Energy Determination of Superconducting Vortex Lattices with Stochastic Methods Calculated on GPUs

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Abstract—**By fabricating Nb films on top of array of Ni nanodots with different geometries, the vortex lattice for specific values of the external applied magnetic field is modified by the array of periodic pinning potentials. In this work, a GPU-based code developed from scratch simulating this phenomenon is presented. It evaluates the vortex–vortex and the vortex–nanodot interactions providing the total interaction between vortices and pinning sites, as well as the position of the vortices in the array unit cell. This final position is obtained with different stochastic processes being able to simulate square, rectangular, or triangular arrays of nanodefects of different size. A computational performance study is also made.**

Keywords- Superconducting vortices; nanostructures; heuristics; supercomputation; GPU.

I. Introduction

Superconducting vortex lattice dynamics and vortex lattice pinning are strongly modified by arrays of nanodefects embedded in superconducting films. By using arrays of holes (antidotes), which thread the films or dots embedded in the sample, this effect can be studied. Thus, many effects can be observed on these hybrid samples, for example, reconfiguration of the vortex lattice, effects induced by arrays made with different materials, different diameters of the pinning centers, channeling effects, etc.

Magnetoresistance measurements are a perfect tool to study these effects, since resistance vs. applied magnetic fields shows deep minima when the vortex lattice matches the unit cell of the array due to geometric matching occurs when the vortex density is an integer multiple of the pinning center density. These phenomena are ruled by the balance among different interactions, (i) vortex–vortex, (ii) vortex–artificially induced pinning center (array of nanodefects), (iii) vortex–intrinsic and random pinning centers. The magnetoresistance minima show up only when the temperature is close to T_c, since, at these temperatures, the effect of the vortex–array interaction is enhanced. The large roughness of the sample surface precludes the use of standard local probe methods to detect experimentally the vortex position and symmetry of the vortex lattice, which could be only inferred from the experimental matching conditions.

Therefore, theoretical approaches have been undertaken by computer simulation methods. In a pioneering work, in the framework of molecular dynamics, Reichhardt et al. [1], by integrating numerically the Langevin equation of motion, were able to predict some of the matching fields at which commensurate vortex arrangements happen. According to this approach, the superconducting penetration depth is the crucial parameter. These authors use cut-off conditions, pinning strengths and other relevant parameters governed by the penetration superconducting depth. In a similar scenario, Langevin equation of motion of the vortices, Dinis et al. [2] have been able to simulate the rectifier behavior of the vortex lattice in the transverse ratchet effect. In this case, the parameters are taken from the experiment and the random intrinsic pinning of the superconductor plays a crucial role. Simulations of vortex dynamics in superconducting films with pinning array have been also reported by Kato and Enomoto [3], Gropp et al. [4] and Rodríguez-Pascual et al. [5].

In this work, the possibility to simulate the commensurability experiments in the framework of the Langevin equation of motion is explored without any initial conditions neither constraints and using only as input the vortex–vortex interaction and the periodic pinning sites (array unit cell). This process is carried out with genetic algorithms and simulated annealing techniques on GPUs. The experimental magnetoresistance minima permit obtaining the number of vortices in the array unit cell and figuring out the vortices position for different arrays and matching fields, as well as evaluating the vortex lattice interaction.

The article reads as follows. After this Introduction section, the experiment that can measures the energy of superconducting vortex lattices is described. In Section III, the simulation that has been implemented with a code that runs on GPUs is presented, as well as the stochastic methodologies that have been designed. The obtained results are included in Section IV, while the conclusions come in Section V.

II. Experiment

Superconducting/magnetic hybrids have been grown by magnetron sputtering, electron beam lithography and etching techniques, for more details see for example. In brief, the samples are Nb film on top of array of submicrometric Ni dots which have been fabricated by electron beam lithography on Si (100) substrates. Thus, 400×600 nm^2 rectangular arrays of Ni dots have been selected as the artificially fabricated pinning arrays for the present work, though the code can also simulate squares, rectangles, and triangles of any size. The thickness of the Ni dots is 40 nm, while the thickness of the Nb film is 100 nm. The diameter of the Ni dots is 200 nm. The maximum number of vortices that could accommodate one of these pinning sites, i.e., the so-called filling factor could be estimated as one vortex per dot.

