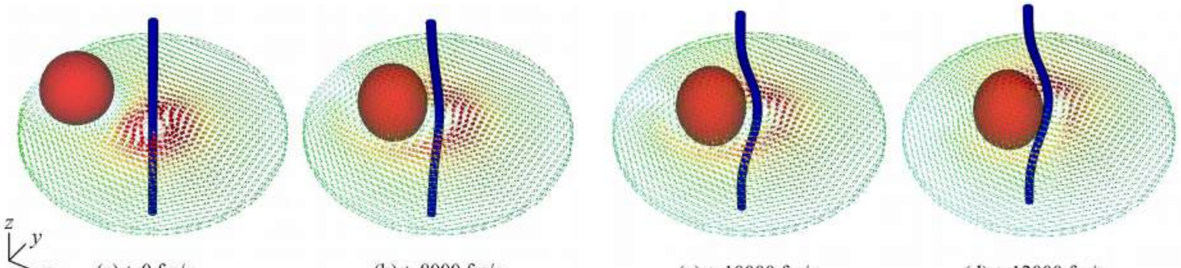
Nuclear density functional theory as a source of microscopic input for pulsar glitch models

Gabriel Wlazłowski

Warsaw University of Technology
University of Washington

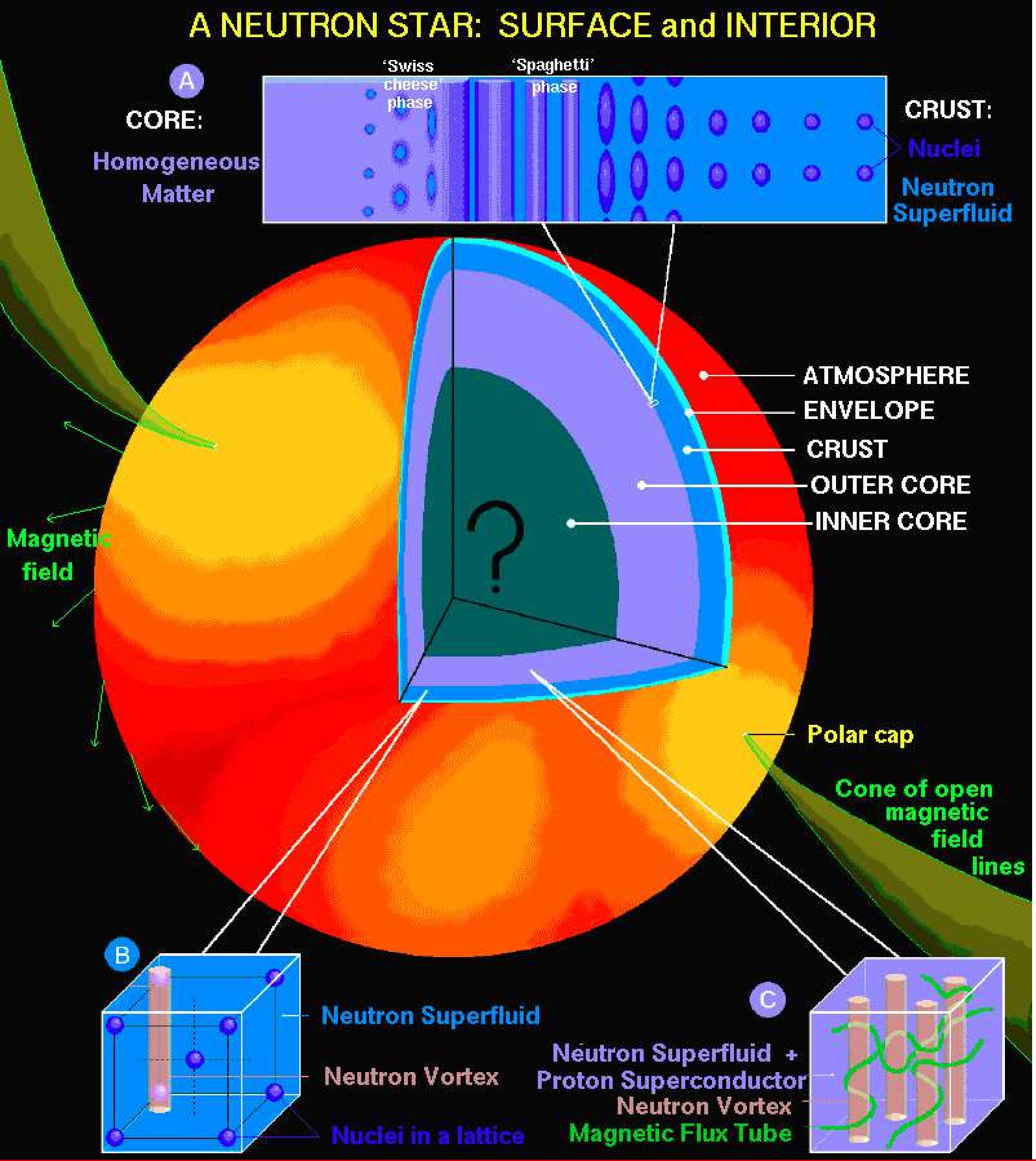
In collaboration with:
- Piotr Magierski (WUT)
- Kazuyuki Sekizawa (Niigata University)
- Michael Forbes(WSU, Pullman)
- Aurel Bulgac (UW, Seattle)



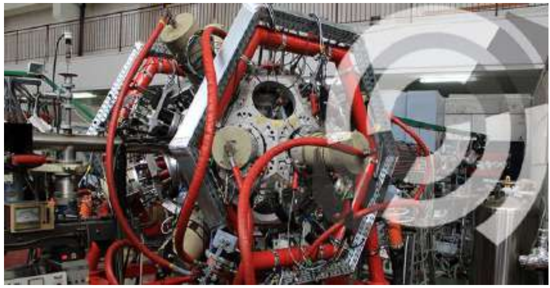
(a) t=0 fm/c (b) t=8000 fm/c (c) t=10000 fm/c (d) t=12000 fm/c

NATIONAL SCIENCE CENTRE
POLAND

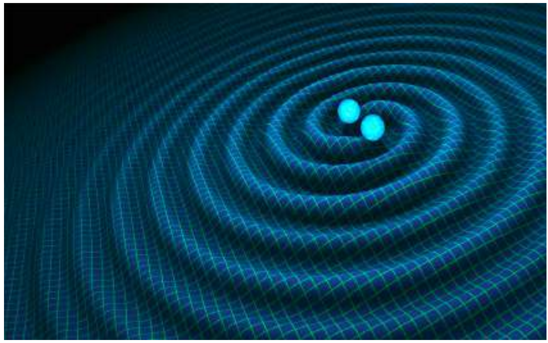
UW, 27-02-2020



Nuclear physics

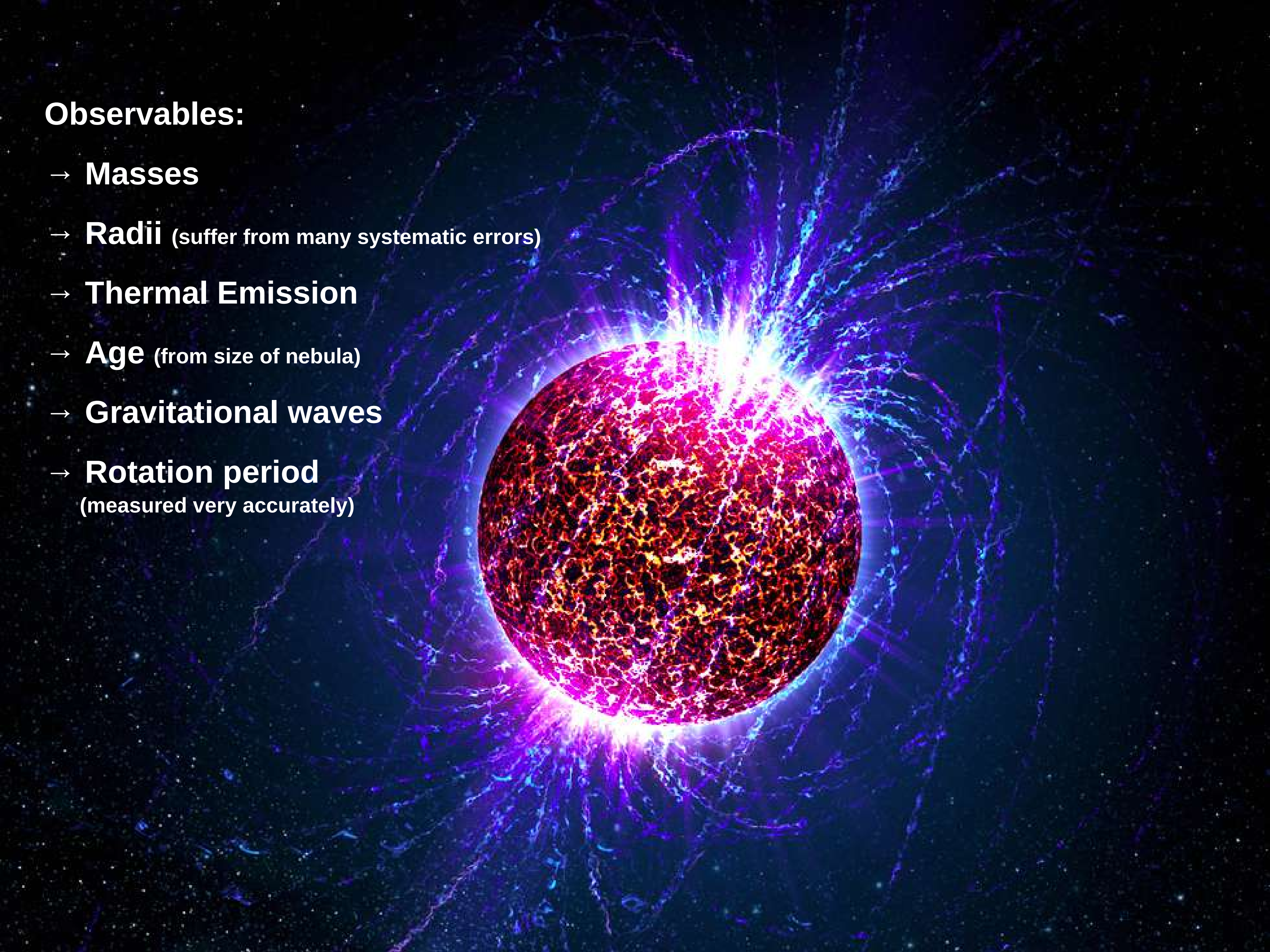


General relativity



Astronomy

Collective effort



Observables:

→ **Masses**

→ **Radii** (suffer from many systematic errors)

→ **Thermal Emission**

→ **Age** (from size of nebula)

→ **Gravitational waves**

→ **Rotation period**
(measured very accurately)

https://www.facebook.com/thecosmicstudio/videos/531504000921818

Observables:

→ **Masses**

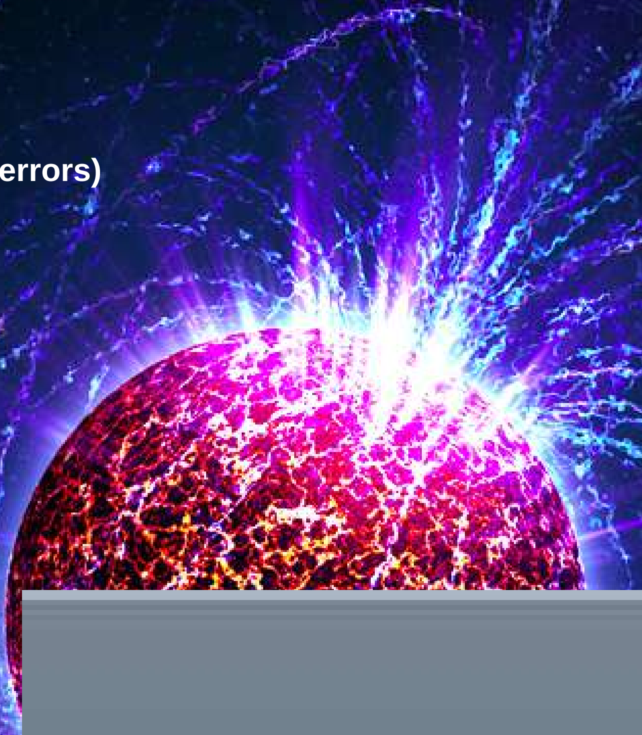
→ **Radii** **(suffer from many systematic errors)**

→ **Thermal Emission**

→ **Age** **(from size of nebula)**

→ **Gravitational waves**

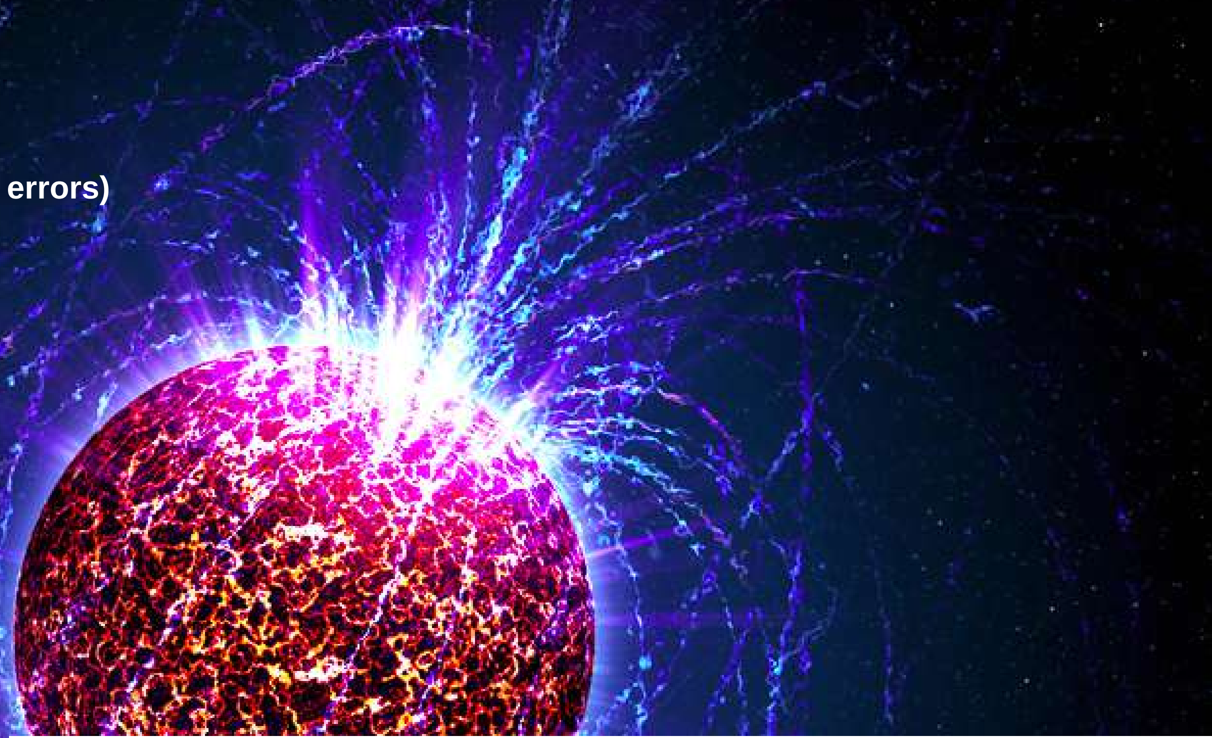
→ **Rotation period**
(measured very accurately)

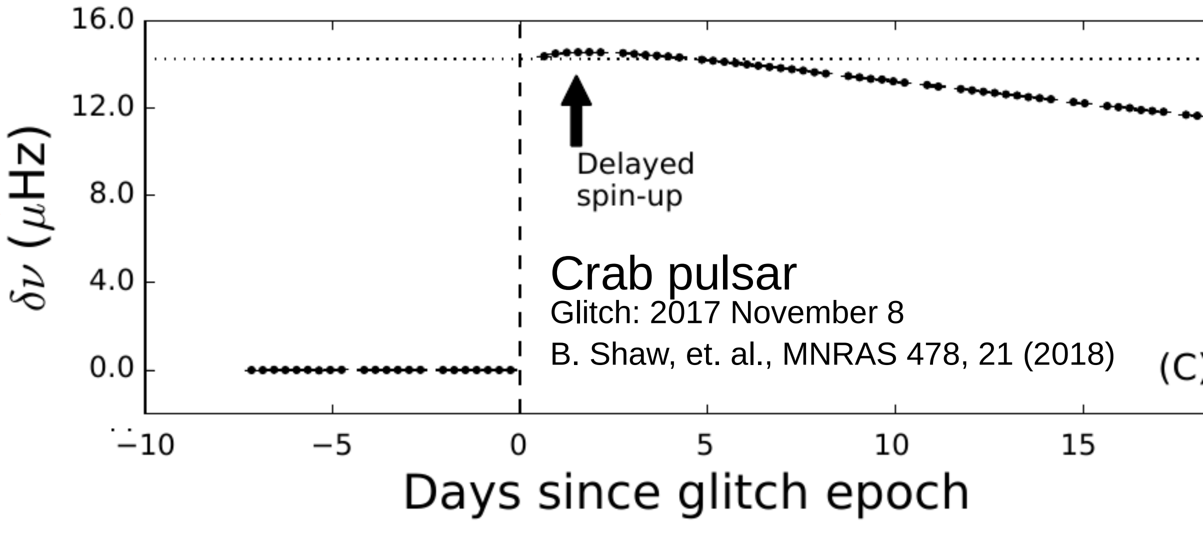


Movie from:
https://www.youtube.com/watch?v=6ttpXxgjyrN

Observables:

- → **Masses**
- → **Radii** (suffer from many systematic errors)
- → **Thermal Emission**
- → **Age** (from size of nebula)
- → **Gravitational waves**
- → **Rotation period** (measured very accurately)





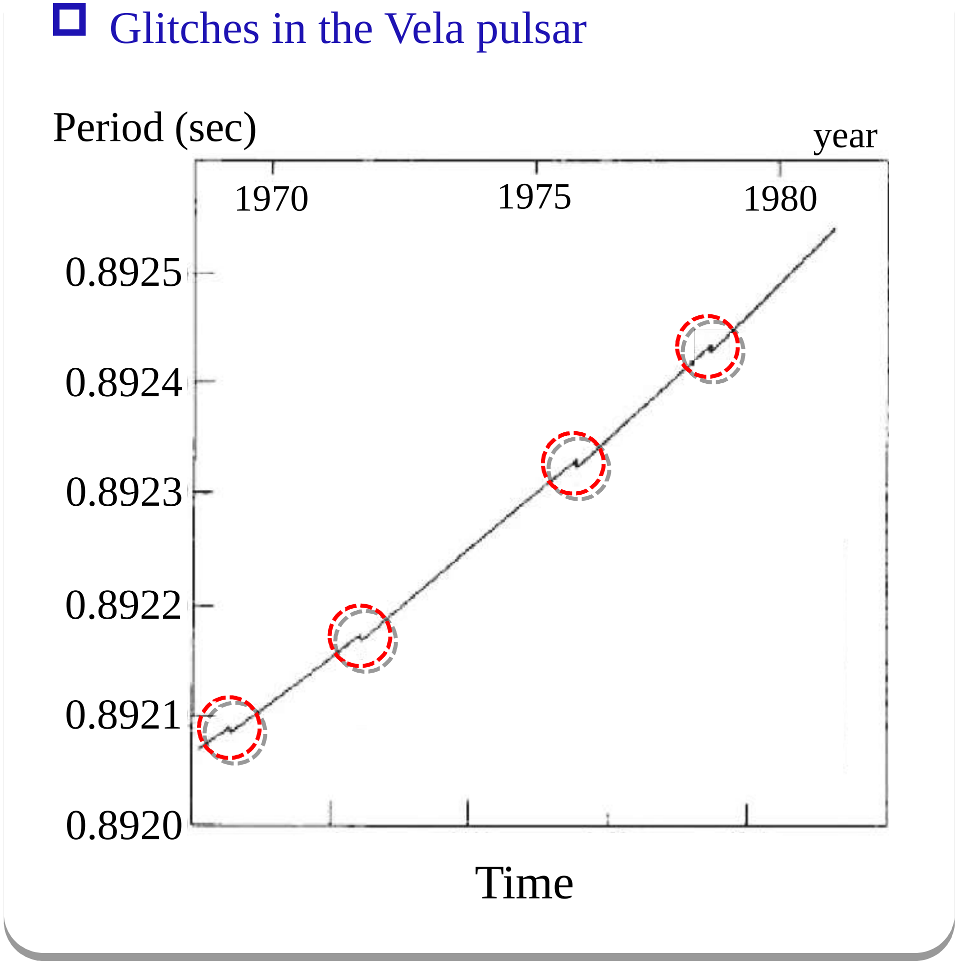
Crab pulsar

Glitch: 2017 November 8

B. Shaw, et. al., MNRAS 478, 21 (2018)

Glitch: a sudden increase of the rotational frequency

- ☐ Glitches in the Vela pulsar



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

- **Vortex model**
  (P. W. Anderson and N. Itoh, Nature 256 (1975))
  - Presently the standard picture for pulsar glitches
  - Can explain: post-glitch relaxation, statistics of the glitching populations...
  - Idea:
    - Superfluid interior contains quantized vortices pinned to the crustal lattice
    - Glitches are believed to occur when a large number of vortices simultaneously unpin and move outward

