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To cite this version:
Stéphane Labbé. Fast computation for large magnetostatic systems adapted for micromagnetism. SIAM Journal on Scientific Computing, Society for Industrial and Applied Mathematics, 2005, 26, pp. 2160-2175, n. 6. <hal-00086968>

HAL Id: hal-00086968
https://hal.archives-ouvertes.fr/hal-00086968
Submitted on 20 Jul 2006

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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 \( \Omega \) 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

\[
\begin{cases}
\nabla \times \mathbf{H} = \mathbf{0} \\
\n\nabla \cdot \mathbf{B} = \mathbf{0} \\
\n\mathbf{B} = \mu_0 (\mathbf{H} + \mathbf{u}),
\end{cases}
\]

(1.1)

where \( \mu_0 \) is the permeability of the vacuum, and \( \mathbf{u} \) vanishes outside \( \Omega \).

The numerical resolution of this system amounts to solve the Poisson equation, namely

\[-\Delta \Phi = \nabla \cdot \mathbf{u}; \quad \nabla \Phi = \mathbf{H}\]

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 \( \Omega \) and such that \( \mathbf{u} \) minimizes the energy \( e(\mathbf{u}) = -\int_{\Omega} \mathbf{u} \cdot H_T(\mathbf{u}) \, dx \). Such minimizers verify

\[\|\mathbf{u} \wedge H_T(\mathbf{u})\|_{0,\Omega} = 0,\]

where \( H_T(\mathbf{u}) \) 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 \( H_h \) might be crucial, otherwise, it may exists regions \( \omega \), included in \( \Omega \), in

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which $\mathbf{H}_h \cdot \mathbf{u}_h > 0$ almost everywhere in $\omega$ 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 where 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. Tyrtyshnikov 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 $\Omega$, $L^2(\Omega)$ 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 $\| \cdot \|_{0,\Omega}$.

$D(\Omega)$ is the space of functions which are infinitely differentiable and compactly supported in $\Omega$. Its dual is the space of distributions, denoted $D'(\Omega)$. For any positive integer $m$, $H^m(\Omega)$ is the Sobolev space of distributions defined in $\Omega$, whose derivates 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, \( H^m(\Omega) \) 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 \( \text{rot} \mathbf{H} = 0 \), there exist a unique \( \phi \) in the weighted Sobolev space \( W^{1}(\mathbb{R}^3) \) such that

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

with

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

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

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

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

\[
\phi(\mathbf{u}) \text{ the unique solution of (2.2)},
\]

and \( \mathbf{A}(\mathbf{u}) = -\text{grad} \phi(\mathbf{u}) \).

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

\[
\mathbf{H} = -\text{grad} \left( G \ast \text{div} (\mathbf{u}) \right)
\]

\[
= -\text{grad} \left( G \ast \sum_{i=1}^{3} \frac{\partial \mathbf{u}_i}{\partial x_i} \right)
\]

\[
= -\text{grad} \left( \sum_{i=1}^{3} \frac{\partial}{\partial x_i} G \ast \mathbf{u}_i \right)
\]

\[
= -\text{grad} \left( \sum_{i=1}^{3} \frac{\partial}{\partial x_i} (G \ast \mathbf{u}) \right)
\]

\[
= -\text{grad} \left( \text{div} (\mathbf{u} \ast G) \right),
\]

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) \[
\mathbf{A}(\mathbf{u}) = -\mathbf{H} = \text{grad} \left( \int_{\Omega} \mathbf{u}(y) \cdot \frac{1}{4\pi|x-y|} \, dy \right).
\]

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

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

\[
(A(u), u)_{0,\mathbb{R}^3} = 0 \iff (\text{grad} \ \phi(u), u)_{0,\mathbb{R}^3} = 0,
\]

\[
\iff - (\phi(u), \text{div} \ u)_{0,\mathbb{R}^3} = 0,
\]

\[
\iff (\phi(u), \Delta \phi(u))_{0,\mathbb{R}^3} = 0,
\]

\[
\iff (\text{grad} \ \phi(u), \text{grad} \ \phi(u))_{0,\mathbb{R}^3} = 0,
\]

\[
\iff \|A(u)\|^2_{0,\mathbb{R}^3} = 0.
\]

