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FAST COMPUTATION FOR LARGE MAGNETOSTATIC SYSTEMS ADAPTED FOR MICROMAGNETISM

STÉPHANE LABBÉ*

Abstract. In this paper, an efficient method is developed for computing the magnetostatic field for ferromagnetic materials on large structured meshes. The problem is discretized using a finite volume approximation. The discrete operator is proved to preserve the main properties of the continuous model, and a lower estimate of its lower eigenvalue is given. Using the fact that the discrete operator has a block-Toeplitz structure for cubic meshes in parallelepipedic domains, a fast solving method is built. Based upon the use of fast Fourier transform, this method allows to reduce the computational cost to from n^2 to $O(n \log(n))$ but also to reduce the storage to $O(n)$ instead of n^2 where n is the number of cells in the mesh.

Key words. finite-volume method, magnetostatics, Maxwell equations, block-Toeplitz matrices

AMS subject classifications. 15A18, 47G20, 47B35, 65M60

1. Introduction. When computing the magnetization of ferromagnetic materials, the theory of micromagnetism uses a non linear evolution equation, the Landau-Lifshitz equation, relating the magnetization field to the excitation field (see [3]). The excitation originates from various physical phenomena, one of them is induced by the stray field \mathbf{H} that appears in the Maxwell equations. In the case where the wavelengths are large compared to the size of the material, the Maxwell system is usually replaced by the so-called quasistatic approximation. If the material fills a domain Ω in \mathbb{R}^3 , the equation of magnetostatics relates the magnetization field \mathbf{u} , the magnetic field \mathbf{B} , and the stray field \mathbf{H} in the following way

$$(1.1) \quad \begin{cases} \operatorname{rot} \mathbf{H} = \mathbf{0} \\ \operatorname{div} \mathbf{B} = 0 \\ \mathbf{B} = \mu_0(\mathbf{H} + \mathbf{u}), \end{cases}$$

where μ_0 is the permeability of the vacuum, and \mathbf{u} vanishes outside Ω . The numerical resolution of this system amounts to solve the Poisson equation, namely

$$-\Delta \Phi = \operatorname{div} \mathbf{u}; \quad \operatorname{grad} \Phi = \mathbf{H}$$

where \mathbf{u} is now considered as a datum. The problem has to be solved in the whole space \mathbb{R}^3 and thus requires very efficient solvers. The purpose of this paper is to propose such a solver adapted to the micromagnetism computations.

In the micromagnetism context, we seek for equilibrium states whose characterization is : find \mathbf{u} in $(L^2(\Omega))^3$, $|\mathbf{u}| = 1$ for almost every points of Ω and such that \mathbf{u} minimizes the energy $e(\mathbf{u}) = - \int_{\Omega} \mathbf{u} \cdot \mathbf{H}_T(\mathbf{u}) \, dx$. Such minimizers verify

$$\|\mathbf{u} \wedge \mathbf{H}_T(\mathbf{u})\|_{0,\Omega} = 0,$$

where $\mathbf{H}_T(\mathbf{u})$ is typically equal to $\mathbf{H} + A \Delta \mathbf{u}$ and $A > 0$ is called the exchange constant. We will see in section 2 that $\mathbf{u} \mapsto \mathbf{H}$ defines a linear negative operator. At this stage, we warn the reader that preserving this property with the discretized operator \mathbf{H}_h might be crucial, otherwise, it may exist regions ω , included in Ω , in

*Université Paris 11, Orsay, Laboratoire de Mathématique, Bât. 425, 91405 Orsay, FRANCE (Stephane.labbe@math.u-psud.fr).

which $\mathbf{H}_h \cdot \mathbf{u}_h > 0$ almost everywhere in ω whereas $\mathbf{H} \cdot \mathbf{u} \leq 0$ for the continuous case. In such regions, it is expected that the discretized solution would be in the opposite direction of the continuous one. Therefore, in this article, we will focus particularly on discretization methods preserving the negativity of the magnetostatic operator.

The first numerical method used to compute the magnetization field (see [18]) was based on the dipolar approximation. Its main drawback was to produce negative eigenvalues of the approximation of a positive operator. Furthermore, the cost was prohibitive for the applications that we have in mind. Improvements using finite volumes were made by Y. Nakatami, Y. Uesaka and N. Hayashi [15], but the two main drawbacks remained.

On the other hand, efficient finite element methods have been used to compute the equilibrium states by minimization of the energy (see [20], [1]). However, in view of further use in computations of susceptibility, we really need to couple (1.1) to the time dependent Landau-Lifshitz equation.

In this paper we introduce a finite volume approximation, which preserves the main properties of the operator given in the continuous model : positivity and symmetry. Furthermore the resulting system has a block-Toeplitz structure, which allows efficient and fast solvers.

In Section 2 we introduce the continuous problem and the notations.

In Section 3, we define the discretization method. It is based on solving the exact problem for piecewise constant functions and then projection of the solution onto the space of piecewise constant functions. Actually the method used is based upon a semi-analytical integration, as it is often the case when solving integral equations. We prove that the properties of the continuous operator are preserved, and we are able to give a lower bound on the eigenvalues.

In Section 4, we present a fast solver using a multilevel block-Toeplitz construction. The notion of Toeplitz matrices has been introduced by G. Strang (see [19]). Thereafter, E.E. Tyrtshnikov studied the spectrum of block-Toeplitz matrices and together with V.L. Ivakhnenko, applied them to solve electromagnetic scattering problems (see [10]). We prove that this method, when applied to our problem, reduces the storage from $O(n^2)$ to $O(n)$ elements and the computation complexity from n^2 to $n \log(n)$ where n is the number of cells in the mesh. At the end of the paper, we show some numerical experiments in order to illustrate the efficiency of the method.

2. The magnetostatic equations. First, we recall some notations used in Sobolev spaces. For any three dimensional domain Ω , $L^2(\Omega)$ is the Hilbert space of square-integrable functions, furnished with the inner product

$$(v, w) = \int_{\Omega} v(x)w(x) dx,$$

and the corresponding norm is denoted by $\|\cdot\|_{0,\Omega}$.

