Numerical models for coupling Navier-Stokes and Gross-Pitaevskii solvers for two-fluid quantum flows

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Special session: Advances in mathematical modelling and numerical simulation of superfluids

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

Joint work with **M. E. Brachet (ENS Paris), Zhentong Zhang (postdoc), Georges Sadaka (postdoc) and Victor Kalt (PhD).**

Agence Nationale de la Recherche

ANR Project QUTE-HPC (01/2019-06/2024)

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**

2. **Models for superfluid helium**
   - ($T \sim 0K$) The Gross-Pitaevskii (GP) model
   - ($T \sim 1K$) Coupling Euler and Navier-Stokes equations
   - ($T \sim 1K$) Coupling Vortex Lines and Navier-Stokes equations

3. **Coupling Gross-Pitaevskii and Navier-Stokes equations**
   - Coupling procedure
   - Numerical validation

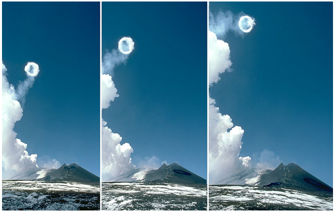
4. **Conclusions**

Vortices in classical (or normal) fluids

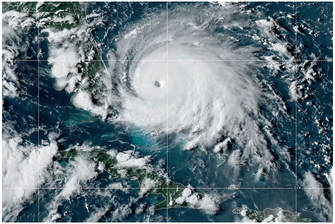
velocity-pressure → vorticity

Aircraft trailing vortices

Niagara Falls 2019



Vortex rings (Etna volcano)



Dorian Hurricane 2019

Classical Turbulence (Navier-Stokes equations)

(movie) normal incompressible fluid

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

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

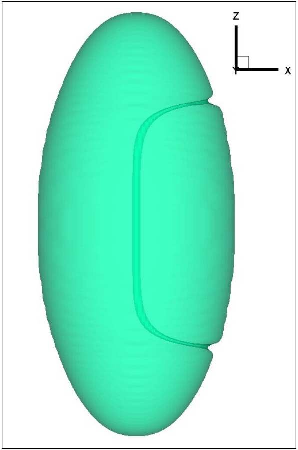
Bow River Falls 2024

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).

Vortices in quantum fluids (BEC)

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



Macroscopic description

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

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

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

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

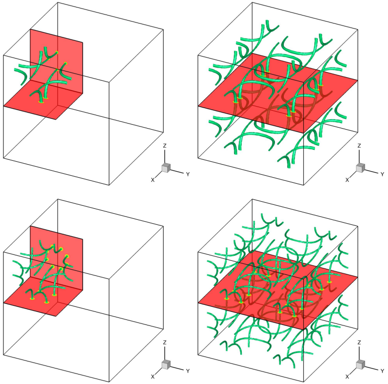
- quantified circulation

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

Super Turbulence (Gross-Pitaevskii)

C. Nore, M. Abid, M. Brachet, Physics of Fluids, 1997.

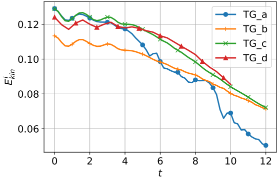
movie



Taylor-Green vortices

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

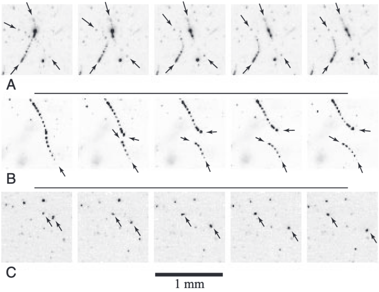
$\psi_{|t=0}$ contains vortices with winding number 3.



