# GPELab: an open source Matlab toolbox for the numerical simulation of Gross-Pitaevskii equations

#### X. Antoine<sup>1</sup> & R. Duboscq<sup>2</sup>

1: Institut Elie Cartan de Lorraine

2: Institut de Mathématiques de Toulouse (IMT) 1,2: ANR BECASIM

New Challenges in Mathematical Modelling and Numerical Simulation of Superfluids June 27 - July 1, 2016

#### INTRODUCTION

COMPUTATION OF STATIONARY STATES WITH GPELAB Stationary states: definition/properties Numerical methods in GPELab Numerical examples with GPELab

COMPUTATION OF THE DYNAMICS WITH GPELAB Numerical methods in GPELab Numerical examples with GPELab

CONCLUSION AND PERSPECTIVES

## WHAT IS THE AIM OF GPELAB?

▶ GPELab (Gross-Pitaevskii Equation Laboratory) is a Matlab toolbox developed for computing the stationary states and dynamics of large classes of GPEs which are time-dependent PDEs that model the evolution of Bose-Einstein Condensates (BECs) (BECs can also be described by other models).



## Description of a BEC by the GPE

Obtained by **Gross & Pitaevskii** (1961), the GPE is a nonlinear Schrödinger equation modeling the real-time dynamics of the **wave function**  $\psi$  of the BEC

The "basic" Gross-Pitaevskii equation

$$\left\{ \begin{array}{l} i\partial_t\psi(\boldsymbol{x},t) = -\frac{1}{2}\Delta\psi(\boldsymbol{x},t) + V(\boldsymbol{x})\psi(\boldsymbol{x},t) + \beta f(\psi)\psi(\boldsymbol{x},t), \ t > 0, \\ \psi(\boldsymbol{x},0) = \psi_0(\boldsymbol{x}), \ \boldsymbol{x} \in \mathbb{R}^d, \end{array} \right.$$

where

- $\blacktriangleright$  V is a (confining) potential corresponding to the trapping device,
- $f(\psi) = |\psi|^2$  is a nonlinear term corresponding to the interaction between the particles in the BEC.

## Some conserved physical quantities

► The mass

$$N(\psi) = \int_{\mathbb{R}^d} |\psi(\boldsymbol{x},t)|^2 d\boldsymbol{x} = \int_{\mathbb{R}^d} |\psi_0(\boldsymbol{x})|^2 d\boldsymbol{x} = ||\psi_0||_{L^2}^2 = 1.$$

► The energy

$$E(\psi) = \int_{\mathbb{R}^d} \left[ \frac{1}{2} |\nabla \psi|^2 + V |\psi|^2 + \frac{1}{2} \beta |\psi|^4 \right] d\boldsymbol{x}.$$

## Additional models: rotating condensate

The Gross-Pitaevskii equation with a rotation term

$$\begin{split} i\partial_t \psi(\boldsymbol{x},t) &= -\frac{1}{2} \Delta \psi(\boldsymbol{x},t) + V(\boldsymbol{x})\psi(\boldsymbol{x},t) + \beta |\psi(\boldsymbol{x},t)|^2 \psi(\boldsymbol{x},t) \\ &- \boldsymbol{\Omega} \cdot \mathbf{L} \psi(\boldsymbol{x},t), \ t > 0, \\ \psi(\boldsymbol{x},0) &= \psi_0(\boldsymbol{x}), \ \boldsymbol{x} \in \mathbb{R}^d, \end{split}$$

where

- the vector  $\Omega$  corresponds to the axis of rotation (direction) and its speed (modulus),
- ▶ the operator  $\mathbf{L} = (p_x, p_y, p_z)^t = x \wedge \mathbf{P}$  is the angular momentum operator with  $\mathbf{P} = -i\nabla$  the impulsion,
- here, we consider a rotation along the z-axis with a speed  $\Omega$  (*i.e.*  $\Omega = (0, 0, \Omega)$ ). This gives:  $\Omega \cdot \mathbf{L} = \Omega L_z := -i\Omega(x\partial_y - y\partial_x)$



Figure: Vortex nucleation by rotating a Bose-Einstein condensate.

