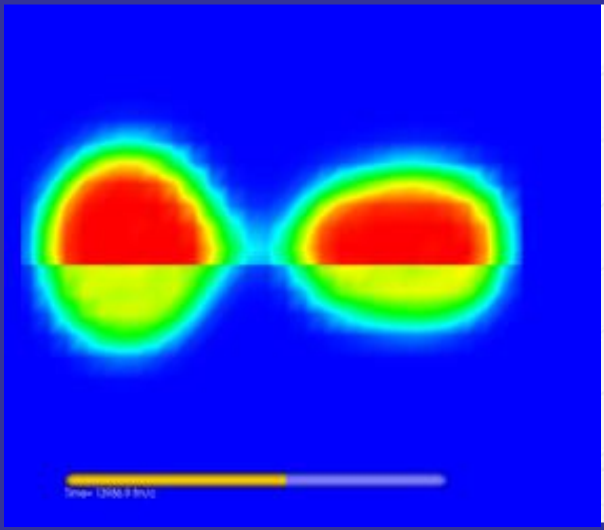
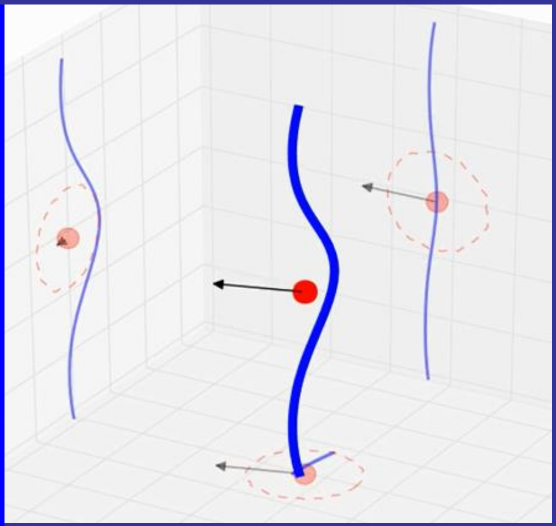
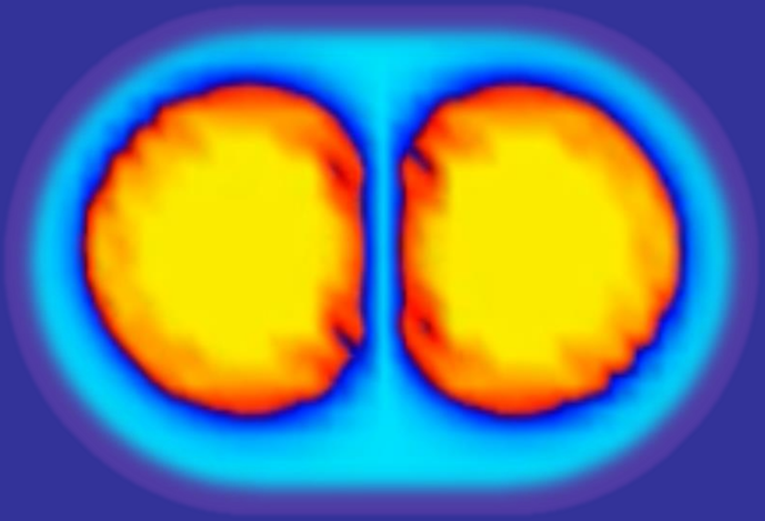
Modelling quantum superfluids - how supercomputers help us understand mechanisms of nuclear processes.







Piotr Magierski (Warsaw University of Technology)

100 years of superconductivity and superfluidity in Fermi systems

Discovery: H. Kamerlingh Onnes in 1911 cooled a metallic sample of mercury at T<4.2K

20 orders of magnitude over a century of (low temperature) physics

- ✓ Dilute atomic Fermi gases $T_c \approx 10^{-12} - 10^{-9}$ eV
- ✓ Liquid ^{3}He $T_c \approx 10^{-7}$ eV
- ✓ Metals, composite materials $T_c \approx 10^{-3} - 10^{-2}$ eV
- ✓ Nuclei, neutron stars $T_c \approx 10^{5} - 10^{6}$ eV
- QCD color superconductivity $T_c \approx 10^{7} - 10^{8}$ eV

units (1 eV $\approx 10^4$ K)

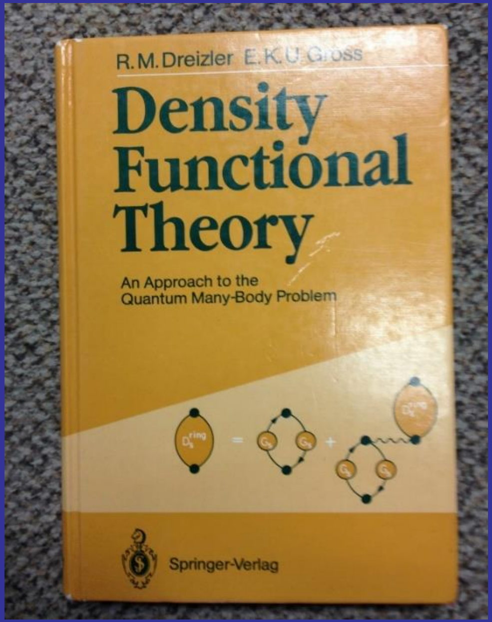
Robert B. Laughlin, Nobel Lecture, December 8, 1998:

One of my favorite times in the academic year occurs [..] when I give my class of extremely bright graduate students [..] a take home exam in which they are asked <u>TO DEDUCE SUPERFLUIDITY FROM FIRST PRINCIPLES.</u>
There is no doubt a special place in hell being reserved for me at this very moment for this mean trick, for the task is <u>IMPOSSIBLE</u>. Superfluidity [..] is an EMERGENT phenomenon – a low energy collective effect of huge number of particles that <u>CANNOT</u> be deduced from the microscopic equations of motion in a <u>RIGOROUS WAY</u> and that <u>DISAPPEARS</u> completely when the system is taken apart.