Vortices in quantum flows (He)

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

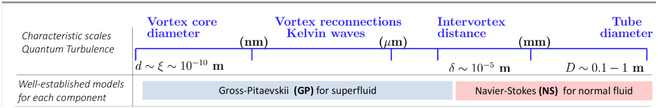
Reconnection of vortex lines (Maryland, USA, Bewley et al., PNAS, 2008)



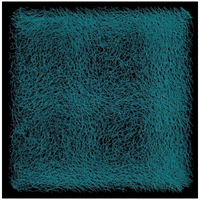
(movie)

Quantum Turbulence (QT) in ^{4}He

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

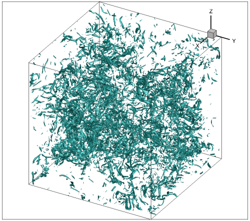


GP Super-Turbulence ST

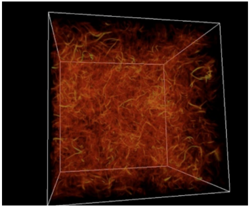


(courtesy M. Brachet)

Two-fluid Quantum Turbulence QT



CT (Navier-Stokes)



(courtesy E. Lévêque)

Outline

1 From vortices to turbulence

2 Models for superfluid helium
- ($T \sim 0K$) The Gross-Pitaevskii (GP) model
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- ($T \sim 1K$) Coupling Vortex Lines and Navier-Stokes equations

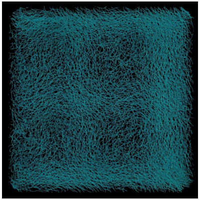
3 Coupling Gross-Pitaevskii and Navier-Stokes equations
- Coupling procedure
- Numerical validation

4 Conclusions

Models for superfluid helium

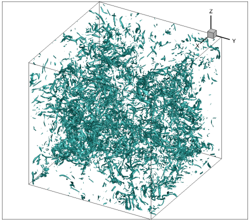
$T \sim 0.3K$

GP Super-Turbulence ST



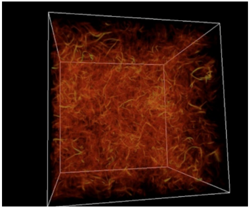
$T \sim 1K$

Two-fluid Quantum Turbulence QT



$T \sim 2.K$

CT (Navier-Stokes)



GP Super-Turbulence ... revisited

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

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

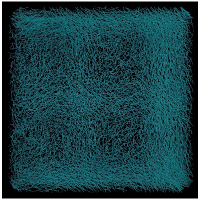
Michikazu Kobayashi [a], Philippe Parnaudeau [b], Francky Luddens [c], Corentin Lothodé [c], Luminita Danaila [d], Marc Brachet [e], Ionut Danaila [c,*]

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

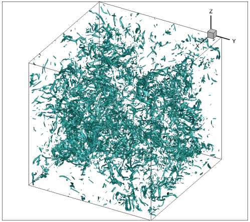
Models for superfluid helium

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

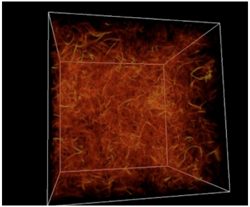
$T \sim 0.3K$
GP Super-Turbulence ST



$T \sim 1K$
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:

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

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

HVBK Quantum-Turbulence

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,†]

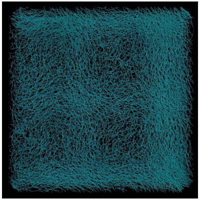
- apply statistical tools used in CT
- transport equations for the third-order moments

Models for superfluid helium

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

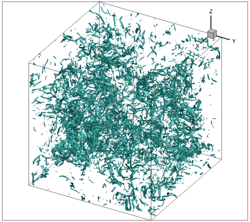
$T \sim 0.3K$

GP Super-Turbulence ST



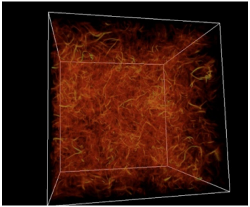
$T \sim 1K$

Two-fluid Quantum Turbulence QT



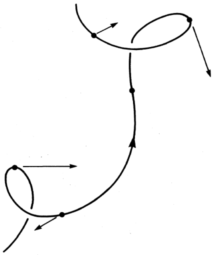
$T \sim 2.K$

CT (Navier-Stokes)



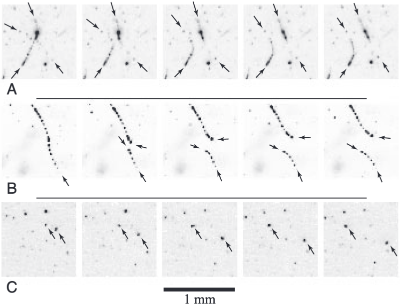
Vortex lines (filaments in superfluid helium)

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



Vortex filaments dynamics (Schwartz, PRB, 1995).