## Additional models: random fluctuations

The Gross-Pitaevskii equation with a stochastic potential

$$\begin{split} i\partial_t \psi(\boldsymbol{x},t) &= -\frac{1}{2} \Delta \psi(\boldsymbol{x},t) + V(\boldsymbol{x})\psi(\boldsymbol{x},t)(1+\boldsymbol{\dot{w}}_t) \\ &+ \beta |\psi(\boldsymbol{x},t)|^2 \psi(\boldsymbol{x},t), \ t > 0, \\ \psi(\boldsymbol{x},0) &= \psi_0(\boldsymbol{x}), \ \boldsymbol{x} \in \mathbb{R}^d, \end{split}$$

where the white noise  $(\dot{w}_t)_{t\in\mathbb{R}^+}$  corresponds to the formal derivative of the brownian motion  $(w_t)_{t\in\mathbb{R}^+}$ .



Figure: Evolution of the density of a 1D BEC with random fluctuations in the trapping device.

## Additional models: spinor BEC

A system of Gross-Pitaevskii equations with spin-orbit coupling

$$\begin{split} & (i\partial_t\psi_1(\boldsymbol{x},t) = \left(\mathcal{L} + \beta_1|\psi_1|^2 + \beta_{12}|\psi_2|^2\right)\psi_1(\boldsymbol{x},t) + \mathcal{S}_1\psi_2(\boldsymbol{x},t), \ t > 0, \\ & (i\partial_t\psi_2(\boldsymbol{x},t) = \left(\mathcal{L} + \beta_2|\psi_2|^2 + \beta_{12}|\psi_1|^2\right)\psi_2(\boldsymbol{x},t) + \mathcal{S}_2\psi_1(\boldsymbol{x},t), \ t > 0, \\ & (\psi_1(\boldsymbol{x},0) = \psi_{1,0}(\boldsymbol{x}) \text{ and } \psi_2(\boldsymbol{x},0) = \psi_{2,0}(\boldsymbol{x}), \ \boldsymbol{x} \in \mathbb{R}^d, \end{split}$$

where

- $\mathcal{L} = \left(-\frac{1}{2}\Delta + V(\boldsymbol{x})\right), \beta_{12} = \text{intensity of interaction between the two-components.}$
- ►  $S_1 = \kappa(-i\partial_x + \partial_y)$  and  $S_2 = \kappa(-i\partial_x \partial_y)$  are the spin-coupling operators



Figure: Density of each (3) component of the spinor BEC: (a) initial state and (b) after applying a magnetic field gradient.

## About the numerical simulation: motivations

#### Motivations

- Since the system is quantum, it is technically extremely complex and expensive to perform an experiment and to observe the physical phenomena: the numerical simulation can be a cheap way for experimenting complex configurations
- ▶ Many complex BECs models exist and so the numerical simulation can help in understanding the validity of these models and how to improve them
- Managing BECs is crucial for future highly technological applications (quantum computer, GPS,...)

#### References.

[1] W. Bao and Y. Cai, Mathematical Theory and Numerical Methods for Bose-Einstein Condensation, Kinet. Relat. Mod., Vol. 6, pp. 1-135, 2013 (An Invited Review Paper).

[2] X.A. and R. Duboscq, Modeling and Computation of Bose-Einstein Condensates: Stationary States, Nucleation, Dynamics, Stochasticity, in Nonlinear Optical and Atomic Systems: at the Interface of Mathematics and Physics, Lecture Notes in Mathematics, 2146, pp. 49-145, Springer.

## About the numerical simulation: difficulties

## Difficulties for the numerical simulation

- ▶ The system of GPEs is a 3D nonlinear system.
- One can be interested in computing the stationary (ground/excited) states or the dynamics.
- ▶ It can couple some wave functions.
- ▶ The potential can be general, for example it can be nonlocal (convolution).
- ▶ The creation of vortices by the rotation term (or other gradient terms) is a very difficult numerical challenge.
- ▶ Stochastic effects arise in the modeling...