$\mathcal{D}(\Omega)$ is the space of functions which are infinitely differentiable and compactly supported in Ω . Its dual is the space of distributions, denoted $\mathcal{D}'(\Omega)$. For any positive integer m , $H^m(\Omega)$ is the Sobolev space of distributions defined in Ω , whose derivatives up to order m belong to $L^2(\Omega)$, furnished with the inner product

$$(u, w)_{m,\Omega} = \sum_{|k| \leq m} (D^k u, D^k w)_{0,\Omega},$$

and the corresponding norm is denoted $\|\cdot\|_{m,\Omega}$ (as usual, $H^0(\Omega)$ is identical to $L^2(\Omega)$). Furthermore, we denoted

$$|u|_{m,\Omega} = \sum_{|k|=m} \|D^k v\|_{0,\Omega}.$$

The notations $(\cdot, \cdot)_{m,\Omega}$ and $\|\cdot\|_{m,\Omega}$ will be applied to $H^m(\Omega)$ or $(H^m(\Omega))^3$. It is well known (see [5]), that for \mathbf{H} in $(L^2(\Omega))^3$ satisfying $\mathbf{rot} \mathbf{H} = 0$, there exist a unique ϕ in the weighted Sobolev space $W^1(\mathbb{R}^3)$ such that

$$(2.1) \quad \mathbf{H} = \mathbf{grad} \phi \text{ in } \mathbb{R}^3,$$

with

$$W^1(\mathbb{R}^3) = \{\varphi \in \mathcal{D}'(\mathbb{R}^3), \mathbf{grad} \varphi \in L^2(\mathbb{R}^3), \frac{\varphi}{\sqrt{1+r^2}} \in L^2(\mathbb{R}^3)\}.$$

By (1.1) we derive an equation for $\phi \in W^1(\mathbb{R}^3)$

$$(2.2) \quad \Delta \phi(\mathbf{u}) = -\mathbf{div} \mathbf{u} \text{ in } \mathbb{R}^3.$$

And we set, for all \mathbf{u} in $(L^2(\mathbb{R}^3))^3$,

$$\begin{aligned} \phi(\mathbf{u}) & \text{ the unique solution of (2.2),} \\ & \text{and } \mathbf{A}(\mathbf{u}) = -\mathbf{grad} \phi(\mathbf{u}). \end{aligned}$$

By (2.1) and (2.2) we can write \mathbf{H} as :

$$\begin{aligned} \mathbf{H} &= -\mathbf{grad} (G * \mathbf{div}(\mathbf{u})) \\ &= -\mathbf{grad} \left(G * \sum_{i=1}^3 \frac{\partial \mathbf{u}_i}{\partial x_i} \right) \\ &= -\mathbf{grad} \left(\sum_{i=1}^3 G * \frac{\partial \mathbf{u}_i}{\partial x_i} \right) \\ &= -\mathbf{grad} \left(\sum_{i=1}^3 \frac{\partial}{\partial x_i} (G * \mathbf{u}) \right) \\ &= -\mathbf{grad} (\mathbf{div}(\mathbf{u} * G)), \end{aligned}$$

where G is the fundamental solution for the Laplace equation in \mathbb{R}^3 :

$$\forall x, y \in \mathbb{R}^3 \quad G(x, y) = \frac{-1}{4\pi|x-y|}.$$

Throughout this paper we shall use the notation

$$(2.3) \quad \mathbf{A}(\mathbf{u}) = -\mathbf{H} = \mathbf{grad} \left(\mathbf{div} \left(\int_{\Omega} \mathbf{u}(y) \cdot \frac{1}{4\pi|x-y|} dy \right) \right).$$

The operator \mathbf{A} is a linear operator from $(L^2(\mathbb{R}^3))^3$ into $(L^2(\mathbb{R}^3))^3$. It is positive, symmetric, and its norm is bounded by 1 (see [8]). Furthermore, it is singular ; its kernel is given by the following lemma

LEMMA 2.1. *The operator \mathbf{A} satisfies the following properties*

(i) *For any \mathbf{u} in $(L^2(\mathbb{R}^3))^3$, $(\mathbf{A}(\mathbf{u}), \mathbf{u})_{0,\mathbb{R}^3} = 0 \iff \mathbf{A}(\mathbf{u}) = 0$.*

(ii) $\text{Ker}(\mathbf{A}) = \{\mathbf{u} \in (L^2(\mathbb{R}^3))^3, \text{div } \mathbf{u} = 0 \text{ in } \mathbb{R}^3\}$.

Proof. (i) for any \mathbf{u} in $(L^2(\mathbb{R}^3))^3$, we have the following relations

$$\begin{aligned} (\mathbf{A}(\mathbf{u}), \mathbf{u})_{0, \mathbb{R}^3} = 0 &\iff (\mathbf{grad } \phi(\mathbf{u}), \mathbf{u})_{0, \mathbb{R}^3} = 0, \\ &\iff -(\phi(\mathbf{u}), \text{div } \mathbf{u})_{0, \mathbb{R}^3} = 0, \\ &\iff (\phi(\mathbf{u}), \Delta \phi(\mathbf{u}))_{0, \mathbb{R}^3} = 0, \\ &\iff (\mathbf{grad } \phi(\mathbf{u}), \mathbf{grad } \phi(\mathbf{u}))_{0, \mathbb{R}^3} = 0, \\ &\iff \|\mathbf{A}(\mathbf{u})\|_{0, \mathbb{R}^3}^2 = 0. \end{aligned}$$

(ii) For any \mathbf{u} in $(L^2(\mathbb{R}^3))^3$ such that $\text{div } \mathbf{u} = 0$, the uniqueness of solutions of (2.2) proves that $\phi(\mathbf{u}) = 0$, so $\mathbf{A}(\mathbf{u}) = 0$.

For all \mathbf{u} in $\text{Ker}(\mathbf{A})$, since $\text{div } \mathbf{A}(\mathbf{u}) = \text{div } \mathbf{u}$ we have $\text{div } \mathbf{u} = 0$. \square

3. The finite-volume discretisation.

3.1. Space discretisation. The domain Ω is broken down in n cubes Ω_i of length h . A function in $(L^2(\Omega))^3$ will be approximated by piecewise constant functions (constant on each cube Ω_i). \mathbb{R}^3 is equipped with the euclidian product \cdot and norm $\|\cdot\|$. We introduce $(\mathbb{R}^3)^n$ made of functions $u = (\mathbf{u}_1, \dots, \mathbf{u}_n)$, each \mathbf{u}_i belonging to \mathbb{R}^3 . The space $(\mathbb{R}^3)^n$ is furnished with the canonical euclidian structure written as follows

$$\begin{aligned} \forall (u, v) \in (\mathbb{R}^3)^n : \\ (u, v)_h &= \sum_{i=1}^n |\Omega_i| \mathbf{u}_i \cdot \mathbf{v}_i, \\ \|u\|_h^2 &= \sum_{i=1}^n |\Omega_i| |\mathbf{u}_i|^2, \end{aligned}$$