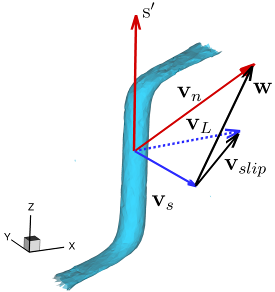
Superfluid Helium
$(T < T_\lambda = 2.17K)$



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

Coupling Vortex Lines with NS dynamics (1)

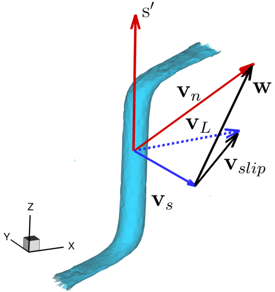
- (UK-France) Galantucci, Baggaley, Barenghi & Krstulovic, *A new self-consistent approach of quantum turbulence in superfluid helium*, Eur. Phys. J. Plus, 2020.
- (Japan) Inui & Tsubota, *Coupled dynamics of quantized vortices and normal fluid in superfluid ^{4}He based on lattice Boltzmann method*,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

Coupling Vortex Lines with NS dynamics (2)

$\mathcal{L} = s(\xi, t)$
$\mathbf{s}' = \partial s / \partial \xi$



Equilibrium of forces: $\boldsymbol{f}_{md} + \boldsymbol{f}_{ns} = 0$

- Magnus force $\boldsymbol{f}_{md}$.
- Friction force $\boldsymbol{f}_{ns}$.

$$\frac{\partial s}{\partial t} = \boldsymbol{v}_s + \alpha \mathbf{s}' \times \mathbf{w} - \alpha' \mathbf{s}' \times (\mathbf{s}' \times \mathbf{w})$$

Friction force in Navier-Stokes equations:

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

$$\frac{\partial \mathbf{v_n}}{\partial t} + (\mathbf{v_n} \cdot \nabla)\mathbf{v_n} = -\frac{\mathbf{1}}{\rho_\mathbf{n}} \nabla \mathbf{p_n} + \frac{\mathbf{1}}{\rho_\mathbf{n}} \mathbf{F_{ns}} + \nu_\mathbf{n} \nabla^2 \mathbf{v_n}.$$

The friction force: distributed around the vortex line

$$\mathbf{F_{ns}} = \oint_{\mathcal{L}} \mathbf{f_{ns}}(s) \delta(\mathbf{x} - s) d\xi.$$

Outline

1. From vortices to turbulence

2. Models for superfluid helium
   - ($T \sim 0K$) The Gross-Pitaevskii (GP) model
   - ($T \sim 1K$) Coupling Euler and Navier-Stokes equations
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3. **Coupling Gross-Pitaevskii and Navier-Stokes equations**
   - Coupling procedure
   - Numerical validation

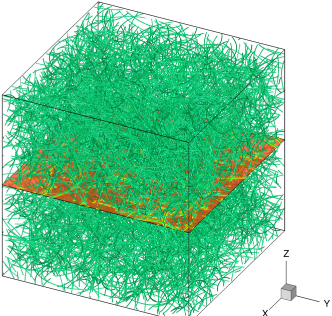
4. Conclusions

Our new model: idea

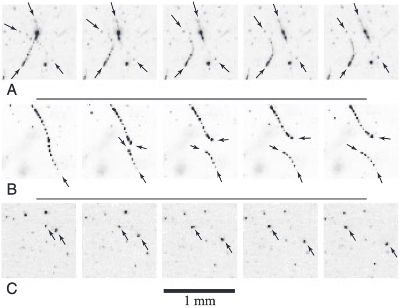
GP includes complete vortex dynamics (with nucleation and reconnections)

Superfluid vortex dynamics:

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

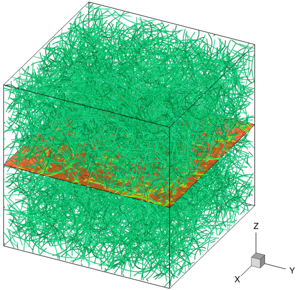


Superfluid Helium ($T < T_\lambda = 2.17K$)



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 $\boldsymbol{v}_{\rm slip}$.
3. (new) Modify the GP equation to move the vortices with the correct $\boldsymbol{v}_{\rm slip}$. External driving of the GP dynamics.
4. (as in HVBK) Evaluate the volumetric friction force to be included in the NS equations.

