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WASP the wide angle neutron spin echo instrument

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ILL

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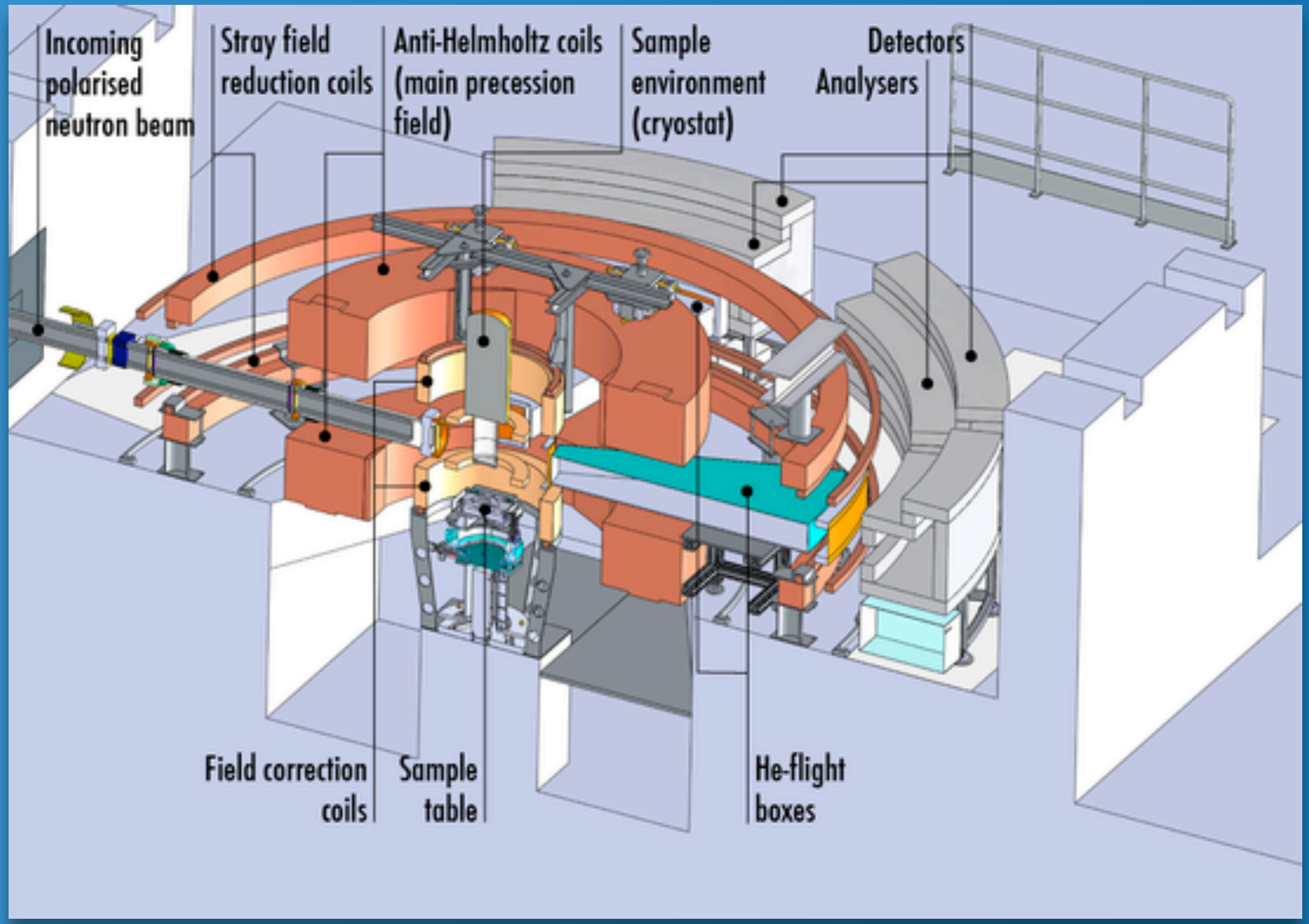


