Numerical simulation of Bose-Einstein Condensates based on Gross-Pitaevskii Equations

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Funded by ANR BECASIM

Conference in Honor of Abderrahmane BENDALI
12th-14th december 2017

Outline

What is a BEC

Definition of a BEC

A Bose-Einstein condensate (BEC) is a state of matter of a dilute gas of bosons cooled to temperatures very close to absolute zero. Under such conditions, a large fraction of bosons occupy the lowest quantum state, at which point microscopic quantum phenomena, particularly wavefunction interference, become apparent. A BEC is formed by cooling a gas of extremely low density, about one-hundred-thousandth the density of normal air, to ultra-low temperatures.

Expected applications to come

- Atom lasers
- High precision GPS
- Quantum computers...

Figures in the history of BECs

Predicted by Satyendra Nath Bose and Albert Einstein (1924-25).

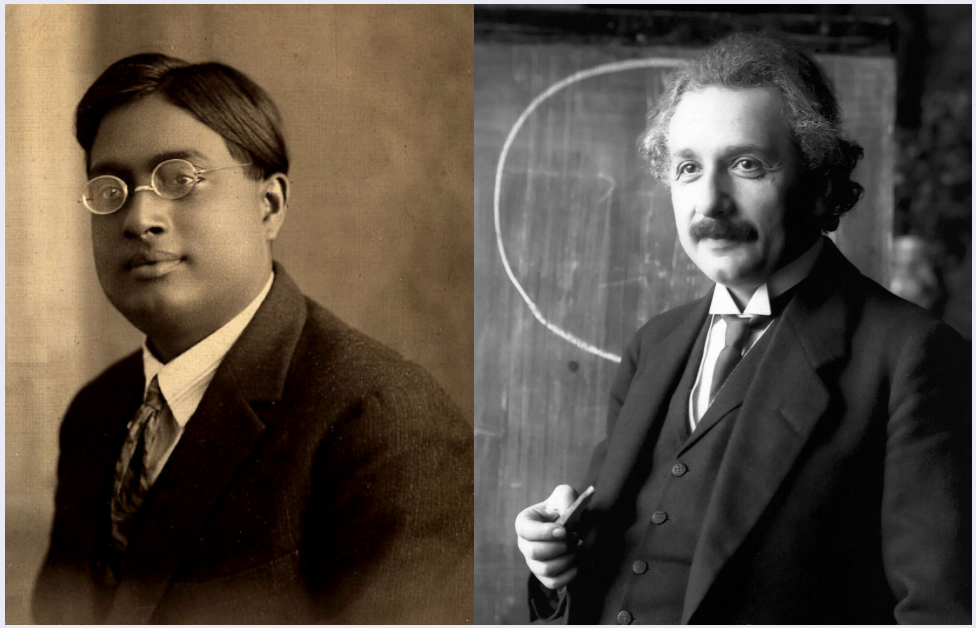

Figure: Bose and Einstein.

Figures in the history of BECs

First experiments (1995) by Cornell, Wieman (Boulder) and Ketterle (MIT) who received the 2001 Nobel Prize in Physics

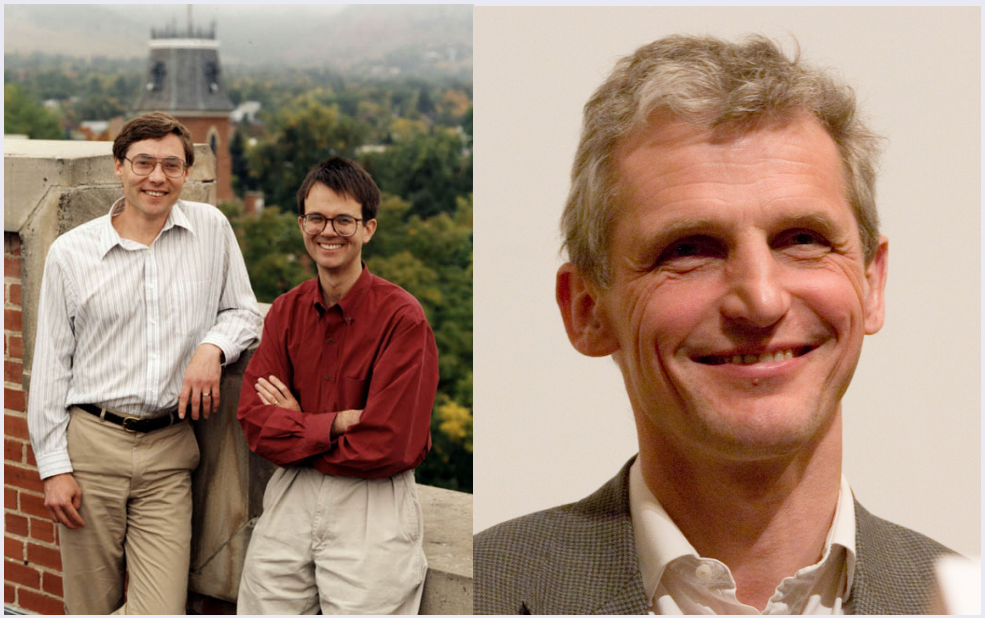

Figure: Wieman, Cornell and Ketterle.

