A FreeFem++ toolbox for computing rotating stationary states of Bose-Einstein condensates

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Plan

1. Program architecture
2. Gross-Pitaevskii (GP) energy and stationary GP equation
3. Approximations
   - Thomas-Fermi approximation
   - Axisymmetric approximation in 2D ($\Omega = 0$)
   - Solution without rotation as an approximation
   - Vortex ersatz
4. Methods
   - Sobolev gradient method
   - Adaptive mesh
   - Using Ipopt
5. Examples in 3D
6. Other results in 2D
7. Other results in 3D

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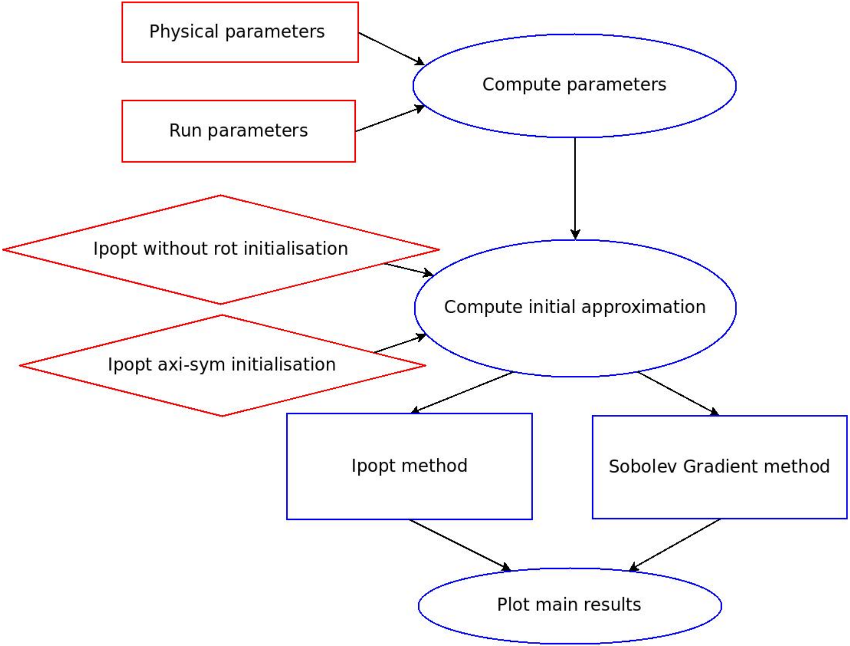
Physical parameters
Run parameters
Compute parameters
Ipopt without rot initialisation
Ipopt axi-sym initialisation
Compute initial approximation
Ipopt method
Sobolev Gradient method
Plot main results

Outline

Let $\mathcal{D} \subset \mathbb{R}^3$ be an open and bounded domain.
The wave function of the BEC $u \in H^1(\mathcal{D}, \mathbb{C})$ minimizes GP energy :

$$E(u) = \int_{\mathcal{D}} \left[\frac{1}{2} |\nabla u|^2 + V_{trap} |u|^2 + \frac{1}{2} C_g |u|^4 \right] - C_\Omega L_z,$$

where

$$V_{trap} = \frac{1}{2}(a_x x^2 + a_y y^2 + a_z z^2) : \text{ harmonic trapping potential,}$$
$$\text{ou } V_{trap} = \frac{1}{2}(a_x x^2 + a_y y^2 + a_z z^2 + a_4 r^4) : \text{ quartic/quadratic potential,}$$

C_g and C_Ω are constants, and

$$L_z = -\int_{\mathcal{D}} \mathcal{I}m \left[\overline{u} \left(y \frac{\partial u}{\partial x} - x \frac{\partial u}{\partial y} \right) \right] = \int_{\mathcal{D}} \mathcal{R}e \left[i\overline{u} \left(y \frac{\partial u}{\partial x} - x \frac{\partial u}{\partial y} \right) \right].$$

u is normalized and the mass conservation can be wrote as :

$$\int_{\mathcal{D}} |u|^2 = 1.$$

Stationary GP equation to find critical points :

$$-\frac{1}{2}\Delta u + V_{trap} u + C_g |u|^2 u - iC_\Omega (y\partial_x u - x\partial_y u) = \mu u,$$

μ is the chemical potential and play the role of a Lagrange multiplier.

