Finite-element tools for the simulation of Bose-Einstein condensates

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joint work with F. Hecht, G. Vergez (Paris 6),
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B. Protas (McMaster, Canada)

12th AIMS conference, Taipei, July 7, 2018.

Outline

Outline

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

LMRS

Matlab toolbox: GPELab

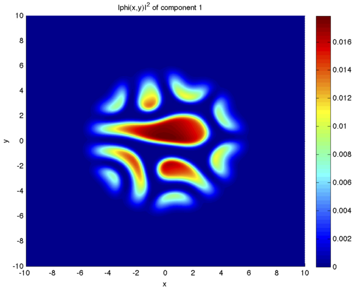
GPELab (Fourier spectral, FFT)

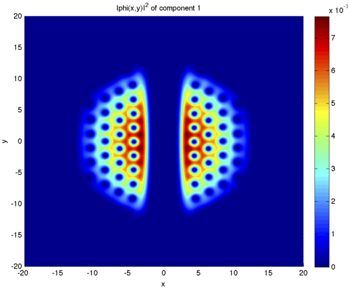
Developers : R. Duboscq, X. Antoine.

- 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



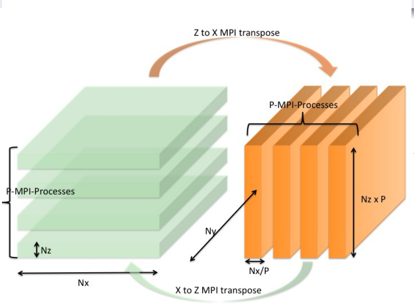


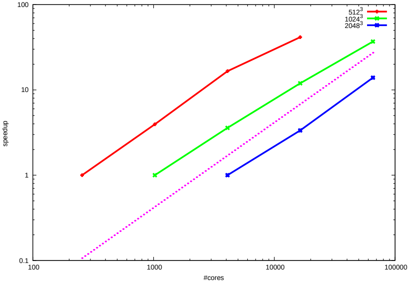
MPI-OpenMP code (GPS): spectral or 6th order FD

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.





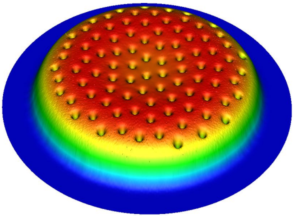
FreeFem++ Toolbox (www.freefem.org)

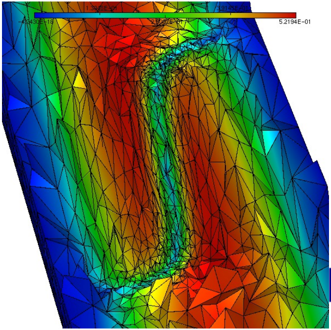
Developers: G. Vergez, I. Danaila, F. Hecht.
Computer Physics Communications, 2016 (with programs)!

GPFEM: finite element solver

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

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





FreeFem++ Toolbox: Gross-Pitaevskii (GP) models

Unsteady GP → real time dynamics

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V_{\text{trap}}\psi + g|\psi|^2\psi - i\hbar\Omega\mathbf{A}^t\cdot\boldsymbol{\nabla}\psi$$

Steady GP → ground and meta-stable states

$$\psi = \phi\exp(-i\mu t/\hbar), \qquad -\frac{\hbar^2}{2m}\nabla^2\phi + V_{trap}\,\phi + Ng_{3D}|\phi|^2\phi - \mu\phi = 0$$

Bogoliubov - de Gennes → stability of stationary states

$$\delta\psi = \left(a(\mathbf{x})e^{-i\omega t} + b^*(\mathbf{x})e^{i\omega^* t}\right),$$

$$\begin{pmatrix} H(\Omega) & g\phi^2 \\ -g(\phi^*)^2 & -H(-\Omega) \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \hbar\omega\begin{pmatrix} a \\ b \end{pmatrix}$$

$$H(\Omega) = -\frac{\hbar^2}{2m}\nabla^2 - \mu(\phi) + V_{\text{trap}} + 2g|\phi|^2 - i\hbar\Omega\mathbf{A}^t\cdot\boldsymbol{\nabla}$$