A cross-shaped bridge of 40 μm is patterned in the hybrids for magnetotransport measurements by means of standard photolithography and etching techniques. The magnetic fields are applied perpendicular to the sample and magnetoresistance measurements have been done in a commercial cryostat with superconducting solenoid.

Minima appear at applied magnetic fields $H_n = n \cdot \varphi_0/(a \cdot b)$, where *a* and *b* are the lattice parameters of the rectangular array and $\varphi_0 = 2.07 \cdot 10^{-15}$ Wb is the fluxoid. The number of vortices *n* per array unit cell can be known by simple inspection of the magnetoresistance curves, in which the first minimum corresponds to one vortex per unit cell, the second minimum to two vortices per unit cell, and so on.

III. Simulations

The next step is to model these behaviors by computer simulation. This have been done by implementing the DiVoS code. Computer simulation with DiVoS reproduces the aforementioned experimental effects, but different geometries of lattices have been also evaluated by calculating the interaction of each possible vortices configuration and choosing the most convenient, i.e., the one with the lowest energy according to the desired specifications (physical parameters) used as input data. This code has been implemented from scratch; it does not take advantages neither of matching conditions with respect to the vortices lattices nor computational cutoff approximations to place the vortices. Several interactions are present and the code obtains the configuration with the lowest energy, so the interactions in the overdamped equation of vortex motion can be described as follows:

$$fi = f_i^{vv} + f_i^{vp} = \Sigma_{j=1}{}^{N}{}_{V} f_0 K_0(\mid r_i - r_j \mid / \lambda) + \\ + \Sigma_{k=1}{}^{N}{}_{p} (f_p/rp)|r_i - r_k| \, \Theta[(r_p - |r_i - r_k| / \lambda)]\boldsymbol{r}_{ik} \qquad (1)$$

where f_i is the total force per unit length acting on vortex *i*, f_i^{vv} is caused by the vortex–vortex interaction and f_i^{vp} is the pinning force.

The first sum runs up to the total number of vortices N_v and K_0 is the zero order modified Bessel function, which depends on the distance r_{ij} and the penetration depth λ, being λ (at $0.99T_c$) = 2.6 μm in the experiment. Specifically, f_0 is $3.08 \cdot 10^{-6}$ T^2nm in our experiment.

In addition, the second sum related to pinning force has *k* as the index referring to the different pinning sites in the system, *Θ* as the Heaviside step function, f_p as the maximum pinning force (it has been considered as 0.5 times the constant f_0) and r_p as the pinning radius (100 nm in our experiment).

The DiVoS code represents the following physical model: Surface is represented as a 2D grid; pinning sites define either rectangular or triangular cells; there are 1,2...n vortices per cell; and, vortex-vortex and vortex-pinning site interactions rule the system according to the previous formula (1).

As for the previous experiments, the number of cells sums up to 60x60. Considering each cell could contain up to 3 vortices, for example, the problem to be tackled results in 7,200 vortices. The interaction of 2 vortices is simulated by calculating the distance first and applying the Bessel Modified Function afterwards. Doing so, the vortices dynamics is performed as a vortex in a given position moves by looking at the interactions with all the others and the pinning sites and moving to the less energetic adjacent position. Thus, there are about 25 million interactions to be calculated in every simulation step; in other words, considering for example a rectangular cell size of 400x600 nm (simulated points), there are 240,000 positions for each vortex.

Altogether, an efficient way of calculating the system energy and algorithms to discard most of the possible configurations is needed, which results in stochastic processes such as Genetic Algorithm and/or Simulated Annealing in this work. Stochastic processes have demonstrated their correct approach [6].

A. *Genetic algorithm*

A genetic algorithm has been implemented as part of the code. As it is well known, a population of candidate solutions (called genes) to an optimization problem is evolved toward better solutions. Each candidate solution has a set of properties which can be mutated and altered randomly as the process goes on.

The evolution starts from a population of randomly generated individuals, and is an iterative process. In each generation, the fitness of every individual in the population is evaluated; the fitness is usually the value of the objective function in the optimization problem being solved, i.e. previous formula (1). The more fit individuals are stochastically selected from the current population, and each individual's genome is modified (recombined and possibly randomly mutated) to form a new generation. The new generation of candidate solutions is then used in the next iteration of the algorithm. The algorithm terminates when either a maximum number of generations has been produced, or a satisfactory fitness level has been reached for the population.