Models

Mathematical modeling

- Different mathematical models to describe the complex physics behind BECs.[a] [b]
- Here, we consider the Gross-Pitaevskii Equation (GPE) which is an approximation model for BECs based on averaging

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[a] L. Pitaevskii & S. Stringari, Bose-Einstein Condensation, Oxford Science Publication, 2003.

[b] C.J. Pethick & H. Smith, Bose-Einstein Condensation in Dilute Gases, Cambridge University Press, 2001.

Figures in the history of BECs

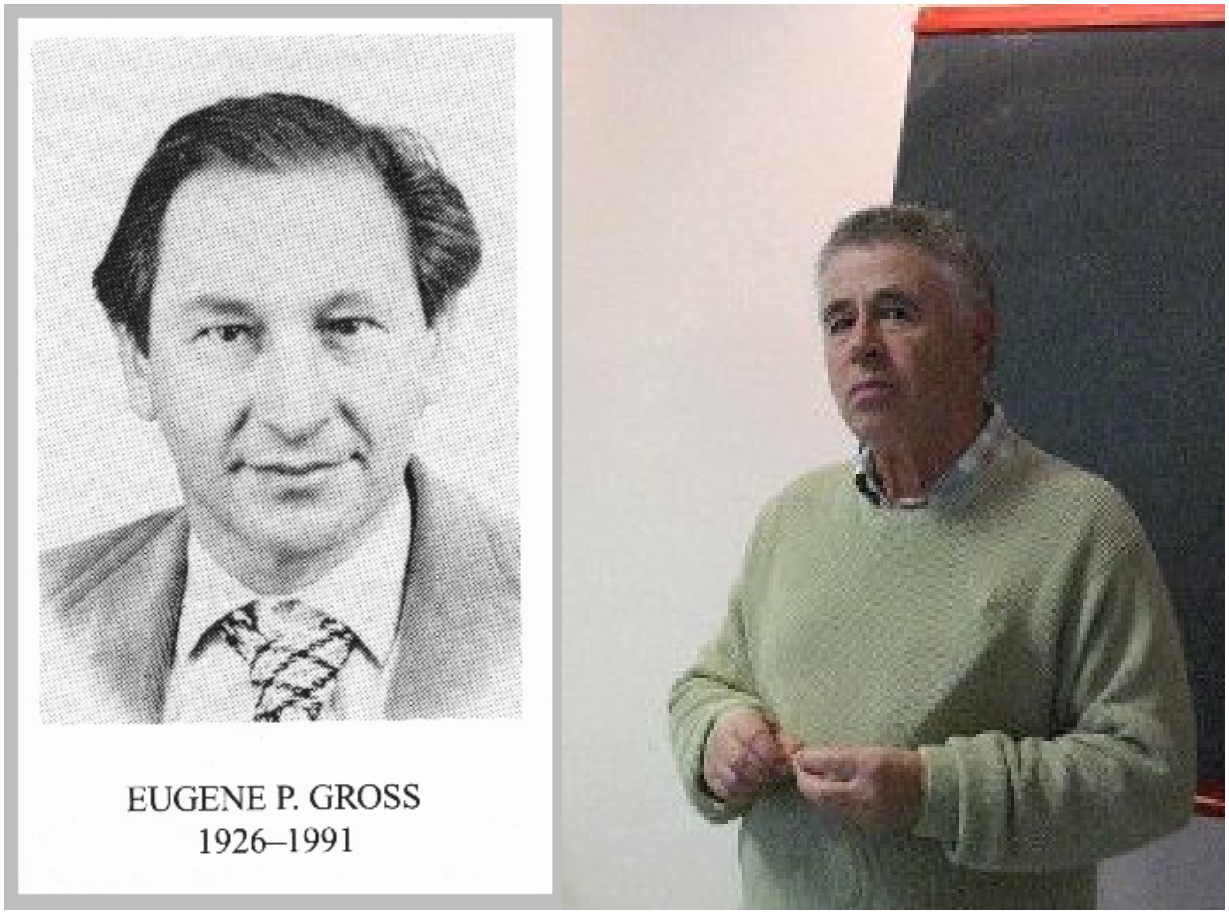

Figure: Gross and Pitaevskii.

Why numerics?

