An overview of the BECASIM project: open source numerical simulators for the Gross-Pitaevskii equation

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New challenges in mathematical modelling and numerical simulation of superfluids, CIRM, June 27, 2016.

ANR project BECASIM: BEC Advanced SIMulations

ANR Agence Nationale de la Recherche

ANR Project BECASIM (Numerical Methods, 2013-2017)

25 French mathematicians from 10 different labs

- develop new methods for real and imaginary time GP,
- mathematical theory, numerical analysis,
- (HPC) parallel codes:: open source,
- huge simulations of physical configurations (turbulence in BEC).

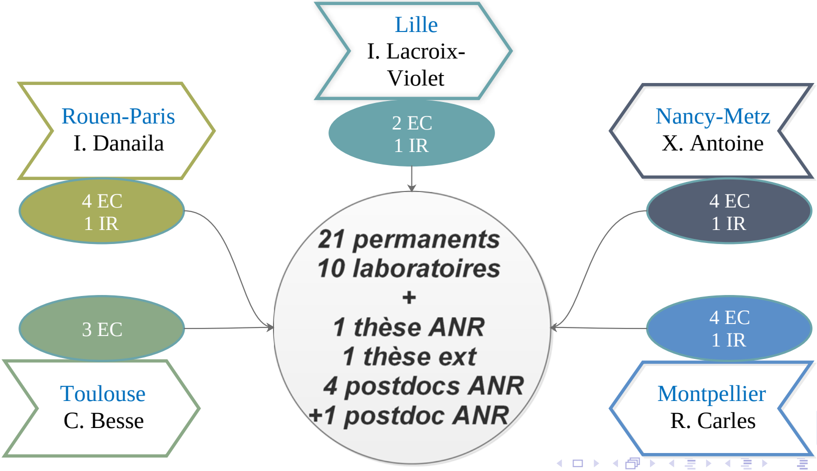
becasim.math.cnrs.fr

Outline

1. **ANR project BECASIM**
   - BECASIM team
   - Mathematical models
   - Program of the BECASIM session
   - Numerical tools

BECASIM team: 9 labs, 25 researchers

- complementary skills: theory of PDEs /numerical analysis/algorithms/ HPC, etc.



Gross-Pitaevskii (GP) equation(s)

Unsteady GP $\rightarrow$ real time dynamics

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + Ng_{3D}|\psi|^2\psi + V_{trap}\,\psi$$

- mean field theory : ψ order parameter,
- nonlinear Schrödinger equation (cubic nonl, defocusing),
- conservation laws: number of atoms $\int|\psi|^2$ and energy $\mathcal{E}(\psi)$.

Steady GP $\rightarrow$ ground and meta-stable states

$\psi = \phi\exp(-i\mu t/\hbar)$, μ is the chemical potential

$$-\frac{\hbar^2}{2m}\nabla^2\phi + V_{trap}\,\phi + Ng_{3D}|\phi|^2\phi - \mu\phi = 0$$

- nonlinear eigenvalue problem,

Gross-Pitaevskii (GP) equation(s)

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But also (see becasim.math.cnrs.fr)

- two-component BEC, non-local potentials,
- stochastic GP, fractional GP, etc

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$$-\frac{\hbar^2}{2m}\nabla^2\phi + V_{trap}\,\phi + Ng_{3D}|\phi|^2\phi - \mu\phi = 0$$

- nonlinear eigenvalue problem,

Program of the BECASIM session

1. X. Antoine: GPELab, an open source Matlab toolbox for the numerical simulation of Gross-Pitaevskii equations
2. Q. Tang: Numerical methods on simulating dynamics of the nonlinear Schrödinger equation with rotation and/or nonlocal interactions
3. C. Besse: High-order numerical schemes for computing the dynamics of nonlinear Schrödinger equation
4. P. Parnaudeau: A hybrid code for solving the Gross-Pitaevskii equation
5. R. Carles: Time splitting methods and the semi-classical limit
6. A. de Bouard: Inhomogeneities and temperature effects in Bose-Einstein condensates

Matlab toolbox: GPELab

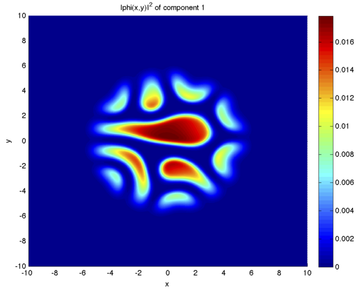
GPELab (Fourier spectral, FFT)

Developers : R. Duboscq, X. Antoine.

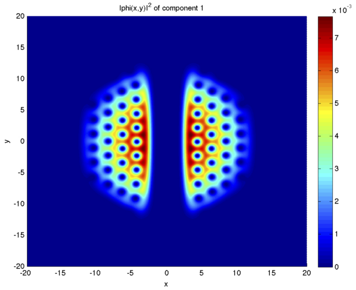
- stationary GP: semi-implicit Euler,
- real-time GP: splitting, relaxation,
- stochastic GP: splitting, relaxation.

