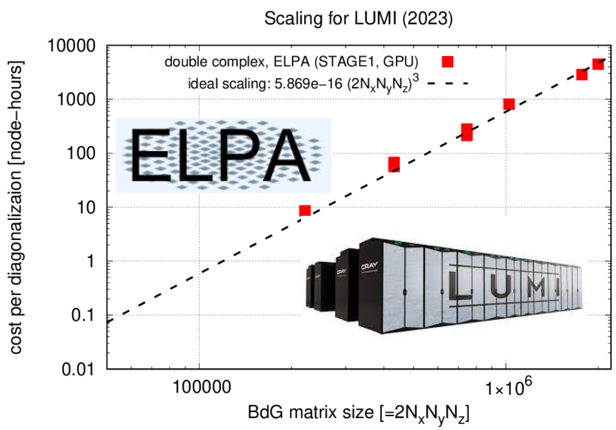
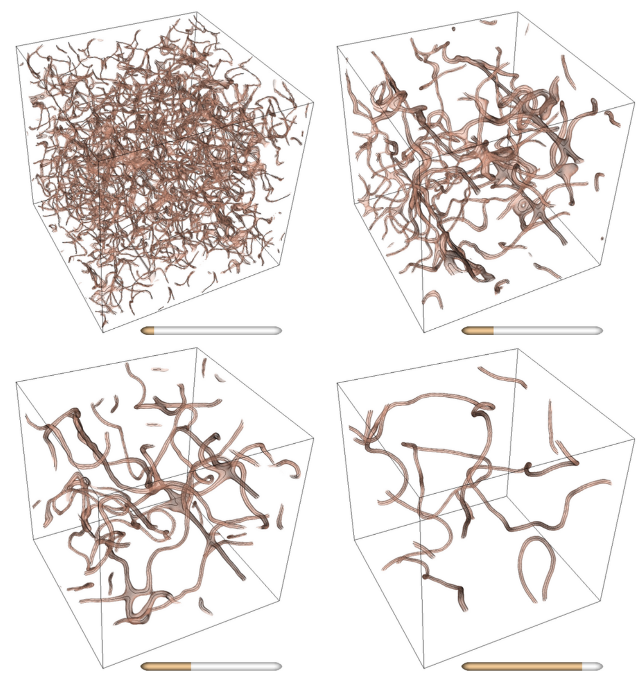
Turbulent dynamics in superfluid Fermi systems

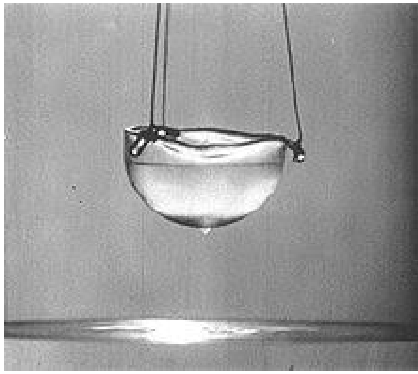
Gabriel Wlazłowski

Warsaw University of Technology

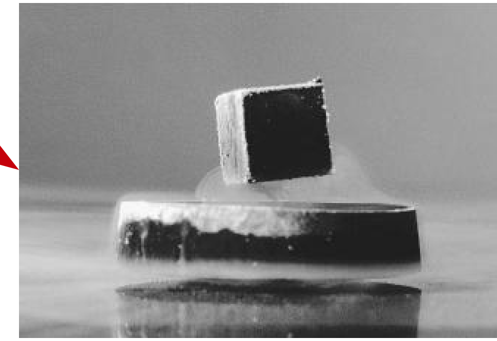




liquid ^3He and ^4He



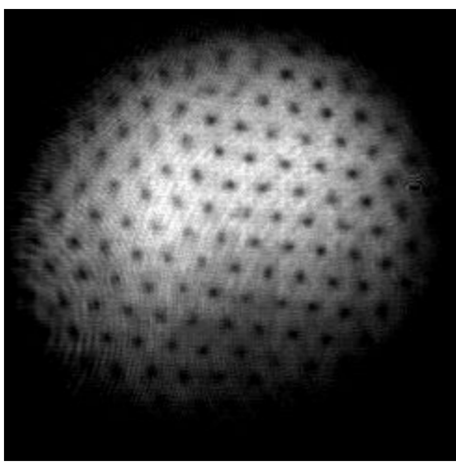
superconductors



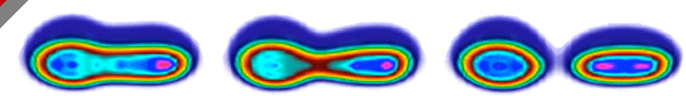
Superfluidity
(Superconductivity)

generic
phenomenon
observed in most
physical systems at
sufficiently low
temperatures.

ultra-cold atomic gases
(bosonic and fermionic)

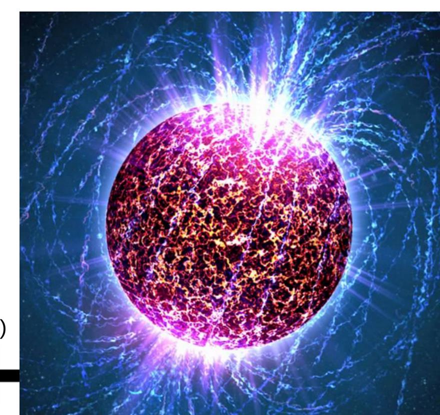


Source: Wolfgang Ketterle - Nobel Lecture:
When Atoms Behave as Waves: Bose-Einstein Condensation and the Atom Laser



nuclear systems such as nuclei...

