Application of OpenCL to numerical study of the Abrikosov vortex system in superconductor with cylindrical hole

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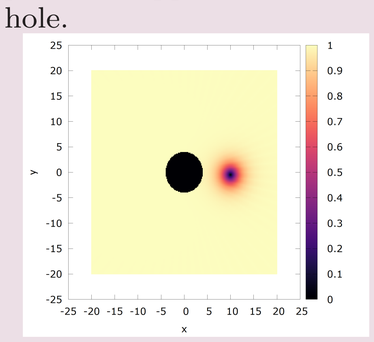
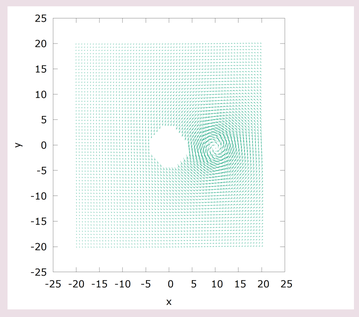
Introduction

We solve numerically the system of Ginzburg-Landau equations describing the superconductor containing Abrikosov vortices in the special geometry essential for practical application: bulk material with a cylindrical hole.



(a) wave function amplitude $\|\Psi|^2$



(b) electrical current $\boldsymbol{j} = -\frac{1}{4\pi}\delta\boldsymbol{A}$

The interaction between the vortex and the hole (absense of a superconductor) defines the potential well needed for correct description and simulation of modern superconducting materials. Depending on the hole radius, we can address such phenomena as vortex pinning (small radius) and interaction with curved surface (large radius).
Taking into account the nonlinearity of the equations, numerical approach is considered the only possible one to describe complex geometries, as well as interaction of several vortices. We apply the GPU OpenCL solver developed especially for vortex-type problems[1].

Here we describe the OpenCL specific tricks and optimizations used for maximal GPU utilization and overall calculation performance.

Ginzburg-Landau equations

$$\left(\frac{i}{\kappa}\nabla + \boldsymbol{A}\right)^2 \Psi - \Psi + |\Psi|^2\Psi = 0,$$

$$\nabla \times (\nabla \times \boldsymbol{A}) + \frac{i}{2\kappa}\left(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*\right) + |\Psi|^2\boldsymbol{A} = 0,$$

where Ψ and $\mathbf{A}$ are the wave function of Cooper pairs and vector potential of the magnetic field.
Boundary conditions on the hole radius

$$\left(\frac{i}{\kappa}\nabla + \boldsymbol{A}\right)\boldsymbol{e}_r\Psi = 0,$$

$$(\nabla \times \boldsymbol{A})_z = \boldsymbol{H}_z$$

and Coulomb gauge for vector potential:

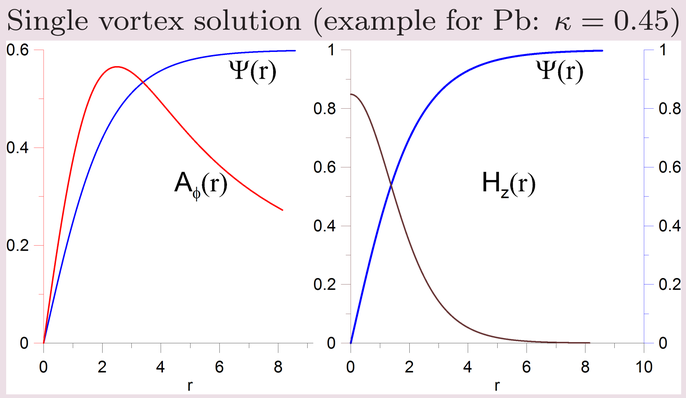
$$\nabla \cdot \boldsymbol{A} = 0$$

Numerical solution

- Reformulation of equations for vortex problem[1]:

$$\Psi(\boldsymbol{\rho}, z) = \Psi_1(\boldsymbol{\rho}) \cdot \Psi_v(\boldsymbol{\rho} - \boldsymbol{\rho}_v),$$
$$\mathbf{A}(\boldsymbol{\rho}, z) = \mathbf{A}_1(\boldsymbol{\rho}) + \mathbf{A}_v(\boldsymbol{\rho} - \boldsymbol{\rho}_v)$$

  where the 2D coordinate $\boldsymbol{\rho}_v = \{x_v, y_v\}$ denotes the center of the vortex.
- Single vortex solution (example for Pb: $\kappa = 0.45$)