## About gpelab

#### GPELab

- ▶ Try to address these modeling questions from the numerical point of view.
- ▶ For 1d, 2d and 3d computations.
- ▶ The toolbox is based on recent numerical methods and some improvements.
- ▶ It is written in Matlab.
- Can be freely downloaded at http://gpelab.math.cnrs.fr/
- ▶ There is a user guide with some extended examples.

#### References.

 X.A. and R. Duboscq, GPELab, a Matlab Toolbox to Solve Gross-Pitaevskii Equations I: Computation of Stationary Solutions, Computer Physics Communications, 185 (11) (2014), pp. 2969-2991.

[2] X.A. and R. Duboscq, GPELab, a Matlab Toolbox to Solve Gross-Pitaevskii Equations II: Dynamics and Stochastic Simulations, Computer Physics Communications 193 (2015), pp. 95-117.

#### INTRODUCTION

#### COMPUTATION OF STATIONARY STATES WITH GPELAB Stationary states: definition/properties

Numerical methods in GPELab Numerical examples with GPELab

#### COMPUTATION OF THE DYNAMICS WITH GPELAB

Numerical methods in GPELab Numerical examples with GPELab

#### CONCLUSION AND PERSPECTIVES

## STATIONARY STATES

Let  $\mathcal{H}(\mathbf{q},\mathbf{p})$  be the **hamiltonian operator** of our quantum system. The Schrödinger equation reads

$$i\partial_t \psi(t, \mathbf{x}) = \mathcal{H}(\mathbf{x}, -i\nabla)\psi(t, \mathbf{x}).$$
(2.1)

#### The stationary states

The stationary states are the **eigenfunctions** of the operator  $\mathcal{H}$ . That is, for each eigenfunction  $\phi$ , we have

$$\mathcal{H}(\mathbf{x}, -i\nabla)\phi(\mathbf{x}) = \mu\phi(\mathbf{x}),$$

where  $\mu$  is the associated eigenvalue.

• 
$$\varphi(t, \mathbf{x}) = \phi(\mathbf{x})e^{-i\mu t}$$
 is a solution of (2.1).

 $\blacktriangleright$  In order to be physically meaningful,  $\phi$  must be normalized

$$\|\phi\|_{L^2}^2 := \int_{\mathbb{R}^d} |\phi(\boldsymbol{x})|^2 d\boldsymbol{x} = 1.$$

# STATIONARY STATES OF THE GPE WITH ROTATION: NONLINEAR EIGENPROBLEM

#### A nonlinear eigenproblem

In the case of the Gross-Pitaevskii equation with rotation, a stationary state is a solution to a **constrained nonlinear eigenproblem** 

$$\begin{cases} -\frac{1}{2}\Delta\phi(\boldsymbol{x}) + V(\boldsymbol{x})\phi(\boldsymbol{x}) + \beta|\phi(\boldsymbol{x})|^2\phi(\boldsymbol{x}) - \Omega L_z\phi(\boldsymbol{x}) = \mu\phi(\boldsymbol{x}), \\ \|\phi\|_{L^2} = 1. \end{cases}$$

We remark that, being given  $\phi$ , we can **directly compute the associated eigenvalue**, also called chemical potential,

$$\mu(\phi) = \int_{\mathbb{R}^d} \frac{1}{2} |\nabla \phi|^2 + V(\mathbf{x}) |\phi|^2 + \beta |\phi|^4 - \Omega \Re \left( \phi^* L_z \phi \right) d\boldsymbol{x}.$$

# STATIONARY STATES OF THE GPE WITH ROTATION: MINIMIZATION UNDER CONSTRAINTS

#### Critical points of the energy

The stationary states are also constrained critical points of the energy function  $E_{\beta,\Omega}$  with

$$E_{\beta,\Omega}(\phi) = \int_{\mathbb{R}^d} \left[ \frac{1}{2} |\nabla \phi|^2 + V |\phi|^2 - \Re \left( \phi^* \Omega L_z \phi \right) + \frac{1}{2} \beta |\phi|^4 \right] d\boldsymbol{x}.$$