Once the genetic representation and the fitness function are defined, the genetic algorithm proceeds to initialize a population of solutions and then to improve it through repetitive application of the mutation, crossover, inversion, and selection operators. The code initializes several genes and let them evolve in a way in which also mutation, crossover, inversion, and selection operators can do cross-fitting.

B. *Simulatted annealing*

Simulated annealing uses a probabilistic technique for approximating the global optimum of the given function (1). It is a metaheuristic to approximate global optimization in a large search space, mainly used when the search space is discrete as it is the case. Simulated annealing is usually preferable to alternatives such as gradient descent for problems where finding an approximate global optimum is more important than finding a precise local optimum in a fixed amount of time.

In the implemented code, f_i moves to f_{i+1} via a proposal, i.e. the vortices move randomly to any of the 8 adjacent positions (N, NE, E, SE, S, SW, W, and NW). If the new state has lower energy, then f_{i+1} is accepted; unlike, f_{i+1} is accepted with probability $A=exp(-\Delta f/KT)$ By doing so, stochastic acceptance of higher energy states allows the process to escape local minima. If the vortices move 1 by 1 and the comparison is made, the code reproduces molecular dynamics processes; if all the vortices move at the same time in the single step, multidimensional Gaussian is carried out. When T is high, the acceptance of these moves is higher, and local minima are discouraged. As T is lowered, more concentrated search near current local minima is performed due to only few moves will be allowed. Thus, if we get the temperature decrease schedule right, it can be hoping that there will be converge to a global minimum.

Reannealing interval, or epoch length (L), is the number of points to accept before reannealing (change the temperature), i.e., L represents the number of iterations at a particular temperature. Larger decreases in T require correspondingly longer L to re-equilibrate. Also, running long L at larger temperatures is not very useful, so T is decreased rapidly at first. Reannealing interval evolves with $L_{k+1}=\beta L_k$ with $\beta>1$.

Thermostat can be simulated in three different ways:

- Linear: Temperature decreases as $T_{k+1}=\alpha T_k$, (with $1<\alpha<0$) or Tk–α (with $\alpha>0$)
- Exponential: Temperature decreases as 0.95^{α} with $\alpha \geqslant 1$
- Logarithmic: Temperature decreases as $1/\log(\alpha)$ with $\alpha \geqslant 10$

IV. RESULTS

In this work, preliminary results of the execution of the code for values of the matching point 1, 2, and 3 are reported. They are simply intended to test the computational performance as well as the behavior of the different stochastic processes.

Regarding the parallelization, the GPU cluster located at CETA was used. Out of the whole amount of resources, several GPU cards were used so the number of Nvidia cores moved between 1,000 and 5,000. Also, several outcomes have been cloncluded:

- Over 99% of the computing time gets into the evaluation of interactions
- Original scalability is of $O(N^2)$, being N the number of vortices
- Parallel scalability is of $O(N^2/2G)$, being G the number of GPU cores
- By using a cache mechanism, a GPU core is faster than a CPU for this problem

With respect to the genetic algorithm, up to 200 individuals were randomly created and allocated in different Nvidia cores in order to be executed independently. This test performed up to 500 generations, i.e., number of steps to allow the individual to evolve. Mutation and crossover rate are constant

The data related to the simulated annealing were as follow:

- Initial value of T was 25,000 K
- Temperature decreased as $T_{k+1} = 0.8*T_k$
- Population in the simulated annealing is 1

Also, an experiment which combined simulated Annealing and Genetic experiment was carried out. It was programmed in a way in which the output of a simulated annealing (20 epochs) was employed as input for the genetic algorithm (population 20).

All experiments have been executed 5 times and the results are the average values. In order to properly depict the obtained results with figures as large as possible, the latter are shown below. As it can be seen in Figs. 1 and 2, that for the genetic algorithm case, there is no influence of the number of individuals in the obtained result of the energy of the system as it is roughly constant. Unlike, the higher the number of generations, the better result.

Regarding the execution time, it increases as the number of generations increases linearly, but it shows a worse behavior with the number of individuals generated. Thus, there is a double reason for not increasing the population unnecessarily.

The simulated annealing case is more interesting (see Fig.3). It provides the best result both in execution time and energy. Also, it can be deducted that the ideal number of epochs is close to 100 as it is the region where the energy decreases significantly. But not only due to the physical interest, which is the higher one in order to obtain valid results, the execution time vs. the number of epochs also demonstrate that from 150 on the system saturates.