... and neutron stars

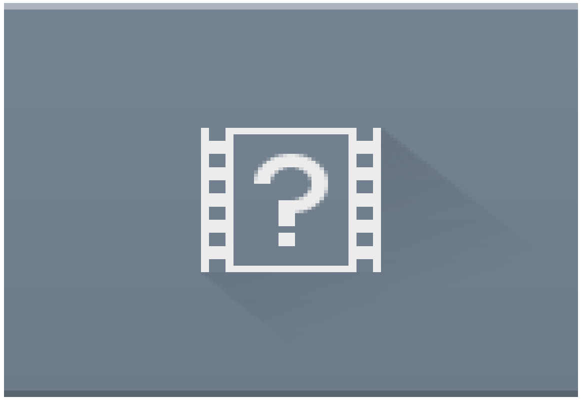


Artist's conception of a neutron star.
(Casey Reed, Penn State University)

Source: https://www.youtube.com/watch?v=w0z8fVrTyzg

Superfluid Hydrodynamics

→ macroscopic description
→ dof: fluid elements



superfluid drop pinching off from a nozzle, T=1.34 Kelvin

Present HPC capabilities allow for this...

towards origin of superfluidity

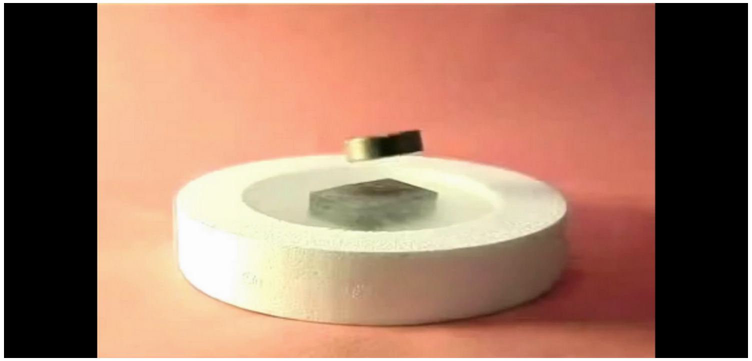
Quantum Mechanics

→ microscopic description
→ dof: particles

Source: https://www.youtube.com/watch?v=nWTSzBWEsms

Superfluid Hydrodynamics

→ macroscopic description
→ dof: fluid elements



Levitating Magnet Over Superconductor

Present HPC capabilities allow for this...

towards origin of superfluidity

Quantum Mechanics

→ microscopic description
→ dof: particles

At microscopic level quantum statistics is important:

- particles with integer spin (bosons): Bose-Einstein condesates, superfluid ^{4}He
- particles with half-integer spin (**fermions**): Superconductors, ultracold Fermi gases, nuclear systems, superfluid ^{3}He...

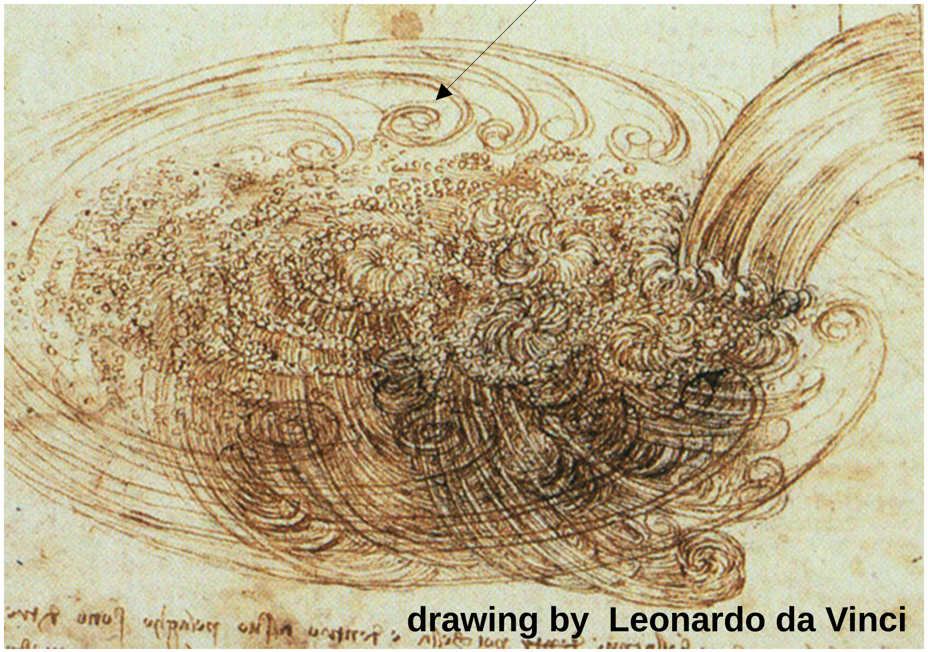
This talk!

