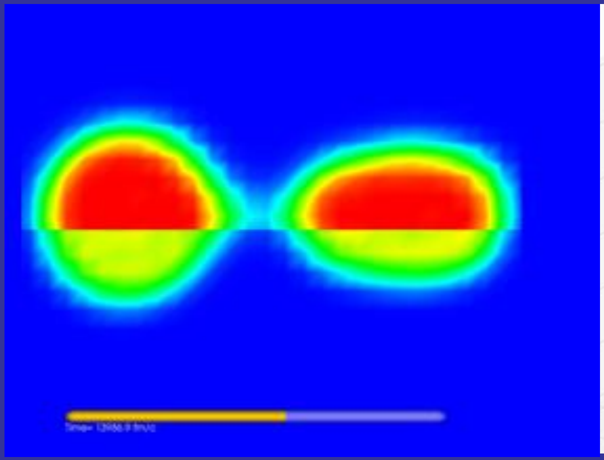
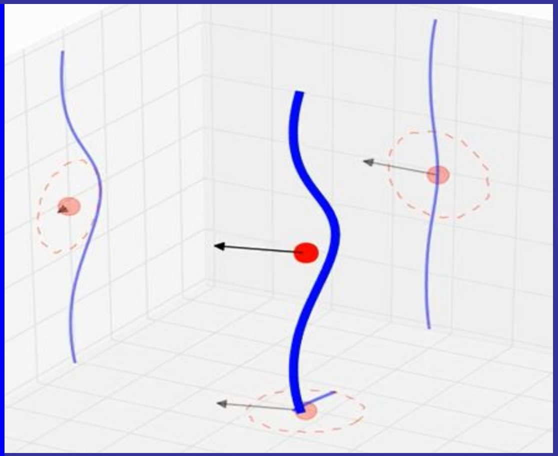
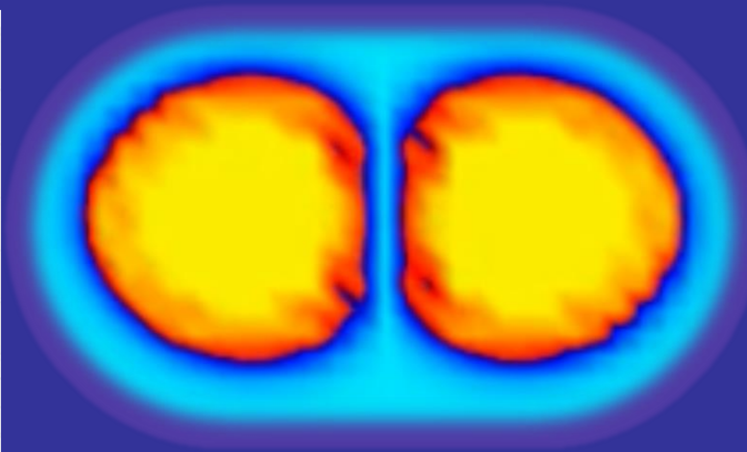
Towards exascale simulations of quantum superfluids far from equilibrium







Piotr Magierski
(Warsaw University of Technology)

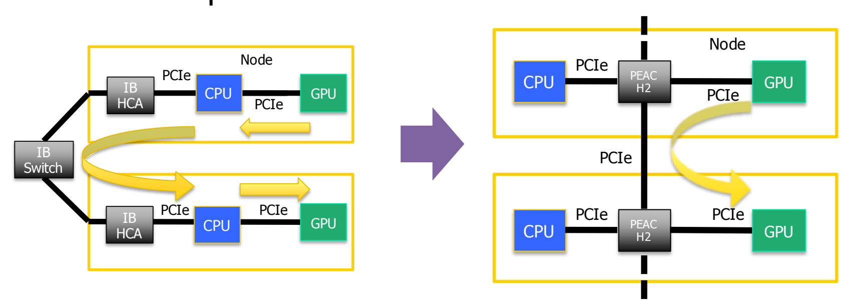
University of Tsukuba
Center for Computational Sciences
筑波大学 計算科学研究センター

Multidisciplinary Cooperative Research
筑波大学計算科学研究センター 学際共同利用

HA-PACS(PACS-VIII) system

Node Spec.	Base Cluster Part	TCA Part
# of nodes	268	64
CPU	Intel Xeon E5-2670, 8 core, 2.6GHz x 2	Intel Xeon E5-2680v2, 10 core, 2.8GHz x 2
GPU	NVIDIA M2090 x4	NVIDIA K20X x4
CPU memory	DDR3 1600 x8, 128GB, 102.4GB/s	DDR3 1866 x8, 128GB, 119.4GB/s
GPU memory	GDDR5, 708GB/s, 24GB	GDDR5, 1000GB/s, 24GB
Peak perf.	332.8GF (CPU) + 2660GF (GPU) = 802 TF	448GF (CPU) + 5240GF (GPU) = 364 TF
Network HCA	InfiniBand QDR x2rail	InfiniBand QDR x2rail
Network b/w	7GB/s	
Net. config.	Fat-Tree with full bisection b/w	
Total perf.	1.166 PFLOPS	
File system	Lustre 500TB with RAID6	

Tightly Coupled Accelerators
with cooperation of NVIDIA



共同利用・共同研究拠点
「先端学際計算科学共同研究拠点」（文部科学省）
Advanced Interdisciplinary Computational Science Collaboration Initiative (the MEXT of Japan)

GOAL:

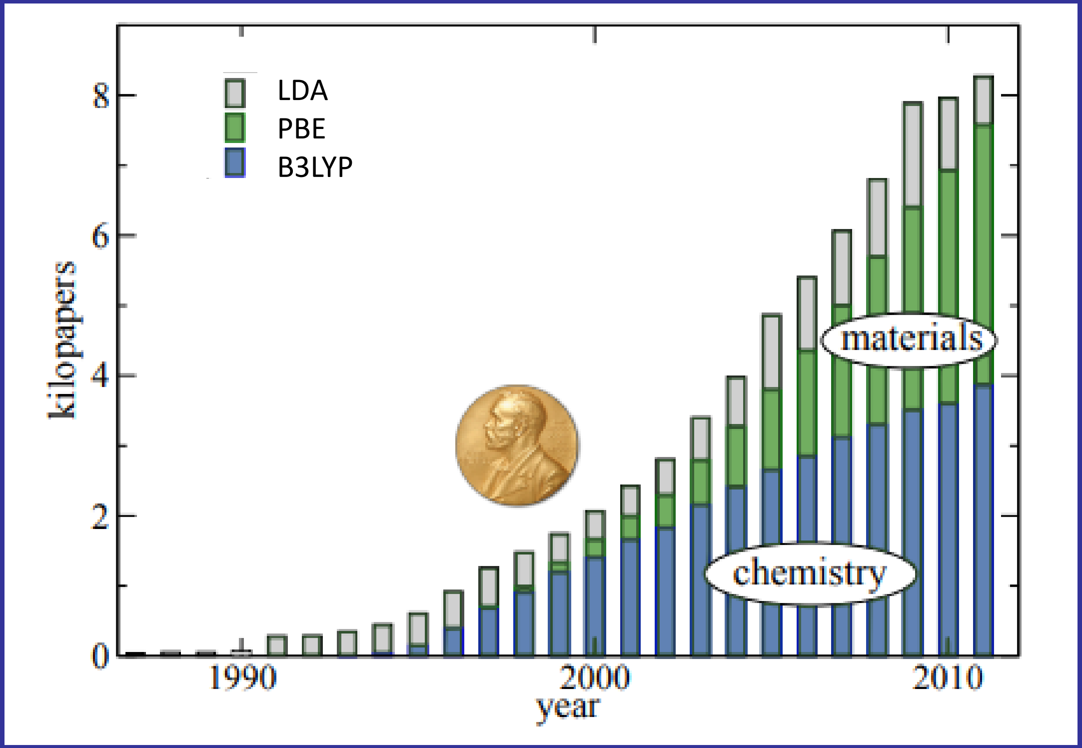
Unified description of superfluid dynamics of fermionic systems far from equilibrium based on microscopic theoretical framework.

Microscopic framework = explicit treatment of fermionic degrees of freedom.

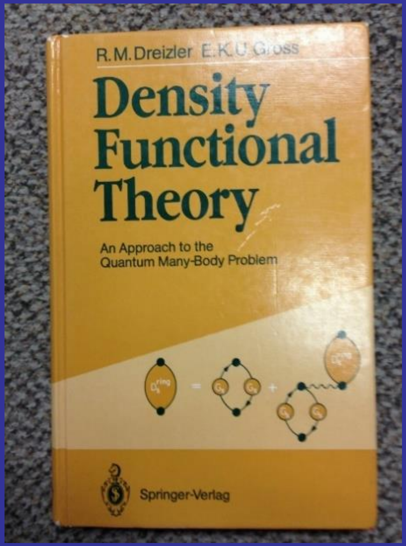
Why Time Dependent Density Functional Theory (TDDFT)?

We need to describe the time evolution of (externally perturbed) spatially inhomogeneous, superfluid Fermi system.

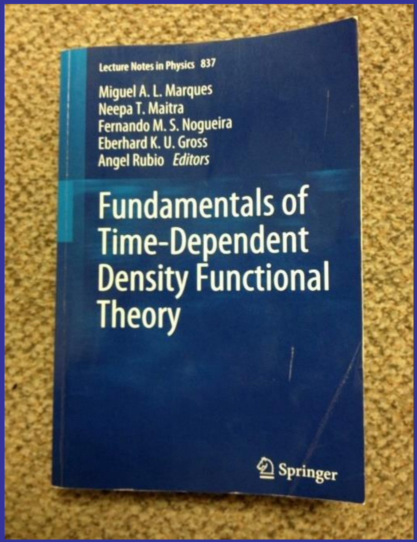
Within current computational capabilities TDDFT allows to describe real time dynamics of strongly interacting, superfluid systems of hundred of thousands fermions.