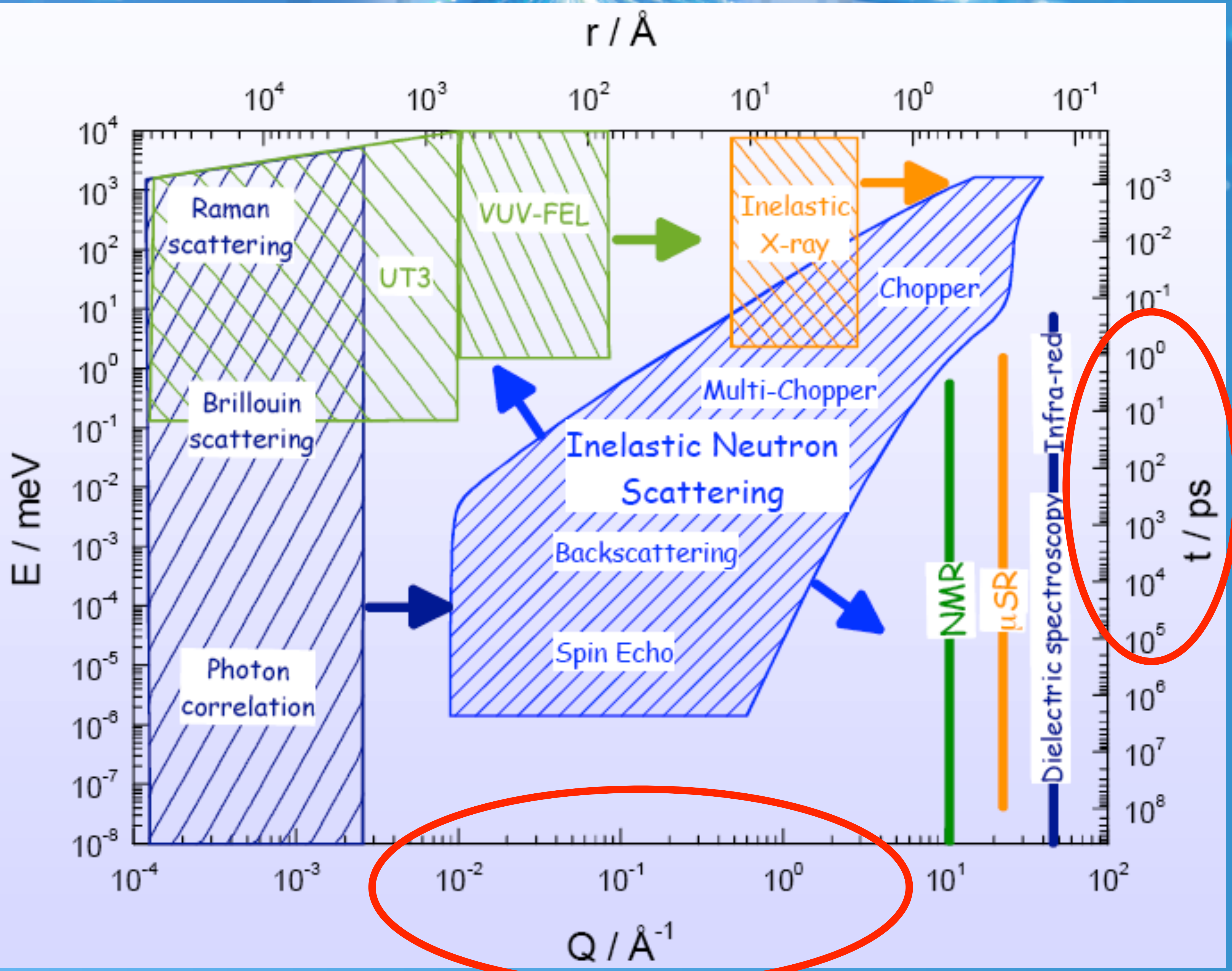
Acknowledgments

Why am here ?

Everything was said the first day:

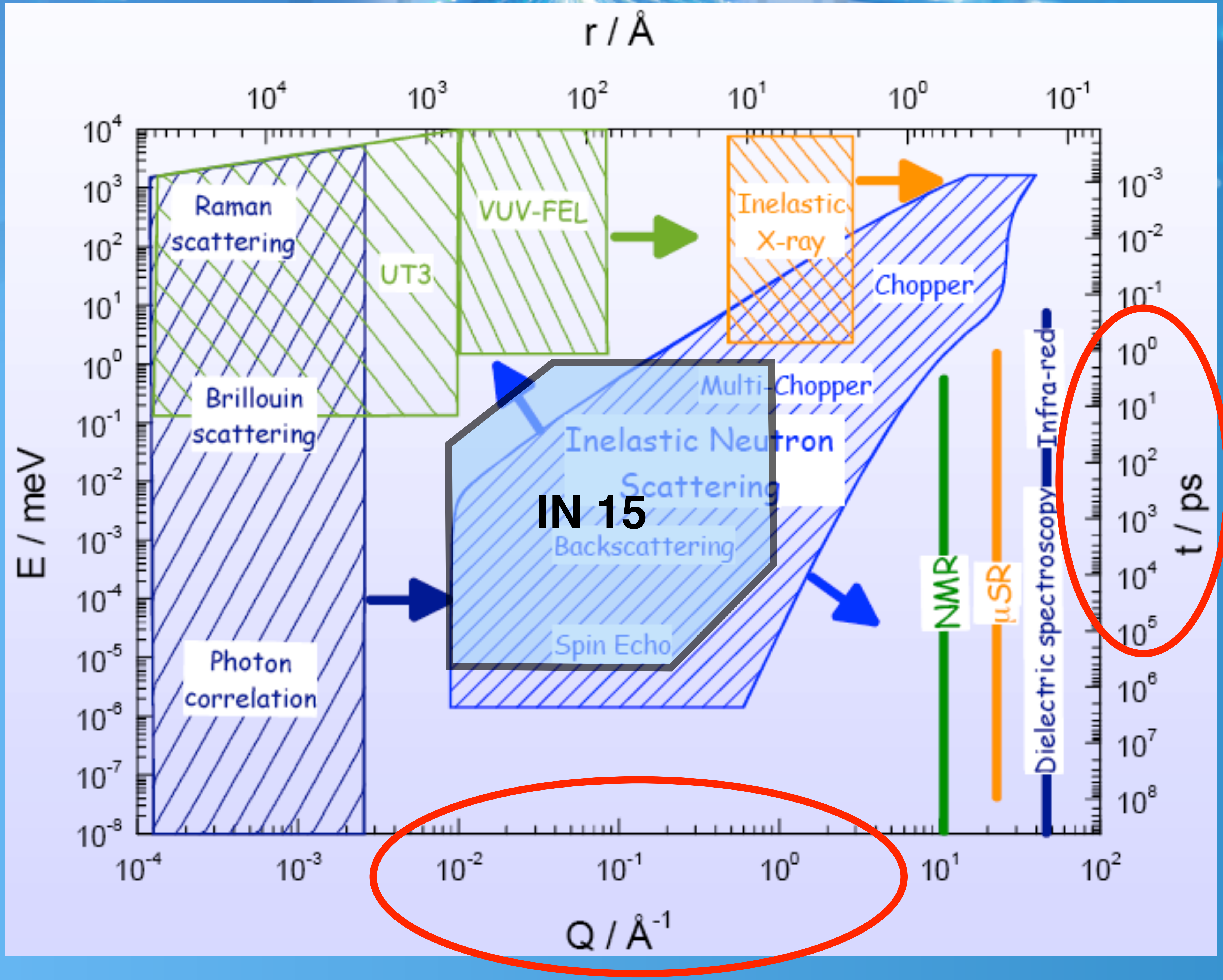
- High resolution techniques with scanning are slow, can we eliminate scanning ? (Martin)
- WASP is ILL's flagship Spin Echo we have the first results (Jacques, Helmut)
- ESS has no NSE 'capability gap' (Andreas)

Why NSE important



- Unmatched Q-t range
- Works in time space not energy space
- Sees difference not sum of coherent and incoherent scattering
- For magnetism XYZ polarisation analysis built in