Outline

Thomas-Fermi approximation

Kinetic energy $\ll$ Interaction forces $\Longrightarrow$

$$E_{TF}(u) = \int_{\mathcal{D}} V^{eff}\,|u|^2 + \frac{C_g}{2}\,|u|^4.$$

where

$$\bar{V}^{eff} = V_{trap} - \frac{C_\Omega^2}{2}(x^2 + y^2).$$

Thomas-Fermi approximation

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Analytic solution :

$$\rho_{TF} = |u|^2 = \frac{1}{(2C_g)}\left(\rho_0 - \bar{V}^{eff}\right),$$

The constant ρ_0 is determined by imposing the unitary norm constraint :

$$\int_{\mathcal{D}} |u|^2 = 1 \Rightarrow \int_{\mathcal{D}} (\rho_0 - \bar{V}_{eff}) = (2C_g).$$

The border $\delta\mathcal{D}$ of the domain containing the condensate can be expressed as the points where :

$$\rho_0 - \bar{V}^{eff} = 0.$$

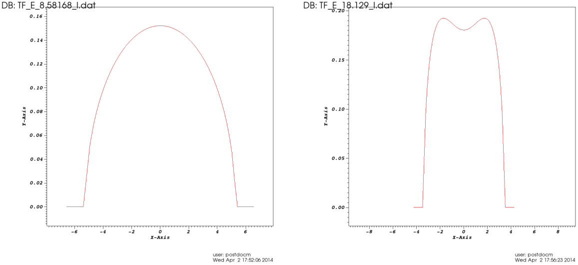

Figure: Thomas-Fermi profile for a harmonic potential and a quartic/quadratic potential.

Axisymmetric approximation in 2D ($\Omega = 0$)

Axisymmetric solution : $\frac{\partial u}{\partial \theta} = 0$.
The energy becomes :

$$E(u) = \int_0^{R_{max}} 2\pi \left[\frac{1}{2} \left| \frac{\partial u}{\partial r} \right|^2 + V_{trap} |u|^2 + \frac{1}{2} C_g |u|^4 \right] r dr,$$

The constraint becomes :

$$C(u) = \int_0^{R_{max}} 2\pi |u|^2 r dr = 1.$$

Initial condition \ Potential	Harmonic	Quartic
Thomas-Fermi	E = 8.58168	E = 18.129
Axisymmetric Ipopt	E = 8.53115	E = 17.9123

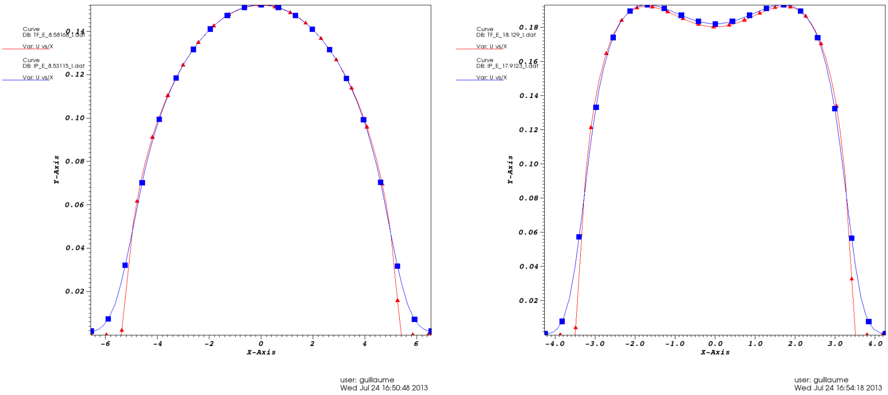

Figure: Compare Thomas-Fermi ▲ and axisymmetric Ipopt ■ for a harmonic potential(left) and a quartic/quadratic potential (right).

Solution without rotation as an approximation

We consider GP energy without rotation :

$$E(u) = \int_{\mathcal{D}} \frac{1}{2}|\nabla u|^2 + V^{eff}\,|u|^2 + \frac{C_g}{2}\,|u|^4.$$

où

$$\bar{V}^{eff} = V_{trap} - \frac{C_\Omega^2}{2}(x^2 + y^2).$$

Initial condition \ Potential	Harmonic	Quartic
Thomas-Fermi	E = 8.58168	E = 18.129
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Ipopt without rot	E = 8.54455	E = 17.9575