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3 Coupling Gross-Pitaevskii and Navier-Stokes equations
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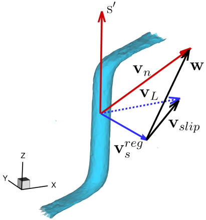
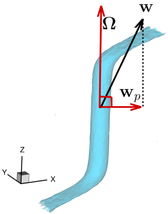
4 Conclusions

Extracting vortex lines, velocity and vorticity

1. (new) Extract vortex lines from the GP field ψ. Define:





a regularised velocity field $\boldsymbol{v}_s^{reg}$

$$\boldsymbol{v}_s^{\epsilon}(\boldsymbol{x},t) = i\frac{\hbar}{2m}\frac{\psi\nabla\overline{\psi} - \overline{\psi}\nabla\psi}{|\psi|^2 + \epsilon^2\bar{\varrho}_s},$$

$$\boldsymbol{v}_s^{reg}(\boldsymbol{x},t) = (1+\epsilon^2)\mathcal{F}^{-1}\left(\exp\left(-\frac{k^2}{k_{\mathrm{reg}}^2}\right)\mathcal{F}(\boldsymbol{v}_s^{\epsilon})\right)$$

a regularised vorticity field $\boldsymbol{\omega}_s$

$$\boldsymbol{\omega}_s(\boldsymbol{x},t) = \nabla\times\boldsymbol{v}_s^{reg},$$

$$\hat{\boldsymbol{\omega}}_s(\boldsymbol{x},t) = F\boldsymbol{\omega}_s = 1 \text{ on VL}, \searrow 0 (\text{far from VL}),$$

a counter-current normal to the VL

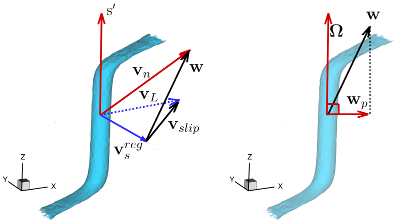
$$\mathbf{w}_p(\boldsymbol{x},t) = \mathbf{w} - \frac{\mathbf{w}\cdot\boldsymbol{\omega}_s}{\boldsymbol{\omega}_s\cdot\boldsymbol{\omega}_s}\boldsymbol{\omega}_s, \quad \text{if } \boldsymbol{\omega}_s > \boldsymbol{\omega}_s^{cut}.$$

Note that $\boldsymbol{\omega}_s\times\mathbf{w}_p = \boldsymbol{\omega}_s\times\mathbf{w}$.

Determine the slip velocity of the vortex line

2. (as in VL-NS) Apply the equilibrium of forces to determine $\boldsymbol{v}_{\mathrm{slip}}$.

- Magnus force $\boldsymbol{F}_{md} = \rho_s(\boldsymbol{v}_L - \boldsymbol{v}_s^{reg}) \times \boldsymbol{\omega}_s$,
- Friction force $\boldsymbol{F}_{ns} = \rho_n B_\star \boldsymbol{\omega}_s \times (\hat{\boldsymbol{\omega}}_s \times (\boldsymbol{v}_n - \boldsymbol{v}_L)) + \rho_n B'_\star \boldsymbol{\omega}_s \times (\boldsymbol{v}_n - \boldsymbol{v}_L)$.



$$\boldsymbol{F}_{md} + \boldsymbol{F}_{ns} = 0$$

results in an equation for $\boldsymbol{v}_{\mathrm{slip}}$

$$\boldsymbol{v}_{\mathrm{slip}} = U_\star \mathbf{w}_p + V_\star \hat{\boldsymbol{\omega}}_s \times \mathbf{w}$$

the expression for the friction force follows

$$\boldsymbol{F}_{ns} = \rho_s \boldsymbol{\omega}_s \times \boldsymbol{v}_{\mathrm{slip}}.$$

Modified GP equation with external driving $\boldsymbol{v}_{\rm slip}$ (1)

3. (new) Modify the GP equation to move the vortices with $\boldsymbol{v}_{\rm slip}$.