Identification of a quantized vortex

Macroscopic description

- $\psi \in \mathbb{C}$ wave function

$$\psi = \sqrt{\rho(r)}e^{i\theta(r)}$$

- vortex :: $\rho = 0$ + rotation
- velocity field

$$v(r) = \frac{h}{m}\nabla\theta$$

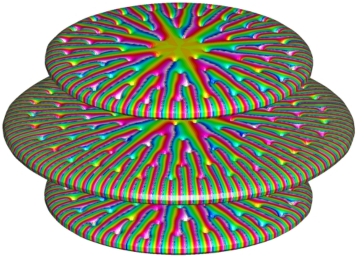
- quantified circulation

$$\Gamma = \int v(s)ds = n\frac{h}{m}$$

Identification of a quantized vortex (2)

- phase portraits

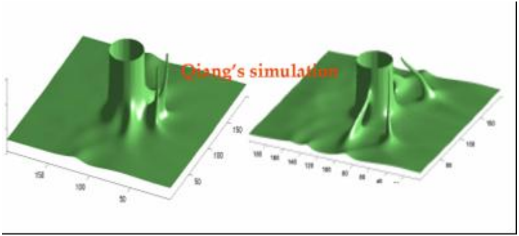
optical lattice



giant vortex

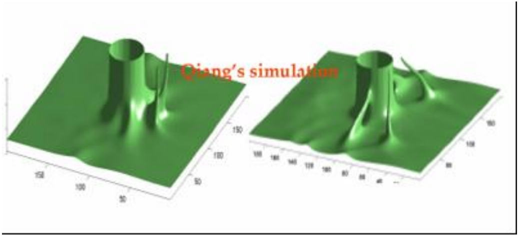
Creating vortices in BEC

Wake of moving objects Q. Du, Penn State

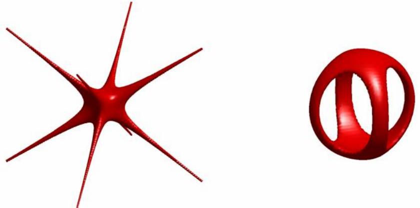


Creating vortices in BEC

Wake of moving objects Q. Du, Penn State

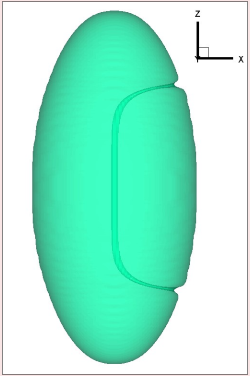


Phase imprint L.-C. Crasovan, V. M. Pérez-García, I. Danaila, D. Mihalache, L. Torner, PRA, 2004.

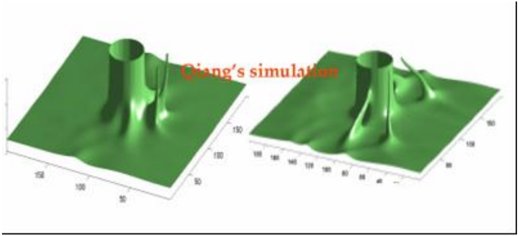


Creating vortices in BEC

Rotation



Wake of moving objects Q. Du, Penn State



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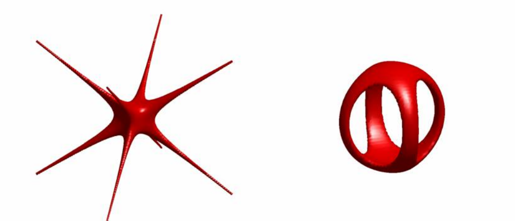
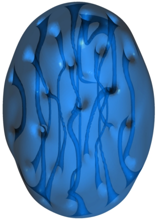


Quantum Turbulence (QT) in BEC

BEC = perfect superfluid system for QT

- pure superfluid system,
- highly controlable (phase imprinting),
- larger vortex cores than in He,
- finite size $\rightarrow$ rotating/oscillating QT.



Recent experiments/Special volumes

- Henn et al., J. Low Temp. Phys., 2010.
- Seman et al., Laser Phys., 2011.
- (Edts) Tsubota & Halperin, Elsevier, 2009.
- (Edts) Barenghi & Sergeev, Springer, 2008.