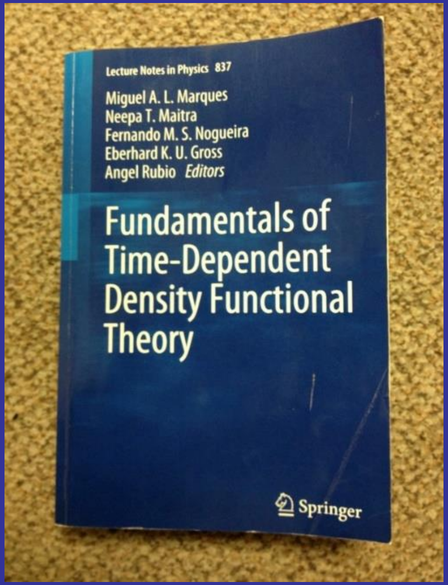
[..]students who stay in physics long enough [..] eventually come to understand that the <u>REDUCTIONIST IDEA IS WRONG</u> a great deal of the time and perhaps <u>ALWAYS.</u>

Main Theoretical Tool

THEOREM: There exist an universal density functional of particle density.



1990



2012

DFT has been developed and used mainly to describe normal (non-superfluid) electron systems – more than <u>50 years old theory</u>:

DFT - Kohn and Hohenberg, 1964
LDA - Kohn and Sham, 1965
Extension for superconductors/superfluids: DFT - Oliveira, Gross, Kohn (1988),
TDDFT - Wacker, Kummel, Gross (1994)
SLDA, TDSLDA – Bulgac (2002)

TDDFT equations with local pairing field (TDSLDA):

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_{k\uparrow}(\mathbf{r},t) \\ u_{k\downarrow}(\mathbf{r},t) \\ v_{k\uparrow}(\mathbf{r},t) \\ v_{k\downarrow}(\mathbf{r},t) \end{pmatrix} = \begin{pmatrix} h_{\uparrow,\uparrow}(\mathbf{r},t) & h_{\uparrow,\downarrow}(\mathbf{r},t) & 0 & \Delta(\mathbf{r},t) \\ h_{\downarrow,\uparrow}(\mathbf{r},t) & h_{\downarrow,\downarrow}(\mathbf{r},t) & -\Delta(\mathbf{r},t) & 0 \\ 0 & -\Delta^*(\mathbf{r},t) & -h^*_{\uparrow,\uparrow}(\mathbf{r},t) & -h^*_{\uparrow,\downarrow}(\mathbf{r},t) \\ \Delta^*(\mathbf{r},t) & 0 & -h^*_{\uparrow,\downarrow}(\mathbf{r},t) & -h^*_{\downarrow,\downarrow}(\mathbf{r},t) \end{pmatrix}\begin{pmatrix} u_{k\uparrow}(\mathbf{r},t) \\ u_{k\downarrow}(\mathbf{r},t) \\ v_{k\uparrow}(\mathbf{r},t) \\ v_{k\downarrow}(\mathbf{r},t) \end{pmatrix}$$

The form of $h(r,t)$ and $\Delta(r,t)$ is determined by EDF (Energy Density Functional)

- **The system is placed on a large 3D spatial lattice.**
- **No symmetry restrictions.**
- **Number of PDEs is of the order of the number of spatial lattice points.**

Table 1: Comparison of profit gained by using GPUs instead of CPUs for two example lattices. The timing was obtained on Titan supercomputer. Note, Titan has 16x more CPUs than GPUs.

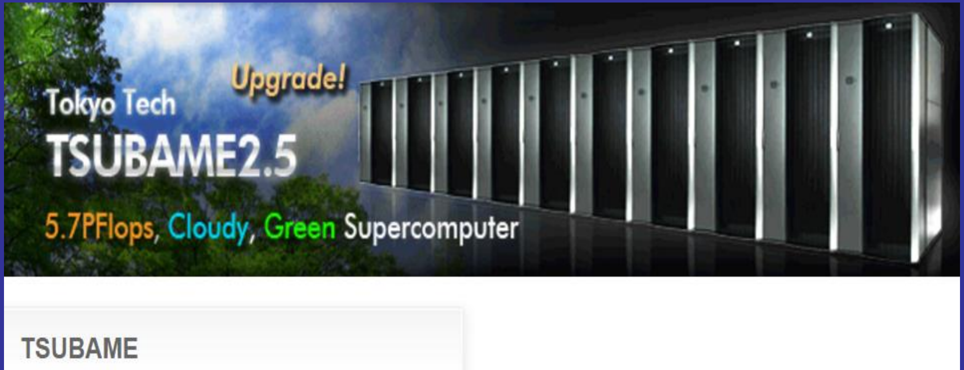
		CPU implementation		GPU implementation		
$N_xN_yN_z$	Number of HFB equations	# of CPUs	time per step	# of GPUs	time per step	***SPEEDUP***
48^3	110,592	110,592	3.9 sec	6,912	0.39 sec	**10**
64^3	262,144	262,144	20 sec	16,384	0.80 sec	**25**

Within current computational capabilities TDDFT allows to describe real time dynamics of strongly interacting, superfluid systems of hundred of thousands fermions.

Selected supercomputers (CPU+GPU) currently in use:

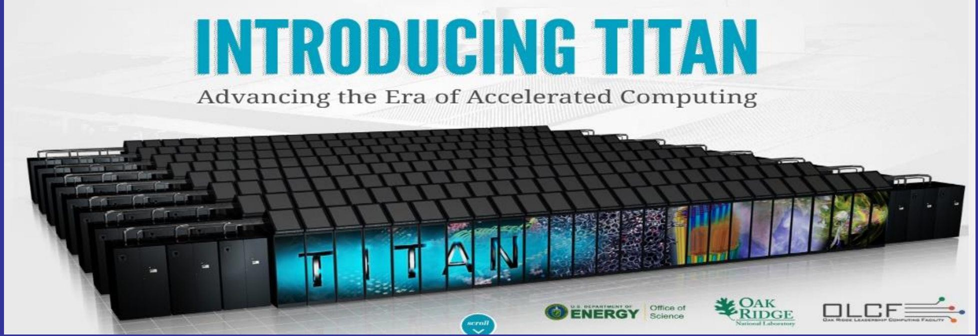
Piz Daint: 7.787 PFlops
(Swiss National Supercomputing Centre)

HA-PACS: 0.802 PFlops
(University of Tsukuba)



Tsubame: 5.7 PFlops
(Tokyo Institute of Technology)

Titan: 27 PFlops
(ORNL Oak Ridge)



Areas of applications

$$\frac{\Delta}{\varepsilon_F} \leq 0.5$$

Ultracold atomic (fermionic) gases. Unitary regime.