Great flexibility to deal with new physical models:

multi-component BEC



BEC with double-well potential



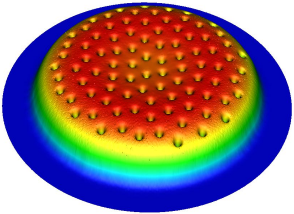
FreeFem++ Toolbox (www.freefem.org)

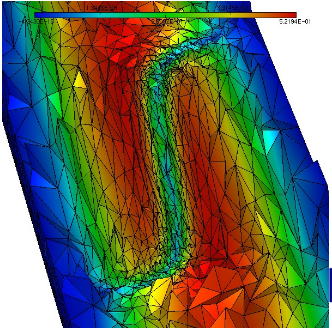
Developers: G. Vergez, I. Danaila, F. Hecht.
paper in revision, CCP (to freely distribute scripts)!

GPFEM: finite element solver

2D/3D anisotropic mesh adaptation, flexibility for boundary conditions,

- stationary GP: different Sobolev gradients.
- instationary GP: splitting, relaxation schemes.





FreeFem++: Bogoliubov-de Gennes modes

Two-component condensate:

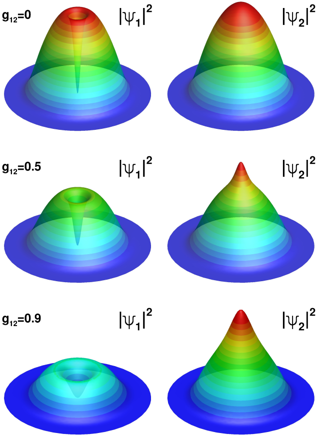
$$
\begin{aligned}
i\hbar\frac{\partial\psi_1}{\partial t} &= \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{trap}}(\mathbf{x}) + g_{11}|\psi_1|^2 + g_{12}|\psi_2|^2\right]\psi_1, \\
i\hbar\frac{\partial\psi_2}{\partial t} &= \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{trap}}(\mathbf{x}) + g_{21}|\psi_1|^2 + g_{22}|\psi_2|^2\right]\psi_2.
\end{aligned}
$$

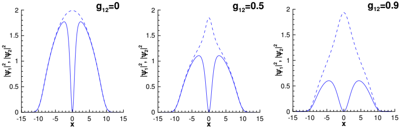
The Bogoliubov-de Gennes model is based on the linearisation:

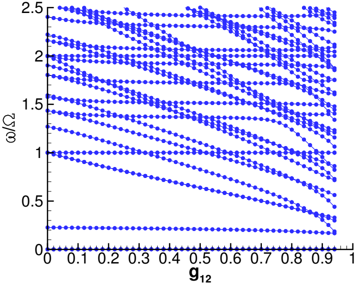
$$
\begin{aligned}
\psi_1(\mathbf{x},t) &= \exp(-i\mu_1 t/\hbar)\left(\phi_1 + a(\mathbf{x})e^{-i\omega t} + b^*(\mathbf{x})e^{i\omega^* t}\right) \\
\psi_2(\mathbf{x},t) &= \exp(-i\mu_2 t/\hbar)\left(\phi_2 + c(\mathbf{x})e^{-i\omega t} + d^*(\mathbf{x})e^{i\omega^* t}\right)
\end{aligned}
$$

BdG 2d: Vortex-Antidark Solitary Waves

I. Danaila, M. A. Khamehchi, V. Gokhroo, P. Engels, P. G. Kevrekidis, http://arxiv.org/abs/1606.05607

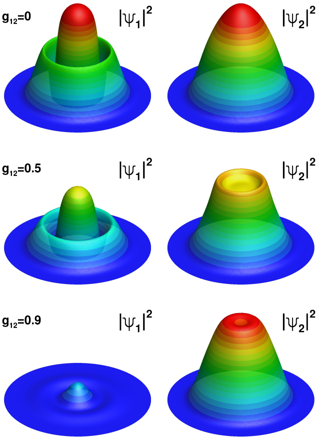


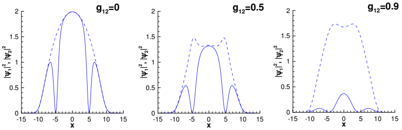


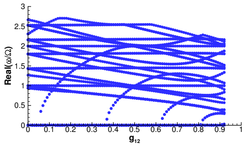


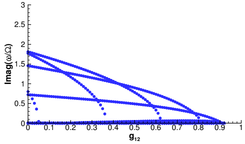
BdG 2d: Ring-Antidark-Ring Solitary Waves

