GPU-based Stochastic Problem Solving and Scalability of Superconducting Vortices

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Physical problem

- Niobium thin films can provide superconducting properties

- Samples are these films on top of a Nickel array of pinning sites can create variations on the potential at certain points (superconducting vortices)

- Each vortice interacts with all the others and the pinning sites till a minimum in the energy is found

- The question is, can we simulate the behavior of vortices? This would provide useful information to the experimentalists

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

- Vortex-Vortex and Vortex-Pinning site interactions rule the system

- Mathematically speaking, the interaction to be minimized is

$$f_i = f_i^{vv} + f_i^{vp} = \sum_{j=1}^{N v} f_0 K_0\left(\frac{|r_i - r_j|}{\lambda}\right)\hat{r}_{ij} + \sum_{k=1}^{N p}\left(\frac{f_p}{r_p}\right)|r_i - r_k|\Theta\left(\frac{r_p - |r_i - r_k|}{\lambda}\right)\hat{r}_{ik}$$

Computational problem

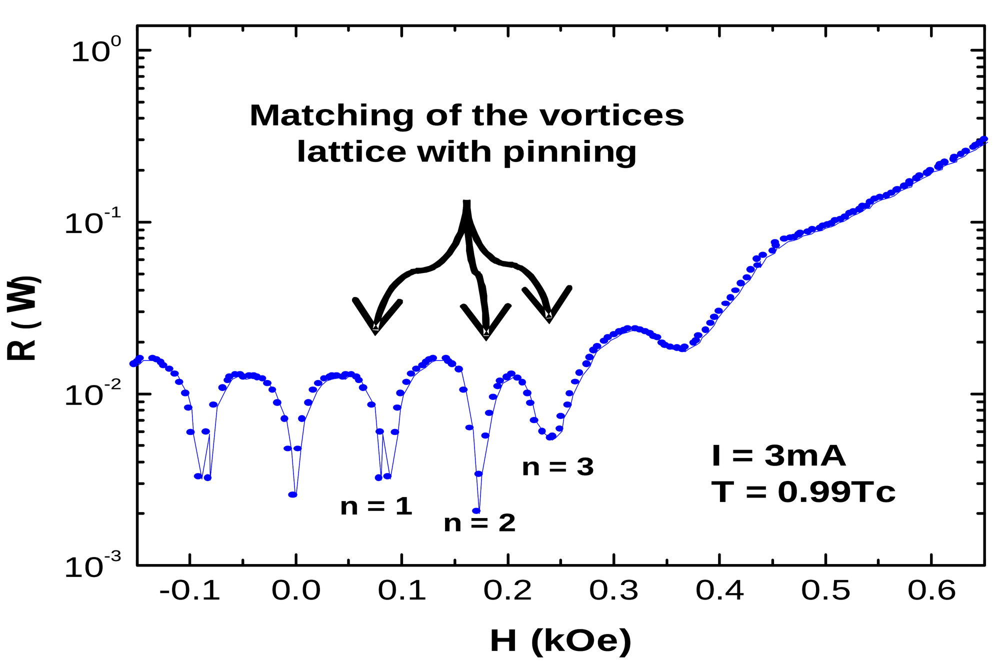
- Number of cells: up to 60x60, each with up to 3 vortices: up to 7,200 vortices

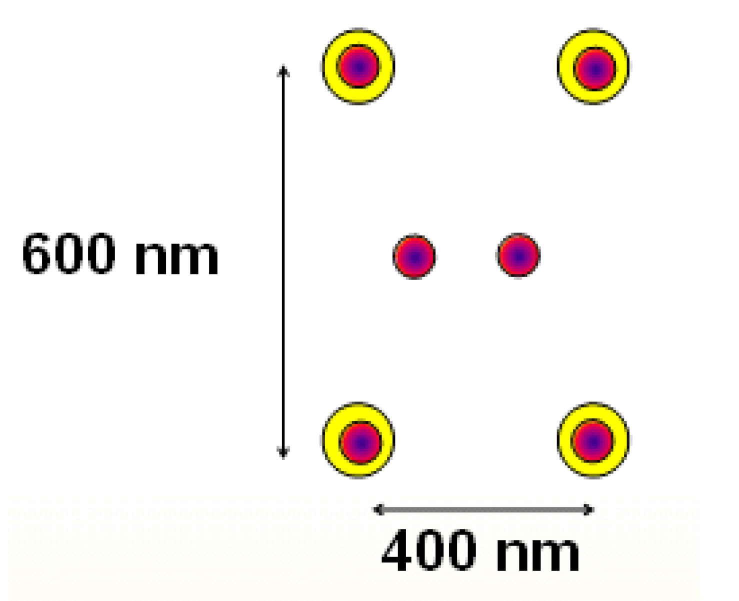
- Interaction of 2 vortices: calculate distance, apply Bessel Modified Function

- 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.
- There are about 25 million interactions to calculate every simulation step!

-- Rectangular cell size: 400x600: 240,000 positions for each vortex

All together, an efficient way of calculating the system energy and algorithms to discard most of the possible configurations is needed (Genetic Algorithm, Simulated Annealing...)

