Numerical tools for superfluids

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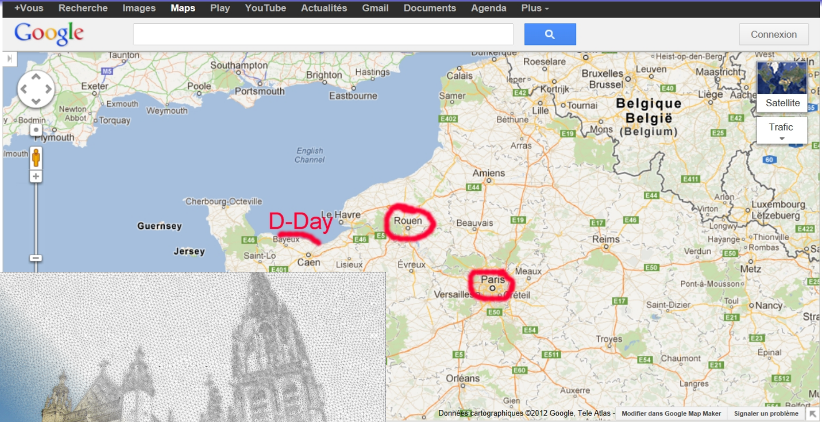
Workshop and Summer School Bridging classical and quantum turbulence, Cargése, July 3-15, 2023.

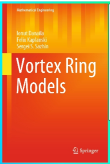
Where is Rouen?



Rouen Cathedral
... meshed with FreeFem++

ANR LMRS

Scientific Computing at LMRS, Rouen Normandy



Fluids: vortex rings

Naviers-Stokes equations

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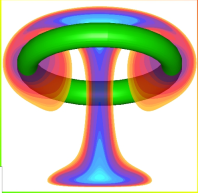
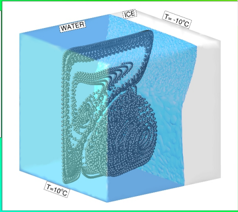


Liquid-solid phase-change systems

Naviers-Stokes-Boussinesq equations

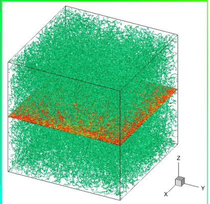
http://lmrs-num.math.cnrs.fr



Super-Fluids : Quantum Turbulence (He)
Bose-Einstein Condensates

Schrödinger/ Gross-Pitaevskii equations

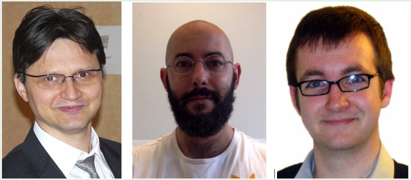
http://qute-hpc.math.cnrs.fr/



Scientific Computing group

Research Group: Numerical methods and Applications

I. Danaila, F. Luddens, C. Lothodé



http://lmrs-num.math.cnrs.fr/

ANR project QUTE-HPC: QUantum Turbulence Exploration by High-Performance Computing

Agence Nationale de la Recherche

ANR Project QUTE-HPC (2019-2023)

10 members, 5 Physics/5 Mathematics

- (HPC) parallel codes for QT :: open source,
- huge simulations of physical configurations (compare with our own experiments).

http://qute-hpc.math.cnrs.fr/

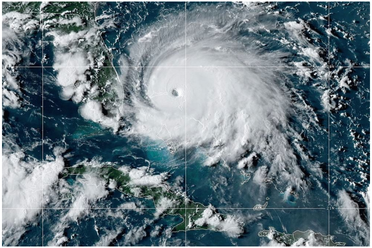
Outline

1. **From vortices to turbulence**
   - Vortices in fluids and superfluids
   - Classical Turbulence vs Quantum Turbulence
2. **Numerical methods for the GP equation**
   - Computation of stationary states of the GP equation
   - Computation of Bogoliubov-de Gennes modes
3. **Adaptive finite-element codes for the GP equation**
4. **Spectral code for the GP equation**
5. **Simulations of Quantum Turbulence with GPS**
6. **Numerical models for superfluid helium**

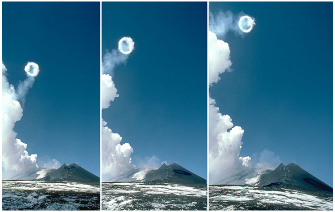
Vortices in classical (or normal) fluids

velocity-pressure $\to$ vorticity

Aircraft trailing vortices



Dorian Hurricane



Vortex rings (Etna volcano)

Niagara Falls 2019

Vortices in fluids and superfluids

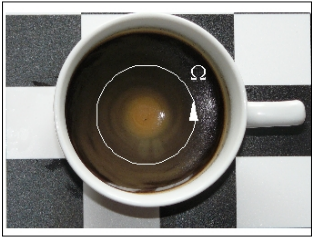
classical fluids

- easy intuition (velocity - pressure)
- complicated math description

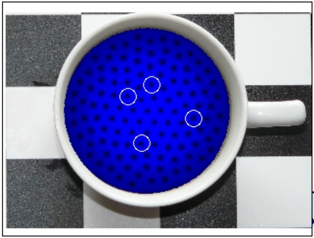
superfluids

- difficult intuition
(vanishing viscosity)
- simple math description
(wave function)

solid rotation



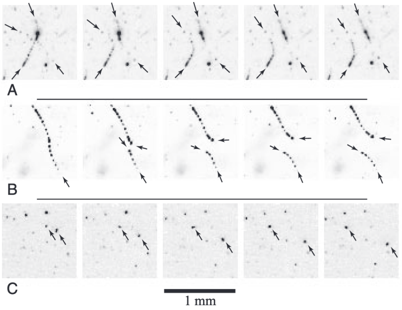
local rotation



Vortices in quantum flows

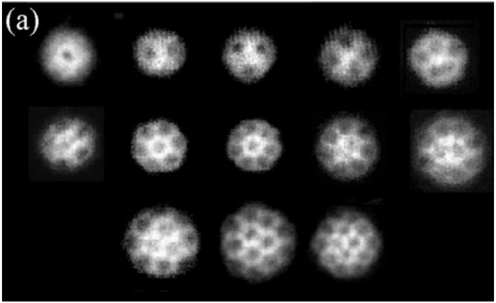
macroscopic wave-function $\rightarrow$ velocity-pressure

Superfluid Helium
$(T < T_\lambda = 2.17K)$



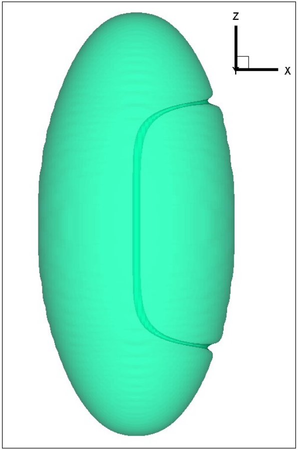
Reconnection of vortex lines (Maryland, USA, Bewley et al., PNAS, 2008).

Bose-Einsten condensate
$(T \sim 500nK)$



Vortices in rotating BEC (LKB, ENS, France, Madison et al., PRL, 2000).

Identification of a quantized vortex



Macroscopic description

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

(Madelung transform) $\psi = \sqrt{\rho(r)/m} e^{i\theta(r)}$

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

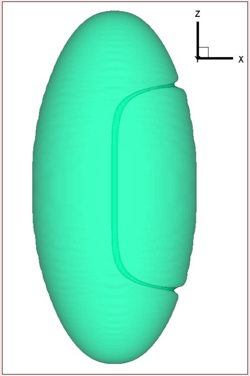
$$v(r) = \frac{\hbar}{m}\nabla\theta = i\frac{\hbar}{2m}\frac{\psi\nabla\overline{\psi} - \overline{\psi}\nabla\psi}{\rho}$$

- quantified circulation

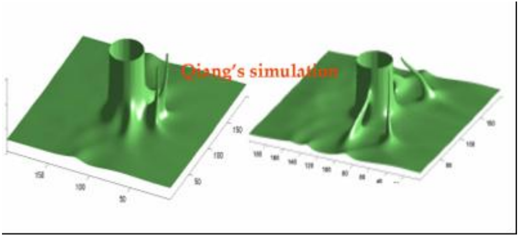
$$\Gamma = \int v(s)ds = n\frac{h}{m}, \quad v|_{r=0} \sim \frac{1}{r}.$$

Creating vortices in Bose Einstein Condensates

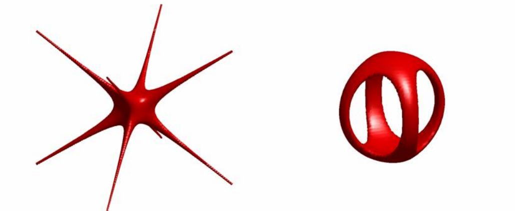
Rotation



Wake of moving objects Q. Du, Penn State

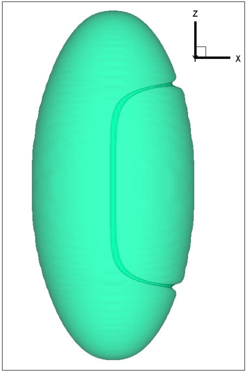


Phase imprint L.-C. Crasovan, V. M. Pérez-Garcia, I. Danaila, D. Mihalache, L. Torner, PRA, 2004.

