Computational Materials Science 102 (2015) 228–233

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Use of supercomputer for modeling coherent processes in magnetic nano-structures

T.S. Belozerova [a], A.G. Demenev [a], V.K. Henner [b,c], P.V. Kharebov [b], E.K. Khenner [a], G.U. Sumanasekera [c,*]

[a] Perm State University, Department of Mechanics and Mathematics, Perm 614990, Russia
[b] Perm State University, Department of Physics, Perm 614990, Russia
[c] University of Louisville, Department of Physics, Louisville, KY 40292, USA

ARTICLE INFO

Article history:
Received 14 September 2014
Received in revised form 2 February 2015
Accepted 9 February 2015
Available online 14 March 2015

Keywords:
High-performance computing
Parallel algorithms
Mathematical modeling
Coherent effects in spin systems
Magnetic nano-structures

ABSTRACT

Multi-scale spin dynamics of systems of nanomagnets is investigated by numerical simulation using parallel algorithms. A FORTRAN program was developed using an application programming interface OpenMP. The parallel code provides following areas of research: study of the possibility of regulation time of switching of magnetization of the nanostructure; study of the role of nanocrystal geometry of coherent relaxation of 1-, 2- and 3-dimensional objects; study of magnetodynamics of spin system coupled with the passive resonator (radiation damping (RD)); application of RD to ultra-fast relaxation in an assembly of single-domain ferromagnetic particles; study of the role of long distant dipole–dipole fields as the origin of the extremely random behavior in hyperpolarized NMR maser, etc. Estimates of speedup and efficiency of implemented algorithms in comparison with sequential algorithms have been obtained. It is shown that the use of supercomputing technology for study of spin dynamics provides simulation power for spin systems which include thousands of magnetic voxels.

1. Introduction

We describe computational model, algorithms and some applications of high-performance and reliable software for computer simulation of spin dynamics of magnetic nanostructures, such as nano-molecules, nano-clusters, molecular crystals. The main difficulty of describing the collective behavior of multi-spin systems is rooted in the presence of long-range spin–spin interactions. For systems consisting of a large number (thousands) of spins, finding of the spectrum of eigenvalues of the quantum Hamiltonian is not possible because computational complexity of the problem grows exponentially as the number of spins increases. However, for large values of the spins of the individual particles quasi-classical approximation may be used, in which the spins are treated as classical vectors. Even in this approximation, the numerical study of the spin dynamics models is accompanied by a non-linear increase in computational complexity with respect to the number of structural elements.

The modeling of thermodynamic [1] and dynamic [2] properties of the systems of interacting spins, including the simulation of coherent processes, was initiated on the mainframes of 3rd generation and continued on personal computers [3]; it was available for systems with a relatively small number of magnetic moments. However, to adequately reflect the real processes of spin dynamics, simulation systems must consist of thousands of magnetic moments, and the problem of the lack of computing power continues to exist. Parallelization of the algorithms and the use of supercomputers show promise of the possibility of potentially significant increase in the number of structural elements of the model and the range of time evolution of the systems that are available for study. However, the parallel computational methods require specific studies for ensuring the correctness of the results and efficiency of mapping of parallel computing algorithms for modern computer architectures.

2. Theoretical model used for numerical simulations

Physical phenomena investigated in this paper using parallel computational methods are different coherent relaxation processes, in particular the problem of super-radiance where the relaxation time can be inversely proportional to the number of spins [4–6].

We consider simulations for two particular problems of coherent spin dynamics. The first is fast magnetic relaxation in a ferromagnet nanoparticle system based on the theory of

* Corresponding author.
E-mail addresses: a-demenev@mail.ru (A.G. Demenev), vkhenner@yandex.ru (V. K. Henner), gamini.sumanasekera@louisville.edu (G.U. Sumanasekera).

http://dx.doi.org/10.1016/j.commatsci.2015.02.013
0927-0256/

superradiation. The dynamics of magnetization inversion of a nanoparticle is governed by the Landau–Lifshitz relaxation and radiation damping. The numeric simulations enable us to account for the interparticle dipole–dipole interactions in a rigorous way. In the second, a numerical simulations based on microscopic approach are used to explore the spin dynamics encountered in the recently reported hyperpolarized ^{129}Xe NMR maser where series of amplitude modulated rf emissions are observed [7].

In both cases the ensemble of magnetic moments (the sample) is placed into a homogeneous magnetic field H_0 aligned with the Oz axis and into a resonator (detection coil) which we model by an LCR circuit, with Ox taken as the coil axis. As soon as the magnetic moments are no longer aligned with Oz, an electromotive force appears in the coil, which in turn, induces an AC current in the circuit. The magnetic field produced by this electrical current acts on the nuclear magnetic moments modifying their individual dynamics.