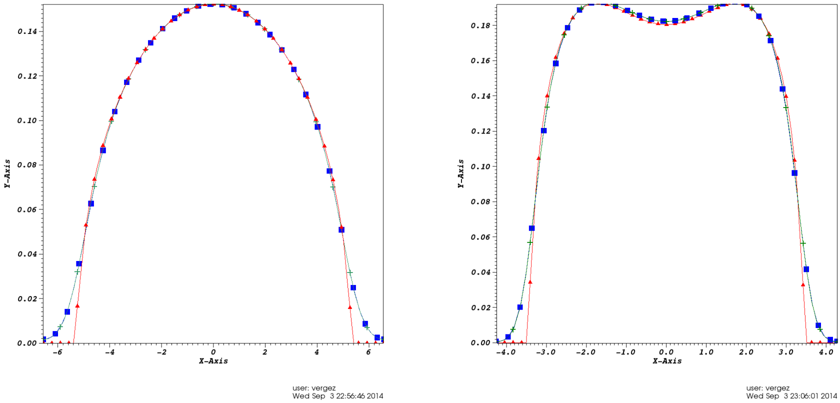


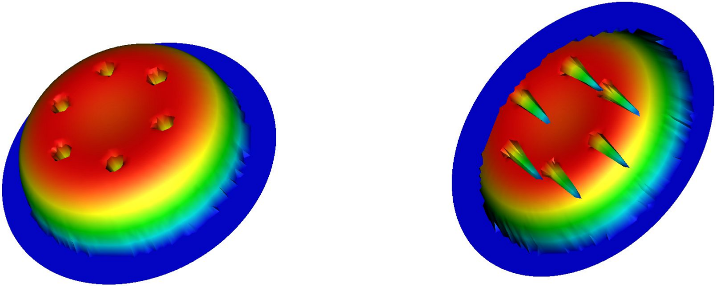
Figure: Compare Thomas-Fermi ▲ and axisymmetric Ipopt ■ and Ipopt without rotation + for a harmonic potential(left) and a quartic/quadratic potential (right).

Vortex ersatz

In 2D we can add vortex ersatz by multiplying u approximation by the function :

$$u_v = \sqrt{\frac{1}{2}\left[1 + tanh\left(\frac{4}{\varepsilon_v}(r_v - \varepsilon_v)\right)\right]} \cdot e^{i\theta_v},$$

where (r_v, θ_v) are the polar coordinates of the vortex centre and ε_v is its radius.



In 3D we can make r_v be a function of z to obtain different shapes of vortex with this formula :

$$\begin{cases} r_v(z) = -1 + \dfrac{tanh\left[\alpha_v\left(1+\frac{z}{\beta_v}\right)\right]}{tanh(\alpha_v)} \,\text{si} z < 0 \\ r_v(z) = 1 + \dfrac{tanh\left[\alpha_v\left(-1+\frac{z}{\beta_v}\right)\right]}{tanh(\alpha_v)} \,\text{si} z \geq 0 \end{cases}$$

where α_v and β_v respectively control curvature and length of the vortex.

Figure: @shape U on the left and @shape S on the right

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Sobolev gradient (SG) method

- Direct Energy minimisation method :

$$u_{n+1} = u_n + \rho\, \mathcal{G}_n,$$

$\mathcal{G}_n$: Descent direction $(D_{u_n} E . \mathcal{G}_n < 0)$
ρ : Descent step.

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  $\mathcal{G}_n$: Descent direction ($D_{u_n} E.\mathcal{G}_n < 0$)
  ρ : Descent step.

- Sobolev gradient method $\Longrightarrow \mathcal{G}_n = -\nabla E(u_n)$.

- Let $(X, \langle \cdot, \cdot \rangle_X)$ be a Hilbert space on which $D_{u_n}E$ is a continuous linear form, then by Riez representation theorem :

$$\exists \, ! \, \mathcal{G}_n \in X \text{ such that } \forall v \in X, \; D_{u_n}E.v = \langle \mathcal{G}_n, v \rangle_X .$$

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$$\forall v \in L^2,\ D_{u_n}E.v = \langle \nabla_{L^2} E(u_n), v \rangle_{L^2} .$$

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$$\forall v \in H^1,\ D_{u_n}E.v = \langle \nabla_{H^1} E(u_n), v \rangle_{H^1}.$$

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$$\forall v \in H^1,\ D_{u_n}E.v = \langle \nabla_{H^1} E(u_n), v \rangle_{H^1}.$$

- I. Danaila and P.Kazemi $\Longrightarrow$ new scalar product on $H^1(\mathcal{D}, \mathbb{C})$:

$$\langle u, v \rangle_{H_A} = \int_{\mathcal{D}} uv + \underbrace{(\nabla u + i\Omega A^T u)}_{\nabla_{H_A} u} \cdot (\nabla v + i\Omega A^T v).$$

Here is the algorithm we finally use :

