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USING GPUS FOR DETERMINING THE ENERGY CONFIGURATION OF SUPERCONDUCTING VORTEX LATTICES WITH STOCHASTIC METHODS

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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 two stochastic processes (simulated annealing, Basin Hopping) being able to simulate square, rectangular, or triangular arrays of nanodefects of different size. A computational performance study is also made.

1 INTRODUCTION

Arrays of nanodefects embedded in superconducting films have the faculty to modify the dynamics of superconducting vortex lattices as well as the effects of vortex lattice pinning. Experimentally, this effect can be observed using arrays of holes (antidotes) due to they thread the films or dots embedded in the sample producing different diameters of the pinning centers, reconfiguration of the vortex lattice, channeling effects, etc.

The way in which these phenomena are studied is by means of magnetoresistance measurements, i.e. resistance vs. applied magnetic field. The minima depicted in the curve corresponds to the moment in which the vortex lattice matches the unit cell of the array. When so, the vortex density is an integer multiple of the pinning center density. According to the literature, this effect is cause by different interactions when the temperature is close to the critical one (T_c): (i) vortex–vortex, (ii) vortex–artificially induced pinning center (array of nanodefects), (iii) vortex–intrinsic and random pinning centers. Because of the roughness of the sample surface, probe methods are unable to detect the vortex position and symmetry of the vortex lattice as only the aforementioned experimental matching conditions can be observed, so numerical simulations can be a tool for inferring these geometries.

Reichhardt and collaborators (Reichhardt et al. 1998) integrated numerically the Langevin equation of motion in order to predict some of the matching fields at which commensurate vortex arrangements happen. In this work, cut-off conditions were integrated in the simulation as well as pinning strengths and other relevant parameters governed by the penetration superconducting depth. Dinis and collaborators (Dinis et al. 2009) simulated the rectifier behavior of the vortex lattice in the transverse ratchet effect with the Langevin equation of motion of the vortices too, but taking experimental parameters as input. Simulations of vortex dynamics in superconducting films with pinning array have been also reported by other authors (Kato and Enomoto 2000, Gropp et al. 1996, and Rodríguez-Pascual et al. 2012).

The aim of this work is to simulate the commensurability experiments in the framework of the Langevin equation of motion without any initial conditions neither constraints. In other words, the main

contribution of this work is to allow vortices to freely evolve within the experimental conditions without any prefixed condition, a fact that was not taken into account in previous works as documented before. By doing so, it is expected to better reproduce the experiment as well as inferring real interactions playing key roles. Thus, only the vortex–vortex interaction and the periodic pinning sites (array unit cell) are implemented in the code as governing conditions. This process is carried out with simulated annealing and Basin Hopping 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 measure the energy of superconducting vortex lattices is briefly described. In Section 3, 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 4, while the conclusions come in Section 5.

2 EXPERIMENTS

Magnetron sputtering, electron beam lithography on Si (100) substrates, and etching techniques are used to grow superconducting/magnetic hybrids. 400 by 600 nm^2 rectangular or 400 nm^2 equilateral triangle arrays of Ni dots (diameter of 200 nm) have been built as samples of Nb films on top of arrays of submicrometric Ni dots. The maximum number of vortices that could accommodate one of these pinning sites, i.e. the so-called filling factor, is defined as one vortex per dot.

In the hybrids for magnetotransport measurements, a cross-shaped bridge is patterned with size of 40 μm by etching and standard photolithography techniques. The magnetic field is perpendicularly applied to the sample and magnetoresistance measurements have been done in a commercial cryostat with superconducting solenoid.

When the applied magnetic field is $H_n = n \cdot \varphi_0/(a \cdot b)$, minima appear, being *a* and *b* the lattice parameters of the rectangular array and $\varphi_0 = 2.07 \cdot 10^{-15}$ Wb the fluxoid. By simply inspecting the magnetoresistance curves, the number of vortices *n* per array unit cell can be known; then, the first minimum corresponds to one vortex per unit cell, the second minimum to two vortices per unit cell, and so on.

