Vortices in classical fluids and superfluid Bose-Einstein condensates: a numerical investigation

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Fluid turbulence Applications in Both Industrial and ENvironmental topics

Marseille, July 8, 2019.

Main message of the talk

Many thanks, Fabien, for the initial scientific impulse!

... back in 1997!

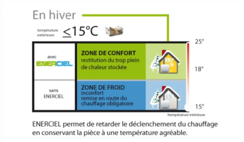
... back in 1997!

Scientific Computing at LMRS and Applications

(hot) Classical fluids: internal combustion engine

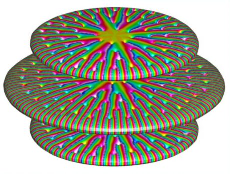
(Continental Automotive)

(hot <-> cold) Solids/Classical fluids: phase change materials



(WINCO Technologies)

(horribly cold) Super-Fluids : Bose-Einstein Condensates



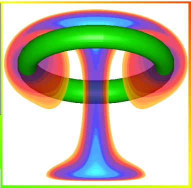
(I Danaila, LMRS)

Scientific Computing at LMRS

Classical fluids: vortex rings

Naviers-Stokes equations

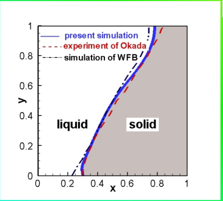
http://ionut.danaila.perso.math.cnrs.fr/



Liquid-solid phase-change systems

Naviers-Stokes-Boussinesq equations

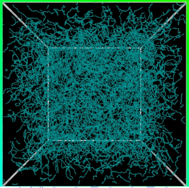
http://lmrs-num.math.cnrs.fr



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

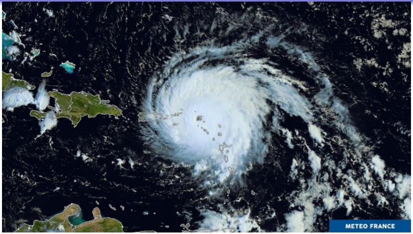
Schrödinger/ Gross-Pitaevskii equations

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

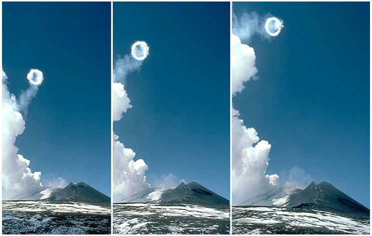


Vortices in classical fluids

Aircraft trailing vortices



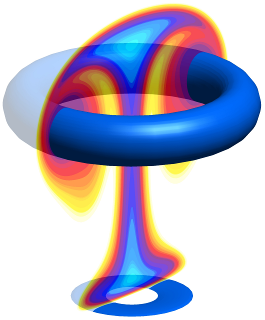
IRMA Hurricane



Vortex rings (Etna volcano)

Niagara Falls 2019

Models for classical vortex rings



New types of gasoline injectors
French project MAGIE

- Rouen
Y. Zhang
F. Luddens

- Paris
F. Hecht

- Brighton (UK)
S. Sazhin
F. Kaplanski
A. Papoutsakis

- Canada
B. Protas
(McMaster)

Contributions in this field (see my web page)

1. use high-resolution DNS for the physics of vortex rings,
   I. Danaila and J. Hélie, Physics of Fluids, 2008.
2. derive analytical and numerical models for the inflow,
   I. Danaila, C. Vadean, S. Danaila, Th. Comput. Fluid Dynamics, 2009.
3. use vortex rings models to reconstruct PIV fields.
   Y. Zhang and I. Danaila, J. of Numerical Mathematics, 2012.
   Y. Zhang and I. Danaila, Applied Mathematical Modelling, 2013.
   I. Danaila and B. Protas, Proc. Royal Soc. A , 2015.
4. derive/test analytical models of confined vortex rings,
   I. Danaila, F. Kaplanski and S. Sazhin, J. Fluid Mechanics, 2015.
   I. Danaila, F. Kaplanski and S. Sazhin, J. Fluid Mechanics, 2017.
   I. Danaila, F. Luddens, F. Kaplanski, A. Papoutsakis, and S. Sazhin, Phys Rev Fluids, 2018.