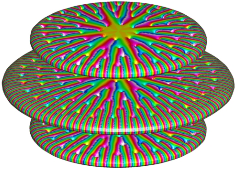


Catalogue of simulated vortices in BEC

rotating, U-vortex



rotating + optical lattice



fast rotating, giant vortex

BEC with (many) vortices

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

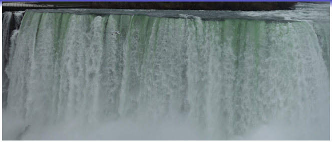
Classical Turbulence (CT)

Navier-Stokes equations

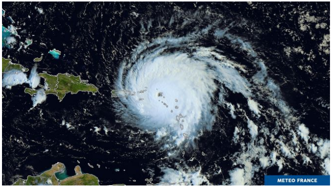
(normal incompressible fluid)

$$\nabla\cdot\mathbf{v}_n = 0,$$

$$\frac{\partial \mathbf{v}_n}{\partial t} + \mathbf{v}_n \cdot \nabla\mathbf{v}_n = -\frac{1}{\rho_n}\nabla p_n + \nu_n \Delta \mathbf{v}_n.$$



Niagara Falls 2019



IRMA Hurricane

Universal definition???

(i) 3D rotational velocity $\omega = \nabla \times \mathbf{v}$,
(ii) random space/time fluctuations,
(iii) turbulent scales $>>$ molecular scales and form a continuum,
(iv) the smallest scale is set by viscosity,
(v) viscous dissipation transforms the kinetic energy of smallest scales into internal energy,
(vi) the diffusivity is increased by turbulence (numerical models).

Super-Turbulence (ST)

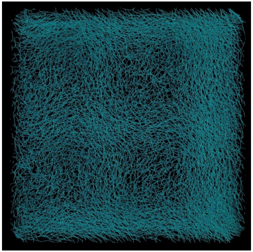
Gross-Pitaevskii equation

(superfluid)

$V(\mathbf{x}) = 0$

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{x},t) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) + g\,|\psi|^2\right)$$

$$\psi \in \mathbb{C},\ \ g = \frac{4\pi\hbar^2 a_s}{m} > 0.$$



ST in Bose-Einstein condensates and superfluid helium ($T \to 0$)
(i) vortex tangle turbulence,
(ii) some similarities with CT (Kolmogorov laws),
(iii) yet many open questions.

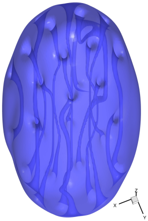
Super-Turbulence (ST) in BEC

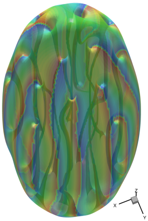
BEC = perfect superfluid system for QT?

$V(\mathbf{x}) \neq 0$

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

Cons
- quantitative measurements?
- pertinence of statistics?
- dissipation/thermal cloud influence?

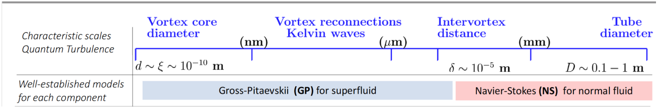




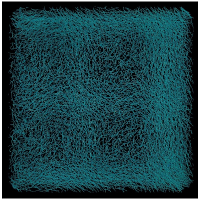
Recent experiments/numerics
- Henn et al., J. Low Temp. Phys., 2010.
- Henn et al., J. Low Temp. Phys., 2010.
- Seman et al., Laser Phys., 2011.
- (Edts) Tsubota & Halperin, Elsevier, 2009.
- Navon et al., Nature, 2016.

Quantum Turbulence (QT) in ^{4}He

- Two-fluid model (Tisza, Landau): normal fluid + superfluid.
- QT = classical turbulence (Navier-Stokes) + vortex tangle turbulence (Gross-Pitaevskii)

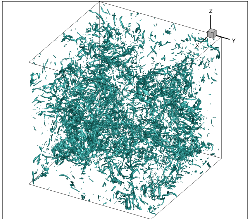


GP Super-Turbulence ST

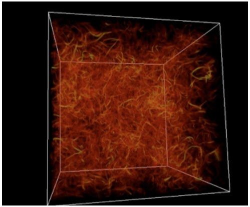


(courtesy M. Brachet)

Two-fluid Quantum Turbulence QT



CT (Navier-Stokes)



(courtesy E. Lévêque)

Outline

ANR LMRS

Models for superfluids (T=0): GP equation

Time-dependent GP → real time dynamics

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

Time-independent 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

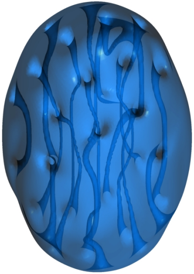
$$\delta\psi = \left(a(\mathbf{x})e^{-i\omega t} + b^*(\mathbf{x})e^{i\omega^* t}\right),$$

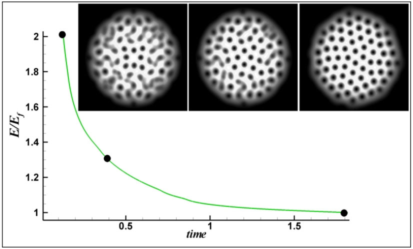
$$\begin{pmatrix} H(\Omega) & g\phi^2 \\ -g(\phi^*)^2 & -H(-\Omega)\end{pmatrix}\begin{pmatrix} a \\ b\end{pmatrix} = \hbar\omega\begin{pmatrix} a \\ b\end{pmatrix}$$

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

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 $\partial\mathcal{D}$

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

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

Normalized gradient flow (Bao and Du, 2004)

- Backward-Euler (BE) semi-implicit method

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

- 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

- 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

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

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

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.

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

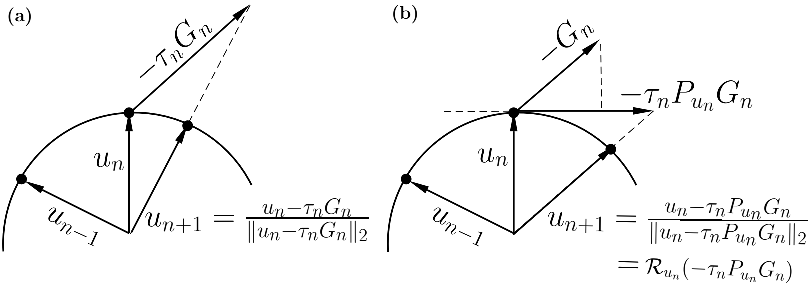
$$\langle u, v\rangle_{H_A} = \int_{\mathcal{D}} \langle u, v\rangle + \langle \nabla_A u, \nabla_A v\rangle, \;\; \nabla_A = \nabla + iC_\Omega \mathbf{A}$$

- equivalence

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

- provides a better preconditioner (other choices possible).

Stay close to the Manifold



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: $u_{n+1} = u_n - \tau_n P_{u_n,X} G_n$,
- Projected gradient

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

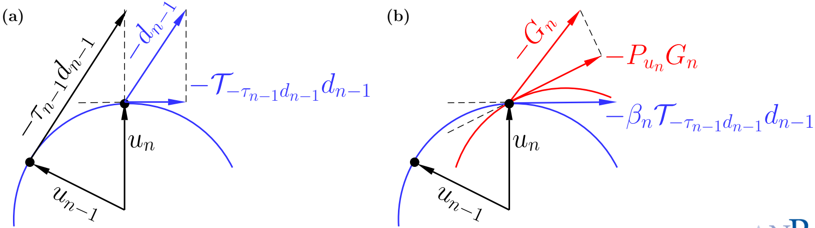
- Explicit formula for the projected gradient

Even better idea: Riemanian gradient method

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

Ideas

- Constrained minimization $\Longrightarrow$ Unconstrained min. on $\mathcal{M}$.
- Adapt the Nonlinear conjugate-gradient (Euclidean case).
- Transport all the vectors to the tangent space $\mathcal{T}_{u_n}\mathcal{M}$.