Turbulence in classical mechanics

The plume from this candle flame goes from laminar to turbulent. The Reynolds number can be used to predict where this transition will take place

Fig. From https://en.wikipedia.org/wiki/Turbulence

Vortices are inherently related to turbulent dynamics



drawing by Leonardo da Vinci

Turbulence is usually an undesirable phenomenon in the context of applications!
(enhanced viscous conversion of mechanical energy to heat)

$$\frac{dE_{\text{flow}}}{dt} = -\frac{1}{2}\eta \int \left(\frac{\partial v_i}{\partial x_k} + \frac{\partial v_k}{\partial x_i} \right)^2 dV$$

(shear) viscosity

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The plume from this candle flame goes from laminar to turbulent. The Reynolds number can be used to predict where this transition will take place

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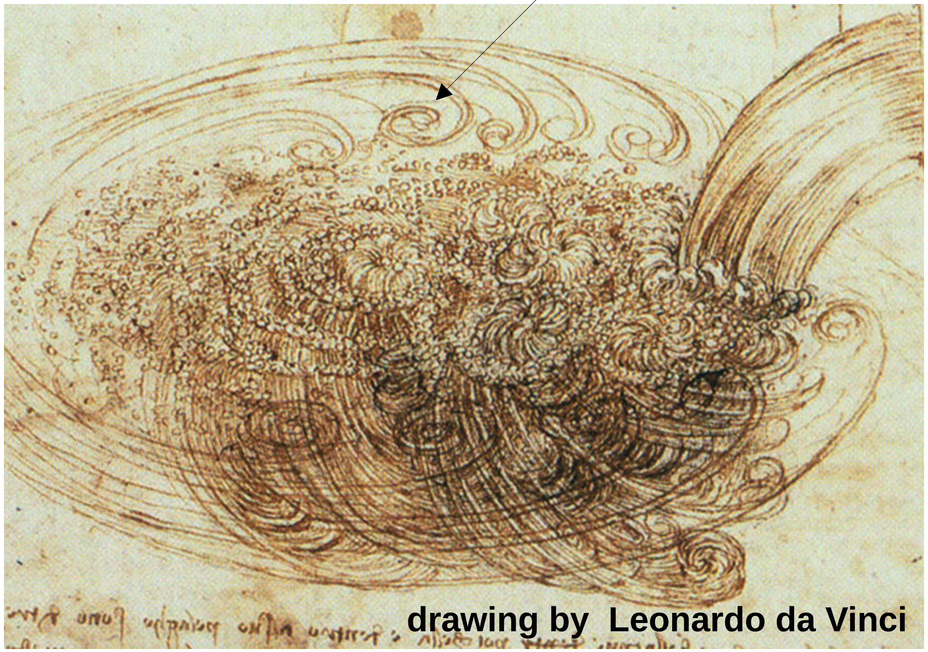

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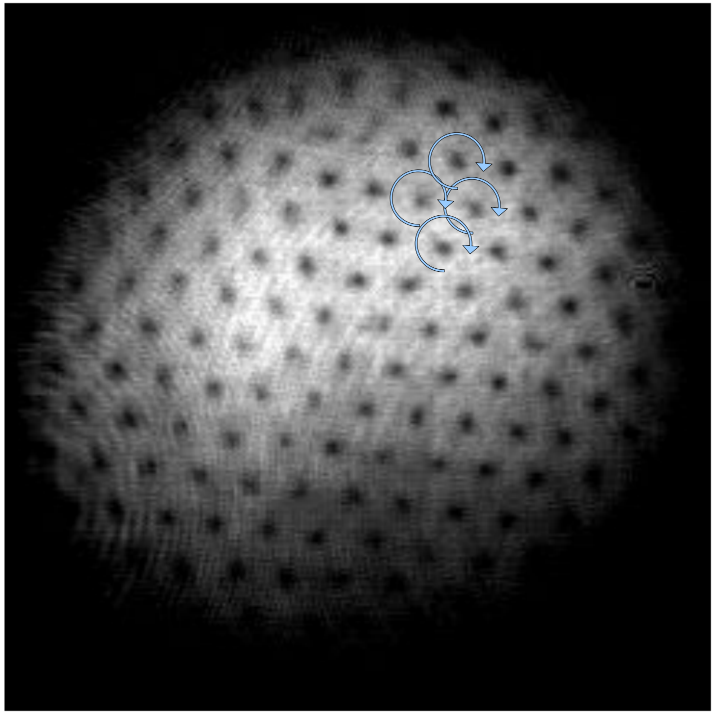
(shear) viscosity

But superfluids have zero viscosity!
... so, no energy looses?

Turbulence in quantum mechanics → Chaotic dynamics of many quantized vortices



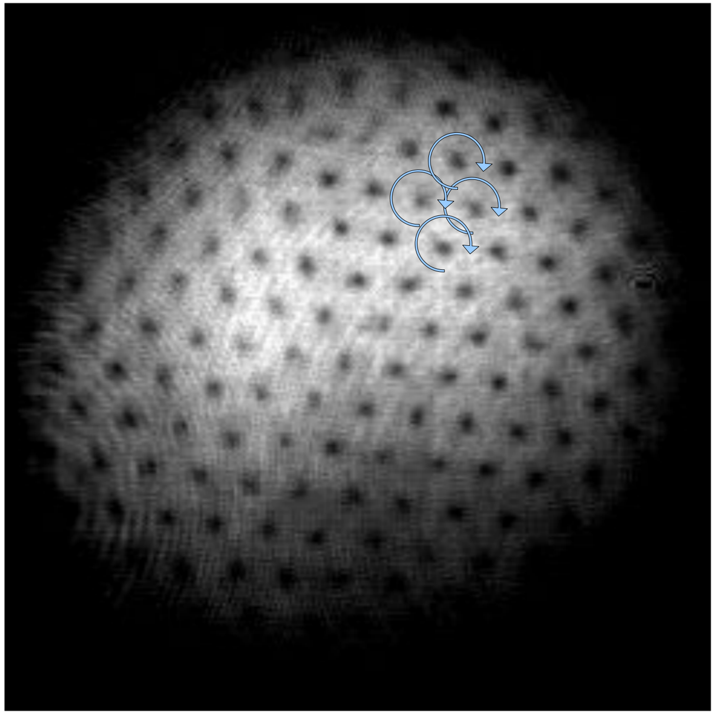
Source: Wolfgang Ketterle
Nobel Lecture: When Atoms Behave as Waves:
Bose-Einstein Condensation and the Atom Laser.