Number of papers using variants of DFT from K.Burke,J.Chem.Phys.136,150901(2012)



1990



2012

TDDFT equations with local pairing field (TDSLDA):

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

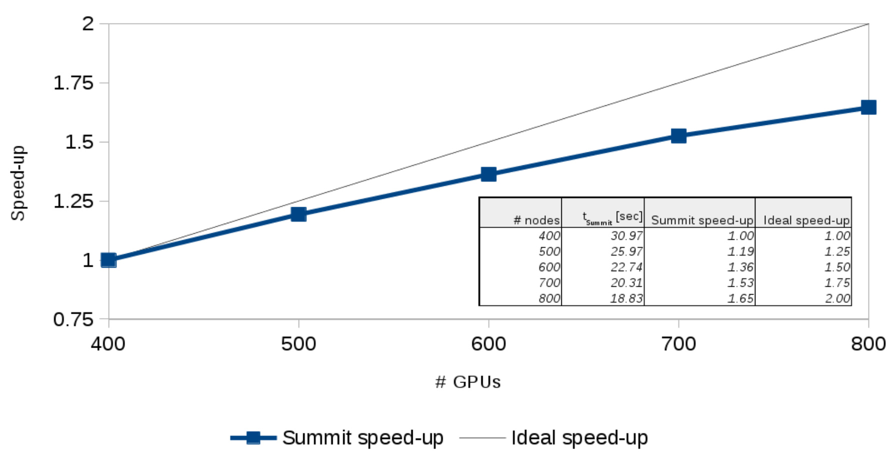
The form of $h(r,t)$ and $\Delta(r,t)$ is determined by EDF (Energy Density Functional)

- **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.**

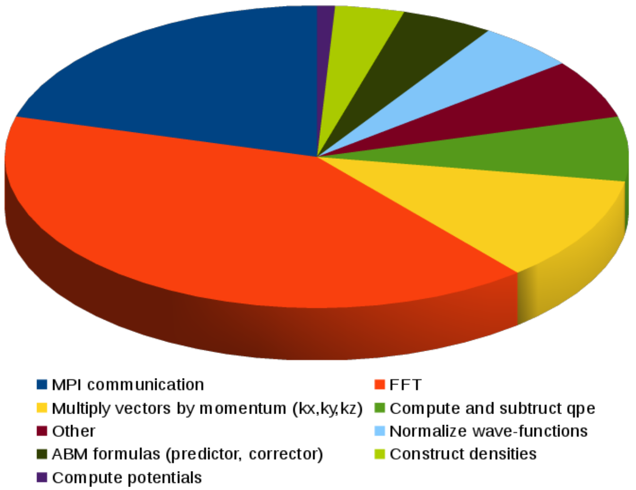
Table 1: Comparison of profit gained by using GPUs instead of CPUs for two example lattices. The timing was obtained on Titan supercomputer. Note, Titan has 16x more CPUs than GPUs.

		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**

Lattice=60^3, nwf=2*226,102



# nodes	t_{Summit} [sec]	Summit speed-up	Ideal speed-up
400	30.97	1.00	1.00
500	25.97	1.19	1.25
600	22.74	1.36	1.50
700	20.31	1.53	1.75
800	18.83	1.65	2.00



Areas of applications

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

Ultracold atomic (fermionic) gases. Unitary regime.

Dynamics of quantum vortices, solitonic excitations, quantum turbulence.

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

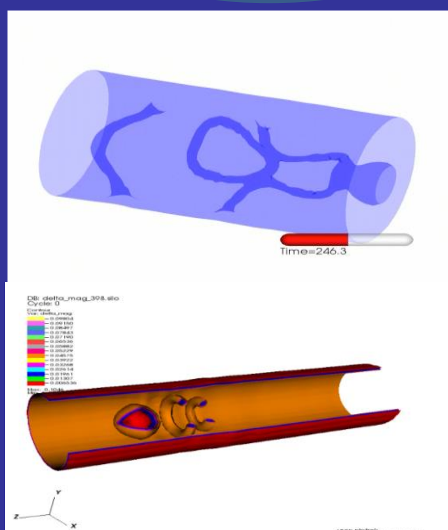
Astrophysical applications.

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

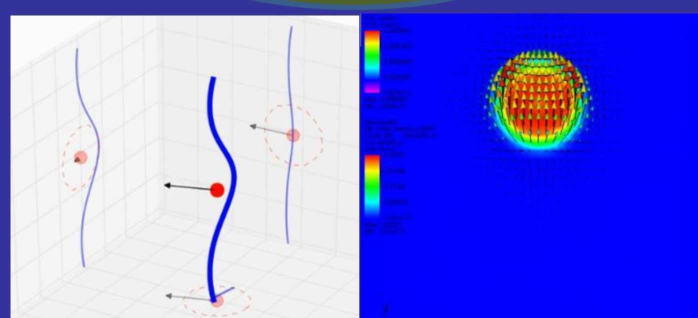
$$\frac{\Delta}{\varepsilon_F} \le 0.03$$

Nuclear physics.

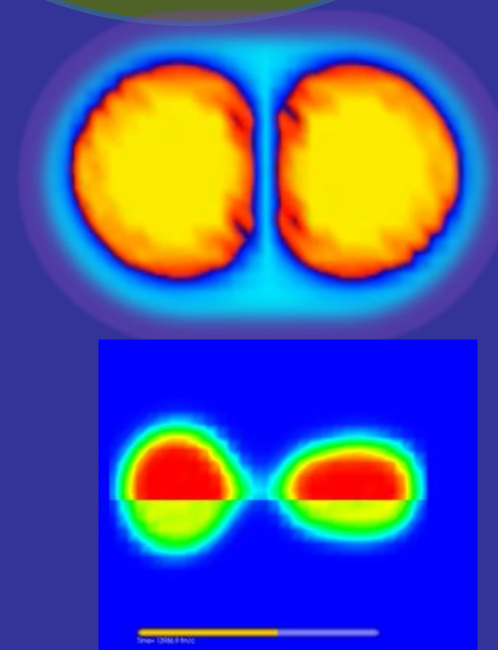
Induced nuclear fission, fusion, collisions.



Phys. Rev. Lett. 120, 253002 (2018)
Phys. Rev. Lett. 112, 025301 (2014)
Science **332**, 1288 (2011).

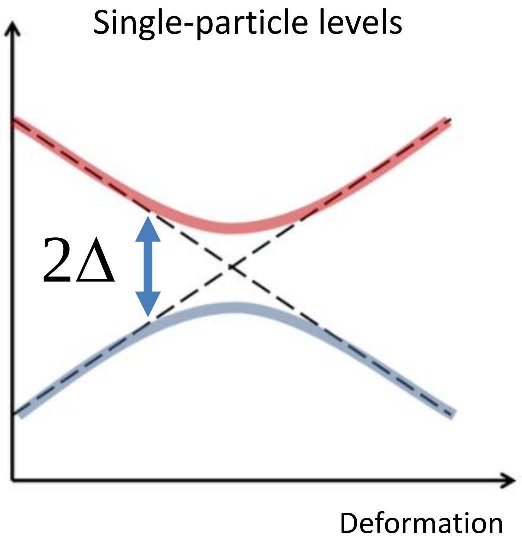


Phys. Rev. Lett. **117**, 232701 (2016)
Phys. Rev. Lett. 110, 241102 (2013)



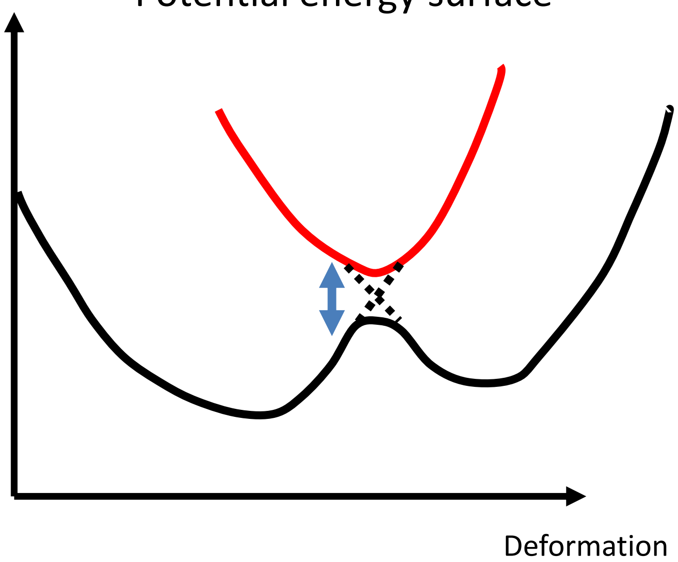
Phys. Rev. Lett. **119**, 042501 (2017)
Phys. Rev. Lett. **116**, 122504 (2016)
Phys. Rev. Lett. **114**, 012701 (2015)

Pairing as an energy gap



Quasiparticle energy:

$$E_{qp} = \sqrt{(\varepsilon - \mu)^2 + |\Delta|^2}$$



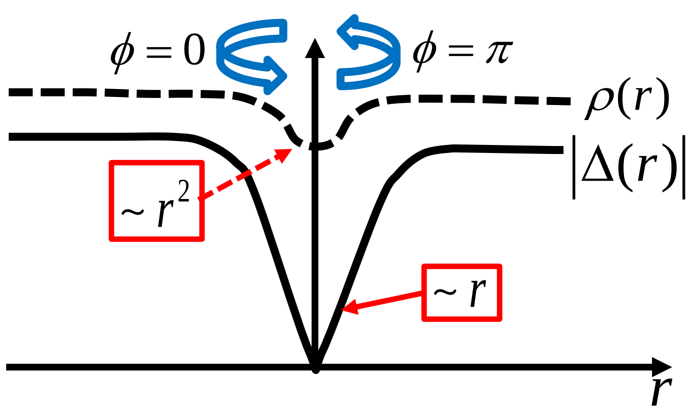
Pairing as a field

$$\Delta(\vec{r}, t) = |\Delta(\vec{r}, t)| e^{i\phi(\vec{r}, t)}$$

Both magnitude and phase may have a nontrivial spatial and time dependence.

Example of a nontrivial spatial dependence: *quantum vortex*

Vortex structure:
section through the vortex core

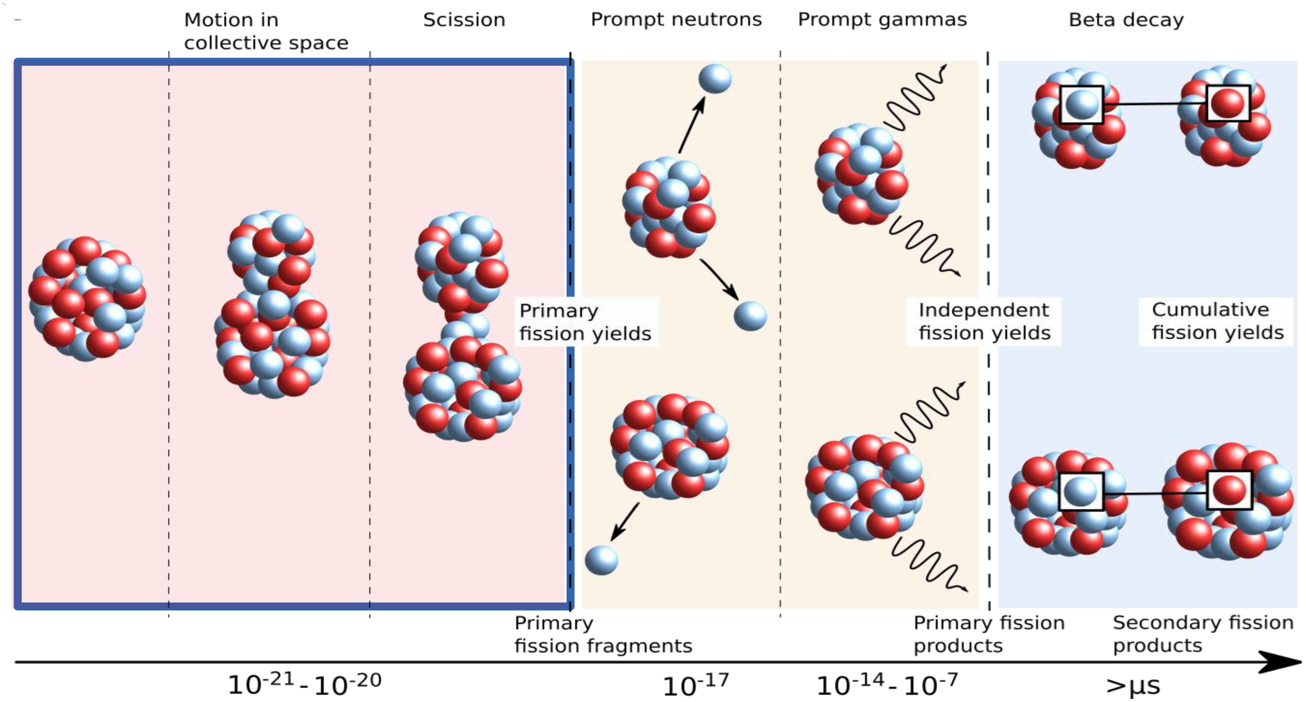


Example of a topological excitation: magnitude of the pairing gap vanishes in the vortex core.

