C05: Numerical simulation of the Gross–Pitaevskii equation by vortex tracking

SFB 1481 Sparsity and Singular Structures

Gaspard Kemlin (PIs: Benjamin Stamm & Christof Melcher)

RWTH AACHEN UNIVERSITY

Universität Stuttgart

Research goal

The Gross–Pitaevskii (GP) equation plays a central role in various models of superfluids and condensed matter physics. A dominating feature is the occurrence of quantized vortices that effectively evolve according to a Hamiltonian system in the limit of point-like vortices. The project aims at placing the well-developed analytical theory of this singular limit in a computational framework that allows to prove accuracy and efficiency of numerical approximations throughout the vortex regime.

Model

The time-dependent GP equation is a fundamental tool to model and understand superfluids. It reads, for given $\varepsilon > 0$ and boundary conditions $g : \partial\Omega \to \mathbb{S}^1$ on a bounded domain $\Omega \subset \mathbb{R}^2$,

$$\begin{cases} \mathrm{i}\dfrac{\partial \psi_\varepsilon}{\partial t} = \Delta\psi_\varepsilon + \dfrac{1}{\varepsilon^2}(1-|\psi_\varepsilon|^2)\psi_\varepsilon \text{ in } \Omega, \\ \psi_\varepsilon(\cdot,t) = g \text{ on } \partial\Omega \text{ and } \psi_\varepsilon(\cdot,0) = \psi_\varepsilon^0. \end{cases} \quad (1)$$

$\psi_\varepsilon : \Omega \times \mathbb{R}^+ \to \mathbb{C} \simeq \mathbb{R}^2$ is called the *wave function* and $|\psi_\varepsilon|^2$ represents the *density* of the superfluid.

Background

We are interested here in the behavior of the solutions in the singular limit $\varepsilon \to 0$. A striking feature is the occurrence of *quantized vortices* that evolve, in the limit $\varepsilon \to 0$, according to Hamiltonian dynamics [3]. These vortices correspond to isolated zeroes of ψ_ε with nonzero winding numbers (or degree). In [6], the authors consider a sequence of initial conditions $(\psi_\varepsilon^0)_{\varepsilon>0}$ made of "almost vortices", in the sense that the *vorticity* $J(\psi_\varepsilon^0) = \det\nabla\psi_\varepsilon^0$ converges, when $\varepsilon \to 0$, to a sum of N Dirac masses, representing vortices locations $X^0 = (\boldsymbol{x}_j^0)_{j=1,\dots,N} \in \Omega^N$ with winding numbers $d = (d_j)_{j=1,\dots,N} = (\pm 1)_{j=1,\dots,N}$. More precisely, ψ_ε^0 is required to satisfy, for some $C > 0$ and $\alpha \in (0,1)$,

$$\forall\ \varepsilon \text{ small enough,} \quad \Big\| J(\psi_\varepsilon^0) - \pi \sum_{1\leqslant j\leqslant N} d_j \delta_{\boldsymbol{x}_j^0} \Big\|_{\dot{W}^{-1,1}} \leqslant C\varepsilon^\alpha,$$

where the $\dot{W}^{-1,1}$ norm is dual to the Lipschitz norm. The main result of [6] is then that the same kind of estimates hold for $J(\psi_\varepsilon(\cdot,t))$ and vortex locations $X(t) = (\boldsymbol{x}_j(t))_{j=1,\dots,N} \in \Omega^N$, where $\boldsymbol{x}_j$ solves the following Hamiltonian ODE:

$$\begin{cases} \dot{\boldsymbol{x}}_j(t) = -\dfrac{1}{\pi} d_j \mathbb{J} \nabla_{\boldsymbol{x}_j} W(X(t), d), \\ \boldsymbol{x}_j(0) = \boldsymbol{x}_j^0, \end{cases} \quad (2)$$

$$\text{where} \quad \mathbb{J} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

Here $W : \Omega^N \times \{\pm 1\}^N \to \mathbb{R}$ is the *renormalized energy* introduced in [2].

The renormalized energy

$$W(X,d) = -\pi \sum_{1\leqslant j\neq i\leqslant N} d_i d_j \log|\boldsymbol{x}_j - \boldsymbol{x}_i| + \text{boundary terms}$$

is the limit of $E_\varepsilon(u_\varepsilon) - N(\pi \log 1/\varepsilon + \gamma)$. Here, γ is a universal constant introduced in [2] and u_ε is a minimizer of the energy conserved by (1):

$$E_\varepsilon(u) = \int_\Omega \frac{1}{2}|\nabla u|^2 + \frac{1}{4\varepsilon^2}(1-|u|^2)^2.$$

W can be seen as the Γ-limit of E_ε minus the self-energy of N vortices of degree ± 1.