Motivations for developing numerical methods

- These developments are now growing rapidly in theoretical and experimental physics because of potential long term revolutionary applications (cold atoms lasers, quantum computers)
- The numerical simulations are then extremely important for predicting the behavior of BECs but also challenging because of the complexity of the phenomenon and the fact that it is almost impossible to compare to experimental results
- In particular, a BEC is extremely fragile in an experimental setting because it can easily be affected through exchanges with the exterior environment, loosing then its interesting features
- Here we try to focus on problems related to BEC in rapid rotation and for strong nonlinearities where giant quantized vortices (topological defects) are created

Giant vortex creation: Abrikosov lattice

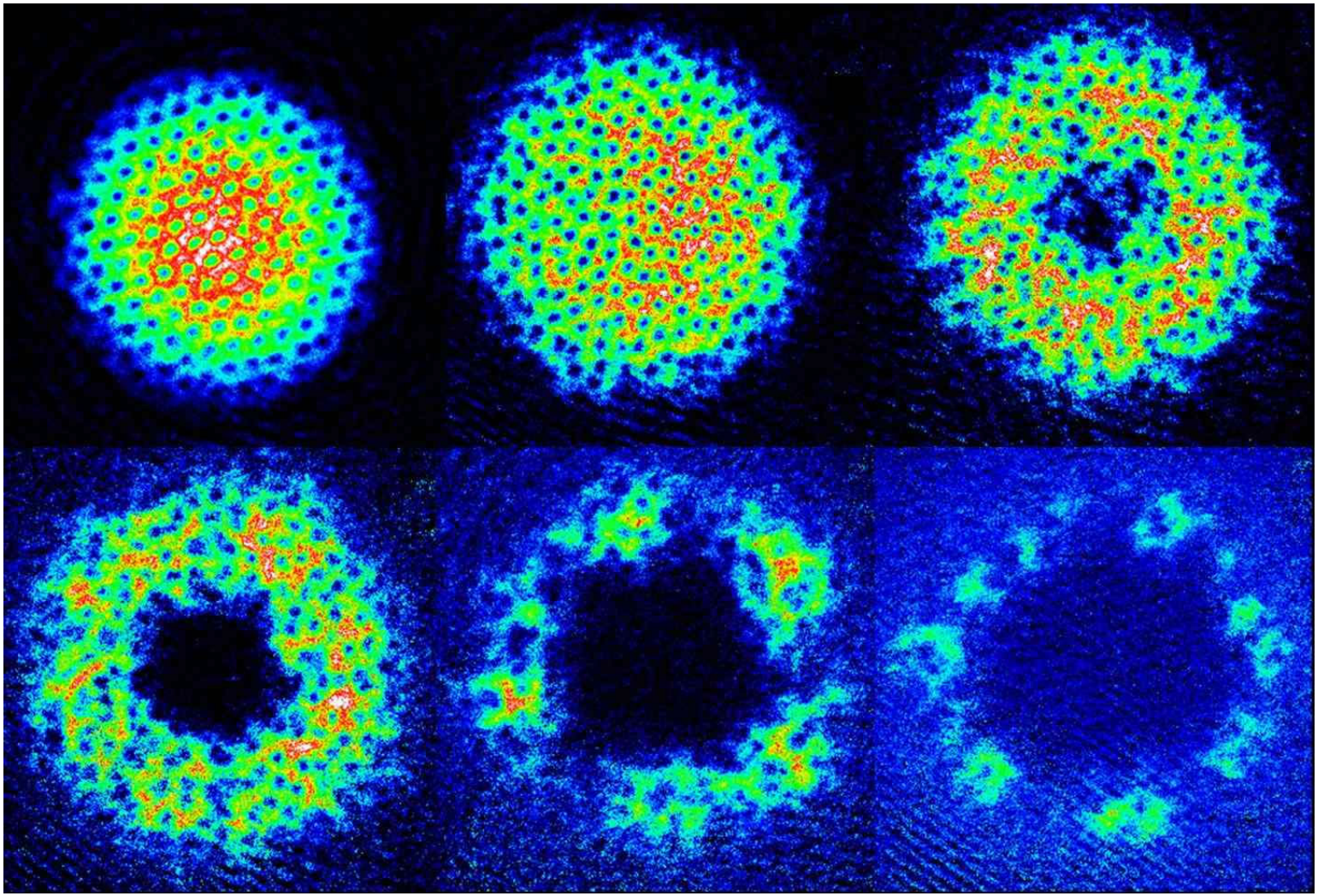

Figure: BEC under rapid rotation (Cornell group, 2010).