The Riemanian conjugate-gradient method

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

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

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

- Polak-Ribière momentum term

$$\beta_n = \beta_n^{PR} := \frac{\left\langle P_{u_n,H_A} G_n, \left(P_{u_n,H_A} G_n - \mathcal{T}_{-\tau_{n-1} d_{n-1}} P_{u_{n-1},H_A} G_{n-1}\right)\right\rangle_{H_A}}{\left\langle P_{u_{n-1},H_A} G_{n-1}, P_{u_{n-1},H_A} G_{n-1}\right\rangle_{H_A}}. \qquad (3)$$

- optimal descent step (Brent's method)

$$\tau_n = \underset{\tau>0}{argmin}\, E\left(\mathcal{R}_{u_n}(-\tau d_n)\right) \qquad (4)$$

The Riemanian conjugate-gradient method

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

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

Implementation with finite-elements

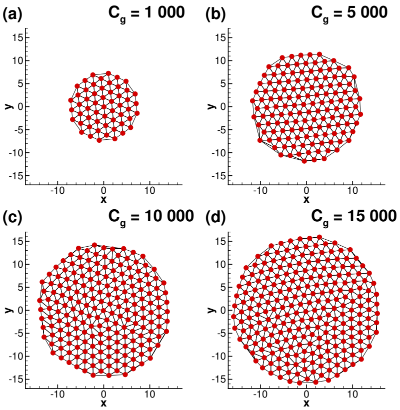
- looks horrible, but ... easy with FreeFem++
- easy and elegant implementation (like the math formulation)!

$$\beta_n = \beta_n^{PR} := \frac{\left\langle P_{u_n,H_A} G_n, \left(P_{u_n,H_A} G_n - \mathcal{T}_{-\tau_{n-1} d_{n-1}} P_{u_{n-1},H_A} G_{n-1}\right) \right\rangle_{H_A}}{\left\langle P_{u_{n-1},H_A} G_{n-1}, P_{u_{n-1},H_A} G_{n-1} \right\rangle_{H_A}}. \qquad (3)$$

- optimal descent step (Brent's method)

$$\tau_n = \underset{\tau>0}{argmin}\, E\left(\mathcal{R}_{u_n}(-\tau d_n)\right) \qquad (4)$$

BEC with dense Abrikosov lattice $\rightarrow$ QT



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.

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

Two-component condensate:

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

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

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

$$\psi_1(\mathbf{x},t) = \exp(-i\mu_1 t/\hbar)\left(\phi_1 + a(\mathbf{x})e^{-i\omega t} + b^*(\mathbf{x})e^{i\omega^* t}\right)$$

$$\psi_2(\mathbf{x},t) = \exp(-i\mu_2 t/\hbar)\left(\phi_2 + c(\mathbf{x})e^{-i\omega t} + d^*(\mathbf{x})e^{i\omega^* t}\right)$$

BdG equations: linear eigenvalue problem

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

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

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

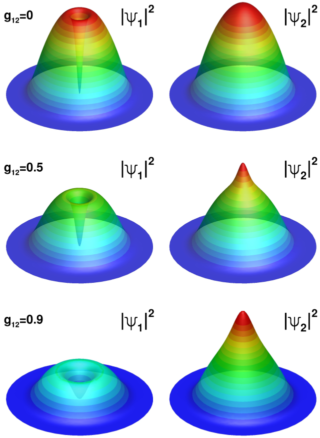
$$H = -\frac{\hbar^2}{2m}\nabla^2 + V_{\text{trap}}$$

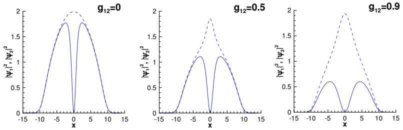
- Interface with ARPACK to solve this problem!

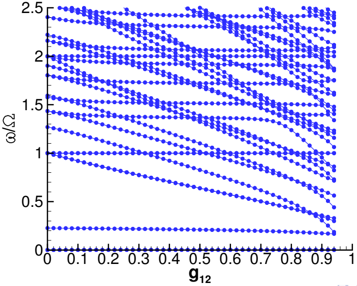
Computation of Bogoliubov-de Gennes modes

BdG 2d: Vortex-Antidark Solitary Waves

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

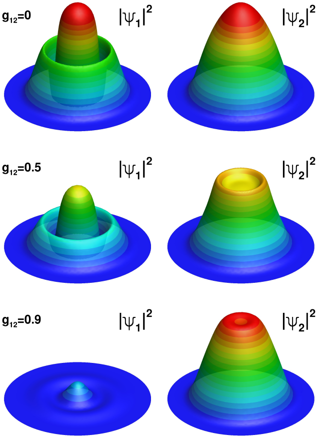


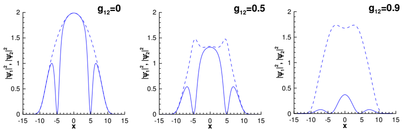


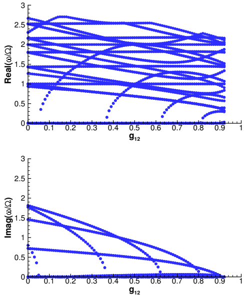


BdG 2d: Ring-Antidark-Ring Solitary Waves

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

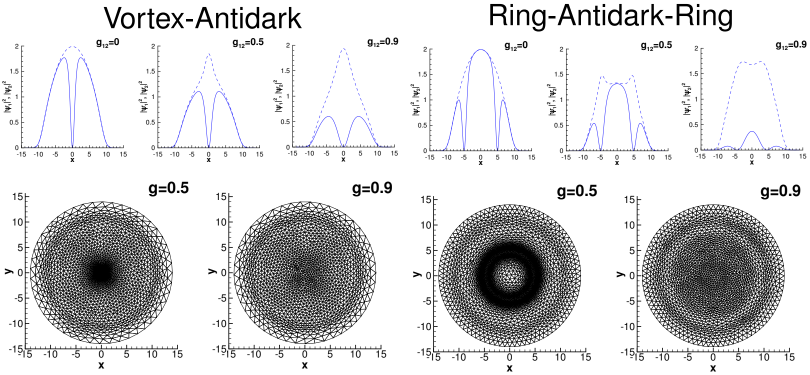






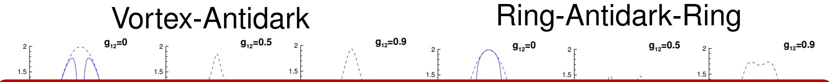
BdG 2d: mesh adaptivity

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



BdG 2d: mesh adaptivity

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



The BdG FreeFem++ toolbox

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

G. Sadaka, V. Kalt, I. Danaila and F. Hecht
A finite element toolbox for the Bogoliubov-de Gennes stability analysis of Bose-Einstein condensates, arXiv:2303.05350 (2023).

Outline

FreeFem++: a generic finite-element solver

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.

FreeFem++ syntax

- create a mesh and a finite element space

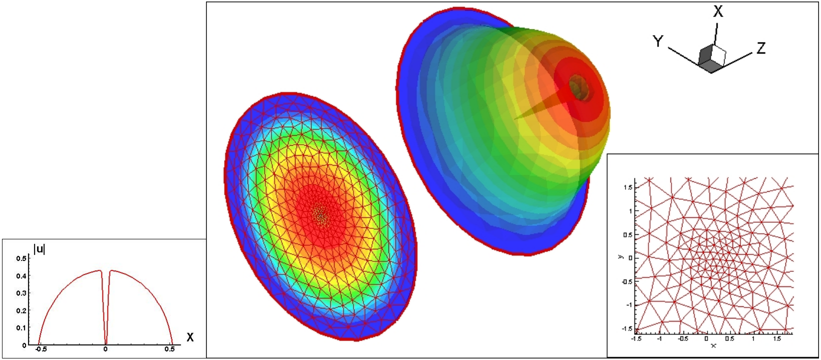
```
border circle(t=0,2*pi)
{label=1;x=Rmax*cos(t);y=Rmax*sin(t);};
mesh Th=buildmesh(circle(100));
fespace Vh(Th,P1);    fespace Vh4(Th,P4);
```