Objectives and questions so far

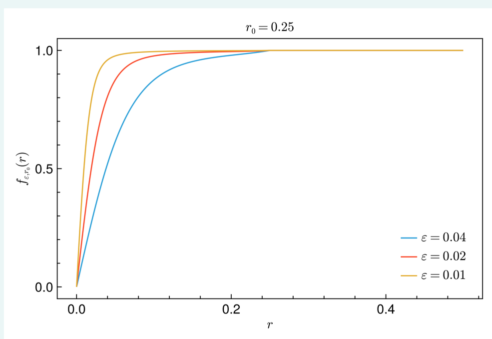
- At the (continuous) PDE level:
  - How to set up numerically well-prepared initial conditions?
  - How to localize the vortices?
  - How to extend the estimates in [6] at the computational level?
- At the (discrete) Hamiltonian level:
  - How to simulate efficiently the Hamiltonian dynamics?
  - Can we recover an approximation of the solution for ε small but finite from the vortex locations $X(t)$ evolving according to (2)?

Well-prepared initial conditions

Well-prepared initial conditions can be set up from the ansatz for a single vortex $f(r)\mathrm{e}^{\mathrm{i}\theta}$ and using [6, Lemma 14]. By inserting this ansatz in (1), we see that f_{ε,r_0} has to solve the following ODE, for a given $r_0 > 0$,

$$\frac{1}{r}\left(r f_{\varepsilon,r_0}'(r)\right)' - \frac{d^2}{r^2} f_{\varepsilon,r_0}(r) + \frac{1}{\varepsilon^2}\left(1 - |f_{\varepsilon,r_0}(r)|^2\right) f_{\varepsilon,r_0}(r) = 0,$$

with boundary conditions $f_{\varepsilon,r_0}(0) = 0$ and $f_{\varepsilon,r_0}(r_0) = 1$.



f_{ε,r_0} for various ε.

Then, define

$$\psi_\varepsilon^0(\boldsymbol{x}) = \mathrm{e}^{\mathrm{i}H(\boldsymbol{x})} \prod_{j=1}^N f_{\varepsilon,r_0}(|\boldsymbol{x} - \boldsymbol{x}_j^0|)\mathrm{e}^{\mathrm{i}d_j\theta(\boldsymbol{x}-\boldsymbol{x}_j^0)},$$

where H is some smooth harmonic function and $\theta(\boldsymbol{x} = (x,y)) = \arg(x + \mathrm{i}y)$. Finally, set accordingly

$$g(\boldsymbol{x}) = \mathrm{e}^{\mathrm{i}H(\boldsymbol{x})}\mathrm{e}^{\mathrm{i}\sum_j d_j\theta(\boldsymbol{x}-\boldsymbol{x}_j^0)}$$

so that ψ_ε^0 satisfies the boundary conditions. Note that $g : \partial\Omega \to \mathbb{S}^1$ has winding number $\sum_j d_j$. ψ_ε^0 can be seen as a smoothing of the harmonic map $\psi_\star : \Omega \to \mathbb{S}^1$ with singularities at locations X^0 with winding numbers d:

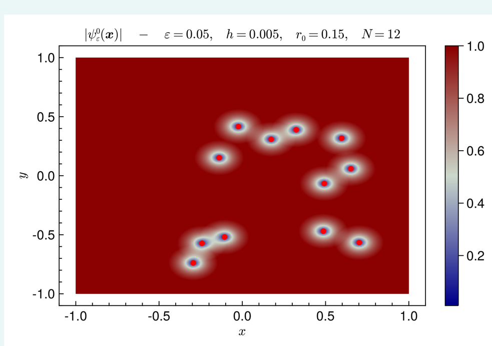
$$\psi_\star(\boldsymbol{x}) = \mathrm{e}^{\mathrm{i}H(\boldsymbol{x})}\mathrm{e}^{\mathrm{i}\sum_j d_j\theta(\boldsymbol{x}-\boldsymbol{x}_j^0)}.$$

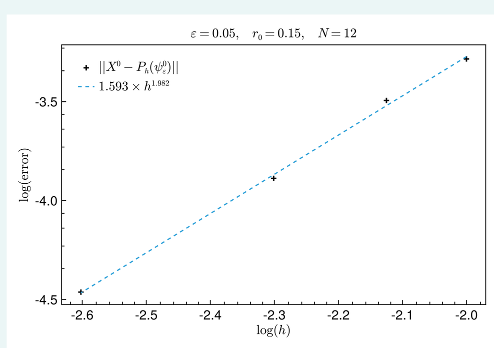
Localizing the vortices

Here is a simple algorithm, inspired from [4, 7], to locate the vortices of a wave function ψ on a triangular finite element mesh $\mathcal{T}_h$ with mesh size h.

