Parallelism in Magnetic Force Microscopy Studies Algorithm and Optimization

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Abstract. *The algorithm of the calculation of the dipole-dipole interaction was formalized and was implemented in C++ code using MPI library. The program package is fully parallelized and has high optimization for computational architecture. Our parallel program allows obtain Magnetic-Force-Microscopy (MFM) images and to establish the magnetic configuration which one correspond given experimental MFM picture.*

Keywords

Parallel processing, MPI, magnetic force microscopy images, supercomputer simulations.

1 Introduction

Nanoscale structures are currently the subject of intense research. Magnetic nanostructures interesting from the viewpoint of applications, since they can be used for a random access memory cells (MRAM), and a highly integrated magnetic electronic devices [1], and also for use in spintronics [2]. From a fundamental point of view of the interest in nanostructures determined by the complexity of building physics correlated state, in particular, are still open questions today, for example, the transition from the individual behavior of isolated magnetic nanoparticles to the collective behavior of nanosystems in general, and the role played by the magnetostatic interaction for such a transition [3], and the mechanisms of reversal of magnetization [4,5]. It is undeniable that the sharp rise in the field of information technology is also connected with progress in the research of magnetic particles, and it is obvious that the further development of magnetic logic will be associated with the use of magnetic nanostructures [6].

Magnetic Force Microscopy (MFM) is used by manufacturers storage media as a method of investigation of nanostructures in order to minimize the work area corresponding to a single bit of information, noise immunity, reduced noise in recording and reading information, as well as development of new principles and devices for magnetic recording. For a complex theoretical and experimental studies of nano-architectures opportunities today provides a modern high-performance computing, which allows to validate and evaluate the adequacy, accuracy and acceptability of conventional models in numerical experiments to obtain data on the magnetic states, the types of ordering the collective behavior [7]. Therefore, interest in research methods of modeling experiments MFM-like ensembles and individual ferromagnetic nanoparticles - parts for nano-structures is clear [8,9].

In this paper we present the scalable computational algorithm of a simulation MFM-images, designed for parallel execution on the supercomputer hardware. The results of a numerical simulation experiment magnetic force obtained by the test specimen copyright software supercomputer (SC) of the cluster.

2 The Samples and Experimental Data

Cobalt films with the thickness 10 nm are deposited in an ultrahigh vacuum 10-10 Torr on naturally oxidized monocrystals (100) Si from effusion cell at a room temperature. From above the film was covered 3 nm Cu layer for oxidizing prevention. Investigations have shown that Co films are polycrystal with the uni-axial induced magnetic anisotropy. Usually assumed, that a radius of the ferromagnetic correlation obtained from MFM images of the films

magnetic structure, has made the order of 600 nm. Then the round and square nanodots with the diameter d=600 nm and the period 3d and 2d are patterned by the focused ion Ga+ beams, in each array was 10x10 nanodots.

The structure of films and arrays was explored by high energy electrons diffraction methods (RHEED), a scanning electronic microscopy (SEM) and atomicforce microscopy. To obtain the magnetic structure image and hysteresis loops of the single nanodot the method of magneticforce microscopy (MFM) and micromagnetic simulation in software package OOMMF [3] are used. Computer simulation of MFM images taking into account the interaction between the tip and nanodot(s).