(1) Suppose solution at step n is built.
We built $\mathcal{G} = \nabla_{H_A} E(u_n)$ solution of the variational problem :

$$\langle \mathcal{G}, v \rangle_{H_A} = \langle \nabla_{L^2} E(u_n), v \rangle_{L^2}, \ \forall v \in H_0^1(\mathcal{D}, \mathbb{C}).$$

where

$$\langle \mathcal{G}, v \rangle_{H_A} = \int_{\mathcal{D}} \left(1 + \Omega^2 (x^2 + y^2)\right) \mathcal{G} v + \nabla \mathcal{G} \nabla v - 2i\Omega A^T \nabla \mathcal{G} v,$$

and

$$\langle \nabla_{L^2} E(u_n), v \rangle_{L^2} = \int_{\mathcal{D}} \nabla u_n \nabla v + \left[2C_{trap} u_n + 2C_g |u_n|^2 u_n - 2i\Omega A^T \nabla u_n\right] v$$

with a finite element method.

(2) we build the projection of $\mathcal{G}$ on T_{u_n,H_A} :

$$P_{u_n,H_A}\mathcal{G} = \mathcal{G} - \frac{\mathcal{R}e\left(\langle u_n, \mathcal{G}\rangle_{L^2}\right)}{\mathcal{R}e\left(\langle u_n, v_{H_A}\rangle_{L^2}\right)} v_{H_A},$$

where v_{H_A} is solution of the variational problem :

$$\langle v_{H_A}, v\rangle_{H_A} = \langle u, v\rangle_{L^2},\ \forall v \in H_A.$$

(3) we build solution at step $n+1$:

$$u_{n+1} = u_n - \rho\ P_{u_n,H_A}\mathcal{G}.$$

Adaptive mesh in 2D

$Th = adaptmesh(Th, [real(un), imag(un)], hmin = hminad, err = erradapt, ratio = 1.3, anisomax = 2, nbvx = 10^6);$

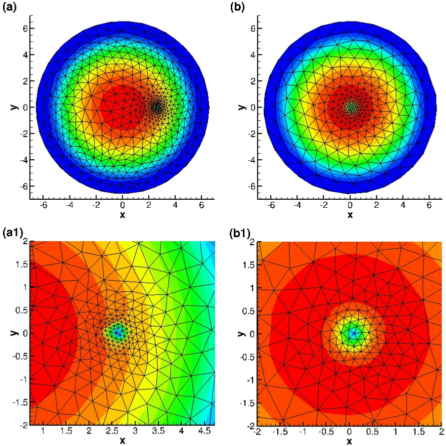

Figure: Initial approximation on the left, solution with Sobolev gradient method on the right.

Adaptive mesh in 3D

$real[int]met = mshmet(Th, uur, uui, hmin = hminad, hmax = hmaxad, err = erradapt, aniso = anisoadapt);$
$Th = mmg3d(Th, metric = met, opt = " - O - 1");$

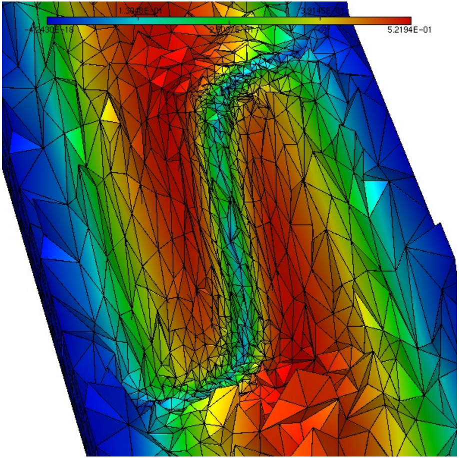

Figure: Solution with S shaped vortex view with Medit

Using Ipopt

- Optimizer developped by Andreas Wächter and Carl Laird.
- Use an interior point method J. Nocedal et Waltz (2008) and Wächter thesis (January 2002)).
- In FreeFem++, load library ff-Ipopt interfaced by S.Auliac.

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It solves minimisation's problems under constraint on the form :

$$\text{find } x_0 = \underset{x \in \mathbb{R}^n}{\text{argmin}}(f(x))$$

$$\text{such that } \begin{cases} \forall i \leq n,\ x_i^{lb} \leq x_i \leq x_i^{ub} \text{ (simple bounds)} \\ \forall i \leq m,\ c_i^{lb} \leq c(x_i) \leq c_i^{ub} \text{ (constraint functions)} \end{cases}$$

- Input arguments :
  1. The functional you want to minimize, its gradient and its Hessian matrix.
  2. The functional defining the constraint, its Jacobian matrix and the upper and lower boundaries.
  3. An error tolerance you want to reach when approximating the solution.

- We add mesh adaptation in a tricky way.

