10 Dec. 2014, LJLL, Paris

FreeFem++ workshop : BECASIM session

Numerical simulation of the Gross-Pitaevskii equation by pseudo-spectral and finite element methods – comparison of GPS code and FreeFem++

Atsushi Suzuki

LJLL, INRIA-Nancy

stationary state of Gross-Pitaevskii equation 1/3

time-dependent Gross-Pitaevskii equation in 2D, $\mathcal{D} \subset \mathbb{R}^2$

$$
\begin{aligned}
&i\frac{\partial}{\partial t}\phi(t) = -\frac{1}{2}\triangle\phi(t) - \Omega i\left(\begin{smallmatrix} y \\ -x \end{smallmatrix}\right)\cdot\nabla\phi(t) + V\phi(t) + \beta|\phi(t)|^2\phi(t) \ \text{ in } \mathcal{D}\times(0,T) \\
&\phi(0,\cdot) = \phi_0
\end{aligned}
$$

stationary state is given by the minimization of the energy

$$
\begin{aligned}
&\phi \in H_0^1(\mathcal{D},\mathbb{C}) \\
&E(\phi) = \int_{\mathcal{D}} \frac{1}{2}|\nabla\phi|^2 + V|\phi|^2 + \frac{\beta}{2}|\phi|^4 - \Omega i\left(\begin{smallmatrix} y \\ -x \end{smallmatrix}\right)\cdot\nabla\phi\,\bar{\phi} \\
&\min_{||\phi||=1} E(\phi).
\end{aligned}
$$

Remark on energy of the angular momentum term

$\int_{\mathcal{D}} \left(\begin{smallmatrix} y \\ -x \end{smallmatrix}\right)\cdot\nabla\phi\,\bar{\phi} \ \in \mathbb{R}$

$$
\int_{\mathcal{D}}(y\partial_x\phi - x\partial_y\phi)\bar{\phi} = -\int_{\mathcal{D}}(\partial_x(y\bar{\phi}) - \partial_y(x\bar{\phi}))\phi + \int_{\partial\mathcal{D}}(y\,n_x - x\,n_y)\phi\bar{\phi}
$$

$\mathcal{D} = \{x\,;\,|x| < R\} \quad \Rightarrow \left(\begin{smallmatrix} n_x \\ n_y \end{smallmatrix}\right) = \left(\begin{smallmatrix} x \\ y \end{smallmatrix}\right)/R$ on $\partial\mathcal{D} \quad \Rightarrow \quad y\,n_x - x\,n_y = 0.$

$$
\mathrm{Re}\int_{\mathcal{D}}(y\partial_x\phi - x\partial_y\phi)\bar{\phi} = 0
$$

stationary state of Gross-Pitaevskii equation 2/3

minimization problem

$$E(\phi) = \int_{\mathcal{D}} \frac{1}{2}|\nabla\phi|^2 + V|\phi|^2 + \frac{\beta}{2}|\phi|^4 - \Omega i \binom{y}{-x} \cdot \nabla\phi\,\bar{\phi}$$

$$\min_{||\phi||=1} E(\phi).$$

equivalent nonlinear eigen value problem

find $\lambda \in \mathbb{R},\ \phi \in H_0^1(\mathcal{D}\,;\,\mathbb{C})$

$$\lambda\phi = -\frac{1}{2}\triangle\phi - \Omega i \binom{y}{-x} \cdot \nabla\phi + V\phi + \beta|\phi|^2\phi$$

$$||\phi|| = 1$$

λ : chemical potential

$$\lambda = \int_{\mathcal{D}} \lambda\phi\,\bar{\phi} = \int_{\mathcal{D}} -\triangle\phi\bar{\phi} - \Omega i \binom{y}{-x} \cdot \nabla\phi\,\bar{\phi} + V\phi\,\bar{\phi} + \beta|\phi|^2\phi\,\bar{\phi}$$