Outline

Implementation of the new method

FreeFem++ (www.freefem.org)

Free Generic PDE solver using finite elements (2D and 3D)

- powerful mesh generator,
- easy to implement weak formulations,
- use combined P1, P2 and P4 elements,
- complex matrices available,
- mesh interpolation and adaptivity.

You are welcome to participate in the:

FreeFem++ Days, Paris, December, every year.
Graduate course at the Fields Institute, March 2016.

FreeFem++: syntax close to mathematics

Switch from one finite-elemnt (P^1) to another (P^4) in one line !

- create a mesh and a finite element space

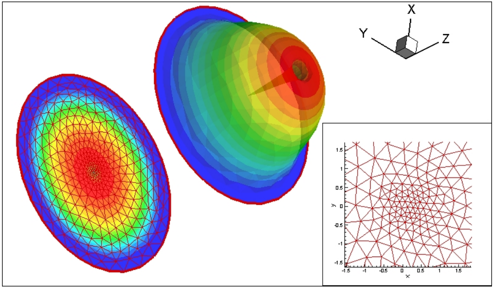
```
border circle(t=0,2*pi)
{label=1;x=Rmax*cos(t);y=Rmax*sin(t);};
mesh Th=buildmesh(circle(nbseg));
fespace Vh(Th,P1);    fespace Vh4(Th,P4);
```

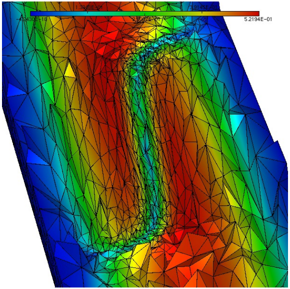
- compute the gradient for $X = H^1$

```
Vh<complex> ug,v ;
problem AGRAD(ug,v) =
int2d(Th)(ug*v + dx(ug)*dx(v)+dy(ug)*dy(v))
- int2d(Th)(Ctrap*un*v)
- int2d(Th)(CN*real(un*conj(un))*un*v)
+ ...
+ on(1,ug=0);

AGRAD;
```

FreeFem++: mesh adaptivity (2D and 3D)





Mesh adaptivity with FreeFem++

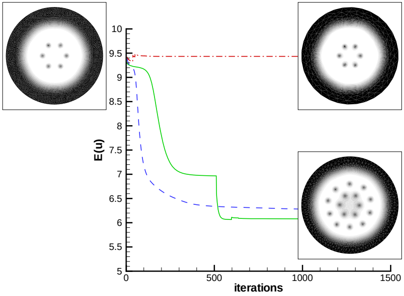
I. Danaila, F. Hecht, J. Computational Physics, 2010.

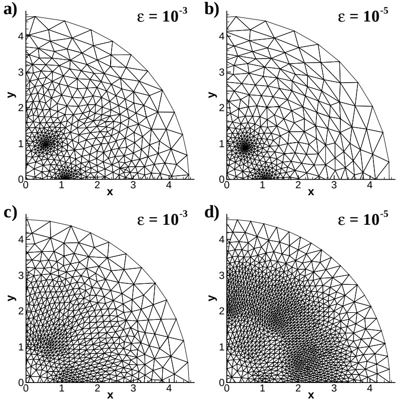
G. Vergez, I. Danaila, S. Auliac, F. Hecht, Comput. Phys. Comm., 2016.

- Good refinement strategy $\chi = [u_r, u_i]$;

$V_{trap} = \frac{1}{2}r^2 + \frac{1}{4}r^4$,

$\Omega = 2 \quad \rightarrow \quad \Omega = 2.5.$

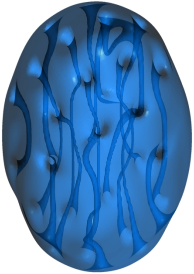


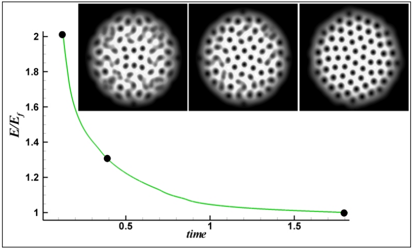


Outline

Computation of stationary states

- used as initial conditions for time-dependent simulations,
- analyse meta-stable states observed in experiments,
- used for stability analysis (Bogoliubov-de Gennes).