First observed in 1969: V. Radhakrishnan and R. N. Manchester, Nature 222, 228–229 (1969);
P. E. Reichley and G. S. Downs, Nature 222, 229–230 (1969);

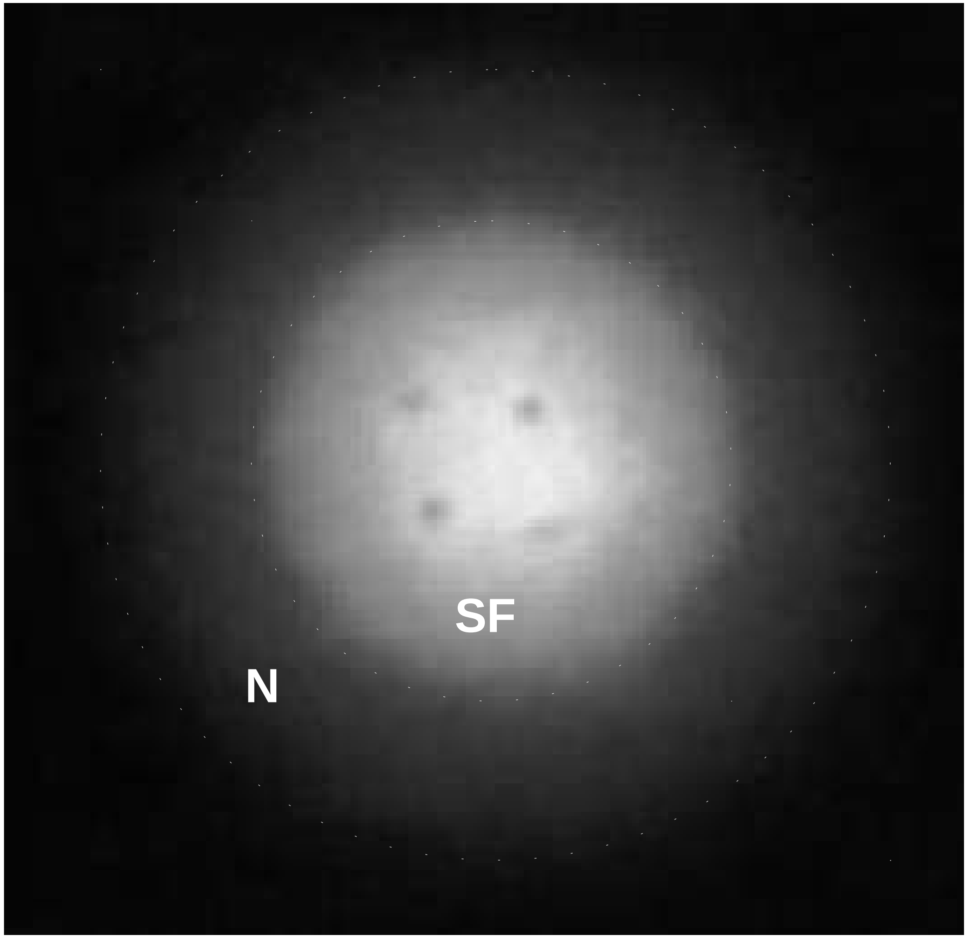


Figure taken from: Zwierlein, et. al, Science 311, 492 (2006)

Normal component
- rigid body rotation

Superfluid component
- can rotate only in form of vortices

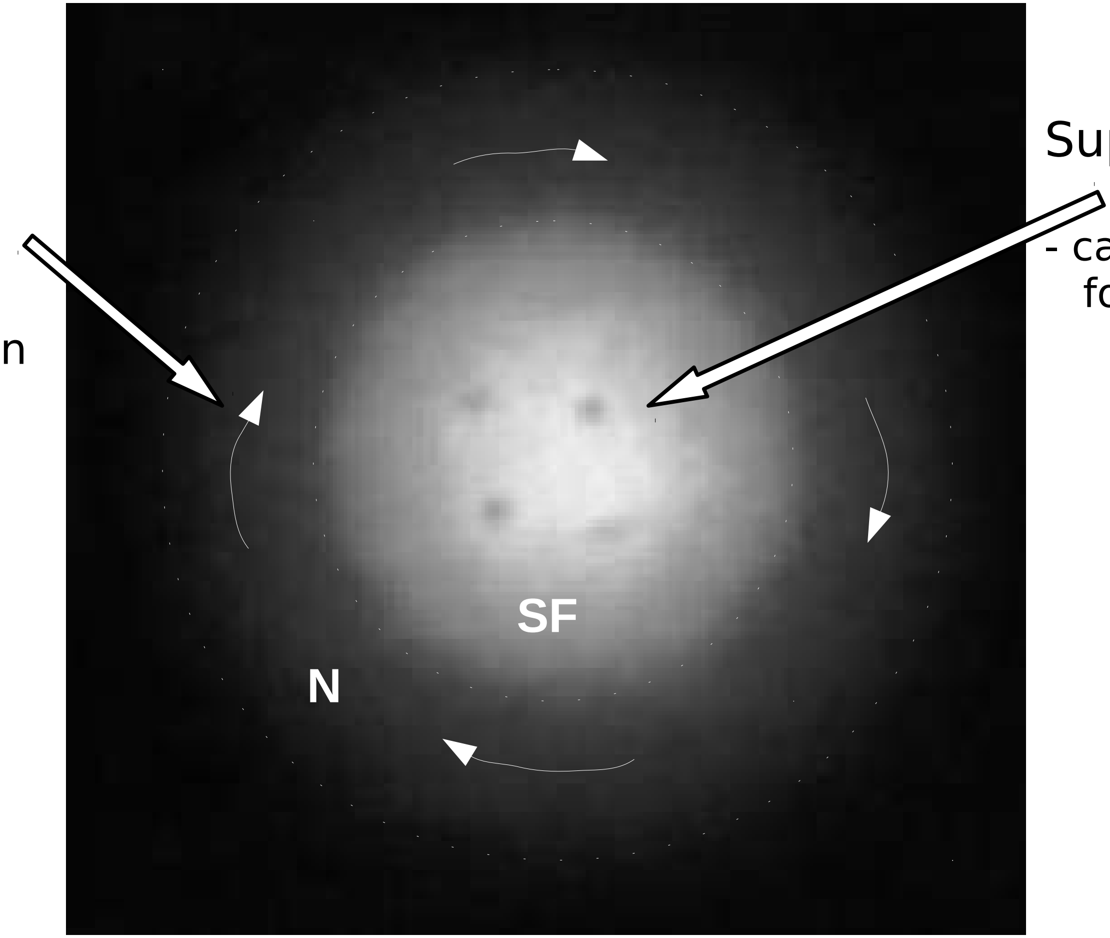
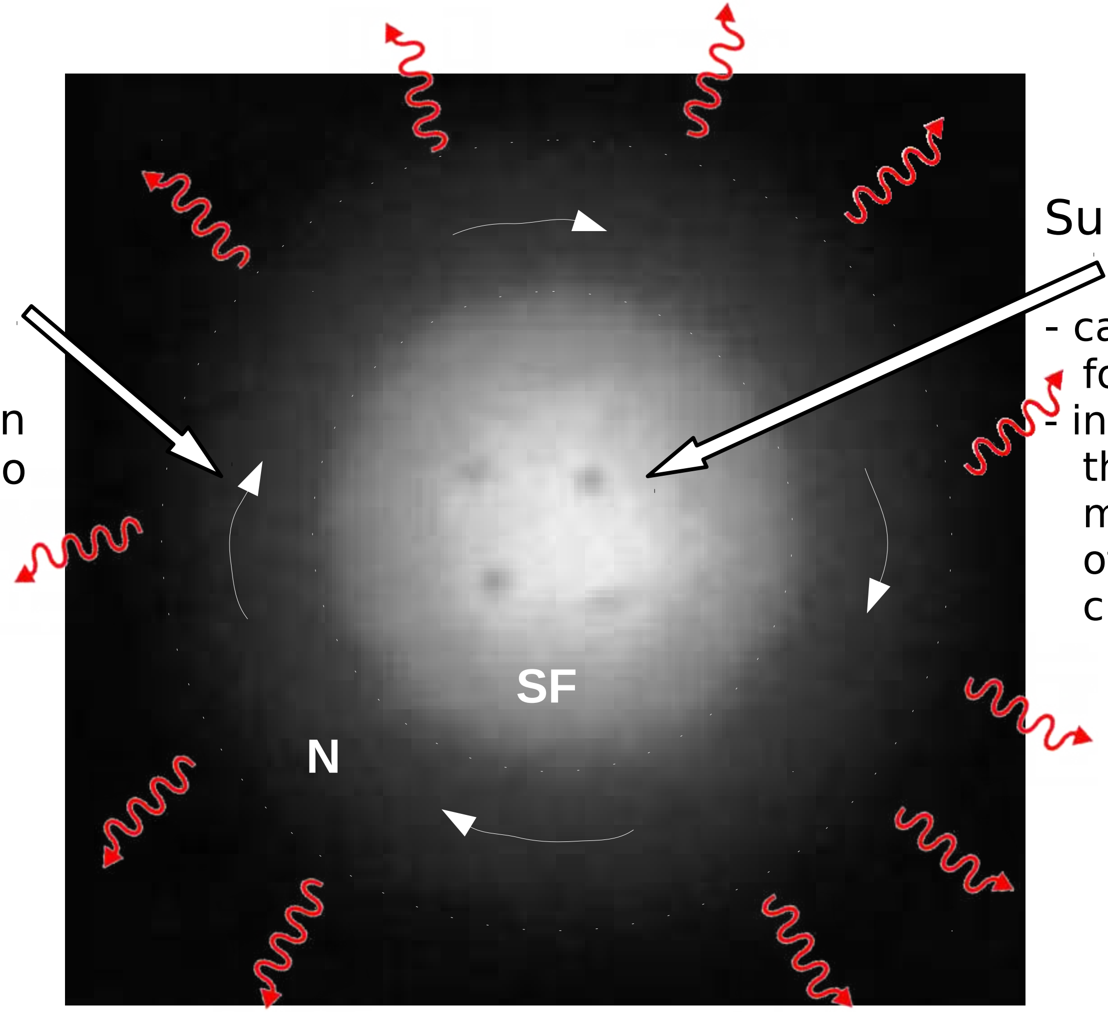


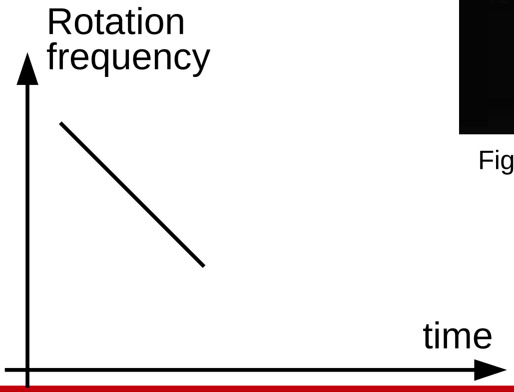
Figure taken from: Zwierlein, et. al, Science 311, 492 (2006)

Normal component
- rigid body rotation
- slows down due to energy radiation



Superfluid component
- can rotate only in form of vortices
- in order to decrease the angular momentum number of vortices must change

Figure taken from: Zwierlein, et. al, Science 311, 492 (2006)



Normal component
- rigid body rotation
- slows down due to energy radiation

Tension between N and SF component is generated!

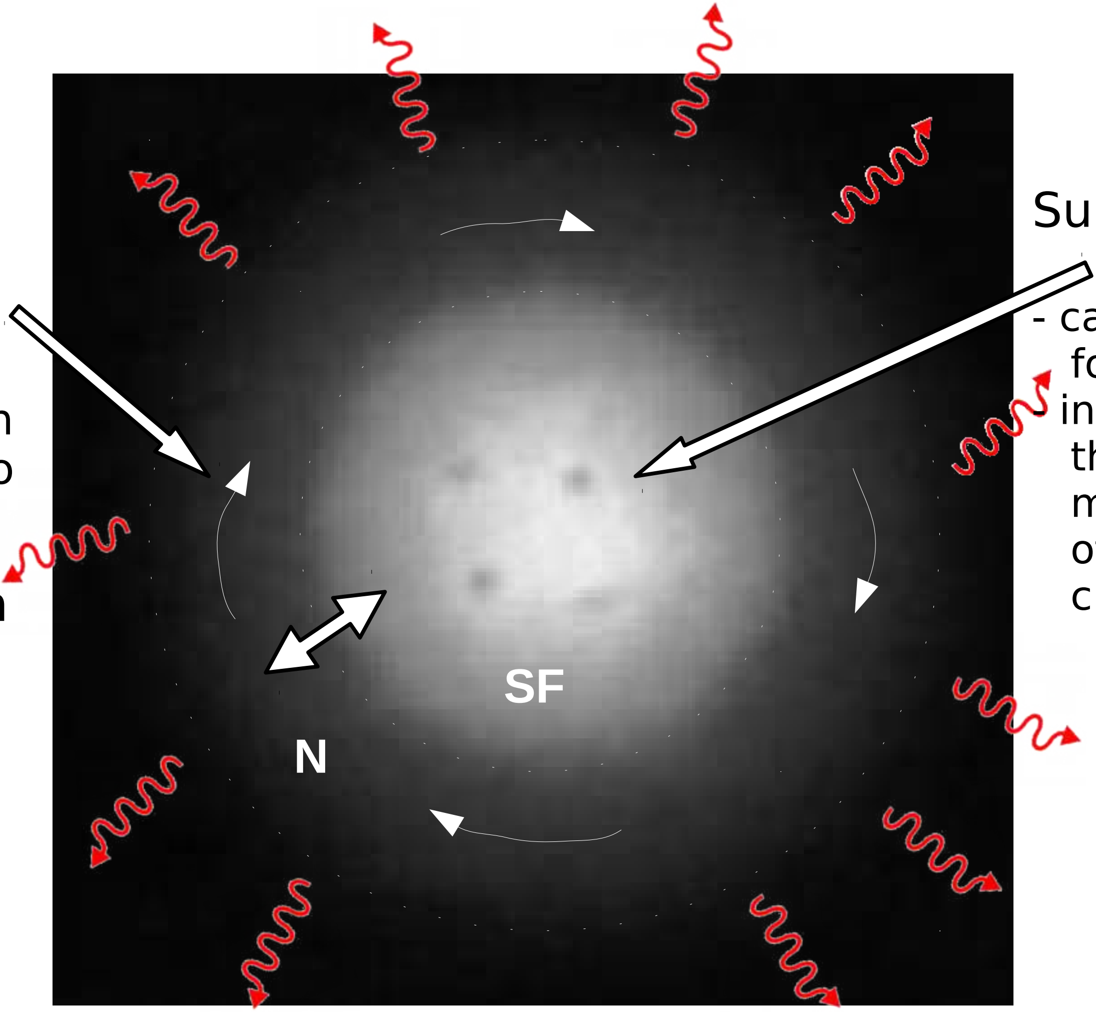
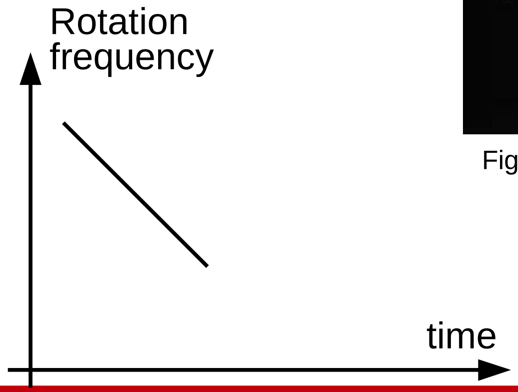
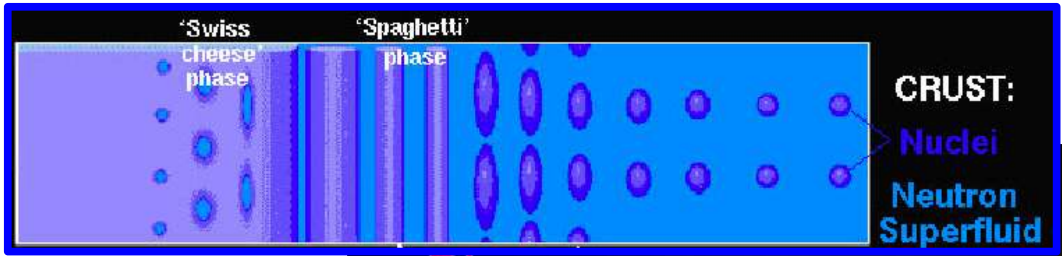


Figure taken from: Zwierlein, et. al, Science 311, 492 (2006)

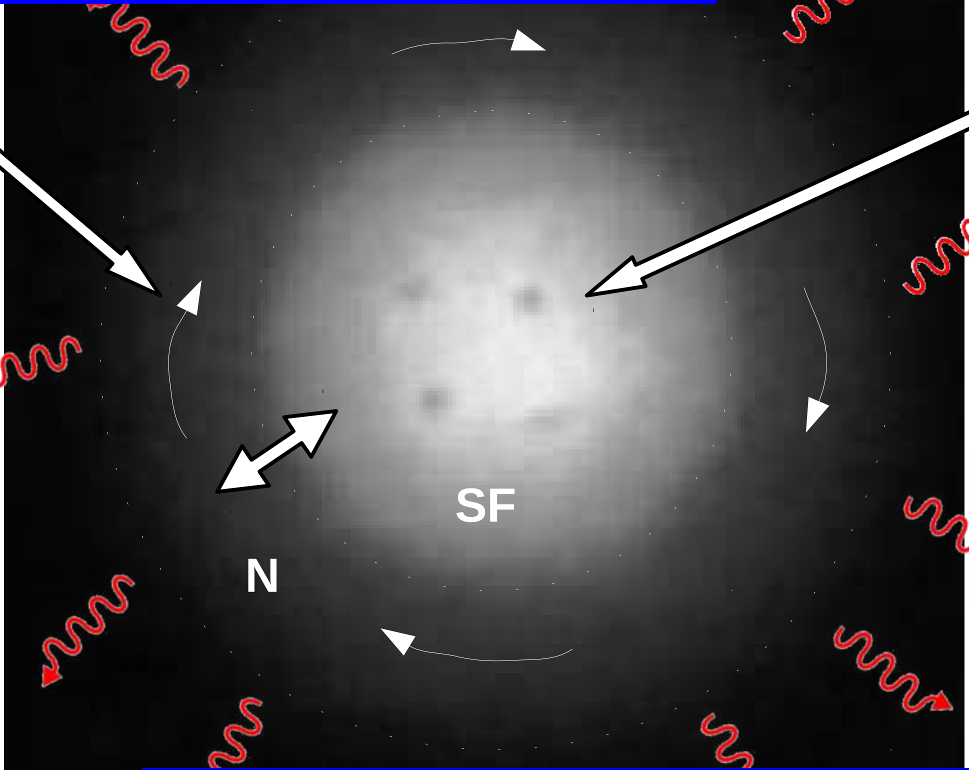
Superfluid component
- can rotate only in form of vortices
- in order to decrease the angular momentum number of vortices must change





Normal component
- rigid body rotation
- slows down due to energy radiation

Tension between N and SF component is generated!