- 2D geometry
- Nonlinear coordinate $r = R \cdot tan(\theta) = R \ldots \infty$
- Pseudoviscosity method:

$$-\frac{\partial\Psi}{\partial t} = GLE_1(\Psi, \mathbf{A}),$$
$$-\frac{\partial\boldsymbol{A}}{\partial t} = GLE_2(\Psi, \mathbf{A})$$

- Special type of implicit Euler method for improved stability
- Boundary conditions using Fourier transform

OpenCL application

1. Iterative approach allows us to use the Production-CL library for iterative scientific calculations [2].
   - Batch of numerical kernels: `inside_2D()`, `boundary_consitions_1D()`, `time_step_2D()`
   - `NS` max. number of iterations, `numSave` between saving the state, `numSelf` between recalculation of currents and magnetic field (for self-consistent solution)
   - possibility to continue the calculation from the saved state
2. During calculation (iterations):
   - simulation of main equations and time step: $N_r \times N_\phi$ points, 3 components (A_r, A_ϕ, Ψ) in parallel;
   - applying boundary conditions: N_ϕ points, 3 components (A_r, A_ϕ, Ψ) in parallel using FFT;
   - parallel calculation of electrical current inside the superconductor volume: $N_r \times N_\phi$ points, 2 components (j_r, j_ϕ) in parallel;
   - self-consistent magnetic field on hole surface: N_ϕ points, 1 component H_z, each needs integration of $N_r \times N_\phi$ terms (parallel reduction);
3. After convergence, to obtain the value of Gibbs free energy:
   - calculate magnetic field inside hole: $N_\phi \times N_r^{(inside)}$ points, each needs integration of $N_\phi \times N_r$ terms.
   - calculate the value of Gibbs free energy: integrate 3 terms – magnetic field energy inside the hole, $|\psi|^4$ and $|curlA|^2$ inside the superconductor. $N_r \times N_\phi$ terms, parallel reduction.