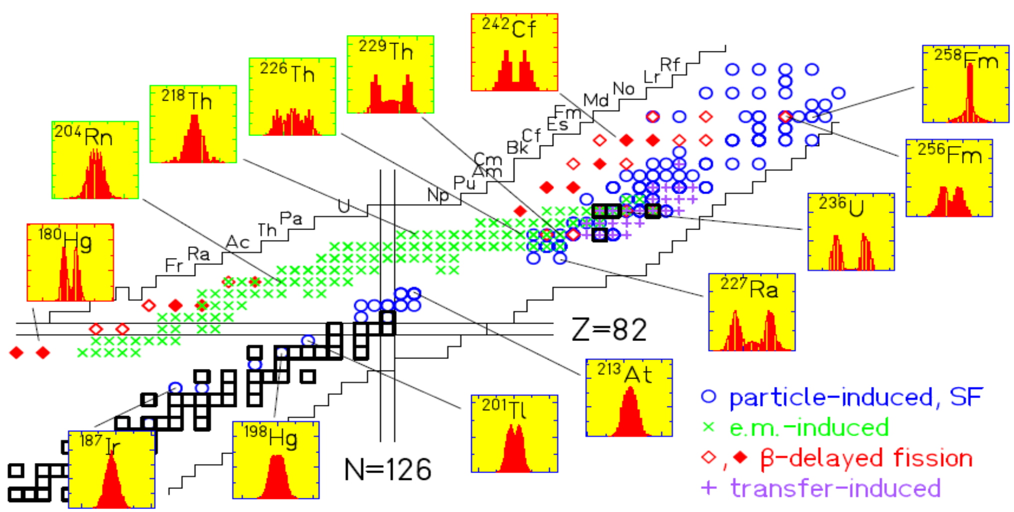
Examples of applications:

- Nuclear induced fission
- Solitonic cascades in ultracold atomic gases
- Collisions of medium or heavy superfluid nuclei
- Spin-polarized impurity stabilized by pairing field
- Quantum turbulence in fermionic atomic gases
- From microscopic dynamics to large scale models of neutron stars.

Time-scales of nuclear fission process



From N. Schunck's lecture (Beijing 2018)

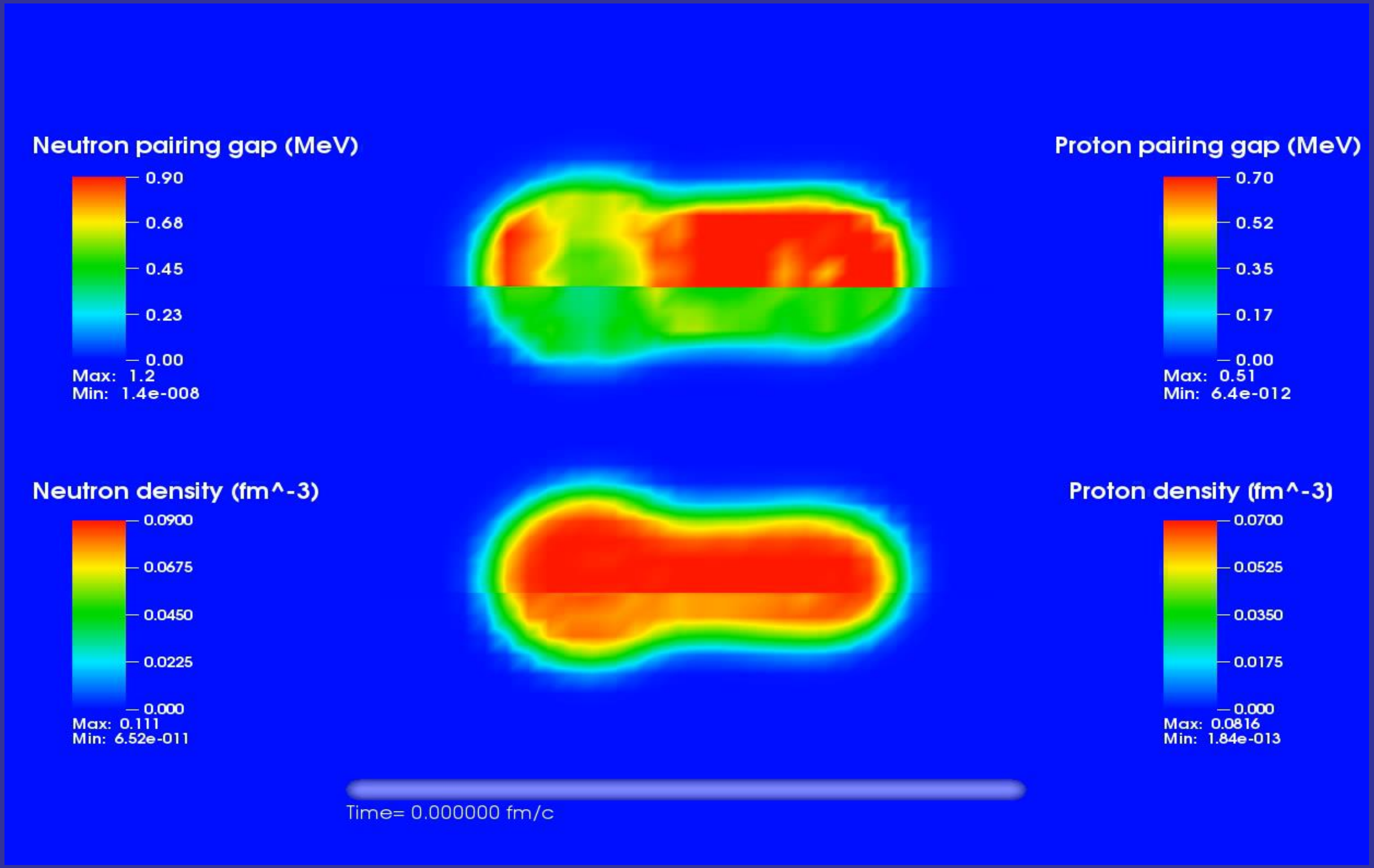


<u>Low energy fission</u> of nuclear systems investigated up to about 2016.

From K.-H. Schmidt, B. Jurado, Rep. Prog. Phys. 81 106301 (2018)

Fission dynamics of ^{240}Pu

Initial configuration of ^{240}Pu is prepared at the barrier (saddle point) at quadrupole Deformation *Q=165b* and excitation energy *E=8.08 MeV*:

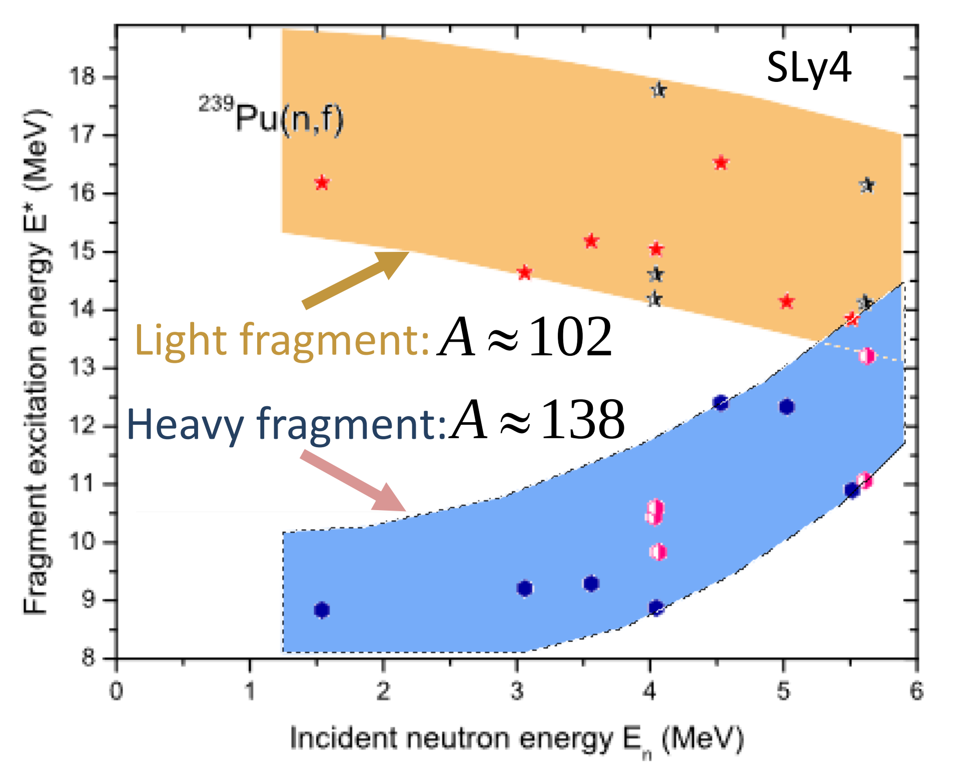


During the process shown, the exchange of about 2 neutrons and 3 protons occur between fragments before the actual fission occurs.

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

The saddle-scission time is considerably longer than in simplified approaches.