Outline

U shaped vortex with Ipopt in 3D

Figure: Anisotropic quadratic potential with $Cg = 1250$ and $C_\Omega = 0.4$.

S shaped vortex with Sobolev Gradient in 3D

Figure: Anisotropic quadratic potential with $Cg = 1250$ and $C_\Omega = 0.35$.

Outline

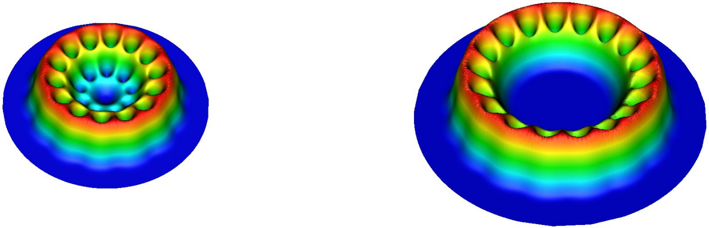

Figure: Quartic+Quadratic potential with $Cg = 500$ and $C_\Omega = 3$ (left) or $C_\Omega = 3.5$ (right).

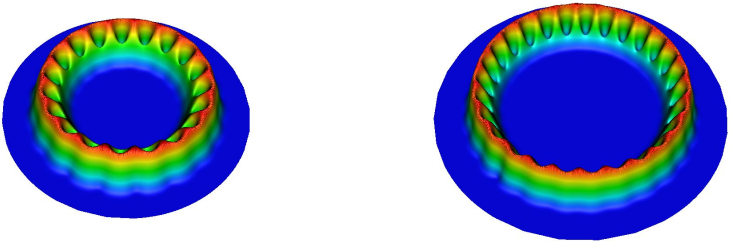

Figure: Quartic+Quadratic potential with $Cg = 500$ and $C_\Omega = 4$ (left) or $C_\Omega = 5$ (right).

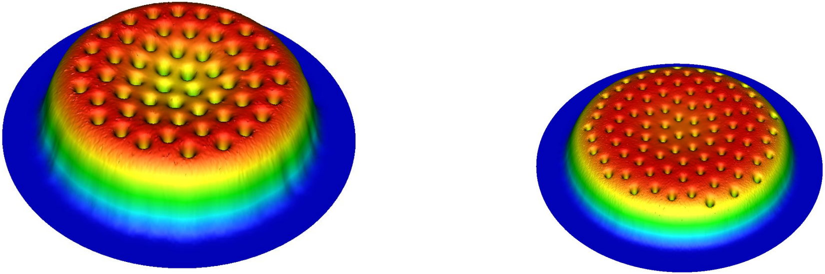

Figure: Quartic+Quadratic potential with $C_\Omega = 3.5$ and $Cg = 5000$ (left) or $Cg = 15000$ (right).

Outline

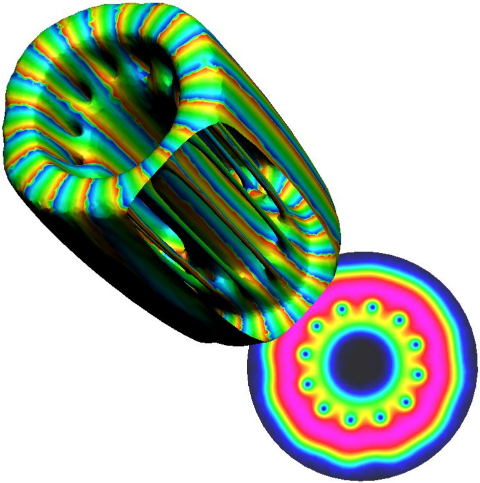

Figure: Quartic-Quadratic potential with $Cg = 1250$ et $C_\Omega = 1.5$.

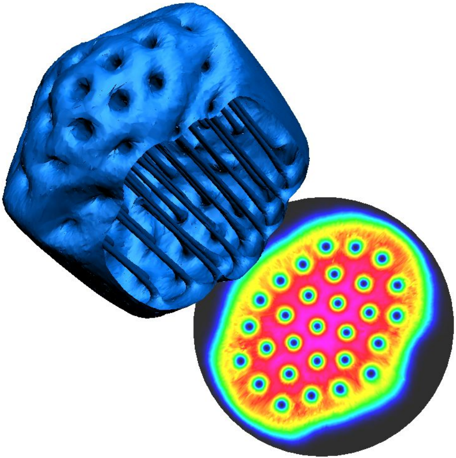

Figure: Anisotropic harmonic potential with $Cg = 5000$ et $C_\Omega = 0.95$.

Thank you for your attention.