By introducing a Lagrange multiplier  $\lambda$ , we can see that critical points are solutions of the equation

$$D_{\psi,\psi^*} E_{\beta,\Omega}(\phi) - \lambda D_{\psi,\psi^*} N(\phi) = 0,$$

where  $N(\psi) = \|\psi\|_{L^2}^2$ . This equation is equivalent to

$$-\frac{1}{2}\Delta\phi(\boldsymbol{x}) + V(\boldsymbol{x})\phi(\boldsymbol{x}) + \beta|\phi(\boldsymbol{x})|^2\phi(\boldsymbol{x}) - \Omega L_z\phi(\boldsymbol{x}) = \lambda\phi(\boldsymbol{x}).$$

#### INTRODUCTION

## COMPUTATION OF STATIONARY STATES WITH GPELAB Stationary states: definition/properties Numerical methods in GPELab

#### COMPUTATION OF THE DYNAMICS WITH GPELAB

Numerical methods in GPELab Numerical examples with GPELab

#### CONCLUSION AND PERSPECTIVES

## VARIOUS NUMERICAL METHODS CAN BE USED

We can either solve the nonlinear eigenproblem or search for critical points of the energy

- ▶ Search for critical points by using a Lagrange multiplier [Bao & Tang, 2003]
- ▶ Optimal damping algorithm [Dion & Cancès, 2007]
- ▶ Continuation method on a Lagrange multiplier [Wang & Chien, 2011]

 ${\tt GPELab}$  considers the imaginary time method

Search for critical points by a Continuous Normalized Gradient Flow (CNGF).

W. Bao and Q. Du, Computing the Ground State Solution of Bose-Einstein Condensates by a Normalized Gradient Flow, SIAM J. Sci. Comput., Vol. 25, No. 5. pp. 1674-1697, 2004.

## FORMULATION

The continuous normalized gradient flow consists in

- ► a gradient flow on a certain time interval (*i.e.* an energy-diminishing step),
- ► then **a projection** on the constraint manifold (*i.e.* a normalization step).

Let  $t_0 < \ldots < t_n < \ldots$  be a uniform time discretization with  $\delta t = t_{n+1} - t_n$ .

## Continuous Normalized Gradient Flow (CNGF)

$$\begin{aligned}
\begin{aligned}
\dot{\phi} &= -D_{\phi^*} E_{\beta,\Omega}(\phi) = \frac{1}{2} \Delta \phi - V \phi - \beta |\phi|^2 \phi \\
&+ \Omega L_z \phi, \ t \in [t_n, t_{n+1}], \\
\phi(\boldsymbol{x}, t_{n+1}) &= \phi(\boldsymbol{x}, t_{n+1}^+) = \frac{\phi(\boldsymbol{x}, t_{n+1}^-)}{||\phi(\boldsymbol{x}, t_{n+1}^-)||_{L^2}}, \\
&\phi(\boldsymbol{x}, 0) &= \phi_0(\boldsymbol{x}), \boldsymbol{x} \in \mathbb{R}^d, \ \text{with } ||\phi||_{L^2} = 1.
\end{aligned}$$
(2.2)

## SUITABLE TIME DISCRETIZATION

## Semi-implicit Backward Euler (BE) scheme

The Euler semi-implicit method leads to

$$\begin{cases} A^{BE,n}\tilde{\phi}(\boldsymbol{x}) = b^{BE,n}(\boldsymbol{x}), \boldsymbol{x} \in \mathbb{R}^{d}, \\ \phi^{n+1}(\boldsymbol{x}) = \frac{\tilde{\phi}(\boldsymbol{x})}{||\tilde{\phi}||_{L^{2}}}, \end{cases}$$
(2.3)

where  $A^{BE}$  and  $b^{BE}$  are given by

$$A^{BE,n} := \left(\frac{I}{\delta t} - \frac{1}{2}\Delta + V + \beta |\phi^n|^2 - \Omega L_z\right),$$
  
$$b^{BE,n} := \frac{\phi^n}{\delta t}.$$
 (2.4)

#### The energy is diminishing without **CFL** on the time step and the nonlinearity is **explicit**.

W. Bao and Q. Du, Computing the Ground State Solution of Bose-Einstein Condensates by a Normalized Gradient Flow, SIAM J. Sci. Comput., Vol. 25, No. 5. pp. 1674-1697, 2004.