How simply describe the BEC?

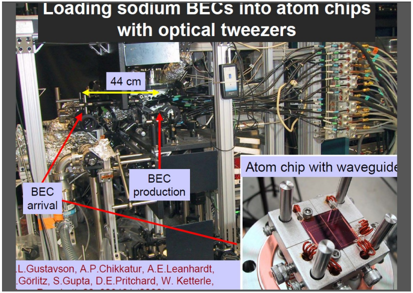
New state of the matter : super-atome

source Science, 2005

A possible new technological revolution!

Highly controlable system

- atomic clocks, interferometry, GPS, microscopy,
- atomic "lasers" for nano-lithography chip imprinting,
- quantic computer.



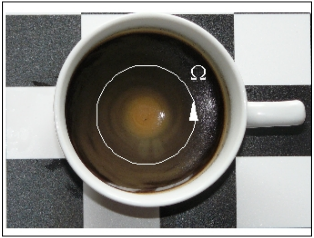
W. Ketterle, Collège de France, 2005

Vortices in fluids and superfluids

classical fluids

- easy intuition (velocity - pressure)

solid rotation



Vortices in fluids and superfluids

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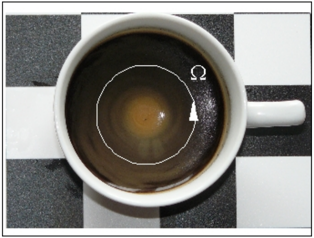
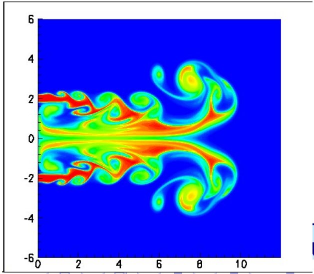
solid rotation





Vortices in fluids and superfluids

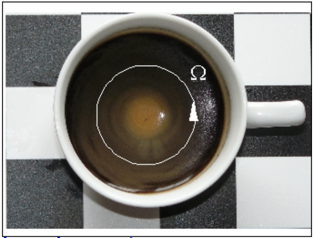
classical fluids

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

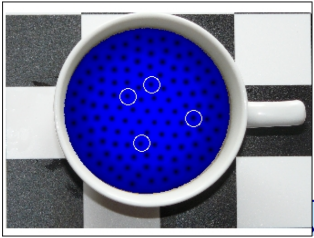
superfluids

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

solid rotation



local rotation



Vortices in fluids and superfluids

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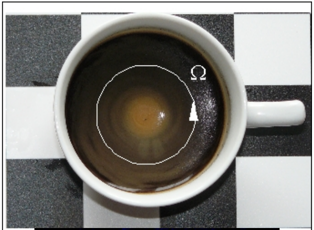
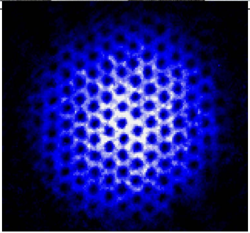




(JILA, Colorado)

Vortices in a Bose-Einstein condensate

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

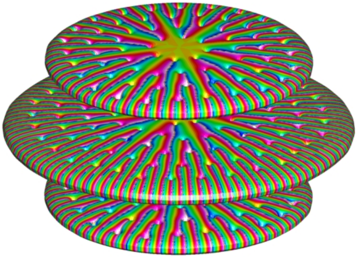
$$\Gamma = \int v(s)ds = n\frac{h}{m}$$

LMRS

Identification of a quantized vortex (2)

- phase portraits

optical lattice

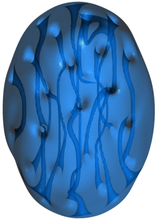


giant vortex

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.

