Quantum turbulence exploration using the Gross-Pitaevskii equation

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Modeling and Simulation for Quantum Condensation, Fluids and Information
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Outline

Introduction
  Quantum turbulence phenomena
  Gross-Pitaevskii equation

GPS code
  Simulation of BECs (trapping potential, rotating BECs)
  Towards QT simulations
  Quantities of interest
  Initial conditions for QT

Numerical illustrations
  Initial data from classical flow
  Initial data by manipulation of the wave function
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Quantum turbulence exploration

- Different successive projects/collaborations...
  - ANR project BECASIM (2013-2017), more focused on Bose-Einstein condensate
  - ANR project QUTE-HPC (2019-2022)
- ... involving many people from different communities
  - I. Danaila, I. Ciotir, C. Lothodé, F. L., P. Parnaudeau, V. Kalt, M. Brachet, L. Danaila, E. Lévêque, Ph.-E. Roche,
  - Collaboration with M. Kobayashi.
ANR Project QUTE-HPC: QUantum Turbulence Exploration by High-Performance Computing

Quantum Turbulence (QT):
- multi-scale, multi-physics phenomenon,
- in (super) cold systems (Bose-Einstein condensate, superfluid Helium),
- coexistence of a "normal" fluid (viscous) and a superfluid (no viscosity).
First step : GP only

Superfluid (very small scales) :

- dimensionless Gross-Pitaevskii equation (non linear Schrödinger)

\[ i \partial_t \psi = -\alpha \Delta \psi + V(x)\psi + \beta |\psi|^2 \psi - i\Omega L_z \psi \]

- GPS code (for Gross-Pitaevskii Simulator) : spectral or high-order compact FD scheme,
- \( V(x) \) : trapping potential,
- \( \alpha, \beta, \Omega \) real constants,
- \( L_z \psi = (x \partial_y \psi - y \partial_x \psi) \),
- with \(|\psi|_{\text{max}} = 1\), we have

\[ c = \sqrt{2\alpha \beta} \quad \text{speed of sound} \]
\[ \xi = \sqrt{\frac{\alpha}{\beta}} \quad \text{healing length} \]
Superfluid = fluid without viscosity?

Gross-Pitaevskii equation (for QT):

\[ i \partial_t \psi = -\alpha \Delta \psi + \beta |\psi|^2 \psi \]

Where are the hydrodynamic quantities?
Superfluid = fluid without viscosity?

Gross-Pitaevskii equation (for QT):

\[ i \partial_t \psi = -\alpha \Delta \psi + \beta |\psi|^2 \psi \]

Where are the hydrodynamic quantities?

Madelung transformation

\[ \psi = \sqrt{\rho} e^{i\theta/(2\alpha)} \]

- \( \rho = |\psi|^2 \) is the density of the fluid,
- \( u := \nabla \theta \) is the velocity,
- in other terms, we have: \( \rho u = 2\alpha \text{Im}(\psi^* \nabla \psi) \),
- recover Euler-like equations

\[ \partial_t \rho + \nabla \cdot (\rho u) = 0, \]
\[ \partial_t (\rho u) + \nabla \cdot (\rho uu) = g, \]

\( g \) more complicated than in Euler equations.
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GPS code:

- spatial: spectral method with periodic BC, or 6th order compact FD scheme (periodic or Dirichlet BC),
- real-time simulations: second order ADI time-splitting,
- imaginary-time simulations: full Newton method or semi-implicit backwards Euler,
- two levels of parallelization: MPI and OpenMP,
- pencil distribution of the grid,
- 2D (OpenMP) or 3D (MPI/OpenMP).
Either solve the (real) time dependent problem

\[ i \partial_t \psi = -\alpha \Delta \psi + V(x)\psi + \beta |\psi|^2 \psi - i\Omega L_z \psi \]

or the stationary state problem (search for ground states) : find \( \psi \) with \( \|\psi\| = 1 \) such that

\[ -\alpha \Delta \psi + V(x)\psi + \beta |\psi|^2 \psi - i\Omega L_z \psi = \mu(\psi)\psi, \]

\( \mu \) is the chemical potential.