Time-dependent GPE with rotating term

A possible model for BECs is the (normalized) GP Equation

Time-dependent GPE with rotating term

$$i\partial_t \psi(\mathbf{x},t) = -\frac{1}{2}\Delta\psi(\mathbf{x},t) + V(\mathbf{x})\psi(\mathbf{x},t) + \eta f(|\psi(\mathbf{x},t)|)\psi(\mathbf{x},t) \\ -\boldsymbol{\Omega}\cdot\mathbf{L}\psi(\mathbf{x},t), (\mathbf{x},t) \in \mathbb{R}^d \times \mathbb{R}^{*+}, \tag{2.1}$$

where

- ψ is the condensate wave function, $d = 2, 3$,
- the Laplace operator is defined as: $\Delta = \nabla^2$, where $\nabla := (\partial_x, \partial_y, \partial_z)^t$ is the gradient operator
- the spatial variable is $\mathbf{x} = (x, y, z)^t \in \mathbb{R}^3$
- for 2d problems we have $\nabla := (\partial_x, \partial_y)^t$ and $\mathbf{x} = (x, y)^t \in \mathbb{R}^2$
- the time is t.

Time-dependent GPE with rotating term

Time-dependent GPE with rotating term

$$i\partial_t\psi(\mathbf{x},t) = -\frac{1}{2}\Delta\psi(\mathbf{x},t) + V(\mathbf{x})\psi(\mathbf{x},t) + \eta f(|\psi(\mathbf{x},t)|)\psi(\mathbf{x},t) \\ -\boldsymbol{\Omega}\cdot\mathbf{L}\psi(\mathbf{x},t), (\mathbf{x},t) \in \mathbb{R}^d \times \mathbb{R}^{*+}, \tag{2.2}$$

where

- Function V is the external confining potential (for example harmonic) (could also be time-dependent in some cases)

Time-dependent GPE with rotating term

Time-dependent GPE with rotating term

$$i\partial_t\psi(\mathbf{x},t) = -\frac{1}{2}\Delta\psi(\mathbf{x},t) + V(\mathbf{x})\psi(\mathbf{x},t) + \eta f(|\psi(\mathbf{x},t)|)\psi(\mathbf{x},t) \\ -\boldsymbol{\Omega}\cdot\mathbf{L}\psi(\mathbf{x},t), (\mathbf{x},t) \in \mathbb{R}^d \times \mathbb{R}^{*+}, \tag{2.3}$$

where

- Parameter η is the nonlinearity strength describing the interaction between atoms of the condensate. This parameter is related to the s-scattering length (a_s) and is positive for a repulsive interaction and negative for attractive interactions.
- Function f describes the nonlinearity arising in the problem, which is fixed e.g. to the cubic case: $f(|\psi|) = |\psi|^2$ (but other cases could be considered like e.g. cubic-quintic problems or integral nonlinearities for dipolar gazes).

Time-dependent GPE with rotating term

Time-dependent GPE with rotating term

$$i\partial_t\psi(\mathbf{x},t) = -\frac{1}{2}\Delta\psi(\mathbf{x},t) + V(\mathbf{x})\psi(\mathbf{x},t) + \eta f(|\psi(\mathbf{x},t)|)\psi(\mathbf{x},t) \\ -\boldsymbol{\Omega}\cdot\mathbf{L}\psi(\mathbf{x},t), (\mathbf{x},t) \in \mathbb{R}^d \times \mathbb{R}^{*+}, \tag{2.4}$$

where

- For vortices creation, a rotating term is added. The vector $\boldsymbol{\Omega}$ is the angular velocity vector and the angular momentum is $\mathbf{L} = (p_x, p_y, p_z)^t = \mathbf{x} \wedge \mathbf{P}$, with the momentum operator $\mathbf{P} = -i\nabla$. In many situations and all along the talk, the angular velocity is such that $\boldsymbol{\Omega} = (0, 0, \omega)^t$ leading to

$$L_x = 0, L_y = 0, L_z = -i(x\partial_y - y\partial_x). \tag{2.5}$$

Time-dependent GPE with rotating term

Invariants

- The mass:

$$N(\psi) = \int_{\mathbb{R}^d} |\psi(\mathbf{x}, t)|^2 d\mathbf{x} = \int_{\mathbb{R}^d} |\psi(\mathbf{x}, 0)|^2 d\mathbf{x} = ||\psi||_0^2 = 1, \tag{2.6}$$

  for $t > 0$, where $||\psi||_0$ is the $L^2(\mathbb{R}^d)$-norm of ψ.

- The energy (for a cubic nonlinearity here) is

$$E(\psi) = \int_{\mathbb{R}^d} \frac{1}{2}|\nabla\psi|^2 + V|\psi|^2 + \frac{1}{2}\eta|\psi|^4 - \omega\,\mathrm{Re}\left(\psi^* L_z \psi\right) d\mathbf{x} \tag{2.7}$$

  where ψ^* is the conjugate of ψ. Then the energy for the non rotating part is conserved and sometimes the whole energy

GPE equation with rotating term

Questions here before considering the dynamics: computing the stationary states

- Need for a fast, accurate and robust method for computing the stationary states
- The numerical methods can be adapted to more general GPEs
- Computing stationary solutions corresponds to stable/metastable physical solutions (ground states, excited states)
- In the sequel, we are also interested in the question of considering strong general nonlinearities as well as fast rotations: much more complicate to obtain numerically

The second question is then: what is the real dynamics of a BEC through the GPE (not discussed in the talk)

- High resolution schemes, efficient,...
- Need to preserve the physical invariants (mass, energy,...)