Superfluid component
- can rotate only in form of vortices
- in order to decrease the angular momentum number of vortices must change

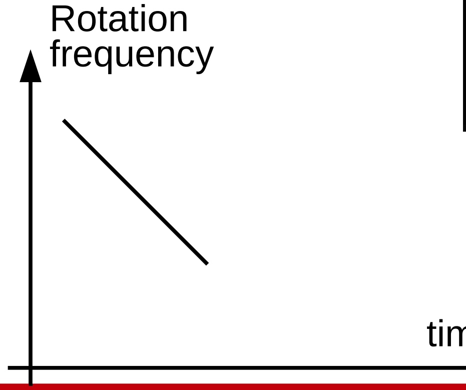


Figure tak

Normal component
- rigid body rotation
- slows down due to energy radiation

Tension between N and SF component is generated!

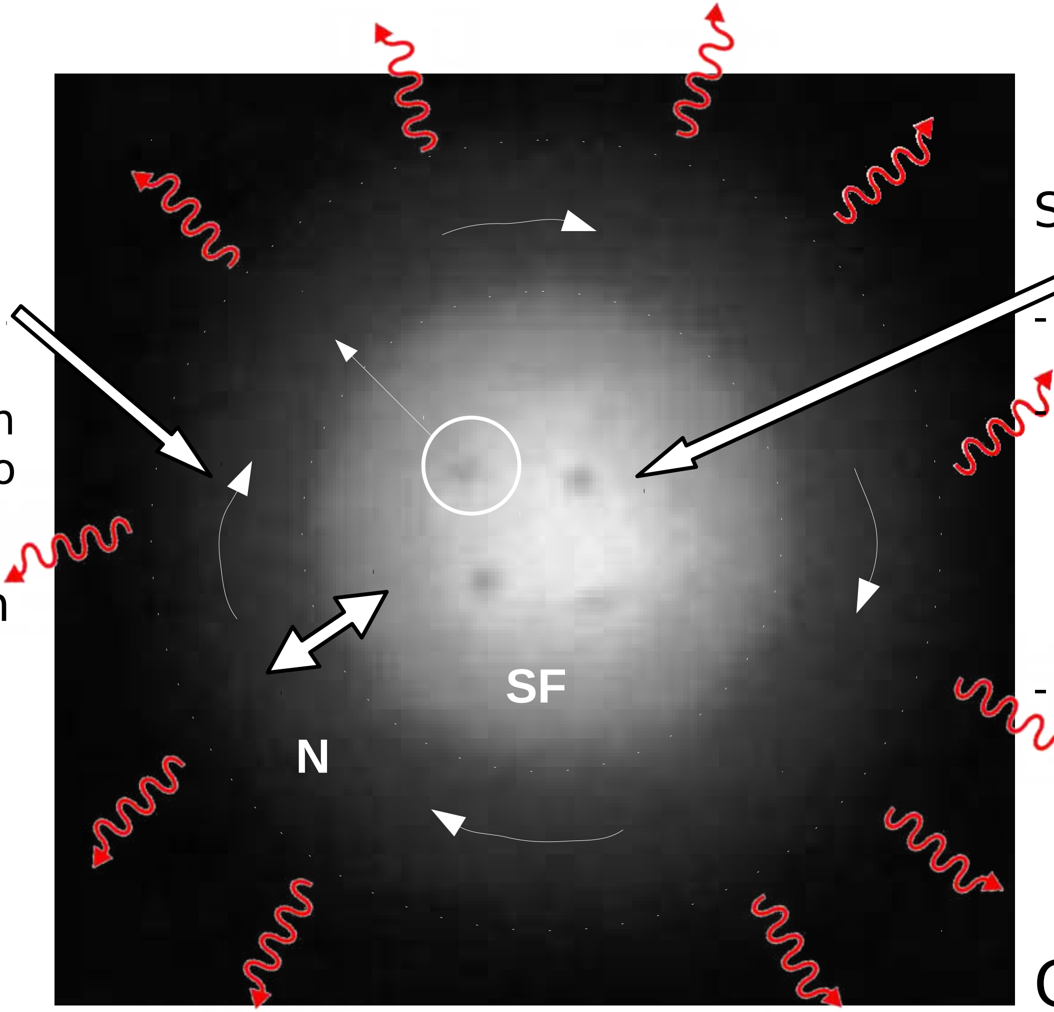
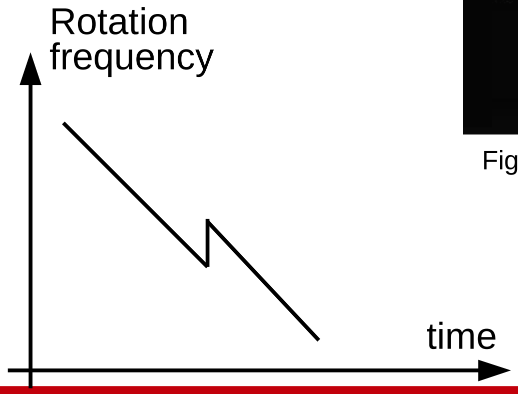


Figure taken from: Zwierlein, et. al, Science 311, 492 (2006)

Superfluid component
- can rotate only in form of vortices in order to decrease the angular momentum number of vortices must change

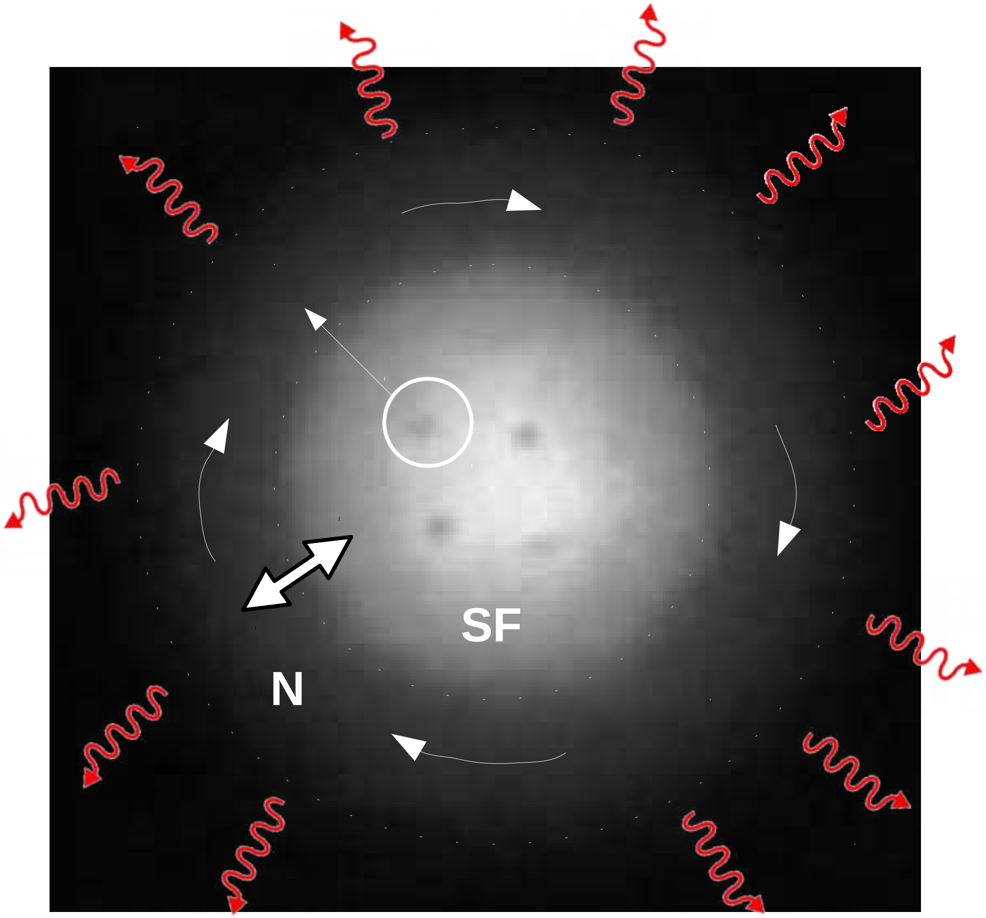
- when vortices are ejected they transfer its angular momentum to N component

GLITCH!



A lot of open problems:

- ...
- ...
- origin of pinning mechanism?
- regular lattice of vortices
  or tangle of vortices?
- ...
- ...



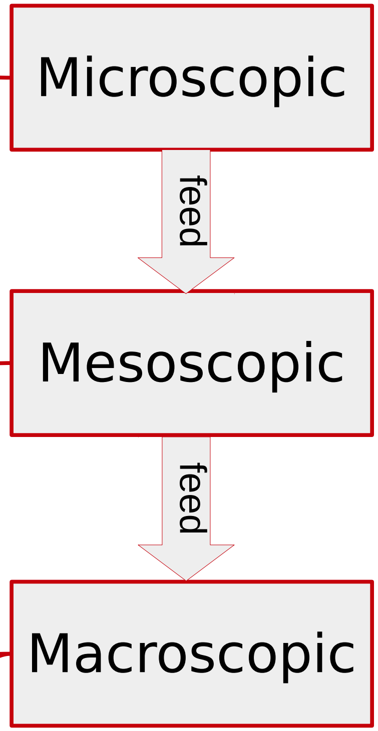
→ neutron star ≈ 10^{17} vortices
→ up to ≈ 10^{13} involved in a glitch

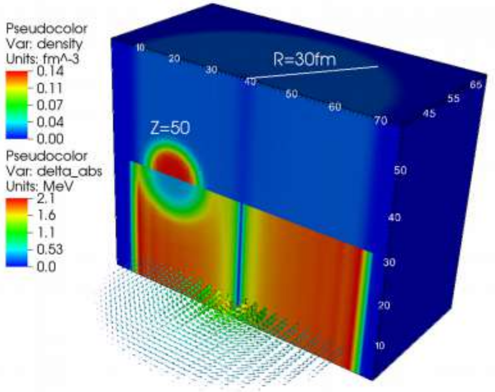
→ size of vortex ξ_c ≈ 10 fm
→ separated by a distance dv ≈ 10^{-3} cm

A lot of open problems:

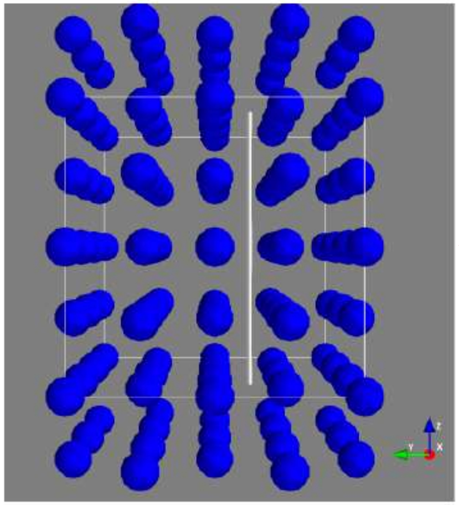
- ...
- ...
- origin of pinning mechanism?
- regular lattice of vortices or tangle of vortices?
- ...
- ...
- vortex avalanche trigger mechanism?

Hierarchy of theories:

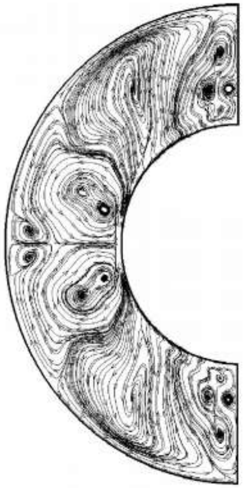




Method: TDDFT
DoF: fermionic
(neutrons, protons...)

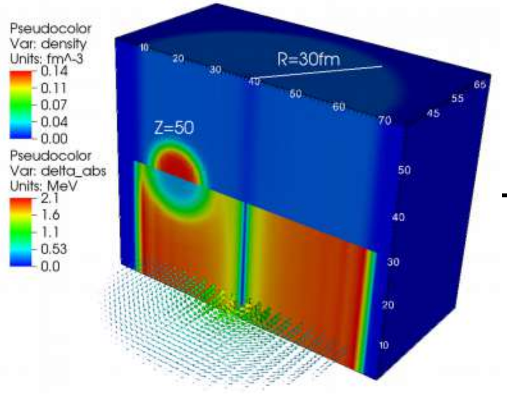


Method: Vortex filament model
DoF: impurities and vortices

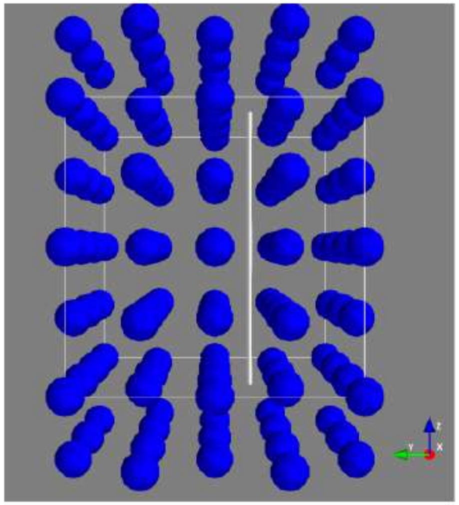


Method:
Hydrodynamics
DoF: fluid elements

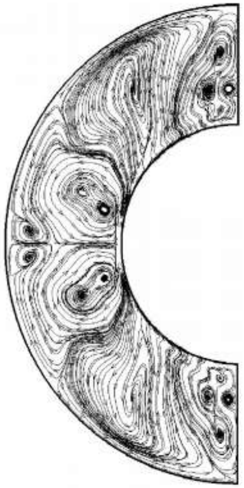
Observations



Method: TDDFT
DoF: fermionic
(neutrons, protons...)



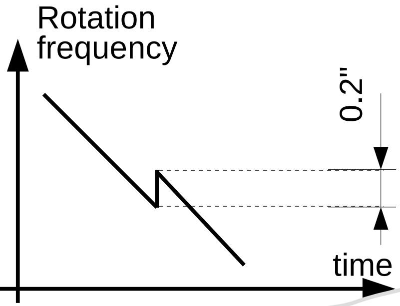
Method: Vortex filament model
DoF: impurities and vortices



Method:
Hydrodynamics
DoF: fluid elements

Matching theories is hard..

- ...
- scaling problem...
- output → input conversion
- ...
- collective effort...
- ...



Observed relative sizes of glitches:

$$\Delta\nu/\nu \sim 10^{-11} - 10^{-5}$$

maximum glitch amplitude

$$\Delta\Omega_{\mathrm{max}} = \frac{\pi^2}{\kappa\, I}\int_0^{R_d} dr\, r^3\, f_P(r)$$

quantum of circulation

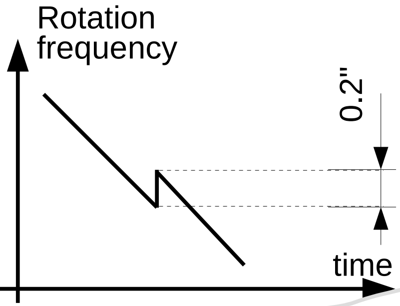
moment of inertia

pinning force

(force needed to move a vortex through the medium with "impurities")

Result is weakly sensitive to various assumptions of a model...

- P. Pizzochero, M. Antonelli, B. Haskell, S. Seveso, Nature Astronomy 1, 0134 (2017)
- M. Antonelli, P. Pizzochero, Journal of Physics: Conf. Series 861 (2017) 012024
- M. Antonelli, A. Montoli, P. M. Pizzochero, MNRAS 475, 5403 (2018)



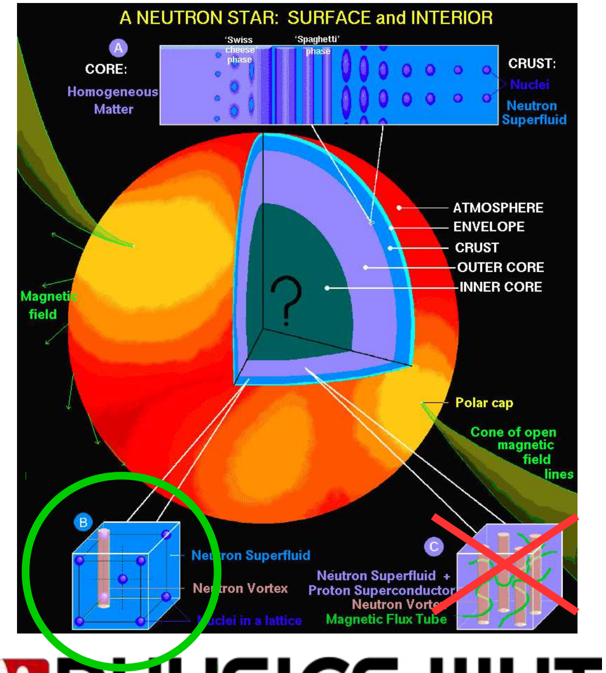
maximum glitch amplitude

Observed relative sizes of glitches:

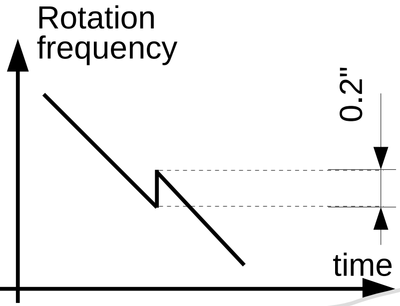
$$\Delta\nu/\nu \sim 10^{-11} - 10^{-5}$$

$$\underbrace{\Delta\Omega_{\mathrm{max}}}_{\textit{Observation}} = \underbrace{\frac{\pi^2}{\kappa\, I}\int_0^{R_d} dr\, r^3\, f_P(r)}_{\textit{Theory}}$$

Assumption: only crust contributes



… now also quantity matters (not only quality) … → … reliable theory needed!



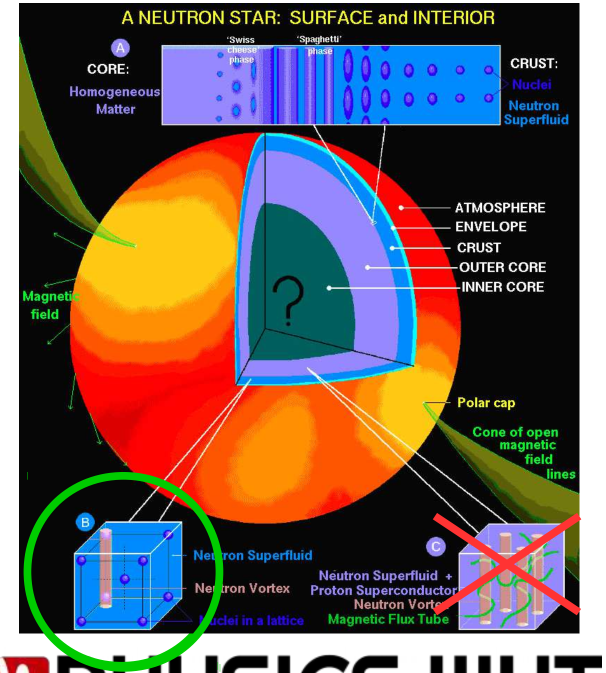
maximum glitch amplitude

Observed relative sizes of glitches:

$$\Delta\nu/\nu \sim 10^{-11} - 10^{-5}$$

$$\underbrace{\Delta\Omega_{\max}}_{\textit{Observation}} = \underbrace{\frac{\pi^2}{\kappa I}\int_0^{R_d} dr\, r^3}_{\textit{Theory}} f_P(r)$$

Assumption: only crust contributes



… now also quantity matters (not only quality) … → … reliable theory needed!