Or 3D cases "VisIt a giant vortex" (not as big as the "Rain Vortex" though).
3D case with $512^3$, $1024^3$ and $2048^3$ grid points; [256 : 64536] MPI processes and 1, 2 or 4 OpenMP threads. Top left: scalability of the code. Bottom left: efficiency of the code. Top right: speedup results. Bottom right: results of the hybrid code MPI-OpenMP.
What kind of diagnostics?

**Energy related**

\[
E_{\text{kin}} = \frac{1}{2} \int_{\Omega} \rho |\mathbf{u}|^2 = E_{\text{kin}}^i + E_{\text{kin}}^c
\]

\[
E_q = 2\alpha^2 \int_{\Omega} |\nabla (\sqrt{\rho})|^2, \quad E_{\text{int}} = \alpha \beta \int_{\Omega} (\rho - 1)^2
\]

- accurately compute these energies,
- time evolution, spectra.

**Structure functions**

\[
S_{\parallel}^p (r) = \int \left( (\mathbf{v}(x + r\mathbf{e}_x) - \mathbf{v}(x)) \cdot \mathbf{e}_x \right)^p
\]

(or replace \( \mathbf{e}_x \) by any unit vector).

- comparisons with classical turbulence,
- helicity,
- conserved quantities?
What kind of initial conditions?

Artificial initial condition

- use a near solution of GP equation to create turbulence (initial vortex tangle),
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- use random phase in $\psi$ without vortex to see QT generation.
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**Mimicking classical flows**
- ARGLE procedure, given $u^{adv}$ a "target velocity"
- Gradient flow method: introduce imaginary-time (pseudo time) and solve the following problem until steady state is achieved:

\[
\frac{\partial}{\partial t} \phi = \alpha \Delta \phi - \beta |\phi|^2 \phi + \left( \beta - \frac{||u^{adv}||^2}{4\alpha} \right) \phi + i \frac{u^{adv} \cdot \nabla \phi}{V(x)} = 0.
\]

- Use $\phi$ as initial state for real-time GP.
Imaginary time scheme

\[ \partial_t \phi = \alpha \Delta \phi - \beta |\phi|^2 \phi + \left( \beta - \frac{\|u^{adv}\|^2}{4\alpha} \right) \phi + iu^{adv} \cdot \nabla \phi = 0. \]

is equivalent to minimizing the following (modified) energy:

\[ \mathcal{J}(\phi) := \int_{\Omega} \alpha \left| \nabla \phi - i \frac{u^{adv}}{2\alpha} \phi \right|^2 + \frac{\beta}{2} \left( |\phi|^2 - 1 \right)^2. \]
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With the hydrodynamics analogy:

\[ \phi = \sqrt{\rho} \exp(i\theta/(2\alpha)), \quad u = \nabla \theta, \]

\[ \nabla \phi = \nabla (\sqrt{\rho}) \exp(i\theta/(2\alpha)) + i \frac{\phi}{2\alpha} u \]

\[ \mathcal{J}(\rho, u) = \int_{\Omega} \alpha \left| \nabla (\sqrt{\rho}) \right|^2 + \frac{1}{4\alpha} \rho \left| u - u^{adv} \right|^2 + \frac{\beta}{2} (\rho - 1)^2 \]

- suitable (in principle for any \( u^{adv} \), even not divergence-free),
- unconstrained minimization problem, hence no renormalization,
- competition between a uniform distribution \( \rho \equiv 1 \) and a phase accommodating \( u^{adv} \).
Imaginary time scheme

Originally in GPS:

- Semi-implicit backwards Euler (Bao et al.)

\[
\frac{\phi_{n+1} - \phi_n}{\delta t} - \alpha \Delta \phi_{n+1} + \beta |\phi_n|^2 \phi_{n+1} - \beta \phi_n + \frac{\|u^{adv}\|^2}{4\alpha} \phi_{n+1} - iu^{adv} \cdot \nabla \phi_{n+1} = 0.
\]

- Full Newton method

\[
\frac{\phi_{n+1} - \phi_n}{\delta t} - \alpha \Delta \phi_{n+1} + \beta |\phi_{n+1}|^2 \phi_{n+1} - \beta \phi_{n+1} + \frac{\|u^{adv}\|^2}{4\alpha} \phi_{n+1} - iu^{adv} \cdot \nabla \phi_{n+1} = 0.
\]

- Systems preconditionned by diagonal terms in physical space (Antoine & Dubosq),

- + renormalization (for BEC).