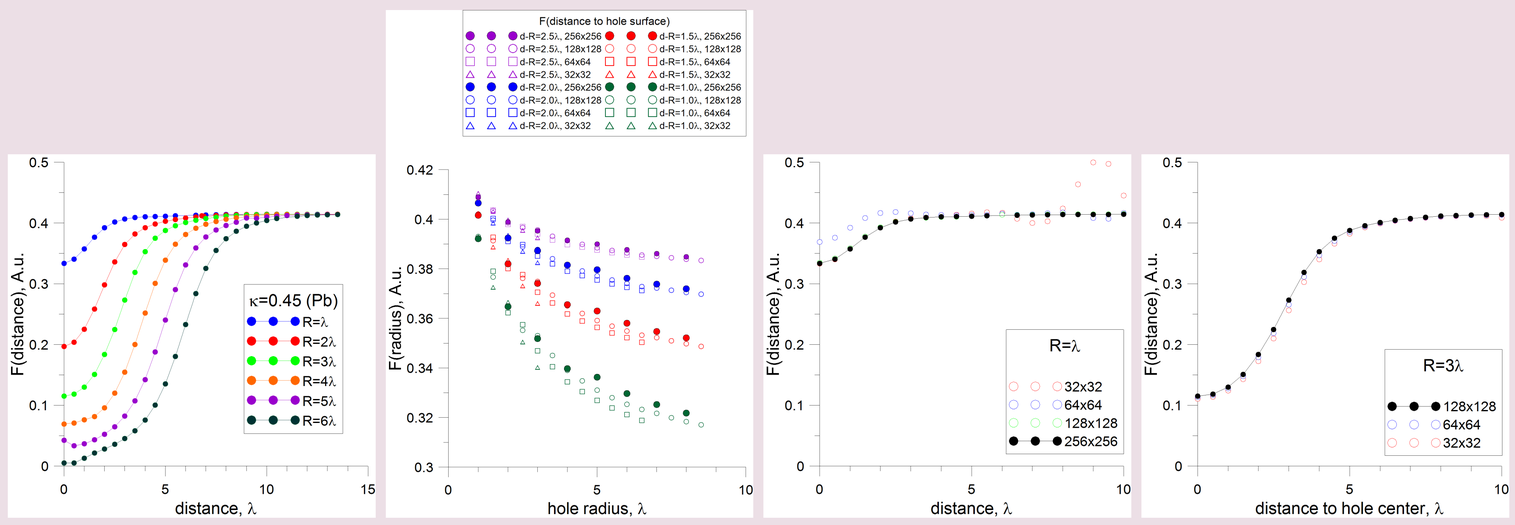
OpenCL/GPU specific tricks

- **local memory** storage of data when calculating finite-difference derivatives
- **immediate in-place calculation** of nonlinear coordinate metrics, instead of reading from memory
- **several simulations for different parameters simultaneously**, to maximize GPU occupancy

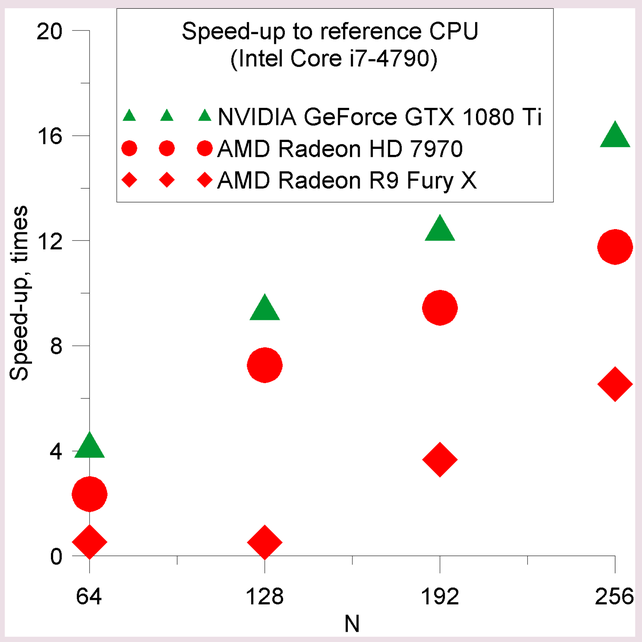
First two optimizations are specific for scientific calculations which are memory-bound; the last one takes into account the fact that the amount of actual calculations which can be done in parallel is not enough to occupy all the compute units (CUs) of the GPU. For the grid of 128x128 points which is fine enough for obtaining stable and reliable results, we can estimate that the saturation is achieved for approximately 10÷12 simultaneous calculations. This value can be derived from the number of parallel workgroups (128) and amount of local memory per workgroup (4 KiB).

Results of simulation

1: Vortex pinning, 2: Surface curvature, 3,4: convergence control
As expected, we see the potential well profile $U(d)$ for the so-called vortex pinning on the hole, depending on the hole radius R:



Speed-up



It is noticeable that even rather old accelerator AMD Radeon HD 7970 still shows decent results which can be probably explained by the highest FP64 performance of it among these GPUs.

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Bibliography

1. P.F.Kartsev, IWOCL 2018 Proceedings, DOI: 10.1145/3204919.3204944
2. P.F.Kartsev, IWOCL 2017 Proceedings, DOI: 10.1145/3078155.3078162
3. V.A.Kashurnikov *et al.*, Superconductor Science and Technology **31**(11), 115003 (2018).