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Periodic Boundary Conditions for Finite-Differentiation-Method Fast-Fourier-Transform Micromagnetics *

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We describe an accurate periodic boundary condition (PBC) called the symmetric PBC in the calculation of the magnetostatic interaction field in the finite-differentiation-method fast-Fourier-transform (FDM-FFT) micromagnetics. The micromagnetic cells in the regular mesh used by the FDM-FFT method are finite-sized elements, but not geometrical points. Therefore, the key PBC operations for FDM-FFT methods are splitting and relocating the micromagnetic cell surfaces to stay symmetrically inside the box of half-total sizes with respect to the origin. The properties of the demagnetizing matrix of the split micromagnetic cells are discussed, and the sum rules of demagnetizing matrix are fulfilled by the symmetric PBC.

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Micromagnetics are the mainstream theory in computational applied magnetism to calculate the nano-sized domains and hysteresis loops.[1,2] The main idea is to find the stable magnetization distribution by locally minimizing the free energy, which includes the crystalline anisotropy energy, exchange energy, magnetostatic energy, magnetoelastic energy and the Zeeman energy.[3] Since the magnetostatic interaction is long-range, the calculation of this term is the most time-consuming process, often occupying 95% of the whole computational time. In 1988, Bertram *et al.* introduced the FDM-FFT micromagnetic method, largely decreasing the time consumption.[4] Generally, the Fourier transformation requires the micromagnetic cells forming an infinite regular mesh as a Bravais lattice, and consequently, the periodic boundary conditions (PBC) have to be utilized in a mesh with the finite-sized total computation area or a finite number of micromagnetic cells.

The ordinary PBC in a finite total-sized mesh of geometrical points is quite simple: transform all the points whose displacement to the origin is greater than or equal to half the total size in a dimension by a negative total size in this dimension. However, micromagnetic cells are not geometrical points, and they have finite sizes. If the ordinary PBC are utilized in FDM-FFT micromagnetics, the sum rule that the demagnetizing field in a regular mesh with PBC should be zero with uniform magnetization (because there are no magnetic poles) cannot be satisfied. The first PBC suitable for FDM-FFT micromagnetics was found by Wang *et al.* in 2005.[5] This treatment is accurate in a 3D bulk, but it is not 100% accurate in a very thin film because of the asymmetry of the PBC, and the in-plane component of the demagnetizing field in a uniformly magnetized thin film is not exactly zero.

In this Letter, we improve our first PBC for the FDM-FFT method with a full consideration of symmetry, and the sum rule in a uniformly magnetized 3D bulk or a thin film can both be satisfied. This symmetric PBC is accurate for any computational method using the fast-Fourier-transform for finite sized cells, and it is important especially for the small sized 2D model.

In FDM, the magnetostatic or demagnetizing field generated by a cell at $\boldsymbol{r}_i$ in a micromagnetic cell at $\boldsymbol{r}_j$ is given by $\boldsymbol{H}(\boldsymbol{r}_j) = -\tilde{N}(\boldsymbol{r}_j - \boldsymbol{r}_i) \cdot 4\pi \boldsymbol{M}(\boldsymbol{r}_j)$, where $\tilde{N}$ is the demagnetizing matrix, and $\boldsymbol{M}$ is the magnetization vector. Since $\tilde{N}$ depends only on the relative position vector $\boldsymbol{r}_j - \boldsymbol{r}_i$, the Fourier transformation can be utilized in a regular mesh with PBC. The ordinary PBC of geometrical points is given by

$$\boldsymbol{r}_i - \boldsymbol{r}_j \to \begin{cases} \boldsymbol{r}_i - \boldsymbol{r}_j - L_1 D_1 \boldsymbol{e}_1, & \text{if } i_1 - 1 \geqslant L_1/2, \\ \boldsymbol{r}_i - \boldsymbol{r}_j - L_2 D_2 \boldsymbol{e}_2, & \text{if } i_2 - 1 \geqslant L_2/2, \\ \boldsymbol{r}_i - \boldsymbol{r}_j - L_3 D_3 \boldsymbol{e}_3, & \text{if } i_3 - 1 \geqslant L_3/2, \end{cases} \quad (1)$$

where D_1, D_2 and D_3 are the sizes of a micromagnetic cell, and L_1, L_2 and L_3 are the numbers of cells in the respective dimensions in a cuboid regular mesh. If the ordinary PBC are utilized in the FDM-FFT method, the sum rule that the demagnetizing field in an infinite bulk should be zero with uniform magnetization cannot be satisfied.