Microscopic level: DFT and TDDFT

Qualitatively and **quantitatively** accurate

Unified description of static and dynamic properties of **large Fermi systems**

$$\boxed{i\hbar\frac{\partial}{\partial t}\psi = \hat{H}\psi}$$

$$\begin{cases} [h(\mathbf{r})-\mu]u_k(\mathbf{r}) + \Delta(\mathbf{r})v_k(\mathbf{r}) = E_k u_k(\mathbf{r}),\\ \Delta^*(\mathbf{r})u_k(\mathbf{r}) - [h(\mathbf{r})-\mu]v_k(\mathbf{r}) = E_k v_k(\mathbf{r}),\end{cases}$$

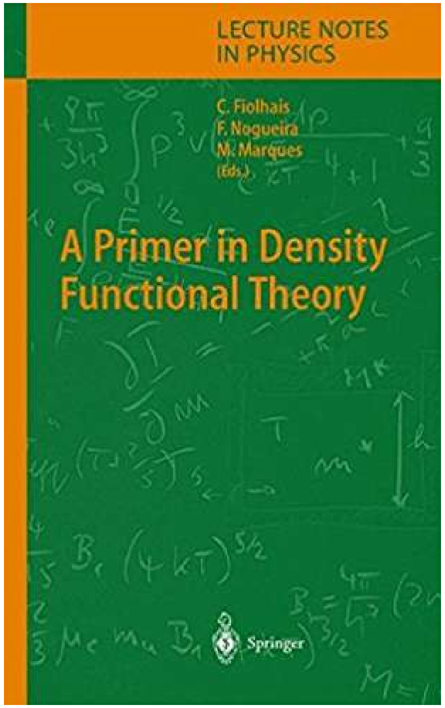
HFB equations

$$h(\mathbf{r}) = -\boldsymbol{\nabla}^2/2m + v_{\mathrm{KS}}(\mathbf{x})$$

$$v_{KS} = \frac{\delta E_{\mathrm{int}}}{\delta\rho} + U_{\mathrm{ext}} \qquad \Delta = -\frac{\delta E_{\mathrm{int}}}{\delta\nu^*}$$

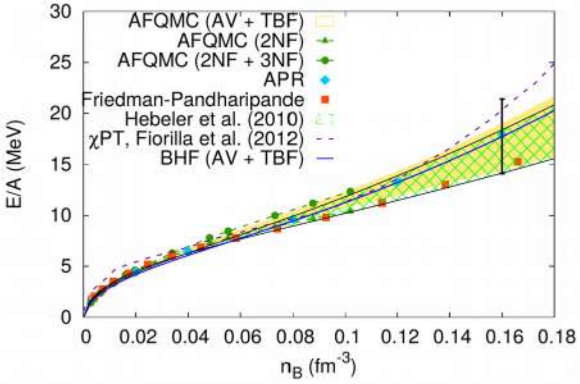
$$E_k \rightarrow i\hbar\frac{\partial}{\partial t}$$

Input: E_{int}
energy density functional

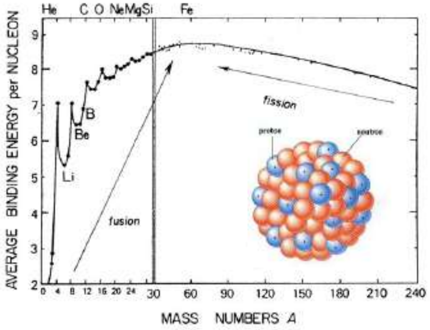


LECTURE NOTES IN PHYSICS
C. Fiolhais
F. Nogueira
M. Marques
(Eds.)
A Primer in Density Functional Theory
Springer

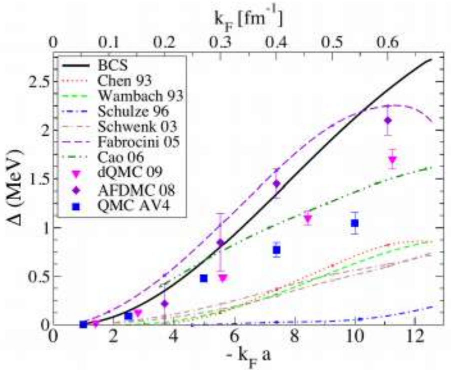
EoS (typically from QMC)



Exp. data for nuclei
(masses, radii, ...)



Pairing gap (s-wave)



Input 1

Input 2

Input 3

Dimensional arguments, renormalizability, Galilean invariance, and symmetries (translational, rotational, gauge, parity)

Postulate

Energy Density Functional
E[n,...]

Validation against other quantities

Predictions...

Quality of DFT results strongly depend on quality of the functional!

Which functional should we choose?

The nuclear energy density functional theory has been very successfully applied to describe the structure and the dynamics of medium-mass and heavy nuclei.

However, many functionals encounter problems when applied to neutron stars:

- they yield unrealistic neutron-matter equation of state
- they yield unrealistic pairing gaps in nuclear matter
- they lead to spurious instabilities in nuclear matter
  (e.g. speed of sound exceeds *c*, feromagnetic transition)

Brussels-Montreal Skyrme functionals (BSk)

These functionals were fitted to both experimental data and N-body calculations using realistic forces.

Experimental data:

- all atomic masses with $Z, N \geq 8$ from the Atomic Mass Evaluation (root-mean square deviation: 0.5-0.6 MeV)
  `http://www.astro.ulb.ac.be/bruslib/`
- charge radii
- incompressibility $K_v = 240 \pm 10$ MeV (ISGMR)
  Colò et al., Phys.Rev.C70, 024307 (2004).

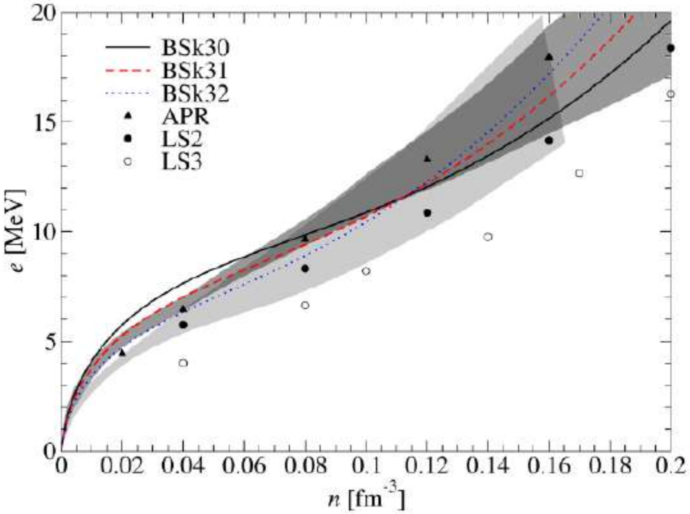
N-body calculations using realistic forces:

- equation of state of pure neutron matter
- ${}^1S_0$ pairing gaps in nuclear matter
- effective masses in nuclear matter

From: Nicolas Chamel talk,
Buffalo, March 2016

Brussels-Montreal Skyrme functionals (BSk)

These functionals were fitted to both experim
calculations using realistic forces.

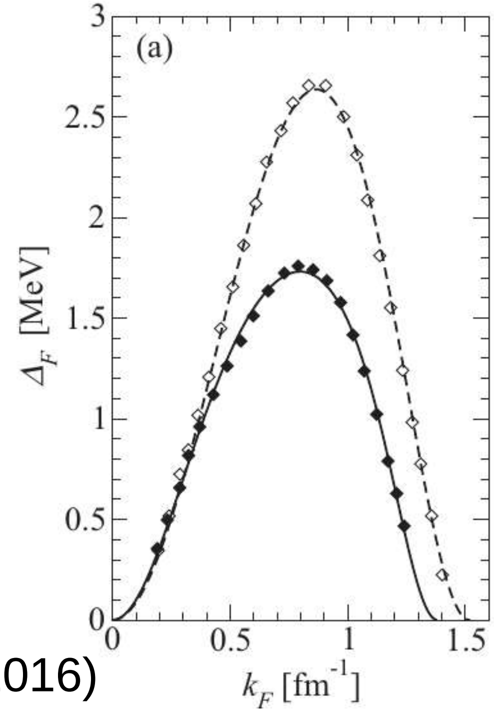


Experimental data:

- all atomic masses with $Z, N \geq 8$ from the
  Evaluation (root-mean square deviation:
  `http://www.astro.ulb.ac.be/bruslib/`
- charge radii
- incompressibility $K_v = 240 \pm 10$ MeV (ISGMR)
  Colò et al., Phys.Rev.C70, 024307 (2004).

N-body calculations using realistic forces:

- equation of state of pure neutron matter
- $^1S_0$ pairing gaps in nuclear matter
- effective masses in nuclear matter

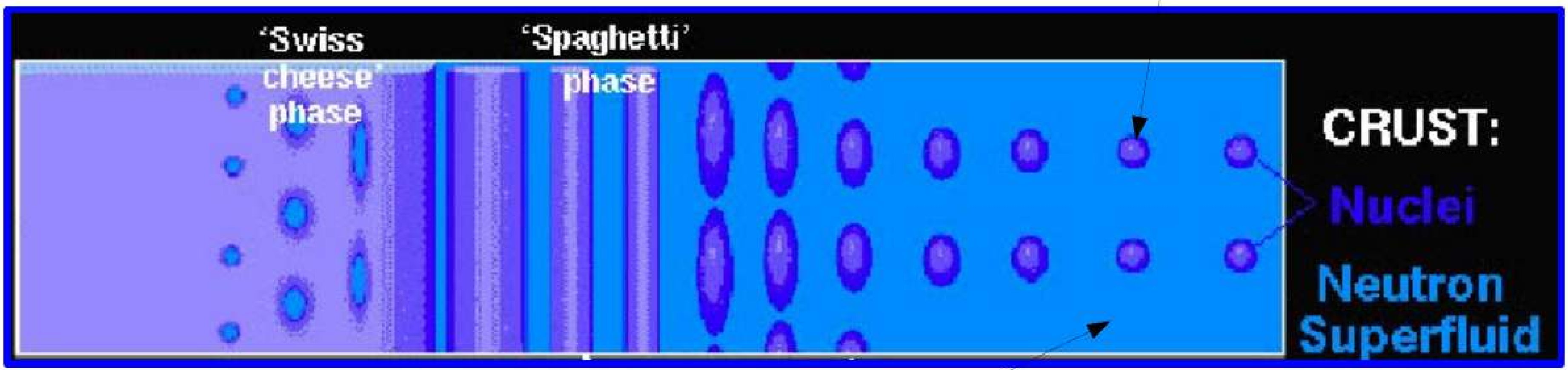


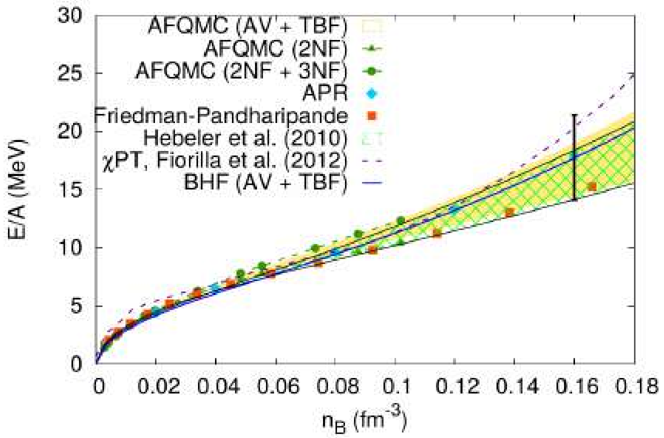
PRC 93, 034337 (2016)

From: Nicolas Chamel talk,
Buffalo, March 2016

EDF for NS crust is well constrained..

Nuclei - terrestrial experiments.

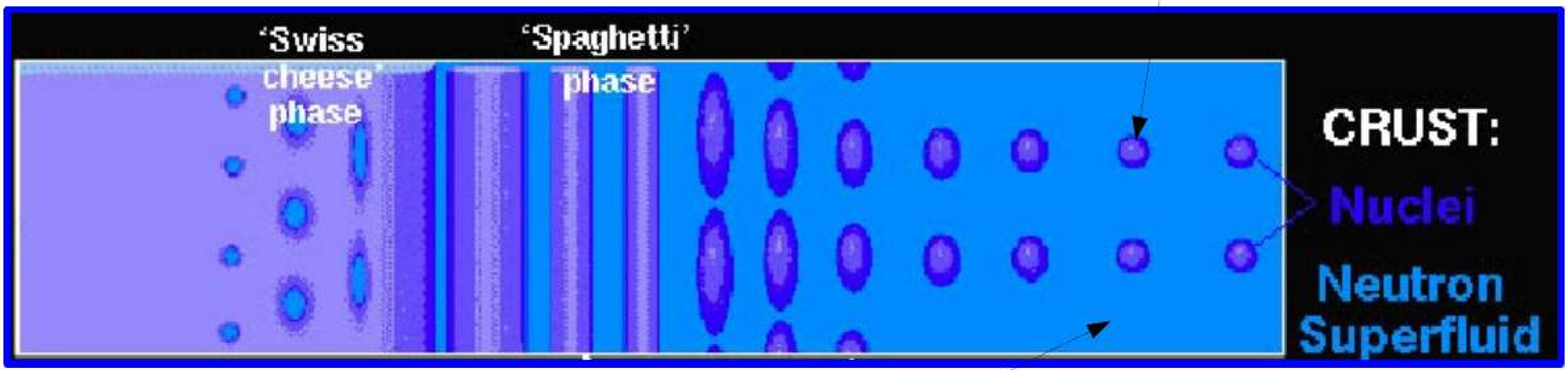


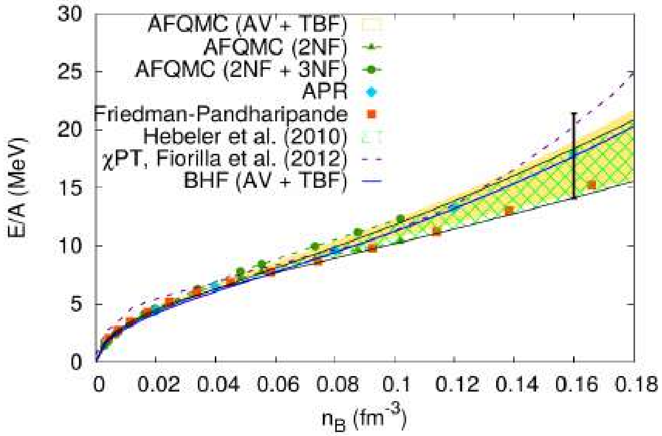


Dilute neutron matter very well constrained by QMC calculations.

EDF for NS crust is well constrained..

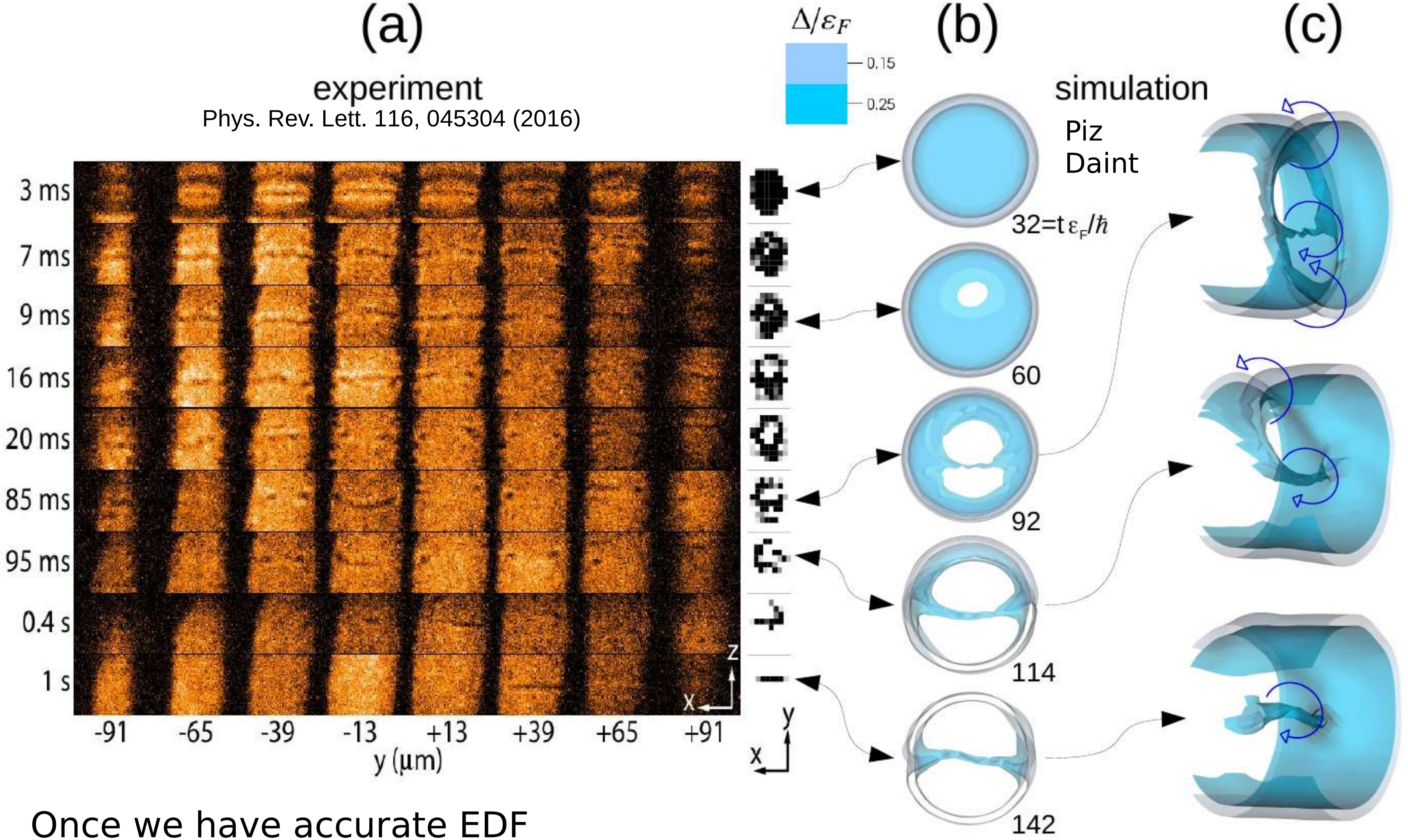
Nuclei - terrestrial experiments.





Dilute neutron matter very well constrained by QMC calculations.