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,
- huge simulations of physical configurations (compare with our own experiments).

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

ANR Project BECASIM (2013-2017)

25 members from Mathematics

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

Models for superfluids (T=0)

Time-dependent GP $\rightarrow$ real time dynamics

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

Time-independent GP $\rightarrow$ 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 $\rightarrow$ stability of stationary states

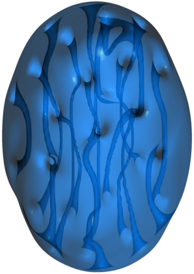
$$\delta\psi = \left(a(\mathbf{x})e^{-i\omega t} + b^*(\mathbf{x})e^{i\omega^* t}\right),$$

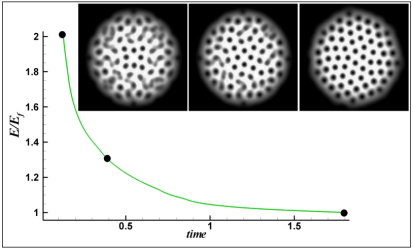
$$\begin{pmatrix} H(\Omega) & g\phi^2 \\ -g(\phi^*)^2 & -H(-\Omega) \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \hbar\omega\begin{pmatrix} a \\ b \end{pmatrix}$$

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

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 $\partial\mathcal{D}$

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

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.

Sobolev gradient descent method

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.

Riemanian conjugate-gradient method

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

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

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

- Polak-Ribière momentum term

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

- optimal descent step (Brent's method)

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

Riemanian conjugate-gradient method

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

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

$d_0 = -P_{u_0} G_0$

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

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

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

- optimal descent step (Brent's method)

$$\tau_n = \operatorname{argmin} E\left(\mathcal{R}_{u_n}(-\tau d_n)\right) \tag{4}$$

BEC with dense Abrikosov lattice (2)

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

FreeFem++ Toolbox (www.freefem.org)

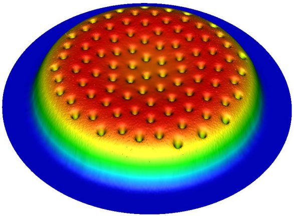
Developers: G. Vergez, I. Danaila, F. Hecht.

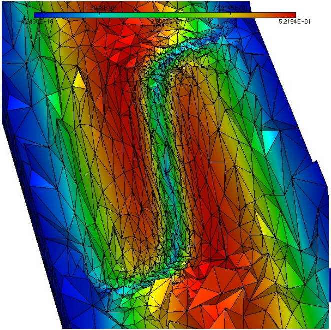
Computer Physics Communications, 2016 (with programs)!