In the first problem the dynamics of the particles that make up the ensemble, can be described by a system of equations for classical magnetic moment of each particle $\boldsymbol{\mu}^{(k)}$:

$$\frac{d\boldsymbol{\mu}^{(k)}}{dt} = -|\gamma|(\boldsymbol{\mu}^{(k)} \times \boldsymbol{\mathcal{H}}^{(k)}) - \frac{\alpha|\gamma|}{\mu}(\boldsymbol{\mu}^{(k)} \times (\boldsymbol{\mu}^{(k)} \times \boldsymbol{\mathcal{H}}^{(k)})). \tag{1}$$

In (1) α is dimensionless parameter of the spin–lattice relaxation, γ – gyromagnetic ratio for electrons, $\boldsymbol{\mathcal{H}}^{(k)}$ – magnetic field acting on the k-th spin. $\boldsymbol{\mathcal{H}}^{(k)}$ includes:

(1) a constant external field $\boldsymbol{H}_0 \| Oz$,
(2) a single-axle anisotropic field $\boldsymbol{H_A} = (H_A/\mu)(\boldsymbol{\mu}\boldsymbol{n})\boldsymbol{n}$, $H_A = 2E_A/\mu$, where $\boldsymbol{n}$ is unit vector of the easy axis, E_A is anisotropy energy,
(3) the field of feedback $\boldsymbol{H} = (H, 0, 0)$ induced in the resonant coil,
(4) dipole magnetic field $\mathbf{H}_d^{(k)}$ induced by pair dipole–dipole interactions of the k-th particle with all the others.

Let us define dimensionless parameters

$$p_A = \frac{\omega_A}{\omega_0} = \frac{H_A}{H_0}, \quad p_H = \frac{\omega_H}{\omega_0} = \frac{H}{H_0}, \quad p_d = \frac{\omega_d}{\omega_0} = \frac{\mu}{a^3 H_0}, \tag{2}$$

where $\omega_0 = |\gamma|H_0$, $\omega_H = |\gamma|H$, $\omega_d = |\gamma|\mu/a^3$, $\omega_A = |\gamma|H_A$ are the frequencies related with the field $\boldsymbol{H}_0$ (Larmor frequency), field of feedback and dipole (local) magnetic field. Here a is the average distance between particles.

As a result Eq. (1) for the unit vectors $\boldsymbol{e}^{(k)} = \boldsymbol{\mu}^{(k)}/\mu$ take the form [8]

$$\begin{aligned}
\dot{e}_x^{(k)} &= -(1 + \omega_i + p_A e_z^{(k)})e_y^{(k)} - p_{di}(e_y^{(k)}\tilde{H}_{dz}^{(k)} - e_z^{(k)}\tilde{H}_{dy}^{(k)}) \\
&\quad + \alpha(p_H + p_{di}\tilde{H}_{dx}) \times e_y^{(k)2} + e_z^{(k)2}) \\
&\quad - \alpha(1 + p_A e_z^{(k)} + p_{di}\tilde{H}_{dz})e_x^{(k)}e_z^{(k)} - \alpha p_{di}\tilde{H}_{dy}e_x^{(k)}e_y^{(k)} - \Gamma_2 e_x^{(i)}, \\
\dot{e}_y^{(k)} &= (1 + \omega_i + p_A e_z^{(k)})e_x^{(k)} - p_H e_z^{(k)} - p_{di}(e_z^{(k)}\tilde{H}_{dx}^{(k)} - e_x^{(k)}\tilde{H}_{dz}^{(k)}) \\
&\quad - \alpha(p_H + p_{di}\tilde{H}_{dx}) \times e_x^{(k)}e_y^{(k)} - \alpha(1 + p_{di}\tilde{H}_{dz} + p_A e_z^{(k)})e_y^{(k)}e_z^{(k)} \\
&\quad + \alpha p_{di}\tilde{H}_{dy}(e_x^{(k)2} + e_z^{(k)2}) - \Gamma_2 e_y^{(i)}, \\
\dot{e}_z^{(k)} &= p_H e_y^{(k)} - p_{di}(e_x^{(k)}\tilde{H}_{dy}^{(k)} - e_y^{(k)}\tilde{H}_{dx}^{(k)}) - \alpha(p_H + p_{di}\tilde{H}_{dx})e_x^{(k)}e_z^{(k)} \\
&\quad + \alpha(1 + p_A e_z^{(k)} + p_{di}\tilde{H}_{dz})(e_x^{(k)2} + e_y^{(k)2}) - \alpha p_{di}\tilde{H}_{dy}e_y^{(k)}e_z^{(k)}.
\end{aligned} \tag{3}$$