Quantized circulation:

$$\oint \boldsymbol{v} \cdot d\boldsymbol{\ell} = h/M$$

These vortices cannot decay
(topological defect)
→ lifetime of this configuration ~
lifetime of the setup

Turbulence in quantum mechanics → Chaotic dynamics of many quantized vortices

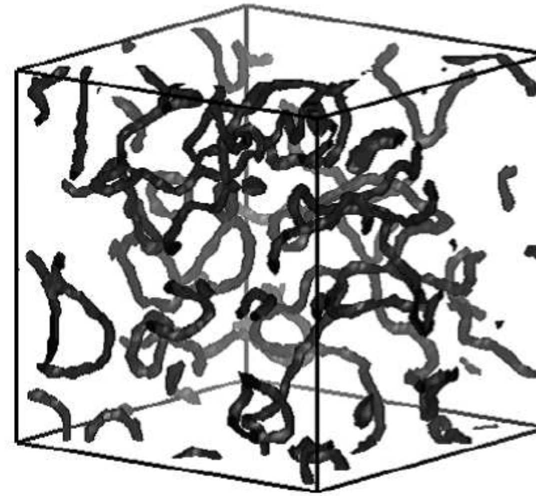


Source: Wolfgang Ketterle
Nobel Lecture: When Atoms Behave as Waves: Bose-Einstein Condensation and the Atom Laser.

There exists other (than viscosity) mechanisms than can lead to the energy dissipation!

→ effective viscosity

Example: energy can be dissipated during vortex reconnection.



Phys. Rev. Lett. 97 (2006) 145301

Quantized circulation:

$$\oint \boldsymbol{v} \cdot d\boldsymbol{\ell} = h/M$$

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→ lifetime of this configuration ~ lifetime of the setup

Phys. Rev. A 103, L051302 (2021)

Quantum mechanical description

Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \Psi(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N, t) = \hat{H} \Psi(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N, t)$$

Practical (and accurate) method of solving:

Density Functional Theory (DFT)

Self-Consistent Equations Including Exchange and Correlation Effects

W. Kohn and L. J. Sham

Phys. Rev. **140**, A1133 – Published 15 November 1965

Physics

Most frequently cited paper in physics
(within Physical Review journals)

Article	References	Citing Articles (46,542)	PDF	Export Citation

The Nobel Prize in Chemistry 1998 was divided equally between Walter Kohn "for his development of the density-functional theory" and John A. Pople "for his development of computational methods in quantum chemistry."

Credit: https://www.nobelprize.org/

Density-Functional Theory for Superconductors

L. N. Oliveira, E. K. U. Gross, and W. Kohn
Phys. Rev. Lett. **60**, 2430 – Published 6 June 1988

…triggered by…

The Nobel Prize in Physics 1987 was awarded jointly to J. Georg Bednorz and K. Alexander Müller "for their important break-through in the discovery of superconductivity in ceramic materials."

Credit: https://www.nobelprize.org/

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In general superfluid DFT results with integro-differential equations...

Beyond reach even for exascale systems...

Unless approximation is used...

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Phys. Rev. Lett. **73**, 2915 – Published 21 November 1994

Local density approximation for systems with pairing correlations

Aurel Bulgac
Phys. Rev. C **65**, 051305(R) – Published 25 April 2002

SLDA: crucial for numerical treatment...

Results with many PDEs...

In practice at least petascale performance is required...

In general superfluid DFT results with integro-differential equations...

Beyond reach even for exascale systems...

Unless approximation is used...

Solving time-dependent problem for superfluids...

The real-time dynamics is given by equations, which are formally equivalent to the Time-Dependent HFB (TDHFB) or Time-Dependent Bogolubov-de Gennes (TDBdG) equations

$$h \sim f_1(n,\nu,\ldots)\nabla^2 + \boldsymbol{f}_2(n,\nu,\ldots)\cdot\nabla + f_3(n,\nu,\ldots)$$

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_{n,\uparrow}(\boldsymbol{r},t) \\ v_{n,\downarrow}(\boldsymbol{r},t)\end{pmatrix} = \begin{pmatrix} h_\uparrow(\boldsymbol{r},t)-\mu_\uparrow & \Delta(\boldsymbol{r},t) \\ \Delta^*(\boldsymbol{r},t) & -h^*_\downarrow(\boldsymbol{r},t)+\mu_\downarrow \end{pmatrix}\begin{pmatrix} u_{n,\uparrow}(\boldsymbol{r},t) \\ v_{n,\downarrow}(\boldsymbol{r},t)\end{pmatrix}$$