Dynamics of quantum vortices, solitonic excitations, quantum turbulence.

$$\frac{\Delta}{\varepsilon_F} \leq 0.1-0.2$$

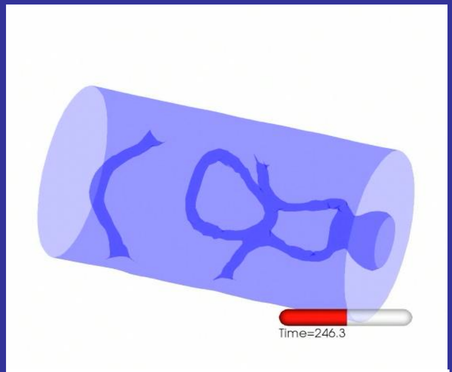
Astrophysical applications.

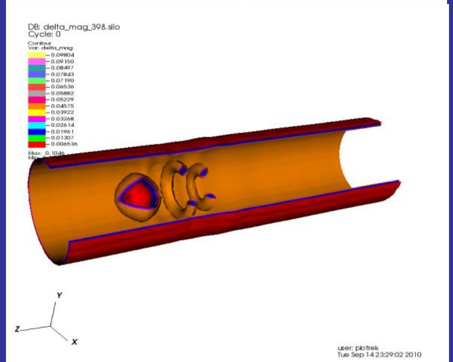
Modelling of neutron star interior (glitches): vortex dynamics, dynamics of inhomogeneous nuclear matter (in strong magnetic fields).

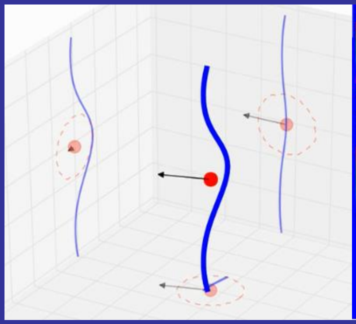
$$\frac{\Delta}{\varepsilon_F} \leq 0.03$$

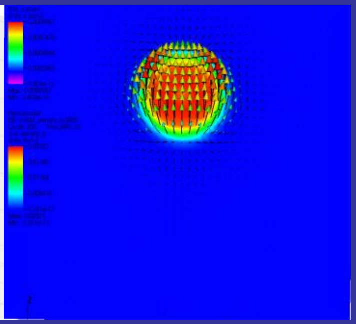
Nuclear physics.

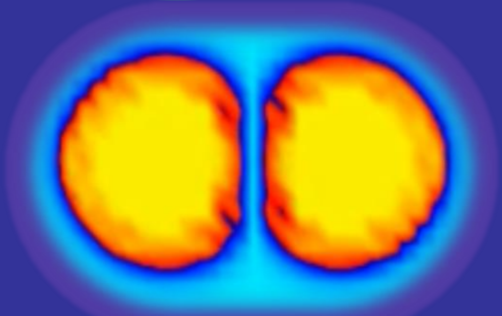
Induced nuclear fission, fusion, collisions.