In order to define the discrete problem, we introduce the following operators : R_h maps $(\mathbb{R}^3)^n$ into $(L^2(\Omega))^3$ and is defined by

$$\forall v \in (\mathbb{R}^3)^n, \quad R_h(v) = \sum_{i=1}^n \chi_i v_i,$$

P_h maps $(L^2(\Omega))^3$ into $(\mathbb{R}^3)^n$ and is defined by

$$\forall \mathbf{u} \in (L^2(\Omega))^3, \quad P_h(\mathbf{u})_i = \frac{1}{|\Omega_i|} \int_{\Omega_i} \mathbf{u}(x) dx,$$

where χ_i is defined for x in \mathbb{R}^3 by : $\chi_i(x) = 1$ if x belongs to Ω_i , $\chi_i(x) = 0$ otherwise. We shall use three main properties of these operators (see [4], [7])

PROPOSITION 3.1. *Operators R_h and P_h satisfy the following properties :*

- (i) *there exists C in \mathbb{R}^+ , such that for all \mathbf{u} in $(H^1(\Omega))^3$*

$$\|\mathbf{u} - R_h(P_h(\mathbf{u}))\|_{0, \Omega} \leq C h \|\mathbf{u}\|_{1, \Omega},$$
- (ii) $\forall v \in (\mathbb{R}^3)^n; \quad \|R_h(v)\|_{0, \Omega} = \|v\|_h$
- (iii) $\forall \mathbf{u} \in (L^2(\Omega))^3; \quad \|P_h(\mathbf{u})\|_h \leq \|\mathbf{u}\|_{0, \Omega}$

This allows us to approximate the operator \mathbf{A} by the following finite volume operator

$$(3.1) \quad \mathbf{A}_h = P_h \circ \mathbf{A} \circ R_h.$$

\mathbf{A}_h is an operator from $(\mathbb{R}^3)^n$ into $(\mathbb{R}^3)^n$. We introduce the notation

$$(3.2) \quad (\mathbf{A}_h(u))_i = \sum_{j=1}^n K_i^j(\mathbf{u}_j).$$

where $\forall u \in (\mathbb{R}^3)^n$, $u = (\mathbf{u}_i)_{i \in \{1, \dots, n\}}$ and

$$(3.3) \quad \forall \mathbf{u} \in \mathbb{R}^3, \quad K_i^j(\mathbf{u}) = \frac{1}{4\pi|\Omega_i|} \int_{\Omega_i} \left[\mathbf{grad} \operatorname{div} \cdot \int_{\Omega_j} \mathbf{u}(y) \frac{-1}{|y-x|} dy \right] dx.$$

Each K_i^j is a 3 by 3 real matrix. These matrices characterise the interaction between two cells Ω_i and Ω_j .

3.2. Properties of the approximate operator \mathbf{A}_h . We start with the elementary properties of \mathbf{A}_h

THEOREM 3.2. *For all real $h > 0$, the discrete operator \mathbf{A}_h is symmetric and a positive contraction in $\mathcal{L}((\mathbb{R}^3)^n)$; furthermore, there exists C in \mathbb{R}_*^+ such that for all \mathbf{u} in $(H^1([0, T] \times \Omega))^3$*

$$\|R_h \circ \mathbf{A}_h \circ P_h(\mathbf{u}) - \mathbf{A}(\mathbf{u})\|_{0,\Omega} \leq C h \|\mathbf{u}\|_{1,\Omega}.$$

The proof is straightforward and will be omitted (see [13]).

We saw in Lemma 2.1 that \mathbf{A} is singular. On the contrary, the discretised operator \mathbf{A}_h is regular. To prove that result we will use an intermediate lemma

LEMMA 3.3. *For all u in $(\mathbb{R}^3)^n$, one can write*

$$\operatorname{div} R_h(u) = 0 \iff \forall i \in \{1, \dots, n\}, \quad \mathbf{u}_i = 0.$$

Proof. We first write that $\operatorname{div} R_h(\mathbf{u})$ vanishes if and only if the normal component of $R_h(\mathbf{u})$ is continuous on the interfaces $\bar{\Omega}_i \cap \bar{\Omega}_j$. So, starting from one edge, since $R_h(\mathbf{u})$ vanishes outside of Ω , $R_h(\mathbf{u})$ vanishes everywhere. \square

With this result, we can prove

THEOREM 3.4. *For every $h > 0$, the discrete operator \mathbf{A}_h is regular, i.e. $\mathbf{Ker} \mathbf{A}_h = \{0\}$.*

Proof. Let u in $(\mathbb{R}^3)^n$ such that $\mathbf{A}_h(u) = 0$. Then, for every i in $\{1, \dots, n\}$ we have the following sequence of relations

$$\begin{aligned} \int_{\Omega_i} (\mathbf{A}(R_h(u))) dx = 0 &\Rightarrow \sum_{i=1}^n \left(\int_{\Omega_i} \mathbf{A}(R_h(u)) dx \right) \mathbf{u}_i = 0 \\ &\Rightarrow \int_{\Omega} \mathbf{A}(R_h(u)) R_h(u) dx = 0 \end{aligned}$$

This implies by Lemma 2.1 that $\mathbf{A}(\mathbf{R}_h(u)) = 0$. Then $\mathbf{A}_h(u)$ vanishes if and only if $\mathbf{A}(\mathbf{R}_h(u))$ vanishes ; that is, if and only if $\mathbf{R}_h(\mathbf{u})$ is in $\mathbf{Ker}\mathbf{A} \cap \{\mathbf{v} \in (\mathbf{L}^2(\mathbb{R}^3))^3 | v = 0 \text{ a.e. in } \mathbb{R}^3 \setminus \Omega\}$. So, thanks to Lemma 3.3, we conclude that $\mathbf{A}_h(u)$ vanishes if and only if $u = 0$. \square

We shall now prove an estimate on the smallest eigenvalue of \mathbf{A}_h .

THEOREM 3.5. *The smallest eigenvalue $\lambda_{h,min}$ of \mathbf{A}_h is such that*

$$(3.4) \quad \lambda_{h,min} \geq \frac{1}{4\sqrt{34}} \frac{h^{5/2}}{d(\Omega)},$$

where $d(\Omega)$ is the diameter of Ω , i.e. $d(\Omega) = \sup_{\mathbf{x}, \mathbf{y} \in \Omega} (|\mathbf{x} - \mathbf{y}|)$.

Proof. The main idea is to use the variational formulation to estimate the Rayleigh quotient.

