ESAIM: PROCEEDINGS, Vol. ?, 2006, 1-10
Editors: Will be set by the publisher
DOI: (will be inserted later)

NUMERICAL SIMULATIONS OF FERROMAGNETIC MATERIALS

Stéphane Labbé[1]

Abstract. In this article, we give a glimpse on our last works in simulation of ferromagnetism phenomena. The main problems encountered in this type of computation are the demagnetization field and the microwave susceptibility computations. Difficulties for the demagnetization field come principally form the fact that the operator is nonlocal and the discretized operator gives a full matrix, we will focus here on the periodic case ; the microwave susceptibility computation requests the resolution of many ill-conditionned linear systems.

Résumé. Dans cet article, nous présentons des travaux récents concernant la simulation de phénomènes ferromagnétiques. Les principaux problèmes rencontrés sont le calcul du champ démagnétisant et de la susceptibilité. En ce qui concerne le calcul du champ démagnétisant, il s'agit de discrétiser un opérateur non-local. Nous nous concentrerons sur le cas périodique. Quant à la susceptibilité, il s'agit ici de résoudre plusieurs systèmes linéaires mal conditionn és.

Mathematics Subject Classification. 35Q60,65Z05.

Introduction

Ferromagnetic materials are of high importance for applications, they are used, for example, in nano electronic, telephony or magnetic data recording. All these applications needs the creation of expensive samples whose have long time processes f built. Then, in order to optimize these objects, if becomes necessary to be able to simulate the behavior of magnetic objects before their effective conception. When simulations of static and dynamic sates are acquired, the comparison with experiments is a crucial point. It is solved by computing the microwave susceptibility the magnetic objects. In this article, we will remind quickly the notion microwave susceptibility.

The model used in this article for ferromagnetism is the micromagnetism, introduced by W.-F. Brown in 60'. This model, based upon a thermodynamic analysis of the ferromagnetism phenomena, can be modelized using a static approach or a dynamic approach. In fact, at least formally, the time asymptotic solutions of the dynamical approach are local minimizers of the energy used in the static approach.

In a first part we will give a quick reminder of the micromagnetism problem (see also [2,4,5]). In a second part we will recall the principles of the dynamic simulation [6, 9] and of the magnetostatic computation in the non-periodic and periodic case [3,7]. The last part will be dedicated to the microwave susceptibility computations [8] and particularly to the strategy adopted to treat the ill-conditionning of the systems to solve for each frequence.

Keywords and phrases.

[1] Laboratoire de Mathématiques, Bât. 425, Université Paris-Sud 11, 91405 Orsay cedex.

1. A model for ferromagnetism: the micromagnetism

Let Ω be an open bounded set of $\mathbb{R}^3$, we designate by m in $H^1(\Omega, \mathbb{S}^2)$ the magnetization (here, $\mathbb{S}^2 = \{x \in \mathbb{R}^3 \mid |x| = 1\}$). The energy functional is given by:

$$E(m) = A \int_\Omega |\nabla m|^2 \, dx + \int_{\mathbb{R}} |\nabla \varphi(m)|^2 \, dx + \int_\Omega \phi(m) \, dx - 2 \int_\Omega h_{\text{ext}} \cdot m \, dx,$$

the first integral is called the exchange contribution and modelizes the microscopic spin-spin interaction on the crystal net, $\varphi(m)$ is the potential of the demagnetization contribution and verifies $\triangle \varphi(m) = -\text{div}(\tilde{m})$ ($\tilde{m}$ is the padding to zero of m in the whole space), the third integral modelizes the anisotropy effects of the crystal. Minimizers of this energy are called equilibrium states of the system. There exists also local equilibrium states, these states are those most commonly observed and can be obtained as time-limits of a dynamical system. This system, introduced by Landau and Lifchitz, is the following:

$$\frac{\partial m}{\partial t} = -m \wedge h_{\text{tot}}(m) - \alpha m \wedge (m \wedge h_{\text{tot}}(m)) + h_{\text{ext}}, \tag{1}$$

where $h_{\text{tot}}(m) = A \triangle m + h_{\text{d}}(m) + \frac{\partial \varphi}{\partial m}(m)$, the differential in m of the concentration of energy. This dynamical system preserves the magnitude of the magnetization m and ensures, if the external field is not dependent of time, the decreasing of the energy. Formally, this properties leads to conclude that time limits of the solution of (1) are local minimizers of the energy $E(m)$.
The tool used in order to compare the three dimensional simulations and experimental results is the microwave susceptibility. The main idea is to light a sample with a monochromatic light, in the three direction of space, and retrieve the energy emitted by the sample. Mathematically, the problem is written as follows: given an equilibrium state m_{eq}, (h_1, h_2, h_3) an orthogonal basis of $\mathbb{R}^3$, for each ω in $\mathbb{R}_*^+$, a pulsation, m_j in $L^2(\Omega, \mathbb{R}^3)$, for j in $\{1, ..., 3\}$ is such that $m_{\text{eq}} + m_j e^{i\omega \, t}$ is the solution of the linearised system (1) (first order in h_j, m_j) for $h_{\text{ext}} = h_j e^{i\omega \, t}$,