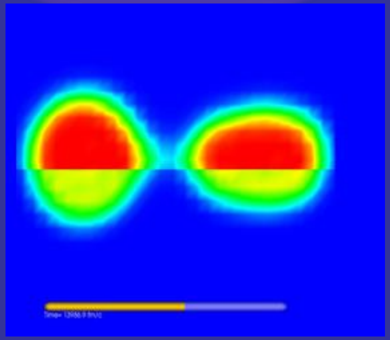










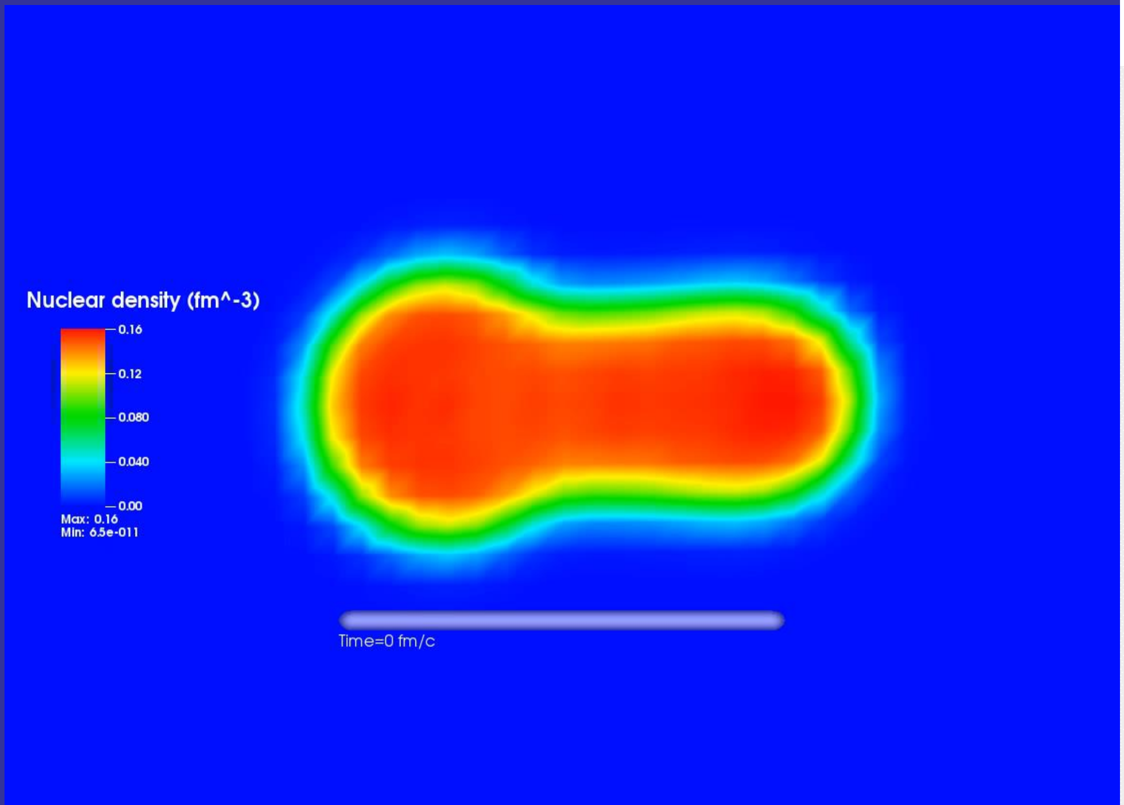


Examples of applications:

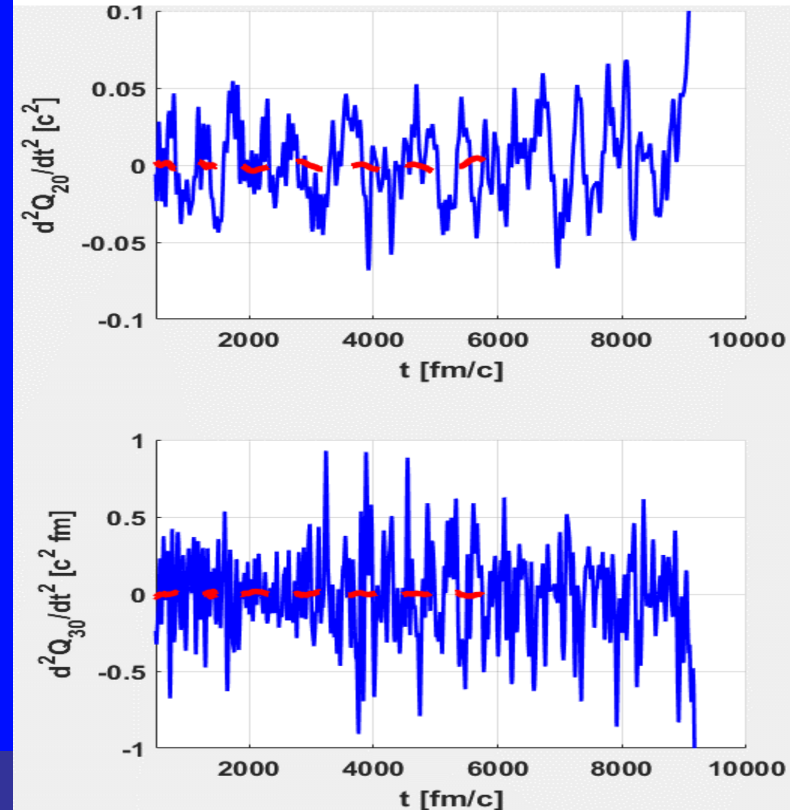
- *Nuclear induced fission*
- *Collisions of medium or heavy superfluid nuclei*
- *Dynamics of quantum vortices in the neutron star crust*

Fission dynamics of ^{240}Pu

Initial configuration of ^{240}Pu is prepared beyond the barrier at quadrupole deformation *Q=165b* and excitation energy *E=8.08 MeV*:



Accelerations in quadrupole and octupole moments along the fission path

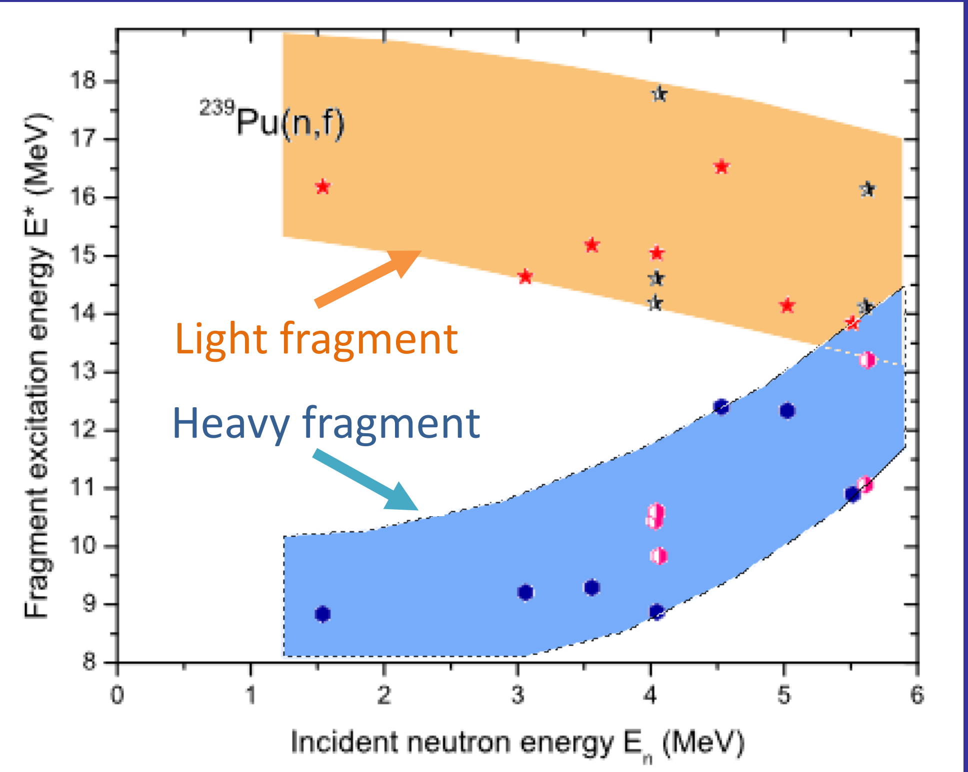


During the process shown, the exchange of about 2 neutrons and 3 protons occur between fragments before the actual fission occurs.