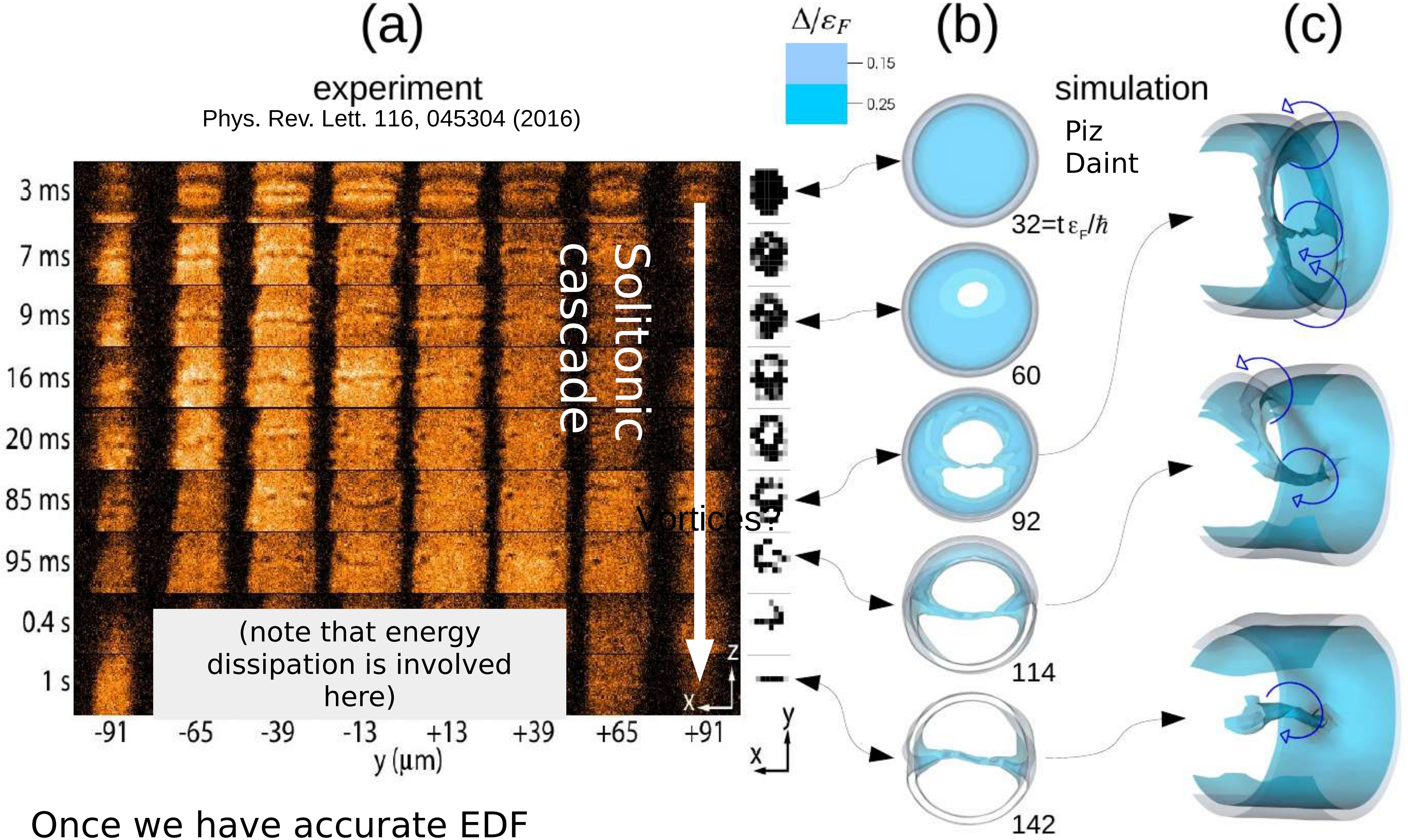
Vortices?



Once we have accurate EDF
→ remarkable agreement between theory and data!

No adjusting parameters to the experiment!

G. Wlazłowski, K. Sekizawa, M. Marchwiany, P. Magierski, PRL 2018 (arXiv:1711.05803)



experiment
Phys. Rev. Lett. 116, 045304 (2016)

simulation

Piz
Daint

Solitonic cascade

Vortices?

(note that energy dissipation is involved here)

Once we have accurate EDF
→ remarkable agreement between theory and data!

No adjusting parameters to the experiment!

G. Wlazłowski, K. Sekizawa, M. Marchwiany, P. Magierski, PRL 2018 (arXiv:1711.05803)

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

Spatial derivatives hidden here...

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

We explicitly track fermionic degrees of freedom!

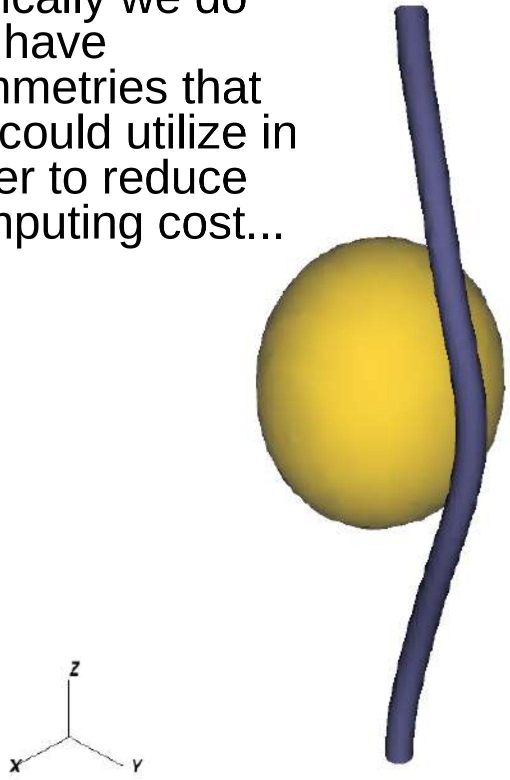
where *h* and Δ depends on “densities”:

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

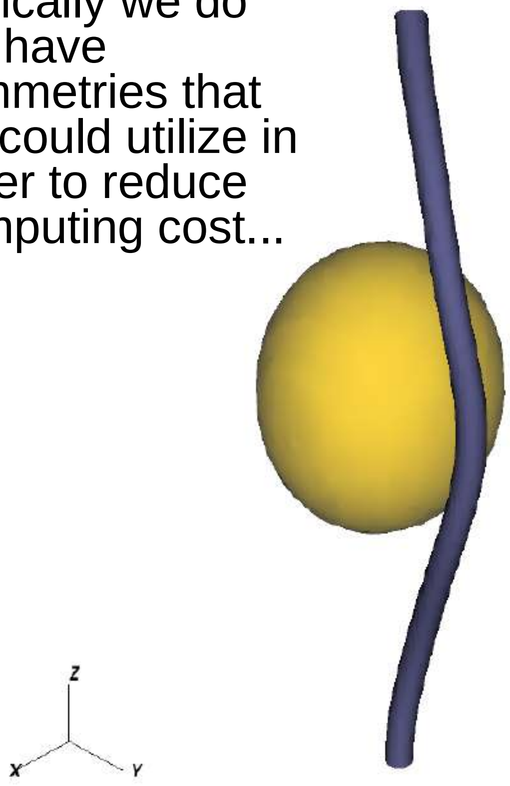
$$\nu(\boldsymbol{r},t) = \sum_{E_n<E_c} u_{n,\uparrow}(\boldsymbol{r},t)v^*_{n,\downarrow}(\boldsymbol{r},t), \qquad \boldsymbol{j}_\sigma(\boldsymbol{r},t) = \sum_{E_n<E_c} \mathrm{Im}[v^*_{n,\sigma}(\boldsymbol{r},t)\nabla v_{n,\sigma}(\boldsymbol{r},t)],$$

a lot of nonlinear coupled 3D
Partial Differential Equations
(in practice 10^5 - 10^6)

Typically we do not have symmetries that we could utilize in order to reduce computing cost...



Typically we do not have symmetries that we could utilize in order to reduce computing cost...



Present computing capabilities:

- full 3D (unconstrained) superfluid dynamics
- Volume ~ $(100\text{fm})^3$
- number of particles ~10^4-10^5
- Time trajectory length ~10^4-10^5 fm/c

  (10^{-20}-10^{-19}s)

Piz Daint @ Swiss National Supercomputing Centre (Switzerland) - presently the fastest European computing system. Access is granted thanks to PRACE.

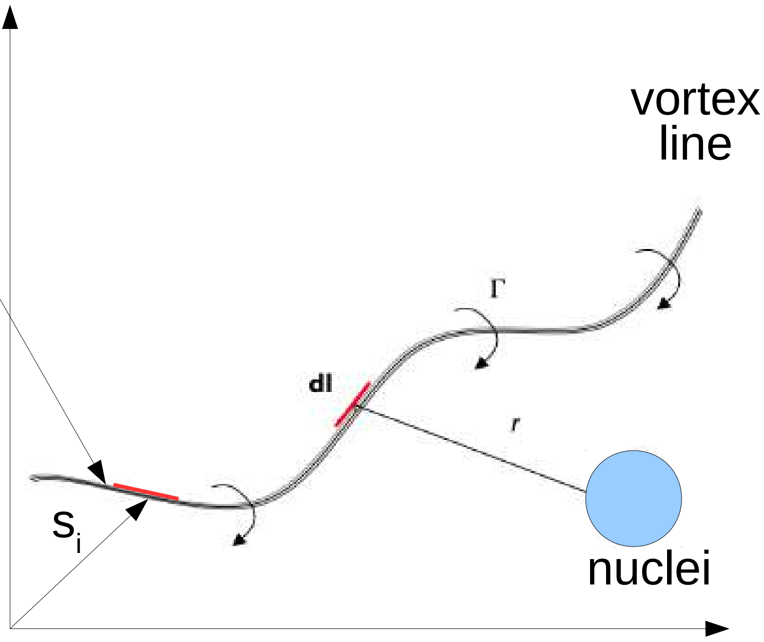
Summit @ Oak Ridge National Laboratory (USA) - presently the fastest world computing system. Access is granted thanks to INCITE grant.

Tsubame3.0 @ Global Scientific Information and Computing Center, Tokyo Institute of Technology (Japan)

Okeanos @ Interdisciplinary Centre for Mathematical and Computational Modelling (Poland)

Vortex Filament Model

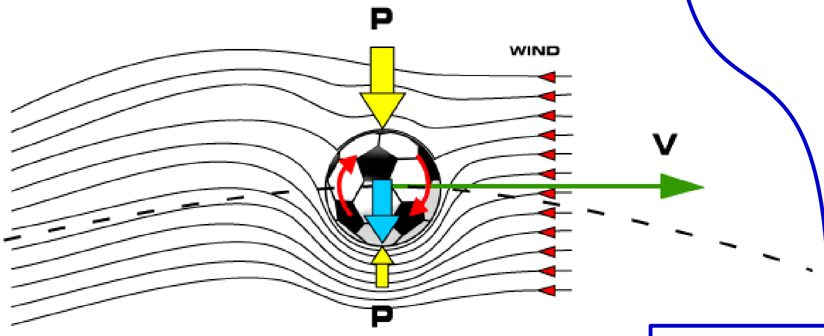
- *Each filament of the vortex line generates rotational flow around it,*
- *The total flow at arbitrary position can be calculated by means of Biot-Savart,*



<u>Equation of motion for the vortex line:</u>

Balance of forces (mass of vortex negligible):

$$\underbrace{\kappa\rho_s \hat{\boldsymbol{t}}\times(\dot{\boldsymbol{s}}-\boldsymbol{v}_{ind}-\boldsymbol{v}_{ext})}_{\text{Magnus force}}+\boldsymbol{f}^{VN}+\boldsymbol{f}^{D}=0$$



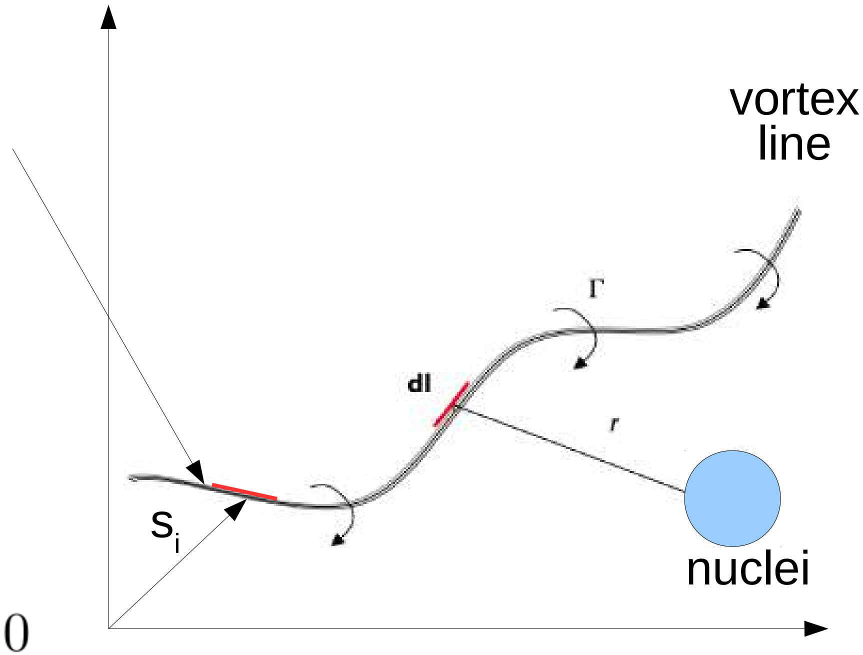
Vortex – nucleus interaction

“Dissipation” force

Example: $\boldsymbol{f}^D = -\eta\dot{\boldsymbol{s}}$

Vortex Filament Model (VFM)

- *Each filament of the vortex line generates rotational flow around it,*
- *The total flow at arbitrary position can be calculated by means of Biot-Savart,*



Equation of motion for the vortex line:

Balance of forces (mass of vortex negligible):

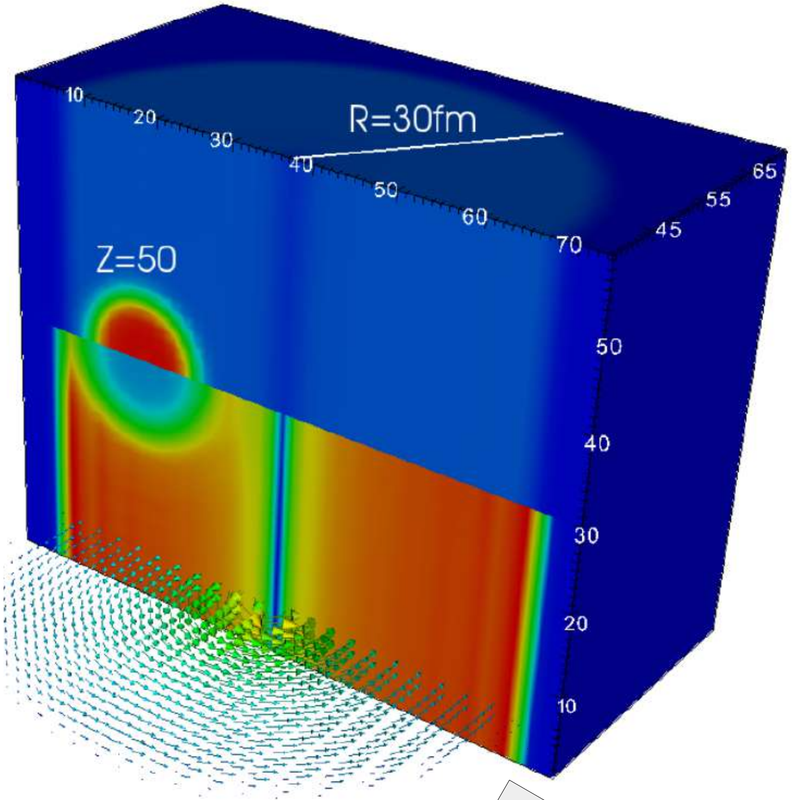
$$\kappa\rho_s\hat{\boldsymbol{t}}\times(\dot{\boldsymbol{s}}-\boldsymbol{v}_{ind}-\boldsymbol{v}_{ext})+\boldsymbol{f}^{VN}+\boldsymbol{f}^{D}=0$$

Our aim:

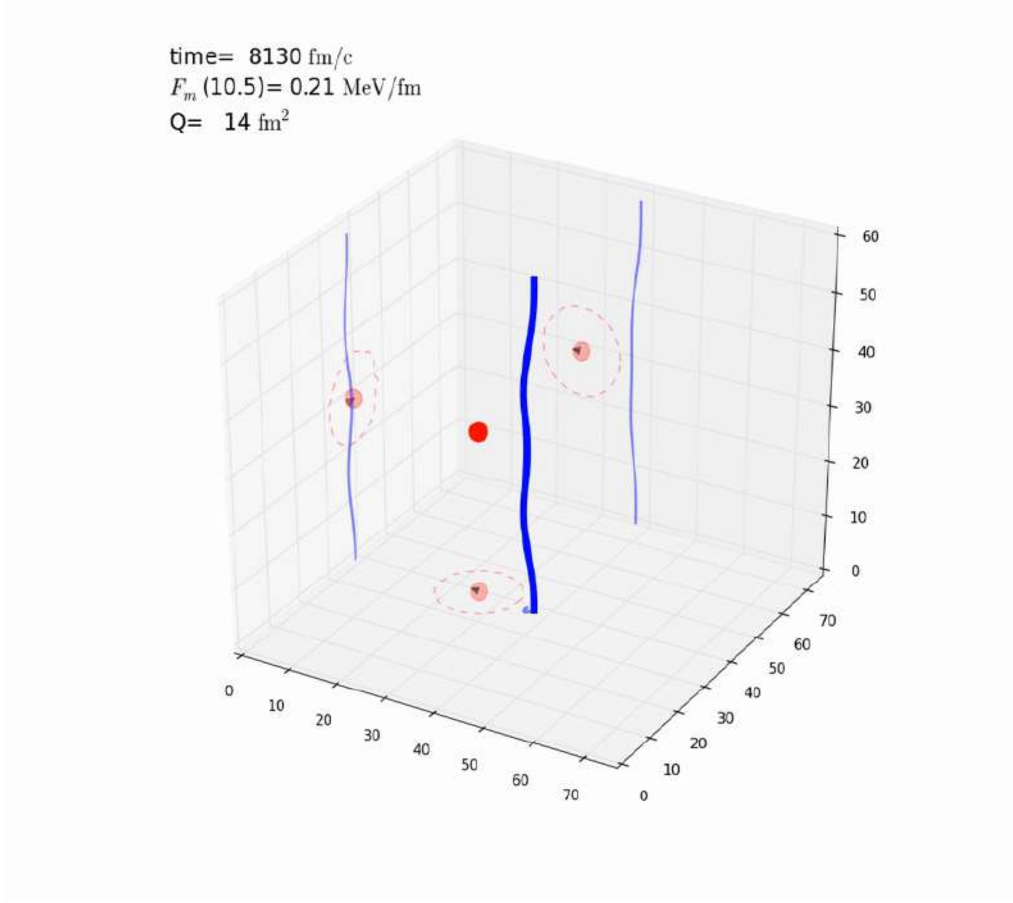
Construct such VFM that reproduces dynamics seen in microscopic simulations