For the cells that satisfy the identifier conditions $i_n - 1 > L_n/2$ ($n = 1$, 2 and 3), the PBC is the same as the ordinary PBC for geometrical points as in Eq. (1). However, for the cells that satisfy one or more identifier conditions $i_n - 1 = L_n/2$, an extra operation should be taken to avoid the accumulation of magnetic poles on the edge of the simulated area, as shown in Fig. 1(a). It should be noted that schematics of the periodic boundary conditions are plotted in two dimensions (2D) in Fig. 1, and in computations the PBC can be applied in 2D or three dimensions (3D). The ith cell (the index i means (i_1, i_2 and i_3) in 3D) has six surfaces, which all contribute to the $\tilde{N}$ of a uniformly magnetized cell where magnetic poles

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only exist on its surfaces

$$\begin{aligned}\tilde{N}(\boldsymbol{r}_j,\boldsymbol{r}_i) &= -\frac{1}{4\pi}\int_S^{(i)} d^2r' \frac{(\boldsymbol{r}_j-\boldsymbol{r}')\hat{n}'}{|\boldsymbol{r}_j-\boldsymbol{r}'|^3} \\ &= -\frac{1}{4\pi}\int_S^{(i)} d^2r' \frac{((\boldsymbol{r}_j-\boldsymbol{r}_i)-(\boldsymbol{r}'-\boldsymbol{r}_i))\hat{n}'}{|(\boldsymbol{r}_j-\boldsymbol{r}_i)-(\boldsymbol{r}'-\boldsymbol{r}_i)|^3} \\ &= \tilde{N}(\boldsymbol{r}_j-\boldsymbol{r}_i). \end{aligned} \tag{2}$$

However, since the jth cell is fixed at the origin with identifier (111), in the ith cell with $i_n - 1 = L_n/2$, the center of one of the six surfaces is closer to the origin than the criteria $L_nD_n/2$ marked by the dashed-dotted thin line large box in Fig. 1(a). Therefore, these surfaces should not be translated by the ordinary PBC in Eq. (1) to a new position as marked by the dashed lines in Fig. 1(a), and the contributions to $\tilde{N}$ from these special surfaces marked by dashed lines should be subtracted, and added back to $\tilde{N}^i = N(\boldsymbol{r}_j = 0, \boldsymbol{r}_i)$ after these surfaces are moved back by a dimension size L_nD_n. This modified PBC can calculate the demagnetizing field correctly in a 3D bulk, and there are no accumulated magnetic poles when the magnetization is uniform. However, it is obvious that in Fig. 1(a) the cell distribution is asymmetric with respect to the origin cell $j = (111)$, and this PBC will not be 100% accurate in a thin film.

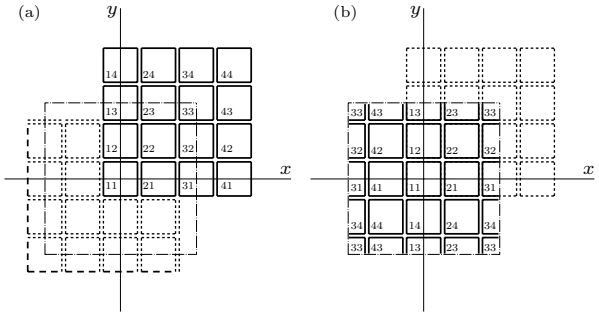

Fig. 1. Schematics of the modified PBC and symmetric PBC for FDM-FFT micromagnetics in 2D. The demagnetizing field is calculated for the cell at the origin. (a) The first modified PBC found in 2005.[5] The solid lines refer to the original cell arrangement. The dotted lines refer to the relocated cells. The dashed lines mark the special surfaces that should be split from a cell and moved back to the original place. (b) The symmetric PBC for FDM-FFT micromagnetics. The solid lines refer to the surface arrangement after the symmetric PBC operation, where the number marked on a cell is with respect to the cell number before the PBC operation in (a). In both (a) and (b), the large thin dashed-dotted lines mark the half-total-sized boundary $\pm L_nD_n/2$.