3 SIMULATIONS

The next step is to model these behaviors by computer simulation. This has been done by implementing the DiVoS code. DiVoS is implemented in PyCUDA, the library for implementing Nvidia's CUDA API with Python. Computer simulations with DiVoS reproduce the aforementioned experimental effects, though the code can define squares, rectangles, and triangles of any size. Different geometries of lattices have been 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 takes advantages neither of matching conditions with respect to the vortices lattices nor computational cutoff approximations to place the vortices, being this one the main contribution of this work. 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:

$$f_i = f_{vv} + f_{vp} = \sum_{j=1}^{Nv} f_0 K_0\left(\frac{|r_i - r_j|}{\lambda}\right)\boldsymbol{r_{ij}} + \sum_{k=1}^{Np} \frac{f_p}{r_p}|r_i - r_k|\Theta\left[\frac{(r_p - |r_i - r_k|)}{\lambda}\right]\boldsymbol{r_{ik}} \quad (1)$$

where f_i is the total force per unit length acting on vortex *i*, f_{vv} is caused by the vortex–vortex interaction, f_{vp} is the pinning force, and $\boldsymbol{r_{ij}}$ and $\boldsymbol{r_{ik}}$ are the vectors from vortex *i* to vortex *j* and from vortex *i* to pinning *k* respectively.

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 $\lambda(\text{at } 0.99T_c) = 2.6$ μm in the experiment. Specifically, f_0 is $3.08 \cdot 10^{-6}$ T^2nm in the 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 Equation (1).

As for the previous experiments, the number of cells sums up to 60 by 60. 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 400 by 600 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 simulated annealing or Basin Hopping in this work. Stochastic processes have demonstrated their correct approach (Van Kampen 2007).

3.1 Simulated Annealing

Simulated annealing uses a probabilistic technique for approximating the global optimum of the given function. 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 a single step, multidimensional Gaussian is carried out. When the temperature 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 according to the previous statements, there will be higher possibilities of converging 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 L 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 $T_k-\alpha$ (with $\alpha>0$).
- Exponential: Temperature decreases as 0.95^{α} with $\alpha \geq 1$.
- Logarithmic: Temperature decreases as $1/log(\alpha)$ with $\alpha \geq 1$.

3.2 Basin Hopping

The Basin Hoping methodology is similar to the one applied to simulated annealing, though it represents an improvement. It was introduced by Wales and Doye (Wales and Doye 1997)

The following general characteristics can be mentioned with respect to the previous technique:

- Random perturbation of coordinates (location on error surface).
- Local minimization – find best (lowest) error locally.
- Acceptation/rejection of new position based on function value at that point.
- Acceptance test is usually Metropolis criterion from Monte Carlo (Metropolis-Hastings) methods.
- It is more generally used to generate random samples from a probability distribution from which direct sampling is difficult (it might not be known what it looks like).

The literature accounts on some comparison available among different algorithms (Rios and Sahinidis 2013).

4 RESULTS

In this work, preliminary results of the execution of the code for values of the matching point are reported. They were simply intended to test the computational performance as well as the behavior of the different stochastic processes, though one physical result of interest arose. In order to properly compare both stochastic approximations as well as reproducing the experiment, the simulation is ended when the measured critical temperature (T_c) is reached.

The evolution of the system in the model can follow a molecular dynamic approach or a multidimensional Gaussian one. In the former, one vortex is moved L times and then the system makes the comparison; in the latter, all the vortices are moved L times and then the comparison is made.

Regarding the parallelization, the GPU cluster located at CETA-CIEMAT 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 (in particular, Tesla K20). Also, several outcomes have been concluded:

- 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.