GPFEM: finite element solver

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

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

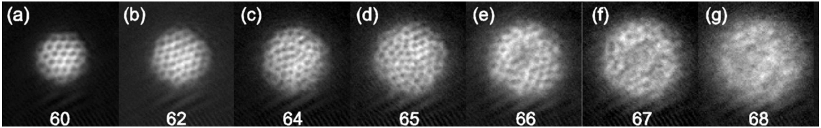




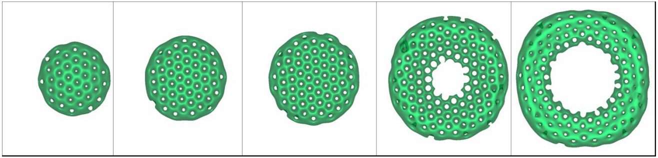
Simulation of fast rotating condensates

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

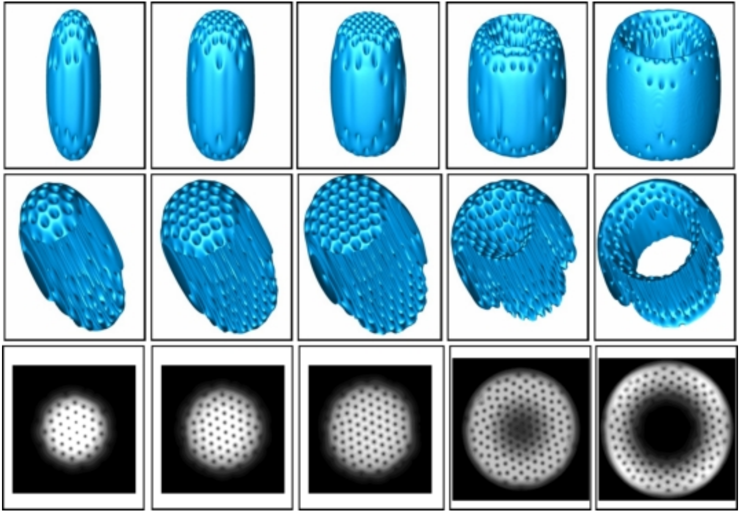
V. Bretin, S. Stock, Y. Seurin, J. Dalibard, Phys. Rev. Lett. 2003.



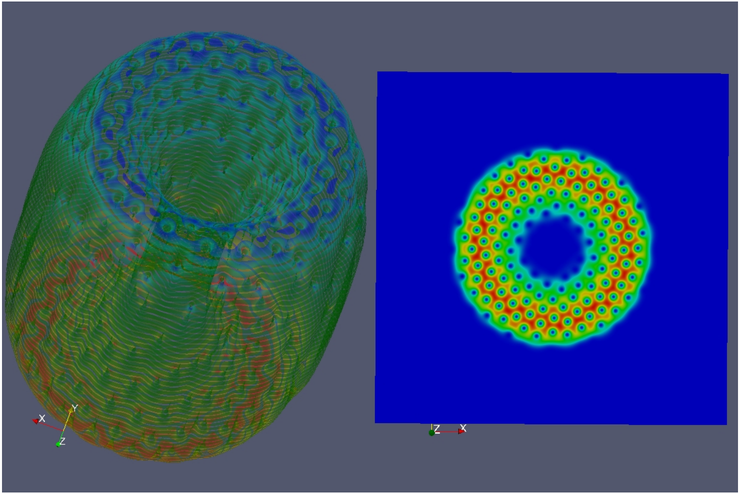
I. Danaila, Phys. Rev. A, 2005.



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



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



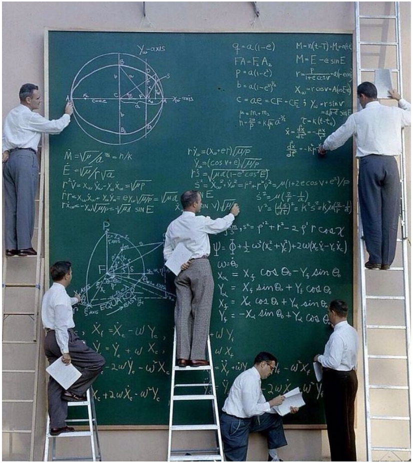
ANR project QUTE-HPC: QUantum Turbulence Exploration by High-Performance Computing

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

Post-doc position available immediately in Rouen

Modelling and HPC numerical simulations of Quantum Turbulence. Models for coupling Gross-Pitaevskii and Navier-Stokes equations.

Collaborators



- QUTE-HPC

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F. Luddens
Ph. Parnaudeau
Ph. Roche

- FreeFem++

F. Hecht
G. Vergez
P.-E. Emmeriau

- Physics (ENS)

F. Chevy
S. Laurent

- International

R. Carretero (San Diego)
P. Kevrekidis (UMas Amherst)
M. Kobayashi (Kyoto)
B. Protas (McMaster)

Conclusion

Thanks Fabien for the initial scientific impulse and your human guidance!

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```
int i=60;
while (i)
{        cout<<" Many happy returns !" << i << endl;
       i++;
}
```