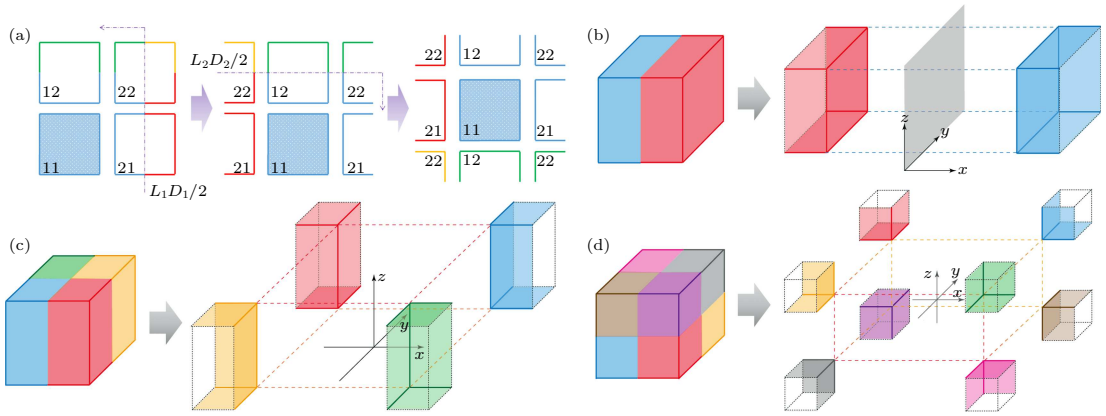

Fig. 2. (a) The 2D sketches of the construction process of the symmetric PBC. (b)–(d) The 3D sketches of split micromagnetic cells. Each of those cells satisfy one (b), two (c) or three (d) identifier equations $i_n - 1 = L_n/2$. After the symmetric PBC operation, the blue part of a cell keeps its position unchanged, while the parts in other colors are moved by the dimension size L_nD_n.

In the symmetric FDM-FFT PBC, only the cell surfaces (solid lines in Fig. 1(a)) located outside the dashed-dotted line half-total-sized box should be relocated in the way of being transformed by the total simulation size L_nD_n as in Eq. (1). The final arrangement of cell surfaces is totally symmetric with respect to the origin, as shown in Fig. 1(b). Before the PBC operation, the cells that satisfy one or more identifier conditions ($i_n - 1 = L_n/2$) must be split equally into 2, 4 or 8 pieces, as shown in Figs. 2(b)–2(d). Then, only one split piece located originally inside the half-total-sized box of $L_nD_n/2$ keeps its position unchanged after the symmetric PBC operation, while the other pieces should be moved by one or more total size L_nD_n until they are relocated inside the box of $L_nD_n/2$, as shown in Fig. 2(a). Specifically, the surfaces of cells that satisfy one identifier equation ($i_n - 1 = L_n/2$) will be split into two pieces (Fig. 2(b)). The contribution to the demagnetizing matrix from the red half piece should be subtracted and added back after moving, which can be written as

$$\tilde{N}_\mathrm{b} = \tilde{N}_0 - \tilde{N}_{1/2} + \tilde{N}'_{1/2}. \tag{3}$$

For the cells that satisfy two identifier equations, the cell should be split into four pieces and three of them will be moved (Fig. 2(c)). Here $\tilde{N}$ is described by

$$\tilde{N}_\mathrm{c} = \tilde{N}_0 - \sum\nolimits_3 \tilde{N}_{1/4} + \sum\nolimits_3 \tilde{N}'_{1/4}. \tag{4}$$

For the only cell that satisfies three identifier equations, the cell should be split into eight pieces and then rearranged at the vertexes of the large cube with

the total simulation size L_nD_n (Fig. 2(d)). Thus $\tilde{N}$ is written as

$$\tilde{N}_{\rm d} = \tilde{N}_0 - \sum\nolimits_7 \tilde{N}_{1/8} + \sum\nolimits_7 \tilde{N}'_{1/8}. \tag{5}$$