Interestingly the fragment masses seem to be relatively stiff with respect to changes of the initial conditions.

A. Bulgac, P. Magierski, K.J. Roche, and I. Stetcu, Phys. Rev. Lett. 116, 122504 (2016)

Excitation energy of the fragments from TDDFT



E^* (MeV)	E_n (MeV)	$t_{fission}$ (fm/c)	TKE (MeV)	Z_L	N_L
8.08	1.542	8517	173.81	40.825	62.246
9.60	3.063	9215	174.73	40.500	61.536
10.10	3.560	9287	179.09	41.625	62.783
10.57	4.032	7243	173.67	40.092	61.256
10.58	4.043	7287	173.39	40.146	61.388
10.58	4.047	7134	175.11	40.313	61.475
10.60	4.065	7737	174.75	40.904	62.611
11.07	4.534	6444	176.46	41.495	63.134
11.56	5.024	6261	175.15	40.565	61.894
12.05	5.515	5898	176.75	40.412	61.809
12.15	5.610	6100	176.36	40.355	61.695
12.16	5.626	7404	176.10	41.386	62.764

The lighter fragment is more excited (and strongly deformed) than the heavier one.

Energies are not shared proportionally to mass numbers of the fragments!

$$\mathrm{TKE} = 177.80 - 0.3489 E_n \quad [\text{in MeV}],$$

Nuclear data evaluation, Madland (2006)

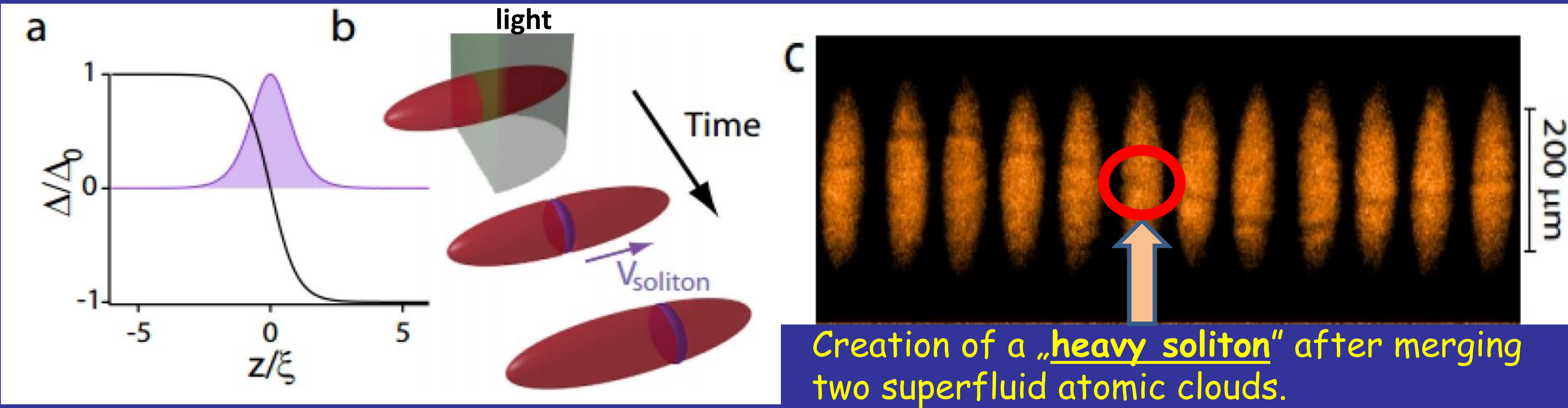
Calculated TKEs slightly underestimate the observed values by no more than: 1 - 3 MeV !

J. Grineviciute et al. (in preparation)

Nuclear collisions

Collisions of superfluid nuclei having different phases of the pairing fields

Motivated by experiments on ultracold atomic gases: merging two 6Li clouds



Creation of a „**heavy soliton**" after merging two superfluid atomic clouds.
T. Yefsah et al., Nature 499, 426 (2013).

Sequence of decays of topological excitations is reproduced by TDSLDA:
Wlazłowski, et al.,Phys. Rev. A91, 031602 (2015)

In the context of nuclear systems the main questions are:
- how a possible solitonic structure can be manifested in nuclear system?
- what observable effect it may have on heavy ion reaction:
  kinetic energies of fragments, capture cross section, etc.?

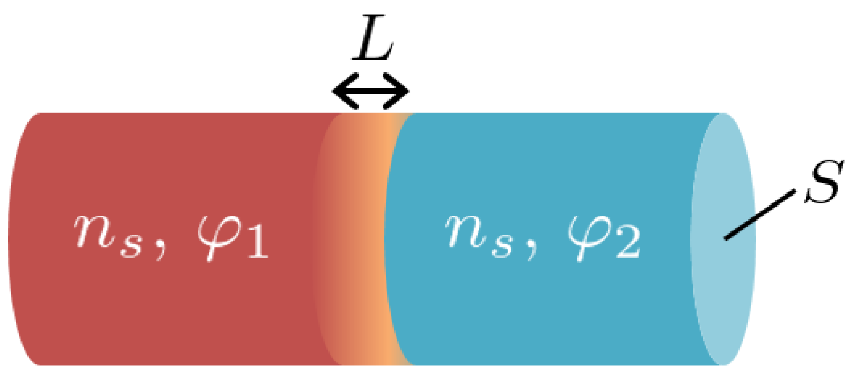
Clearly, we cannot control phases of the pairing field in nuclear experiments and the possible signal need to be extracted after averaging over the phase difference.