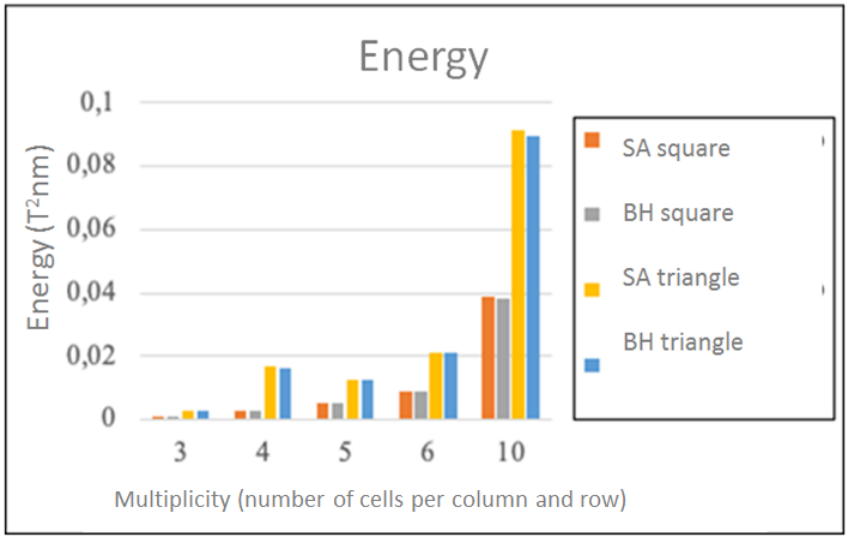

Figure 1: Value of the energy according to the stochastic method used and how the pinning sites are located (multidimensional Gaussian).

The data related to the experiment have been swiped in order to better test how the code performs, though an initial fixed value of $T=25{,}000\ K$ was kept. Otherwise indicated, linear decrease is selected with $\alpha=0.8$.

When possible, i.e. those experiments devoted to obtain a final value of the final energy, all experiments have been executed 5 times and the results are the average values. For those cases in which the evolution of the system is made according to how a parameter evolves, no average is calculated at the end.

According to the results of the simulations, the following outcomes can be derived:

- The Basin Hopping method provides better results than the simulated annealing algorithm, despite using more execution time.
- Using the same execution values, targets divided into rectangular cells requires shorter execution times than films divided into triangles.
- The exponential thermostat method is the most optimal method of temperature decrease, since it allows obtaining an optimal configuration in less time than the logarithmic one. It is also possible to combine the execution of the code with a linear decrement and then with an exponential one to obtain the optimal solution on this respect.
- It is more advisable to use the molecular dynamics simulation method, although another equally valid option is to combine the execution of the code using the multidimensional Gaussian simulation and then apply the molecular dynamics method to obtain the optimal solution.
- The energy evolves in the expected way thanks to the decrease in temperature, initially checking large regions so, as it evolves, focus on specific areas until finding the global minimum.
- The tests carried out demonstrate the existence of configurations that are much more optimal than those theoretically proposed up to now, so the introduction of new interactions into the model is needed in order to properly reproduce the experiment.

To substantiate the previous bullets, some figures are depicted along the text. Figure 1 shows the value of the energy according to the stochastic method used and how the pinning sites are located using the multidimensional Gaussian method. As it can be seen, the Basin Hopping method provides lower values of the temperature.

On the other side, Figure 2 depicts the energy according to the number of vortices per cell and the time needed for the calculi. In this case, cells of 400 by 600 nm^2 size are simulated with a multidimensional Gaussian movement.