1. Compute the winding number of all the cells using the discrete winding number formula:
$$\forall\ K \in \mathcal{T}_h, \quad w(K) = \frac{1}{2\pi}\sum_{i=1}^3 \theta(\psi(\boldsymbol{a}_{i-1}), \psi(\boldsymbol{a}_i)),$$
where $\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3 = \boldsymbol{a}_0$ are the three vertices of the cell K and $\theta(\boldsymbol{x},\boldsymbol{y}) = \theta(\boldsymbol{y}) - \theta(\boldsymbol{x})$. Build the list L_{cells} of cells that have nonzero winding number.
2. For all cells in L_{cells}, compute the approximate location of the vortex using barycentric coordinates.

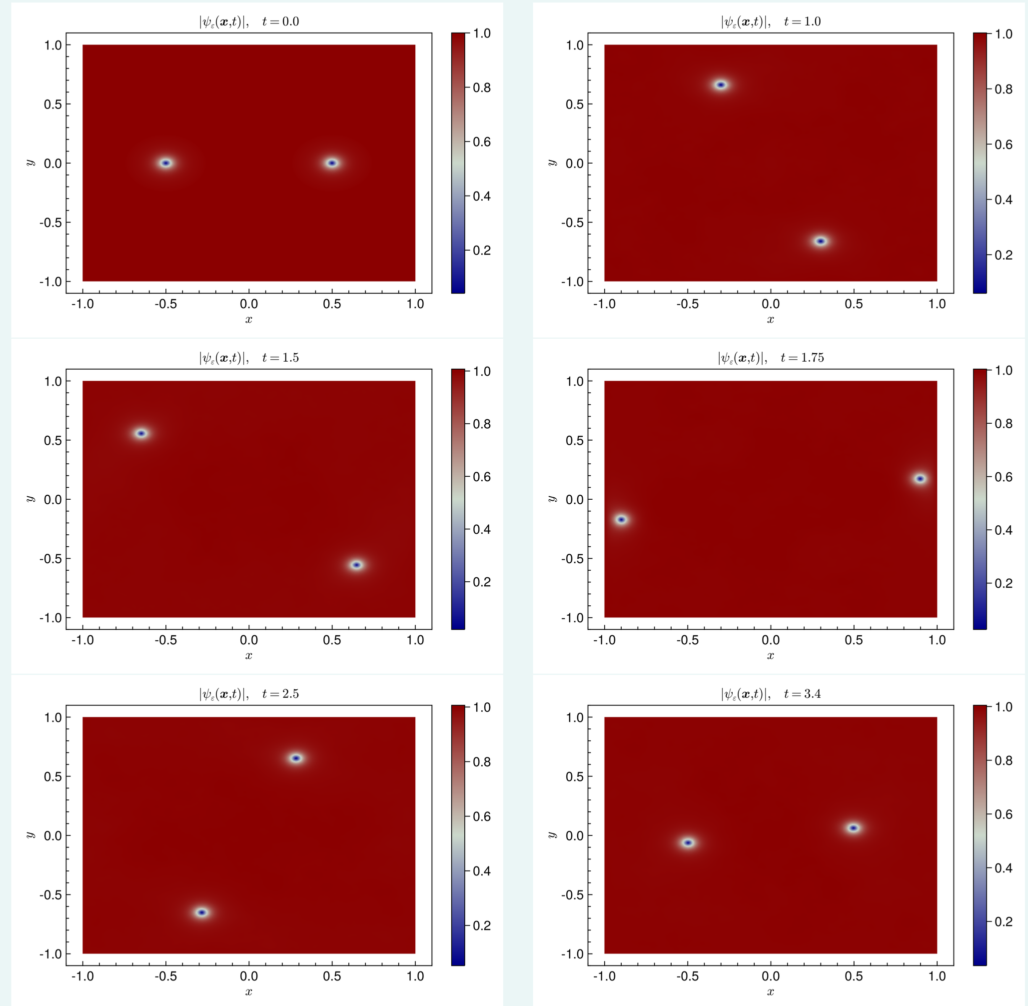
Then, such an algorithm localizes the vortices of ψ_ε^0 with accuracy h^2.