Minimisation of the GP energy

$\mathcal{D} \subset \mathbb{R}^3$ et $u = 0$ on $\partial\mathcal{D}$

$$E(u) = \int_{\mathcal{D}} \frac{1}{2}|\nabla u|^2 + C_{trap}(\mathbf{r})|u|^2 + \frac{C_g}{2}|u|^4 - iC_\Omega \int_{\mathcal{D}} u^* \mathbf{A}^t \cdot \nabla u$$

under the unitary norm constraint

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

(meta-)stable states :: local minima of the energy min $E(u)$

Numerical methods for the stationary GP equation

- Imaginary time propagation.
- Direct minimization of the energy $\longrightarrow$ Sobolev gradients.

Imaginary time propagation (1)

Normalized gradient flow (Bao and Du, 2004)

Aftalion & Du, 2001; Bao & Tang, 2003; Bao & Zhang, 2005; Bao & Shen, 2008. (review paper).

$$\frac{\partial u}{\partial t} = -\frac{1}{2}\nabla_{L^2} E(u)$$

$$\frac{\partial u}{\partial t} - \frac{1}{2}\Delta u + C_{trap} u + C_g |u|^2 u - i C_\Omega \mathbf{A}^t \cdot \nabla u = 0$$

Remark on the associated numerical method

- Conserve the gradient flow structure $\Longrightarrow$ explicit Euler method (very poor convergence)!

$$\frac{u_{n+1} - u_n}{\delta t} = -\frac{1}{2}\nabla_{L^2} E(u_n)$$

Imaginary time propagation (2)

Backward-Euler (BE) method (Bao and Du, 2004)

- Use semi-implicit integration methods $\Longrightarrow$ pseudo-time integration (or imaginary-time methods)!

$$\frac{\tilde{u} - u_n}{\delta t} = \frac{1}{2}\Delta \tilde{u} - C_{\text{trap}}\tilde{u} - C_g |u_n|^2 \tilde{u} + iC_\Omega \mathbf{A}^t \cdot \boldsymbol{\nabla} \tilde{u}$$

- Impose the constraint : $\|u\|_2 = \int_{\mathcal{D}} |u|^2 = 1$ $\Longrightarrow$ normalization

$$u_{n+1} = \frac{\tilde{u}(t_{n+1})}{\|\tilde{u}(t_{n+1})\|_2}$$

Remarks: implemented in FreeFem++!

- The gradient flow structure is lost at the discrete level!
- The solution evolves far from the manifold of the constraint!

Sobolev gradient descent method (1)

Normalized gradient flow

$$\frac{\partial u}{\partial t} = -\nabla E(u)$$

$$-\frac{1}{2}\nabla_{L^2} E(u) = \frac{1}{2}\Delta u - C_{trap} u - C_g |u|^2 u + i C_\Omega \mathbf{A}^t \cdot \boldsymbol{\nabla} u$$

New ideas

1. Define a "better gradient" for the descent method.
2. Evolve the iterates close to the spherical manifold.
3. Use Riemannian Optimization for the conjugate-gradient.

(1) Sobolev gradient: a better gradient

I. Danaila and P. Kazemi, SIAM J. Sci Computing, 2010.

- physical insight from another form of the energy

$$E(u) = \int_{\mathcal{D}} \frac{1}{2}|\nabla u + iC_\Omega \mathbf{A} u|^2 + \left(C_{trap} - \frac{C_\Omega^2 r^2}{2}\right)|u|^2 + \frac{c_g}{2}|u|^4$$

- mathematical proof for a new inner product

$$\langle u, v\rangle_{H_A} = \int_{\mathcal{D}} \langle u, v\rangle + \langle \nabla_A u, \nabla_A v\rangle, \ \ \nabla_A = \nabla + iC_\Omega \mathbf{A}$$

- equivalence

$$H_A(\mathcal{D}, \mathbb{C}) = H^1(\mathcal{D}, \mathbb{C}) \subset L^2(\mathcal{D}, \mathbb{C})$$

- provides a better preconditioner.