- solve the Poisson eq: $-\Delta u = f \Longrightarrow \int_{\mathcal{D}} \nabla u \nabla v - \int_{\mathcal{D}} fv = 0$

```
func f=4;  // RHS (source) function
fespace Vh(Th, P1);// FE space
Vh u,v;    // u=unknown, v=test function
// Variational (weak formulation)
problem Poisson(u,v)= int2d(Th)(dx(u)*dx(v)+dy(u)*dy(v))
- int2d(Th)(f*v)
+ on(1,u=0); // Dirichlet boundary condition
Poisson;  // Solve the problem
plot(u,dim=2,fill=1);// plot the solution
```

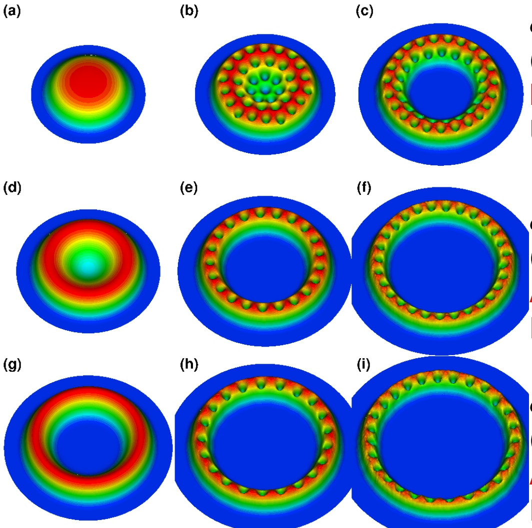
- write the weak formulation:: FreeFem will take care of the rest!

Mesh adaptivity



BEC with giant vortex (1)

$$C_{\text{trap}}(x,y) = (1-\alpha)r^2 + \frac{1}{4}kr^4,\ C_g = 1000,\ k = 1,\ C_\Omega = 0, 3, 4.$$



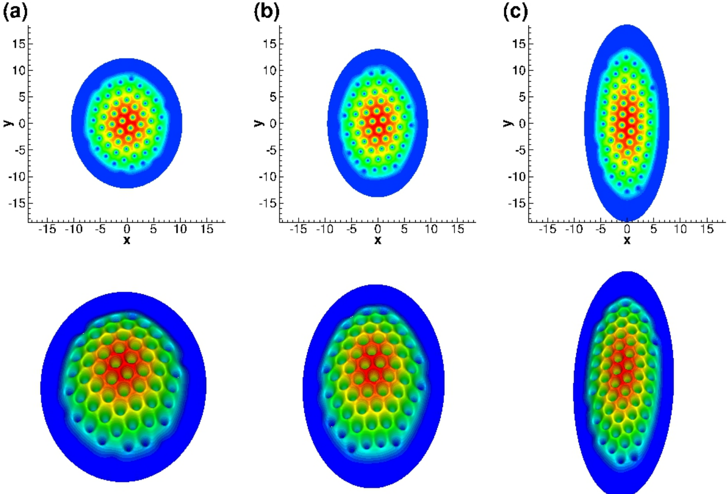
$\alpha = 1/2$ (Regime 1), Kasamatsu, Tsubota, Ueda, PRA, 2002.

$\alpha = 11/2$, (Regime 2), Aftalion, Danaila, PRA, 2004.

$\alpha = 9$, (Regime 3) Aftalion, Danaila, PRA, 2004.

BEC with anisotropic traps

$C_{\text{trap}}(x,y) = \frac{1}{2}\left[(1+\eta^2)x^2 + (1-\eta)y^2\right], \quad \eta = 2(1-C_\Omega)\epsilon,$
$\epsilon = 0.15, 0.35, 0.65,\ C_\Omega = 0.9.$



FreeFem++ Toolbox (www.freefem.org)

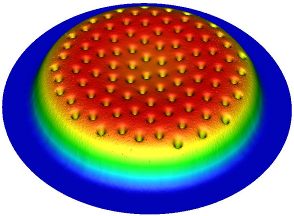
Developers: G. Vergez, I. Danaila, F. Hecht.

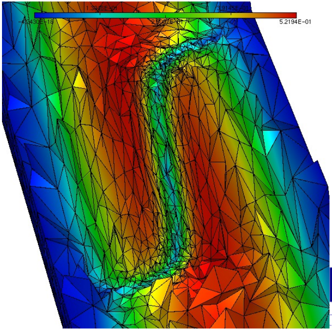
Computer Physics Communications, 2016 (with programs)!

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 for vortex identification

Developers: V. Kalt, G. Sadaka, I. Danaila, F. Hecht.

Computer Physics Communications 284 (2023) 108606

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COMPUTER PHYSICS COMMUNICATIONS

Identification of vortices in quantum fluids: Finite element algorithms and programs ☆,☆☆

Check for updates

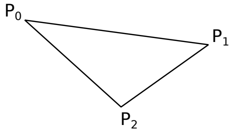
Victor Kalt [a], Georges Sadaka [a], Ionut Danaila [a,*], Frédéric Hecht [b]

[a] Univ Rouen Normandie, CNRS, LMRS, Laboratoire de Mathématiques Raphaël Salem, UMR 6085, F-76000 Rouen, France
[b] Sorbonne Université, CNRS UMR 7598, Laboratoire Jacques-Louis Lions, F-75005, Paris, France

ANR LMRS

Simple idea for vortex identification

- Discretisation of $\psi = \psi_r + i\psi_i$ with P1 finite-elements.



- Vortex found if:

$$\min(\psi_r(P_0), \psi_r(P_1), \psi_r(P_2)) < 0,$$
$$\min(\psi_i(P_0), \psi_i(P_1), \psi_i(P_2)) < 0,$$
$$\max(\psi_r(P_0), \psi_r(P_1), \psi_r(P_2)) > 0,$$
$$\max(\psi_i(P_0), \psi_i(P_1), \psi_i(P_2)) > 0.$$

- Winding number approximated from:

$$\kappa = \frac{1}{2\pi}\Im\left(\log\left(\frac{\psi(P_1)}{\psi(P_0)}\right) + \log\left(\frac{\psi(P_2)}{\psi(P_1)}\right) + \log\left(\frac{\psi(P_0)}{\psi(P_2)}\right)\right).$$

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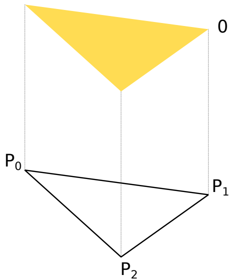

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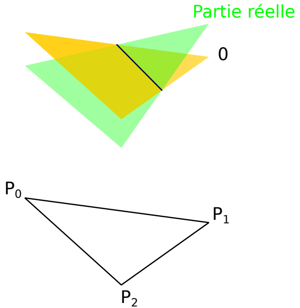

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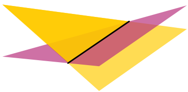

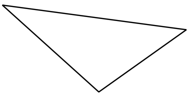

- Vortex found if:

$$
\begin{aligned}
\min(\psi_r(P_0), \psi_r(P_1), \psi_r(P_2)) &< 0,\\
\min(\psi_i(P_0), \psi_i(P_1), \psi_i(P_2)) &< 0,\\
\max(\psi_r(P_0), \psi_r(P_1), \psi_r(P_2)) &> 0,\\
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\end{aligned}
$$

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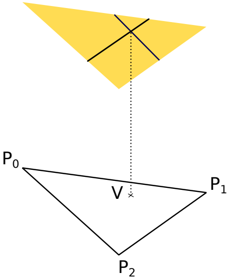

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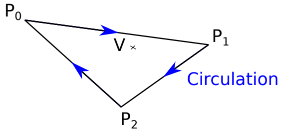

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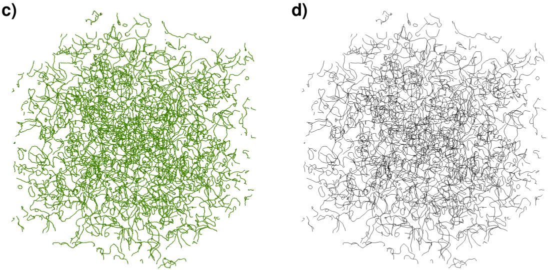
Helium: identification of vortices in QT

- QT simulation with the spectral code GPS.