Why NSE important



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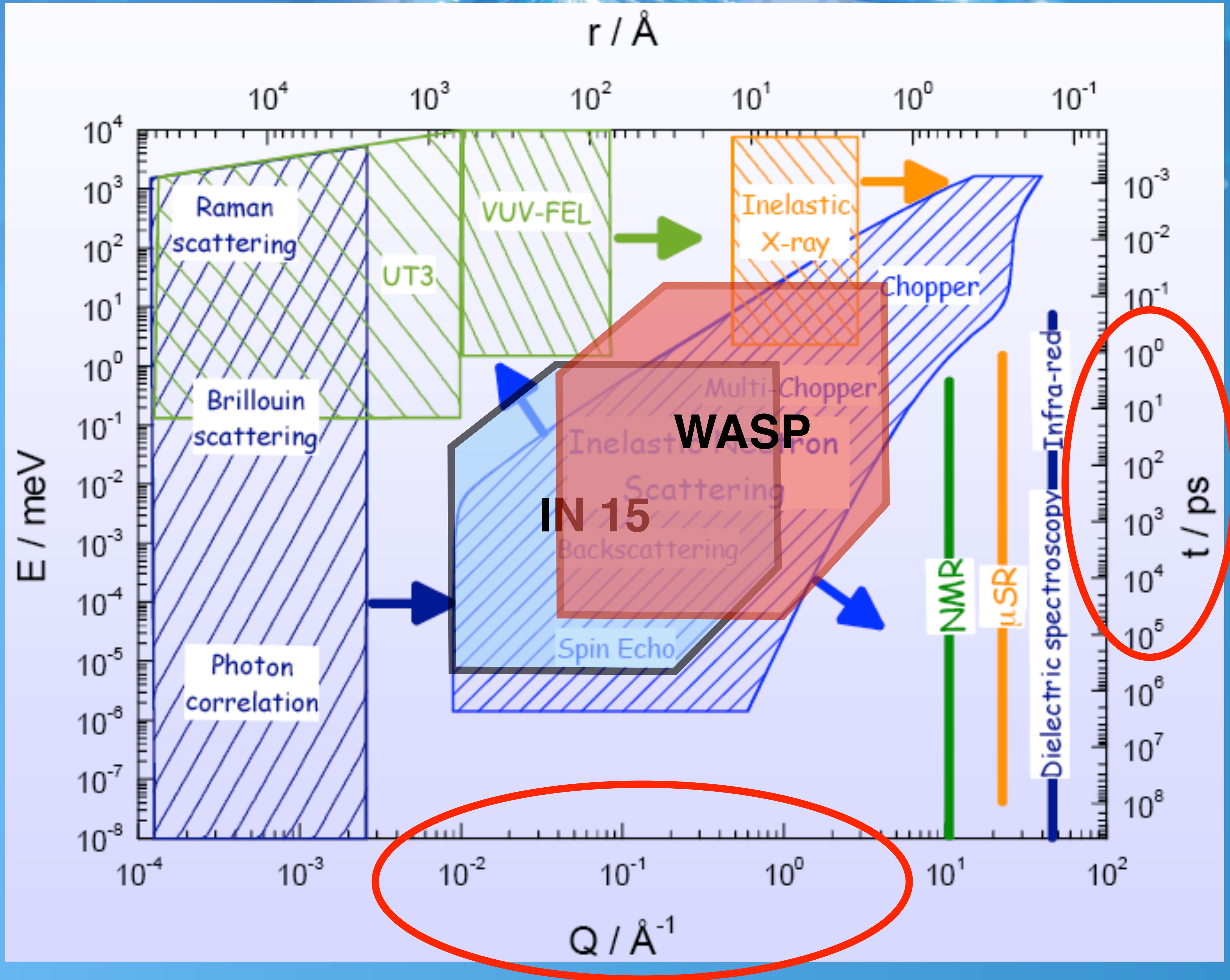
- **IN 15** is optimized for **molecular length scales 0.01-1 Å^{-1}, 5ps-1000 ns**

Why NSE important



- Unmatched Q-t range
- Works in time space not energy space
- Sees difference not sum of coherent and incoherent scattering
- For magnetism XYZ polarisation analysis built in

- **WASP** is optimized for **atomic to molecular length scales 0.1-4 Å^{-1}, 0.2 ps-100 ns**

- **IN 15** is optimized for **molecular length scales 0.01-1 Å^{-1}, 5ps-1000 ns**