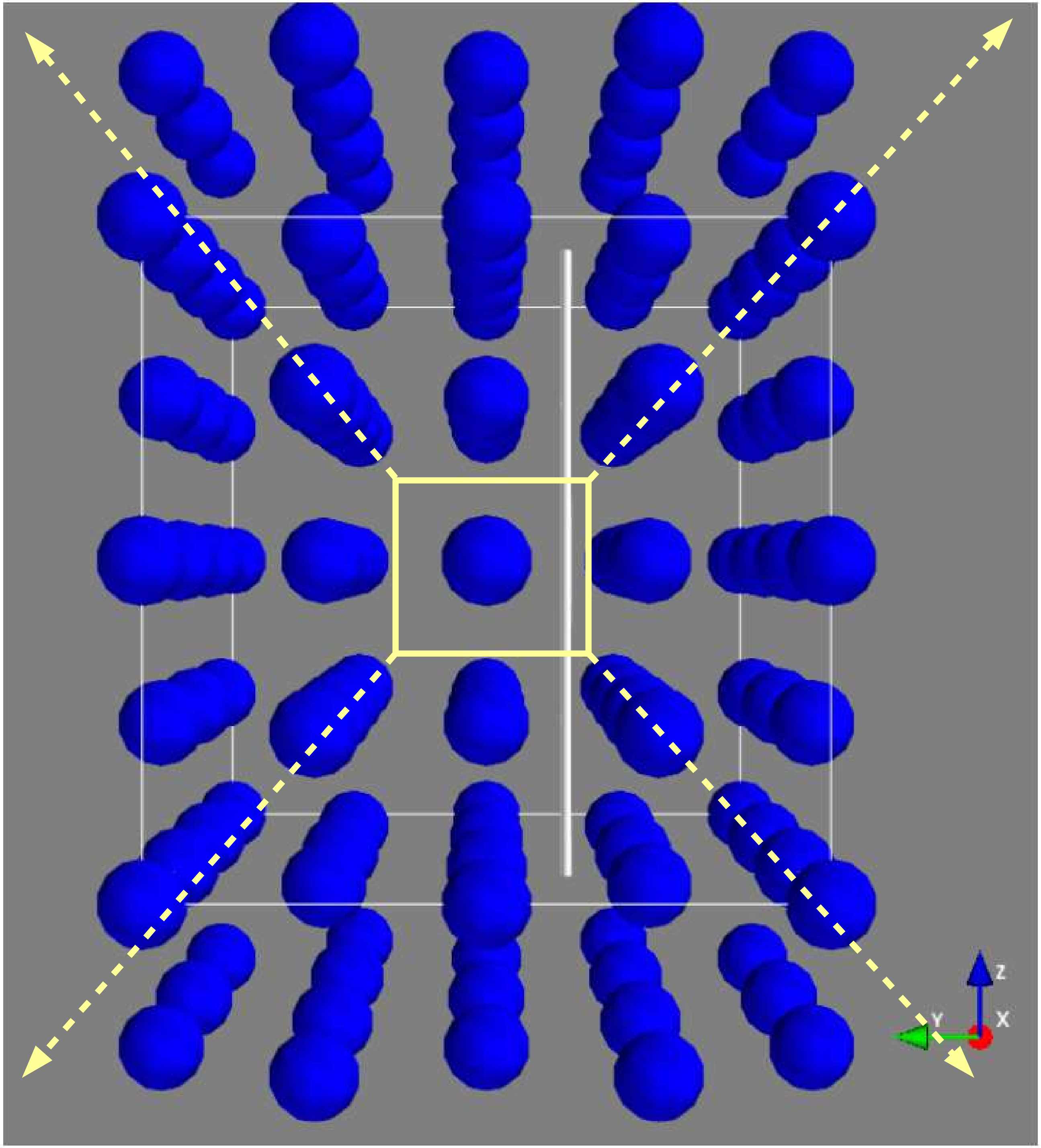
Vortex Filament Model should reproduce it

(at qualitative and quantitative level)



REDUCTION

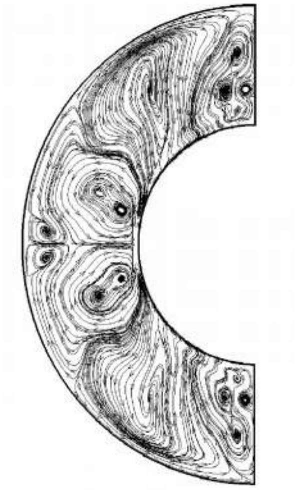




“Fluid element”

feed

Two-fluid hydrodynamics



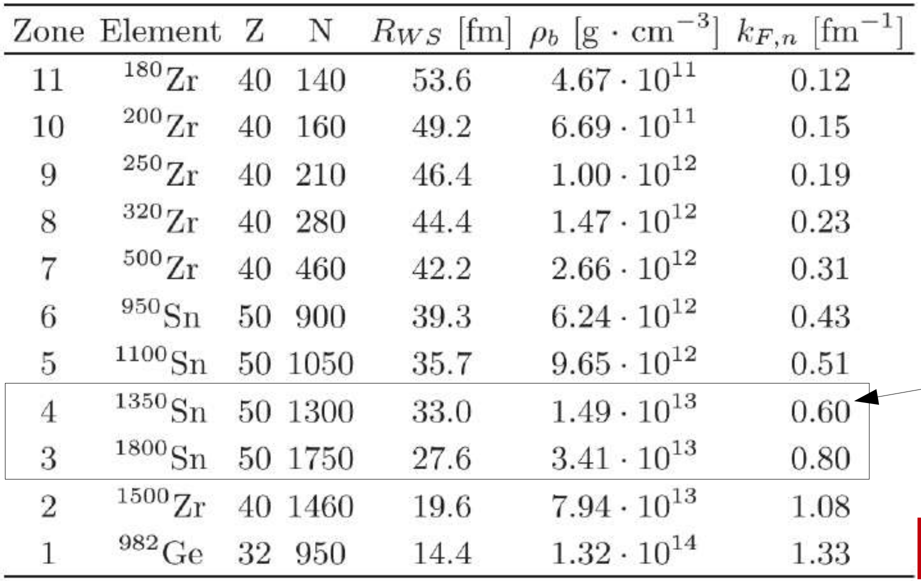
Proof of concept: *extraction of vortex-nucleus force*

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

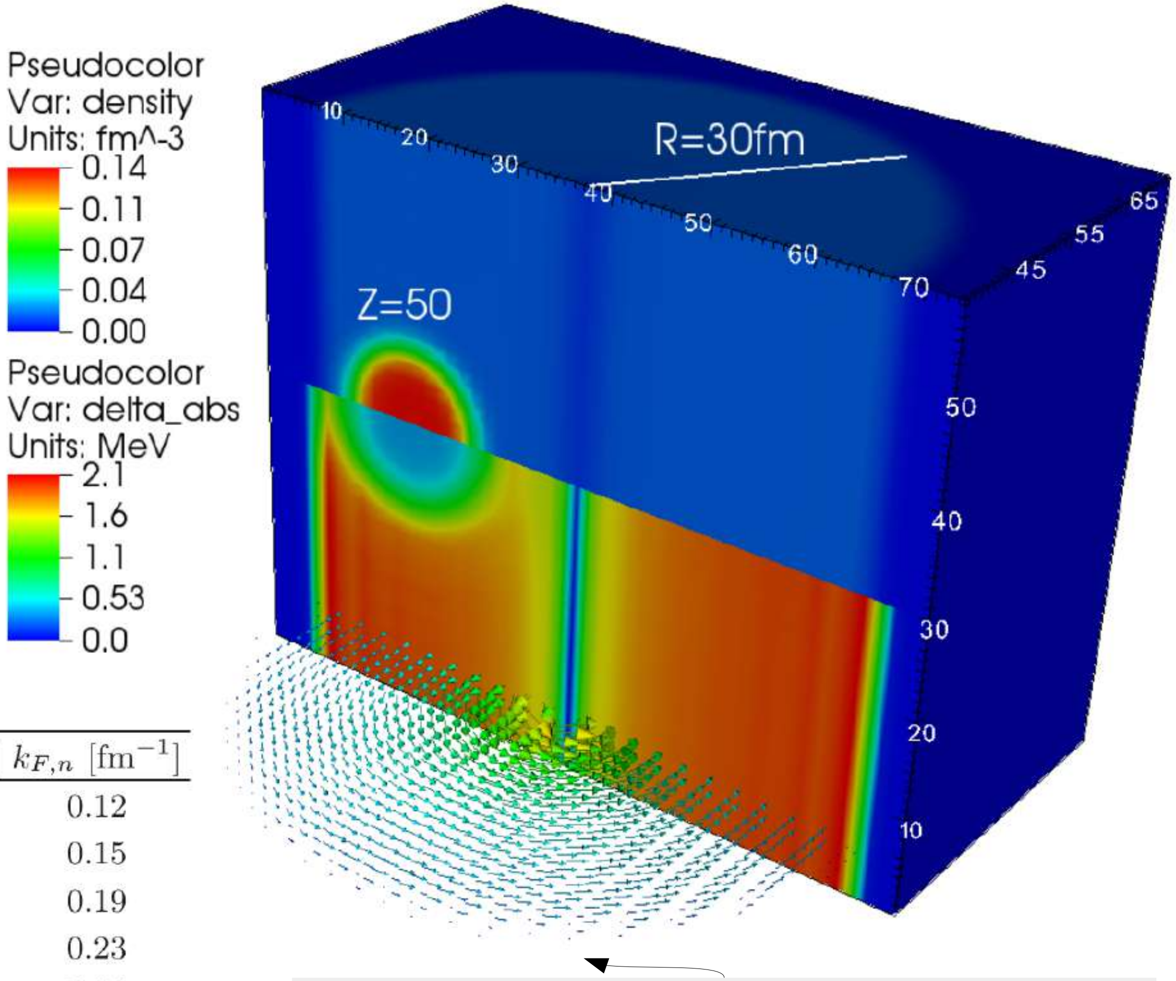
Self-consistent solution of static problem with constraints:

- fixed center of mass of protons
- nonzero total angular momentum of neutrons

J. Negele and D. Vautherin,
Nucl. Phys. A 207, 298 (1973)

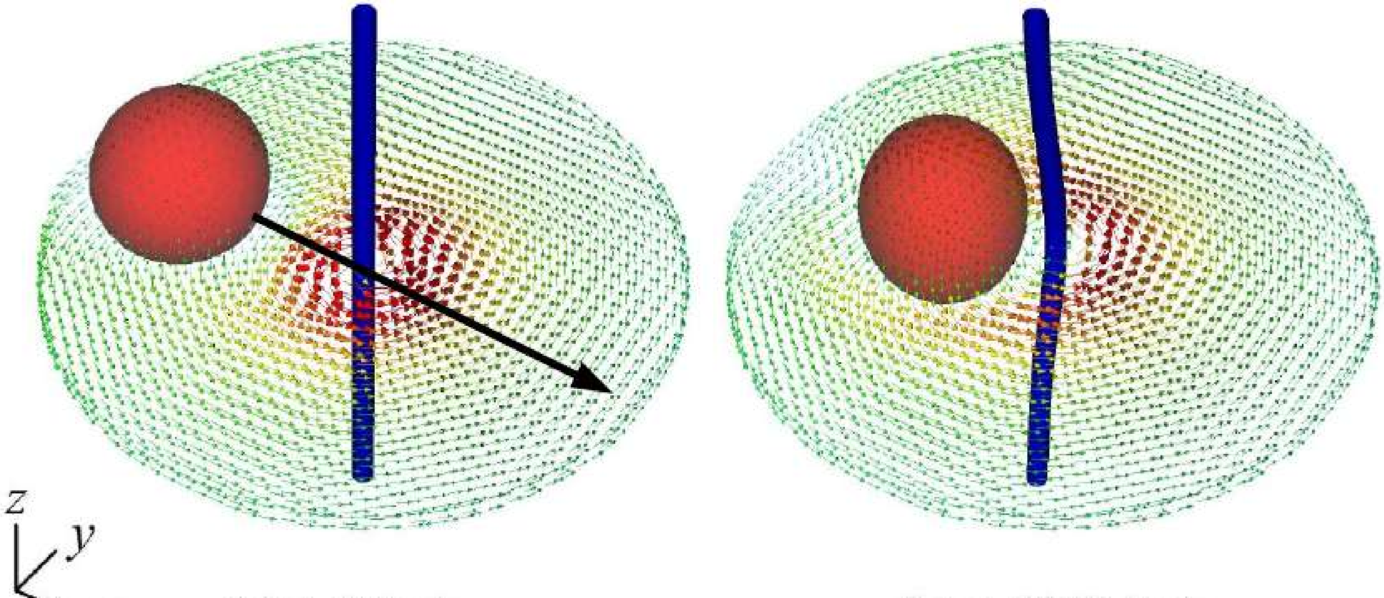


Zone	Element	Z	N	R_{WS} [fm]	ρ_b [$\mathrm{g \cdot cm^{-3}}$]	$k_{F,n}$ [$\mathrm{fm^{-1}}$]
11	^{180}Zr	40	140	53.6	$4.67 \cdot 10^{11}$	0.12
10	^{200}Zr	40	160	49.2	$6.69 \cdot 10^{11}$	0.15
9	^{250}Zr	40	210	46.4	$1.00 \cdot 10^{12}$	0.19
8	^{320}Zr	40	280	44.4	$1.47 \cdot 10^{12}$	0.23
7	^{500}Zr	40	460	42.2	$2.66 \cdot 10^{12}$	0.31
6	^{950}Sn	50	900	39.3	$6.24 \cdot 10^{12}$	0.43
5	^{1100}Sn	50	1050	35.7	$9.65 \cdot 10^{12}$	0.51
4	^{1350}Sn	50	1300	33.0	$1.49 \cdot 10^{13}$	0.60
3	^{1800}Sn	50	1750	27.6	$3.41 \cdot 10^{13}$	0.80
2	^{1500}Zr	40	1460	19.6	$7.94 \cdot 10^{13}$	1.08
1	^{982}Ge	32	950	14.4	$1.32 \cdot 10^{14}$	1.33



Lowest energy state (constrained) for Z=50 and N=2,530 confined in tube of radius R=30fm

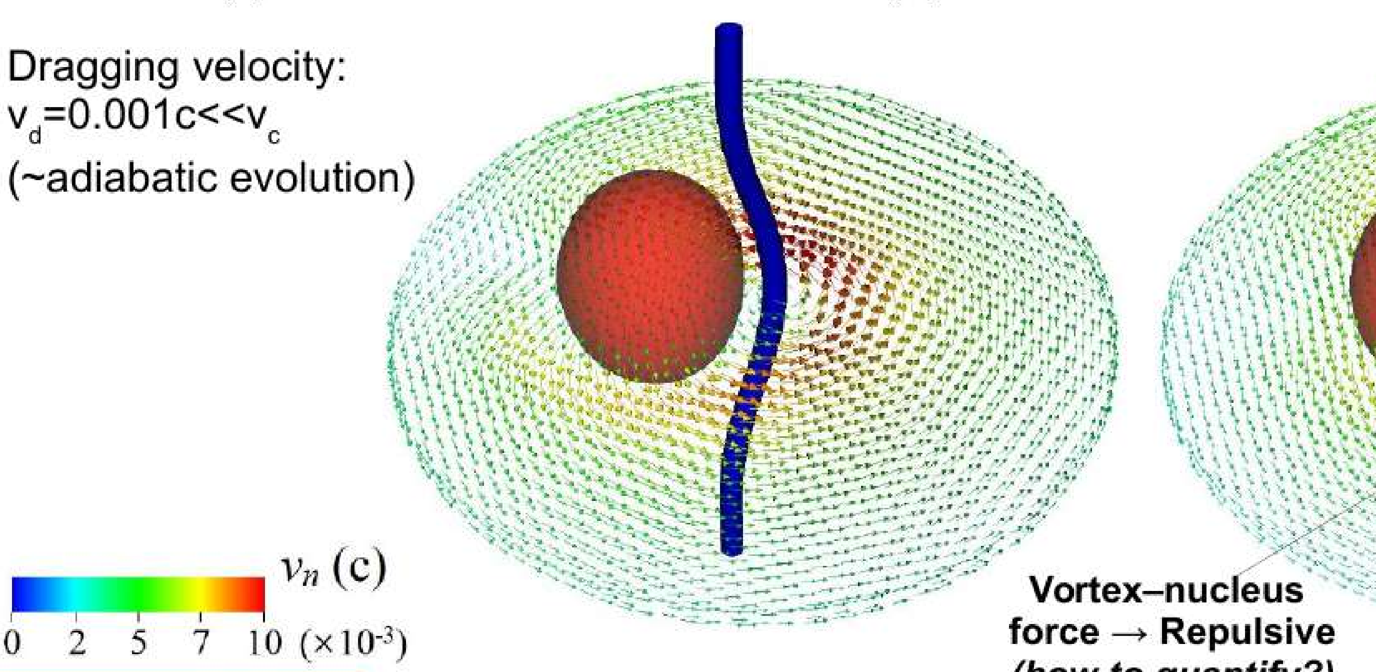
$(n = 0.031\ \mathrm{fm}^{-3})$



(a) t=0 fm/c (b) t=8000 fm/c

We drag the impurity along a line and observe the vortex response...

Dragging velocity:
$v_d=0.001c \ll v_c$
(~adiabatic evolution)



Vortex–nucleus force → Repulsive
(how to quantify?)

(c) t=10000 fm/c (d) t=12000 fm/c

Figures from:
JPS Conf. Proc. 14, 010807 (2017)

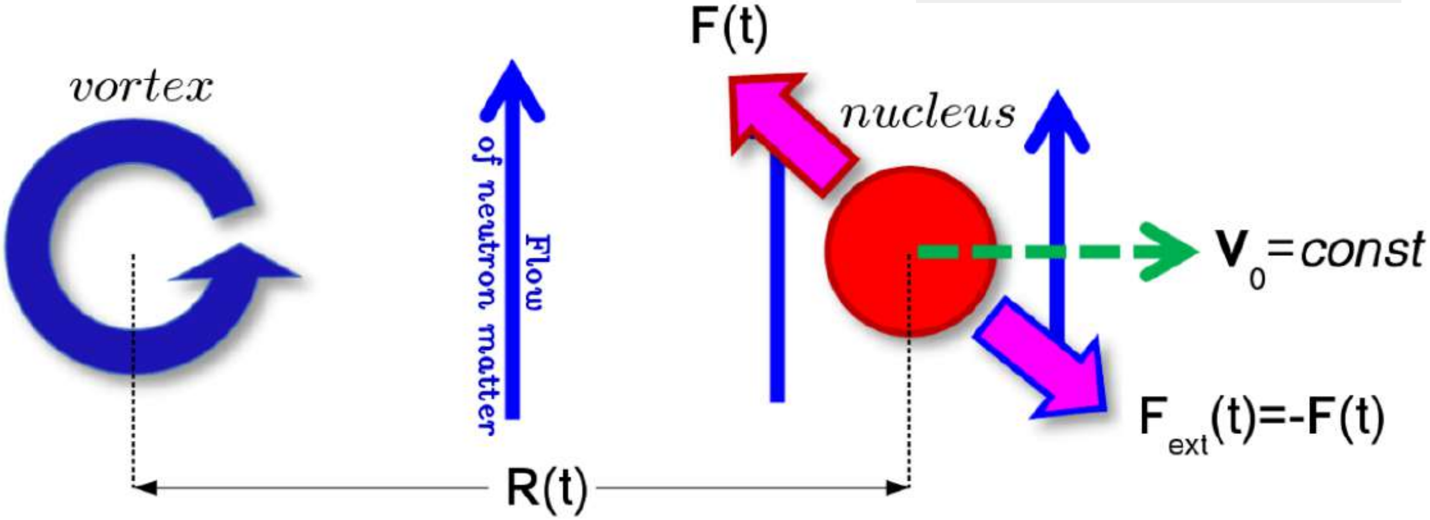
We use Newton's 3rd law and extract the force from motion of the nucleus.....

Consider Eq. of motion for impurity:

Vortex-nucleus interaction

$$M\frac{d\boldsymbol{v}}{dt} = \boldsymbol{F}_{\text{tot.}} = \boldsymbol{F} + \boldsymbol{F}_{\text{ext.}} = 0 \Leftrightarrow \boldsymbol{v} = \text{const}$$

Uniform electric field that we control



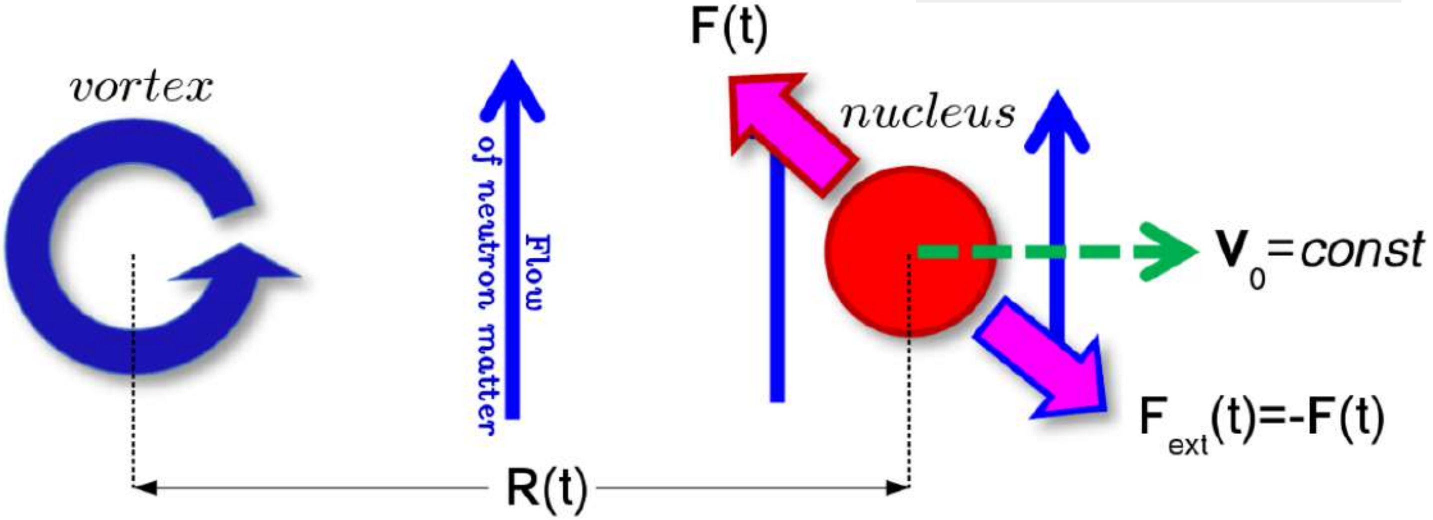
We use Newton's 3rd law and extract the force from motion of the nucleus.....