Estimates for the magnitude of the effect

At first one may think that the magnitude of the effect is determined by the nuclear pairing energy which is of the order of MeV's in atomic nuclei (according to the expression):

$$\frac{1}{2} g(\varepsilon_F)|\Delta|^2; \quad g(\varepsilon_F) \text{ - density of states}$$

On the other hand the energy stored in the junction can be estimated from Ginzburg-Landau (G-L) approach:

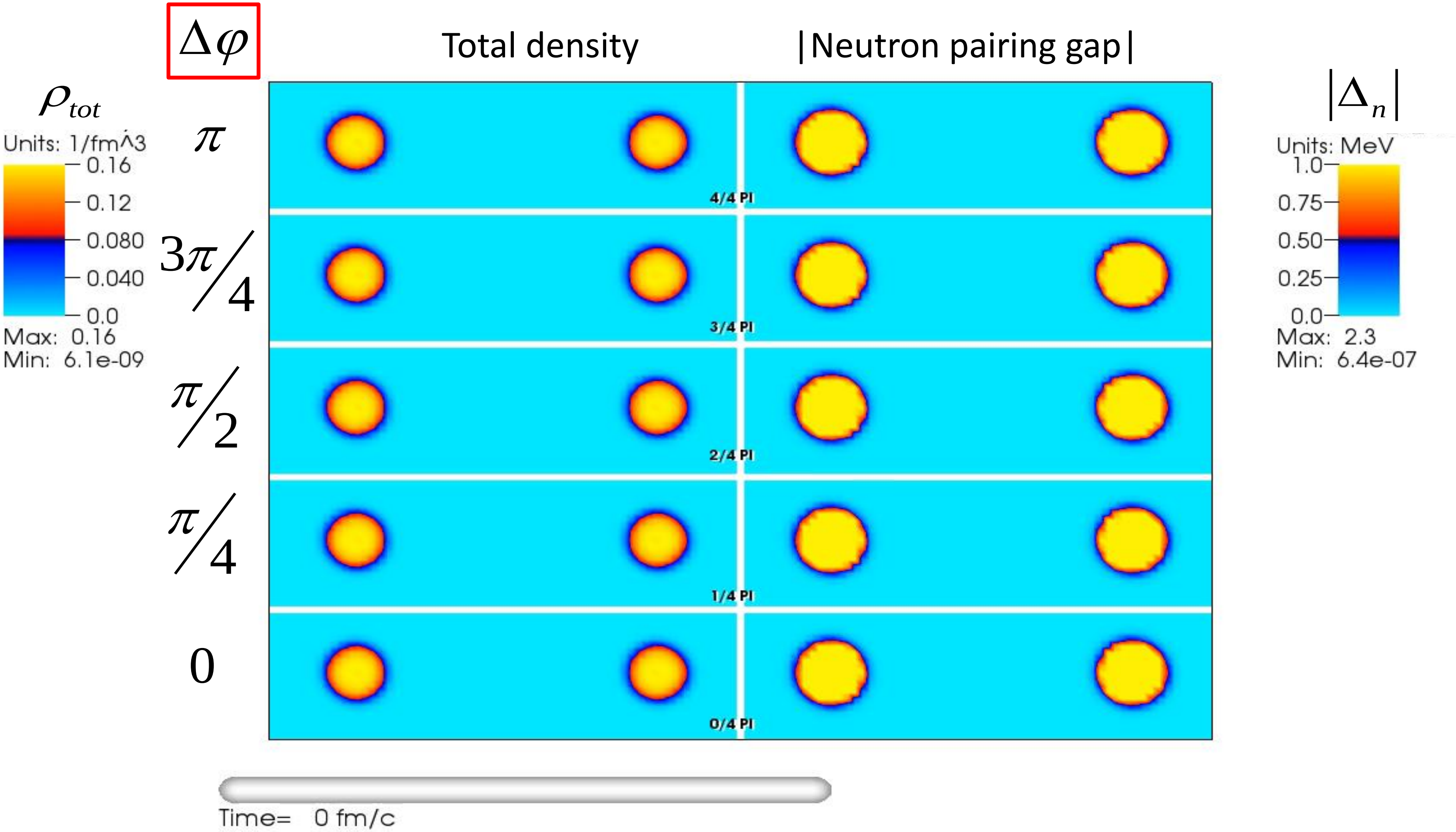


$\Delta\varphi \ (\equiv \varphi_1 - \varphi_2)$

$$E_j = \frac{S}{L}\frac{\hbar^2}{2m} n_s \sin^2 \frac{\Delta\varphi}{2}$$

For typical values characteristic for two heavy nuclei: $E_j \approx 30 MeV$