$|u_{n\sigma}|^2$ – probability for the hole in the n-th state
$|v_{n\sigma}|^2$ – probability for the particle in the n-th state

where *h* and Δ depends on "densities":

$$n_\sigma(\boldsymbol{r},t) = \sum_{E_n<E_c} |v_{n,\sigma}(\boldsymbol{r},t)|^2, \qquad \tau_\sigma(\boldsymbol{r},t) = \sum_{E_n<E_c} |\nabla v_{n,\sigma}(\boldsymbol{r},t)|^2,$$

$$\nu(\boldsymbol{r},t) = \sum_{E_n<E_c} u_{n,\uparrow}(\boldsymbol{r},t)v^*_{n,\downarrow}(\boldsymbol{r},t), \qquad \boldsymbol{j}_\sigma(\boldsymbol{r},t) = \sum_{E_n<E_c} \mathrm{Im}[v^*_{n,\sigma}(\boldsymbol{r},t)\nabla v_{n,\sigma}(\boldsymbol{r},t)],$$

+ orthogonality of states:

$$\sum_{\sigma=\uparrow,\downarrow}\int \left(v_{m,\sigma}(\boldsymbol{r},t)v^*_{n,\sigma}(\boldsymbol{r},t) + u_{m,\sigma}(\boldsymbol{r},t)u^*_{n,\sigma}(\boldsymbol{r},t)\right)d\boldsymbol{r} = \delta_{mn}$$

a lot of nonlinear coupled 3D Partial Differential Equations
(in practice n=1,2,..., 10^5 - 10^6)

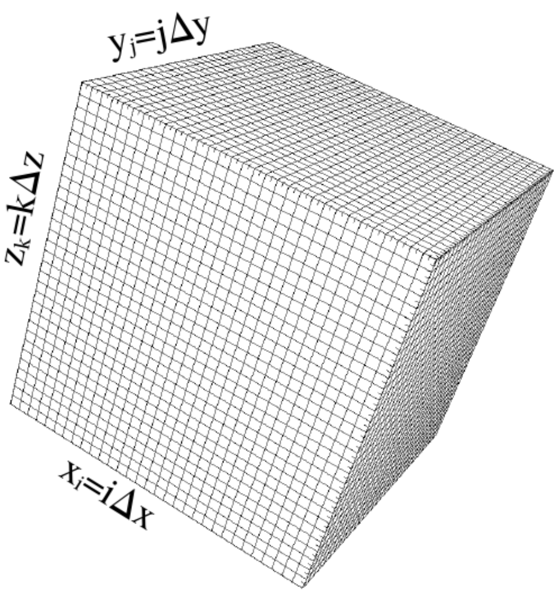
To start the time-dependent problem, we need provide the initial state...

$$\begin{pmatrix} h_{\uparrow}(\boldsymbol{r}) - \mu_{\uparrow} & \Delta(\boldsymbol{r}) \\ \Delta^{*}(\boldsymbol{r}) & -h_{\downarrow}^{*}(\boldsymbol{r}) + \mu_{\downarrow} \end{pmatrix} \begin{pmatrix} u_{n,\uparrow}(\boldsymbol{r}) \\ v_{n,\downarrow}(\boldsymbol{r}) \end{pmatrix} = E_n \begin{pmatrix} u_{n,\uparrow}(\boldsymbol{r}) \\ v_{n,\downarrow}(\boldsymbol{r}) \end{pmatrix}$$

It is eigenvalue problem, where we need to extract all eigenvectors with energy range $E_n \in [0, E_c]$

We solve the problem on a Cartesian mesh: $N_x \times N_y \times N_z$.

Then the matrix size is $(2N_x \times N_y \times N_z)^2$



In our case, we used:
$N_x = N_y = N_z = 100$...
… so the matrix is $2M \times 2M$
… that we diagonalize in double complex precision

ELPA

(Eigenvalue soLvers for Petaflop Applications)

PHYSICS.WUT

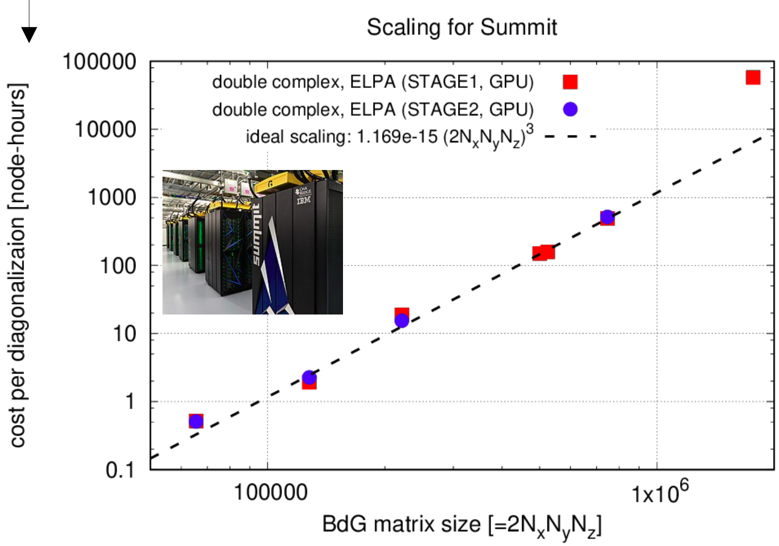
» List of Records https://elpa.mpcdf.mpg.de/ELPA_RECORDS.html

LIST OF RECORDS

We would like to give a short overview of some records achieved with the ELPA-library on HPC systems.