(2) Stay closed to the manifold: projected gradient

I. Danaila and P. Kazemi, SIAM J. Sci Computing, 2010.

- Spherical manifold $\mathcal{M} := \left\{ u \in H_0^1(\mathcal{D}) \ : \ \|u\|_2 = 1 \right\}$.
- Gradient method

$$u_{n+1} = u_n - \tau_n G_n, \quad n = 0, 1, \dots,$$

$$\|u_{n+1}\|_2^2 = \|u_n - \tau_n G_n\|_2^2 = \|u_n\|_2^2 - 2\tau_n \Re\langle u_n, G_n \rangle_{L^2} + \tau_n^2 \|G_n\|_2^2,$$

- Projected gradient

$P_{u_n,X} G_n \in \mathcal{T}_{u_n}\mathcal{M} = \left\{ v \in H_0^1(\mathcal{D}) \ : \ \langle u_n, v \rangle_{L^2} = 0 \right\}$

$$P_{u_n,X} G_n = G_n - \lambda v_X, \qquad \lambda = \frac{\Re\langle u_n, G_n \rangle_{L^2}}{\Re\langle u_n, v_X \rangle_{L^2}},$$

$$\langle v_X, v \rangle_X = \langle u_n, v \rangle_{L^2}, \quad \forall v \in X$$

(3) Riemanian gradient method

P.-A. Absil, R. Mahony and R. Sepulchre, Optimization Algorithms on Matrix Manifolds, Princeton (2008).

Retraction operator: $\mathcal{R}_u \; : \; \mathcal{T}_u\mathcal{M} \to \mathcal{M} \; \mathcal{R}_u(\xi) = \frac{u+\xi}{\|u+\xi\|_2}$

Riemanian gradient method

$$\text{(RG)} \qquad u_{n+1} = \mathcal{R}_{u_n}\left(-\tau_n P_{u_n,H_A} G_n\right), \qquad n = 0, 1, \ldots . \qquad (1)$$

$$\tau_n = \underset{\tau>0}{argmin}\, E\left(\mathcal{R}_{u_n}(-\tau P_{u_n,H_A} G_n)\right). \qquad (2)$$

Constrained minimization $\Longrightarrow$ Unconstrained minimization on $\mathcal{M}$!!!

(3) Riemanian conjugate-gradient method

I. Danaila, B. Protas, SIAM J. Sci. Computing, 2017.

$$\text{(RCG)} \qquad u_{n+1} = \mathcal{R}_{u_n}\left(-\tau_n d_n\right), \qquad n = 0, 1, \ldots, \tag{3}$$

$$\begin{aligned} d_0 &= -P_{u_0,H_A} G_0, \\ d_n &= -P_{u_n,H_A} G_n + \beta_n \mathcal{T}_{-\tau_{n-1} d_{n-1}}(d_{n-1}), \qquad n = 1, 2, \ldots \end{aligned} \tag{4}$$

- Polak-Ribière momentum term

$$\beta_n = \beta_n^{PR} := \frac{\left\langle P_{u_n,H_A} G_n, \left(P_{u_n,H_A} G_n - \mathcal{T}_{-\tau_{n-1} d_{n-1}} P_{u_{n-1},H_A} G_{n-1}\right) \right\rangle_{H_A}}{\left\langle P_{u_{n-1},H_A} G_{n-1}, P_{u_{n-1},H_A} G_{n-1} \right\rangle_{H_A}}. \tag{5}$$

- optimal descent step (Brent's method)

$$\tau_n = \underset{\tau > 0}{argmin}\, E\left(\mathcal{R}_{u_n}(-\tau d_n)\right) \tag{6}$$

(3) Riemanian conjugate-gradient method

I. Danaila, B. Protas, SIAM J. Sci. Computing, 2017.

$$\text{(RCG)} \qquad u_{n+1} = \mathcal{R}_{u_n}\left(-\tau_n\, d_n\right), \qquad n = 0, 1, \ldots, \qquad (3)$$

$$d_0 = -P_{u_0,H_A} G_0$$

Implementation in the FreeFem++ toolbox ... in progress!