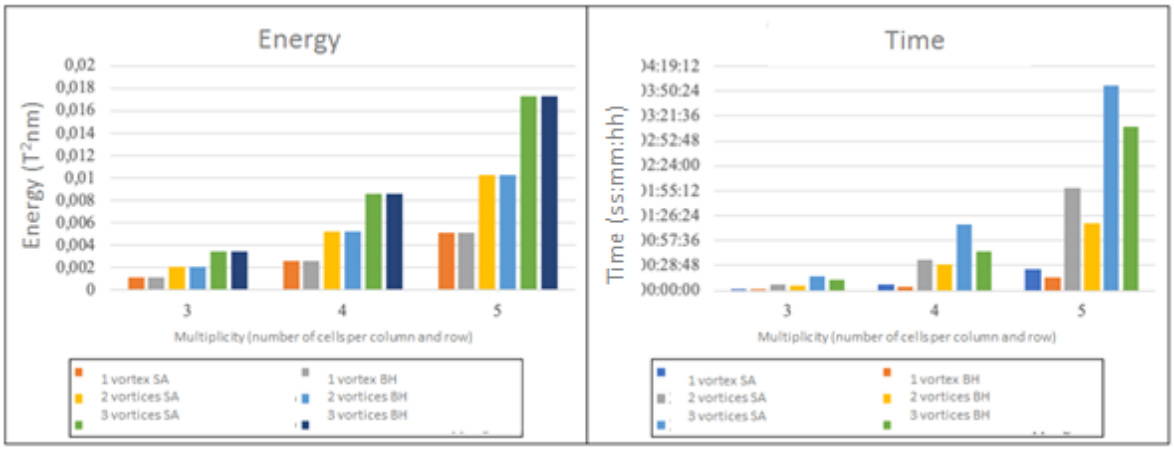

Figure 2: Value of the energy according to the number of vortices per cell and the time needed for the calculi (400 by 600 nm^2 configuration, multidimensional Gaussian).

Figure 3 shows the value of the energy as the epoch parameter evolves, finding out that 50 steps is a threshold value from which no improvement is achieved. In Figure 4, the execution time depending on the thermostat method used is depicted. Both figures correspond to a 400 by 600 nm^2 configuration with a multidimensional Gaussian approach.

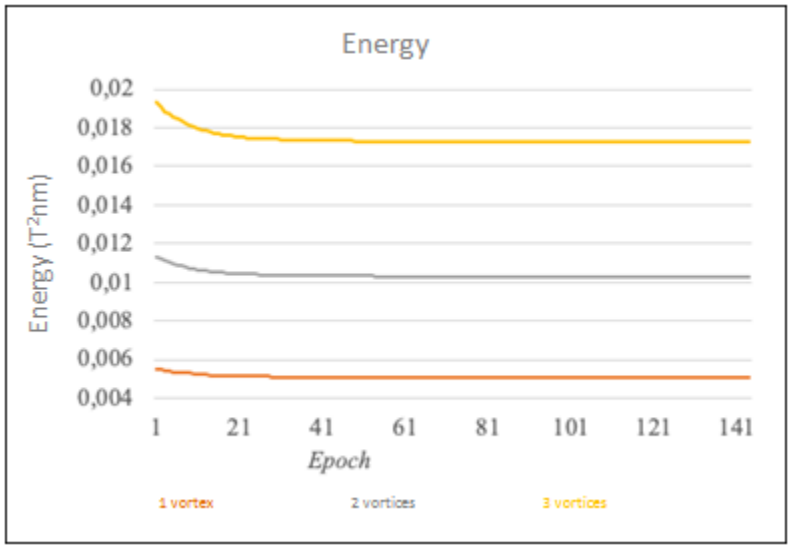

Figure 3: Value of the energy as the epoch parameter evolves (400 by 600 nm^2 configuration, multidimensional Gaussian).