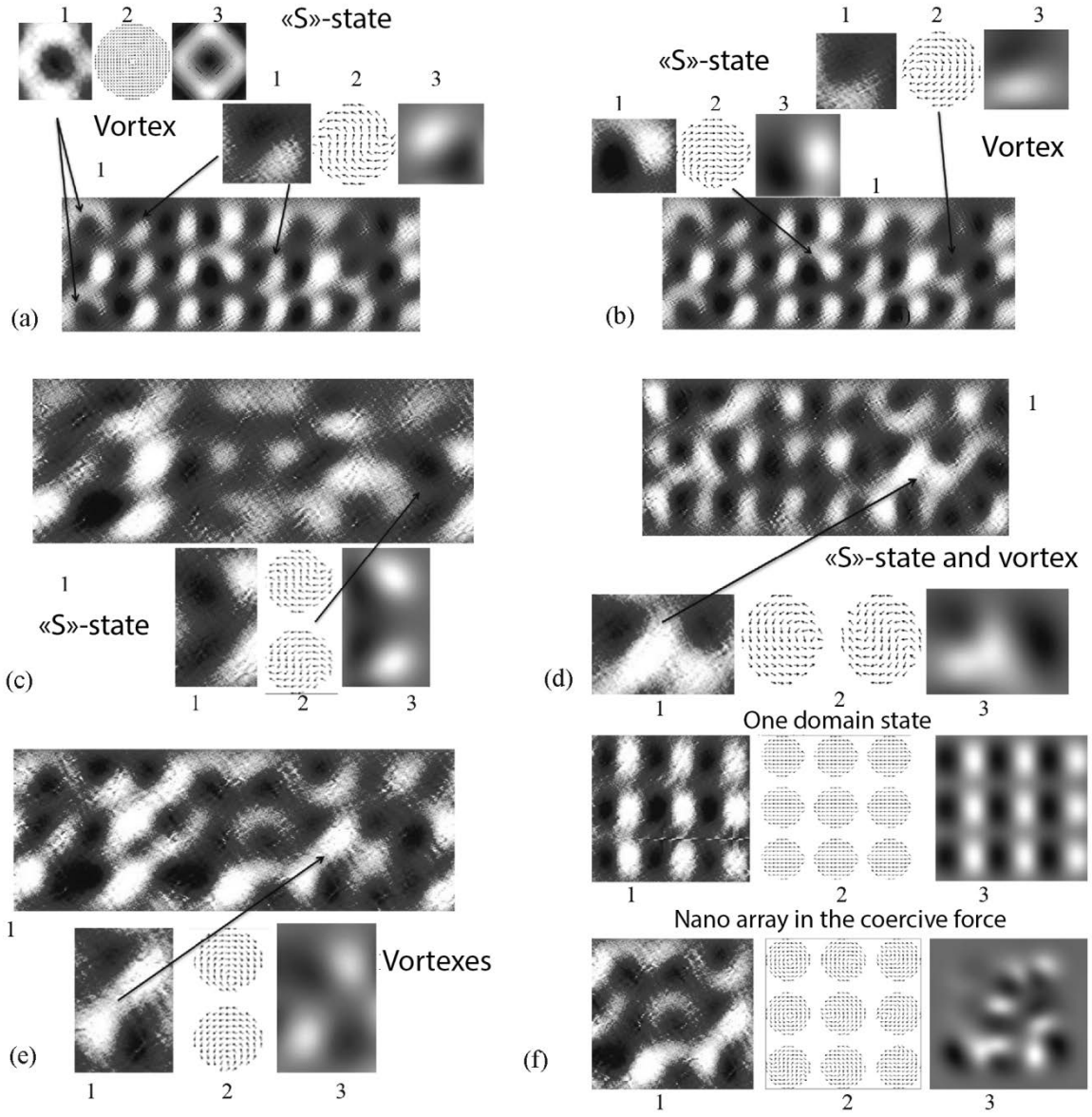

Fig.1. The interpretation of the experimental MFM-image magnetic structures of selected magnetic nanodots simulation state by authoring software for the supercomputer computing cluster. Images from the index "1" - experimental MFM-image, with the index "2" simulated configuration of the magnetic dipoles, "3" – calculated MFM-images, which ones is corresponded to the given configuration of the magnetization. (a-d) - the external magnetic field a) $H = 2H_c$; b) $H = 1.5\ H_c$; c) $H = H_c$; d) $H = 1.75\ H_c$, where H_c is corrective force, which one was obtained in nature experiments.

Fig. 1 shows examples of modeling the magnetic states of individual elements and their groups in an ordered array of quasi-reversal of cobalt nanodisks with a diameter of 600 nm, related to the strong dipole-dipole interaction in a variety of external magnetic fields. The interpretation of the experimental data of MFM-magnetic states of individual elements of nanosystems, located in different magnetic fields is shown in Figures 1a-d. Simulation 3 x 3 array of magnetic structure of cobalt nanoparticles in the saturation and coercive field strength is shown in Figure 1e, respectively. For the ordered single-domain state is observed good agreement between the simulated MFM contrast

with the experimentally observed, which is not the modeling of magnetic ordering in the coercive force, where collective interactions play a key role in the choice of the magnetic state of nanoparticles in general and each nanoparticle separately.

3 Software Description

3.1 The Formalism

The model of the classical macrospin was used. We made simulation with authoring program which one allows to interpret MFM pictures from nature experiments.

The form of polycrystal is nanodisk with following size 10 nm in height and 600 nm in diameter, for square nanodots linear sizes were 600x600x10 (nm3). The microstructure of the nanodot is the random distribution of grains, which ones grow out on total height of nanodot. The mean diameter of crystalline grain is 5 nm. In this model the nanosquare consists from 100x100 subdots. The partitions are in the nodes of the simple square lattice. Thus each macrospin has four nearest neighbors in the lattice. For detailed description of formalism see [4].