- looks horrible, but ...
- easy and elegant implementation (like the math formulation)!

$$\beta_n = \beta_n^{PR} := \frac{\left\langle P_{u_n,H_A} G_n, \left(P_{u_n,H_A} G_n - \mathcal{T}_{-\tau_{n-1} d_{n-1}} P_{u_{n-1},H_A} G_{n-1}\right) \right\rangle_{H_A}}{\left\langle P_{u_{n-1},H_A} G_{n-1}, P_{u_{n-1},H_A} G_{n-1} \right\rangle_{H_A}}. \qquad (5)$$

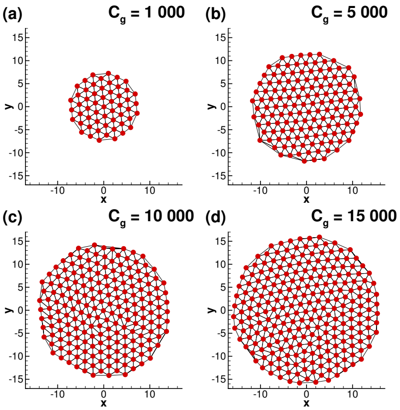
- optimal descent step (Brent's method)

$$\tau_n = \underset{\tau > 0}{argmin}\, E\left(\mathcal{R}_{u_n}(-\tau d_n)\right) \qquad (6)$$

BEC with dense Abrikosov lattice (2)

Harmonic potential and high angular velocities:
$C_{\text{trap}} = r^2/2$, $C_g = 1000$, $C_\Omega = 0.9$.

BEC with dense Abrikosov lattice (3)



Harmonic potential and high angular velocities: $C_{\text{trap}} = r^2/2$, $C_g = 1000, 5000, 10000, 15000$, $C_\Omega = 0.9$.

- Identification of vortices with FreeFem++.
- Post-processing measuring r_v and b_v.
- Can be used with experimental data.

Outline

Bogoliubov-de Gennes modes: linearisation of the GP time-dependent equation

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 equations: linear eigenvalue problem

$$[A_1 A_2] \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \hbar\omega \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix}$$

$$A_1 = \begin{pmatrix} H - \mu_1 + 2g_{11}|\phi_1|^2 + g_{12}|\phi_2|^2 & g_{11}\phi_1^2 \\ -g_{11}(\phi_1^*)^2 & -\left(H - \mu_1 + 2g_{11}|\phi_1|^2 + g_{12}|\phi_2|^2\right) \\ g_{21}\phi_1^*\phi_2 & g_{21}\phi_1\phi_2\phi_2^2 \\ -g_{21}\phi_1^*\phi_2^* & -g_{21}\phi_1\phi_2^* \end{pmatrix}$$

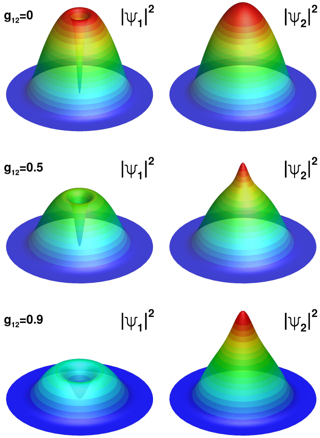
$$A_2 = \begin{pmatrix} g_{12}\phi_1\phi_2^* & g_{12}\phi_1\phi_2 \\ -g_{12}\phi_1^*\phi_2^* & -g_{12}\phi_1^*\phi_2 \\ H - \mu_2 + g_{21}|\phi_1|^2 + 2g_{22}|\phi_2|^2 & g_{22}\phi_2^2 \\ -g_{22}(\phi_2^*)^2 & -\left(H - \mu_2 + g_{21}|\phi_1|^2 + 2g_{22}|\phi_2|^2\right) \end{pmatrix}$$

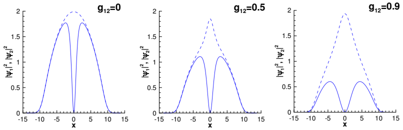
$$H = -\frac{\hbar^2}{2m}\nabla^2 + V_{\text{trap}}$$

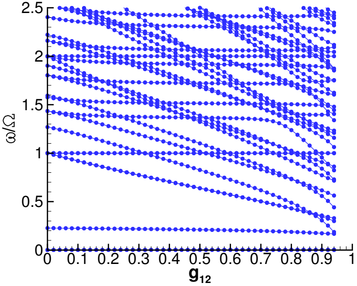
- Interface with ARPACK to solve this problem!