$$i\omega m_j - (D_1(m_{\text{eq}}) \circ h_{\text{tot}} + D_2(m_{\text{eq}}))m_j = D_1(m_{\text{eq}})h_j, \tag{2}$$

where, for every w in $\mathbb{R}^3$

$$\begin{aligned} D_1(m_{\text{eq}})w &= -m_{\text{eq}} \wedge w - \alpha m_{\text{eq}} \wedge (m_{\text{eq}} \wedge w), \\ D_2(m_{\text{eq}})w &= h_{\text{tot}}(m_{\text{eq}}) \wedge w - \alpha m_{\text{eq}} \wedge (w \wedge h_{\text{tot}}(m_{\text{eq}})). \end{aligned}$$

2. Dynamical simulations

The dynamical simulation of solution of system (1) is obtained by a finite difference discretization in time and a finite volumes discretization in space. The main difficulty of the space discretization is to dicretize the demagnetization field. The demagnetization contribution is given by the following representation formula:

$$h_{\text{d}}(m) = \text{grad div } \triangle^{-1} \tilde{m}.$$

In order to discretize this formula, we use a finite volumes like scheme. Let u be an element of $L^2(\Omega)$ and $(\omega_i)_{i \in \{1,\ldots,N\}}$ a regular cubic mesh of Ω, we define

$$P(u) = \sum_{i \in \{1,\ldots,N\}} \chi_i \frac{1}{|\omega_i|} \int_{\omega_i} u(x) dx,$$

where χ_i is the characteristic function of ω_i, and P^* is the canonical injection of the piecewise functions into $L^2(\Omega)$. Then, the discrete demagnetizing field $h_{\mathrm{d},h}$ is defined by

$$h_{\mathrm{d},h} = P \circ h_{\mathrm{d}} \circ P*,$$

this approximation is convergent and the spectrum of the discrete operator preserves the properties of positivity and contraction. Using the regular mesh structure, we prove that the demagnetization matrix associated to the discrete operator is a block-Toeplitz matrix, then we can develop a fast computation algorithm such that the complexity of the demagnetization evaluation is reduced to $O(N\log(N))$ and the storage is in $O(N)$ [7]. It is possible to also compute the demagnetization field for a domain periodic in one or two directions of space. In order compute this contribution, we choose to mesh the whole space with a dyadic mesh built on the central mesh (see fig. 1). In fact, using the scale independence of the demagnetization field, we see that the computation of the demagnetization contribution on each level is the same, then, we can use the fast algorithm developed for one domain. The algorithm accuracy is good (see fig. 2). For details see [3].

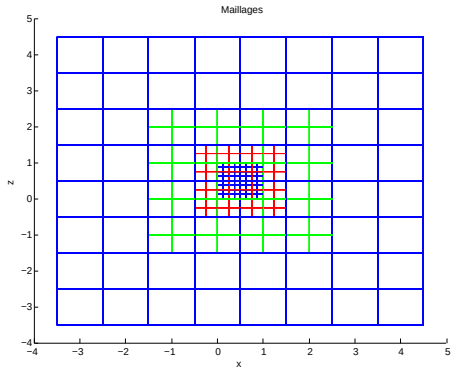

FIGURE 1. Dyadic mesh for a periodic domain in two direction ($8 \times 8 \times 8$ mesh of the core domain).

The exchange contribution and anisotropy contribution discretization are classical. In time, we use an explicit finite difference scheme with a time step optimization in order to ensure the convergence of the scheme. The time step optimization is automatic and ensure the optimal decreasing of the energy [6, 9].

3. The microwave susceptibility

In order to compute the discretized microwave susceptibility, we replace in equation 2 the continuous version of operators by the discretized one. The equilibrium states, $m_{\mathrm{eq},h}$ are obtain by computing time limits of

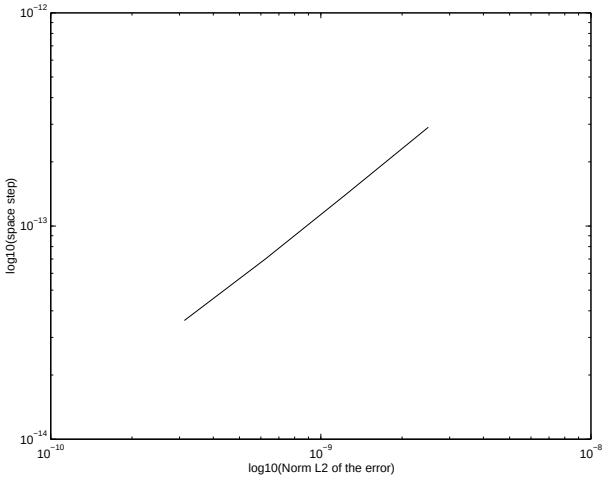

FIGURE 2. Accuracy of the multilevels algorithm.