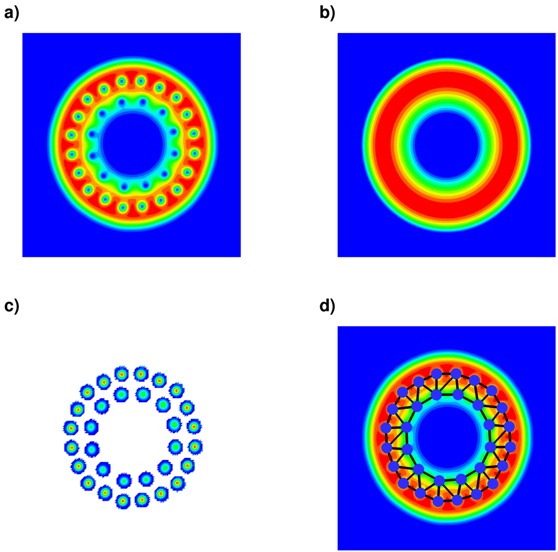
Grid resolution 256^3.

c) Isosurfaces of density

d) 640 identified vortices.

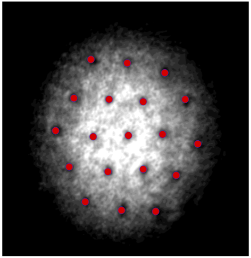
- CPU necessary = 12 minutes
- Similar case in Villois et al., J. Phys. A: Math. Theor., 2016 with 576 vortices = 6 hours (with 64 MPI procs).

BEC: Identification of a giant vortex



a) Initial density (simulation with GPFEM),
b) Thomas-Fermi density,
c) Vortex zones,
d) Identified vortices.

BEC: Identification of vortices in experimental images



Coddington et al., *Experimental studies of equilibrium vortex properties in a Bose-condensed gas*, PRA, 2004.

Outline

ANR project QUTE-HPC: QUantum Turbulence Exploration by High-Performance Computing

Agence Nationale de la Recherche

ANR Project QUTE-HPC (2019-2022)

10 members, 5 Physics/5 Mathematics

- (HPC) parallel codes for QT :: open source,

http://qute-hpc.math.cnrs.fr/

ANR Project BECASIM (2013-2017)

25 members from Mathematics

- numerics for real and imaginary time GP,
- mathematical theory, numerical analysis.

http://becasim.math.cnrs.fr/

GPS code: Gross Pitaevskii Simulator

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

Solver for the stationary GP

- imaginary-time propagation: Krylov preconditioned Backward Euler (Bao, 2003; Antoine & Duboscq, 2014).
- direct minimization of the GP-energy by Sobolev gradients (Danaila & Kazemi, 2010).
- Newton method.

Solver for the real-time GP

- relaxation scheme (Besse, 2004).
- Lie/Strang splitting scheme.
- Crank-Nicolson scheme.

GPS code: Spatial discretisation

Differential operators

- pseudo-spectral Fourier (FFTW 1D),
- 6th order compact finite-difference schemes.

Linear system solvers (in house)

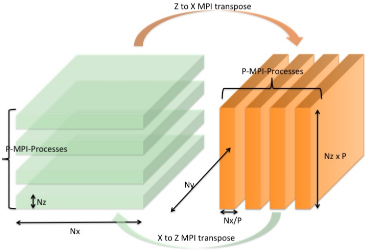
- BiCGStab,
- Generalized Conjugate Residual (GCR).

Boundary conditions, initial conditions

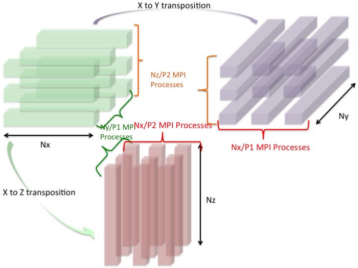
- BC: periodic (spectral), Dirichlet (FD).
- initial conditions: Thomas-Fermi, vortex ansatz, etc.

GPS code: MPI decomposition

- Slab decomposition



- Pencil decomposition

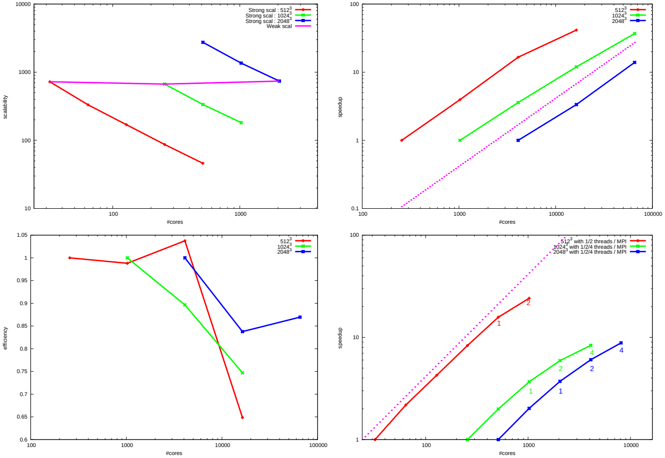


Step 1-Computation 1D **FFT** or **CS** to compute ∂_x^2 and ∂_x;
Step 1- X to Y transposition *Pencil* decomposition.
Step 2-Computation 1D **FFT** or **CS** to compute ∂_y^2 and ∂_y;.
Step 2- X to Z transposition *Pencil* or *Slab* decomposition.
Step 3-Computation 1D **FFT** or **CS** to compute ∂_z^2;.

GPS code: hybrid MPI - OpenMP

- **2 hybrid MPI-OpenMP parallelization schemes**, based on a transpose algorithm: slab and pencil decompositions.
- Hybrid parallelization schemes are similar for both space discretizations: FFT or CS.
- **OpenMP parallelization** consists in an inner loop optimization, and an intensive use of ”collapse” directives in order to optimize it.
- In order to **avoid the cost of the collective communications**, a **non-blocking collective communication** may be used (LibNBC/MPI-3).

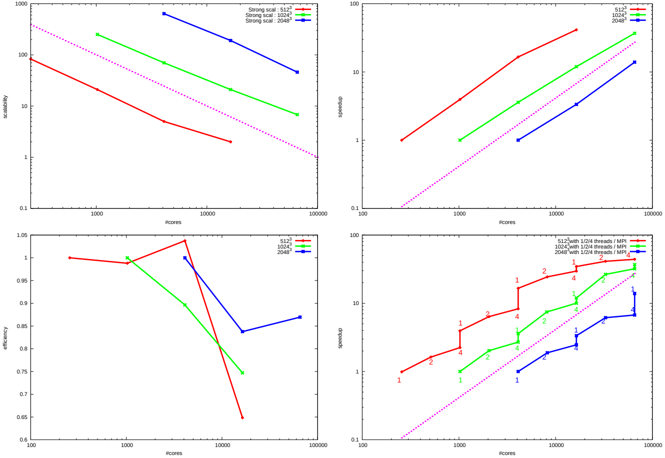
GPS code: scalability for the slab decomposition



3D case with 512^3, 1024^3 and 2048^3 grid points

With [64 : 2048] MPI processes and 1, 2, or 4 threads by MPI processes

GPS code: scalability for the pencil decomposition



3D case with 512^3 and 1024^3 grid points

[256 : 64536] MPI processes and 1, 2 or 4 threads by OpenMP

GPS code: summary

GPS is an **accurate, robust, efficient and high performance code to simulate Bose-Einstein condensates on a large choice of computing architectures.**

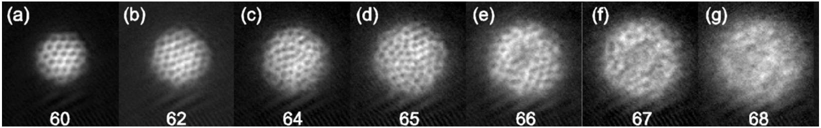
- quasi-linear scaling with both decompositions,
- good efficiency in term of runtime performance,
- 4 threads per process results in a smooth gain using OpenMP.

The Input/Output are performed using ADIOS (Oak Ridge)
Developers of the GPS-IO: Ph. Parnaudeau, A. Mouton.

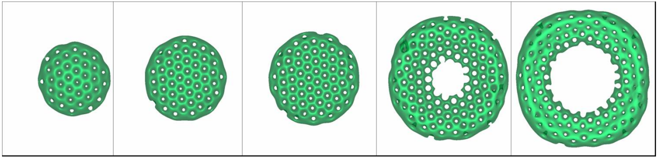
Simulation of fast rotating condensates

- (stationary GP) 3D simulation of the experimental configuration (10^7 grid points).