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



E^* (MeV)	E_n (MeV)	TKE_{TDSLDA} (MeV)	TKE_{syst} (MeV)	err (%)	Z_L	N_L
8.08	1.542	173	177.26	1.95	40.825	62.246
9.60	3.063	174	176.73	1.13	40.500	61.536
10.10	3.560	179	176.56	1.43	41.625	62.783
10.57	4.032	173	176.39	1.55	40.092	61.256
10.58	4.043	173	176.39	1.70	40.146	61.388
10.58	4.047	175	176.39	0.72	40.313	61.475
10.60	4.065	174	176.38	0.92	40.904	62.611
11.07	4.534	176	176.22	0.14	41.495	63.134
11.56	5.024	175	176.05	0.51	40.565	61.894
12.05	5.515	176	175.88	0.49	40.412	61.809
12.15	5.610	176	175.84	0.29	40.355	61.695
12.16	5.626	176	175.84	0.15	41.386	62.764

Induced fission of 240Pu

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

Excitation 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 reproduce experimental data with accuracy < 2%

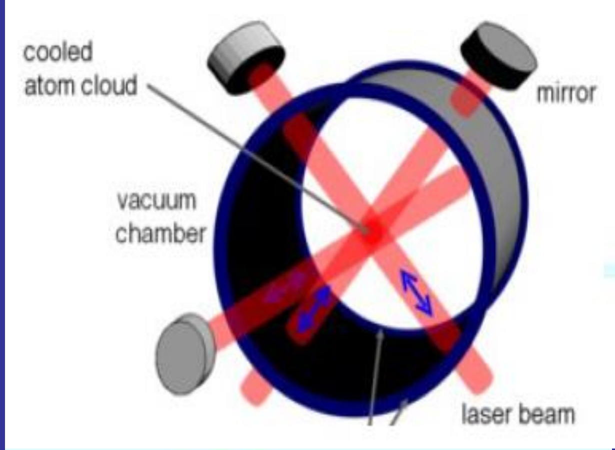
J. Grineviciute, et al. (in preparation)

see also:

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

Ultracold atomic gas:

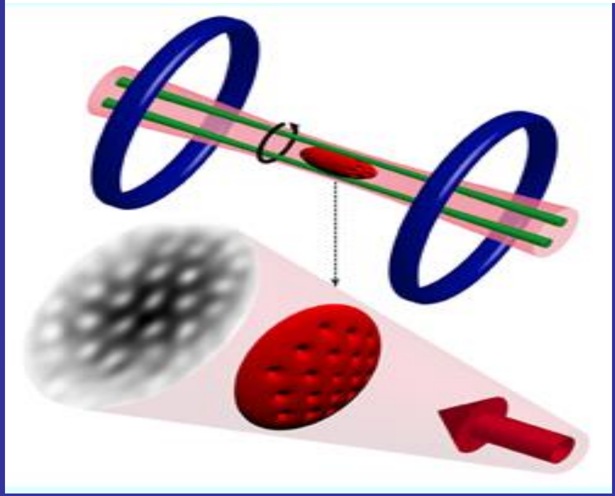
Very cold (T of the order of (1-100)nK),
very dilute (interparticle distance: ≈1000 Bohr radii)
gas of atoms (fermionic or bosonic) confined in an external potential.
System is metastable: lifetime is of the order of minutes.



Important dates:

✓In 1999 DeMarco and Jin created a degenerate atomic Fermi gas.

✓In 2005 Zwierlein/Ketterle group observed quantum vortices which survived when passing from BEC to unitarity – evidence for superfluidity!



system of fermionic ^{6}Li atoms for various interatomic interaction strengths (various values of ext. magnetic field)

BEC side: a>0

BCS side: a<0

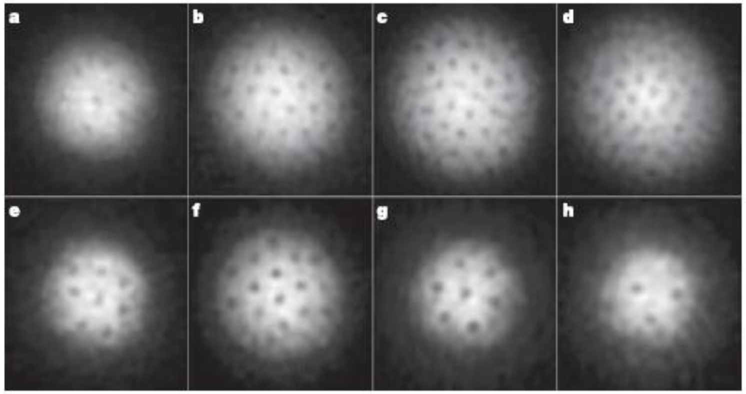


Figure 2 | Vortices in a strongly interacting gas of fermionic atoms on the BEC- and the BCS-side of the Feshbach resonance. At the given field, the cloud of lithium atoms was stirred for 300 ms (**a**) or 500 ms (**b**–**h**) followed by an equilibration time of 500 ms. After 2 ms of ballistic expansion, the magnetic field was ramped to 735 G for imaging (see text for details). The magnetic fields were 740 G (**a**), 766 G (**b**), 792 G (**c**), 812 G (**d**), 833 G (**e**), 843 G (**f**), 853 G (**g**) and 863 G (**h**). The field of view of each image is 880 μm × 880 μm.

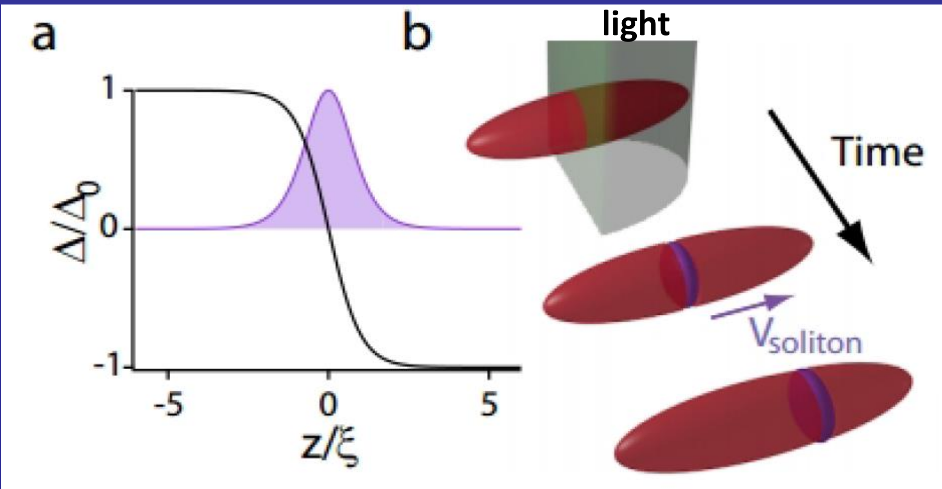
In dilute atomic systems experimenters can control nowadays almost anything:

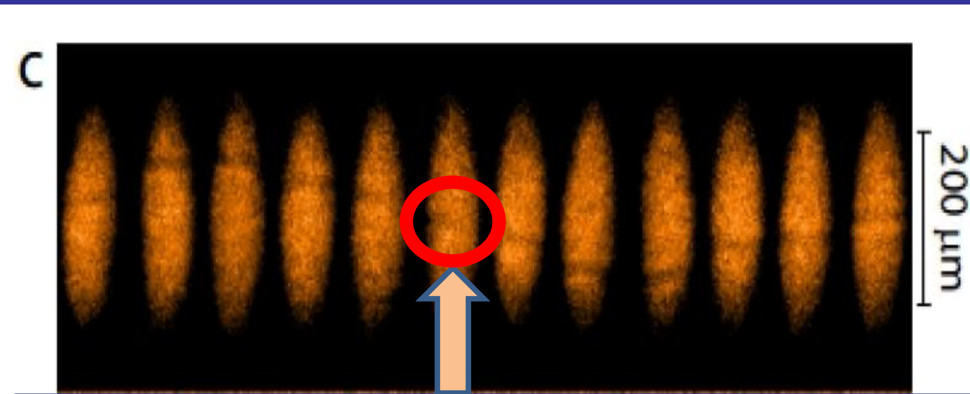
- The number of atoms in the trap: typically about 10^5-10^6 atoms
- Shape of confining potential, dimensionality
- The density of atoms
- Mixtures of various atoms
- The temperature of the atomic cloud
- The strength of this interaction is fully tunable!

M.W. Zwierlein *et al.*, Nature, 435, 1047 (2005)

Solitonic cascades

Merging of two superfluid atomic clouds with different phases of pairing fields:





Creation of a „**heavy soliton**" after merging two superfluid atomic clouds.

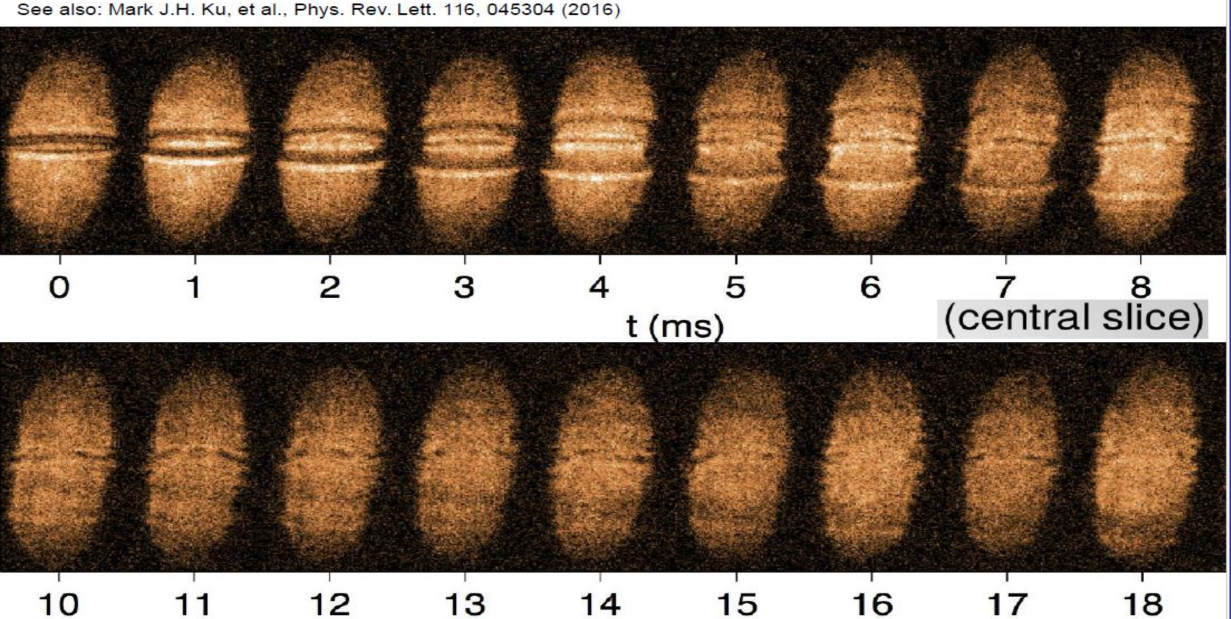
T. Yefsah et al., Nature 499, 426 (2013).