Consider Eq. of motion for impurity:

$$M\frac{d\boldsymbol{v}}{dt} = \boldsymbol{F}_{\text{tot.}} = \boldsymbol{F} + \boldsymbol{F}_{\text{ext.}} = 0 \Leftrightarrow \boldsymbol{v} = \text{const}$$

Vortex-nucleus interaction

Uniform electric field that we control



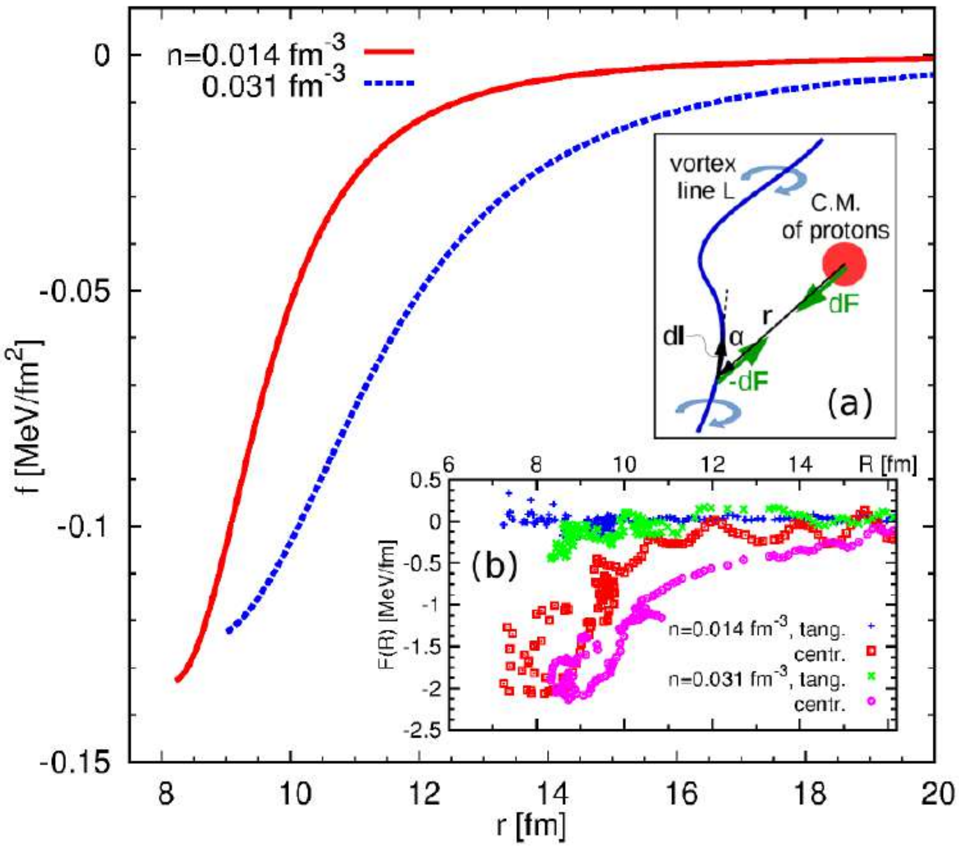
$$\boxed{\boldsymbol{F}(R)}$$

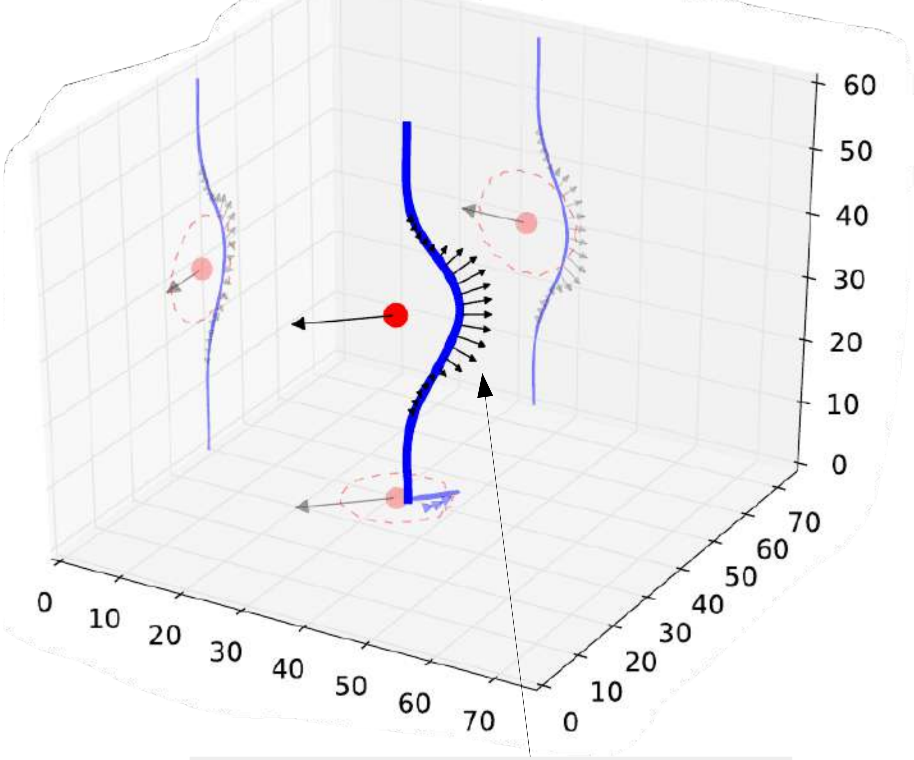
We construct F_{ext} dynamically:

$$\boldsymbol{F}_{\text{ext}}(t+\Delta t) = \boldsymbol{F}_{\text{ext}}(t) - \alpha\left[\boldsymbol{v}(t) - \boldsymbol{v}_0\right]$$

Force per unit length

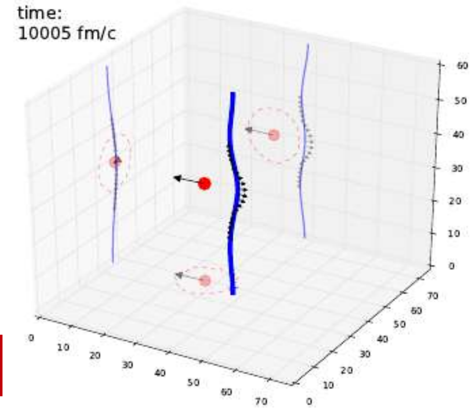
Phys. Rev. Lett. 117, 232701 (2016)



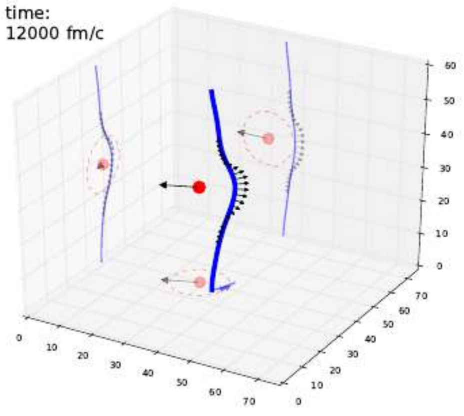


Only part close to nucleus surface contributes...

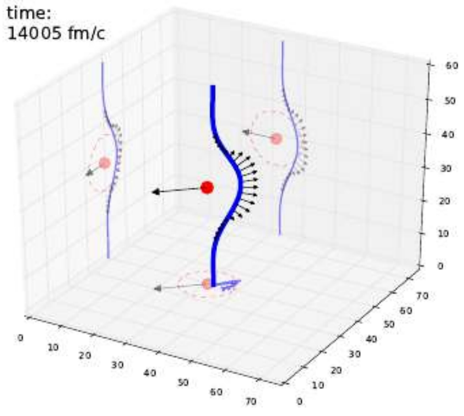
time: 10005 fm/c



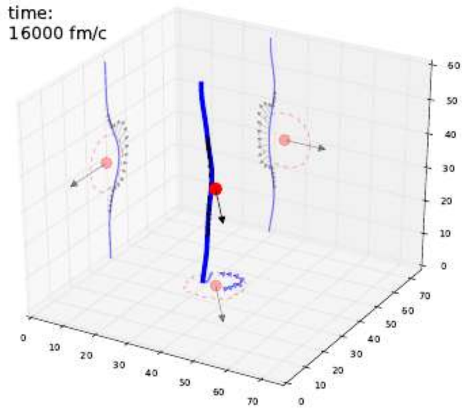
time: 12000 fm/c



time: 14005 fm/c

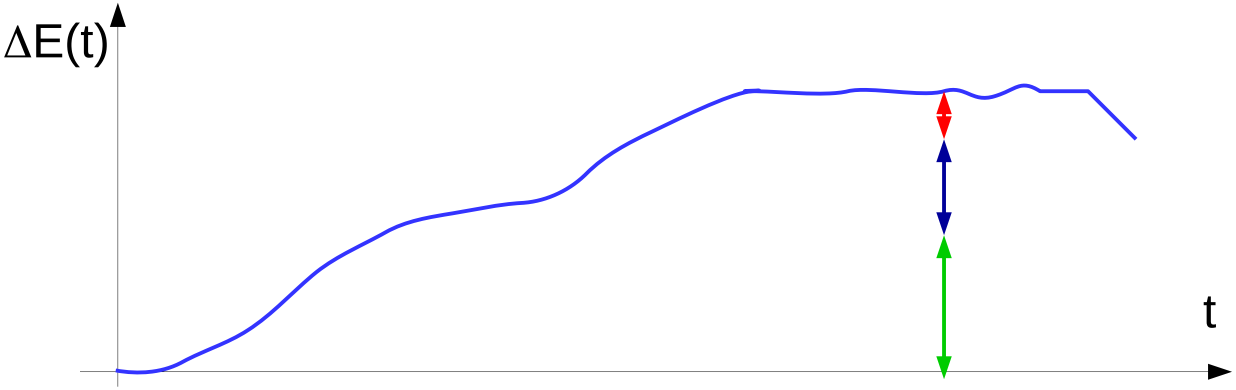


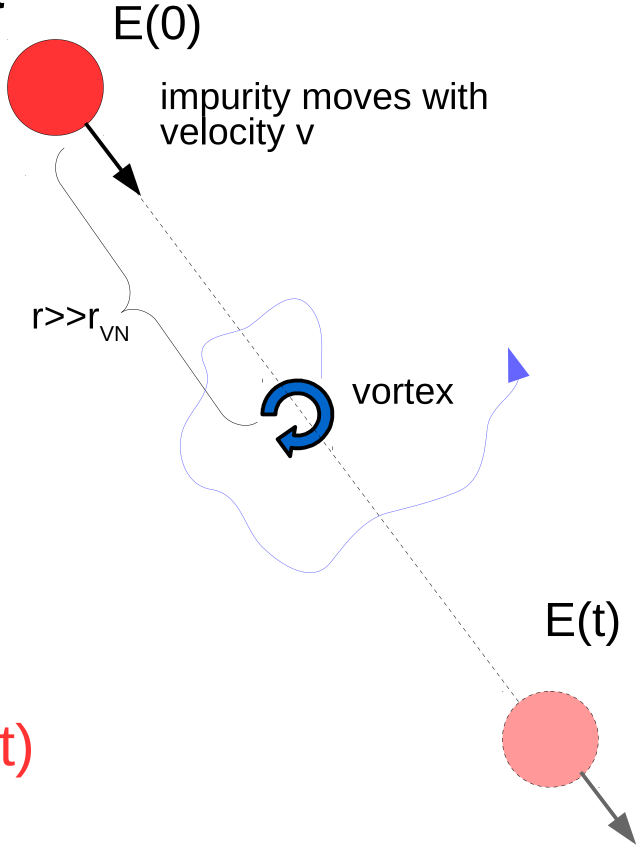
time: 16000 fm/c



Extraction of the dissipation force – idea

- drag impurity with various velocities...
- look at excitation energy...

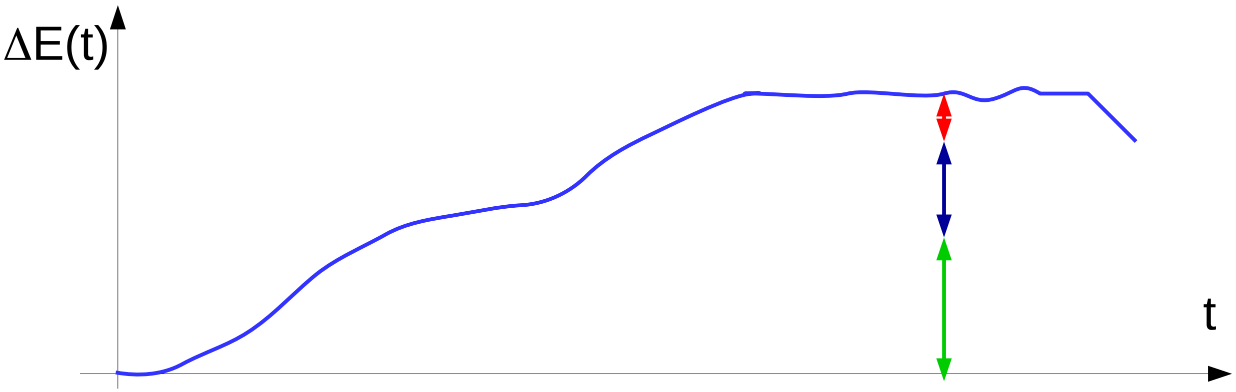


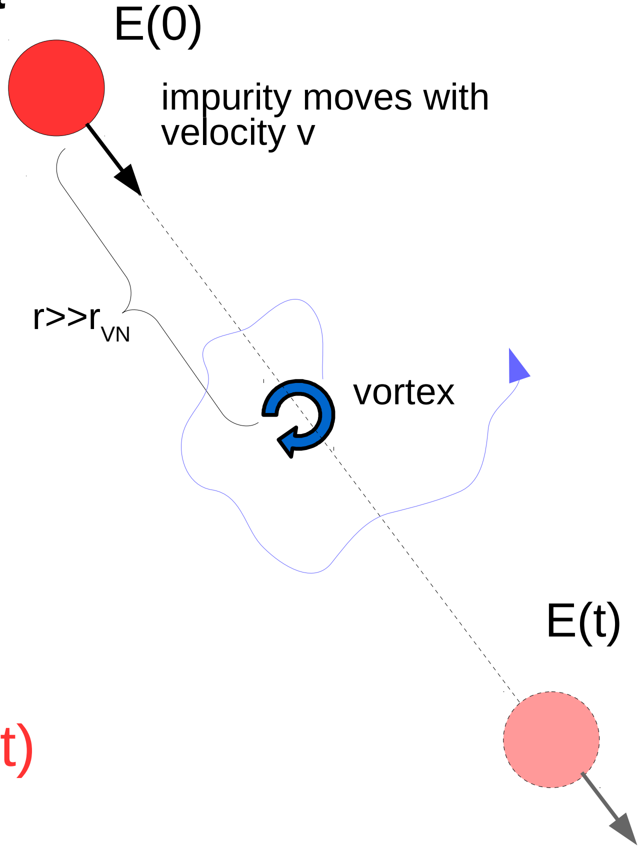


$$\Delta E(t) = \Delta E_{\mathrm{vortex}}(t) + \Delta E_{\mathrm{compressible}}(t) + \Delta E_{\mathrm{internal}}(t)$$

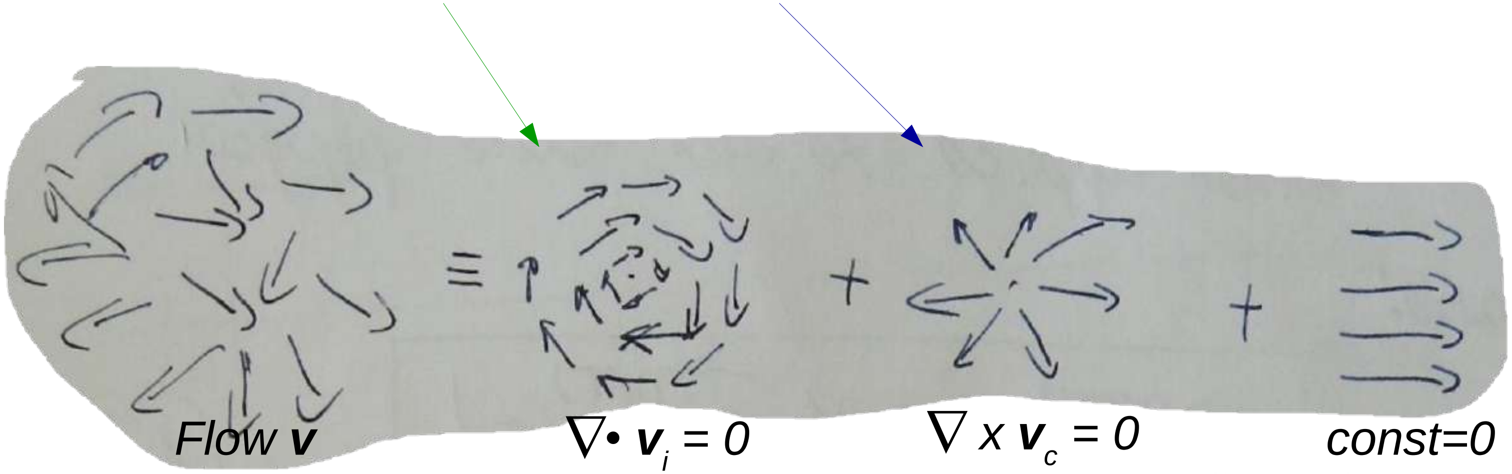
Extraction of the dissipation force – idea

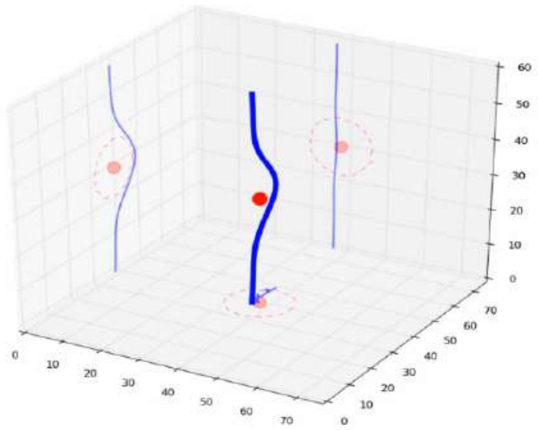
- drag impurity with various velocities...
- look at excitation energy...





$$\Delta E(t) = \Delta E_{vortex}(t) + \Delta E_{compressible}(t) + \Delta E_{internal}(t)$$





$$\boldsymbol{f}^D = -\eta_1(\dot{\boldsymbol{s}} - \boldsymbol{v}_{\text{nuclei}}) - \eta_2(\dot{\boldsymbol{s}} - \boldsymbol{v}_{\text{ext}})$$

Use “ansatz” here for the dissipation force, and try to reproduce $W_d(t)$...

