International PhD position
Applied and Computational Mathematics

Accurate and efficient computational methods for the HPC simulation of Bose-Einstein Condensates

Ph.D. advisors:
• Professor Xavier ANTOINE (Université de Lorraine, France)
• Professor Qinglin TANG (Sichuan University, P.R. China)
Title: Accurate and efficient computational methods for the HPC simulation of Bose-Einstein Condensates

Advisors:
Professor Xavier ANTOINE, Institut Elie Cartan de Lorraine, UMR 7502, Université de Lorraine, France & Inria SPHINX team. Email: xavierantoine@univ-lorraine.fr
Website: https://iecl.univ-lorraine.fr/membre-iecl/antoine-xavier/
Professor Qinglin TANG, College of Mathematics, Sichuan University, Chengdu, P.R. China. Email: qinglin_tang@163.com; Website: http://www.qinglin-tang-scu.com

Framework-skills-salary. We are hiring a Ph.D. student with good knowledges in applied mathematics/computational physics/scientific computing. A second-year master degree in applied mathematics or related topic is necessary to start the Ph.D thesis. The applicant must be able to speak and write correctly in english for the scientific production and the discussions with the two advisors (B2 level expected). Speaking French or Chinese is a plus but is not mandatory. The Ph.D. position is funded for at least three years. This is an international collaboration. Therefore, the Ph.D. student will spend half of his/her time in France and China. During the three first years, the income salary of the Ph.D. student will be 1800 euros (1400 euros after taxes). In addition, an important funding will help the student to move between the two countries and to participate to international conferences. Do not hesitate to contact the two advisors for further details. To apply see the footnote.

Abstract: The first scientific objective of this Ph.D. thesis concerns the development of new efficient and accurate numerical methods for computing the stationary states and dynamics of Gross-Pitaevskii equations (fast rotation; multi-component; dipolar interactions) that arise in Bose-Einstein condensation. A second objective is related to the HPC implementation of these schemes in the solver BEC2HPC. Finally, a third objective is the application of the full methodology and enriched BEC2HPC solver to simulate some simple problems related to the complex physics behind quantum turbulence.

Scientific context. Since its first experimental realization in 1995 [1, 2, 3], the Bose-Einstein Condensation (BEC) phenomena provides an incredible glimpse into the macroscopic quantum world and has opened a new era in atomic and molecular physics as well as in condensed matter physics. It regains vast interests and has been extensively studied both experimentally and theoretically [4, 5, 6, 7, 8]. In particular, future high-tech applications are expected like for example for high precision GPS, atomic lasers or quantum computers. At temperatures $T$ much smaller than the critical temperature $T_c$, the properties of a rotating BEC is well described by a macroscopic complex-valued wave function $\psi(x, t)$ whose evolution is governed by the three-dimensional (3D) Gross-Pitaevskii equation (GPE). Solving the $d$-dimensional ($d = 2$ or 3) dimensionless GPE with a rotation term $\omega L_z$ [9] leads to the following initial-value problem: for a given initial state $\psi_0$, find the complex wave function $\psi(x, t)$ solution to

\[
\begin{align*}
 i\partial_t \psi(x, t) &= \left[ -\frac{1}{2} \nabla^2 + V(x, t) - \omega L_z + \beta |\psi|^2 \right] \psi(x, t), \\
\psi(x, t = 0) &= \psi_0(x), \quad x \in \mathbb{R}^d, \quad t \geq 0,
\end{align*}
\]

where $x := (x, y, z) := (x, y)$ in 2D and $t$ are the space and time variables, respectively. Denoting by $\nabla$ the gradient operator, $\nabla^2$ is then the laplacian operator, and $V(x, t)$ is a function corresponding to the potential. The real-valued constants $\beta$ and $\omega$ respectively represent the nonlinear interaction strength and the rotating frequency. In addition, $L_z = i(y \partial_x - x \partial_y)$ is the $z$-component of the angular momentum [9]. When $\omega = 0$, the GPE is also often called nonlinear cubic Schrödinger equation. Being able to simulate BEC through the GPE is crucial since the experimental realization of a condensate is complex but also very fragile since the quantum behavior is destroyed almost instantaneously when the system interacts with the exterior (for example when imaging the BEC). Therefore, the numerical simulation of such complex structures is a serious experimental way to understand and manipulate BECs. As an

\[1\] http://doctorat.univ-lorraine.fr/fr/les-ecoles-doctorales/iaem/offres-de-these/methodes-numeriques-rapides-et-precises-pour-la
\[2\] http://team.inria.fr/bec2hpc/
\[3\] https://en.wikipedia.org/wiki/Bose%E2%80%93%Einstein_condensate
\[4\] https://www.nature.com/articles/d41586-018-05111-2
example, we provide in the frontpage (left) an example of BEC imaging in a Physics Lab where we can see the quantum vortex lattice, and the result of a computation of a 2D BEC based on numerical methods for the fast rotation case (right).

**Objectives of the Ph.D. thesis.** The goal of the Ph.D. thesis is to develop accurate and efficient numerical methods for solving the GPE and to contribute to implement the methods in a HPC solver. Most specifically, we will consider the rotating GPE (0.1) as a first model. Indeed, solving this problem is already extremely challenging, most particularly for large nonlinearities $\beta$ and fast rotations $\omega$. In these situations, the BEC has many vortices, translating the multiscale nature of the quantum problem, which are extremely delicate to capture. For the stationary states, the problem can be recast as a constrained optimization problem of the associated nonconvex and strongly nonlinear energy functional $[9]$. In particular, we are often interested in computing the ground state, which is the global minimum of the energy, or the first excited states, corresponding to higher energy local minima. Since small features must be captured, high-order discretization techniques are required. Here, we will focus on pseudospectral FFT-based methods where we have a strong expertise, preconditioned normalized gradient flows and conjugate gradients, accelerated by multi-grid algorithms. Another problem is to compute the dynamics of the GPE. Then, one has to derive high-order time and space adaptive schemes that also conserve some physical quantities like e.g. the mass or energy $[9]$. We have a strong knowledge in methods that can achieve this goal for the rotating GPE but which still need to be further investigated in a HPC (High Performance Computing) environment. Even if the rotating GPE already includes some complicated problems related to quantum physics, mathematics and parallel computing, other more advanced BEC models will be further investigated, investigating multi-components gasses and nonlocal nonlinear interactions for dipolar gasses. In addition, most of the time, open systems must be considered. For this reason (and also computational aspects), we will develop new Perfectly Matched Layer algorithms in pseudospectral techniques for simulating the unbounded characteristic of the spatial domain. Let us remark that we already have a well-developed HPC solver called BEC2HPC but it is limited to the computation of the stationary states of the 2D/3D rotating GPE. All the numerical developments during the thesis will be first written in Matlab/Python and next implemented in the BEC2HPC solver, with the help of a CNRS research engineer in HPC at IECL. Applications will be considered in quantum turbulence $[10]$. 

**References.**