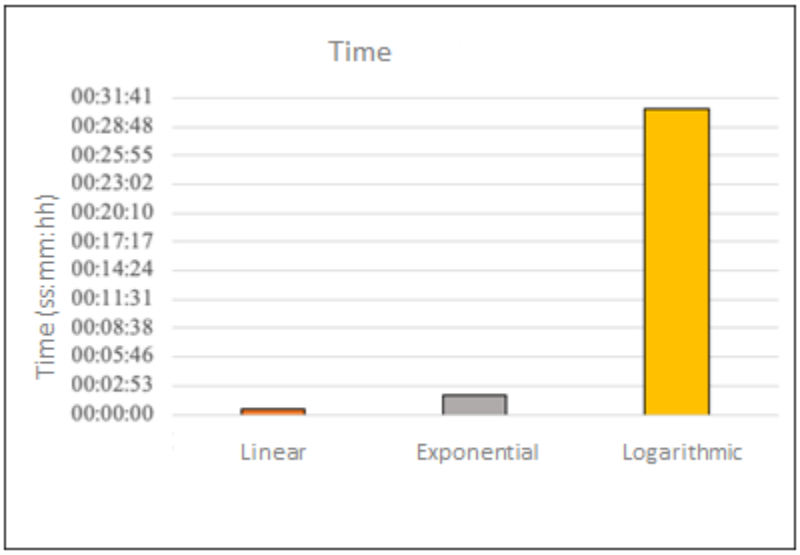

Figure 4: Execution time depending on the thermostat method used (400 by 600 nm^2 configuration, multidimensional Gaussian).

The most interesting result of this work is presented in Figure 5, i.e. the final result of the energy and how the vortices allocate for producing such a value of the energy. In this case, the experimental well-known result is compared with the result provided by the simulation with the simulated annealing and the Basin Hopping methods. As the simulated results provide a lower value of the energy with respect to the experimental result (Exp=544,258, SA=510,725, and BH=510,723, all units in 10^{-8} T^2nm), it can be concluded that more interactions and effects must be taken into account for reproducing the experimental result.

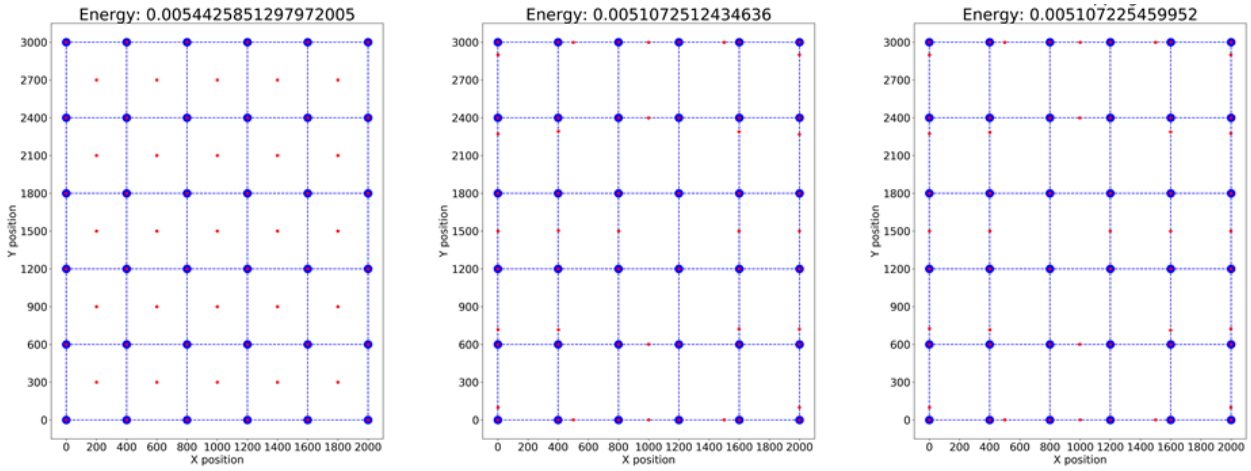

Figure 5: Final result of the energy. On the left, the experimental well-known result; in the middle (SA) and on the right (BH), results of the simulation providing a *lower* value of the energy (10^{-3} T^2nm).

5 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 were 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. 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 two different stochastic methodologies: simulated annealing and Basin Hopping. The best results are provided by the latter 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 as it has been demonstrated that only relying on the vortex-vortex and the vortex-pinning interaction, experimental results are not reproduced, but rather different positions with even lower energy. As the tests have been executed 5 times, with actually a large reproducibility, up to 30 independent runs will be performed in order to provide better statistical confidence as well as to evaluate normality of the samples and parametric vs non-parametric tests.

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