In a micromagnetic program, after the ordinary PBC, $\tilde{N}$ of each of the split cells should be calculated by adding or subtracting the demagnetizing matrix of a rectangle surface at proper positions following Eqs. (3)–(5)[6,7] to achieve the accurate symmetric PBC. To check the errors that may occur, some properties of the $\tilde{N}$ elements could be used. Firstly, $\tilde{N}$ of a split cell in Fig. 2 is always a symmetric matrix, the same as a complete cuboid cell written as Eq. (2). Moreover, the symmetric distribution of the split cell surfaces leads to a simplification of $\tilde{N}$ elements. For those that satisfy one identifier equation (Fig. 2(b)) for example $i_1 - 1 = L_1/2$, the cells have a symmetric plane y–z. Suppose that the magnetostatic field is calculated by

$$\begin{pmatrix} H_1 \\ H_2 \\ H_3 \end{pmatrix} = - \begin{pmatrix} N_{11} & N_{12} & N_{13} \\ N_{12} & N_{22} & N_{23} \\ N_{13} & N_{23} & N_{33} \end{pmatrix} \cdot 4\pi \begin{pmatrix} M_1 \\ M_2 \\ M_3 \end{pmatrix}. \tag{6}$$

Following the reflection symmetry with respect to the y–z plane

$$\begin{pmatrix} -H_1 \\ H_2 \\ H_3 \end{pmatrix} = - \begin{pmatrix} N_{11} & N_{12} & N_{13} \\ N_{12} & N_{22} & N_{23} \\ N_{13} & N_{23} & N_{33} \end{pmatrix} \cdot 4\pi \begin{pmatrix} -M_1 \\ M_2 \\ M_3 \end{pmatrix}. \tag{7}$$

Based on Eqs. (6) and (7), we find $0 = N_{12}4\pi M_2 + N_{13}4\pi M_3$. Considering the arbitrariness of M_2 and M_3, we find $N_{12} = N_{13} = 0$ and $H_1 = -N_{11}4\pi M_1$. This indicates the fact that the direction perpendicular to the symmetric plane is the principle axis of the demagnetizing matrix, and one could further find $N_{11} < 0$.

For the cells that satisfy two identifier equations (Fig. 2(c)), two symmetric planes result in two principle axes with negative matrix elements. Correspondingly, the remaining direction should also be a principle axis but with a positive matrix element. For the cell that satisfies three identifier equations (Fig. 2(d)), the demagnetizing matrix is a negative diagonal matrix. The results are concluded by

$$\tilde{N}_{\rm b} = \begin{pmatrix} N_{11} < 0 & 0 & 0 \\ 0 & N_{22} & N_{23} \\ 0 & N_{23} & N_{33} \end{pmatrix}, \tag{8}$$

$$\tilde{N}_{\rm c} = \begin{pmatrix} N_{11} < 0 & 0 & 0 \\ 0 & N_{22} < 0 & 0 \\ 0 & 0 & N_{33} > 0 \end{pmatrix}, \tag{9}$$

$$\tilde{N}_{\rm d} = \begin{pmatrix} N_{11} < 0 & 0 & 0 \\ 0 & N_{22} < 0 & 0 \\ 0 & 0 & N_{33} < 0 \end{pmatrix}, \tag{10}$$

where y–z is the symmetric plane for $\tilde{N}_{\rm b}$, and x–z and $y-z$ are the symmetric planes for $\tilde{N}_{\rm c}$. In FDM-FFT, the FFT calculation of the demagnetizing field should be performed within the total cell number $L_1L_2L_3$ with the 3D-PBC, but not directly performed within the cell number $N_xN_yN_z$ that can cover the device. The model under the conditions $L_1 = N_x$, $L_2 = N_y$ and $L_3 = N_z$ has PBC in three dimensions, for simulations in a bulk device with infinite size. The model under the conditions $L_1 = N_x$, $L_2 = N_y$ and $L_3 = 2N_z$ has PBC in x and y directions, and it can be approximated as a thin film with infinite in-plane size and mesoscopic thickness.