$$= E(\phi) + \int_{\mathcal{D}} \frac{\beta}{2}|\phi|^4$$

stationary state of Gross-Pitaevskii equation 3/3

minimization problem

$$E(\phi) = \int_{\mathcal{D}} \frac{1}{2}|\nabla\phi|^2 + V|\phi|^2 + \frac{\beta}{2}|\phi|^4 - \Omega i \binom{y}{-x} \cdot \nabla\phi\,\bar{\phi}$$

$$\min_{||\phi||=1} E(\phi).$$

normalized gradient flow (imaginary time method : $i\,t \;\rightarrow\; \tilde{t}$)

$$\frac{\partial\phi}{\partial t} = -\frac{1}{2}\frac{\partial E(\phi)}{\partial\phi} = +\frac{1}{2}\triangle\phi + \Omega i \binom{y}{-x} \cdot \nabla\phi - V\phi - \beta|\phi|^2\phi \quad t \in [t_n, t_{n+1})$$

$$\phi(t_{n+1}, \cdot) = \frac{\phi(t_{n+1}^-, \cdot)}{||\phi(t_{n+1}^-, \cdot)||}$$

$$\phi(0, \cdot) = \phi_0, \quad ||\phi_0|| = 1$$

potential

$$V(x,y) = \frac{1-\alpha}{2}(x^2+y^2) + \frac{\kappa}{4}(x^2+y^2)^2$$

$\alpha = 1.2$, $\kappa = 0.3$

appropriate initial condition : Thomas-Fermi approximation

discretization scheme

semi-implicit Euler scheme for time discretization

$$\frac{\tilde{\phi}^{n+1} - \phi^n}{\Delta t} = +\frac{1}{2}\triangle\tilde{\phi}^{n+1} + \Omega i \begin{pmatrix} y \\ -x \end{pmatrix} \cdot \nabla\tilde{\phi}^{n+1} - V\tilde{\phi}^{n+1} - \beta|\phi^n|^2\tilde{\phi}^{n+1}$$

$$\phi^{n+1} = \frac{\tilde{\phi}^{n+1}}{||\tilde{\phi}^{n+1}|}$$

$$\phi^0 = \phi_0, \quad ||\phi_0|| = 1$$

Space discretization

- pseudo-spectral method

  expansion by Fourier basis + collocation method

- finite element method

  P1 element + mesh adaptation by FreeFem++

pseudo-spectral method 1/2

$\mathcal{D} = (-\pi, \pi) \times (-\pi, \pi)$ and assume ϕ is periodic in x- and y-directions

expansion by Fourier basis

$$\phi(x, y) \equiv \sum_{-N/2 \leq k < N/2} \hat{\phi}_k(y) e^{i\, kx}$$

$$\hat{\phi}_k(y) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \phi(x, y) e^{-i\, kx}$$

$$\sim \frac{1}{2\pi} \frac{2\pi}{N} \sum_{0 \leq p < N} \phi(x_p, y) e^{-i\, kx_p}, \quad x_p = -\pi + \frac{2\pi}{N} p$$

$$\partial_x^2 \phi(x, y) = \partial_x^2 \sum_k \hat{\phi}_k(y) e^{i\, kx} = \sum_k (-k^2) \hat{\phi}_k(y) e^{i\, kx}$$

$$y \partial_x \phi(x, y) = y \partial_x \sum_k \hat{\phi}_k(y) e^{i\, kx} = y \sum_k i\, k \hat{\phi}_k(y) e^{i\, kx}$$

at collocation points (x_r, y_s) (same as integration points)

$$\frac{1}{\Delta t} - \frac{1}{2} \triangle - \Omega i \begin{pmatrix} y_r \\ -x_s \end{pmatrix} \cdot \nabla + V(x_r, y_s) + \beta |\phi_{r,s}^n|^2$$

acts to $\phi_{r,s}^{n+1}$ and it is evaluated using

$$\partial_x^2 \phi(x, y)|_{(x_r, y_s)} = \sum_k (-k^2) \frac{1}{N} \sum_p \phi_{p,s} e^{-i\, kx_p} e^{i\, kx_r}$$