Experimental results – Cascade of Solitary Waves

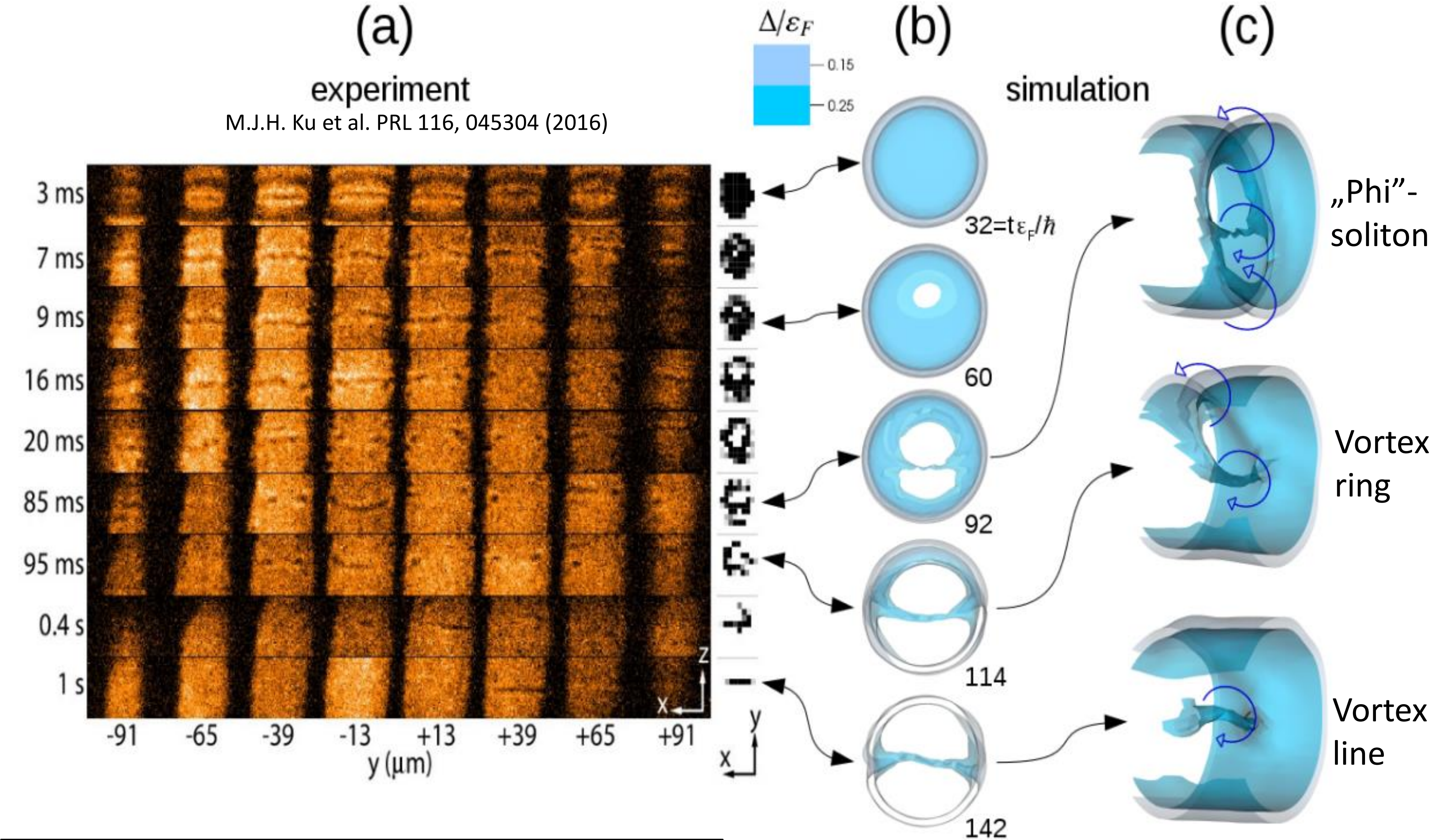
Figures taken from: M. Zwierlein talk, (http://en.sif.it/activities/fermi_school/mmxiv)

School of Physics E. Fermi – Quantum Matter at Ultralow Temperatures Varenna, July 9th , 2014

See also: Mark J.H. Ku, et al., Phys. Rev. Lett. 116, 045304 (2016)



Later it turned out that the cascade of solitons has been observed



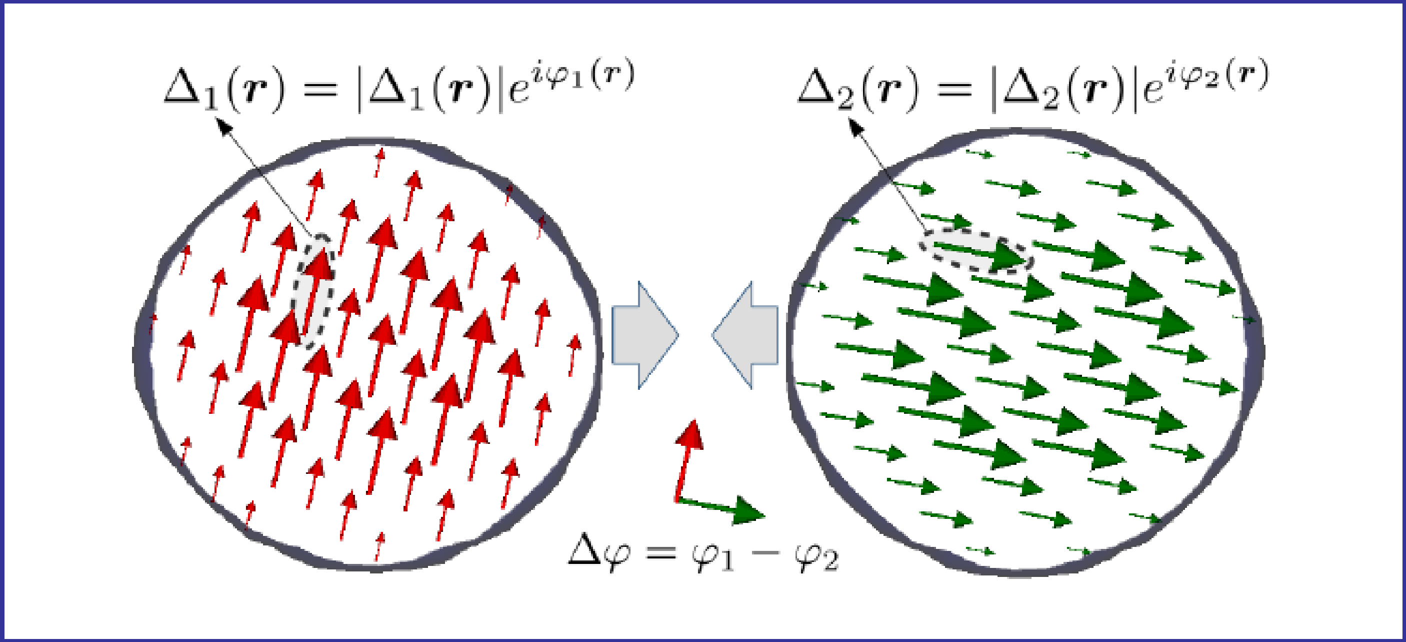
We can reproduce all stages of the experimentally observed solitonic cascade within time dependent SLDA.

G.Wlazłowski, K.Sekizawa, M.Marchwiany, P.Magierski, Phys. Rev. Lett. 120, 253002 (2018)