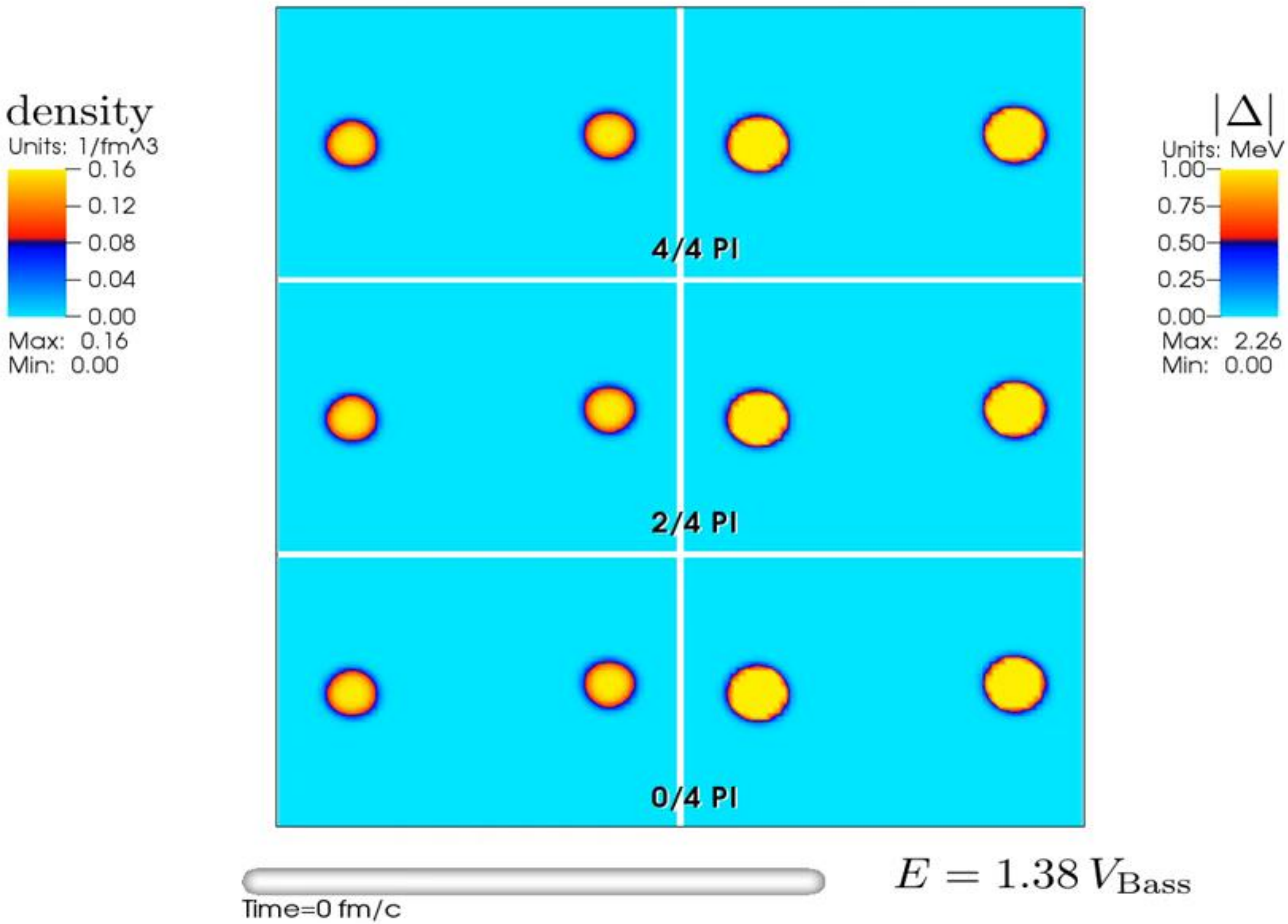
$^{90}Zr + ^{90}\mathrm{Zr}$ at energy $E \simeq V_{Bass}$



Modification of the capture cross section!

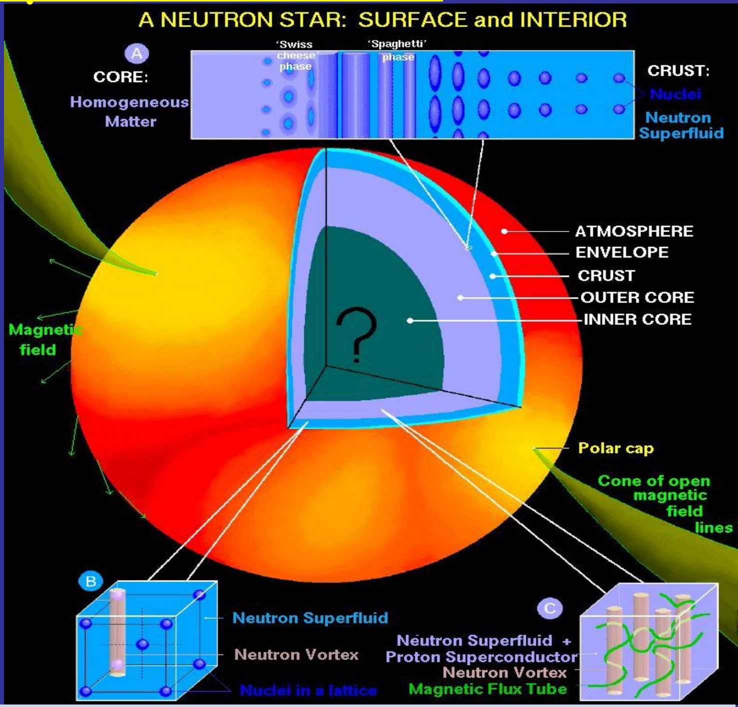
P. Magierski, K. Sekizawa, G. Wlazłowski, Phys. Rev. Lett. 119 042501 (2017)

Noncentral collisions: $^{90}Zr + {}^{90}Zr$



P. Magierski, K. Sekizawa, G. Wlazłowski, Phys. Rev. Lett. 119 042501 (2017)

Modelling neutron star interior – towards microscopic foundations of the neutron star crust dynamics

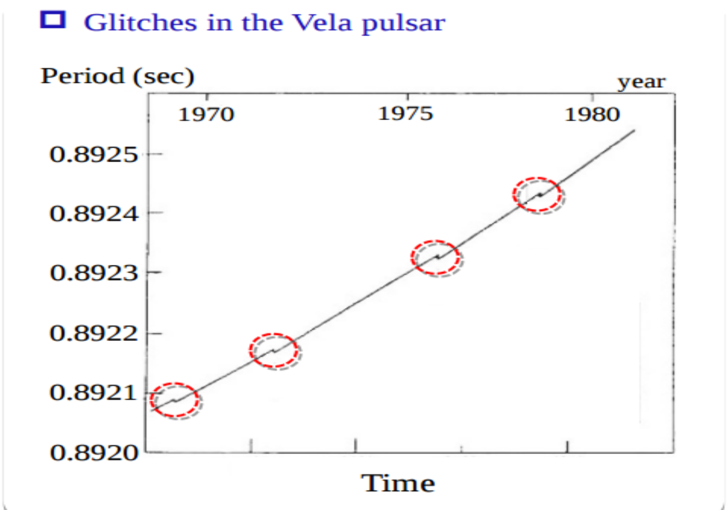


GOAL: Construct large scale model of neutron star interior (in particular neutron star crust), based on microscopic input from nuclear theory.