## SUITABLE SPATIAL DISCRETIZATION

#### BESP scheme

► The spatial derivative operators are **efficiently and accurately** discretized thanks to the Fast Fourier Transform (FFT)

W. Bao and Q. Du, Computing the Ground State Solution of Bose-Einstein Condensates by a Normalized Gradient Flow, SIAM J. Sci. Comput., Vol. 25, No. 5. pp. 1674-1697, 2004.

► In addition, a **robust and efficient** matrix-free solution of the linear systems is obtained by using preconditioned Krylov subspace solvers (BICGStab, GMRES)

X.A. and R. Duboscq, Robust and Efficient Preconditioned Krylov Spectral Solvers for Computing the Ground States of Fast Rotating and Strongly Interacting Bose-Einstein Condensates, Journal of Computational Physics, 258 (1) (2014), pp. 509-523.

#### INTRODUCTION

#### Computation of stationary states with ${\tt gpelab}$

Stationary states: definition/properties Numerical methods in GPELab Numerical examples with GPELab

#### COMPUTATION OF THE DYNAMICS WITH GPELAB

Numerical methods in GPELab Numerical examples with GPELab

#### CONCLUSION AND PERSPECTIVES

## WHAT GPELAB CAN SOLVE

### All along the talk but without being explicit, GPELab can

- $\blacktriangleright$  Solve 1d-2d-3d cases
- ► Consider an arbitrary number of coupled equations (multicomponents)
- ▶ Integrate any GPEs with gradient terms
- ▶ Define general nonlinearities, user-defined potentials
- ▶ The user can define his own equations by simply calling built-in functions
- ▶ And can compute and manipulate any physical quantity that he defines

The same for the dynamics... + stochastic effects in time

## Example 1: double-well potential

#### 2D case

► Double-well potential

$$V(\boldsymbol{x}) = \frac{1}{2} ||\boldsymbol{x}||^2 + 40e^{-||\boldsymbol{x}||^2}$$

- Cubic nonlinearity with  $\beta = 150$ .
- Computational domain  $] 20, 20[^2.$
- ▶ Discretization parameters

• 
$$\delta t = 0.5$$
,

•  $2^9 \times 2^9$  grid points for the FFT.

CONCLUSION

## Example 1: double-well potential



Figure:  $|\psi|^2$  ( $\Omega = 0$  (left) and  $\Omega = 0.7$  (right)).

## Example 2: Quadratic-Quartic Potential

#### 2D case

• Quadratic-quartic potential ( $\alpha = 1.2$  and  $\kappa = 0.3$ )

$$V(\mathbf{x}) = (1 - \alpha) \|\mathbf{x}\|^2 + \kappa \|\mathbf{x}\|^4$$

- Cubic nonlinearity with  $\beta = 1000$ .
- Computational domain  $] 10, 10[^2.$
- ▶ Discretization parameters

• 
$$\delta t = 10^{-3}$$
,

•  $2^8 \times 2^8$  grid points for the FFT.

## EXAMPLE 2: QUADRATIC-QUARTIC POTENTIAL



Figure:  $|\psi|^2$  ( $\Omega = 0$  (left) and  $\Omega = 3.5$  (right)).