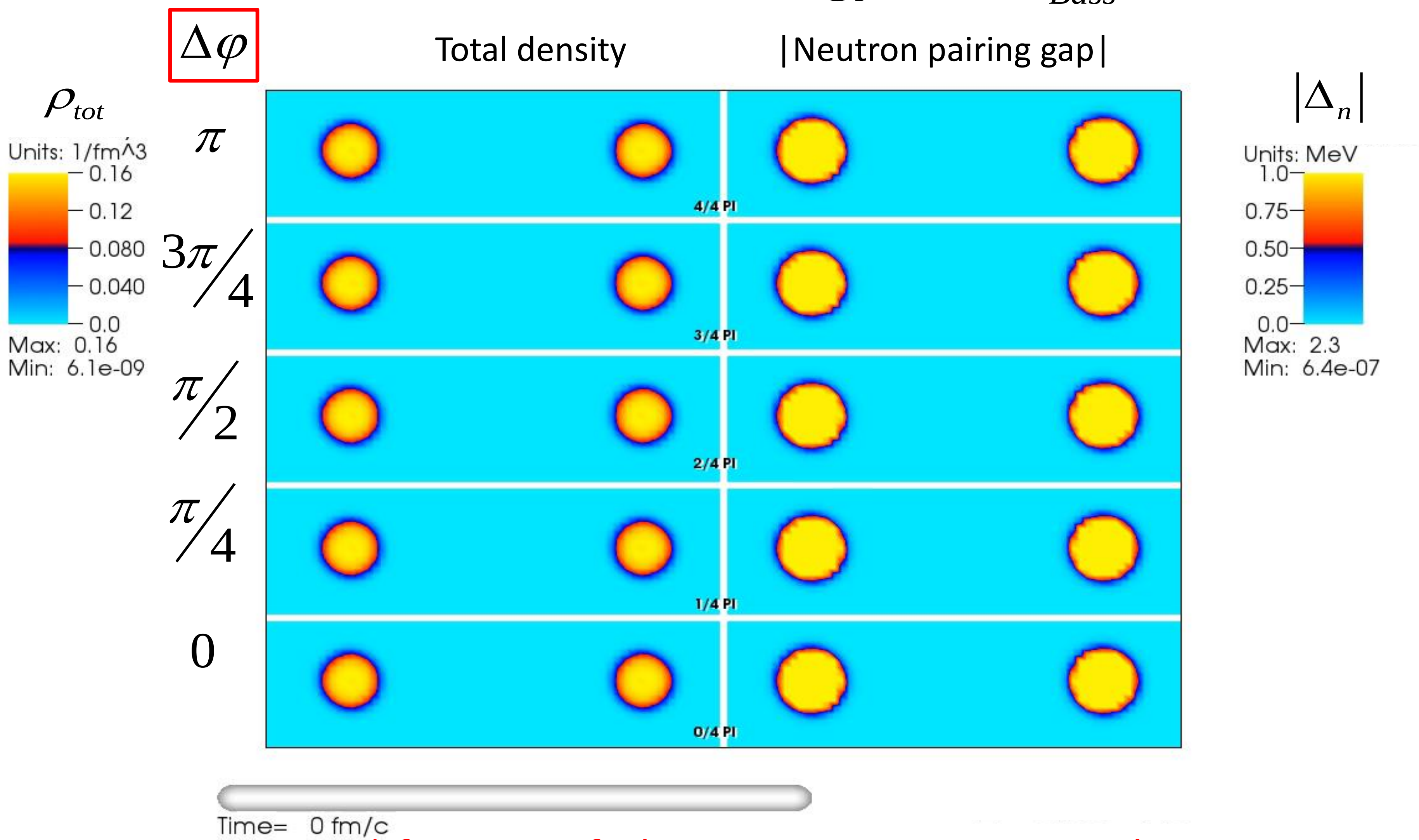
Nuclear collisions

Collisions of superfluid nuclei having different phases of the pairing fields

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



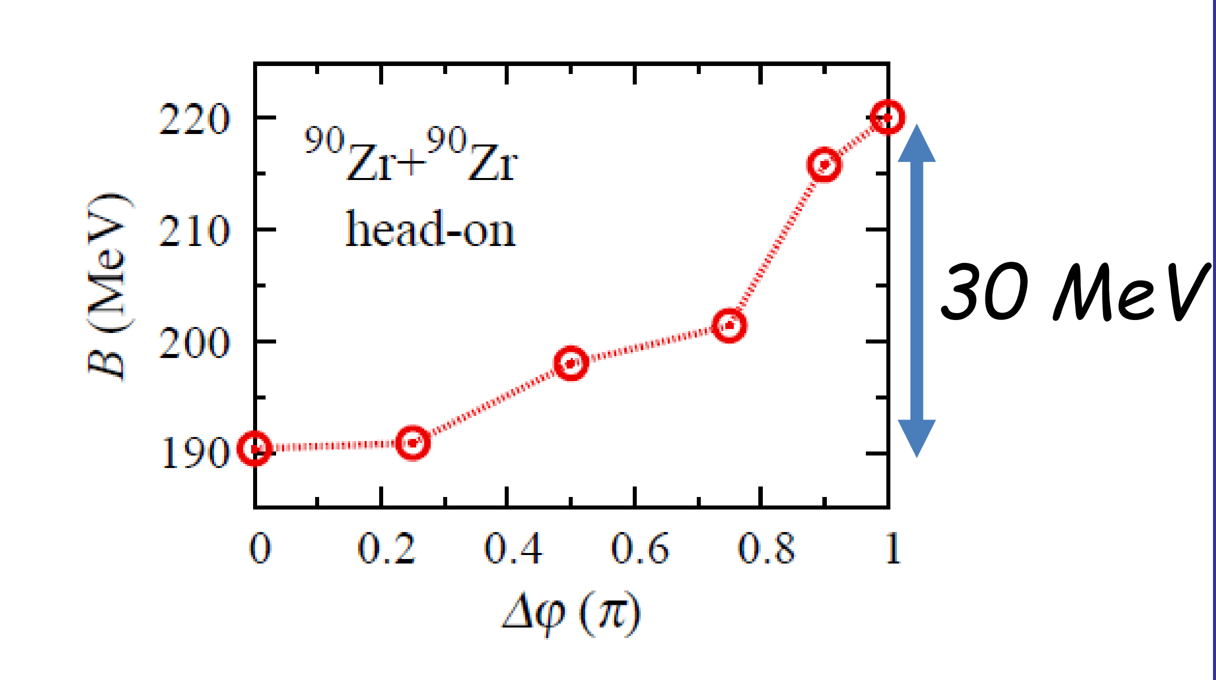
$^{90}Zr + ^{90}Zr$ at energy $E \simeq V_{Bass}$



Modification of the capture cross section!

P. Magierski, K. Sekizawa, G. Wlazłowski, Phys. Rev. Lett. 119 042501 (2017)
See also for light nuclei: Y. Hashimoto, G. Scamps, Phys. Rev. C94, 014610 2016)

Effective barrier height for fusion as a function of the phase difference



What is an average extra energy needed for the capture?

$$E_{extra} = \frac{1}{\pi}\int_0^{\pi}\left(B(\Delta\varphi) - V_{Bass}\right) d(\Delta\varphi) \approx 10 MeV$$

The phase difference of the pairing fields of colliding medium or heavy nuclei produces a similar solitonic structure as the system of two merging atomic clouds.
The energy stored in the created junction is subsequently released giving rise to an increased kinetic energy of the fragments. The effect is found to be of the order of 30MeV for medium nuclei and occur for energies up to 20-30% of the barrier height.

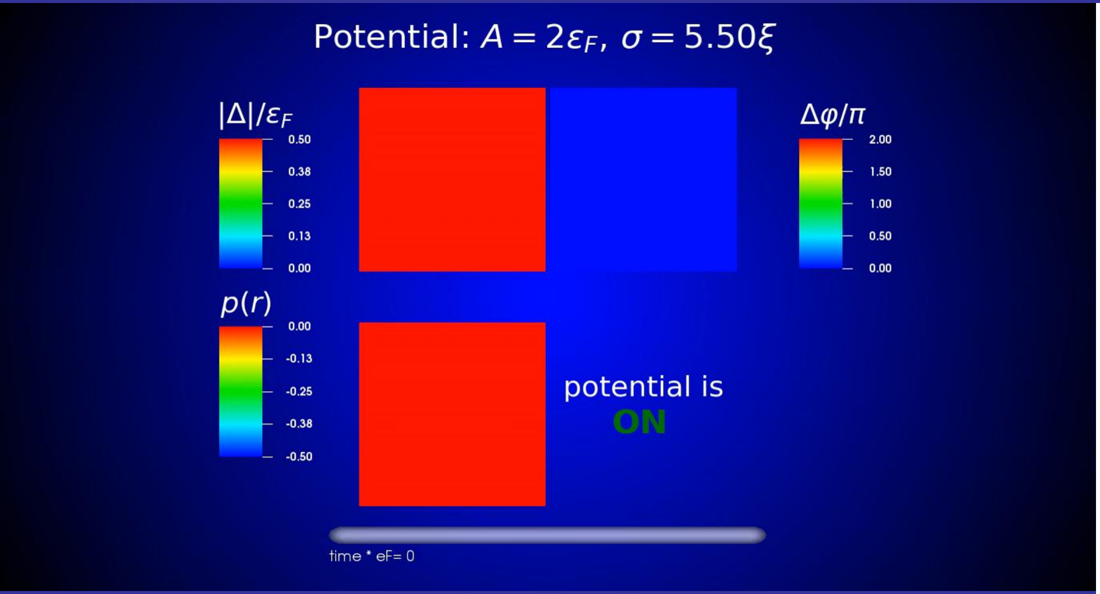
P. Magierski, K. Sekizawa, G. Wlazłowski, Phys. Rev. Lett. 119 042501 (2017)

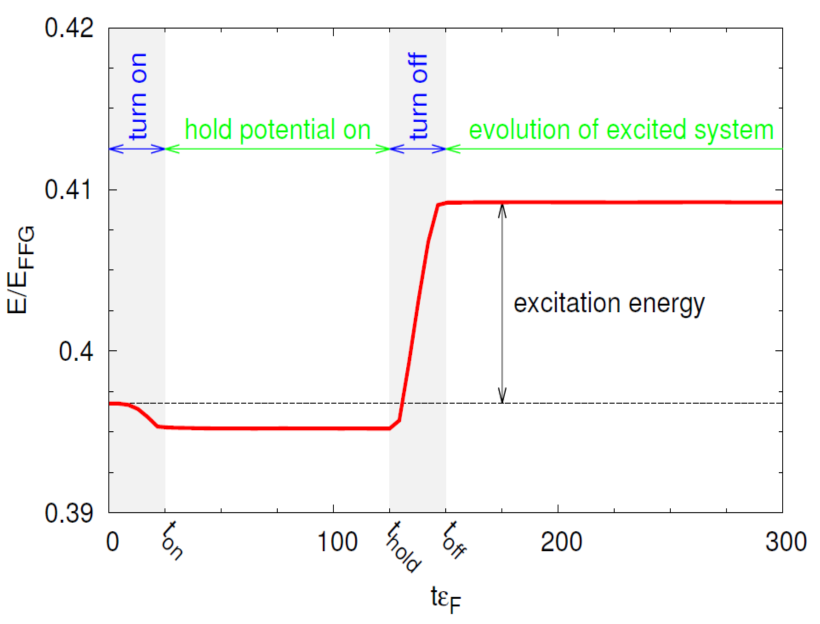
G. Scamps, Phys. Rev. C 97, 044611 (2018): the effect may be weaker than predicted by TDDFT

Stable polarized droplets in the unitary Fermi gas

Can the pairing field stabilize the spin-polarized impurity?

Let's induce locally the spin-polarized region in the unitary Fermi gas:
(unitary Fermi gas: $k_F \to 0,\ k_F a \to \pm\infty$)



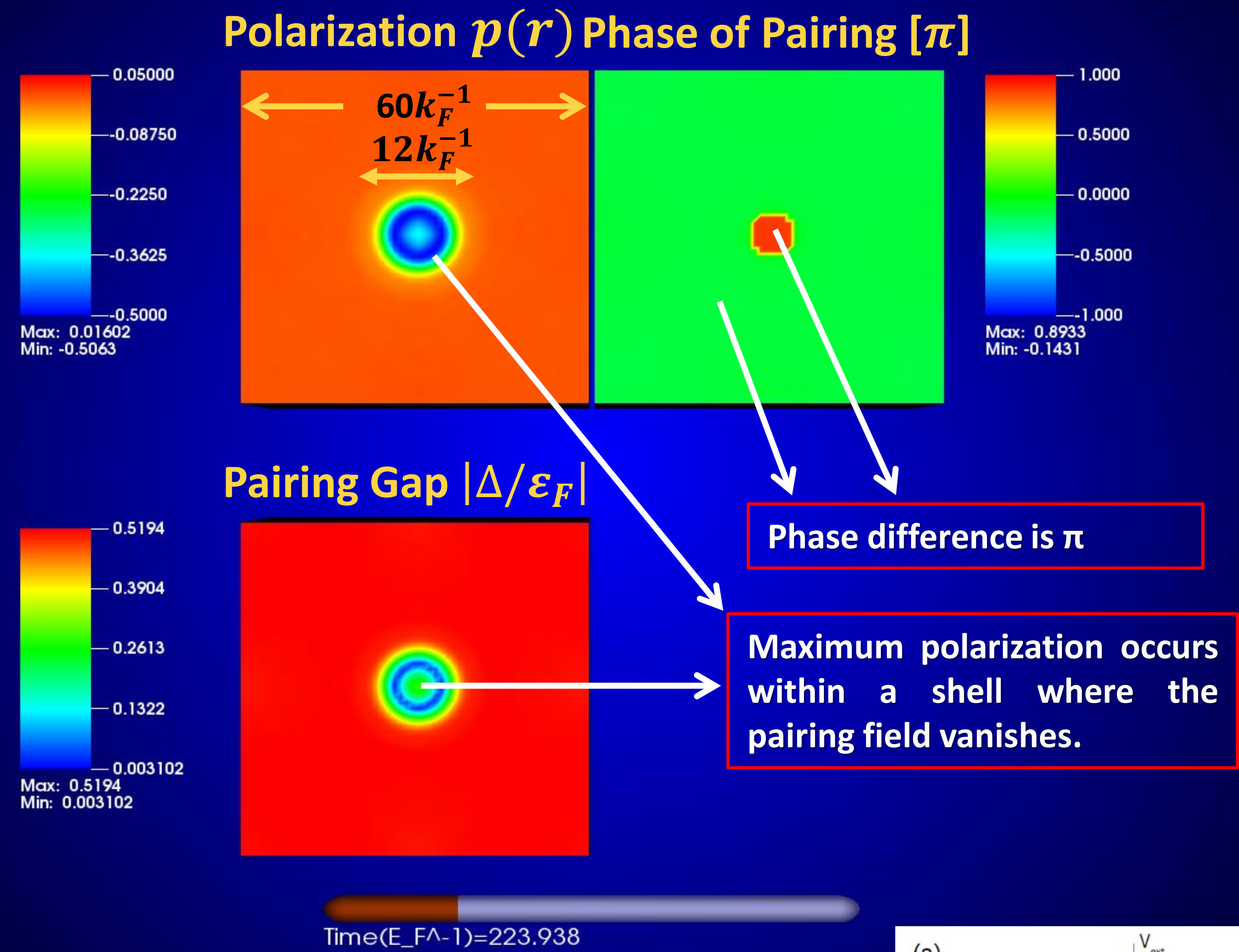


Why the spin-polarized region does not vanish?!