- Mai 2021: Solution of a **real** (double) **20k** matrix (full eigenvector spectrum) in ~2.1 seconds on 250 nodes (18.000 CPUs) on the RAVEN HPC system of MPCDF
- Feb. 2021: Solution of a **complex** (double) **1769k** matrix (full eigenvector spectrum) in ~52.000 seconds on 4000 nodes (24.000 GPUs) on the Summit system of the Oak Ridge National Laboratory
- Jan. 2018: Solution of a **real** (double) **20k** matrix (full eigenvector spectrum) in ~3 seconds on 5120 cores of a Intel Skylake system
- Nov. 2016: Solution of a **real** (double) **1048k** matrix (full eigenvector spectrum) in less than 15000 seconds on 200.000 cores of a Intel KNL system of the Argonne National Laboratory
- Feb. 2011: Solution of a **real** (double) **260k** matrix in less than 800 seconds on 295.000 cores of a IBM Bluegene/P of the Forschungszentrum Jülich

Previous Next



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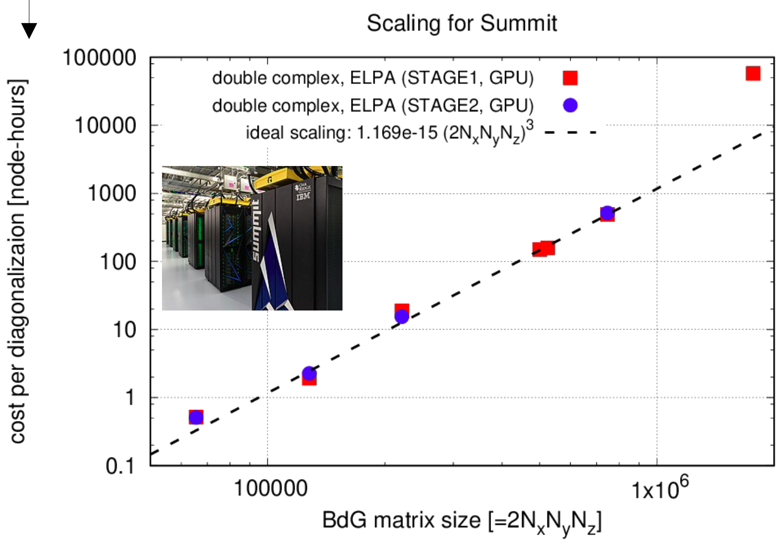
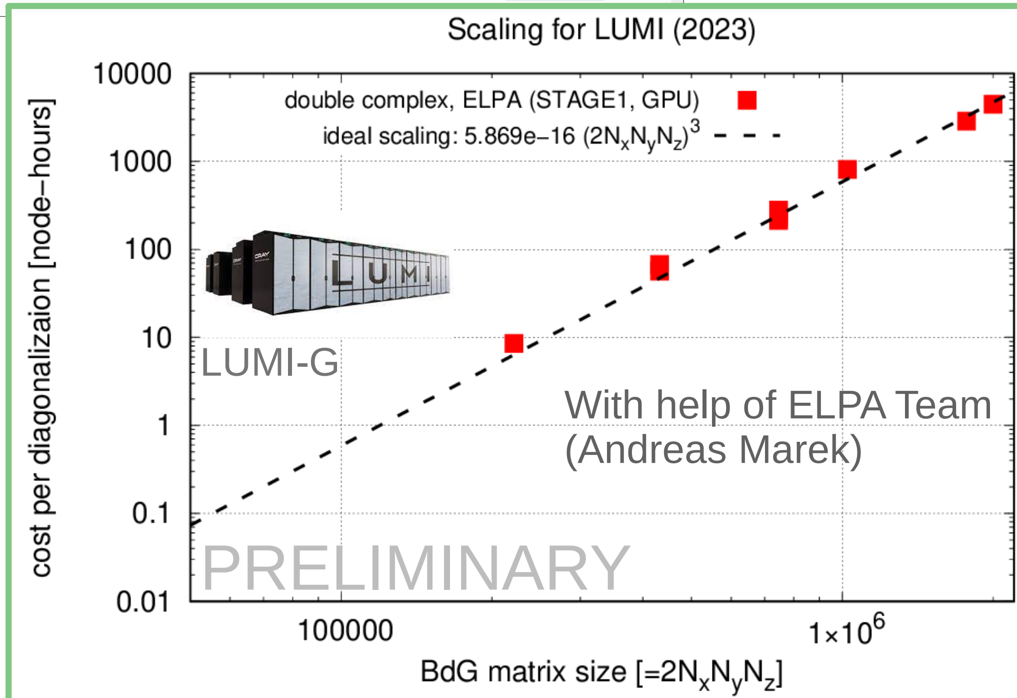




https://wslda.fizyka.pw.edu.pl/
for modeling ultracold atoms

Ongoing extensions:
→ Bose-Fermi mixtures
→ Fermi-Fermi mixtures (like nuclear systems: protons+neutrons)

Functionalities | Download | Gallery | Publications and Materials | Related projects | Info | EN

Warsaw University of Technology | W-SLDA Toolkit

W-SLDA Toolkit

Self-consistent solver of mathematical problems which have structure formally equivalent to Bogoliubov-de Gennes equations.