$$y \partial_x \phi(x, y)|_{(x_r, y_s)} = y_s \sum_k i\, k \frac{1}{N} \sum_p \phi_{p,s} e^{-i\, kx_p} e^{i\, kx_r}$$

these computations are realized by 1D FFT (`fftw` library)

pseudo-spectral method 2/2

The operator on collocation points (x_r, y_s)

$$(\frac{1}{\Delta t} - \frac{1}{2}\triangle - \Omega i\binom{y_r}{-x_s} \cdot \nabla + V(x_r, y_s) + \beta|\phi^n_{r,s}|^2)\phi^{n+1}_{r,s}$$

- collocation method for angular momentum, potential and nonlinear interaction terms simplifies the code

- there is no explicit matrix expression of the linear operator. The matrix is dense because of forward and backward FFTs.

Linear solver
Krylov subspace method with “Thomas-Fermi preconditioner” (X. Antoine, R. Duboscq)

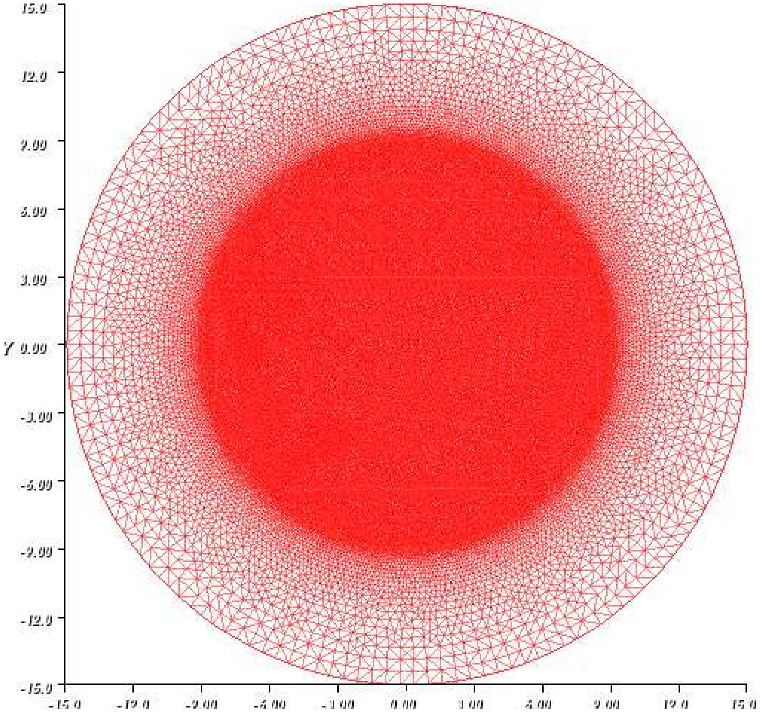
$$(P_{r,s})^{-1} = (\frac{1}{\Delta t} + V(x_r, y_s) + \beta|\phi^n_{r,s}|^2)^{-1}$$