Fundamentals of NSE

$$\hbar\omega = m\upsilon'^2/2 - m\upsilon^2/2$$

final velocity

initial velocity

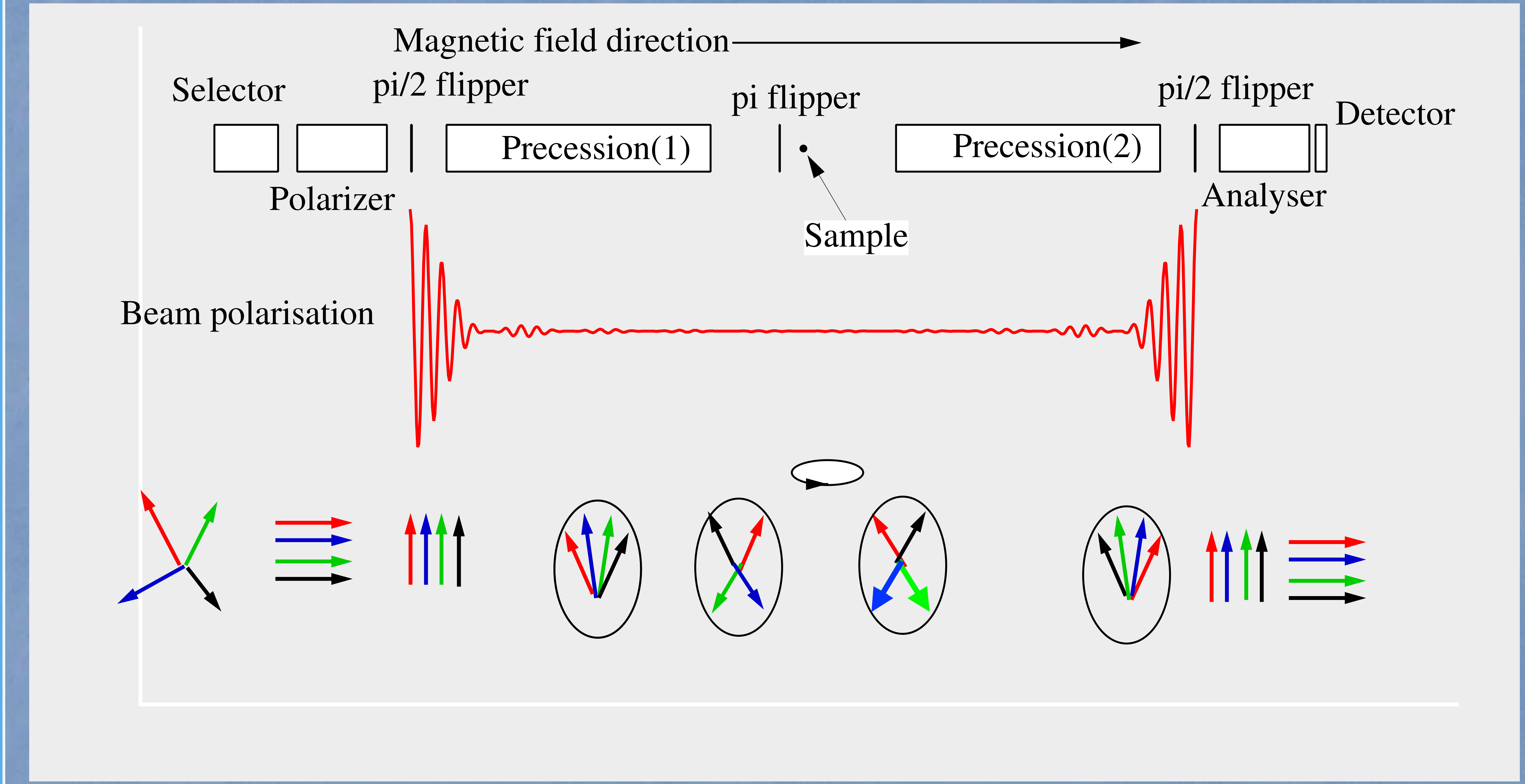
We want to measure the difference
The classical method is defining the final <u>and</u> initial velocity

Defining 2x== throwing away all other neutrons 2x
High resolution== very few neutrons remain ☹☹☹

Can we use all neutrons without defining/monochromatizing ?

Yes ! We will use the neutron spin (Feri Mezei 1972)

NSE basics



$$\omega_L = \gamma_L \cdot B$$

NSE basics

For elastic scattering: $\varphi_{tot} = \frac{\gamma B_1 l_1}{v_1} - \frac{\gamma B_2 l_2}{v_2}$ = 0

For omega energy exchange: $\varphi_{tot} = \frac{\hbar\gamma B l}{m v^3}\omega + o\left(\left(\frac{\omega}{1/2mv^2}\right)^2\right)$

The probability of omega energy exchange: $S(q,\omega)$

The final polarization: $\langle\cos\varphi\rangle = \frac{\int \cos(\frac{\hbar\gamma B l}{m v^3}\omega) S(q,\omega) d\omega}{\int S(q,\omega) d\omega} = S(q,t)$

NSE basics

Echo condition:

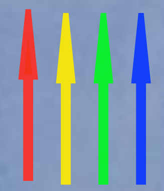
$$\int_{\pi/2}^{\pi} B_1 d\ell = \int_{\pi}^{\pi/2} B_2 d\ell$$

The measured quantity is: S(q,t)/S(q,0)
where

$$t \propto \lambda^3 \int B d\ell$$

For elastic scattering:

$$\varphi_{tot} = \frac{\gamma B_1 l_1}{v_1} - \frac{\gamma B_2 l_2}{v_2} = 0$$



For omega energy exchange:

$$\varphi_{tot} = \frac{\hbar\gamma B l}{m v^3}\omega + o\left(\left(\frac{\omega}{1/2mv^2}\right)^2\right)$$

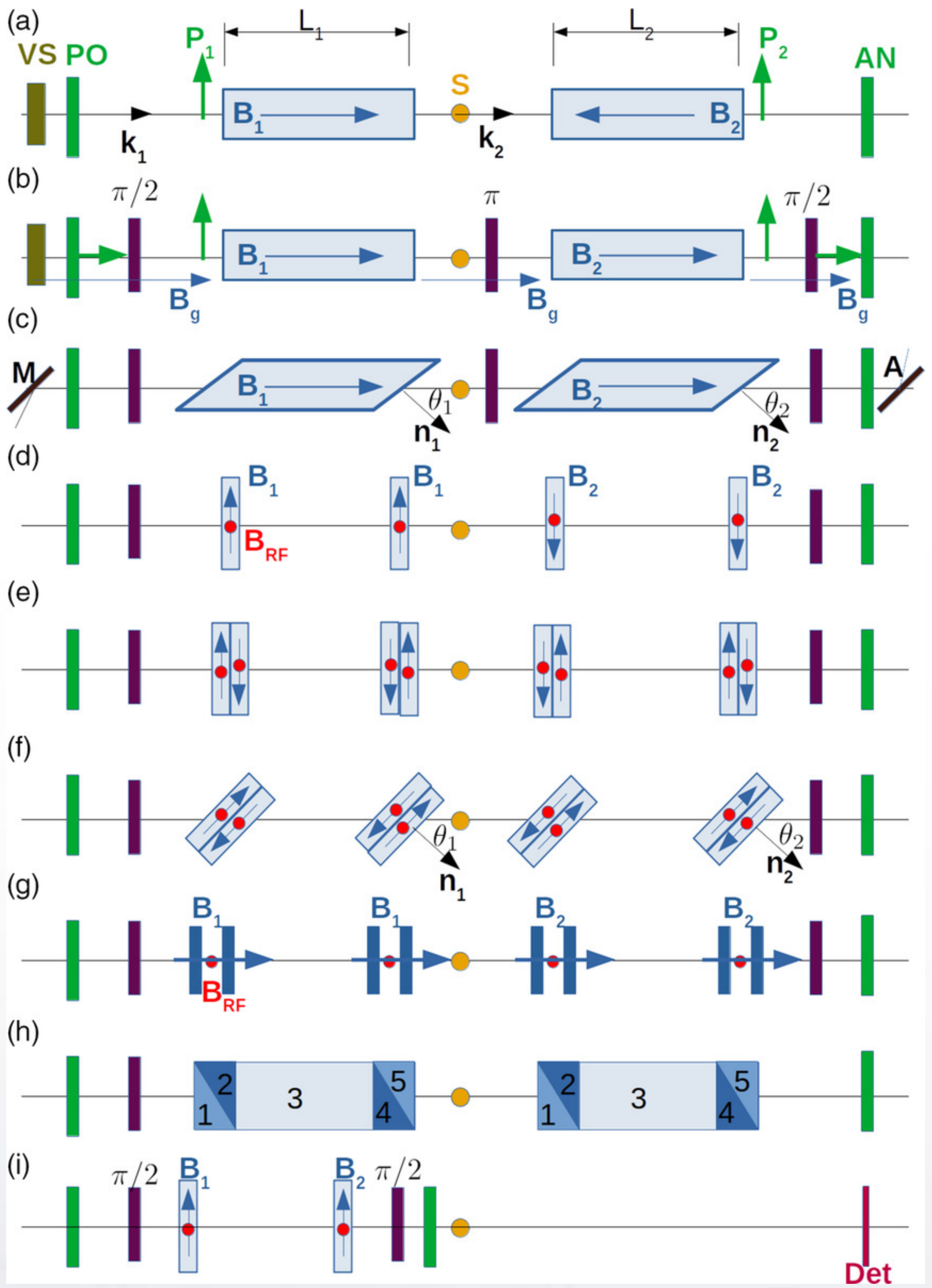
The probability of omega energy exchange:

$$S(q,\omega)$$

The final polarization:

$$\langle\cos\varphi\rangle = \frac{\int \cos\left(\frac{\hbar\gamma B l}{m v^3}\omega\right) S(q,\omega)\, d\omega}{\int S(q,\omega)\, d\omega} = S(q,t)$$

Other Echo methods

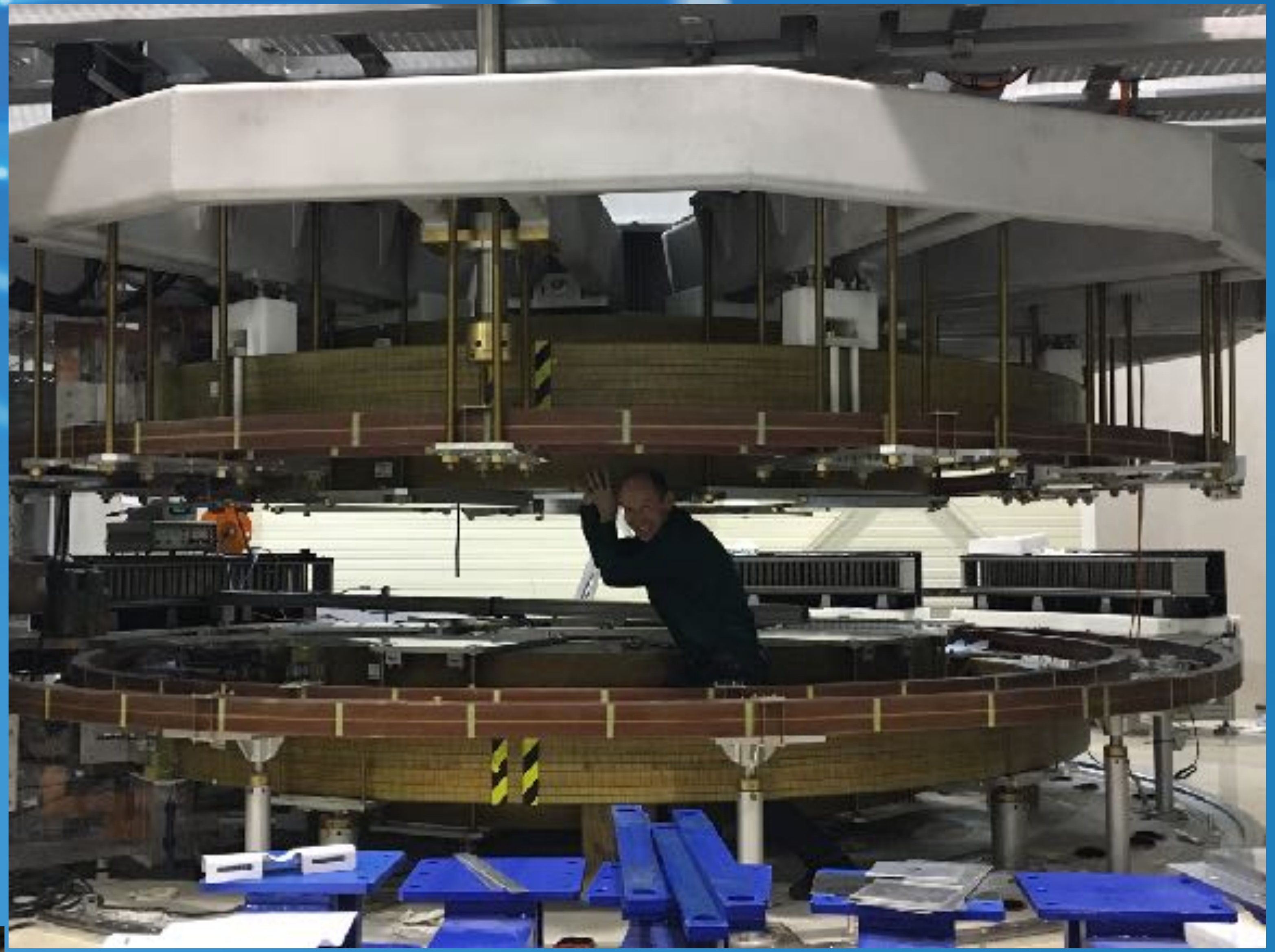


We can code energy or angle or any combination of the two.