With respect to the hybrid case, it does not provide a significant enhancement as the genetic algorithm behavior penalize the simulated annealing one.

V. CONCLUSIONS

Hybrid superconducting/magnetic samples are fabricated with superconducting films on top of array of pinning centers. The magnetoresistance of these hybrids, close to critical temperature, shows deep and equal spaced minima which are due to commensurability effects between the vortex lattice and the unit cell of the array. The first minimum appears when the density of the pinning centers equals the density of the vortex lattice, upper order minima take place at $H_n = n(\Phi_0/S)$, where $n>1$ is an integer number and Φ_0 is the quantum fluxoid. Taking into account the vortex–vortex and the vortex–pinning center interactions, a GPU-based computing simulation code has been implemented. This code can calculate different values and positions for different lattices in size, matching field values, and geometry of the pinning sites, which allows having a picture of the different vortex lattices.

The position of the vortices, as well as the minimum energy are obtained with three different stochastic methodologies: genetic algorithm, simulated annealing, and, a combination of the former. The best results are provided by the simulated annealing version.

Further tests are needed to be carried out in order to properly match experiment and simulation switching different parameters for the simulated annealing case.

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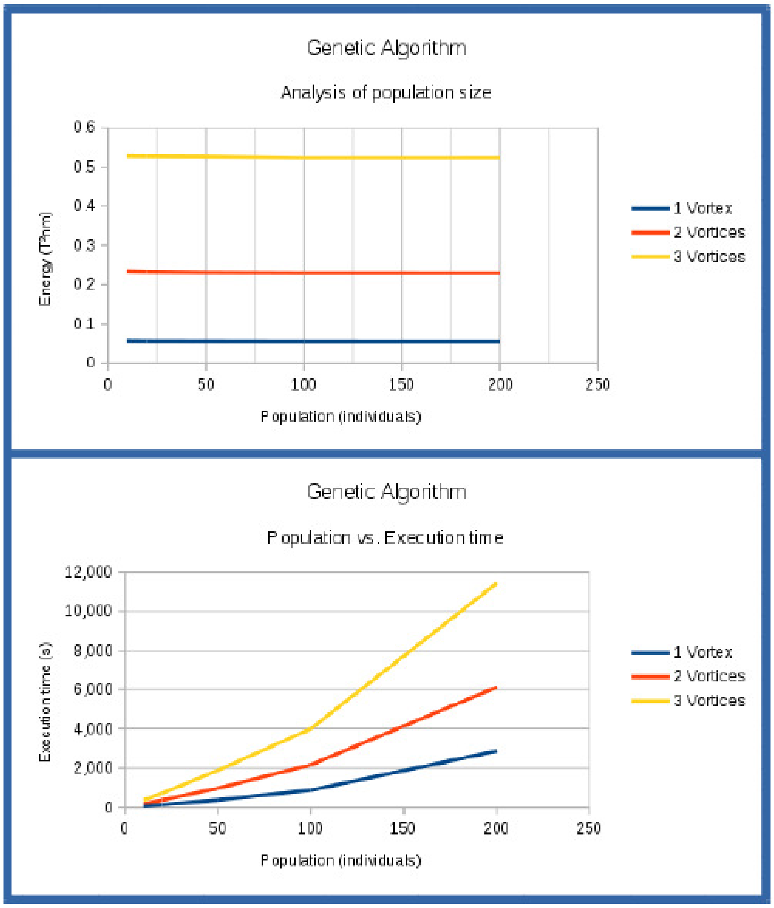

Figure 1. Genetic algorithm version of the code. Influence of the population on the energy obtained and the executiont time.