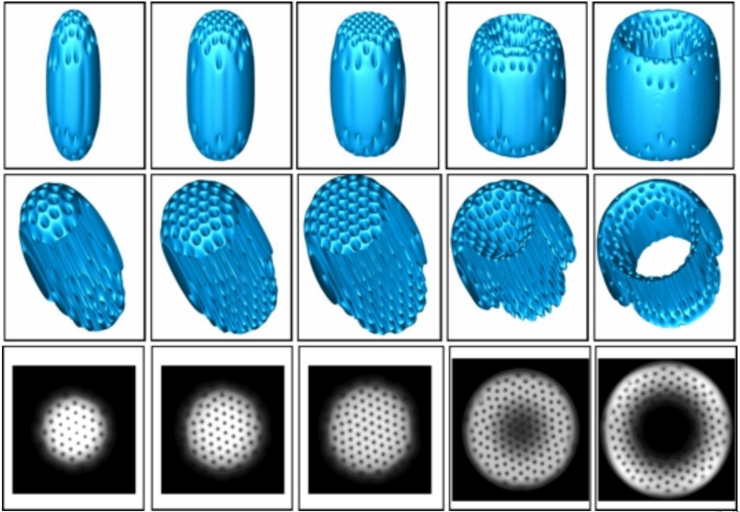
V. Bretin, S. Stock, Y. Seurin, J. Dalibard, Phys. Rev. Lett. 2003.



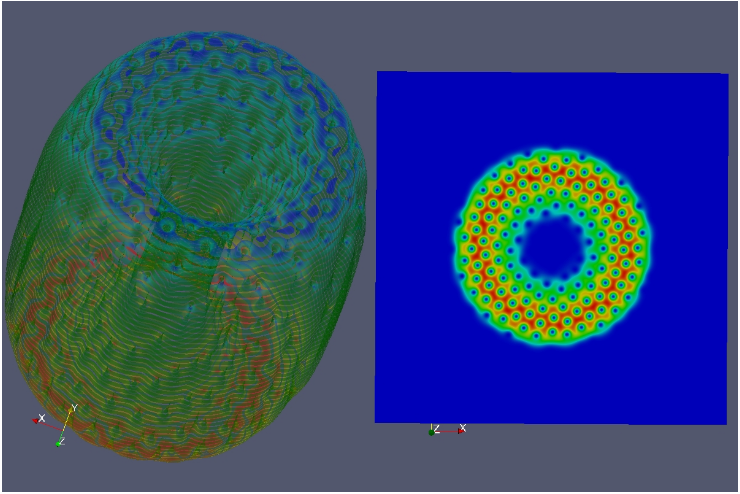
I. Danaila, Phys. Rev. A, 2005.



2005 3D Simulation: grid 240^3 = 2 weeks of CPU



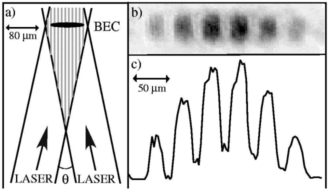
3D Simulation: grid 512^3 = 1 day of CPU



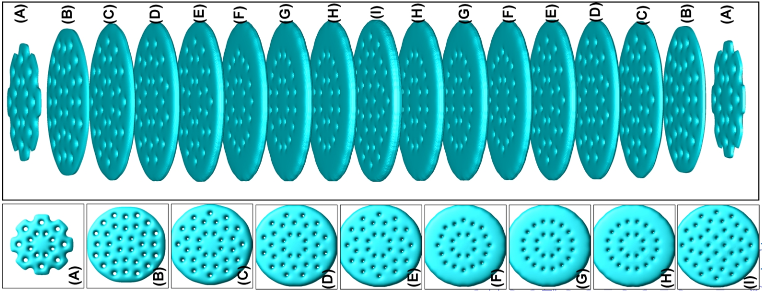
Optical lattice potential: $V_{trap} = r^2 + U \sin^2(\pi z/d)$

- Non rotating BEC in optical lattices

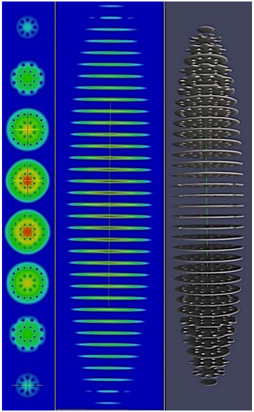
Z. Handzibababic, S. Stock, B. Battelier, V. Bretin, J. Dalibard, Phys. Rev. Lett. 2004.



- 3D simulation



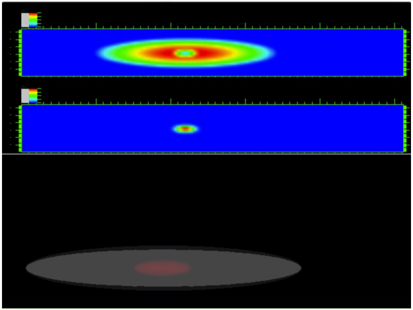
3D Simulation with GPS = 1 day of CPU



Interaction between two BEC (bosons vs fermions)

S. Laurent, Ph. Parnaudeau, F.Chevy, I. Danaila, Nonlinear dynamics of coupled superfuids, xarchiv 1904.07040, 2019.

movie 1
movie 2



Outline

ANR project QUTE-HPC: QUantum Turbulence Exploration by High-Performance Computing

Joint work with:
M. Kobayashi (Kyoto), M. E. Brachet (ENS Paris), Ph. Parnaudeau (Poitiers), C. Lothodé, F. Luddens, L. Danaila (Rouen)

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Quantum turbulence simulations using the Gross–Pitaevskii equation: High-performance computing and new numerical benchmarks☆

Michikazu Kobayashi [a], Philippe Parnaudeau [b], Francky Luddens [c], Corentin Lothodé [c], Luminita Danaila [d], Marc Brachet [e], Ionut Danaila [c,*]

GP model and hydrodynamic analogy

$$i\hbar \frac{\partial}{\partial t}\psi(\mathbf{x}, t) = \left(-\frac{\hbar^2}{2m}\nabla^2 + g\,|\psi(\mathbf{x}, t)|^2\right)\psi(\mathbf{x}, t), \quad g = \frac{4\pi\hbar^2 a_s}{m}$$

Madelung transform: $\psi = \sqrt{n(\mathbf{x}, t)}\, e^{i\theta(\mathbf{x},t)}$

- n is the atomic density, $\rho = mn$ the mass density,
- the velocity

$$\mathbf{v}(\mathbf{x}, t) = \frac{\hbar}{m}\nabla\theta(\mathbf{x}, t) = \frac{\hbar}{\rho}\frac{\psi^*\nabla\psi - \psi\nabla\psi^*}{2i}.$$

- Euler equations (zero-viscosity fluid)

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\mathbf{v}) = 0,$$

$$\frac{\partial \mathbf{v}}{\partial t} + \frac{1}{2}\nabla(\mathbf{v}^2) = -\frac{1}{\rho}\nabla\left(\frac{g\rho^2}{2m^2}\right) + \frac{\hbar^2}{2m^2}\nabla\left(\frac{1}{\sqrt{\rho}}\nabla^2(\sqrt{\rho})\right).$$

Physical parameters for QT

Periodic boundary conditions: Background flow $\rho = \rho_0$.

Typical scales

- sound velocity c and Mach number

$$c = \sqrt{\frac{\partial P_0}{\partial \rho_0}} = \frac{\sqrt{g\rho_0}}{m} = \sqrt{\frac{g n_0}{m}} \Longrightarrow M = \frac{v}{c} \ll 1.$$

- healing length ξ (size of a vortex)

$$\xi = \frac{\hbar}{\sqrt{2mgn_0}} = \frac{\hbar}{\sqrt{2m\mu_0}} = \frac{1}{\sqrt{2}}\frac{\hbar}{mc}.$$

- dispersion relation ($a(\mathbf{x}) = ue^{i\mathbf{k}\cdot\mathbf{x}}, \quad b(\mathbf{x}) = ve^{i\mathbf{k}\cdot\mathbf{x}}$):

$$\delta\psi = a(\mathbf{x})e^{-i\omega t} + b^*(\mathbf{x})e^{i\omega^* t}, \Longrightarrow \omega = ck\sqrt{1 + \frac{\xi^2 k^2}{2}} \Longrightarrow (k\xi \ll 1).$$

LMRS

GPS code for Quantum Turbulence

Developers: C. Lothodé (Rouen), F. Luddens (Rouen), Ph. Parnaudeau (Poitiers), M. Kobayashi (Kyoto).