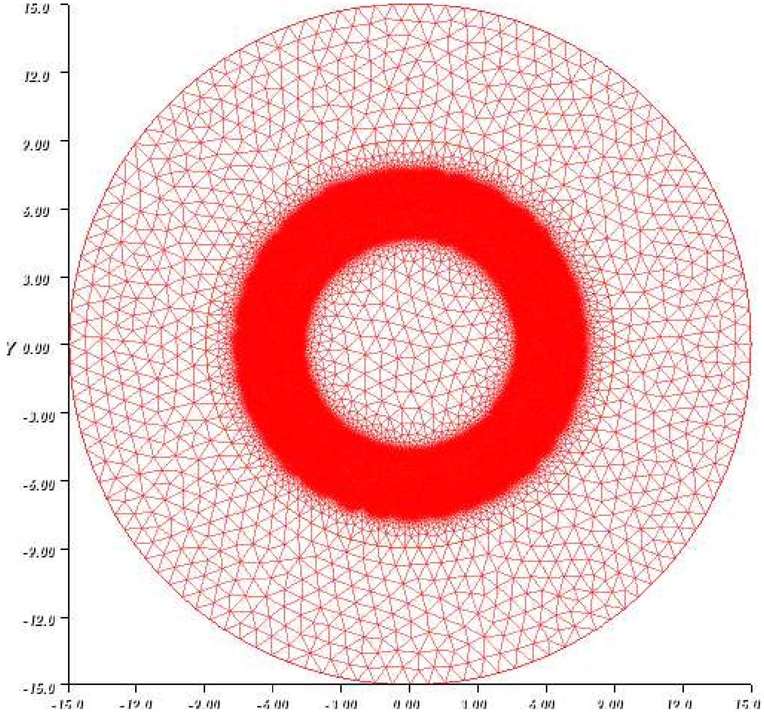
GPS code (P. Parnaudeau, J-M. Sac-Epée, A. Suzuki)
BiCGStab, GCR solver
written by Fortran90 using `fftw` and `OpenMP` + `MPI` (for 3D)
cut-off with some radius to satisfy homogeneous Dirichlet boundary conditions
parallelization technique is encapsulated in vector-matrix product and inner product

finite element method

```
real dt=0.005, alpha=1.2,kappa=0.3;
func V=(1.0-alpha)/2.0*(x*x+y*y)+kappa/4.0*(x*x+y*y)*(x*x+y*y);
real Omega=3.5, beta=1000.0;
func Vtrap=(x*x+y*y)*0.5;
real muTF=sqrt(beta/pi);
func rhoTF=max(0.0,(muTF-Vtrap)/beta);
fespace Vh(Th,P1);
Vh<complex> u,v,u0;
Vh zz;
u0=sqrt(rhoTF);
varf gpe(u,v)=int2d(Th)(1.0/dt*u*conj(v)
                        +0.5*(dx(u)*conj(dx(v))+dy(u)*conj(dy(v)))
                        -Omega*1i*(y*dx(u)-x*dy(u))*conj(v)
                        +(V+beta*u0*conj(u0))*u*conj(v))+on(1,u=0.0);
varf rhs(u,v)=int2d(Th)(1.0/dt*u0*conj(v))+on(1,u=0.0);
for (int it=0; it < 10000; ++it) {
  matrix<complex> A=gpe(Vh,Vh,tgv=-1);
  set(A,solver=sparsesolver,tgv=-1);
  complex[int] b=rhs(0,Vh,tgv=-1);
  complex[int] w=A^-1*b;
  zz=real(u0)*real(u0)+imag(u0)*imag(u0);
  u0=u0/sqrt(int2d(Th)(zz));
}
```

mesh adaptation after some time steps





Comparison of performance

FreeFem++, `UMFPACK` $\Delta t = 0.005$, $n = 274,059 \sim 523^2$

matrix build	RHS build	factorization	fw/bw subst.	energy comput.	# CPU
7.362	0.732	2.767	0.436	5.562	1
FreeFem++, `dissection` $\Delta t = 0.005$, $n = 274,059 \sim 523^3$					
7.468	0.689	1.884	0.107	4.665	1
7.316	0.711	0.805	0.112	4.670	4
GPS/`fftw`, $\Delta t = 0.005$, $n = 512^2$, #itr GCR=42					
7.1965				0.0835	1
3.254/12.974				0.049/0.197	4
GPS/`fftw`, $\Delta t = 0.0005$, $n = 512^2$, #itr GCR=8					
0.527				0.0809	1
0.332/1.319				0.047/0.198	4

mac mini 2012, Intel Core i7 i7-3615QM @ 2.3GHz + 16G mem.

Intel ifort 14.0.4

Newton-Raphson method for nonlinear eigen value problem 1/3

Is stationary state obtained by gradient flow?

- dependence of stationary state on the initial condition seems to be not clear.
- How to understand stationary state?