The sum rules of the demagnetizing matrix elements of all regular mesh cells in the model are related to the demagnetizing field with uniform magnetization, i.e.,

$$\begin{pmatrix} H_1 \\ H_2 \\ H_3 \end{pmatrix} = -4\pi \left\{ \sum\nolimits_i \begin{pmatrix} N^i_{11} & N^i_{12} & N^i_{13} \\ N^i_{12} & N^i_{22} & N^i_{23} \\ N^i_{13} & N^i_{23} & N^i_{33} \end{pmatrix} \right\} \cdot \begin{pmatrix} M_1 \\ M_2 \\ M_3 \end{pmatrix}, \tag{11}$$

where the sum of the index goes over regular mesh cells ($L_1L_2L_3$), and M_i outside the regular mesh ($N_xN_yN_z$) in reality is set as zero. For a uniformly magnetized model with correct 3D-PBC, there should be no accumulated magnetic poles anywhere in the model. Thus the demagnetizing field should be zero. Considering the arbitrariness of M_1, M_2 and M_3 in Eq. (11), one can find the sum rule of the demagnetizing matrix elements over all cells $N_xN_yN_z$,

$$\sum\nolimits_i N^i_{mn} = 0, \ m, n = 1, 2, 3. \tag{12}$$

Table 1 lists the calculations results for different 3D-PBC models. Both the previous FDM-FFT PBC in 2005 and the symmetric PBC satisfy the sum rules in Eq. (12).

In a uniformly magnetized thin film, the 2D in-plane PBC should be utilized, and the magnetic poles uniformly accumulated on the film surface. Thus $\boldsymbol{H}_{\rm d}$ inside the film should be perpendicular to the plane, i.e., the in-plane component is precisely zero. By utilizing $\tilde{N}$ of two rectangle surface, one can find the sum of the demagnetizing matrix elements (supposing that the z-axis is perpendicular to the film plane)

$$\sum\nolimits_i N^i_{mn} = \begin{cases} \sum_{j=1,2} \frac{1}{\pi} \arctan \frac{ab}{2z_j\sqrt{a^2+b^2+4z_j^2}}, \\ m = n = 3, \\ 0, \ \text{others}, \end{cases} \tag{13}$$

where $a = N_xD_1$ and $b = N_yD_2$ are the in-plane sizes of the calculated magnetic thin film, $z_1 = D_3/2$ and $z_2 = (N_z - 1/2)D_3$ refer to the distances from the origin to the two film surfaces, respectively. When the in-plane size of model is large enough or the thickness is small enough ($a, b \gg z_1 + z_2$), the demagnetizing field is close to $-4\pi M_3$.

Table 2 lists the calculation results in a thin film with 2D PBC, where only the symmetric PBC gives the correct sum rules as Eq. (13). The model with a total mesh size such as $N_x \times N_y \times N_z = 16 \times 16 \times 8$

is often utilized to debug or to test simulation parameters, due to the lesser time consumption. When studying the M–H loop of film, usually a model with a total mesh size of $N_x \times N_y \times N_z = 64 \times 64 \times 16$ or larger is needed to include the polycrystalline structure or other microstructures. For the small model, the difference between the first PBC and the symmetric PBC is non-negligible. We have observed totally different magnetization distributions using these two PBCs. Meanwhile, the difference will decrease in a larger sized system. We found that, for the loop simulations with $64 \times 64 \times 16$ cells, the results of the two PBCs have no difference.

Table 1. Demagnetizing matrix and demagnetizing field $\boldsymbol{H}_{\rm d}$ calculated by 3D-PBC with uniform magnetization. Cell size is $1 \times 1 \times 1\,{\rm nm}^3$. Magnetization is 1000 emu/cc in (111) direction. The field is in units of Oe.