Initial condition for QT simulation

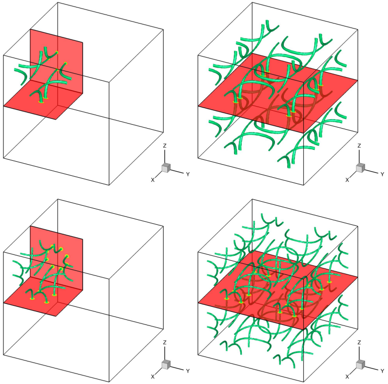
1. Taylor-Green vortices.
2. ABC-flow.
3. Random-phase field.
4. Random vortex rings.

Post-processing of data

- Visualisation of vortices (movies).
- Spectra of the kinetic energy.
- Scaling laws.

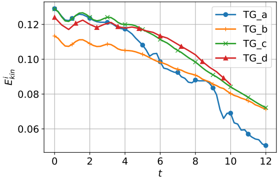
Initial condition 1: Taylor-Green vortices

Pioneering work: C. Nore, M. Abid, M. Brachet, Physics of Fluids, 1997.



$$\mathbf{u}^{adv} = \begin{pmatrix} \sin(x)\cos(y)\cos(z) \\ \cos(x)\sin(y)\cos(z) \\ 0 \end{pmatrix}$$

$\psi_{|t=0}$ contains vortices with winding number 3.

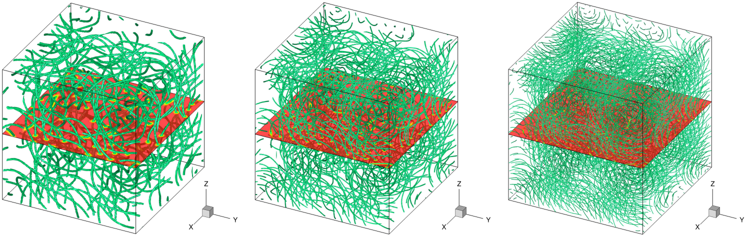


Initial condition 1: Taylor-Green vortices

movie

Initial condition 2: ABC-flow

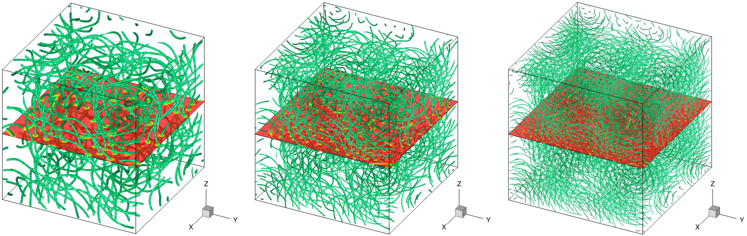
P. C. di Leoni, P. D. Mininni and M. Brachet, Phys. Rev. A, 2017.



$$\mathbf{u}^{adv} = \begin{pmatrix} B(cos(y) + cos(2y)) + C(sin(z) + sin(2z)) \\ C(cos(z) + cos(2z)) + A(sin(x) + sin(2x)) \\ A(cos(x) + cos(2x)) + B(sin(y) + sin(2y)) \end{pmatrix}$$

Initial condition 2: ABC-flow

P. C. di Leoni, P. D. Mininni and M. Brachet, Phys. Rev. A, 2017.

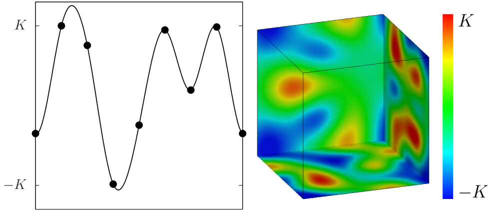


$$\mathbf{u}^{adv} = \begin{pmatrix} B(cos(y) + cos(2y)) + C(sin(z) + sin(2z)) \\ C(cos(z) + cos(2z)) + A(sin(x) + sin(2x)) \\ A(cos(x) + cos(2x)) + B(sin(y) + sin(2y)) \end{pmatrix}$$

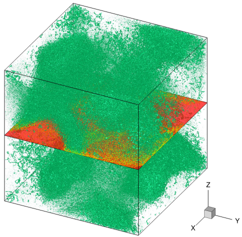
Initial condition 3: Smoothed Random Phase

original

initial



final

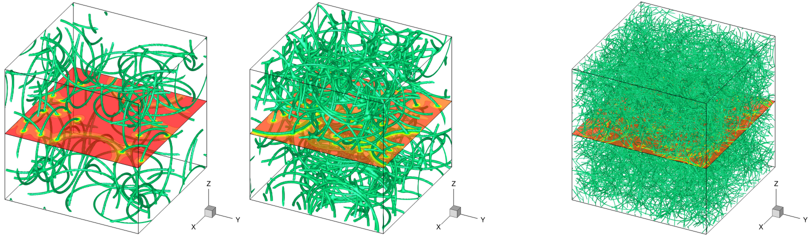


$$\psi_{\mathrm{SRP}} = e^{i\theta(\mathbf{x})}, \quad \theta_{i,j,k} \in [-K, K].$$

Initial condition 4: Random Vortex Rings

original

initial | final



$$\psi_{\mathrm{VR}}(x,y,z,R) = f\left(\sqrt{(r-R)^2+\tilde{z}^2}\right)\, e^{\pm i \tan^{-1}\left(\frac{\tilde{z}}{r-R}\right)}$$

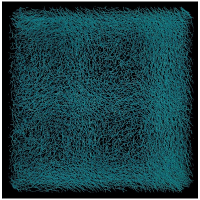
Outline

Models for superfluid helium

$T \sim 0.3K$

GP Super-Turbulence

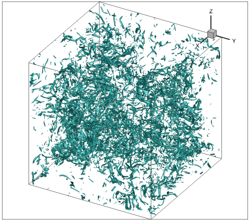
ST



$T \sim 1K$

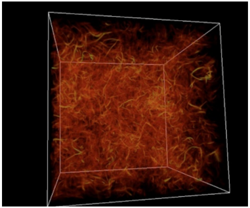
Two-fluid Quantum

Turbulence QT



$T \sim 2.K$

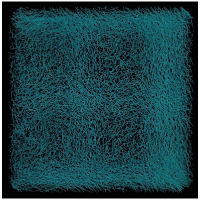
CT (Navier-Stokes)



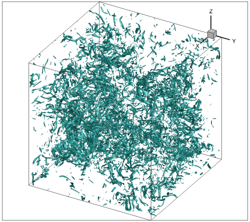
Navier-Stokes type two-fluid models

Idea: couple the Euler equation (superfluid) and Navier-Stokes equations (normal fluid).

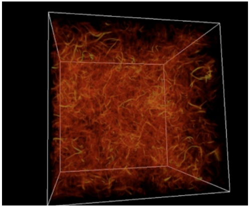
$T \sim 0.3K$
GP Super-Turbulence
ST



$T \sim 1K$
Two-fluid Quantum
Turbulence QT



$T \sim 2.K$
CT (Navier-Stokes)



The HVBK model for QT

Hall-Vinen-Bekharevich-Khalatnikov (HVBK) model:

$$\nabla \cdot \mathbf{v_n} = 0, \ \nabla \cdot \mathbf{v_s} = 0,$$

$$\frac{\partial \mathbf{v_n}}{\partial t} + (\mathbf{v_n} \cdot \nabla)\mathbf{v_n} = -\frac{1}{\rho_n}\nabla \mathbf{p_n} + \frac{1}{\rho_n}\mathbf{F_{ns}} + \nu_n \nabla^2 \mathbf{v_n},$$

$$\frac{\partial \mathbf{v_s}}{\partial t} + (\mathbf{v_s} \cdot \nabla)\mathbf{v_s} = -\frac{1}{\rho_s}\nabla \mathbf{p_s} - \frac{1}{\rho_s}\mathbf{F_{ns}},$$

Coupling friction force:

$$\mathbf{F_{ns}} = -\frac{B}{2}\frac{\rho_s \rho_n}{\rho|\omega_s|}\omega_s \times (\omega_s \times \underbrace{(\mathbf{v_s} - \mathbf{v_n})}_{\mathbf{w}}) - \frac{B'}{2}\frac{\rho_s \rho_n}{\rho}\omega_s \times \underbrace{(\mathbf{v_s} - \mathbf{v_n})}_{\mathbf{w}},$$

where $\omega_s = \nabla \times \mathbf{v_s}$ is the coarse-grained superfluid vorticity.

HVBK Quantum-Turbulence

... talk by Luminita Danaila, next week.