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

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

3. The finite-volume discretisation.

3.1. Space discretisation. The domain \( \Omega \) is broken down in \( n \) cubes \( \Omega_i \) of length \( h \). A function in \((L^2(\Omega))^3\) will be approximated by piecewise constant functions (constant on each cube \( \Omega_i \)). \( \mathbb{R}^3 \) is equipped with the euclidian product '.' and norm \( | | \). We introduce \((\mathbb{R}^3)^n\) made of functions \( u = (u_1, \ldots, u_n) \), each \( u_i \) belonging to \( \mathbb{R}^3 \). The space \((\mathbb{R}^3)^n\) is furnished with the canonical euclidian structure written as follows

\[
\forall \ (u, v) \in (\mathbb{R}^3)^n : 
\]

\[
(u, v)_h = \sum_{i=1}^{n} |\Omega_i| \ u_i, v_i,
\]

\[
\|u\|^2_h = \sum_{i=1}^{n} |\Omega_i| \ |u_i|^2,
\]

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

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

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

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

where \( \chi_i \) is defined for \( x \in \mathbb{R}^3 \) by : \( \chi_i(x) = 1 \) if \( x \) belongs to \( \Omega_i \), \( \chi_i(x) = 0 \) 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 \( u \) in \((H^1(\Omega))^3\)

\[
\|u - R_h(P_h(u))\|_{0,\Omega} \leq C \ h \ |u|_{1,\Omega},
\]

(ii) \( \forall v \in (\mathbb{R}^3)^n; \ \|R_h(v)\|_{0,\Omega} = \|v\|_h \)

(iii) \( \forall u \in (L^2(\Omega))^3; \ \|P_h(u)\|_h \leq \|u\|_{0,\Omega} \)
This allows us to approximate the operator $A$ by the following finite volume operator

$$A_h = P_h \circ A \circ R_h. \tag{3.1}$$

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

$$\langle A_h(u) \rangle_i = \sum_{j=1}^{n} K^j_i(u_j). \tag{3.2}$$

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

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

Each $K^j_i$ is a 3 by 3 real matrix. These matrices characterise the interaction between two cells $\Omega_i$ and $\Omega_j$.

### 3.2. Properties of the approximate operator $A_h$. We start with the elementary properties of $A_h$

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

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

The proof is straightforward and will be omitted (see [13]). We saw in Lemma 2.1 that $A$ is singular. On the contrary, the discretised operator $A_h$ is regular. To prove that result we will use an intermediate lemma

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

$$\text{div} \, R_h(u) = 0 \iff \forall i \in \{1, \ldots, n\}, \quad u_i = 0.$$

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

With this result, we can prove

**Theorem 3.4.** For every $h > 0$, the discrete operator $A_h$ is regular, i.e. $\text{Ker}A_h = \{0\}$.

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

$$\int_{\Omega_i} (A(R_h(u))) \, dx = 0 \Rightarrow \sum_{i=1}^{n} \left( \int_{\Omega_i} A(R_h(u)) \, dx \right) \, u_i = 0 \Rightarrow \int_{\Omega} A(R_h(u)) R_h(u) \, dx = 0.$$
This implies by Lemma 2.1 that \( A(R_h(u)) = 0 \). Then \( A_h(u) \) vanishes if and only if \( A(R_h(u)) \) vanishes; that is, if and only if \( R_h(u) \) is in \( \text{Ker}A \cap \{ v \in (L^2(\mathbb{R}^3))^3 | v = 0 \text{ a.e. in } \mathbb{R}^3 \setminus \Omega \} \). So, thanks to Lemma 3.3, we conclude that \( A_h(u) \) vanishes if and only if \( R_h(u) \) is in \( \text{Ker}A \cap \{ v \in (L^2(\mathbb{R}^3))^3 | v = 0 \text{ a.e. in } \mathbb{R}^3 \setminus \Omega \} \). So, thanks to Lemma 3.3, we conclude that \( A_h(u) \) vanishes if and only if \( u = 0 \).

We shall now prove an estimate on the smallest eigenvalue of \( A_h \).