	Models	Sum of $\tilde{N}$ elements in all cells	$\boldsymbol{H}_{\rm d}$ at origin
Cell number 16×16×16	Original geometric PBC in Eq. (1)	$\begin{pmatrix} 0.33333 & -0.00956 & -0.00956 \\ -0.00956 & 0.33333 & -0.00956 \\ -0.00956 & -0.00956 & 0.33333 \end{pmatrix}$	$\begin{pmatrix} -2404.53 \\ -2404.53 \\ -2404.53 \end{pmatrix}$
	First FDM-FFT PBC in Fig. 1(a)	$\begin{pmatrix} 0.00000 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 \end{pmatrix}$	$\begin{pmatrix} 0.00000 \\ 0.00000 \\ 0.00000 \end{pmatrix}$
	Symmetric PBC in Fig. 1(b)	$\begin{pmatrix} 0.00000 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 \end{pmatrix}$	$\begin{pmatrix} 0.00000 \\ 0.00000 \\ 0.00000 \end{pmatrix}$
Cell number 64×64×64	Original geometric PBC in Eq. (1)	$\begin{pmatrix} 0.33333 & -0.00006 & -0.00006 \\ -0.00006 & 0.33333 & -0.00006 \\ -0.00006 & -0.00006 & 0.33333 \end{pmatrix}$	$\begin{pmatrix} -2417.53 \\ -2417.53 \\ -2417.53 \end{pmatrix}$
	First FDM-FFT PBC in Fig. 1(a)	$\begin{pmatrix} 0.00000 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 \end{pmatrix}$	$\begin{pmatrix} 0.00000 \\ 0.00000 \\ 0.00000 \end{pmatrix}$
	Symmetric PBC in Fig. 1(b)	$\begin{pmatrix} 0.00000 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 \end{pmatrix}$	$\begin{pmatrix} 0.00000 \\ 0.00000 \\ 0.00000 \end{pmatrix}$

Table 2. Demagnetizing matrix and demagnetizing field $\boldsymbol{H}_{\rm d}$ calculated by the 2D-PBC models with uniform magnetization. The z-axis is perpendicular to the plane. Cell size is $1\times1\times1\,{\rm nm}^3$. Magnetization is 1000 emu/cc in (111) direction. The field is in units of Oe.

	Models	Sum of $\tilde{N}$ elements in all cells	$\boldsymbol{H}_{\rm d}$ at origin
Cell number 16×16×8	Original geometric PBC in Eq. (1)	$\begin{pmatrix} 0.17505 & -0.00050 & 0.00778 \\ -0.00050 & 0.17505 & 0.00778 \\ 0.00778 & 0.00778 & 0.64990 \end{pmatrix}$	$\begin{pmatrix} -1209.92 \\ -1209.92 \\ -4602.29 \end{pmatrix}$
	First FDM-FFT PBC in Fig. 1(a)	$\begin{pmatrix} 0.00000 & 0.00000 & 0.00778 \\ 0.00000 & 0.00000 & 0.00778 \\ 0.00000 & 0.00000 & 0.64990 \end{pmatrix}$	$\begin{pmatrix} 56.4394 \\ 56.4394 \\ -4715.17 \end{pmatrix}$
	Symmetric PBC in Fig. 1(b)	$\begin{pmatrix} 0.00000 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.65055 \end{pmatrix}$	$\begin{pmatrix} 0.00000 \\ 0.00000 \\ -4719.90 \end{pmatrix}$
Cell number 64×64×16	Original geometric PBC in Eq. (1)	$\begin{pmatrix} 0.10328 & -0.00002 & 0.00082 \\ -0.00002 & 0.10328 & 0.00082 \\ 0.00082 & 0.00082 & 0.79344 \end{pmatrix}$	$\begin{pmatrix} -743.231 \\ -743.231 \\ -5744.63 \end{pmatrix}$
	First FDM-FFT PBC in Fig. 1(a)	$\begin{pmatrix} 0.00000 & 0.00000 & 0.00082 \\ 0.00000 & 0.00000 & 0.00082 \\ 0.00000 & 0.00000 & 0.79344 \end{pmatrix}$	$\begin{pmatrix} 5.95796 \\ 5.95796 \\ -5756.54 \end{pmatrix}$
	Symmetric PBC in Fig. 1(b)	$\begin{pmatrix} 0.00000 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.79348 \end{pmatrix}$	$\begin{pmatrix} 0.00000 \\ 0.00000 \\ -5756.87 \end{pmatrix}$

In conclusion, we have described an accurate symmetric PBC for the FDM-FFT micromagnetics. It is theoretically significant, since for both bulk and film models, the symmetric PBC strictly satisfies all the demagnetizing field rules in uniformly magnetized material, as well as the demagnetizing matrix sum rules. We should emphasize that this symmetric PBC is general for all computational methods, not just restricted in the area of computational magnetics, using the FFT in a regular mesh with finite-sized cells.

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