- Physical input:

$$\boldsymbol{F}_{ns} = \underbrace{U_\star \rho_s \omega_s \times \mathbf{w}}_{\text{normal to } \mathbf{w} \text{ = no dissipation}} + \underbrace{V_\star \rho_s \omega_s \times (\hat{\omega}_s \times \mathbf{w})}_{\text{parallel to } \mathbf{w} \text{ = dissipation}}$$

$$\boldsymbol{v}_{\rm slip} = \underbrace{U_\star \mathbf{w}_p}_{\text{conserves energy in GP}} + \underbrace{V_\star \hat{\omega}_s \times \mathbf{w}}_{\text{removes energy from GP}}$$

Modified GP equation with external driving v_{slip} (2)

3. (new) Modify the GPE to move the vortices with $\boldsymbol{v}_{\mathrm{slip}}$.

- Mathematical input: GP=Gross-Pitaevskii, GL=Ginzburg-Landau

(original GP): $$\frac{\partial \psi}{\partial t} = i\left(\frac{\hbar}{2m}\nabla^2\psi - \frac{g}{\hbar}|\psi|^2\psi\right),$$

(dissipative GP): $$\frac{\partial \psi}{\partial t} = (i+\eta_D)\left(\frac{\hbar}{2m}\nabla^2\psi - \frac{g}{\hbar}|\psi|^2\psi\right),$$

(non-dissipative GP): $$\frac{\partial \psi}{\partial t} + \boldsymbol{U}^{\mathrm{adv}}\cdot\nabla\psi = i\left(\frac{\hbar}{2m}\nabla^2\psi - \frac{g}{\hbar}|\psi|^2\psi\right),$$

equiv. to $\nabla \to \nabla + \frac{i}{2\alpha}\mathbf{v}$, *Coste*, 1998

(Advective Real GL): $$\frac{\partial \psi}{\partial t} - i\boldsymbol{U}_{\perp}^{\mathrm{adv}}\cdot\nabla\psi = i\left(\frac{\hbar}{2m}\nabla^2\psi - \frac{g}{\hbar}|\psi|^2\psi\right),$$

damped GP/Schrödinger, *Bao&Cai*, 2013

identify $\mathbf{U}^{adv}$ and $\mathbf{U}_{\perp}^{adv}$ from v_{slip}.

Modified GP equation with external driving v_{slip} (3)

3. (new) Modify GPE to move the vortices with $\boldsymbol{v}_{\text{slip}}$.

• use the convective gradient (Coste, 1998) $\nabla \to \nabla + \frac{i}{2\alpha}\mathbf{v}_{\text{slip}}^{cpl}$,

$$\mathbf{v}_{\text{slip}}^{cpl} = (U_\star + iV_\star|\hat{\mathbf{\Omega}}|)\mathbf{w}_p$$

• add a dissipation η_D to remove sound waves and make the coupling compatible to incompressible NS
• add a "chemical potential" μ to conserve mass in GP

$$\begin{aligned} \partial_t\psi &= i\left(\alpha\nabla^2\psi - \gamma(|\psi|^2 - \overline{\rho}_s)\psi - \frac{1}{\alpha}\frac{(\mathbf{v}_{\text{slip}}^{cpl})^2}{4}\psi\right) \\ &- (\mathbf{v}_{\text{slip}}^{cpl}\cdot\nabla)\psi - \frac{1}{2}(\nabla\cdot\mathbf{v}_{\text{slip}}^{cpl})\psi \\ &+ \eta_D(\alpha\nabla^2\psi - \gamma(|\psi|^2 - \overline{\rho}_s)\psi + \mu\psi). \end{aligned} \tag{1}$$

Friction force and GP-NS coupling

4. (as in HVBK) Evaluate the friction force to be included in NS eqs.