1 – Estimate of $\lambda_{h,min}$ through Rayleigh quotient :

To estimate the lowest eigenvalue of \mathbf{A}_h we use the characterisation of $\lambda_{h,min}$ by Rayleigh quotient

$$\min_{u \in (\mathbb{R}^3)^n} \frac{(\mathbf{A}_h(u), u)_h}{\|u\|_h^2} = \lambda_{h,min},$$

or, by definition of \mathbf{R}_h ,

$$\begin{aligned} \lambda_{h,min} &= \min_{u \in (\mathbb{R}^3)^n} \frac{(\mathbf{R}_h(\mathbf{A}_h(u)), \mathbf{R}_h(u))_{0,\Omega}}{\|u\|_h^2} \\ &= \min_{u \in (\mathbb{R}^3)^n} \frac{\|\mathbf{grad} \phi(\mathbf{R}_h(u))\|_{0,\Omega}^2}{\|u\|_h^2}. \end{aligned}$$

2 – Definition of a convenient subset of trial functions :

We set a variational formulation for (2.2) :

$$(3.5) \quad \begin{aligned} &\phi \in \mathbf{W}^1(\mathbb{R}^3), \forall \psi \in \mathbf{W}^1(\mathbb{R}^3) ; \mathbf{u} \in \mathcal{I}m(\mathbf{R}_h) \text{ we have :} \\ &\int_{\mathbb{R}^3} \mathbf{grad} \psi \cdot \mathbf{grad} \phi \, d\mathbf{x} = \int_{\mathbb{R}^3} \mathbf{u} \cdot \mathbf{grad} \psi \, d\mathbf{x}, \end{aligned}$$

To define trial functions, we have to set some notations. The mesh is cubic and we denote \mathbf{X} , \mathbf{Y} and \mathbf{Z} the three main directions. For two adjacent cells in direction \mathbf{X} and for the face between, we shall denote by $\Omega_j^{i,\mathbf{X}}$ the first cell, $\Omega_{j+1}^{i,\mathbf{X}}$ the following and $\Sigma_j^{i,\mathbf{X}}$ the face between.

Then, for two adjacent cells $\Omega_j^{i,\mathbf{X}}$ and $\Omega_{j+1}^{i,\mathbf{X}}$, we define $\psi_j^{i,\mathbf{X}}$ such that

$$\begin{aligned} \psi_j^{i,\mathbf{X}} &\in \mathbf{W}^1(\mathbb{R}^3) \\ \psi_j^{i,\mathbf{X}}|_{\partial(\bar{\Omega}_j^{i,\mathbf{X}})} &= 0 \\ \int_{\Sigma_j^{i,\mathbf{X}}} \psi_j^{i,\mathbf{X}}(x, y, z) \, dy \, dz &= (\mathbf{u}_{j+1}^{i,\mathbf{X}} - \mathbf{u}_j^{i,\mathbf{X}}) \cdot \mathbf{X} \end{aligned}$$

Construction of a well chosen space of $\psi_j^{i,\mathbf{X}}$ is extensively given in [13].

3 – Estimates :

We apply (3.5) for trial functions defined above. for $n_j^{i,x}$ the normal to face $\Sigma_j^{i,x}$ in direction \mathbf{X} and u an element of $(\mathbb{R}^3)^n$ such that $R_h(u) = \mathbf{u}$, it comes using Green formula

$$\begin{aligned} \int_{\mathbb{R}^3} \mathbf{grad} \phi(\mathbf{u}) \cdot \mathbf{grad} \psi_j^{i,x} d\mathbf{x} &= \int_{\mathbb{R}^3} \mathbf{u} \cdot \mathbf{grad} \psi_j^{i,x} d\mathbf{x} \\ &= \int_{\Sigma_j^{i,x}} [R_h(u) \cdot n_j^{i,x}]_{|\Sigma_j^{i,x}} \psi_j^{i,x} d\mathbf{x}, \\ &= ((\mathbf{u}_{j+1}^{i,x} - \mathbf{u}_j^{i,x}) \cdot \mathbf{X}) \cdot \int_{\Sigma_j^{i,x}} \psi_j^{i,x} d\mathbf{x}, \end{aligned}$$

by construction of $\psi_j^{i,x}$ we have

$$((\mathbf{u}_{j+1}^{i,x} - \mathbf{u}_j^{i,x}) \cdot \mathbf{X}) \cdot \int_{\Sigma_j^{i,x}} \psi_j^{i,x} d\mathbf{x} = ((\mathbf{u}_{j+1}^{i,x} - \mathbf{u}_j^{i,x}) \cdot \mathbf{X})^2.$$

At this point of the proof, using the Cauchy-Schwarz inequality and expression of $\psi_j^{i,x}$, it comes

$$(3.6) \quad \|\mathbf{grad} \phi\|_{(\mathbb{L}^2(\bar{\Omega}_j^{i,x}))^3}^2 \geq \frac{9 h^3}{272} ((\mathbf{u}_{j+1}^{i,x} - \mathbf{u}_j^{i,x}) \cdot \mathbf{X})^2$$

This results is also valid for directions \mathbf{Y} and \mathbf{Z} . Now we add a layer of cells on the border of Ω in which we consider that u vanishes. Thanks to that “null layer” we can obtain by summation of (3.6) a global estimate :

$$(3.7) \quad 6 \|\mathbf{grad} \phi\|_{(\mathbb{L}^2(\mathbb{R}^3))^3}^2 \geq \frac{9 h^3}{272} \sum_{i,j,k;l,n,m} \left(((u_{l+1}^{i,x} - u_l^{i,x}) \cdot \mathbf{X})^2 + ((u_{n+1}^{j,y} - u_n^{j,y}) \cdot \mathbf{Y})^2 + ((u_{m+1}^{k,z} - u_m^{k,z}) \cdot \mathbf{Z})^2 \right).$$

On an other hand, by a succession of discrete Cauchy-Schwartz inequalities, we can prove that

$$(3.8) \quad \|u\|_h^2 = \sum_{i=1}^n |u_i|^2 \leq \left(\frac{d(\Omega)}{h} \right)^2 \sum_{i,j,k;l,n,m} \left(((u_{l+1}^{i,x} - u_l^{i,x}) \cdot \mathbf{X})^2 + ((u_{n+1}^{j,y} - u_n^{j,y}) \cdot \mathbf{Y})^2 + ((u_{m+1}^{k,z} - u_m^{k,z}) \cdot \mathbf{Z})^2 \right).$$

So, by (3.7) and (3.8) we get

$$\|\mathbf{grad} \phi\|_{0,\Omega} \geq \frac{1}{4\sqrt{34}} \frac{h^{5/2}}{d(\Omega)} \|u\|_h,$$

which gives (3.4) and ends the proof of the theorem. \square

3.3. Construction of the semi-analytical operator $\mathbf{A}_{h,N}$. The two successive integrals in \mathbf{A}_h practically forbid its use in real computations. Instead we introduce the semi-analytical operator $\mathbf{A}_{h,N}$: it is obtained by analytical integration of $\mathbf{A} \circ \mathbf{R}_h$, followed by a discrete projection $\mathbf{P}_{h,N}$ computed with a N -points Gauss quadrature formula (it is a classical method in integral equations computation, see [16]). So we define the approximate discretised operator by

$$(3.9) \quad \mathbf{A}_{h,N} = \mathbf{P}_{h,N} \circ \mathbf{A} \circ \mathbf{R}_h.$$