Even though the spin current is suppressed due to the pairing field the „impurity" should eventually dissolve

P. Magierski, B. Tuzemen, G. Wlazłowski, in preparation

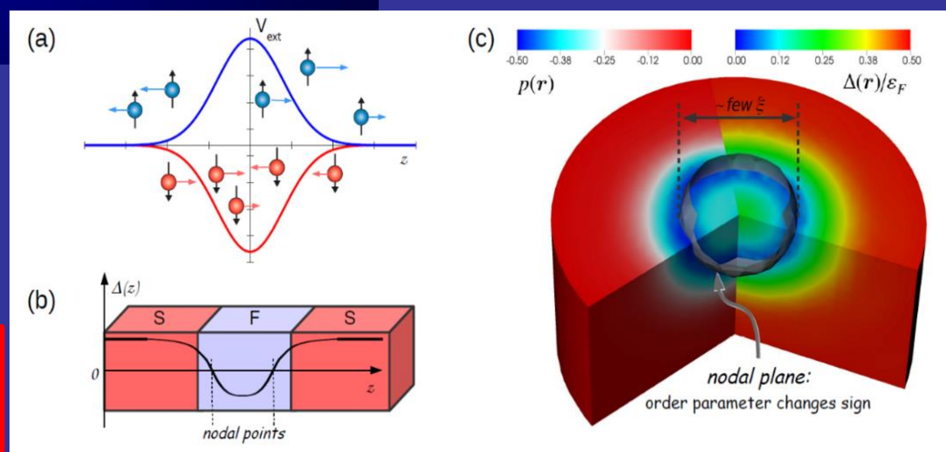
Pairing structure of the impurity



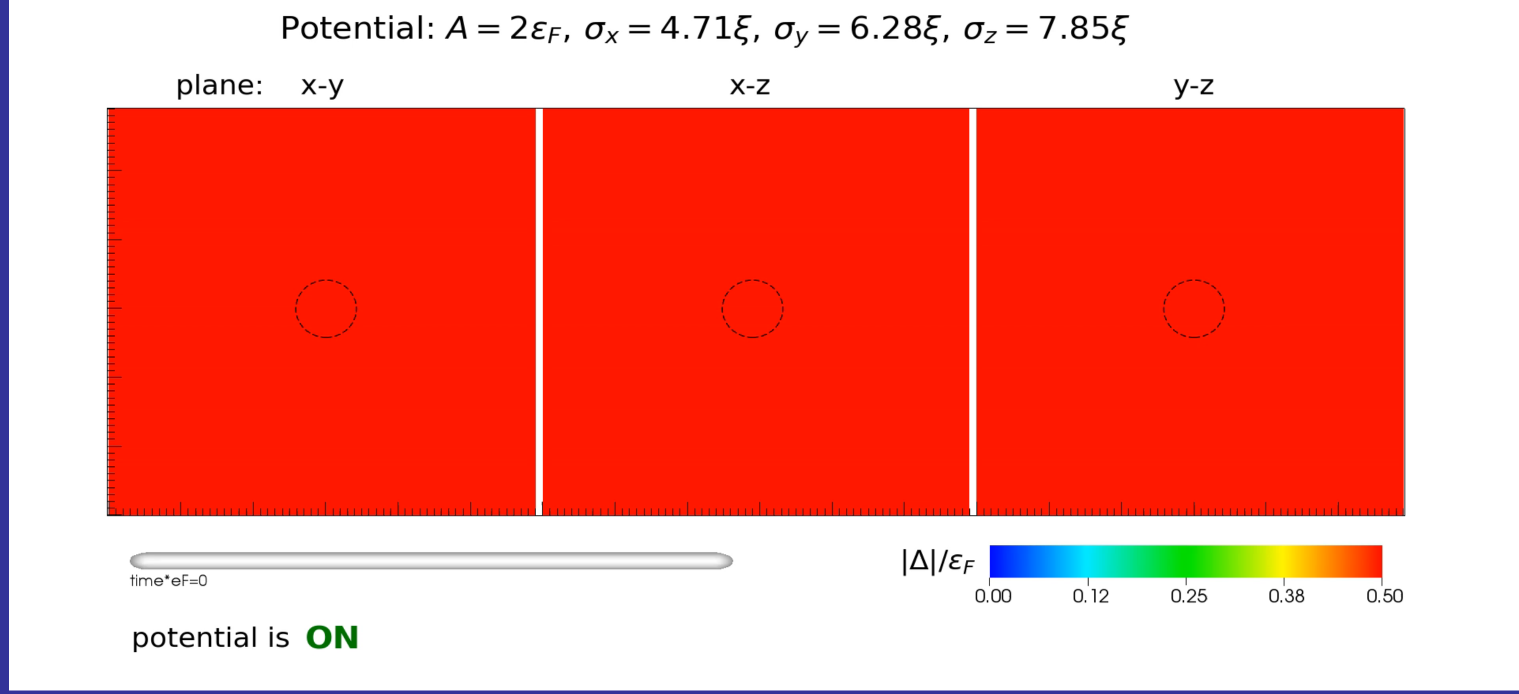
Due to the difference in chemical potentials of spin-up and spin-down particles the pairing field starts to oscillate giving rise to the pairing phase inversion in the center of the impurity.
(similar to the „pi” Josephson junction)

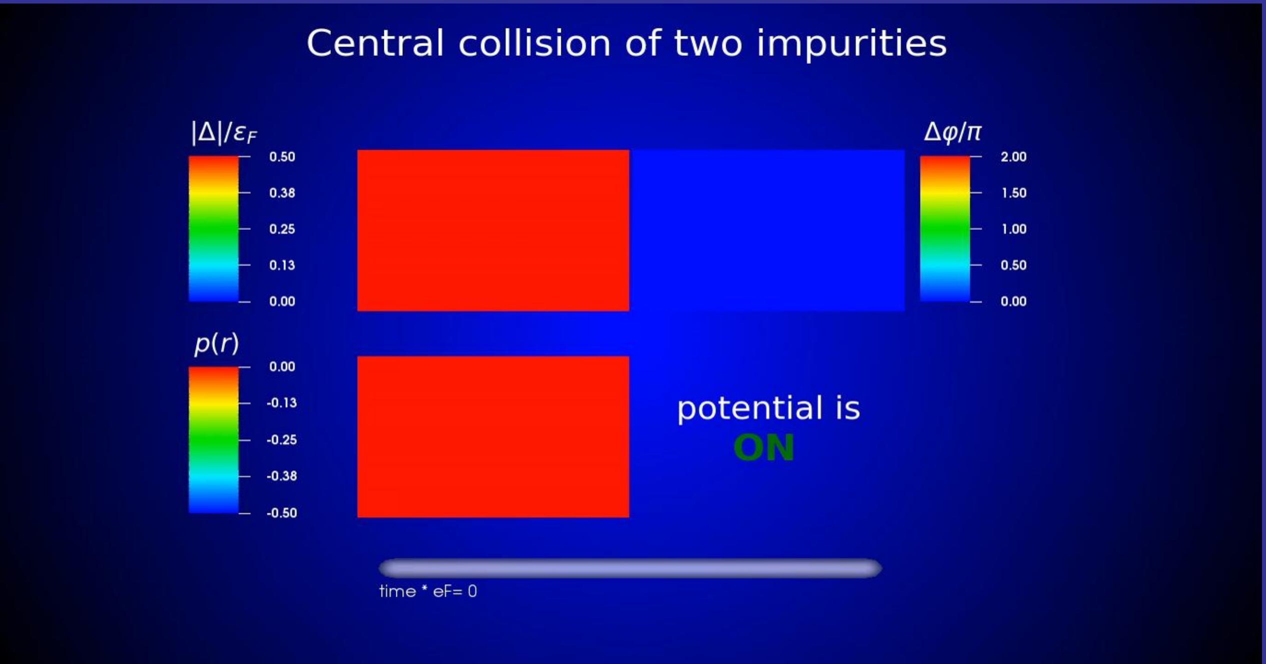
The impurity cannot collapse because it would require to destroy the nonzero pairing field inside, which has an inverted phase.

As a result one obtains the collective excitation stabilized by the pairing field.



Impurity tends to be spherical irrespective of initial deformation.



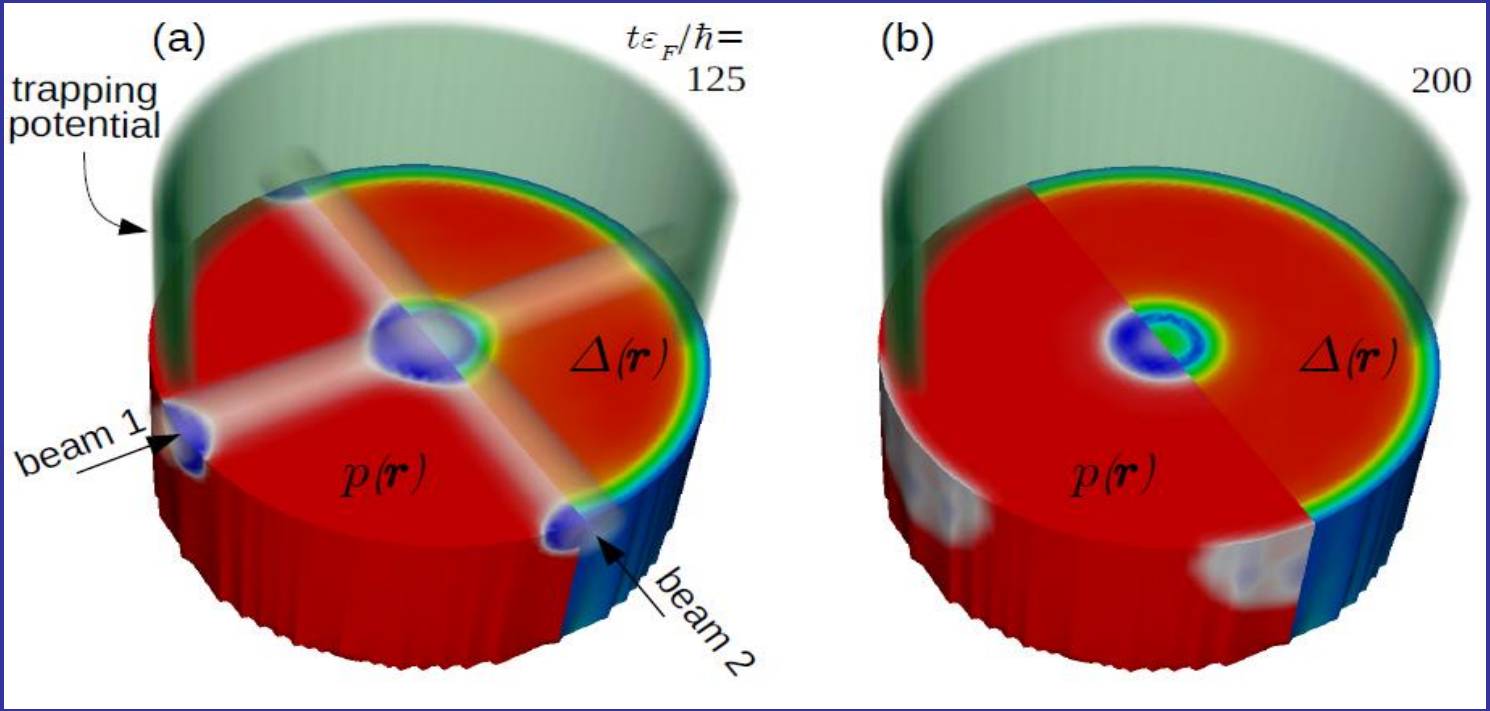


Suggestion for experimental detection

Two crossing laser beams, each polarizing the atomic cloud with the strength of approx. Fermi energy should be applied.
Separately these two beams are two weak to produce the long-lasting, spin-polarized region.