static problems: st-wslda

$$\begin{pmatrix} h_a(\boldsymbol{r}) - \mu_a & \Delta(\boldsymbol{r}) \\ \Delta^*(\boldsymbol{r}) & -h_b^*(\boldsymbol{r}) + \mu_b \end{pmatrix} \begin{pmatrix} u_n(\boldsymbol{r}) \\ v_n(\boldsymbol{r}) \end{pmatrix} = E_n \begin{pmatrix} u_n(\boldsymbol{r}) \\ v_n(\boldsymbol{r}) \end{pmatrix}$$

time-dependent problems: td-wslda

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} u_n(\boldsymbol{r},t) \\ v_n(\boldsymbol{r},t) \end{pmatrix} = \begin{pmatrix} h_a(\boldsymbol{r},t) - \mu_a & \Delta(\boldsymbol{r},t) \\ \Delta^*(\boldsymbol{r},t) & -h_b^*(\boldsymbol{r},t) + \mu_b \end{pmatrix} \begin{pmatrix} u_n(\boldsymbol{r},t) \\ v_n(\boldsymbol{r},t) \end{pmatrix}$$

Speed-up calculations by exploiting High Performance Computing

Functionals for studies of BCS and unitary regimes

Integration with VisIt: visualization, animation and analysis tool

Speed-up calculations by exploiting High Performance Computing

W-SLDA is designed to exploit capabilities of leadership-class supercomputers.

Depending on the type of the code the toolkit can be executed on:

static codes: standard CPU machines, GPU accelerated machines,
time-dependent codes: only GPU accelerated machines.

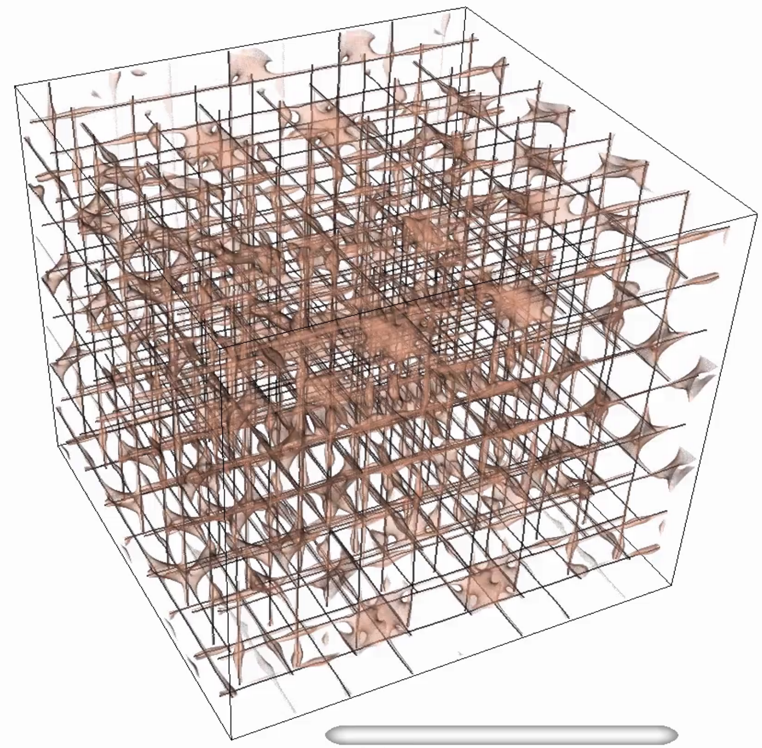
To learn more about a computer that you need for calculations see Requirements

ALL FUNCTIONALITIES →

Dimensionalities of problems: 3D, 2D and 1D

Solvers for spin symmetric and spin imbalanced systems

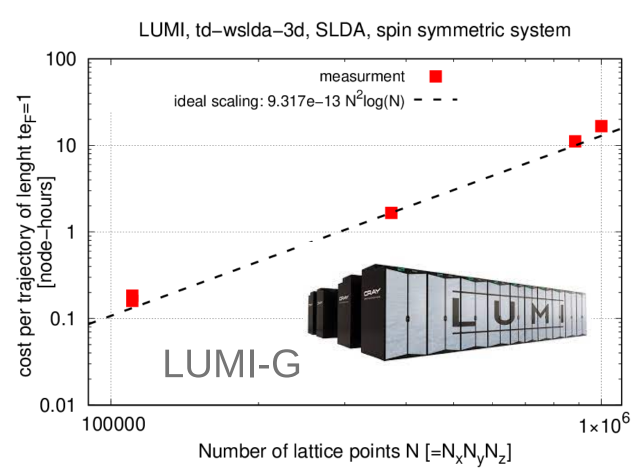
Unified solvers for static and time-dependent problems