The interaction energy of tip with the magnetic nanodot (Zeeman energy) can be estimated by well-known rule

$$E = \int_{V_p} M(r)H(r)dV, \tag{1}$$

where M(r) – summary magnetic moment of probe in field H(r). This field was created by the whole nanodot, notably by summary magnetic field of the each partition. In this case in common view the force, which act to probe, can be calculated as

$$F = -\nabla E = -\int_V \nabla M(r)H(r)dV. \tag{2}$$

Magnetic-force-microscopy can record only z-component of tip deviation, or z-component of force

$$F_z = \int_V \left(M_x \frac{\partial H_x(r)}{\partial z} + M_y \frac{\partial H_y(r)}{\partial z} + M_z \frac{\partial H_z(r)}{\partial z} \right) dV. \tag{3}$$

Thus, the intensity of the picture pixel correspond to scalar value

$$\frac{\partial F_z}{\partial z} = \int_V \left(M_x \frac{\partial^2 H_x(r)}{\partial z^2} + M_y \frac{\partial^2 H_y(r)}{\partial z^2} + M_z \frac{\partial^2 H_z(r)}{\partial z^2} \right) dV. \tag{4}$$

In case of small number of partitions it is possible to change integration by summation. The form and size of modeling tip have strong value on the result of simulation. In our model we use approach of the magneto-hard tip of the pyramid form, fig. 2.

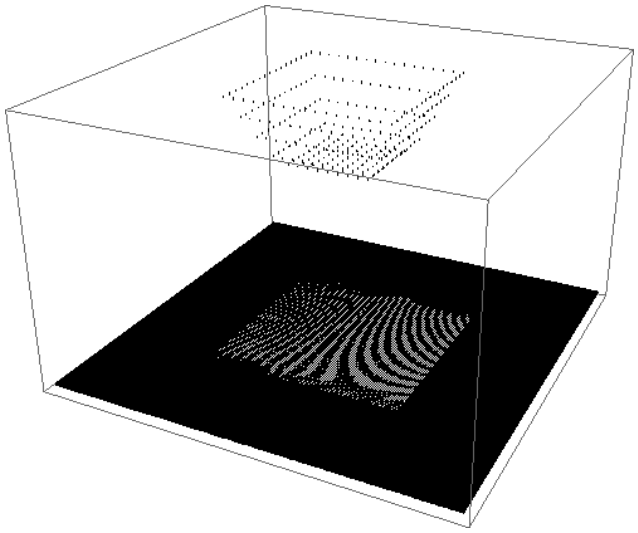

Fig. 2. Simulation of the square nanodot and tip.

The magnetic material of the real probe is distributed on surface of pyramid, the same distribution we had in our model. The magneto-hard approach means that the interaction between the tip and nanodot does not influence on magnetic structure it magnetic states.

3.2 Input and output data

Input data were prepared in OOMMF package. This array of double numbers which ones correspond to components vectors magnetization with given coordinates. By means of file stream data redirect into buffer of RAM which one is the dynamical vector. Using of dynamical memory is specified by large number of elements array. Magnetic tip was simulated similar to real form of tip which one used in physical experiment. So tip had form truncated pyramid. Next the in 6 inserted cycles over coordinates of nanodot (x,y,z) and coordinates of tip (x,y,z) the values gradients of force were calculated using formula (4) and store in array. Outcomes of calculations were written in files with formats “nb” and “bmp”. The maximal time costs demand for a calculation of execution of cycles. The tip has to interact with all partition of nanodot and has visit more points than the number of partition for calculation of dispersion fields. Therefore the parallelization was need.

3.3 The Parallelization and Execution

Program takes file from software package OOMMF with magnetic configuration (it is possible to specify magnetic state by hand), then it calculates MFM image in format of Matematica file (*.nb), additionally the components of nanodot magnetization is calculating.

Variables “sizex”, “sizey” and “sizez” mean number of nodes over direction x, y and z correspondingly. In the result of program code executing we have so many processes so much we set in the “mpirun” command specification, and each process take part from linear size over “x”.

In first version of our program for the simple access to partitions (to value of gradient of force and to components magnetization vector) we have used Cartesian coordinates “x”, “y” and “z” which ones were indexes of the double type fourdimensional array with name “kna”. Interesting to note that if number of free cores were not in corresponding with required number of processes all processes were in “slipping” (wait the generation of other process). After generation of given number of process the calculations were started, and results of calculations summed also in fourdimensional vector “knar”; In frame of optimization we change the four-dimensional vector to 1D array, exclude mathematical functions from “math.h” library, such for example as “pow()”, change “double” to “float”. In addition in this step we used Local Area Multicomputer (LAM) as well as keys for “mpirun” (machinefile) for total loading of nodes of cluster.