Either magnetic filed is static and neutron rotates or neutron is static in 0 field and magnetic field rotates

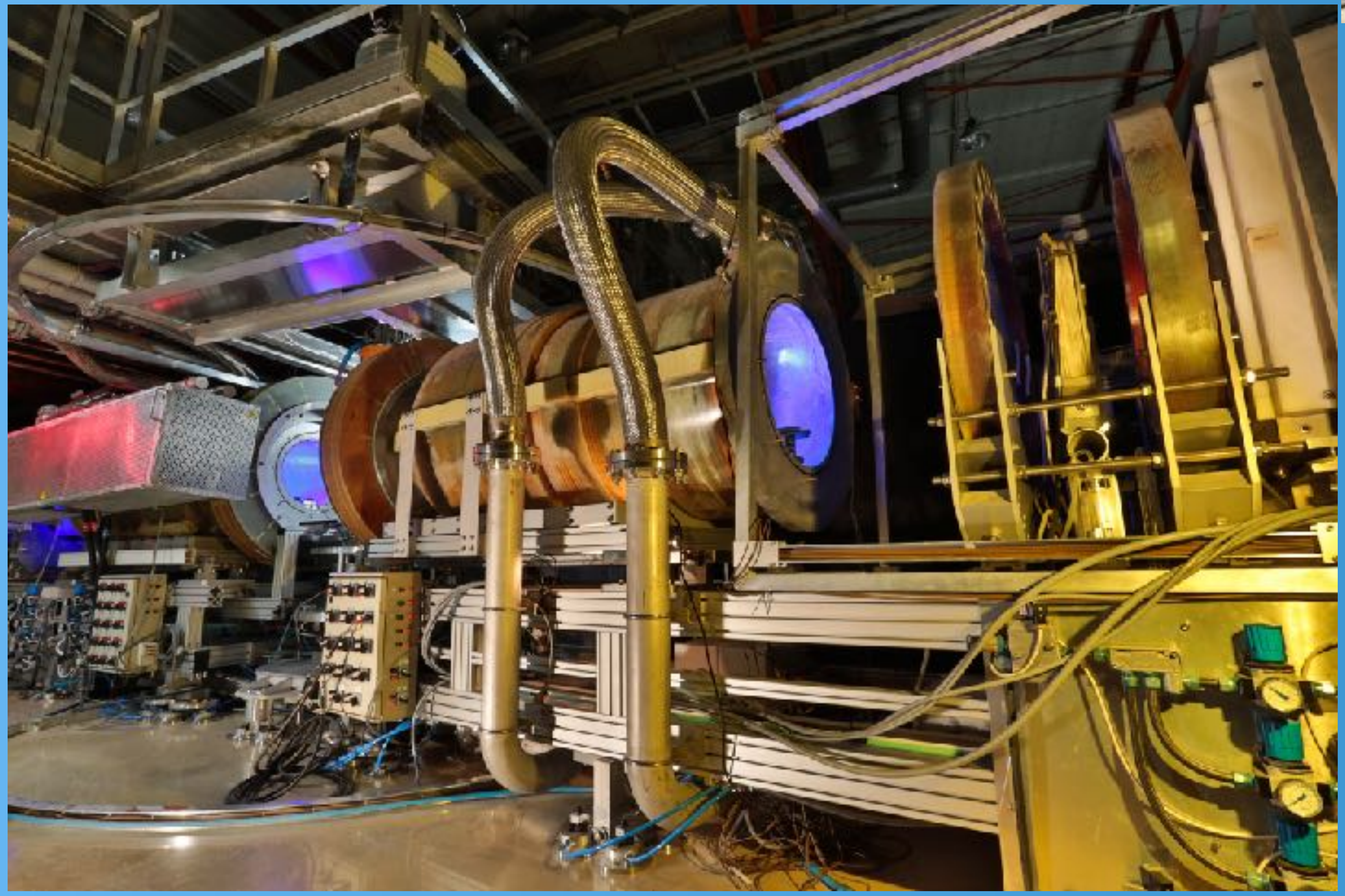
Keller T et al. Physica Status Solidi (b), Volume: 259, Issue: 5, (2021), DOI: (10.1002/pssb.202100164)