For our cases, sufficient to use simpler semi-implicit scheme, and no renormalization:

\[
\frac{\phi_{n+1} - \phi_n}{\delta t} - \alpha \Delta \phi_{n+1} + \beta |\phi_n|^2 \phi_n - \beta \phi_n + \frac{\|u^{adv}\|^2}{4\alpha} \phi_{n} - iu^{adv} \cdot \nabla \phi_{n} = 0.
\]
Real time evolution

- second order Strang splitting in time,

\[ \psi_{n+1} = S \left( \frac{\Delta t}{2}, i\alpha \Delta \right) S(\Delta t, N) S \left( \frac{\Delta t}{2}, i\alpha \Delta \right) \psi_n, \]

\( S(\cdot, H) \) is the exact integrator associated with operator \( H \).

- no dealiasing,
Real time evolution

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- impulsion not conserved (sorry Marc).
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Taylor-Green flow: imaginary time procedure

$u^{adv}$ defined by:

$$u^{adv} = \begin{pmatrix}
\sin(x) \cos(y) \cos(z) \\
\cos(x) \sin(y) \cos(z) \\
0
\end{pmatrix}$$

$\psi|_{t=0}$ contains vortices with winding number 3.

ref. [Nore, Abid & Brachet, 1997]
<table>
<thead>
<tr>
<th></th>
<th>$E_k^i$</th>
<th>$E_k^c$</th>
<th>$E_q$</th>
<th>$E_i$</th>
</tr>
</thead>
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<td>GPS</td>
<td>0.129 567</td>
<td>0.000 272</td>
<td>0.007 804 1</td>
<td>0.013 0279</td>
</tr>
<tr>
<td>MB</td>
<td>0.129 570</td>
<td>0.000 272</td>
<td>0.007 804</td>
<td>0.013 028</td>
</tr>
</tbody>
</table>

Energies computed at the end of imaginary time run: GPS computation (top) vs. data from M. Brachet (bottom).
Unsteady Taylor-Green
Time evolution of kinetic energy

Left: incompressible kinetic energy $E_{kin}^i$. Right: compressible kinetic energy $E_{kin}^c$. 
Energy and structure functions

Left: Spectra of $E_{kin}^i$ for different times. Right: Structure function of order 2.

$\epsilon$ used in the left picture is defined as for the classical turbulence as

$$\epsilon = - \frac{dE_{kin}^i}{dt}.$$ 

Encouraging results, but we need to make sure it works for others physical quantities of interest, e.g. helicity.
ABC flow : check helicity statistics

$u^{adv}$ defined by:

$$
\begin{align*}
    u^{adv} &= \left( 
    B(\cos(y) + \cos(2y)) + C(\sin(z) + \sin(2z)) 
    
    C(\cos(z) + \cos(2z)) + A(\sin(x) + \sin(2x)) 
    
    A(\cos(x) + \cos(2x)) + B(\sin(y) + \sin(2y))
    \right) \\
    \psi_{t=0} &= e^{\theta_0} \text{ with } \theta_0 = \left[ \frac{u^{adv}_x}{2\alpha} \right] x + \left[ \frac{u^{adv}_y}{2\alpha} \right] y + \left[ \frac{u^{adv}_z}{2\alpha} \right] z
    \end{align*}
$$

- No vortex at beginning of imaginary time procedure,
- Flow with helicity,
- Control on the Mach number by changing the values of $A$, $B$ and $C$.

ref. [di Leoni, Mininni & Brachet, 2017]

Relative fluctuation of the ARGLE energy

$$
\frac{|E_V(\phi^{n+1}) - E_V(\phi^n)|}{\Delta t E_V(\phi^n)}.
$$

QT with GP (Singapore, 11/2019) (23/35)
Unsteady ABC
Energy and helicity

[Graphs showing energy and helicity plots with various time intervals and length scales.]
Mass conservation is perfect,

Energy conservation looks nice.