**Theorem 3.5.** The smallest eigenvalue \( \lambda_{h,\text{min}} \) of \( A_h \) is such that

\[
\lambda_{h,\text{min}} \geq \frac{1}{4\sqrt{\frac{34}{5}}} \left( \frac{d(\Omega)}{d(\Omega)} \right)^{5/2},
\]

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

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

1. **Estimate of \( \lambda_{h,\text{min}} \) through Rayleigh quotient:**

To estimate the lowest eigenvalue of \( A_h \) we use the characterisation of \( \lambda_{h,\text{min}} \) by Rayleigh quotient

\[
\min_{u \in (\mathbb{R}^3)^n} \frac{(A_h(u), u)_h}{||u||^2_h} = \lambda_{h,\text{min}},
\]

or, by definition of \( R_h \),

\[
\lambda_{h,\text{min}} = \min_{u \in (\mathbb{R}^3)^n} \frac{(R_h(A_h(u)), R_h(u))_{0,\Omega}}{||u||^2_h} = \min_{u \in (\mathbb{R}^3)^n} \frac{||\text{grad} \phi(R_h(u))||^2_{0,\Omega}}{||u||^2_h}.
\]

2. **Definition of a convenient subset of trial functions:**

We set a variational formulation for (2.2):

\[
\phi \in W^1(\mathbb{R}^3), \forall \psi \in W^1(\mathbb{R}^3); u \in \mathcal{I}m(R_h) \text{ we have }: \int_{\mathbb{R}^3} \text{grad} \psi \cdot \text{grad} \phi \; dx = \int_{\mathbb{R}^3} u \cdot \text{grad} \psi \; dx.
\]

To define trial functions, we have to set some notations. The mesh is cubic and we denote \( X, Y \) and \( Z \) the three main directions. For two adjacent cells in direction \( X \) and for the face between, we shall denote by \( \Omega^i,\bar{X}_j \) the first cell, \( \Omega^{i+1,\bar{X}_j} \) the following and \( \Sigma^i,\bar{X}_j \) the face between.

Then, for two adjacent cells \( \Omega^i,\bar{X}_j \) and \( \Omega^{i+1,\bar{X}_j} \), we define \( \psi^{i,\bar{X}_j}_j \) such that

\[
\psi^{i,\bar{X}_j}_j \in W^1(\mathbb{R}^3) \quad \psi^{i,\bar{X}_j}_j |_{\partial \Omega^i,\bar{X}_j} = 0 \\
\int_{\Sigma^i,\bar{X}_j} \psi^{i,\bar{X}_j}_j(x, y, z) \; dy \; dz = (u^{i,\bar{X}_j}_j - u^{i,\bar{X}_j}_{j+1}) \cdot X
\]

Construction of a well chosen space of \( \psi^{i,\bar{X}_j}_j \) is extensively given in [13].
3 – Estimates:

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

\[
\int_{\mathbb{R}^3} \text{grad} \, \phi(u) \cdot \text{grad} \, \psi^i_j \, dx = \int_{\mathbb{R}^3} u \cdot \text{grad} \, \psi^i_j \, dx
= \int_{\Sigma_j^i_X} [\text{R}_h(u), n^i_j] \cdot \psi^i_j \, dx,
= ((u^i_j - u^i_{j+1}) \cdot X) \cdot \int_{\Sigma_j^i_X} \psi^i_j \, dx,
\]

by construction of \( \psi^i_j \) we have

\[
((u^i_j - u^i_{j+1}) \cdot X) \cdot \int_{\Sigma_j^i_X} \psi^i_j \, dx = ((u^i_j - u^i_{j+1}) \cdot X)^2.
\]

At this point of the proof, using the Cauchy-Schwarz inequality and expression of \( \psi^i_j \), it comes

\[
\| \text{grad} \, \phi \|_{L^2((\hat{\Omega})^i_j)}^2 \geq \frac{9 \, h^3}{272} ((u^i_{j+1} - u^i_j \cdot X)^2.
\]

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

\[
6 \| \text{grad} \, \phi \|_{L^2(\mathbb{R}^3)}^2 \geq \sum_{i,j,k,l,n,m} ((u^i_j - u^i_{j+1}) \cdot X)^2 + ((u^j_n - u^j_{n+1}) \cdot Y)^2 + ((u^k_m - u^k_{m+1}) \cdot Z)^2.
\]

On another hand, by a succession of discrete Cauchy-Schwarz inequalities, we can prove that

\[
\| u \|_{h}^2 = \sum_{i=1}^{n} |u_i|^2 \leq \left( \frac{d(\Omega)}{h} \right)^2 \sum_{i,j,k,l,n,m} ((u^i_j - u^i_{j+1}) \cdot X)^2 + ((u^j_n - u^j_{n+1}) \cdot Y)^2 + ((u^k_m - u^k_{m+1}) \cdot Z)^2.
\]