Notations/ground states/rotating GPE*

Ground states/rotating GPE

The minimization problem is the following: find $\phi \in L^2(\mathbb{R}^d)$ such that

$$\phi \in \underset{\|\phi\|=1}{\arg\min}\, E(\phi). \tag{3.1}$$

We write $\|\phi\| = \int_{\mathbb{R}^d} |\phi|^2$ for the standard L^2-norm and the energy functional E is defined by

$$E(\phi) = \int_{\mathbb{R}^d} \left[\frac{1}{2}|\nabla\phi|^2 + V(\mathbf{x})|\phi|^2 + \frac{\eta}{2}|\phi|^4 - \omega\phi^* L_z \phi \right]$$

*with A. Levitt and Q. Tang, JCP 2017

Notations/ground states/rotating GPE

First-order derivative of the energy

A direct computation leads to

$$\nabla E(\phi) = 2H_\phi \phi, \quad \text{with} \quad H_\phi = -\frac{1}{2}\nabla^2 + V + \eta|\phi|^2 - \omega L_z$$

the mean-field Hamiltonian.

Notations

We introduce

- $\mathcal{S} = \{\phi \in L^2(\mathbb{R}^d), \|\phi\| = 1\}$ as the spherical manifold associated to the normalization constraint.
- Its tangent space at a point $\phi \in \mathcal{S}$ is

$$T_\phi \mathcal{S} = \{h \in L^2(\mathbb{R}^d), \mathrm{Re}\,\langle \phi, h\rangle = 0\}$$

- The orthogonal projection onto this space is given by

$$M_\phi h = h - \mathrm{Re}\,\langle \phi, h\rangle\, \phi$$

Notations/ground states/rotating GPE

First-order condition

The Euler-Lagrange equation (1st-order necessary condition) associated with the problem (3.1) states that, at a minimum $\phi \in \mathcal{S}$, the projection of the gradient onto the tangent space is zero, which is equivalent to

$$H_\phi \phi = \lambda \phi,$$

where $\lambda = \langle H_\phi \phi, \phi \rangle$ is the Lagrange multiplier associated to the spherical constraint.

First-order condition/eigenvalue problem

Therefore, the minimization problem can be seen as a nonlinear eigenvalue problem.

Imaginary Time Method (ITM) (Conjugate Normalized Gradient Flow)

ITM: Principle

- Solve the GPE in imaginary times through the gradient flow

$$\partial_t \phi = -\frac{1}{2} M_\phi \nabla E(\phi) = -(H_\phi \phi - \lambda(\phi)\phi). \qquad (4.1)$$

- The oscillatory behavior of the eigenmodes of the Schrödinger equation is damped thus decreasing the energy.
- The Lagrange multiplier λ ensures $\|\phi\| = 1$
- We consider the following semi-implicit Backward Euler (BE) scheme (Bao & Du, 2004)

$$\frac{\widetilde{\phi}^{\mathsf{BE}}_{n+1} - \phi_n}{\Delta t} = -(H\widetilde{\phi}^{\mathsf{BE}}_{n+1} - \lambda(\phi_n)\phi_n),$$

Imaginary Time Method (ITM) (CNGF)

ITM: discretization and solution

- This discretization decreases the energy when $\Delta t > 0$ is small enough, but does not preserve the norm $\rightarrow$ followed by a projection step

$$\phi_{n+1} = \frac{\widetilde{\phi}_{n+1}}{||\widetilde{\phi}_{n+1}||}.$$

- To be combined with the PseudoSpectral FFT-based discretization (= BESP), the solution to the linear system (implicit scheme) for each n needs a preconditioned iterative MINRES with the tuning parameter Δt that can be small and not easy to fix[a]
- Stopping criterion: we always use

$$\mathcal{E}_{\text{err}}^{n} := |E(\phi_{n+1}) - E(\phi_n)| \leq \varepsilon$$

which is more adapted for rotating BEC (to include the non uniqueness of the minimum up to a rotation) ($\varepsilon = 10^{-12}$)

[a] X.A. and R. Duboscq, JCP 2014

Optimization on manifolds

Nonlinear gradient/conjugate gradients on manifolds

- The previous approach is based on the point of view of discretizing a PDE and may not converge, or converge slowly for strongly nonlinear problems and for high rotations (since Δt must be small)
- Nevertheless, the problem can also be solved as an optimization problem on a manifold (because of the normalization constraint)
- Such optimization techniques are developed since many years (and applied for example in electronic structure computations since about 20 years) but not investigated for the GPE
- Here, we apply these methods (nonlinear gradient/conjugate gradient) which are accelerated by a preconditioner P