3.3.1. Description of the numerical integration. We first introduce the integration of each sub-matrix \mathbf{K}_i^j of \mathbf{A}_h :

$$\mathbf{K}_i^j(\mathbf{u}) = \frac{1}{|\Omega_i|} \left(\int_{\Omega_i} \mathbf{k}_j(\mathbf{x}) \mathbf{u} \, d\mathbf{x} \right),$$

where \mathbf{u} is an element of \mathbb{R}^3 and \mathbf{k}_j is a 3×3 matrix defined by

$$\mathbf{k}_j(\mathbf{x}) \mathbf{u} = \frac{1}{4\pi} \mathbf{grad} \operatorname{div} \int_{\Omega_j} \mathbf{u} \frac{-1}{|\mathbf{y} - \mathbf{x}|} \, d\mathbf{y}.$$

First of all, we remark that for $i = j$, $\mathbf{K}_i^j(\mathbf{u}) = \frac{1}{3} \mathbf{Id}_3$. Indeed, we have

$$\begin{aligned} \mathbf{k}_{i,xx}(\mathbf{x}) &= \frac{1}{4\pi} \frac{\partial^2}{\partial x^2} \int_{\Omega_i} \frac{-1}{|\mathbf{y} - \mathbf{x}|} \, d\mathbf{y}, \\ \mathbf{k}_{i,xy}(\mathbf{x}) &= \frac{1}{4\pi} \frac{\partial^2}{\partial x \partial y} \int_{\Omega_i} \frac{-1}{|\mathbf{y} - \mathbf{x}|} \, d\mathbf{y}, \end{aligned}$$

then, by symmetry, we obtain that the integral of the extra diagonal terms of $\mathbf{k}_j(\mathbf{x})$ over Ω_i vanish and

$$\int_{\Omega_i} \mathbf{k}_{i,xx} \, d\mathbf{x} = \int_{\Omega_i} \mathbf{k}_{i,yy} \, d\mathbf{x} = \int_{\Omega_i} \mathbf{k}_{i,zz} \, d\mathbf{x},$$

but

$$\int_{\Omega_i} (\mathbf{k}_{i,xx} + \mathbf{k}_{i,yy} + \mathbf{k}_{i,zz}) \, d\mathbf{x} = \int_{\Omega_i} \int_{\Omega_i} \Delta \left(\frac{-1}{4\pi |\mathbf{x} - \mathbf{y}|} \mathbf{xy} \right) = |\Omega_i|,$$

then we conclude that $\mathbf{K}_i^i(\mathbf{u}) = \frac{1}{3} \mathbf{Id}_3$ and we set $\tilde{\mathbf{K}}_i^i = \frac{1}{3} \mathbf{Id}_3$.

When $i \neq j$, we have to perform a numerical integration on each $\mathbf{k}_j(\mathbf{x})$ (which are obtained by analytical integration on Ω_j). As pointed out in [15], items of matrix $\mathbf{k}_j(\mathbf{x})$ are linear combinations of functions of the following type

$\forall i, j \in \{1, \dots, n\}$ and $i \neq j$ and $r, s, t \in \{0, 1\}$ we set :

$$\begin{aligned} g_{i,j}^{rst}(x, y, z) &= \tan^{-1} \left(\frac{((y - (y_i - y_j) - sh) \cdot (z - (z_i - z_j) - th))}{(x - (x_i - x_j) - rh) r_{r,s,t}} \right) \\ f_{i,j}^{rst}(x, y, z) &= \operatorname{sh}^{-1} \left(\frac{(z - (z_i - z_j) - th)}{\sqrt{(x - (x_i - x_j) - rh)^2 + ((y - (y_i - y_j) - sh))^2}} \right), \end{aligned}$$

where $r_{r,s,t} = \sqrt{((x_i - x_j) - rh)^2 + ((y_i - y_j) - sh)^2 + ((z_i - z_j) - th)^2}$ and h is the mesh step.

For each (i,j) , $g_{i,j}^{rst}$ is an element of $C^\infty([0, h]^3)$ and for each (i,j) such that Ω_i and Ω_j are non-adjacent, $f_{i,j}^{rst}$ is also an element of $C^\infty([0, h]^3)$.

But, when (i,j) is such that Ω_i and Ω_j are adjacent cells, $f_{i,j}^{rst}$ is no longer an element of $C^\infty([0, h]^3)$, it is an element of $H^1([0, h]^3)$. So, we split $k_j(\mathbf{x})$ in two parts, a singular one denoted $k_j^s(\mathbf{x})$, element $H^1([0, h]^3)$, and a regular one denoted $k_j^r(\mathbf{x})$, element of $C^\infty([0, h]^3)$. This splitting is such that the singular part $k_j^s(\mathbf{x})$ can be integrated analytically.

We recall the Gauss quadrature formula and error estimates. For any function f sufficiently regular, we set

$$\int_{[0,1]^3} f(x) dx \approx \mathcal{Q}_{N,i}(f) = h^3 \sum_{j_1=1}^N \sum_{j_2=1}^N \sum_{j_3=1}^N \left(\prod_{k=1,2,3} \alpha_{j_k} \right) f(h \zeta_{j_1} - x_i, h \zeta_{j_2} - z_i, h \zeta_{j_3} - z_i),$$

where $(\alpha_j, \zeta_j)_{j=1, \dots, N}$ are weights and points for the one-dimensional Gauss quadrature formula. We set an error formula. for all $\sigma \geq 3$ (see [2], [13]) :

$$E_{N,i}(f(x)) = \int_{\Omega_i} f(x) dx - \mathcal{Q}_{N,i}(f).$$

For $f(x)$ in $C^\infty(\Omega_i)$ we have the following error estimate

$$(3.10) \quad |E_{N,i}(f(x))| \leq \frac{C}{N^\sigma} \|f\|_{\mathbf{H}^\sigma(\Omega_i)}.$$

So, we define \tilde{K}_i^j for $i \neq j$:

If Ω_j and Ω_i are non-adjacent we set

$$\tilde{K}_i^j = \frac{1}{|\Omega_i|} \mathcal{Q}_{N,i}(\mathbf{k}_j),$$

else

$$\tilde{K}_i^j = \frac{1}{|\Omega_i|} \left[\mathcal{Q}_{N,i}(\mathbf{k}_j^r) - \int_{\Omega_i} \mathbf{k}_j^s(x) dx \right].$$