System: *strongly interacting Fermi gas*
3D simulation on lattice 100^3

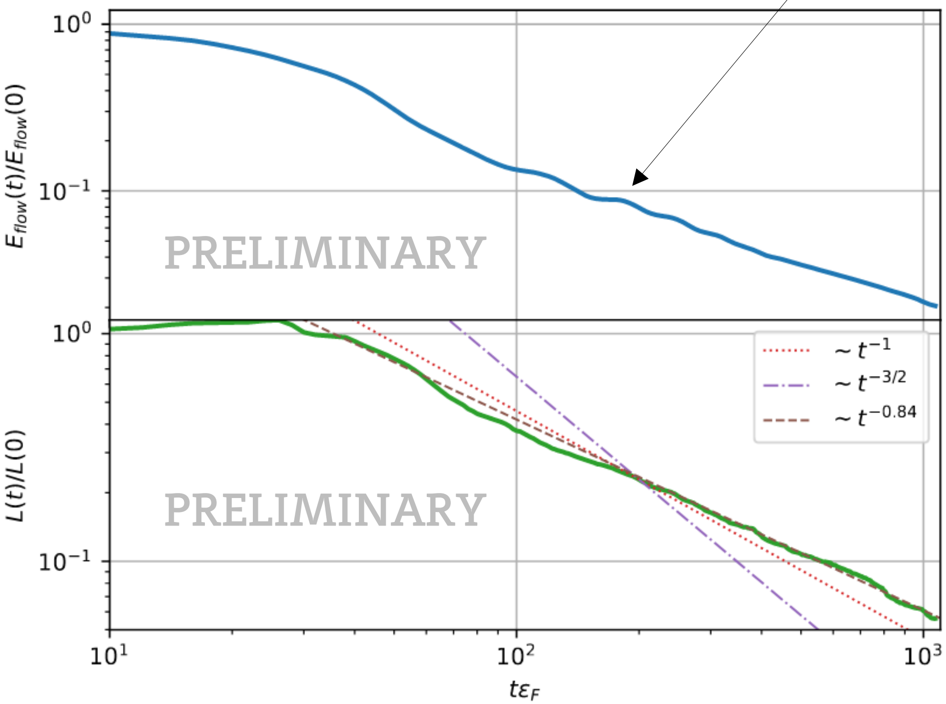
number of atoms = 26,790
number of quasi-particle states = 582,898
number of PDEs = 1,165,796

PRELIMINARY:
quantum turbulence
in the unitary Fermi gas



Conversion CUDA→HIP with the help of Maciej Szpindler (LUST)

We observe energy dissipation, although the underlying system is superfluid!
→ effective viscosity



$$E_{\text{flow}}(t) = \int \frac{\rho(\boldsymbol{r},t)\boldsymbol{v}^2(\boldsymbol{r},t)}{2}\, d\boldsymbol{r}$$

$L(t)$ - total vortex length

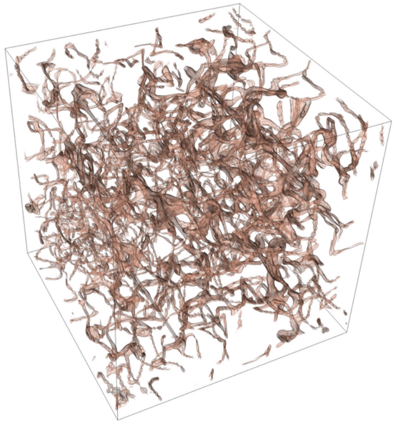
$$E_{\text{total}} = E_{\text{kin}} + E_{\text{interaction}} + E_{\text{flow}} + \ldots = \text{const}$$

Work in progress:

→ identification of mechanisms that lead to the effective viscosity...

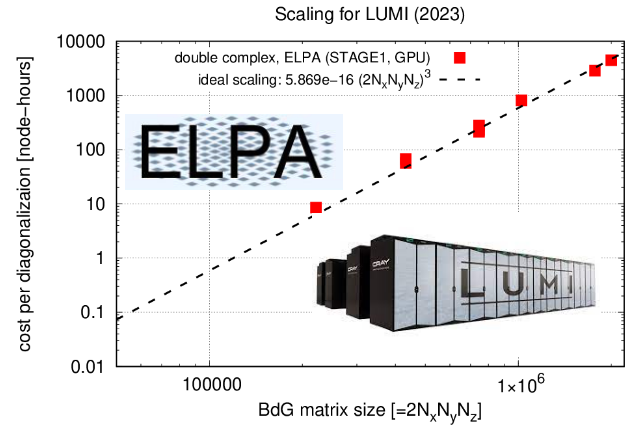
→ ...conditions under which they are triggered.

SUMMARY



- A microscopic theoretical framework (DFT) capable of describing fermionic superfluids and implementable in realistic calculations has become possible recently. Developments of HPC techniques played an important role in this progress.

- (TD)DFT for superfluids/superconducting systems involves:
  → diagonalization of large matrices *(ELPA running on LUMI can diagonalize efficiently matrices of sizes measured in millions!)*
  → solving of large sets of coupled 3D PDEs



- LUMI allowed us to explore regimes that were not accessible for us before *(quantum dynamics of collection of abut 26k particles)*.

- Even short-time access (Pilot phase 1 & 2) resulted in collection of valuable results.

New J. Phys. **25** (2023) 033013 https://doi.org/10.1088/1367-2630/acc26b

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IOP Institute of Physics
Published in partnership with: Deutsche Physikalische Gesellschaft and the Institute of Physics

Pilot 1

PAPER

Disordered structures in ultracold spin-imbalanced Fermi gas

Buğra Tüzemen[1,2,*], Tomasz Zawiślak[2], Gabriel Wlazłowski[2,3] and Piotr Magierski[2,3]

Pilot phase 1 & 2 team: Piotr Magierski, Andrzej Makowski, Bugra Tuzemen, Tomasz Zawiślak (WUT), Andreas Marek, Erwin Laure (MPCDF→ELPA), Maciej Szpindler (ICM→LUST)

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