# EXAMPLE 3: MULTI-COMPONENTS BEC WITH RASHBA COUPLING [AFTALION & MASON, 2013]

#### 2D case

System of two coupled GPEs

$$\begin{cases} i\partial_t\psi_1(t,\mathbf{x}) = -\frac{1}{2}\Delta\psi_1(t,\mathbf{x}) - \kappa\left(i\frac{\partial}{\partial x} + \frac{\partial}{\partial y}\right)\psi_2(t,\mathbf{x}) \\ + \left(\frac{|\mathbf{x}|^2}{2} + g_1|\psi_1|^2 + g_{12}|\psi_2|^2\right)\psi_1(t,\mathbf{x}), \\ i\partial_t\psi_2(t,\mathbf{x}) = -\frac{1}{2}\Delta\psi_2(t,\mathbf{x}) - \kappa\left(i\frac{\partial}{\partial x} - \frac{\partial}{\partial y}\right)\psi_1(t,\mathbf{x}) \\ + \left(\frac{|\mathbf{x}|^2}{2} + g_2|\psi_2|^2 + g_{12}|\psi_1|^2\right)\psi_2(t,\mathbf{x}). \end{cases}$$

# EXAMPLE 3: MULTI-COMPONENTS BEC WITH RASHBA COUPLING [AFTALION & MASON, 2013]

#### 2D case

- Coupled cubic nonlinearities  $g_1 = 1000$ ,  $g_2 = 2000$  and  $g_{12} = 500$ .
- Rashba coupling  $\kappa = 10$ .
- Computational domain  $] 10, 10[^2.$
- ▶ Discretization parameters

• 
$$\delta t = 10^{-2}$$
,

•  $2^8 \times 2^8$  grid points for the FFT.

CONCLUSION

# Example 3: Multi-components BEC with Rashba coupling [Aftalion & Mason, 2013]



Figure:  $|\psi_j|^2$  (j = 1, 2).

These computations are obtained via the following GPELab script...

#### STATIONARY STATES

Dynamics

Example Rashba-2.m:1:1 %%% This file is an example of how to use GPELab (FFT version) %% GROUND STATE COMPUTATION WITH A ROTATING TERM AND COUPLED NONLINEARITIES <u>%</u>\_\_\_\_\_ % Setting the data s-----%% Setting the method and geometry 10 11 Computation = 'Ground'; Ncomponents = 2; 12 13 Type = 'BESP': 14 Deltat = 1e-2: Stop\_time = []; 16 Stop crit = {'MaxNorm', 1e-6}; Method = Method Var2d(Computation, Ncomponents, Type, Deltat, Stop time, Stop crit); 18 Method.Precond = 'FLaplace': 19 xmin = -10: xmax = 10: 20 ymin = -10;22 ymax = 10: 23  $Nx = 2^{8+1}$ : 24 Ny = 2^8+1; 25 Geometry2D = Geometry2D\_Var2d(xmin,xmax,ymin,ymax,Nx,Ny); 26 27 %% Setting the physical problem 28 Delta = 0.5: Beta = 1000: 29 30 Beta coupled = [1.0.5:0.5.2]; 31 Kappa = 10: 32 Physics2D = Physics2D\_Var2d(Method, Delta, Beta); RashbaDispersion{1,1} = @(FFTX, FFTY) Delta\*(FFTX.^2+FFTY.^2); 33 RashbaDispersion{1,2} = @(FFTX,FFTY) Kappa\*FFTX - 1i\*Kappa\*FFTY; 34 RashbaDispersion{2,1} = @(FFTX,FFTY) Kappa\*FFTX + 1i\*Kappa\*FFTY; 35 36 RashbaDispersion{2,2} = @(FFTX,FFTY) Delta\*(FFTX.^2+FFTY.^2); 37 Physics2D = Dispersion\_Var2d(Method, Physics2D, RashbaDispersion); 38 Physics2D = Potential\_Var2d(Method, Physics2D); 39 Physics2D = Nonlinearity Var2d(Method, Physics2D, Coupled Cubic2d(Beta coupled).... 40 [].Coupled Cubic energy2d(Beta coupled)); 41 42 %% Setting the initial data 43 InitialData Choice = 1; 44 Phi 0 = InitialData Var2d(Method, Geometry2D, Physics2D, InitialData Choice); 45 46 %% Setting informations and outputs Save = 0: 48 Outputs = OutputsINI Var2d(Method, Save): 40 Printing = 1: 50 Evo = 100: Draw = 1: 52 Print = Print\_Var2d(Printing,Evo,Draw); 53 54 %<u>-----</u> 55 % Launching simulation 56 %-----58 [Phi, Outputs] = GPELab2d(Phi 0.Method.Geometry2D.Physics2D.Outputs.[].Print):