NSE Spectrometers at the ILL

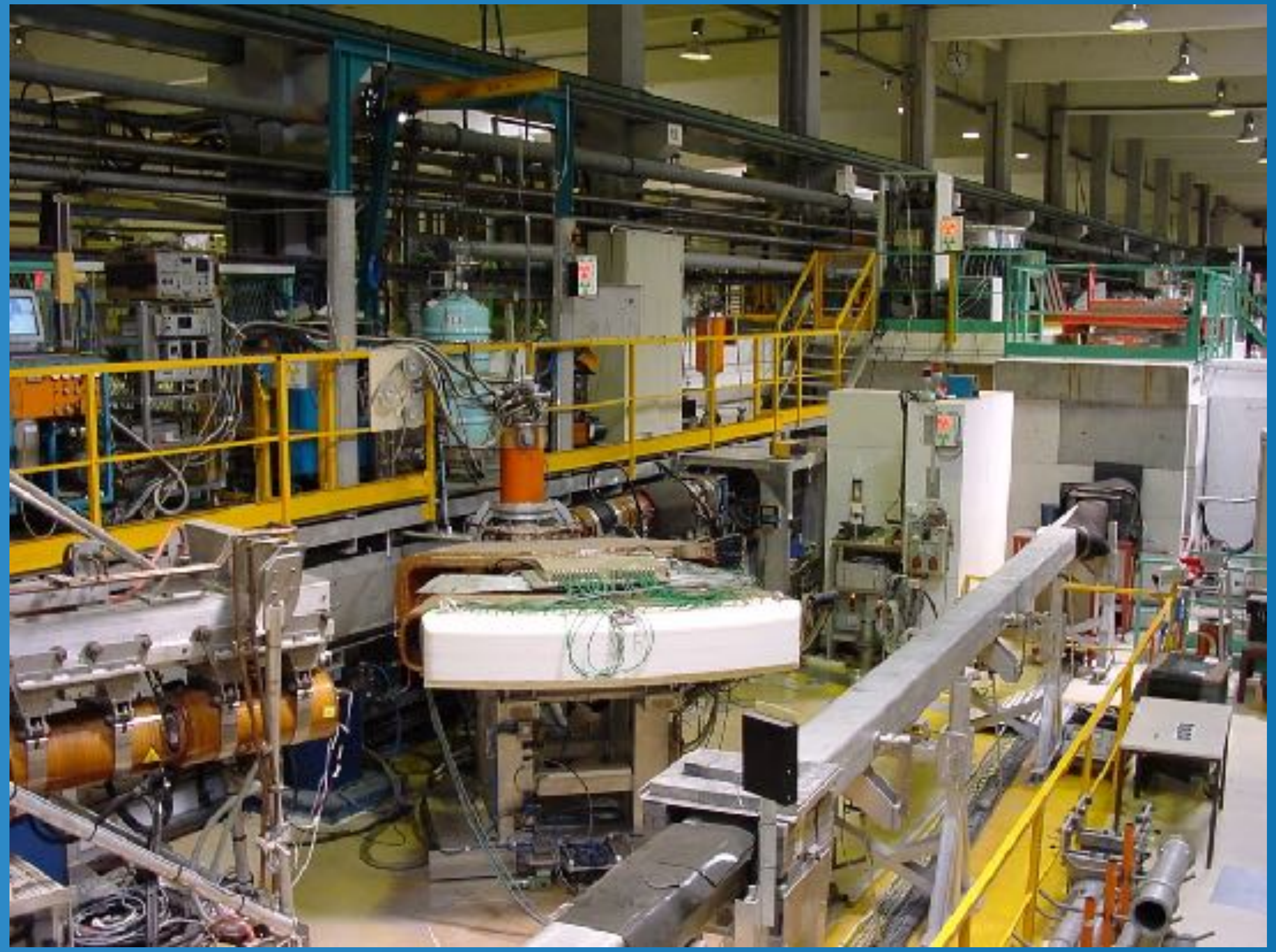


WASP

IN15

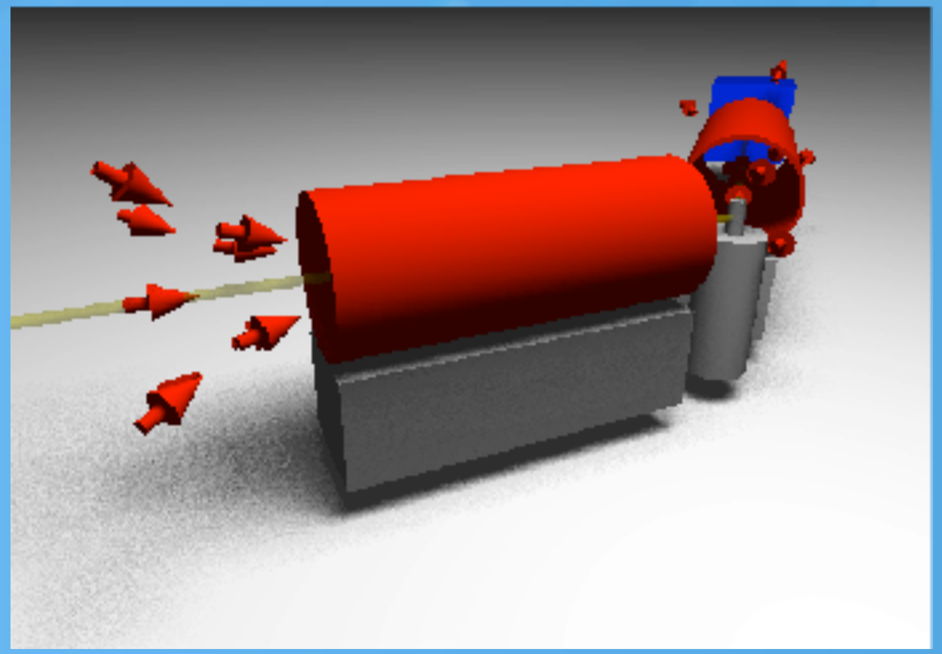


IN11 (1972-2020)