We can therefore apply formula (3.10) to estimate the quadrature error $E_{N,i,j}$ between

K_i^j and \tilde{K}_i^j :

for $i = j$ we have

$$E_{N,i,j} = 0,$$

if $i \neq j$ and Ω_j, Ω_i non-adjacent cells,

$$(3.11) \quad E_{N,i,j} \leq \frac{C}{N^\sigma |\Omega_i|} \|\mathbf{k}_j\|_{\mathbf{H}^\sigma(\Omega_i)},$$

else, if Ω_j and Ω_i are adjacent cells,

$$(3.12) \quad E_{N,i,j} \leq \frac{C}{N^\sigma |\Omega_i|} \|\mathbf{k}_j^r\|_{\mathbf{H}^\sigma(\Omega_i)}.$$

3.3.2. Estimate of the lowest eigenvalue. Now, thanks to the error estimate of the Gauss quadrature, we can establish a lower bound for the lowest eigenvalue of \mathbf{A}_h .

THEOREM 3.6. *Let $\sigma \geq 3$, for k_j belonging to $H^\sigma(\Omega_i)$, a sufficient condition for the positiveness of $\mathbf{A}_{h,N}$ is the existence of a real positive constant α_σ such that*

$$\alpha_\sigma N^\sigma \geq \frac{1}{h^{5/2}},$$

where N is the number of Gauss points in each space direction.

Proof. We denote by E_h the error, i.e. $\mathbf{A}_{h,N} = \mathbf{A}_h + E_h$. Eigenvalues of these three operators are numbered increasingly and denoted as

$(\lambda_i)_{i=1,\dots,3n}$ the spectrum of \mathbf{A}_h ,

$(\tilde{\lambda}_i)_{i=1,\dots,3n}$ the spectrum of $\mathbf{A}_{h,N}$,

$(\epsilon_i)_{i=1,\dots,3n}$ the spectrum of E_h .

Classical algebra results allow to write (see [12])

$$(3.13) \quad \sup_{i \in \{1,\dots,3n\}} |\lambda_i - \tilde{\lambda}_i| \leq \sup_{i \in \{1,\dots,3n\}} |\epsilon_i|.$$

Then, we are led to find an upper bound for the eigenvalues of E_h . Since the integration on the diagonal terms (local 3 by 3 matrices) is exact, the diagonal terms in E_h (local 3 by 3 matrices) vanish. Then, the Gershgorin circles theorem gives

$$\sup_{i \in \{1,\dots,3n\}} |\epsilon_i| \leq \sup_{i \in \{1,\dots,n\}} \left(\sum_{j \in \{1,\dots,3n\}} |E_{h,ij}| \right).$$

As a consequence, if we consider the 3 by 3 sub-matrices K_i^j , using error estimate formulae (3.11, 3.12), we have for any $\sigma \geq 3$ existence of a real constant α_σ such that

$$\sum_{j=1, j \neq i}^N \sum_{l=1}^3 |(\tilde{K}_i^j)_{il} - (K_i^j)_{il}| \leq \alpha_\sigma \frac{C}{N^\sigma},$$

with $\alpha_\sigma = \sup_{i \in \{1,\dots,n\}} \left(\frac{1}{|\Omega_j|} \|k_j\|_{H^\sigma(\Omega_j)} \right)$ and we can write

$$(3.14) \quad \sup_{i \in \{1,\dots,3n\}} |\epsilon_i| \leq \alpha_\sigma \frac{C}{N^\sigma}.$$

We now build a sufficient condition for the positiveness of $\mathbf{A}_{h,N}$: the coefficients of k_j belong to $H^\sigma(\Omega)$ ($\sigma \geq 3$), so by Theorem 3.5 and by (3.14), we have

$$\frac{1}{4\sqrt{34}} \frac{h^{5/2}}{d(\Omega)} \geq \alpha_\sigma \frac{C}{N^\sigma}$$

and we can conclude that

$$N^\sigma \geq \alpha_\sigma C 4\sqrt{34}d(\Omega) \frac{1}{h^{5/2}}.$$

□

3.3.3. Symmetrisation of the approximate operator. In order to keep the operator symmetric, we set $A_{h,N}^S = \frac{1}{2}(A_{h,N} + A_{h,N}^t)$, i.e.

$$\forall u \in (\mathbb{R}^3)^n, \quad (A_{h,N}^S(u))_i = \sum_{j=1}^n \frac{1}{2} \left(K_i^j + \tilde{K}_j^i \right) (\mathbf{u}_j).$$

All the results presented here for $A_{h,N}$ extend to $A_{h,N}^S$. In the sequel we will use $A_{h,N}^S$.

3.3.4. Convergence theorem for the Gauss approximated operator. We are now able to give the convergence rate of the Gauss approximated operator :

THEOREM 3.7. *For all u in $H^1(\Omega)$ and N in \mathbb{N}^* such that the condition given in Theorem 3.6 is verified, then there exists C in \mathbb{R}_+^* such that for all h in \mathbb{R}_+^* , we have*

$$\|R_h \circ A_{h,N}^S \circ P_h(u) - A(u)\|_{0,\Omega} \leq Ch|u|_{1,\Omega},$$

and the operator $A_{h,N}^S$ is symmetric, definite and positive.

Proof. The positiveness, symmetry and regularity of $A_{h,N}^S$ is a direct consequence of the hypothesis of Theorem 3.6 and the previous paragraph. The error estimate is obtained by the following estimation :

$$A_{h,N}^S = \frac{1}{2}(A_{h,N} + A_{h,N}^t) = A_h + \frac{1}{2}(E_{h,N} + E_{h,N}^t),$$

then we have

$$\begin{aligned} \|R_h \circ A_{h,N}^S \circ P_h(u) - A(u)\|_{0,\Omega} &= \|R_h \circ A_h \circ P_h(u) - A(u) + \frac{1}{2}R_h(E_{h,N} + E_{h,N}^t)P_h(u)\|_{0,\Omega} \\ &\leq \|R_h \circ A_h \circ P_h(u) - A(u)\|_{0,\Omega} + \frac{1}{2}\|R_h(E_{h,N} + E_{h,N}^t)P_h(u)\|_{0,\Omega} \\ &\leq Ch|u|_{1,\Omega} + \frac{1}{2}C_1|u|_{1,\Omega} \sup_{(i,j) \in \{1,\dots,n\}^2} |E_{h,N,ij}| \\ &\leq (Ch + C_1\alpha_\sigma h^{5/2})|u|_{1,\Omega}. \end{aligned}$$

□

To illustrate the convergence of the approximation, we compute the error between the exact and approximated solution of the problem a uniform field in a cube of length one (see Fig. 3.1).