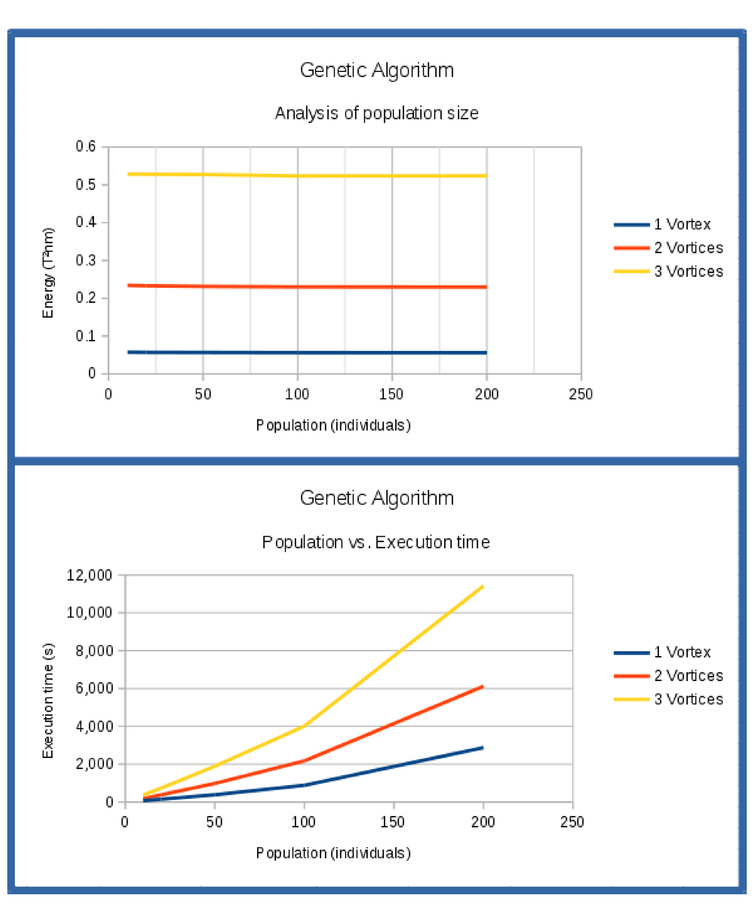


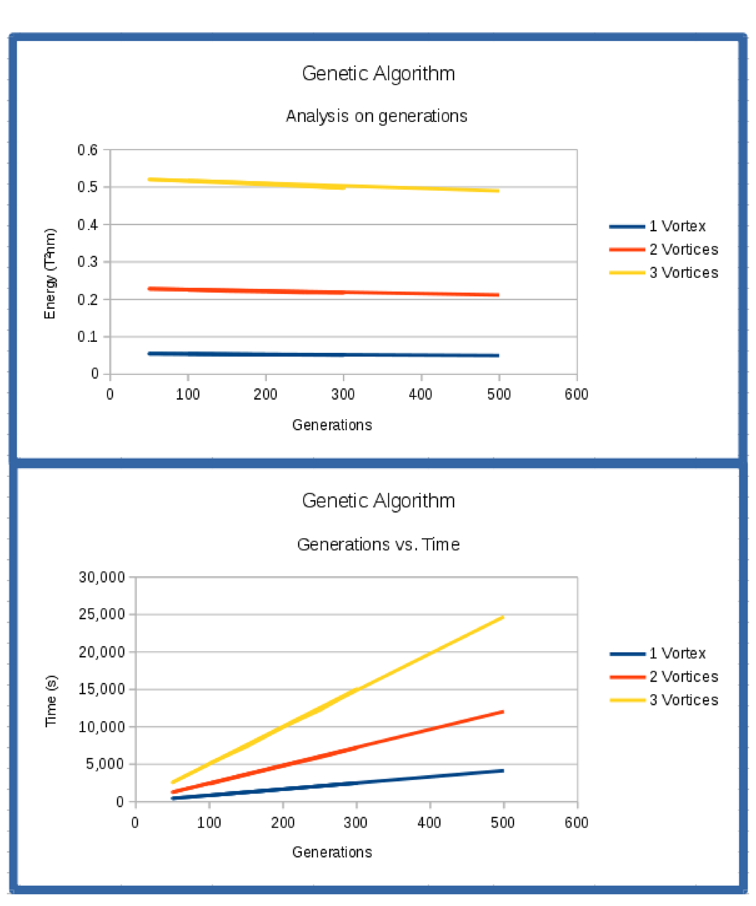


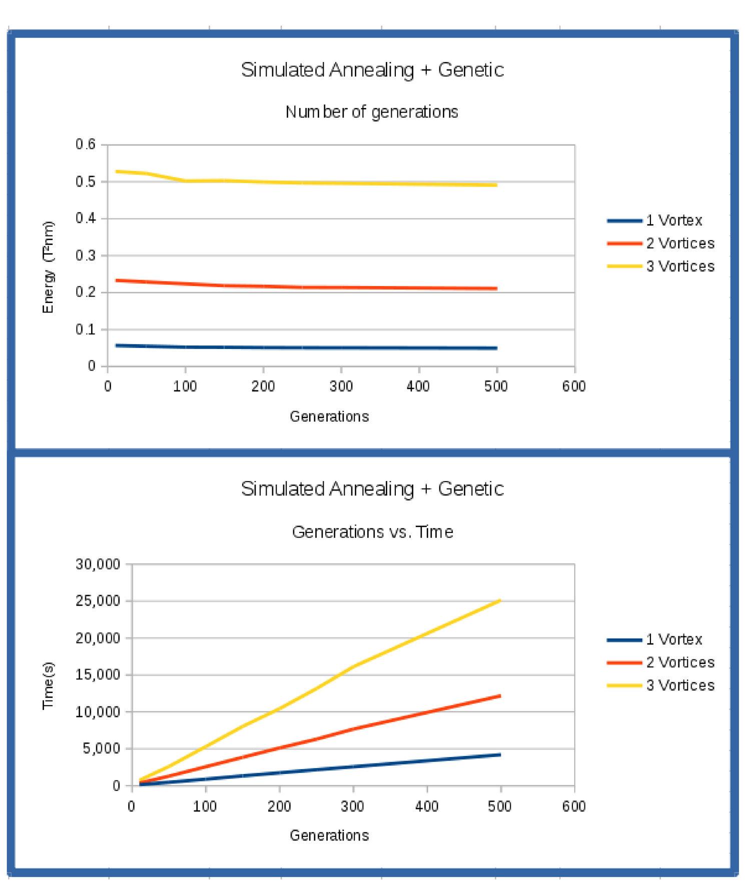
Parallelization

- Over 99% of the computing time gets into the evaluation of interactions
- Original scalability: $O(N^2)$ being N the number of vortices
- Parallel scalability: $O(N^2/2G)$ being G the number of of GPU cores (1K-5K)
- moreover, by using a cache mechanism, a GPU core is faster than a CPU for this problem

Genetic Algorithm





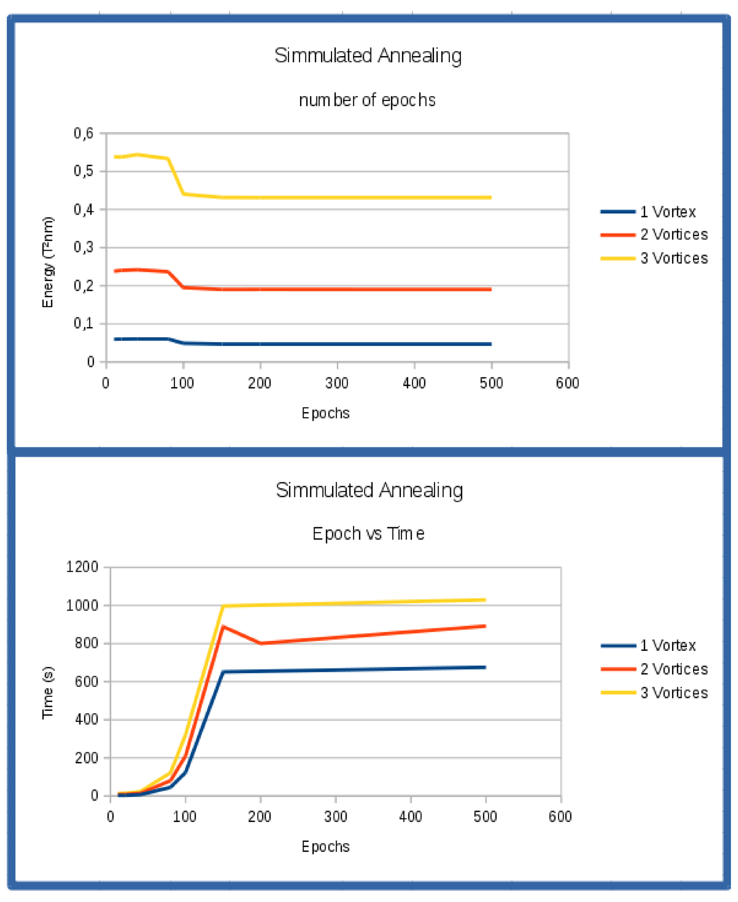


What is the influence of the population size on the results?

And the number of generations?

In all cases, mutation and crosover rate are constant

Simulated Annealing



- Temperature decreases as Tk+1 = 0.8 * Tk

- Population in the simulated annealing is 1

- In the Simulated Annealing + Genetic experiment, the output of a simmulated annealing (20 epochs) is employed as input for the genetic algorithm (population 20)

- All experiments have been executed 5 times. Results shown are the average values.

Result Analysis

Computational analysis
- GPUs are a great tool for this code. Amazing performance, easy to use

Simulation results
- Simulated annealing provides best results in the shortest time

- Genetic algorithm results improve very slowly

- All together, simulation needs further developments for the desired degree of acuracy