Newton-Raphson nonlinear solver approach

$$F_1(\phi,\lambda) := \lambda\phi + \frac{1}{2}\triangle\phi + \Omega\, i\binom{y}{-x}\cdot\nabla\phi - V\phi - \beta|\phi|^2\phi$$

$$F_2(\phi,\lambda) := \lambda(||\phi||^2 - 1)$$

$\binom{\phi^0}{\lambda^0}$: given by gradient flow solution, with computing λ^0 as chemical potential

loop $n = 0, 1, 2, \cdots$

find $\binom{\delta}{\varepsilon}$ by solving a linear system:

$$(\lambda^n + \frac{1}{2}\triangle + \Omega\, i\binom{y}{-x}\cdot\nabla - V - 2\beta|\phi^n|^2)\delta - \beta(\phi^n)^2\bar{\delta} + \varepsilon\phi^n = F_1(\phi^n,\lambda^n)$$

$$\lambda^n \int_{\mathcal{D}} (\bar{\phi}^n\delta + \phi^n\bar{\delta}) + \varepsilon(||\phi^n||^2 - 1) = F_2(\phi^n,\lambda^n)$$

$$\binom{\phi^{n+1}}{\lambda^{n+1}} = \binom{\phi^n}{\lambda^n} - \binom{\delta}{\varepsilon}$$

Newton-Raphson method for nonlinear eigen value problem 2/3

Linear system with $(N+1)\times(N+1)$ matrix

$$(\lambda^n + \frac{1}{2}\triangle + \Omega\, i\binom{y}{-x}\cdot\nabla - V - 2\beta|\phi^n|^2)\delta - \beta(\phi^n)^2\bar{\delta} + \varepsilon\phi^n = F_1(\phi^n,\lambda^n)$$

$$\lambda^n\int_{\mathcal{D}}(\bar{\phi}^n\delta + \phi^n\bar{\delta}) + \varepsilon(||\phi^n||^2 - 1) = F_2(\phi^n,\lambda^n)$$

block factorization strategy using $N\times N$ linear solver:

solve two linear systems

$$(\lambda^n + \frac{1}{2}\triangle + \Omega\, i\binom{y}{-x}\cdot\nabla - V - 2\beta|\phi^n|^2)\sigma - \beta(\phi^n)^2\bar{\sigma} = \phi^n$$

$$(\lambda^n + \frac{1}{2}\triangle + \Omega\, i\binom{y}{-x}\cdot\nabla - V - 2\beta|\phi^n|^2)\gamma - \beta(\phi^n)^2\bar{\gamma} = F_1(\phi^n,\lambda^n)$$