4. Block-Toeplitz matrices, application to the computation of the magnetostatic field. The operator $A_{h,N}^S$ is represented by a full matrix. So, the use of this operator becomes impossible for the huge meshes aimed by simulations as those of micromagnetic systems. To overcome that problem, we use a feature of this matrix : it is a block-Toeplitz matrix. We will start with a general presentation of block-Toeplitz matrices using tensored products. We will then present an application of block-Toeplitz matrices product to compute the magnetostatic field. This fast computation is not built on a truncation of the operator $A_{h,N}^S$: it is an exact method. Effectively, the embedding of Toeplitz matrices in circulant matrices as presented here preserve exactly the matrix vector product.

Number of cells	h	error
64	1/4	0.0546256921
512	1/8	0.0406119569
1736	1/16	0.0264626018
32768	1/32	0.0160913191
262144	1/64	0.0093714246

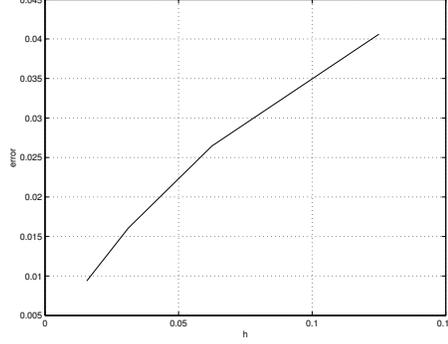


FIG. 3.1. Error between exact and approximated solution of a uniform field in a cube.

4.1. The block-Toeplitz vector-matrix multiplication. We recall briefly the definition of a block-Toeplitz matrix and the main ideas of the block-Toeplitz vector-matrix multiplication. An extensive study of this problem could be found in [9, 17].

DEFINITION 4.1. T_n is a one-level Toeplitz matrix of order n if and only if :

$$T_n = (t_{i-j})_{i,j \in \{1, \dots, n\}} = \begin{pmatrix} t_0 & t_{-1} & \dots & \dots & t_{1-n} \\ t_1 & t_0 & \ddots & & t_{2-n} \\ \vdots & \ddots & \ddots & t_{-1} & \vdots \\ t_{n-2} & & t_1 & t_0 & t_{-1} \\ t_{n-1} & \dots & \dots & t_1 & t_0 \end{pmatrix},$$

with $(t_i)_{i \in \{1-n, \dots, n-1\}} \in \mathbb{R}^{2n-1}$.

The vector $\{t_{1-n}, t_{2-n}, \dots, t_{-1}, t_0, t_1, \dots, t_{n-2}, t_{n-1}\}$ is called generator of T_n .

T_{n_1, \dots, n_p} is called a p -level block-Toeplitz matrix of order $\prod_{i=1}^p n_i$ if and only if, following the notations above, the items $(t_i)_{i \in \{1-n, \dots, n-1\}}$ are $p-1$ block-Toeplitz matrices of order $\prod_{i=2}^p n_i$.

We recall also the definition of circulant matrices

DEFINITION 4.2. C_n is a one-level circulant matrix of order n if and only if C_n is a one-level Toeplitz matrix such that, for all i in $\{1, \dots, n-1\}$, $(C_n)_{i,n} = (C_n)_{i+1,1}$ and $(C_n)_{n,n} = (C_n)_{1,1}$. The multi-level circulant matrices are multi-level block-Toeplitz matrices built using the procedure.

Then, one can demonstrate that you could easily embed Toeplitz matrices in at least 2^p greater circulant matrices where p is the number of level considered. Such an embedding permits to therefore compute the matrix-vector product fastly thanks to Fast-Fourier transformations using the fact that the multiplication between a circulant matrix and a vector is a discrete convolution.

So forth, by applying the fast Fourier transform algorithm to compute the products of Fourier transform of a vector, we have

THEOREM 4.3. *The matrix-vector product algorithm using fast Fourier transforms for p -levels block Toeplitz matrices of order $N_p = \prod_{k=1}^p n_k$ needs*

- $O(3 p 2^p N_p + 3 2^p N_p \log(N_p))$ operations,
- storage of $O(2^p N_p)$ reals numbers.

We keep in mind that a direct computation of the product would have needed $O(N_p^2)$ operations and the storage of $O(N_p^2)$ reals numbers.

Proof. The algorithm requires three p -levels the fast Fourier transforms, two for the embedding (matrix and vector) and one for extraction of the result. A p -levels transform $F_{2^{m_k}}$ needs $2^{m_k} \log(2^{m_k})$ operations. Then, $F_{\otimes p}$, on a grid $\prod_{k=1}^p \{1, \dots, 2^{m_k}\}$ needs a number of operations equal to

$$\left(\prod_{i \neq k, i=1}^p 2^{m_i} \right) 2^{m_k} \log 2^{m_k} = \left(\prod_{i=1}^p 2^{m_i} \right) \log 2^{m_k},$$

where, for any x in \mathbb{R}_*^+ , $\log x$ is the base 2 logarithm.

Using the ‘‘power two’’ FFT, we set $M_p = \prod_{i=1}^p 2^{m_i}$. So, to apply $F_{\otimes p}$ needs $M_p \sum_{k=1}^p \log 2^{m_k} = M_p \sum_{k=1}^p m_k$ operations. Then, using $\text{Fl}(x)$ as a notation for the floor function, we set $m_k = \text{Fl}(\log(n_k)) + 1$ and we have $\forall k \in \{1, \dots, p\} 2^{m_k} \geq n_k$. This allows to bound the number of operations needed for a p -levels FFT by :

$$M_p \sum_{k=1}^p m_k \leq 2^p N_p \log \left(\prod_{k=1}^p 2 n_k \right) = 2^p N_p \log(2^p N_p).$$

And we conclude that the algorithm needs $O(3 p 2^p N_p + 3 2^p \log(N_p))$ operations. We only need to store the generator vectors of the mono-level Toeplitz sub-matrices of the p -levels block Toeplitz matrix. The storage of each mono-level structure needs 2^{m_k} reals, so we can estimate the global storage by

$$\prod_{k=1}^p 2^{m_k} \leq \prod_{k=1}^p 2 n_k \leq 2^p N_p.$$

□

4.2. Application to magnetostatic computations for micromagnetic simulations. Let us come back to problem (1.1). First of all, we have

THEOREM 4.4. *The discretised operator \mathbf{A}_h is a 3-levels block Toeplitz matrix.*

Proof. As we saw precedently,

$$\mathbf{A}_{h,I,J} \mathbf{u} = \frac{1}{4\pi h^3} \int_{\Omega_{\text{ind}_3(I)}} \text{grad}_x \text{div}_x \cdot \int_{\Omega_{\text{ind}_3(J)}} \mathbf{u} \frac{1}{|y-x|} dy dx \quad \forall \mathbf{u} \in \mathbb{R}^3.$$