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

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

which gives (3.4) and ends the proof of the theorem. \( \Box \)
3.3. Construction of the semi-analytical operator \( A_{h,N} \). The two successive integrals in \( A_h \) practically forbid its use in real computations. Instead we introduce the semi-analytical operator \( A_{h,N} \): it is obtained by analytical integration of \( A \circ R_h \), followed by a discrete projection \( P_{h,N} \) 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

\[
A_{h,N} = P_{h,N} \circ A \circ R_h.
\]

(3.9)

3.3.1. Description of the numerical integration. We first introduce the integration of each sub-matrix \( K_{ij} \) of \( A_h \):

\[
K_{ij}(u) = \frac{1}{|\Omega_i|} \left( \int_{\Omega_i} k_j(x) u \, dx \right),
\]

where \( u \) is an element of \( \mathbb{R}^3 \) and \( k_j \) is a 3 \( \times \) 3 matrix defined by

\[
k_j(x) u = \frac{1}{4\pi} \text{grad} \, \text{div} \int_{\Omega_j} u \, \frac{-1}{|y-x|} \, dy.
\]

First of all, we remark that for \( i = j \), \( K_{ii}(u) = \frac{1}{3} \text{Id}_3 \). Indeed, we have

\[
k_{i,xx}(x) = \frac{1}{4\pi} \frac{\partial^2}{\partial x^2} \int_{\Omega_i} \frac{-1}{|y-x|} \, dy,
\]

\[
k_{i,xy}(x) = \frac{1}{4\pi} \frac{\partial^2}{\partial x \partial y} \int_{\Omega_i} \frac{-1}{|y-x|} \, dy,
\]

then, by symmetry, we obtain that the integral of the extra diagonal terms of \( k_j(x) \) over \( \Omega_i \) vanish and

\[
\int_{\Omega_i} k_{i,xx} \, dx = \int_{\Omega_i} k_{i,yy} \, dx = \int_{\Omega_i} k_{i,zz} \, dx,
\]

but

\[
\int_{\Omega_i} (k_{i,xx} + k_{i,yy} + k_{i,zz}) \, dx = \int_{\Omega_i} \int_{\Omega_i} \Delta \left( \frac{-1}{4\pi|x-y|} \right) \, xy \right) = |\Omega_i|,
\]

then we conclude that \( K_{ii}(u) = \frac{1}{3} \text{Id}_3 \) and we set \( \tilde{K}_{ii} = \frac{1}{3} \text{Id}_3 \).

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

\[
\forall i, j \in \{1, \ldots, n\} \text{ and } i \neq j \text{ and } r, s, t \in \{0, 1\} \text{ we set :}
\]

\[
g_{r,s,t}^{i,j}(x, y, z) = \tan^{-1} \left( \frac{(y - (y_i - y_j) - shr)(z - (z_i - z_j) - th)}{(x - (x_i - x_j) - rh)_{r,s,t}} \right)
\]

\[
f_{r,s,t}^{i,j}(x, y, z) = \text{sh}^{-1} \left( \frac{(z - (z_i - z_j) - th)}{\sqrt{(x - (x_i - x_j) - rh) + (y - (y_i - y_j) - shr)^2}} \right),
\]

where \( r_{r,s,t} = \sqrt{(x - x_j)^2 + (y - y_j)^2 + (z - z_j)^2} \) and \( h \) is the mesh step.
For each \((i,j)\), \(g^{rst}_{i,j}\) is an element of \(C^\infty([0,h^3])\) and for each \((i,j)\) such that \(\Omega_i\) and \(\Omega_j\) are non-adjacent, \(f^{rst}_{i,j}\) is also an element of \(C^\infty([0,h^3])\).