However at the crossing region the strength of beams will be sufficient to generate a localized spin-polarized impurity.

For a typical experimental setup the time interval for applying laser beams has to be about 2ms and the predicted lifetime of the impurity: > 12ms.



Quantum tubulence in fermionic ultracold gases

Superfluid turbulence (quantum turbulence): disordered set of quantized vortices. The friction between the superfluid and normal part of the fluid serves as a source of energy dissipation.

Problem: how the energy is dissipated in the superfluid system at small scales at T=0? - „pure" quantum turbulence

Possibility: vortex reconnections → Kelvin waves → phonon radiation

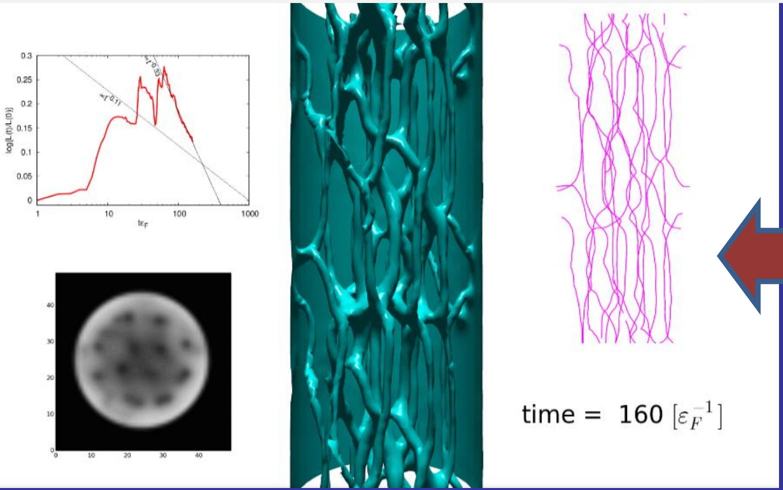
Vortex dynamics is crucial to understand the rate of energy dissipation and the energy distribution stored at various length scales during the turbulent motion (classically the energy distribution obeys the Kolmogorov formula:

$$E(k)=C\,\varepsilon^{2/3}\,k^{-5/3}$$

ε - energy rate (per unit mass) transfered to the system at large scales.

k - wave number (from Fourier transformation of the velocity field).

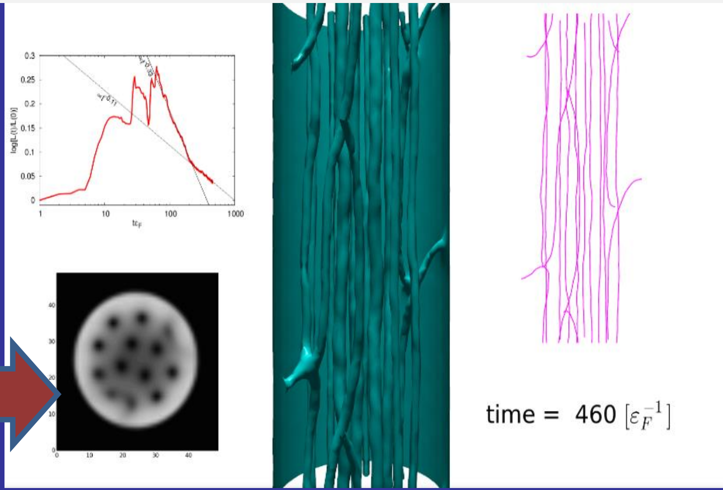
C – dimensionless constant.



Two regimes of the turbulent state decay (preliminary)

Vortex reconnections

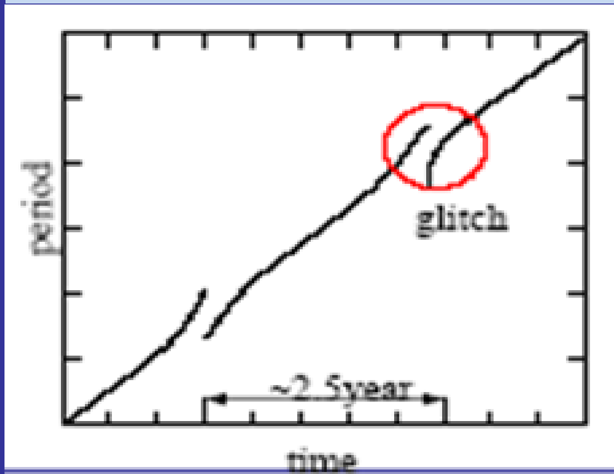
Vortex interactions



Wlazłowski, Sekizawa, Magierski – in preparation

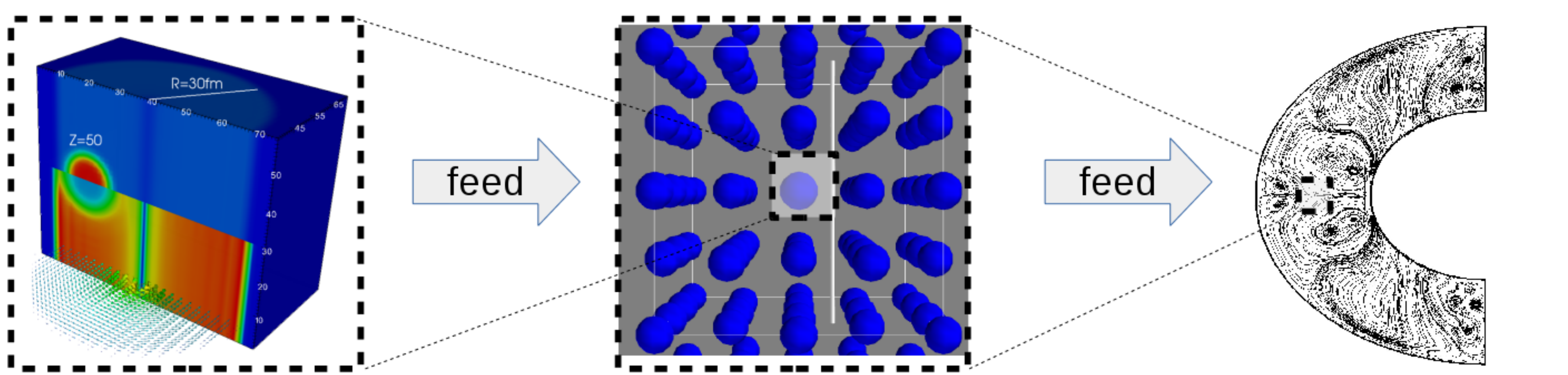
Building the model of turbulent motion in neutron stars

Neutron star is a huge superfluid



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

Hierarchy of theoretical models of neutron star dynamics



Method: TDDFT
DoF: neutrons and protons.
Scale: ~10^{-13}m

Method: Vortex Filament Model
DoF: impurities and vortices
Scale: ~10^{-9}m

Method: Hydrodynamics
DoF: fluid elements
Scale: ~size of star

In collaboration with astrophysical group at CAMK (Warsaw): B. Haskell, M. Antonelli, V. Khomenko

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.

- <u>Future plans</u>:
- Ultracold atoms: investigation of <u>quantum turbulence</u> in Fermi systems;
  topological excitations in <u>spin-polarized</u> atomic gases
  in the presence of <u>LOFF phase</u>.
- Neutron star: Provide a link between <u>large scale models</u> of neutron
  stars and microscopic studies;
  towards the first simulation of the glitch phenomenon
  based on microscopic input.
- Nuclear physics: The dependence of <u>quasifission</u> process on pairing.

University of Tsukuba
Center for Computational Sciences

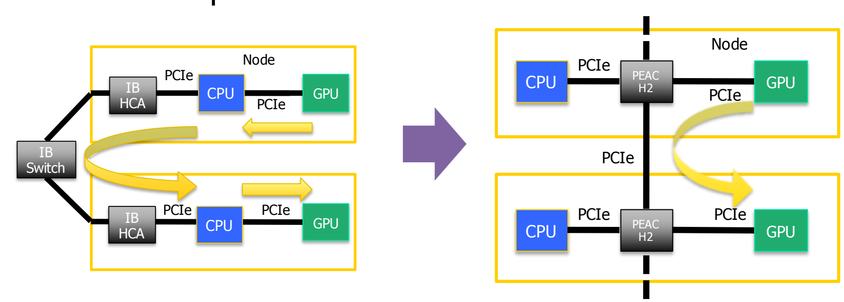
筑波大学
University of Tsukuba

Multidisciplinary Cooperative Research
筑波大学計算科学研究センター 学際共同利用

HA-PACS(PACS-VIII) system

Node Spec.	Base Cluster Part	TCA Part
# of nodes	268	64
CPU	Intel Xeon E5-2670, 8 core, 2.6GHz x 2	Intel Xeon E5-2680v2, 10 core, 2.8GHz x 2
GPU	NVIDIA M2090 x4	NVIDIA K20X x4
CPU memory	DDR3 1600 x8, 128GB, 102.4GB/s	DDR3 1866 x8, 128GB, 119.4GB/s
GPU memory	GDDR5, 708GB/s, 24GB	GDDR5, 1000GB/s, 24GB
Peak perf.	332.8GF (CPU) + 2660GF (GPU) = 802 TF	448GF (CPU) + 5240GF (GPU) = 364 TF
Network HCA	InfiniBand QDR x2rail	InfiniBand QDR x2rail
Network b/w	7GB/s	
Net. config.	Fat-Tree with full bisection b/w	
Total perf.	1.166 PFLOPS	
File system	Lustre 500TB with RAID6	

Tightly Coupled Accelerators
with cooperation of NVIDIA



共同利用・共同研究拠点
「先端学際計算科学共同研究拠点」（文部科学省）
Advanced Interdisciplinary Computational Science Collaboration Initiative (the MEXT of Japan)