We apply to these formula the following change of variables :

$$\begin{aligned} x &= x_{\text{ind}_3(I)} + \hat{x} & \hat{x} &\in [0, h]^3 \\ y &= x_{\text{ind}_3(I)} + \hat{y} & \hat{y} &\in \prod_{k=1}^3 [(i_k - j_k)h, (i_k - j_k + 1)h] = \Omega_{|IJ|}, \end{aligned}$$

$$\text{so that } \mathbf{A}_{h,I,J} \mathbf{u} = \frac{1}{4\pi h^3} \int_{\Omega_{|I,J|}} \text{grad}_x \text{div}_x \cdot \int_{\Omega_{|I,J|}} \mathbf{u} \frac{1}{|\hat{y} - \hat{x}|} d\hat{y} d\hat{x} \quad \forall \mathbf{u} \in \mathbb{R}^3,$$

Then, for all I and J in $\prod_{k=1}^3 \{1, \dots, n_k\}$, $\mathbf{A}_{h,I,J}$ depends only on $(I - J)$. We conclude by using definition (4.1) that \mathbf{A}_h is a 3-levels block Toeplitz matrix. \square

A comparison of the computational for magnetic bricks of various sizes is presented. The time unit used in the tables is $10^{-2}s$.

Number of cells in each direction	Total number of cells	LAPACK	Block Toeplitz algorithm
4×4	16 cells	0,01	0,17
$4 \times 4 \times 2$	32 cells	0,04	0,32
$4 \times 4 \times 4$	64 cells	0,17	0,62
$4 \times 4 \times 8$	128 cells	0,78	1,31
$4 \times 8 \times 8$	256 cells	3,93	2,55
$8 \times 8 \times 8$	512 cells	16,49	5,35
$8 \times 8 \times 16$	1024 cells	70,77	11,03

Computational time

The computations are made with the optimized LAPACK library for full matrices and the fast solving method exposed below. The fast Fourier transform used for the fast solving method is a plain fortran code.

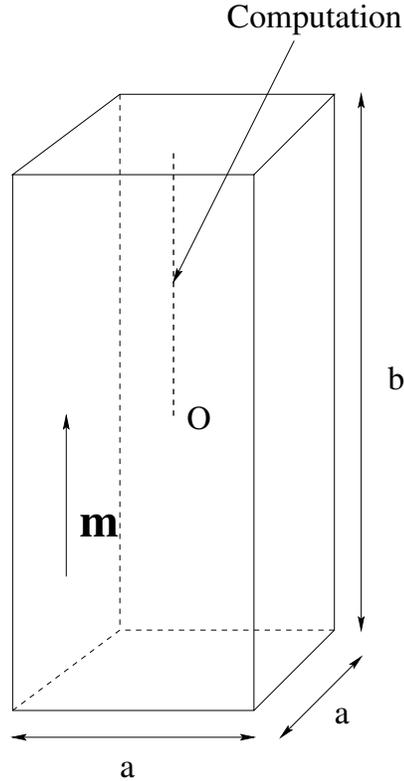
Number of cells in each direction	Total number of cells	Assembly time for a full matrix	Assembly time for a block Toeplitz matrix
4×4	16 cells	52	24
$4 \times 4 \times 2$	32 cells	199	57
$4 \times 4 \times 4$	64 cells	779	133
$4 \times 4 \times 8$	128 cells	3107	290
$4 \times 8 \times 8$	256 cells	12364	611
$8 \times 8 \times 8$	512 cells	49153	1325
$8 \times 8 \times 16$	1024 cells	199938	2725

The assembly time

Assembly has to be made only when the geometry is changed.

5. Some numerical results. In this section, efficiency of the method is performed by comparing numerical and theoretical results. The results, by R.I. Joseph and E. Schlömann (see [11]), are valid for a rectangular magnetic prism whose basis length a is negligible with respect to his height b (see Fig. 5.1); the magnetization field is considered to be uniformly parallel to the height. The authors give the magnetic field along the great axis between two points of the domain : the center of the prism and the center of one of the basis. Figure (5.2) gives the magnetostatic field (projected on the prism height) along the computation line for various ratios $p = \frac{a}{b}$:

$p = \frac{a}{b}$	number of cells on basis	number of cells on length	total number of cells
0.5	16×16	32	8192
0.25	16×16	64	16384
0.125	8×8	64	4096
0.06255	8×8	128	8192

FIG. 5.1. *The magnetic domain Ω .*

The results are quite satisfactory. We see that the theoretical results tend to the numerical results when the length ratio tends to zero.

6. Conclusion. The method developed in this article to compute the magnetostatic field is performant. It is useful for dynamic computations like micromagnetic simulations which needs to compute the magnetostatic field at each time step. For these simulations ([13, 14]), the embedding 3-levels block circulant matrix is computed before the first time step. Then, the only computation at each time step is the matrix-vector block circulant product and the the extraction.

There exist other methods to solve the Poisson equation, one of the most competitive one being the Fast Multipole Method [6]. However, it turns out that this method is not adapted to our problem. The first reason being the non exact preservation of the negativness of the magnetostatic operator ; as explained in the introduction, which is essential to obtain consistant equilibrium states for ferromagnetic problems. The second reason is that the use of a regular grid is an advantage in the context of dynamical simulation ; indeed, the structures we want to catch are very fine and non regular grids may badly influence the results [14]. Eventually, when using regular grids, our method is clearly easier to implement than the Fast Multipole Method for the same complexity.

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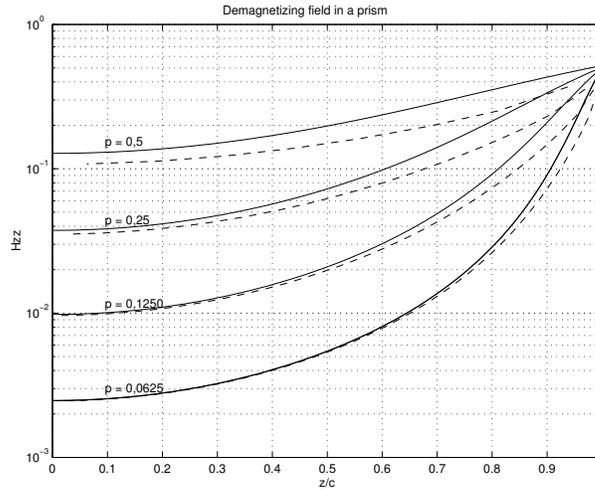


FIG. 5.2. Comparison between theoretical and numerical results.

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