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

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

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

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

\[
E_{N,i}(f(x)) = \int_{\Omega_i} f(x) \, dx - Q_{N,i}(f).
\]

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

\[
(3.10) \quad |E_{N,i}(f(x))| \leq C_N \|f\|_{H^\sigma(\Omega_i)}.
\]

So, we define \(\tilde{K}^j_i\) for \(i \neq j\):

If \(\Omega_j\) and \(\Omega_i\) are non-adjacent we set

\[
\tilde{K}^j_i = \frac{1}{|\Omega_i|} Q_{N,i}(k^j),
\]

else

\[
\tilde{K}^j_i = \frac{1}{|\Omega_i|} \left[ Q_{N,i}(k^j) - \int_{\Omega_i} k^j(x) \, dx \right].
\]

We can therefore apply formula (3.10) to estimate the quadrature error \(E_{N,i,j}\) between \(K^j_i\) and \(\tilde{K}^j_i\):

for \(i = j\) we have

\[
E_{N,i,j} = 0,
\]

if \(i \neq j\) and \(\Omega_j\), \(\Omega_j\) non-adjacent cells,

\[
(3.11) \quad E_{N,i,j} \leq C_N \|k^j\|_{H^\sigma(\Omega_i)}.
\]

else, if \(\Omega_j\) and \(\Omega_j\) are adjacent cells,

\[
(3.12) \quad E_{N,i,j} \leq C_N \|k^j\|_{H^\sigma(\Omega_i)}.
\]
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 $A_h$.

**Theorem 3.6.** Let $\sigma \geq 3$, for $k_j$ belonging to $H^\sigma(\Omega_i)$, a sufficient condition for the positiveness of $A_{h,N}$ is the existence of a real positive constant $\alpha_\sigma$ 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. $A_{h,N} = A_h + E_h$. Eigenvalues of these three operators are numbered increasingly and denoted as $(\lambda_i)_{i=1,\ldots,3n}$ the spectrum of $A_h$,

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

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

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

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

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

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

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

$$\sum_{j=1,j\neq i}^{N} \sum_{l=1}^{3} \left| (K_j^i)_l - (\tilde{K}_j^i)_l \right| \leq \alpha_\sigma \frac{C}{N^\sigma},$$

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

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

We now build a sufficient condition for the positiveness of $A_{h,N}$ : 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

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

\[
\forall u \in (\mathbb{R}^3)^n, \quad (A_{h,N}^S(u))_i = \sum_{j=1}^n \frac{1}{2} \left( K_{i}^j + \tilde{K}_{i}^j \right) (u_j).
\]

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 know 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 \( A_{h,N} \) 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

\[
\| R_h \circ A_{h,N}^S \circ P_h(u) - A(u) \|_{0,\Omega} = \| R_h \circ A_h \circ P_h(u) - A(u) \|_{0,\Omega} + \frac{1}{2} \| R_h(E_{h,N} + E_{h,N}^t)P_h(u) \|_{0,\Omega}
\]

\[
\leq \| R_h \circ A_h \circ P_h(u) - A(u) \|_{0,\Omega} + \frac{1}{2} \| R_h(E_{h,N} + E_{h,N}^t)P_h(u) \|_{0,\Omega}
\]

\[
\leq Ch|u|_{1,\Omega} + \frac{1}{2} C_1 \sup_{(i,j) \in \{1,\ldots,n\}^2} |E_{h,N,ij}| + \alpha_\sigma h^{5/2}|u|_{1,\Omega}.
\]

\( \Box \)

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.
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 find in [9, 17].

**Definition 4.1.** \( T_n \) is a one-level Toeplitz matrix of order \( n \) if and only if:

\[
T_n = (t_{i-j})_{i,j \in \{1, \ldots, n\}} = \left( \begin{array}{cccc}
  t_0 & t_{-1} & \ldots & t_{1-n} \\
  t_1 & t_0 & \ddots & t_{2-n} \\
  \vdots & \ddots & \ddots & \ddots \\
  t_{n-2} & t_{1} & t_0 & t_{-1} \\
  t_{n-1} & \ldots & \ldots & t_{1} & t_0
\end{array} \right),
\]

with \((t_i)_{i \in \{1-n, \ldots, n-1\}} \in \mathbb{R}^{2n-1}\).
The vector \( \{t_{1-n}, t_{2-n}, \ldots, t_{-1}, t_0, t_1, \ldots, t_{n-2}, t_{n-1}\} \) is called generator of \( T_n \).

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

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 \( \{1, \ldots, n-1\} \), \((C_n)_{i,n} = (C_n)_{i+1,1}\) 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 Toeplitx 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 tanks 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 $\prod_{i=1}^{p} \{1, \ldots, 2^{m_i}\}$ needs a number of operations equal to

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

where, far 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 Fl($x$) as a notation for the floor function, we set $m_k = \text{Fl}(\log(n_k)) + 1$ and we have $\forall k \in \{1, \ldots, p\}$, $2 \, n_k \geq 2^{m_k}$.