dynamical solutions. The problem to solve is, for a given set of values of the pulsation ω, to solve:

$$(i\omega Id - M)m = h, \tag{3}$$

where h and m are vectors of $\mathbb{R}^{3N}$, Id is the identity on $\mathbb{R}^{3N}$ and M is a square matrix of order $3N$. M is defined by

$$M = D_1(m_{\mathrm{eq},h}) \circ h_{\mathrm{tot,h}} + D_2(m_{\mathrm{eq},h}).$$

The system 3 is very ill-conditionned, then the built of a preconditioner is crucial. A proposal of preconditioning strategy is proposed in [8]. The main idea is to prove that the matrix M can preconditioned by $(h_{\mathrm{tot,h}})^{-1}$. The cost of the inversion of the complete $h_{\mathrm{tot,h}}$ is to high, then, we use an approximation $\tilde{h}_{\mathrm{tot,h}}$ of this operator computed as the projection of $h_{\mathrm{tot,h}}$ on skew matrices in the sense of the Froebenius norm. The results obtained are good, the implementation for the exchange has been already tested (see fig. 3), the adjunction of the demagnetization term is in tested now.

The computation time obtained using the fast computation algorithms for the demagnetization field simulation and the preconditioning of the susceptibility system allow simulation of huge systems of almost on million degrees of freedom (see [1]).

REFERENCES

[1] F. Boust, N. Vukadinovic, and S. Labbé. Domain wall resonant modes in nanodots with a perpendicular anisotropy. *Journal of Magnetism and Magnetic Materials*, 272-276:708–710, 2004.

[2] W.F. Brown. *Micromagnetics*. Interscience Publishers, 1963.

[3] S. Faure and S. Labbé. Multi-levels computation of the demagnetization field in periodic domains applied to micromagnetism computations. Technical report, Université Paris-Sud 11, Laboratoire de Mathématique, 2006.

[4] L. Halpern and S. Labbé. La théorie du micromagnétisme. Modélisation et simulation du comportement des matériaux magnétiques. *Matapli*, (66):77–92, 2001.

[5] A. Hubert and R. Schäfer. *Magnetic Domains : The Analysis of Magnetic Microstructures*. Springer-Verglag, 2000.

[6] S. Labbé. *Simulation numérique du comportement hyperfréquence des matériaux ferromagnétiques*. PhD thesis, Université Paris 13, Décembre 1998.

[7] S. Labbé. Fast computation for large magnetostatic systems adapted for micromagnetism. *SISC SIAM Journal on Scientific Computing*, 26(6):2160–2175, 2005.

[8] S. Labbé. A preconditioning strategy for microwave susceptibility in ferromagnets. *AES, Advances in Engineering Software*, to appear, 2006.

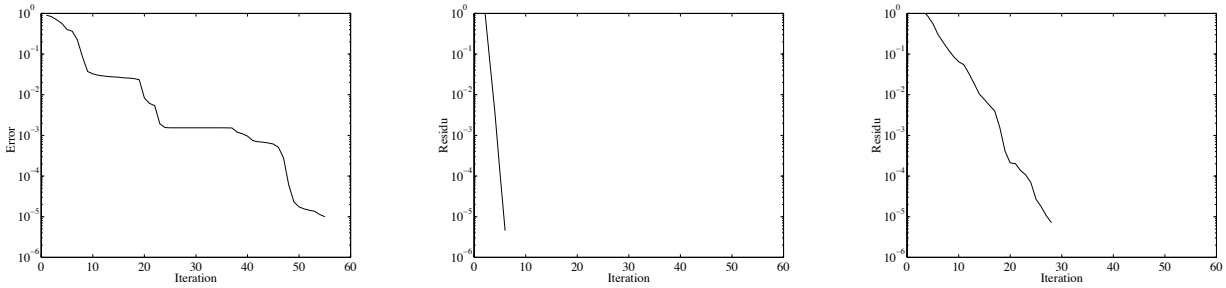

FIGURE 3. Example of convergence curves for non preconditioned system, preconditioned system and approached preconditioned system.

[9] S. Labbé and P.-Y. Bertin. Microwve polarisability of ferrite particles with non-uniform magnetization. *Journal of Magnetism and Magnetic Materials*, 206:93–105, 1999.