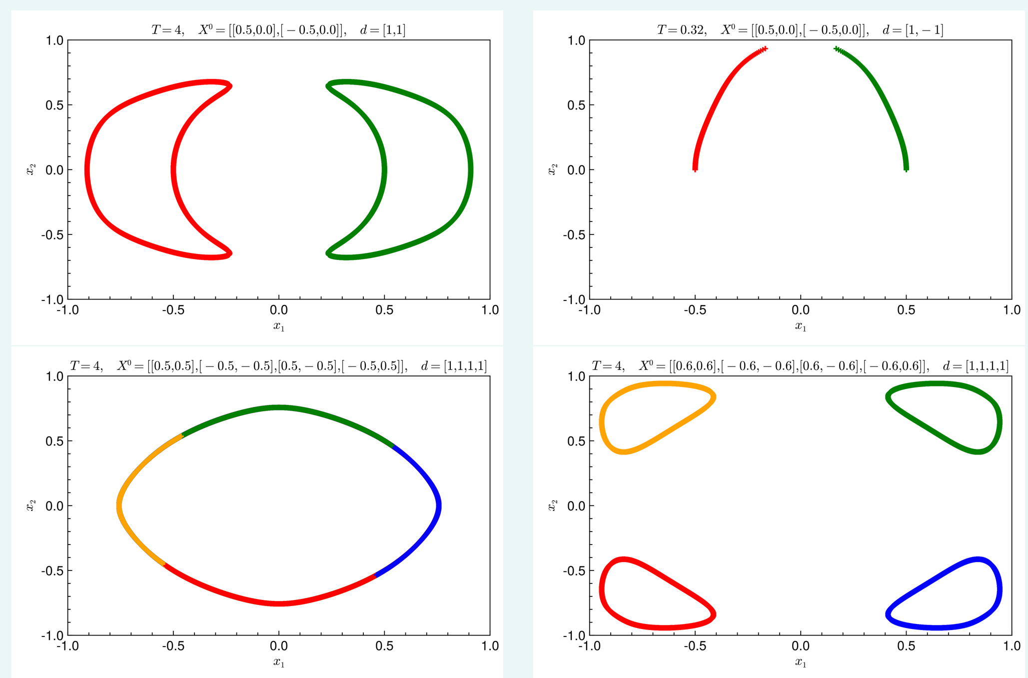
Some simulations of the PDE

Test case from [1]: vortices with identical winding numbers and $\varepsilon = 0.03$, $\Omega = [-1,1]^2$. We used the FEM and a mesh with size $h = 7.5 \cdot 10^{-3}$. The time integration is done with a Strang splitting and $\delta t = 5 \cdot 10^{-5}$.



Hamiltonian dynamics simulation

Solving the Hamiltonian system (2) requires to compute the gradient of the renormalized energy W. This implies solving a harmonic equation at each time step, where only the boundary conditions change. This can be done efficiently using an orthonormal basis of $\partial\Omega$, such as harmonic polynomials. This makes it possible to generate vortex trajectories in a few seconds (*v.s.* several hours for the resolution of the PDE above with the FEM). The plots were generated using a RK4 explicit scheme with $\delta t = 10^{-3}$ and harmonic polynomials up to degree 50.



Connections with other projects

In the past few years, progress has been made regarding the simulation of Hamiltonian dynamics with the help of machine learning and physics-enhanced neural networks [5, 8, 9]. Investigating this within the CRC in order to learn the Hamiltonian dynamics (2) from data obtained with the efficient solver we have set up so far is an interesting opportunity to connect with other projects.

References

[1] W. Bao and Q. Tang. Numerical Study of Quantized Vortex Interactions in the Nonlinear Schrödinger Equation on Bounded Domains. *Multiscale Modeling & Simulation*, 12(2):411–439, 2014.

[2] F. Bethuel, H. Brezis, and F. Hélein. *Ginzburg-Landau Vortices*. Birkhäuser Boston, Boston, MA, 1994.

[3] J. Colliander and R. Jerrard. Vortex dynamics for the Ginzburg-Landau-Schrodinger equation. *International Mathematics Research Notices*, 1998(7):333, 1998.

[4] G. Dujardin, I. Lacroix-Violet, and A. Nahas. A numerical study of vortex nucleation in 2D rotating Bose-Einstein condensates. 2022.

[5] J. Eichelsdörfer, S. Kaltenbach, and P.-S. Koutsourelakis. Physics-enhanced Neural Networks in the Small Data Regime, 2021.

[6] R. L. Jerrard and D. Spirn. Refined Jacobian Estimates and Gross–Pitaevsky Vortex Dynamics. *Archive for Rational Mechanics and Analysis*, 190(3):425–475, 2008.

[7] V. Kalt, G. Sadaka, I. Danaila, and F. Hecht. Identification of vortices in quantum fluids: Finite element algorithms and programs. 2022.

[8] V. Saz Ulibarrena, P. Horn, S. Portegies Zwart, E. Sellentin, B. Koren, and M. X. Cai. A Hybrid Approach for Solving the Gravitational N-Body Problem with Artificial Neural Networks, 2023.

[9] H. Sharma, Z. Wang, and B. Kramer. Hamiltonian Operator Inference: Physics-preserving Learning of Reduced-order Models for Canonical Hamiltonian Systems, 2021.