J. Fluid Mech. (2023), *vol.* 962, A22, doi:10.1017/jfm.2023.235

JFM PAPERS

Higher-order statistics and intermittency of a two-fluid Hall–Vinen–Bekharevich–Khalatnikov quantum turbulent flow

Z. Zhang[1], I. Danaila[1], E. Lévêque[2] and L. Danaila[3,†]

arXiv:2303.06631 (2023).

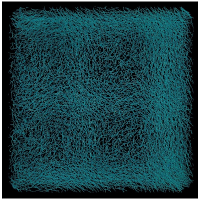
- apply statistical tools used in CT
- transport equations for the third-order moments

ANR LMRS

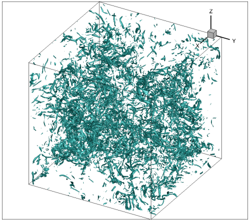
Coupling Vortex Lines and Navier-Stokes equations

Idea: couple the Vortex Lines dynamics (superfluid) and Navier-Stokes equations (normal fluid).

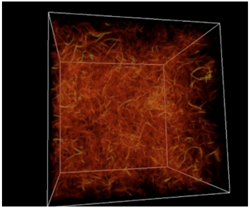
$T \sim 0.3K$
GP Super-Turbulence ST



$T \sim 1K$
Two-fluid Quantum Turbulence QT



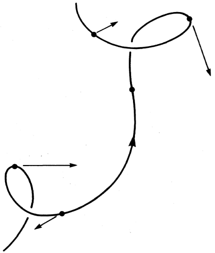
$T \sim 2.K$
CT (Navier-Stokes)



Vortex lines (filaments in superfluid helium)

Superfluid dynamics:

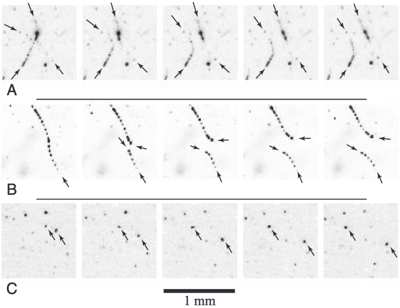
- Biot-Savart-Laplace
- model for reconnection,
- no vortex nucleation.



Vortex filaments dynamics (Schwartz, PRB, 1995).

Superfluid Helium

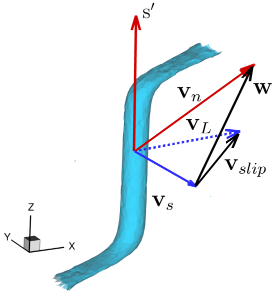
($T < T_\lambda = 2.17K$)



Reconnection of vortex lines (Maryland, USA, Bewley et al., PNAS, 2008).

Coupling Vortex Lines with NS dynamics

- (UK-France) Galantucci, Baggaley, Barenghi & Krstulovic, *A new self-consistent approach of quantum turbulence in superfluid helium*, Eur. Phys. J. Plus, 2020.
- (Japan) Inui & Tsubota, *Coupled dynamics of quantized vortices and normal fluid in superfluid ^{4}He based on lattice Boltzmann method*, PRB, 2021.



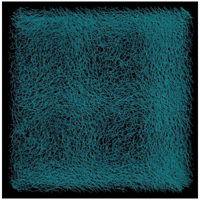
- $\mathbf{v}_s$ superfluid velocity (Biot-Savart)
- $\mathbf{v}_n$ normal velocity (Navier-Stokes)
- $\mathbf{w} = \mathbf{v}_n - \mathbf{v}_s$ counter-current
- $\mathbf{v}_L$ vortex line velocity
- $\mathbf{v}_{slip} = \mathbf{v}_L - \mathbf{v}_s$ slip velocity.

ANR LMRS

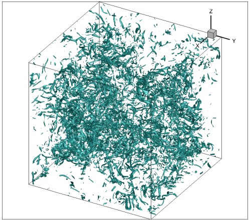
Coupling Gross-Pitaevskii and Navier-Stokes equations

Idea: couple the GP dynamics (superfluid) and Navier-Stokes equations (normal fluid).

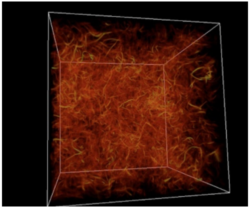
$T \sim 0.3K$
GP Super-Turbulence ST



$T \sim 1K$
Two-fluid Quantum Turbulence QT



$T \sim 2.K$
CT (Navier-Stokes)

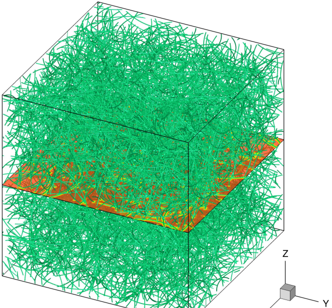


Motivation : initially mathematical and numerical

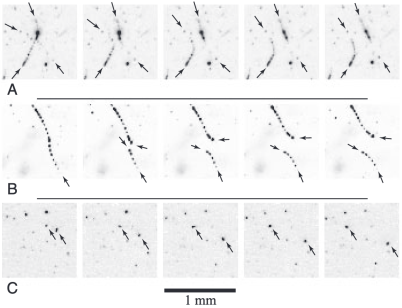
GP includes complete vortex dynamics (with nucleation and reconnections)

Superfluid vortex dynamics:

- ~~Biot-Savart-Laplace~~
- ~~model for reconnection,~~
- ~~no vortex nucleation.~~

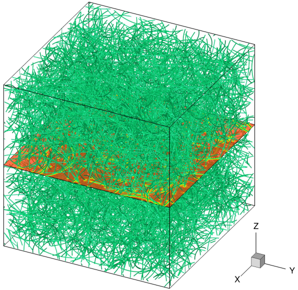


Superfluid Helium ($T < T_\lambda = 2.17K$)



Reconnection of vortex lines (Maryland, USA, Bewley et al., PNAS, 2008).

Main ingredients



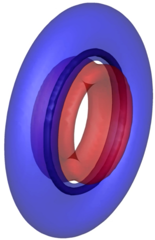
1. (new) Extract vortex lines from the GP field ψ. Define a regularised velocity field $\boldsymbol{v}_s^{reg}$ and vorticity field ω_s.
2. (as in VL-NS) Apply the equilibrium of forces to determine $\boldsymbol{v}_{\mathrm{slip}}$.
3. (new) Modify the GP equation to move the vortices with the correct $\boldsymbol{v}_{\mathrm{slip}}$. External driving of the GP dynamics.
4. (as in HVBK) Evaluate the volumetric friction force to be included in the NS equations.

Numerical code: spectral Fourier

• GPS code used as main framework ⊕ spectral solver for the incompressible Navier-Stokes (as in HVBK).

without normal fluid

with normal fluid



Kivotides, Barenghi et Samuels, *Triple vortex ring structure in superfluid helium II*, Science, 2000.

3D: reconnection of superfluid vortex rings

More details in ...

arXiv:4598109

Journal of Computational Physics 488 (2023) 112193

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Coupling Navier-Stokes and Gross-Pitaevskii equations for the numerical simulation of two-fluid quantum flows

Check for updates

Marc Brachet [a], Georges Sadaka [b], Zhentong Zhang [b], Victor Kalt [b], Ionut Danaila [b,*]

Conclusions

Solvers for the GP equation

- GPS code: spectral, parallel, HPC, using only FFTW.
- FreeFem toolbox for the stationary GPE (published, CPC, 209, 2016).
- FreeFem toolbox for the BdG equations (submitted to CPC).

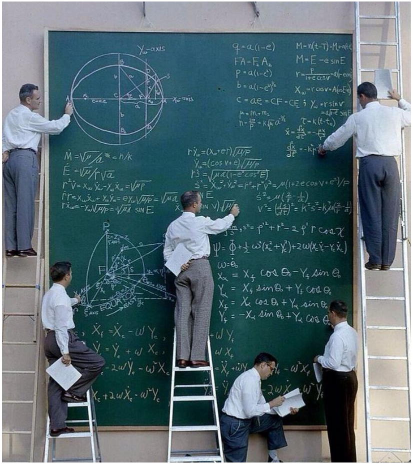
Finite-element post-processing toolbox

- FreeFem toolbox for identifying vortices (published, CPC, 284, 2023).

Solvers for He-II models

- HVBK solver: spectral, HPC, using P3DFFT.
- GP+NS solver: spectral, HPC, using only FFTW.

Collaborators



- QUTE-HPC

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