## EXAMPLE 4: DIPOLE-DIPOLE INTERACTION

#### 3D case

- ▶ Quadratic potential
- ▶ Cubic nonlinearity with  $\beta = 2000 + \text{nonlinear nonlocal interaction}$

$$d^2 \int_{\mathbb{R}^d} \frac{1 - 3\cos^2(\widehat{\mathbf{a}, \widetilde{\mathbf{x}}})}{\|\mathbf{x} - \widetilde{\mathbf{x}}\|^3} |\psi(t, \widetilde{\mathbf{x}})|^2 d\widetilde{\mathbf{x}}.$$

with  $\mathbf{a} = (0, 0, 1)$  and d = 0.5.

- Computational domain  $] 10, 10[^3]$ .
- ► Discretization parameters

• 
$$\delta t = 10^{-2}$$
,

•  $2^6 \times 2^6 \times 2^6$  grid points for the FFT.

CONCLUSION

## EXAMPLE 4: DIPOLE-DIPOLE INTERACTION



Figure: Isovalues( $10^{-3}$ ) of  $|\psi|^2$ .

#### INTRODUCTION

#### Computation of stationary states with ${\tt gpelab}$

Stationary states: definition/properties Numerical methods in GPELab Numerical examples with GPELab

#### COMPUTATION OF THE DYNAMICS WITH GPELAB Numerical methods in GPELab

Numerical examples with GPELab

#### CONCLUSION AND PERSPECTIVES

## DISCRETIZATION SCHEMES

## Time-Splitting SPectral (TSSP) schemes

- ▶  $1^{st}$ ,  $2^{nd}$  and  $4^{th}$ -order in time
- $\blacktriangleright$  + FFT in space

## Relaxation SPectral (ReSP) schemes

- ▶ 2<sup>nd</sup>-order Besse relaxation scheme
- $\blacktriangleright$  + FFT in space + Krylov subspace solvers

#### References.

 W. Bao and Y. Cai, Mathematical Theory and Numerical Methods for Bose-Einstein Condensation, Kinet. Relat. Mod., Vol. 6, pp. 1-135, 2013 (An Invited Review Paper).

[2] X.A., W. Bao and C. Besse, Computational Methods for the Dynamics of the Nonlinear Schrödinger/Gross-Pitaevskii Equations, (A Feature Article) Computer Physics Communications 184 (12), (2013), pp.2621-2633.

## DISCRETIZATION SCHEMES

### Stochastic effects in time in the potential

- ▶ Both TSSP and ReSP are adapted
- ▶ The orders in time of the schemes depend on the regularity of the noise

#### References.

[1] R. Duboscq and R. Marty, Analysis of a time-splitting scheme for a class of random noise partial differential equations, submitted, 2014.

[2] X.A. and R. Duboscq, Modeling and Computation of Bose-Einstein Condensates: Stationary States, Nucleation, Dynamics, Stochasticity, in Nonlinear Optical and Atomic Systems: at the Interface of Mathematics and Physics, Lecture Notes in Mathematics, 2146, pp. 49-145, Springer.

#### INTRODUCTION

#### Computation of stationary states with gpelab

Stationary states: definition/properties Numerical methods in GPELab Numerical examples with GPELab

COMPUTATION OF THE DYNAMICS WITH GPELAB Numerical methods in GPELab Numerical examples with GPELab

CONCLUSION AND PERSPECTIVES

## EXAMPLE 1: PHASE-IMPRINTING OF BLACK SOLITONS

#### Phase-imprinting

Being given the ground state  $\phi$ , we set the initial data as

$$\psi_0(\mathbf{x}) = \phi(\mathbf{x})e^{-i\nu \tanh((x-x_0)/d)}.$$
 (3.1)

This generates an impulsion inside the condensate in the x-direction along the y-axis at the coordinate  $x = x_0$ .