Explanation of parallelization type in our program

```
//declaration of data and functions
. . .
MPI_Init(&argc,&argv);
MPI_Comm_size(MPI_COMM_WORLD,&numprocs);
MPI_Comm_rank(MPI_COMM_WORLD,&myid);
MPI_Get_processor_name(processor_name,&namelen);
fflush(stdout);
while (!done) {
MPI_Bcast(&kna, 1, MPI_DOUBLE, 0, MPI_COMM_WORLD);
done = 1;
for(int x=myid*sizex/numprocs;x <(myid+1)*sizex/numprocs;x++) {
for(int y=0; y<sizey; y++){
for(int z=0; z<sizez; z++){
. . .
//calculations of force gradient
}
MPI_Reduce(&kna,&knar,sizex*sizey*sizez*4, MPI_DOUBLE,
MPI_SUM, 0, MPI_COMM_WORLD);
fflush( stdout );
MPI_Finalize();
. . .
//end of program
```

As you can see from the code in its current format the number of points must be a multiple of the number of cores, or the data will not be calculated. To solve this problem, the code has been modified as follows:

instead of:

```
for(int x=myid*sizex/numprocs; x <(myid+1)*sizex/numprocs;x++)
```

use that:

```
razm=(sizex-1)/numprocs+1;
ibeg=myid*razm;
iend=(myid+1)*razm-1;
if (ibeg>=sizex)iend = ibeg-1;
      else if(iend>=sizex)iend = sizex-1;
for(int x=ibeg; x <=iend;x++)…
```

Such a division of tasks among processors is maximally uniform in terms of computational complexity, for each of the processes set by the user.

In the first versions of the program initialization MPI made immediately before the parallelized loop. As such, the initialization is taking so long as each process reads the source data itself. To avoid this, all the work is the process with rank 0, then the data is synchronized over all processes using the function MPI_Bcast.

Empirically, it was found that for the cluster on which the calculations, the best way to compile represented by the following command:

```
mpicc –o2 –march=core2
```

This method of compilation has reduced the time of the program by about 5%.

After all activities undertaken by optimizing the code was able to reduce the time to perform calculations with 10^5 seconds to $1.76 * 10^3$ seconds on the file 100x100 array. In this way 32 cores (4 nodes with 8 cores each) were used for calculation of 500x500 - array (nanoarchitecture 3x3 magnetic nanodots) and total time of calculation was about 6 hours.

On this development has not stopped since experimentally obtained structure 10x10 nanodots. To calculate this amount of data would require 2-3 weeks on 32 cores. It was noticed that one cannot expect the result at all points, but only such as a 2x2 or 3x3 square, so you can quickly get an approximate result, select the option for a more detailed study and then calculate its entirety.

In order to cluster was loaded permanently into the program adds the ability to pass parameters via command line arguments. This will load the job in a few days and expect results.

4 Conclusion

Thus, parallel programming technologies could be used for numerical simulation of MFM images. The parallelization by means of the MPI library allows essential increase the production of calculations and that important to enlarge the class of solvable physical tasks. The analytical calculation of the space distribution of function $\frac{\partial F}{\partial z}$ values at given array magnetic moments demands serious theoretical efforts. More over exact solution of this task could not be found, whereas numerical simulation relatively gives solution in real time. The developed algorithm has excellent scalability as magnetostatic fields have the property of superposition. The latter implies the possibility of independent calculations of pair interactions. Therefore, the simulation accuracy depends on the number of partitions (the degree of sampling model), ie, the number of cells that are placed in the point dipoles and the lattice structure. The model allows to achieve a very high density of the number of bins needed to achieve the convergence of the obtained results in numerical experiments.

The disadvantage of the method is the fact that the model does not take into account interaction between the dipoles and interference of tip and the object of magnetic force experiment, ie nanodots or film. This interaction can have a significant effect on the calculated magnetic states and, therefore, the distribution of contrast in MFM images. To check the convergence is also needed to experiment with different grid structures of dipoles. All of the simulated magnetic states obtained under the condition that the numerical experiments, a two-dimensional grid. It would be interesting to simulate a two-level sampling, that is, in the case where the dipoles are arranged in the multilayer grid.

Note also that the results obtained based on the existing physical models of the simplification of nanostructures and materials. As a result, solved computational problems appear natural parallelism, which provides scalability to very large scale. Such simplification, however, have their study, at least for quick assessments of properties studied nanomaterials and structures, even sometimes not very accurate in terms of styling subtle effects, especially at the quantum level. The results of numerical simulations have a very good agreement with the results of real experiments.

As a further development of the model and the approach would be a very interesting solution to the inverse problem, ie, task of restoring the magnetization distribution from the known magnetic force image. The inverse problem also allows for a very good scalability and natural parallelism, but requires precise experimental data on the geometry of nano-objects and their arrangement on the MFM image.

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