Nonlinear Preconditioned Gradient (PG) method

Formulation

- An iteration is given by (with $\lambda_n = \lambda(\phi_n)$)

$$\widetilde{\phi}_{n+1} = \phi_n - \alpha_n P\left(H_{\phi_n}\phi_n - \lambda_n\phi_n\right), \quad \phi_{n+1} = \widetilde{\phi}_{n+1} / \left\|\widetilde{\phi}_{n+1}\right\|, \tag{5.1}$$

- which can be recast as

$$\phi_{n+1} = \cos(\theta_n)\phi_n + \sin(\theta_n)\frac{p_n}{\|p_n\|}, \quad p_n = M_{\phi_n} d_n, \tag{5.2}$$

where $d_n = -Pr_n$ is the descent direction, equals to the negative of the preconditioned residual $r_n = H_{\phi_n}\phi_n - \lambda(\phi_n)\phi_n$. The equations (5.1) and (5.2) are equivalent when θ_n or α_n is small enough, with a one-to-one correspondance between θ_n and α_n. To first order, we have: $\alpha_n = \theta_n \|p_n\|$.

Nonlinear Preconditioned Gradient (PG) method

Formulation

- With a constant α_n, and $P = I$ (identity) one gets the Forward Euler approximation of ITM
- Computation of θ_n: various approaches are available but we retain here, after a Taylor's expansion of the energy,

$$\theta_n^{\text{opt}} = \frac{-\operatorname{Re}\langle \nabla E(\phi_n), p_n \rangle \, \|p_n\|}{\operatorname{Re}\left[\nabla^2 E(\phi_n)[p_n, p_n] - \lambda_n\right]}, \tag{5.3}$$

combined with some tests to check that the energy decays

Nonlinear Preconditioned Conjugate Gradient (PCG) method

Formulation

- The PCG method is very similar to PG, but uses an update rule of the form

$$d_n = -Pr_n + \beta_n p_{n-1} \tag{5.4}$$

  instead of simply $d_n = -Pr_n$ (parallel version for linear systems).

- β_n : Polak-Ribière choice $\beta_n = \max(\beta_n^{\mathrm{PR}}, 0)$, where

$$\beta_n^{\mathrm{PR}} = \frac{\langle r_n - r_{n-1}, Pr_n \rangle}{\langle r_{n-1}, Pr_{n-1} \rangle}. \tag{5.5}$$

  We use $\beta_n = \max(\beta_n^{\mathrm{PR}}, 0)$, which is equivalent to restarting the CG method (simply using a gradient step) when $\beta_n^{\mathrm{PR}} < 0$ and is a standard choice in nonlinear CG methods.

Preconditioners

Probably more important than the iterative method itself!

- Kinetic energy preconditioner:

$$P_\Delta = (\alpha_\Delta - \Delta/2)^{-1},$$

with

$$\alpha_\Delta = \widetilde{\lambda}_n := \int \left(\frac{1}{2} |\nabla \phi_n|^2 + V|\phi_n|^2 + \eta |\phi_n|^4 \right) d\mathbf{x} > 0$$

which is positive and represents the characteristic energy of ϕ_n.

- Potential energy preconditioner (with $\alpha_V = \widetilde{\lambda}_n$):

$$P_V = (\alpha_V + V + \eta|\phi_n|^2)^{-1}.$$

- Symmetrized combined preconditioner that is the most robust

$$P_{\mathrm{C}} = P_V^{1/2} P_\Delta P_V^{1/2}.$$

Setting

- We only present $\mathrm{PCG_C}$: PCG with combined preconditioner P_{C} which outperforms all the other methods (e.g. 100 times faster on complicate problems than BESP)
- Harmonic-plus-quartic potential for $d = 3$

$$V(\mathbf{x}) = (1-\alpha) \sum_{\nu=x,y,z} \gamma_\nu \nu^2 + \frac{\kappa\,(x^2+y^2)^2}{4} + \gamma_z^2\, z^2$$

- Cubic nonlinearity and initialization by the Thomas-Fermi ansatz
- 2D: $\gamma_x = \gamma_y = 1$ ($\gamma_z = 0$), $\alpha = 1.2$ and $\kappa = 0.3$. The computational domain and mesh sizes are chosen respectively as $[-16, 16]^2$ and $h = \frac{1}{16}$ ($M = 512$)
- 3D: $\gamma_x = \gamma_y = 1$, $\gamma_z = 3$, $\alpha = 1.4$ and $\kappa = 0.3$. The computational domain is $[-8, 8]^3$ and the mesh size is: $h = \frac{1}{8}$ ($M = 128$).

Example 1: fast rotating and strongly nonlinear 2D BEC in a quadratic-plus-quartic potential

Table 1: CPUs time (*seconds*) for $\mathrm{PCG_C}$ to compute the ground states of the GPE with various ω and η.