Figure: Physical experiment and numerical simulation of a phase-engineered black-soliton [J. Denschlag & *al.*, Science, 2000].

## EXAMPLE 1: PHASE-IMPRINTING OF BLACK SOLITONS

The simulation uses the GPE

$$\begin{cases} i\partial_t \psi(t, \boldsymbol{x}) = -\frac{1}{2} \Delta \psi(t, \boldsymbol{x}) + \frac{1}{2} |\boldsymbol{x}|^2 \psi(t, \boldsymbol{x}) + \beta |\psi|^2 \psi(t, \boldsymbol{x}), \\ \psi(0, \boldsymbol{x}) = \phi_1(\boldsymbol{x}), \end{cases}$$
(3.2)

where  $\phi_1(x,y) = \phi(x,y)e^{-i\nu \tanh((x-x_0)/d)}$ , with  $\nu = -\pi/2$  and d = 0.4.



# Example 2: vortex nucleation induced by stirring

#### Vortex Nucleation in a Stirred Bose-Einstein Condensate

C. Raman, J. R. Abo-Shaeer, J. M. Vogels, K. Xu, and W. Ketterle

Department of Physics, MIT-Harvard Center for Ultracold Atoms, and Research Laboratory of Electronics, MIT, Cambridge, MA 02139 (February 1, 2008)

We studied the nucleation of vortices in a Bose-Einstein condensate stirred by a laser beam. We observed the vortex cores using time-of-flight absorption imaging. By varying the size of the stirrer, we observed either discrete resonances or a broad response as a function of the frequency of the stirrer's motion. Stirring beams small compared to the condensate size generated vortices below the critical rotation frequency for the nucleation of surface modes, suggesting a local mechanism of generation. In addition, we observed the centrifugal distortion of the condensate due to the rotating vortex lattice and found evidence for bent vortices.

PACS 03.75.Fi, 67.40.Vs, 32.80.Pj

CONCLUSION

## EXAMPLE 2: VORTEX NUCLEATION INDUCED BY STIRRING



# EXAMPLE 2: VORTEX NUCLEATION INDUCED BY STIRRING

### The GPE with time-dependent potential

We simulate the following Gross-Pitaevskii equation

$$\begin{cases} i\partial_t \psi(t, \boldsymbol{x}) = -\frac{1}{2} \Delta \psi(t, \boldsymbol{x}) + V(t, \boldsymbol{x}) \psi(t, \boldsymbol{x}) + \beta |\psi|^2 \psi(t, \boldsymbol{x}), \\ \psi(0, \boldsymbol{x}) = \phi(\boldsymbol{x}), \end{cases}$$
(3.3)

where  $V(t, \boldsymbol{x}) = \frac{1}{2} |\boldsymbol{x}|^2 + V_0 e^{-|\boldsymbol{x}-\boldsymbol{x}_s(t)|^2/d^2}$ , with  $V_0 = 100, d = 0.3$  and  $\boldsymbol{x}_s(t) = (x_0 \cos(\eta t)(1 - \sin(\eta t)), y_0 \cos(\eta t) \sin(\eta t)), \eta = 0.74.$ 

CONCLUSION

# EXAMPLE 2: VORTEX NUCLEATION INDUCED BY STIRRING



## Conclusion & Perspectives

#### GPElab: conclusion

- ► An easy-to-use open access Matlab toolbox that solves a large class of 1d-2d-3d GPEs for modeling BECs
- $\blacktriangleright$  Stationary states-Dynamics-Stochastic effects
- ▶ With some flexible, efficient, robust and accurate numerical methods

#### GPElab: perspectives

- ► BECASIM project (http://becasim.math.cnrs.fr/) funded by the National Agency for Research (ANR) (2012-2017)
- ▶ Goal: develop HPC solvers with visualization features to model high fidelity real physics experiments related to BECs
- ► A first version of the solver is being validated and includes the methods developed in GPELab, see Ph. Parnaudeau's talk this morning