I. Danaila, M. A. Khamehchi, V. Gokhroo, P. Engels, P. G. Kevrekidis, http://arxiv.org/abs/1606.05607







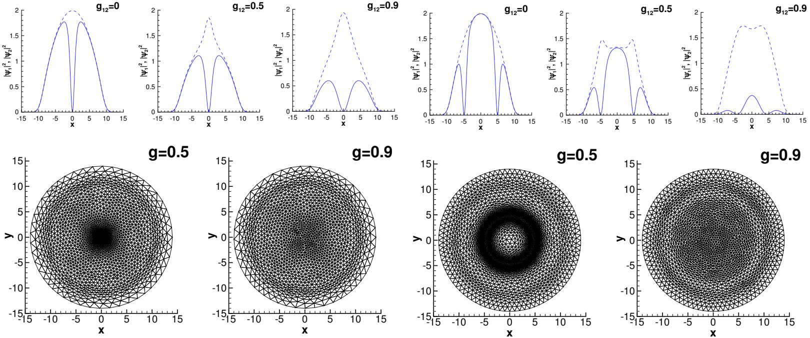


BdG 2d: mesh adaptivity

I. Danaila, M. A. Khamehchi, V. Gokhroo, P. Engels, P. G. Kevrekidis, http://arxiv.org/abs/1606.05607

Vortex-Antidark

Ring-Antidark-Ring

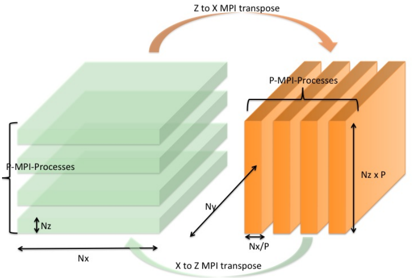


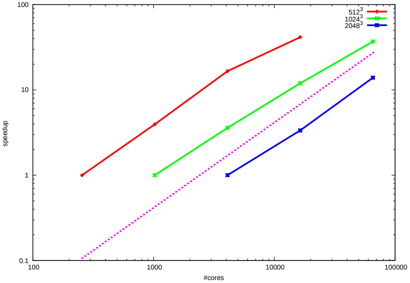
MPI-OpenMP code (GPS): 6th order FD or spectral

Developers: Ph. Parnaudeau, A. Suzuki, J.-M Sac-Epée.

- stationary GP: backward semi-implicit Euler, Sobolev gradients.
- real-time GP: splitting, relaxation, Crank-Nicolson.

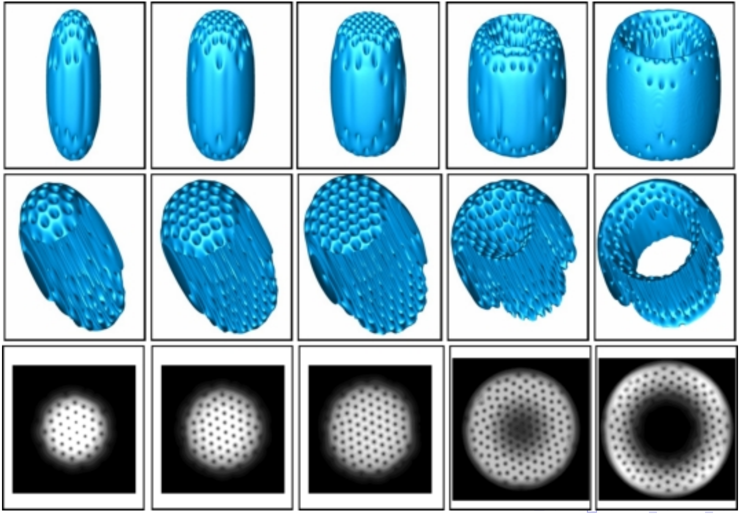
Flexible to run on laptops $\rightarrow$ clusters: 2D/3D grids up to 2048^3, optimized for OpenMP-MPI, from 4 $\rightarrow$ 10^5 cores.





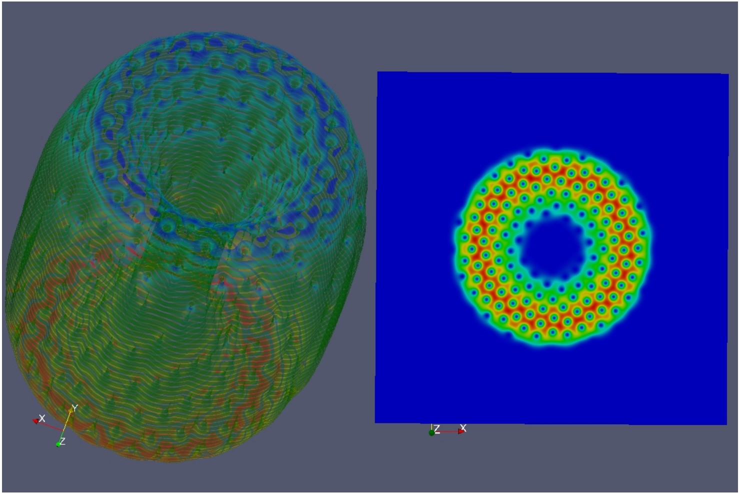
2005 3D Simulation: grid 240^3, 2 weeks)

I. Danaila, Phys. Rev. A, 2005.



2014 3D Simulation: grid 512^3, 1 day

Ph. Parnaudeau, CPC, to be submitted.



Conclusion

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Messages to physicists

We develop new numerical methods and HPC codes:

- currently under intensive tests,
- will be distributed as open source,
- we seek challenging physical applications.