD-SDFT)	Subatomic length scales, computationally heavy. Magnetization density as field **m**(**r**)
Atomistic Spin Dynamics	Nanometer length scales, magnetization density as discrete set of atomic magnetic moments $\mathbf{m}_i$
Micromagnetics	Micron lengths, can simulate complete devices. magnetization density as field **m**(**r**)



Mn doped GaAs as a case study
Hellsvik et al. (submitted to PRB 2008)

Snapshot from simulation of GaAs doped with 5% Mn at T=100 K

Simulations were made for varying As antisite concentration



Our method for atomistic spin dynamics investigates the evolution in time of an atomistic Landau-Lifshitz Equation [1]

Derived from the spin-polarized Kohn-Sham-Hamiltonian, using a separation of time-scales [2]

$$\frac{d\mathbf{m}_i}{dt} = -\gamma \mathbf{m}_i \times [\mathbf{B}_i + \mathbf{b}_i(t)] - \gamma \frac{\alpha}{m} \mathbf{m}_i \times (\mathbf{m}_i \times [\mathbf{B}_i + \mathbf{b}_i(t)])$$

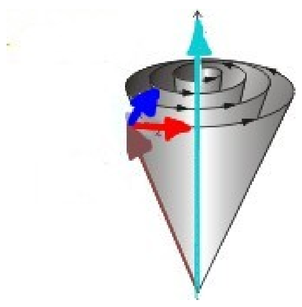
Precession term — Damping term

$\mathbf{m}_i$	atomic magnetic moment	γ	gyromagnetic ratio
$\mathbf{B}_i$	effective magnetic field	α	damping term
$\mathbf{b}_i(t)$	stochastic magnetic field		

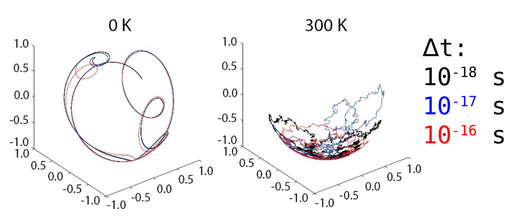
Magnetic exchange is mapped onto a Heisenberg Hamiltonian using the magnetic force theorem

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

The Jij:s can be kept static or be determined self-consistently in each step in time. Simulation cells typically have periodic boundary conditions.



Precession of a single atomic moment in the effective magnetic field.



Finite temperature effects are treated within a Langevin dynamics approach. The fluctuating magnetic field is normal distributed with an amplitude related to the damping parameter.

$$\langle b_{i,\mu}(t) \rangle = 0$$

$$\langle b_{i,\mu}(t) b_{j,\nu}(s) \rangle = 2D\delta_{\mu\nu}\delta_{ij}\delta(t-s)$$

$$D_{SLLG} = \frac{\alpha}{1+\alpha^2} \frac{k_B T}{\gamma m}$$

Motivations for use of atomistic spin dynamics for studies of dilute magnetic systems

- Investigate the magnetization temperature dependence in equilibrium; at varying dopant and defect concentrations.
- Investigate correlation functions, response functions etc.

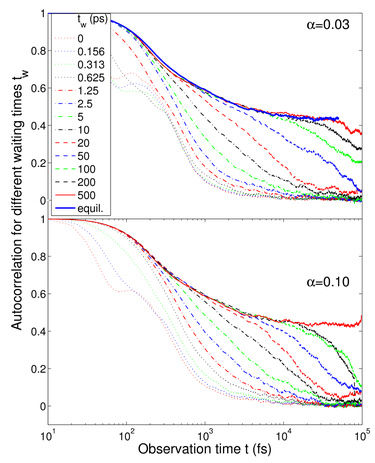
This can be achieved with Monte Carlo simulations – what can be gained with atomistic spin dynamics?

- The (real) time evolution of the magnetization
- Time evolution of correlation functions
- Dynamic response functions
- Simulation of magnetic switching

For magnetic (model Hamiltonian) systems the simplest two-time correlation is the autocorrelation

$$C_0(t_w + t, t_w) = \langle \mathbf{m}_i(t_w) \cdot \mathbf{m}_i(t_w + t) \rangle$$

Autocorrelation C_0 y=1.75%, T=10 K (T_c~30 K)



Quenching simulation:

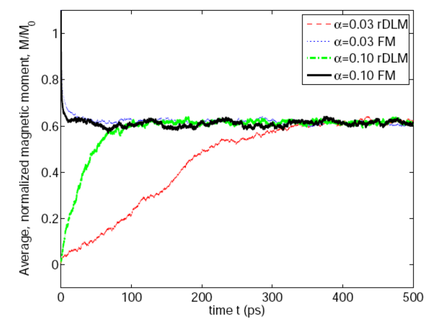
Starts from DLM configuration

Waiting times logarithmically distributed

The autocorrelation is not directly measurable - but relates to the zero (low field) magnetic susceptibility in experiments

The autocorrelation function has been used to study model Heisenberg Hamiltonian spin glass systems with Monte Carlo techniques with the time measured in Monte Carlo steps [3]. In a spin dynamics simulation the (real) time evolution is followed.

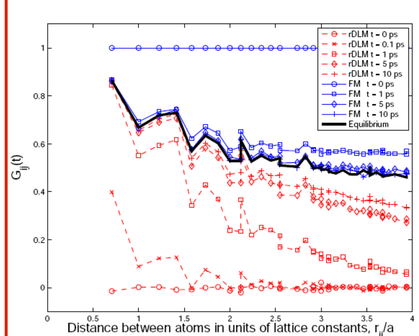
Time evolution of the magnetic order parameter



The time scale is affected by:

Cell size	(as for MC simulations)
T/Tc ratio, crit. slowing down	(as for MC simulations)
The damping parameter	

$$G_{ij}(t) = \langle \mathbf{m}_i(t) \cdot \mathbf{m}_j(t) \rangle = \langle \mathbf{m}(\mathbf{r}_i, t) \cdot \mathbf{m}(\mathbf{r}_j, t) \rangle$$



Time evolution of the equal time pair correlation function, 0.25% As Antisites at T=100 K

[1] B. Skubic, J. Hellsvik, L. Nordström, O. Eriksson, J. Phys.: Condens. Matter **20,** 315203 (2008)

[2] V. P. Antropov, M. I. Katsnelson, B. N. Harmon, M. van Schilfgaarde, D. Kusnezov, Phys. Rev. B **54,** 1019 (1996)

[3] L. Berthier, A.P. Young Phys. Rev. B **69 ,** 184423 (2004)