η	ω=1	1.5	2	2.5	3	3.5	4	4.5
1000	493	551	560	2892	2337	720	966	3249
5000	1006	1706	867	6023	1144	1526	12514	19248
10000	4347	21525	5511	15913	15909	6340	16804	32583

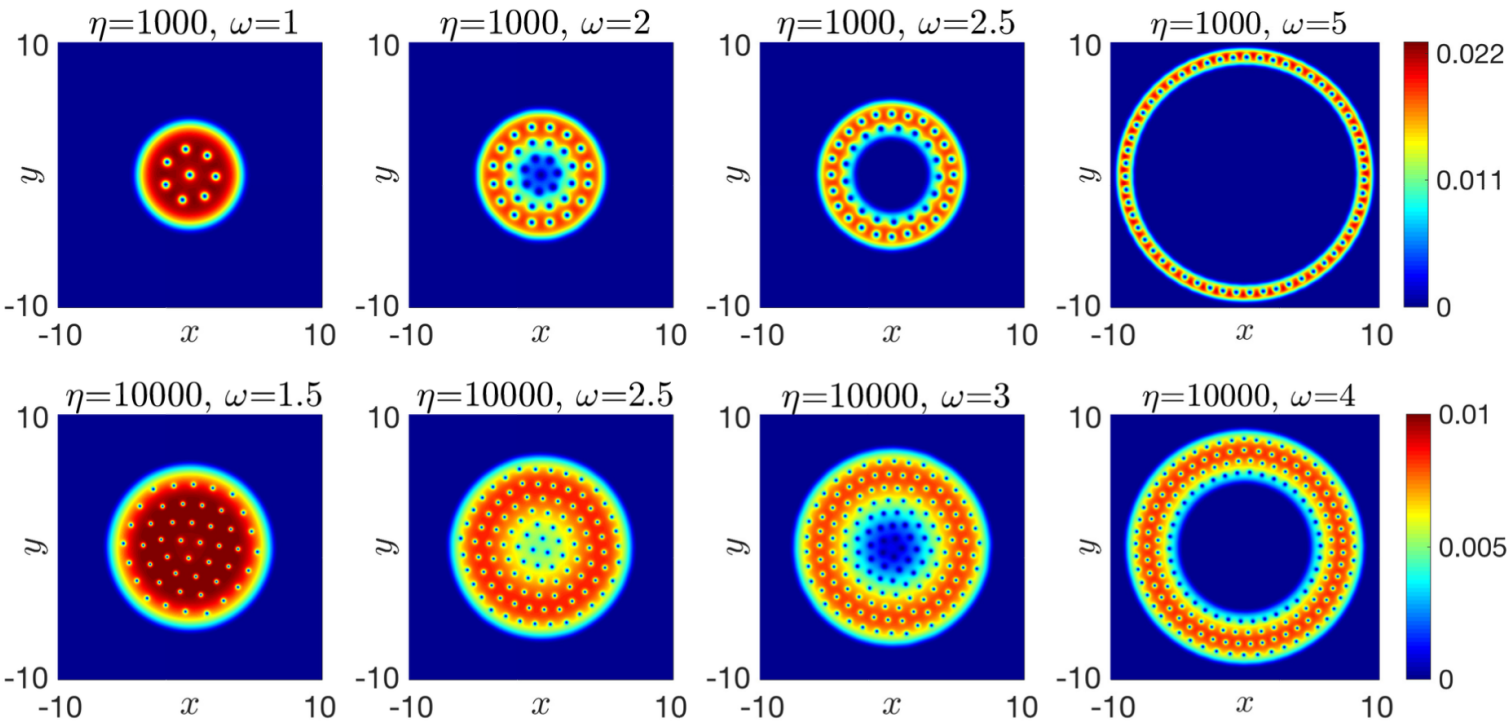

Figure 9: Exemple 6.7. Corresponding contour plots of the density function $|\phi_g(\mathbf{x})|^2$ of Table 1.

Example 2: fast rotating and strongly nonlinear 3D BEC in a quadratic-plus-quartic potential