BdG 2d: Vortex-Antidark Solitary Waves

I. Danaila, M. A. Khamehchi, V. Gokhroo, P. Engels, P. G. Kevrekidis, PRA, 2016.

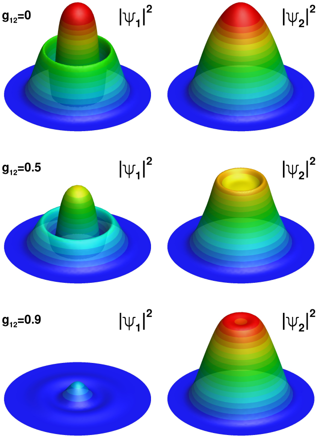


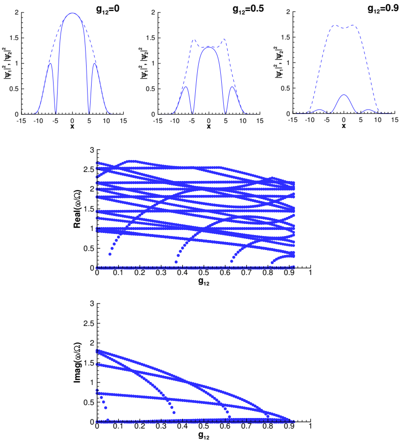




BdG 2d: Ring-Antidark-Ring Solitary Waves

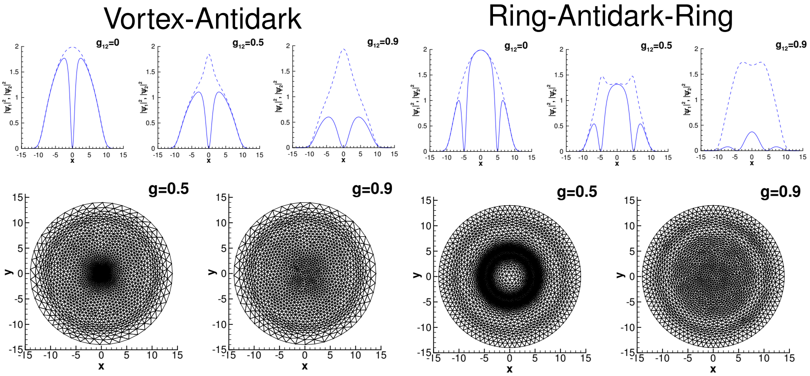
I. Danaila, M. A. Khamehchi, V. Gokhroo, P. Engels, P. G. Kevrekidis, PRA, 2016.





BdG 2d: mesh adaptivity

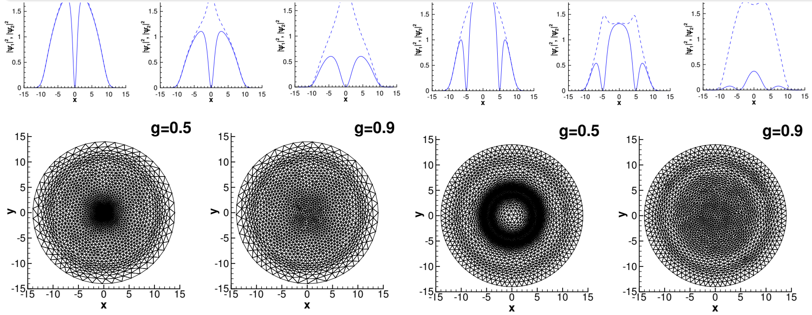
I. Danaila, M. A. Khamehchi, V. Gokhroo, P. Engels, P. G. Kevrekidis, PRA, 2016.



BdG 2d: mesh adaptivity

The BdG FreeFem++ toolbox ... to be submitted to CPC!

- looks horrible, but ...
- easy and elegant implementation (like the math formulation)!