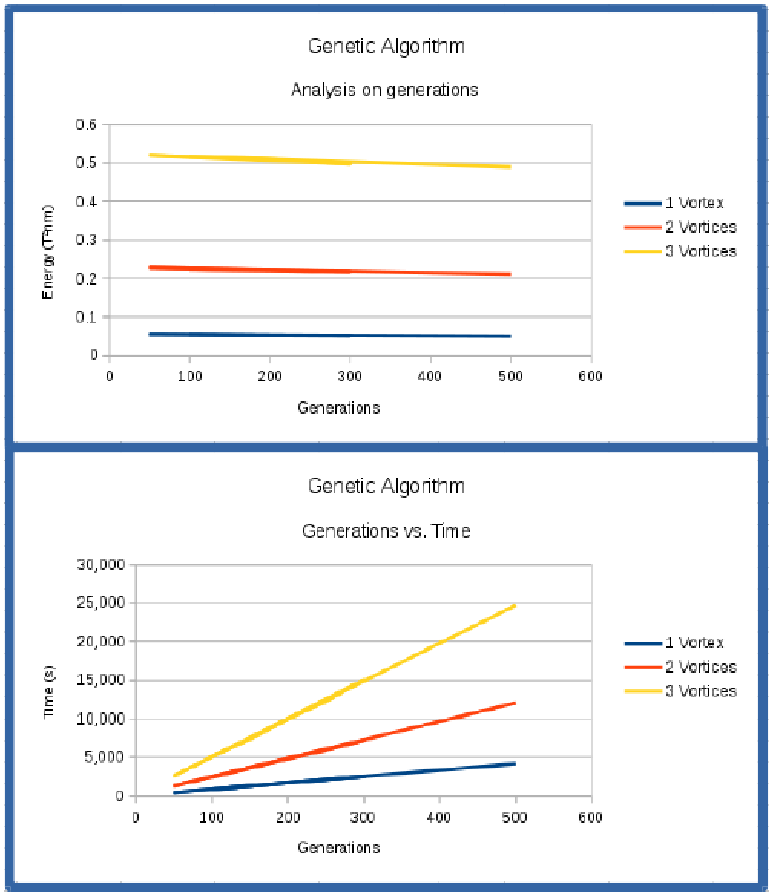

Figure 2. Genetic algorithm version of the code. Influence of the generations on the energy obtained and the executiont time

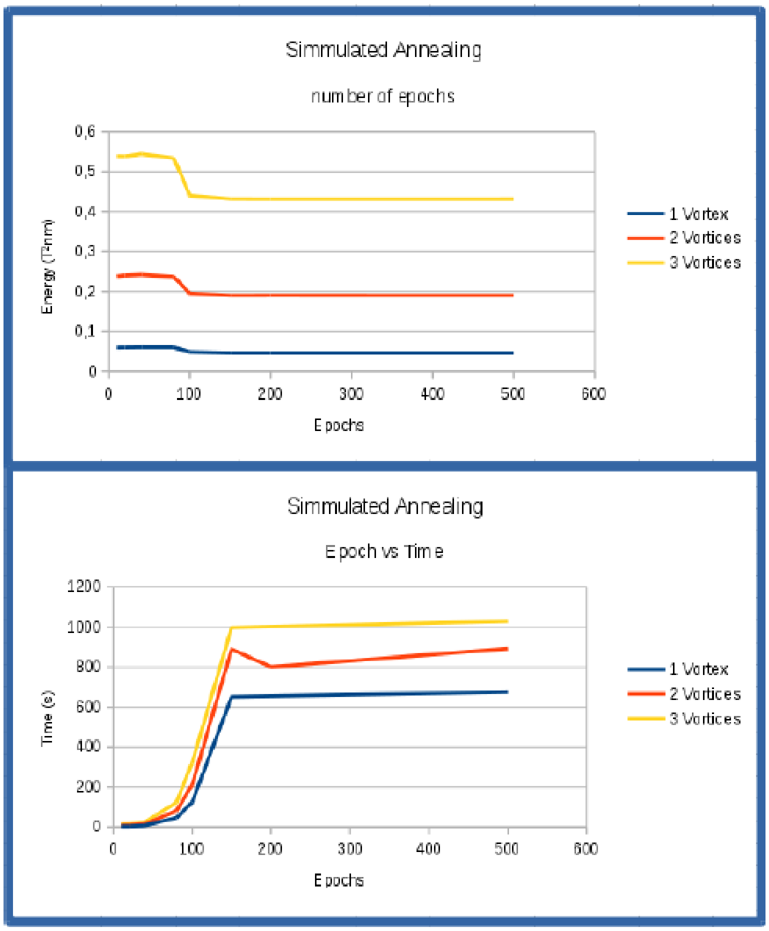

Figure 3. Simulated annealing case. Influence of the number of epochs in the obtained energy amdon the execution time