This allows to bound the number of operations needed for a $p$-levels FFT by:

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

And we conclude that the algorithm needs $O(3 \, p \, 2^p \, N_p + 32^p \, \log(N_p))$ 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

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

\(\Box\)

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 $A_h$ is a 3-levels block Toeplitz matrix.

**Proof.** As we saw precedentely,

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

We apply to these formula the following change of variables:

$$
x = x_{\text{ind}_3(i)} + \hat{x} \quad \hat{x} \in [0, h]^3
$$

$$
y = x_{\text{ind}_3(i)} + \hat{y} \quad \hat{y} \in \prod_{k=1}^{3} [(i_k - j_k)h, (i_k - j_k + 1)h] = \Omega_{|I,J|},
$$

where $I$ and $J$ are the indices of the sub-matrices.
so that \( A_{h,I,J} \mathbf{u} = \frac{1}{4\pi} h^3 \int_{\Omega_{I,J}} \text{grad}_x \text{div}_x \int_{\Omega_{I,J}} \mathbf{u} \frac{1}{|y - \hat{x}|} \, dy \, dx \) \( \forall \mathbf{u} \in \mathbb{R}^3 \),

Then, for all \( I \) and \( J \) in \( \prod_{k=1}^{3} \{1, \ldots, n_k\} \), \( A_{h,I,J} \) depends only on \((I - J)\). We conclude by using definition (4.1) that \( A_h \) 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.

<table>
<thead>
<tr>
<th>Number of cells in each direction</th>
<th>Total number of cells</th>
<th>LAPACK</th>
<th>Block Toeplitz algorithm</th>
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</thead>
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<tr>
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<td>16 cells</td>
<td>0,01</td>
<td>0,17</td>
</tr>
<tr>
<td>4 \times 4 \times 2</td>
<td>32 cells</td>
<td>0,04</td>
<td>0,32</td>
</tr>
<tr>
<td>4 \times 4 \times 4</td>
<td>64 cells</td>
<td>0,17</td>
<td>0,62</td>
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<tr>
<td>4 \times 4 \times 8</td>
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<td>0,78</td>
<td>1,31</td>
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<td>8 \times 8 \times 8</td>
<td>256 cells</td>
<td>3,93</td>
<td>2,55</td>
</tr>
<tr>
<td>8 \times 8 \times 8</td>
<td>512 cells</td>
<td>16,49</td>
<td>5,35</td>
</tr>
<tr>
<td>8 \times 8 \times 16</td>
<td>1024 cells</td>
<td>70,77</td>
<td>11,03</td>
</tr>
</tbody>
</table>

**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.

<table>
<thead>
<tr>
<th>Number of cells in each direction</th>
<th>Total number of cells</th>
<th>Assembly time for a full matrix</th>
<th>Assembly time for a block Toeplitz matrix</th>
</tr>
</thead>
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</tr>
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<td>290</td>
</tr>
<tr>
<td>4 \times 8 \times 8</td>
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</tr>
<tr>
<td>8 \times 8 \times 8</td>
<td>512 cells</td>
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<tr>
<td>8 \times 8 \times 16</td>
<td>1024 cells</td>
<td>199938</td>
<td>2725</td>
</tr>
</tbody>
</table>

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 \( p = \frac{a}{b} \):

<table>
<thead>
<tr>
<th>( p = \frac{a}{b} )</th>
<th>number of cells on basis</th>
<th>number of cells on length</th>
<th>total number of cells</th>
</tr>
</thead>
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<td>16 \times 16</td>
<td>64</td>
<td>16384</td>
</tr>
<tr>
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<td>64</td>
<td>4096</td>
</tr>
<tr>
<td>0.06255</td>
<td>8 \times 8</td>
<td>128</td>
<td>8192</td>
</tr>
</tbody>
</table>
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 need 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 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 consistent 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.

Acknowledgments. I am very grateful to Laurence Halpern, Pierre Leca and François Rogier for their helpful remarks and advises. I want to also thank Pierre-Yves Bertin for his interesting test problems.
Fig. 5.2. Comparison between theoretical and numerical results.

REFERENCES