Outline

Time-dependent GP equation (with rotation)

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V_{\text{trap}}\psi + g|\psi|^2\psi - i\hbar\Omega\mathbf{A}^t\cdot\boldsymbol{\nabla}\psi$$

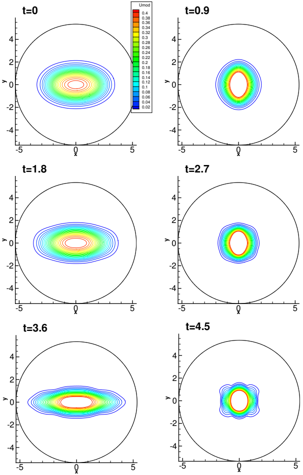
Different numerical schemes

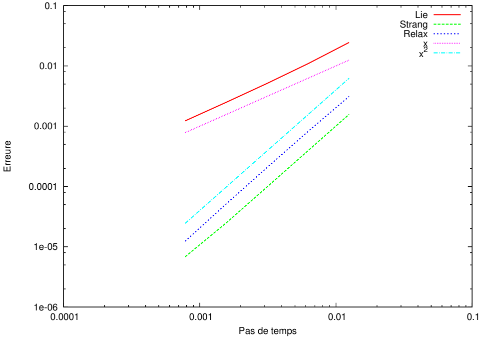
- Splitting schemes: Lie and Strang.
- Relaxation scheme (C. Besse, SIAM J. Num. Analysis, 2004).
- Crank-Nicolson.

P^1 or P^2 finite elements.

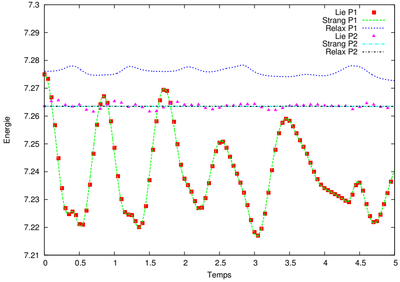
Validation on academic cases (no rotation) (1)

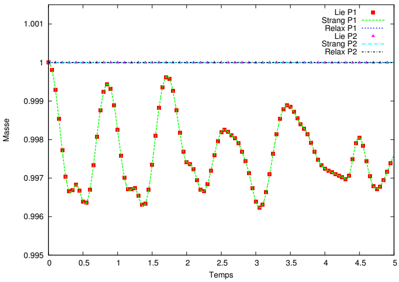
$a_x = 1,\ a_y = 4, \beta = 20 \Longrightarrow (t = 0)$ we set $a_x = 4$ and $a_y = 16$



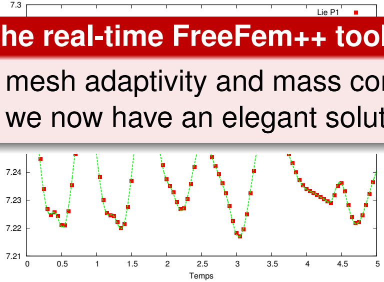


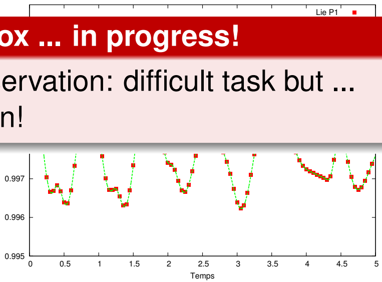
Validation on academic cases (no rotation) (2)





Validation on academic cases (no rotation) (2)





The real-time FreeFem++ toolbox ... in progress!

- mesh adaptivity and mass conservation: difficult task but ...
- we now have an elegant solution!

Outline

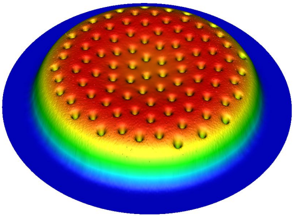
FreeFem++ Toolbox (www.freefem.org)

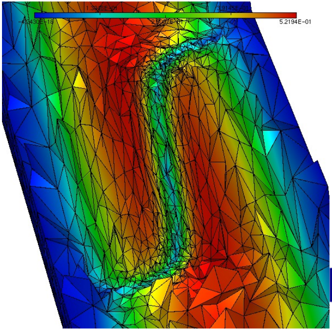
Developers: G. Vergez, I. Danaila, F. Hecht.
Computer Physics Communications, 2016 (with programs)!

GPFEM: finite element solver

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

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





BEC with vortices: GPS + ADIOS

Thanks to A. Mouton.
a psychedelic walk inside a BEC