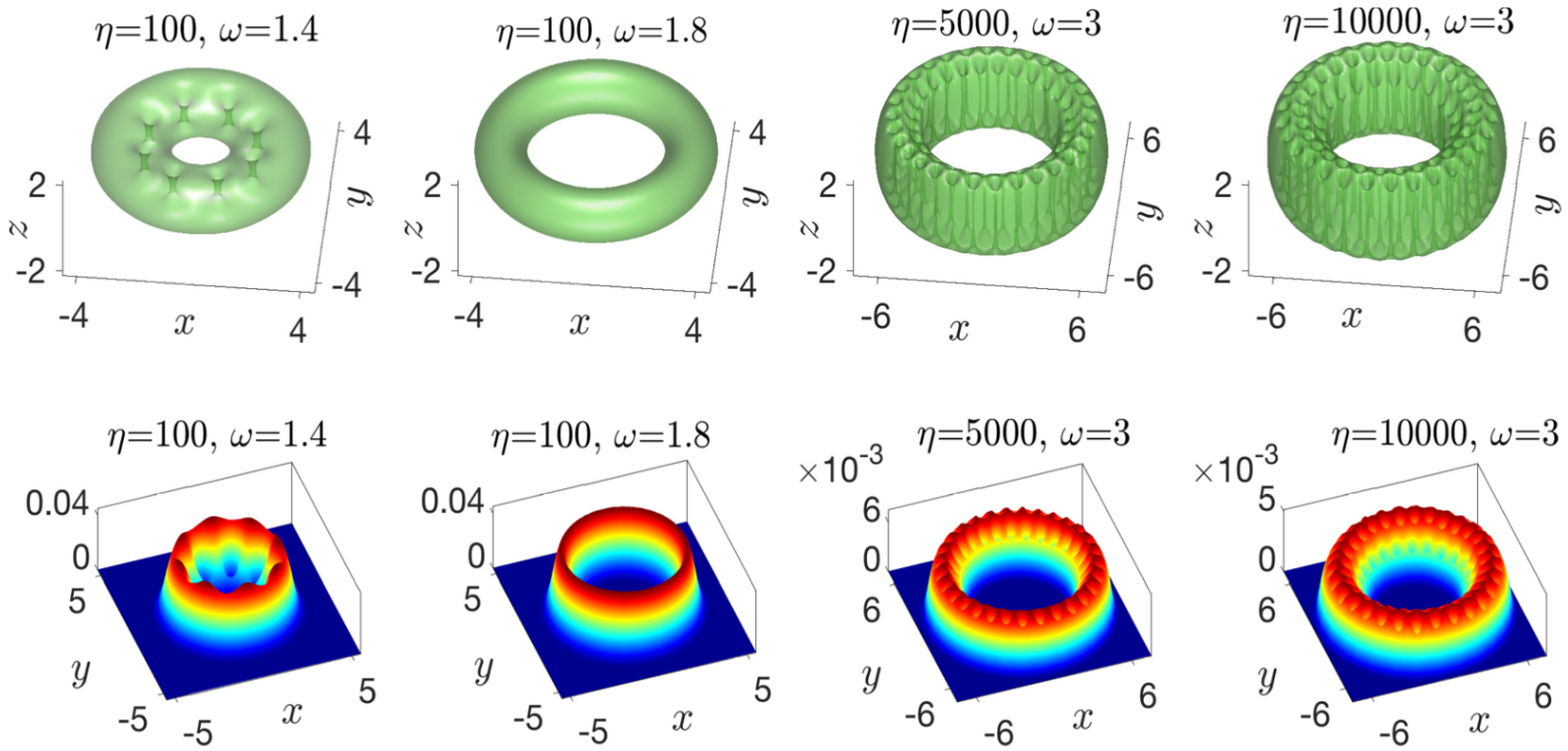

Figure 12: Exemple 6.9. Isosurface $|\phi_g(\mathbf{x})|^2 = 10^{-3}$ (upper) and surface plot of $|\phi_g(x, y, z = 0)|^2$ (lower) in example 6.9. The CPU cost for these four cases are respectively 2256 *(s), 1403 (s), 11694 (s) and 21971 (s).*

Conclusion

What has been done and what we are doing for the stationary states

- Fast iterative preconditioned nonlinear conjugate gradient method for the computation of the ground states of fast rotating and strongly nonlinear GPEs
- Can be again accelerated through IPiano algorithms which are accelerated gradient-type techniques recently introduced for image processing
- A computation with the standard BESP scheme (see GPELab: Matlab) has been reduced from a factor 100 $\rightarrow$ from more than one week to 2-3 hours for complicate cases)
- The parallel HPC implementation is almost ended: 2-3 hours $\rightarrow$ a few minutes: real-time simulations
- The extension to dipolar (nonlocal nonlinear interactions) and to space fractional GPEs is done
- Still need to extend to coupled GP equations (1d is okay) GPELab is used a lot in physics now

Conclusion

Dynamics

- We have a few advanced high-order methods (splitting, IMEX, exponential integrators,...)
- More applications are coming out
- Extensions to time fractional dynamics is ongoing

... about the influence of Abderrahmane in my life

- Huge influence of Abderrahmane on my scientific career always encouraging me to go deeper in my own ideas, since the beginning
- His influence is of course also in terms of scientific topics (OSRCs, ABCs, integral equations, DDM, finite elements...)
- One of the most fundamental elements in a scientific life is people that you meet, and I'm lucky to have met Abderrahmane in 1993, who is at the same time my scientific father, my colleague and my friend