Friction force in Navier-Stokes equations:

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

$$\frac{\partial \mathbf{v_n}}{\partial t} + (\mathbf{v_n} \cdot \nabla)\mathbf{v_n} = -\frac{\mathbf{1}}{\rho_\mathbf{n}}\nabla \mathbf{p_n} + \frac{\mathbf{1}}{\rho_\mathbf{n}}\mathbf{F_{ns}} + \nu_\mathbf{n}\nabla^\mathbf{2}\mathbf{v_n}.$$

$$\boldsymbol{F}_{ns} = \rho_n B_\star \omega_s \times (\hat{\omega}_s \times (\boldsymbol{v}_n - \boldsymbol{v}_L)) + \rho_n B'_\star \omega_s \times (\boldsymbol{v}_n - \boldsymbol{v}_L)$$

NB: In VL-NS models the friction force is distributed around the VL.

Outline

1 From vortices to turbulence

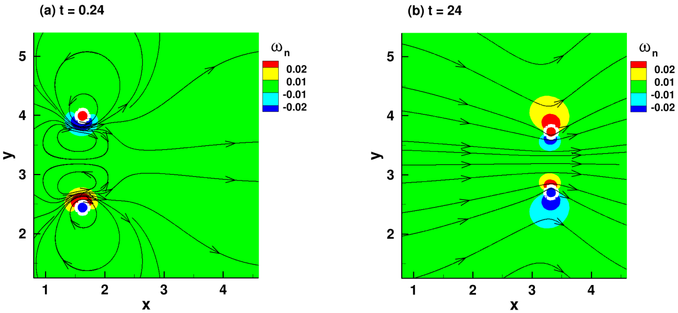
2 Models for superfluid helium
- ($T \sim 0K$) The Gross-Pitaevskii (GP) model
- ($T \sim 1K$) Coupling Euler and Navier-Stokes equations
- ($T \sim 1K$) Coupling Vortex Lines and Navier-Stokes equations

3 Coupling Gross-Pitaevskii and Navier-Stokes equations
- Coupling procedure
- Numerical validation

4 Conclusions

2D: superfluid vortex dipole

- Known case useful to fit numerical parameters:
  - ϵ to avoid division by zero,
  - $k_{reg} \sim 1/\xi$ (spectral) parameter for $\boldsymbol{v}_s^{reg}$,
  - $\eta_D \sim B_{tab}$ dissipation.
- Vortex dipole evolution in a normal fluid



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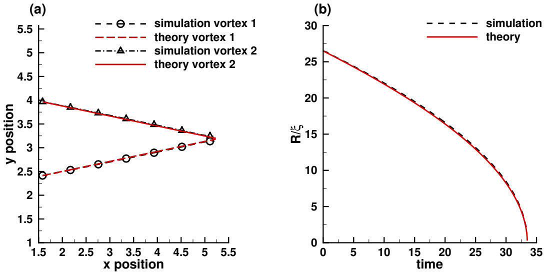
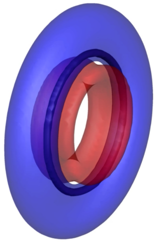


3D: superfluid vortex ring

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

without normal fluid

with normal fluid



3D: reconnection of superfluid vortex rings

Outline

1. From vortices to turbulence
2. Models for superfluid helium
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4. **Conclusions**

Conclusions

Model for coupling GP and NS equations

- First attempt to couple GP and NS. Coste (1998) considered the different case of compressible GP equation, without vortices.
- No assumption on the nucleation/reconnection of vortices.
- Physicall sound method validated for known cases.
- Fourier spectral code (Runge-Kutta integration in time).

New research paths

- Analyse in detail mathematical/numerical aspects.
- Revisit results for Quantum Turbulence obtained with the VL-NS method (the most advanced).

More details in ...

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

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Bridging Classical and Quantum Turbulence

https://eequte2023.sciencesconf.org/

Thank you for your attention!