MICROSCOPIC INPUTS NEEDED:

- vortex-impurity interaction,
- effective masses of nuclear impurities,
- couplings between lattice vibrations and neutron superfluid medium,
- ...

Glitch: a sudden increase of the rotational frequency



V.B. Bhatia, A Textbook of Astronomy and Astrophysics with Elements of Cosmology, Alpha Science, 2001.

glitch phenomenon=a sudden speed up of rotation. To date more than 300 glitches have been detected in more than 100 pulsars

Glitch phenomenon is commonly believed to be related to rearrangement of vortices in the interior of neutron stars (Anderson,Itoh,Nature 256,25 (1975))
It would require however a correlated behavior of huge number of quantum vortices and the mechanism of such collective rearrangement is still a mystery.

Vortex – impurity interaction

Static approach

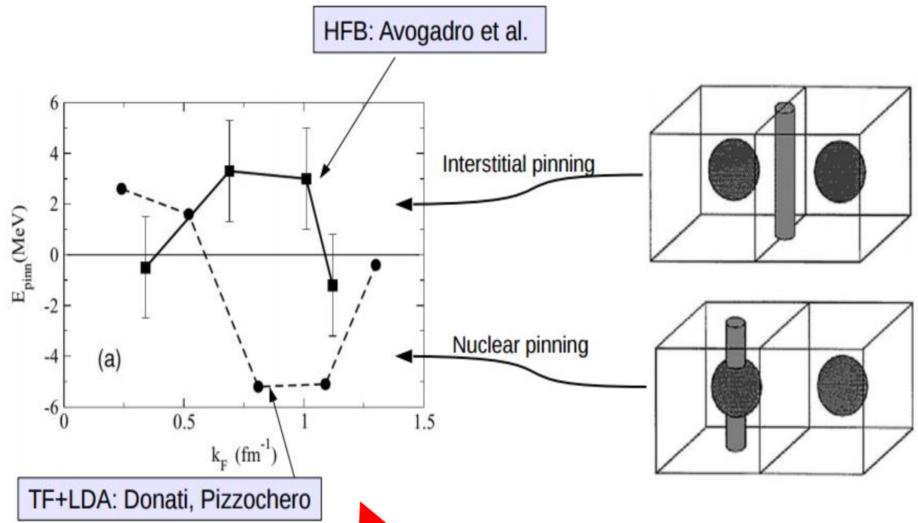
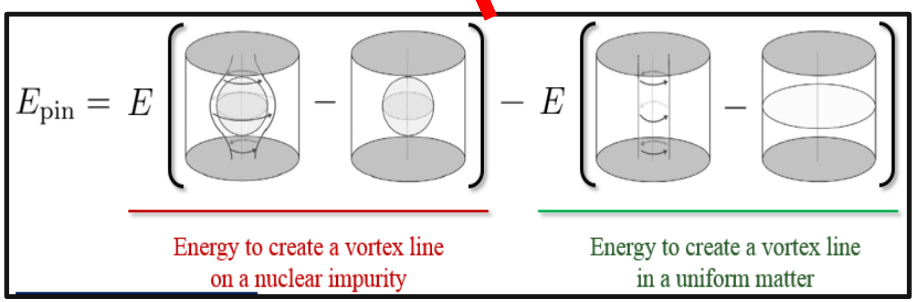


Fig. from: P. Avogadro et al.,
Phys. Rev. C 75, 012805(R) (2007)

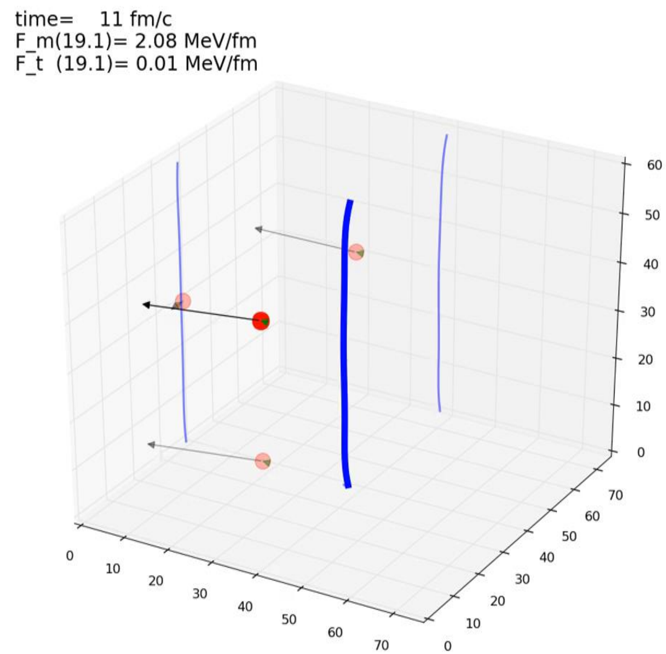
Figs from: P. Donati et al.,
Nuclear Physics A 742 (2004) 363



Pinning energy is obtained as a result of substraction of two large numbers!

Dynamic approach

The external potential keeps the nucleus moving along the straight line with a constant velocity below the critical velocity.



G. Wlazłowski, K. Sekizawa, P. Magierski,
A. Bulgac, M.M. Forbes,
Phys. Rev. Lett. 117, 232701(2016)

Summarizing

- TDDFT extended to superfluid systems and based on the local densities offers a flexible tool to study quantum superfluids far from equilibrium.
- TDDFT offers an unprecedented opportunity to test the nuclear energy density functional for large amplitude collective motion, non-equilibrium phenomena, and in new regions of the collective degrees of freedom.

- **Interesting research topics:**

- Ultracold atoms: investigation of quantum turbulence in Fermi systems; topological excitations in spin-polarized atomic gases in the presence of LOFF phase.
- Neutron star: Provide a link between large scale models of neutron stars and microscopic studies; towards the first simulation of the glitch phenomenon based on microscopic input.
- Nuclear physics: induced fission and fusion processes based directly on Energy Density Functional; search for new effects related to pairing dynamics in nuclear processes.