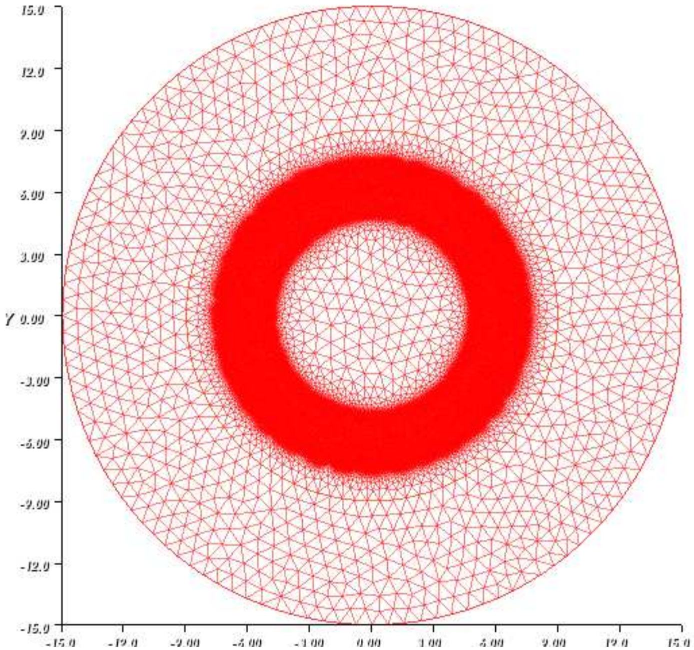
solve Schur complement problem

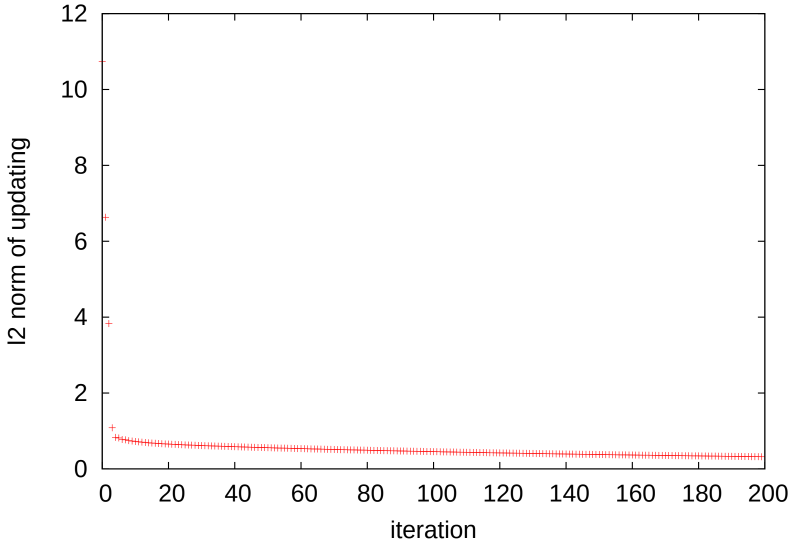
$$s\varepsilon = \lambda^n(||\phi^n||^2 - 1) - \lambda^n\int_{\mathcal{D}}\bar{\phi}^n\gamma + \phi^n\bar{\gamma}$$

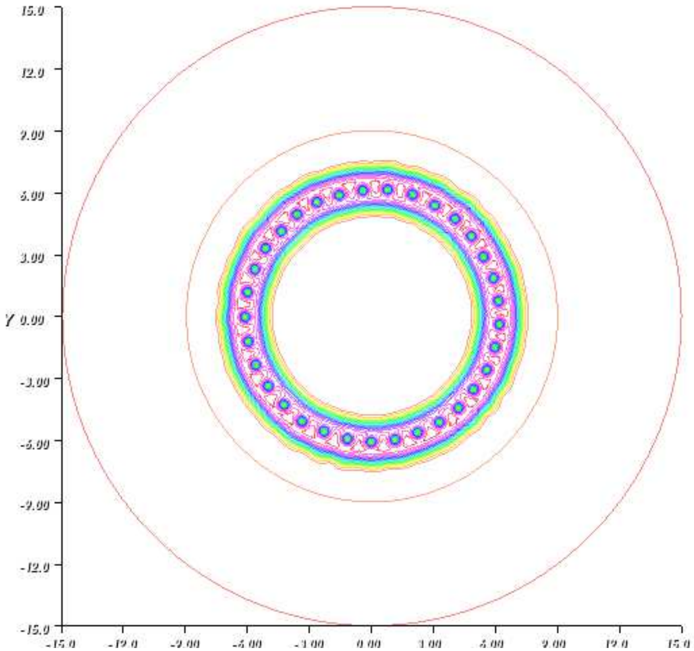
backward substitution

$$(\lambda^n + \frac{1}{2}\triangle + \Omega\, i\binom{y}{-x}\cdot\nabla - V - 2\beta|\phi^n|^2)\gamma - \beta(\phi^n)^2\bar{\gamma} = F_1(\phi^n,\lambda^n) - \varepsilon\phi^n$$

Newton-Raphson method for nonlinear eigen value problem 3/3







	$E(\phi)$	λ	# vortex
GPS	-115.231	-108.223	38
FreeFem++	-108.022	-100.947	33