Time derivatives in (3) are defined with respect to time $\tilde{t} = \omega_0 t$. Here $p_{di} = p_d(1 + \delta_i)$, δ_i is dispersion of precession frequency of spin number i, ω_i is Zeeman frequency of precession of i-th spin (both δ_i and ω_i are distributed under the normal law random variable with zero average value and dispersion σ_δ and σ_ω). Additional relaxation terms $-\Gamma_2 e_{x,y}^{(k)}$ may, in some cases, be caused by short-range dipole interactions.

The equation for magnetic field generated in the resonator in process of spin relaxation is [9,10]:

$$\frac{d^2}{d\tilde{t}^2}p_H + 2\frac{\gamma_r}{\omega_0}\frac{d}{d\tilde{t}}p_H + \left(\frac{\omega_r}{\omega_0}\right)^2 p_H = -4\pi\beta\left(\frac{1}{N}\frac{d^2}{d\tilde{t}^2}\sum_{l=1}^{N} e_x^{(l)}\right). \tag{4}$$

The coefficients in the left-hand side of Eq. (4) can be expressed in terms of the parameters of the circuit $2\gamma_r = R/L = \omega_r/Q$ and $\omega_r = 1/\sqrt{LC}$, where Q is the quality factor. The expression in parentheses on the right hand side of Eq. (4), it makes sense to the ensemble-averaged values of the second derivative of x-projection of the unit vector of the magnetization. Quantity $\beta = \eta N\mu/(VH_0)$ determines the intensity of magnetic coupling between ensemble of the magnetic moments and the inductance coil. The initial conditions for Eq. (4) are zero: $p_H(0) = 0$, $\dot{p}_H(0) = 0$.

3. Method of numerical modeling

In order to solve the equations of motion, a hybrid method for the numerical simulation is utilized, which is often used in the study of the dynamics of spin systems. In this method the spins are regarded as the "classic" (the usual three-dimensional vectors) and the system of differential Eqs. (3) and (4) is solved numerically using the Runge–Kutta method.

Simulation of the dynamics of the spin system with an assigned initial polarization p_0 is performed using the Monte Carlo technique. For this purpose, we construct a random configuration of equiprobable spin directions (first approximation for the Gibbs ensemble sampling). Each direction is characterized by the unit vector $\vec{e}(\vec{x}) = (\vec{i}e^x + \vec{j}e^y + \vec{k}e^z)$, where $(e^x)^2 + (e^y)^2 + (e^z)^2 = 1$. We are looking for a random vector $\vec{e}$ such that $P\{\vec{e} \in \Omega\} = \Omega/4\pi$ for any solid angle Ω. It is easy to see that if x is a random point uniformly distributed in a sphere, the direction of its radius-vector has necessary properties. Thus, we assume $\cos\theta = 2\gamma_1 - 1$, $\varphi = 2\pi\gamma_2$, where γ_1 and γ_2 are independent random variables uniformly distributed in the interval [0,1). Cartesian coordinates of the vector $\vec{e}$ are calculated by the usual formulas: $e^x = \cos\varphi\sqrt{1 - \cos^2\theta}$, $e^y = \sin\varphi\sqrt{1 - \cos^2\theta}$, $e^z = \cos\theta$.

For the resulting configuration the total magnetization p_{init} is calculated. Then, for some randomly selected node a new random direction is defined (as described above) and new total magnetic moment p' is calculated. If $|p' - p_0| < |p_{init} - p_0|$ then modified spin direction is taken as a new member approximation of the ensemble, otherwise discarded. After finding the next configuration of the Gibbs ensemble, this configuration is taken for starting, etc. Thus, the configuration is determined with polarization that is close enough to the initially set. Appropriate array of spin's orientation is selected as the initial configuration.

The condition that each individual spin must maintain its length $l = \sqrt{(e^x)^2 + (e^y)^2 + (e^z)^2} = 1$ is used to control the accuracy of the calculations and to automatically adjust the length of the integration step. If after one integration step l deviates from 1 more than set error ε the step decreased twice. If throughout 10 steps Δt does not change, the step increases twice.

4. Analyses of a potential parallelization of the initial codes

The initial software was created in the environment Borland C ++ Builder (program "Spins") and environment Borland Delphi (program "MagnetoDynamics") for only sequential algorithms under MS Windows. These restrictions prevented the effective use of high performance computing in research of magnetodynamics and coherent processes in nano-magnetic structures.