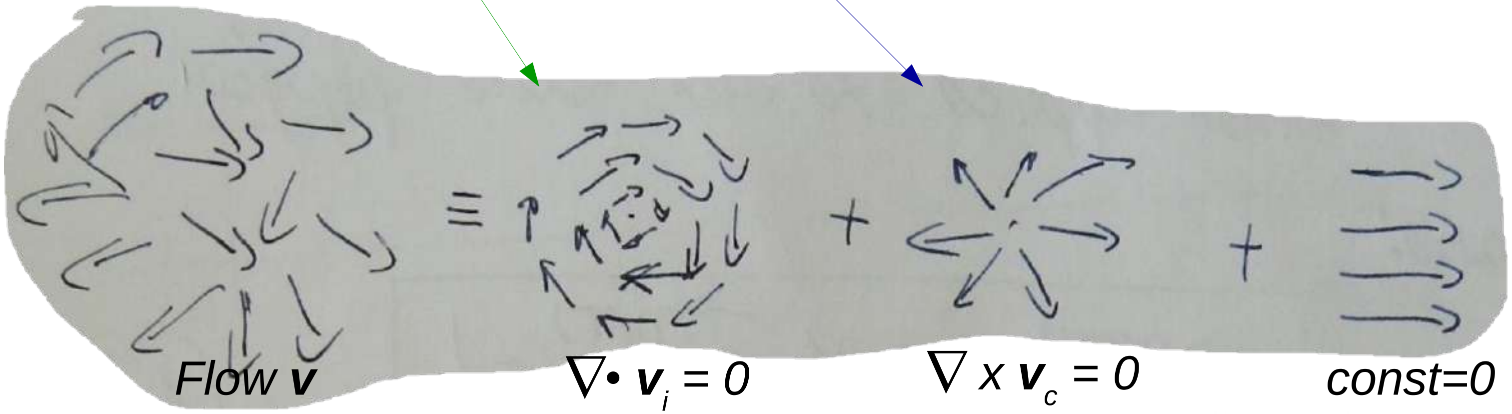
$$W_d(t) = \int_{\mathcal{L}} \left[\int_0^t \boldsymbol{f}^D(t') \cdot \dot{\boldsymbol{s}}_l(t')\, dt' \right] dl$$

Known from simulations...

Reflected by the vortex line deformation in VFM

$W_d(t)$ = Dissipated energy (from point of view of VFM)

$$\Delta E(t) = \Delta E_{\text{vortex}}(t) + \Delta E_{\text{compressible}}(t) + \Delta E_{\text{internal}}(t)$$

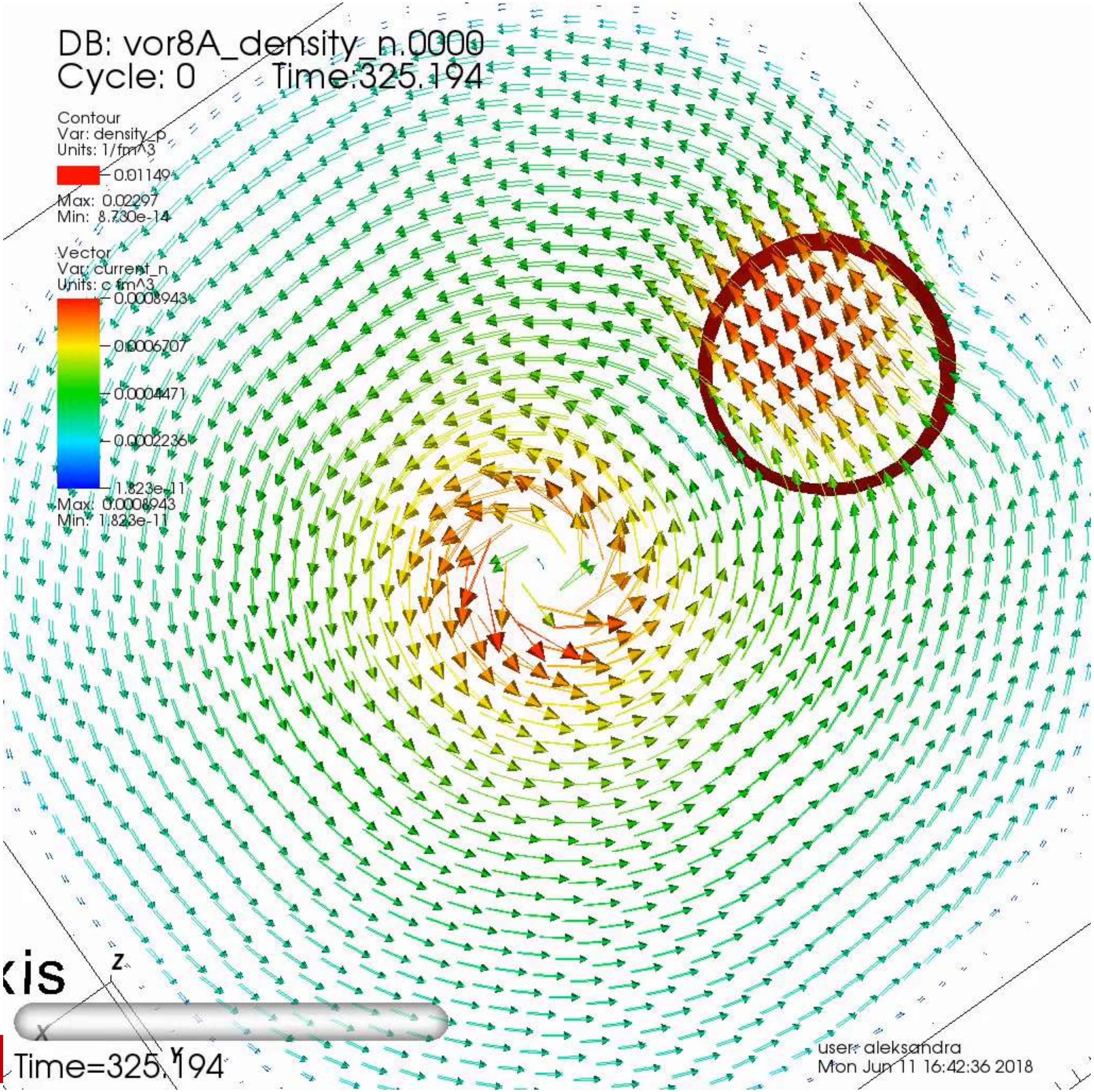


*Flow **v***

$\nabla \cdot \boldsymbol{v}_i = 0$

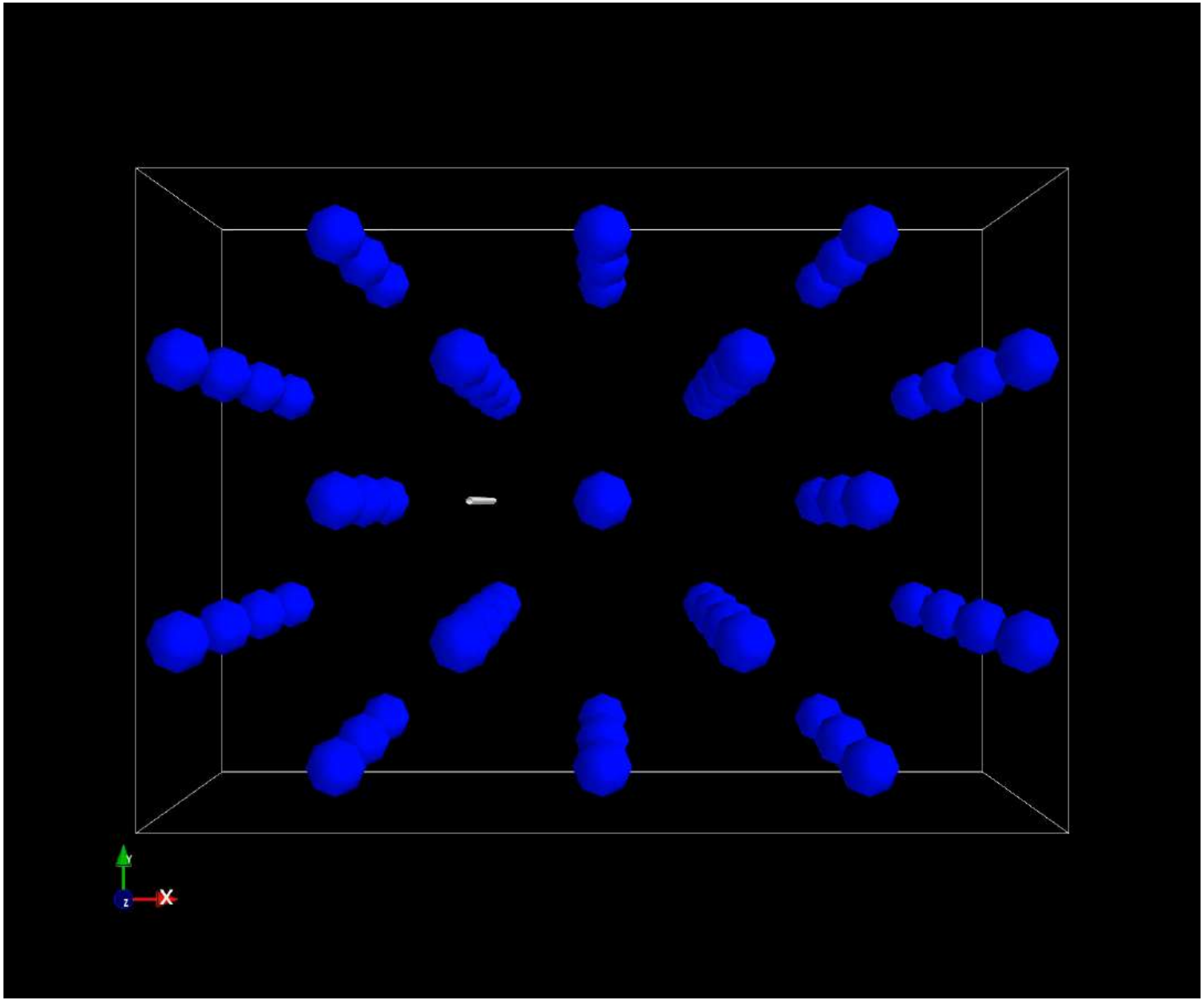
$\nabla \times \boldsymbol{v}_c = 0$

const=0



(movie
created by
A. Olejak)

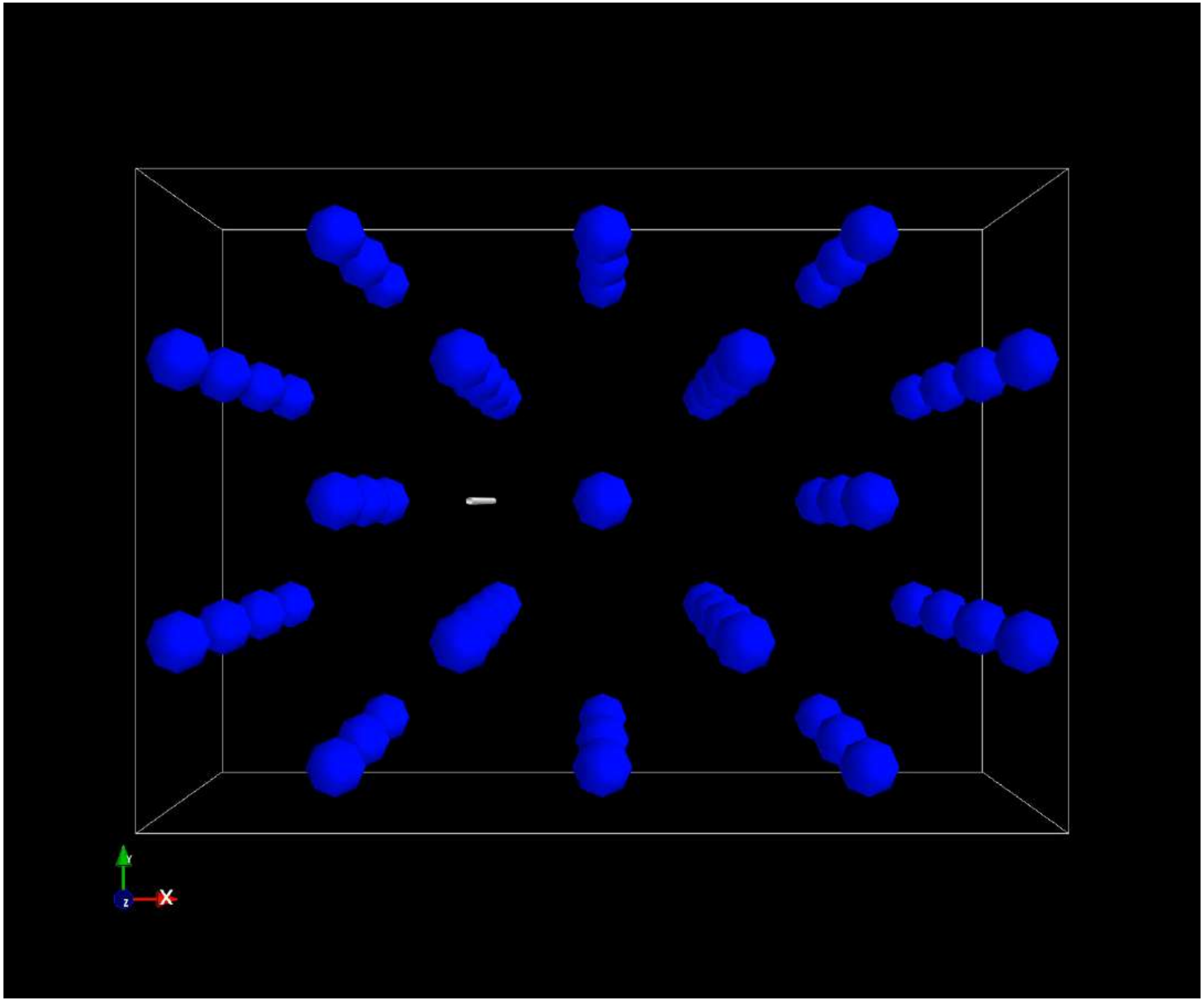
Put all elements together...



→ $V_{ext} < v_{crit}$

From diploma thesis of Konrad Kobuszewski, WUT 2018

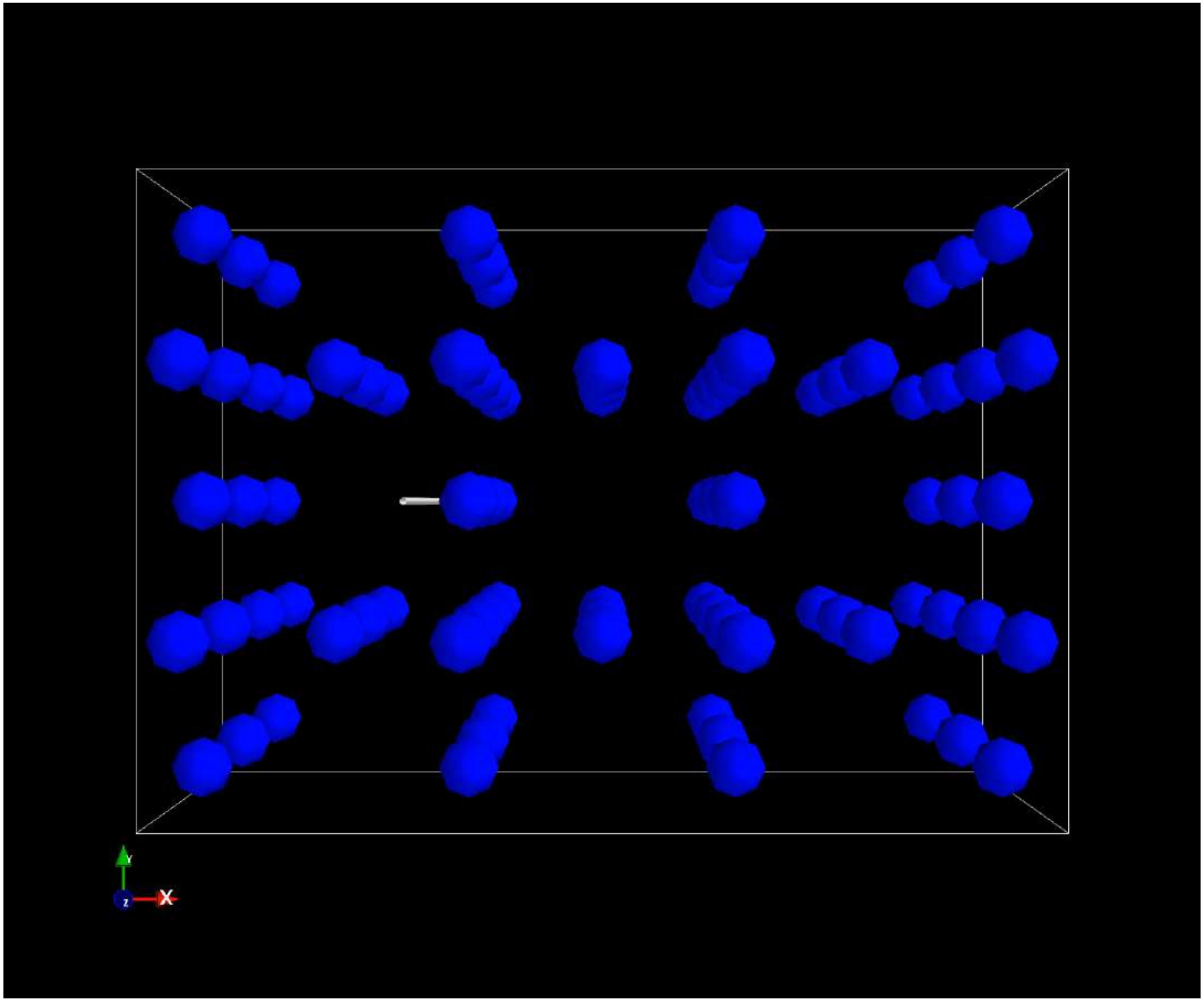
Put all elements together...



$\longrightarrow$ $V_{ext} > v_{crit}$

From diploma thesis of Konrad Kobuszewski, WUT 2018

Put all elements together...



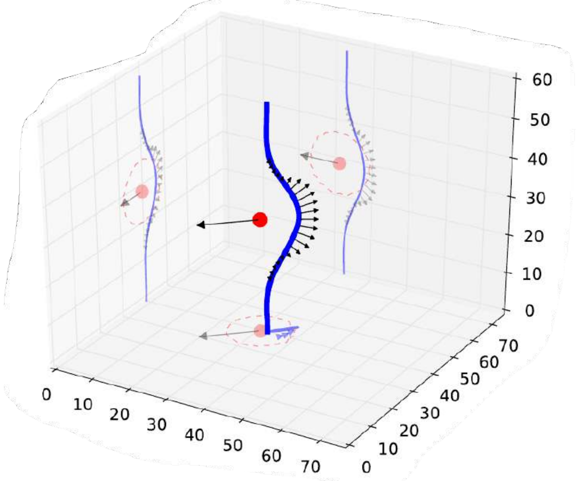
→ $V_{ext} \approx v_{crit}$

From diploma thesis of Konrad Kobuszewski, WUT 2018

CONCLUSIONS

- DFT – route for unified description of static and dynamic properties of large Fermi systems

- TDDFT can be used as a source of microscopic input for pulsar glitch models
  - *We have defined propagation scheme:*
    TDDFT → VFM → Hydro
  - *Proof of concept - yes*



- We plan to execute camping of systematic simulations (scan over densities with modern BSk functional)

- TDDFT has also been applied to other systems
  - *Dynamics in ultracold atoms* (vortex dynamics, quantum turbulence, shock waves...)
  - *Dynamics of nuclear systems* (fission, nuclear reactions, relativistic coulomb excitation...)

Thank you