For flows mimicking classical flows, QT looks like CT.
Random vortex ring pairs (RVR)

\[ \psi_0(\mathbf{x}) = \prod_{i=1}^{N_{vor}} \psi_i(\mathbf{x}, \text{dir}) \]

\[ \psi_R(x, y, z, R) = f \left( \sqrt{(r - R)^2 + z^2} \right) e^{\pm i \tan^{-1} \left( \frac{z}{r - R} \right)}, \]

\[ f(r) = \sqrt{\frac{a_1(r/\xi)^2 + a_2(r/\xi)^4}{1 + b_1(r/\xi)^2 + a_2(r/\xi)^4}}, \]

\[ a_1 = \frac{73 + 3\sqrt{201}}{352}, \quad a_2 = \frac{6 + \sqrt{201}}{528}, \quad b_1 = \frac{21 + \sqrt{201}}{96}, \]

\[ r = \sqrt{x^2 + y^2} \]

- \( \psi_i \) creates a pair of opposite vortex rings (radius of the ring \( L/4 \), inter-vortex distance \( L/4 \), radius of vortex \( \xi \)),

\[ \psi_i(x, z) = \psi_R(x, y, z - L/8, L/4) \psi_R^*(x, y, z + L/8, L/4) \]

- mirror to make \( \psi_i \) periodic, and rotate to have a vortex in any cartesian direction.
Random vortex ring pairs (RVR)

\[ \psi_0(x) = \prod_{i=1}^{N_{vor}} \psi_i(x, \text{dir}) \]

\[ \psi_R(x, y, z, R) = f \left( \sqrt{(r - R)^2 + z^2} \right) e^{\pm i \tan^{-1} \left( \frac{z}{r - R} \right)}, \]

\[ f(r) = \sqrt{\frac{a_1 (r/\xi)^2 + a_2 (r/\xi)^4}{1 + b_1 (r/\xi)^2 + a_2 (r/\xi)^4}}, \]

\[ a_1 = \frac{73 + 3\sqrt{201}}{3\sqrt{201}} \quad 6 + \sqrt{201}, \quad b_1 = \frac{21 + \sqrt{201}}{96}, \]

\[ r = \sqrt{x^2} \]

- \( \psi_i \) creates a pair of opposite vortex rings (radius of the ring \( L/4 \), inter-vortex distance \( L/4 \), radius of vortex \( \xi \)),

\[ \psi_i(x, z) = \psi \quad \text{if} \quad y, z + L/8, L/4 \]

- mirror to make \( \psi_i \) periodic, and rotate to have a vortex in any cartesian direction.
QT seem to appear at early stages \((t < 3)\),

- Dissipation effect for longer times \(E_{\text{kin}}^c\) becomes dominant over \(E_{\text{kin}}^i\).
Conservation of impulse?

Time evolution of \( \int_{\Omega} \rho u_x \) for 4 different runs:

1. \( N_x = 64, \xi k_{max} \approx 2, \Delta t = 0.001 \),
2. \( N_x = 128, \xi k_{max} \approx 4, \Delta t = 0.0005 \),
3. \( N_x = 128, \xi k_{max} \approx 4, \Delta t = 0.00025 \),
4. \( N_x = 256, \xi k_{max} \approx 8, \Delta t = 0.00025 \),
Smooth random phase

\[ \psi_0(x) = \exp(i\theta), \quad \theta \in [-A; A]. \]

- \( \theta \) generated from 64 random values: smoothed by cubic splines,
- \textbf{at } \( t = 0 \), no vortex!
- cubic box of length \( 2\pi \),
- periodic BC,
- choice of \( A \) controls Mach number.
- Vortices are created from random phase,
- QT seem to appear at early stages ($t < 1$),
- Dissipation effect for longer times.
Perspectives

This work was performed using computing resources of CRIANN (Normandie)

- GPS will be able to run interesting cases of QT,
- resolution up to $4096^3$,
- good agreement with other codes (MK, MB),
- good agreement with existing results (ABC flow or Taylor-Green),
- energy conservation is satisfactory for small time steps,
- norm is exactly conserved,
- impulsion not conserved.

A lot of ongoing work :

- structure function : computation OK, but may require averaging,
- total length of vortices is not computed accurately,
- effect of Mach number ?
- links between QT and CT ?
- how to integrate GP+NS ? (at different scales)
Thank you!
Structure functions of order 3 and 4

![Graph of structure functions for order 3 and 4, showing different scales and data points for various times.](image-url)