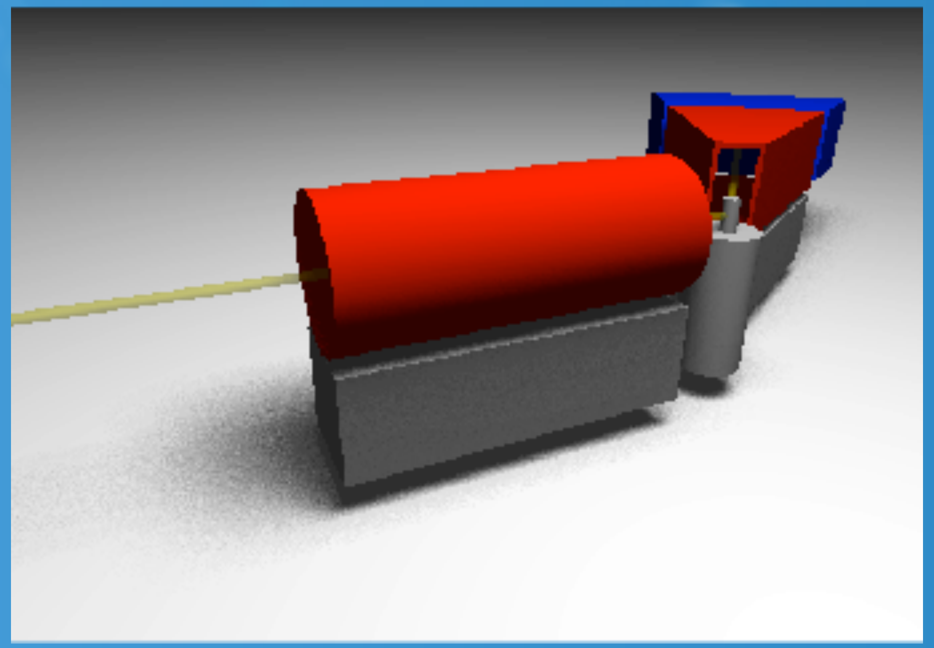
NSE Evolution

IN11A - high res
Mezei ’77, Farago ‘92



x20

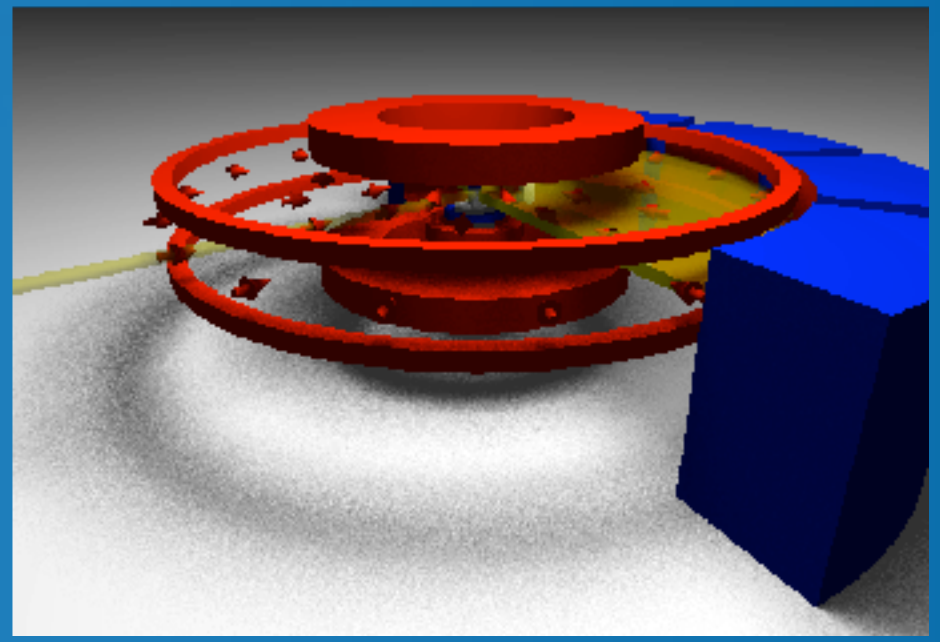
IN11C - 30º detector bank
Farago ‘97



x25

SPAN 30º detector bank
Mezei Pappas ‘99

WASP 90º detectors ‘18



WASP will:

- Provide same **high resolution** as IN11A/ old IN15
- Increase the **sample flux x8**
- Increase the **detection solid angle x3** (90º compared to IN11C)

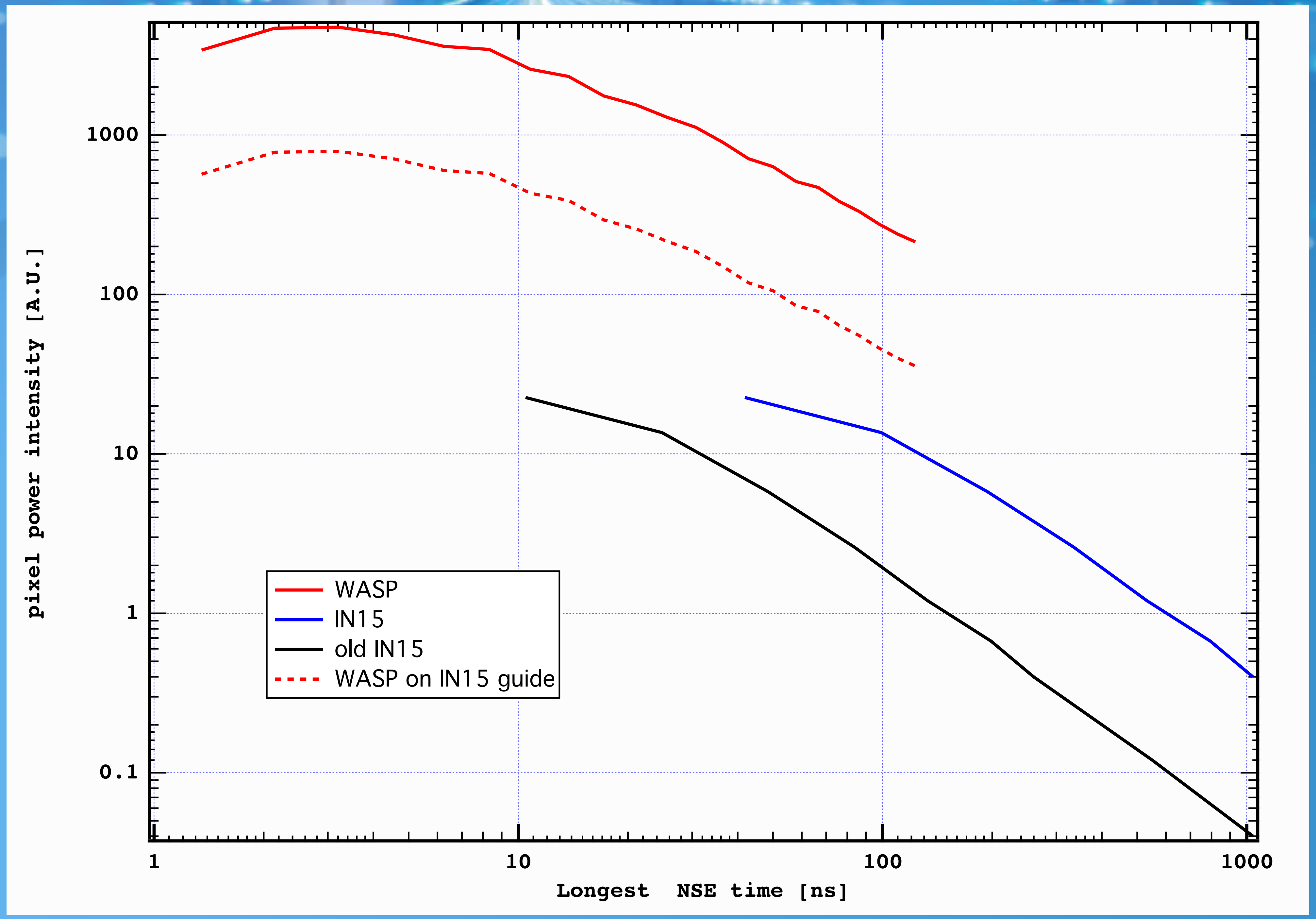
25x higher intensity **and**
6x higher field integral than IN11C

Full q range results on hydrogenated samples in **hours** not weeks

Images Courtesy of P. Fouquet

Reference: J. Neutron Res. **15**, 39 (2007)

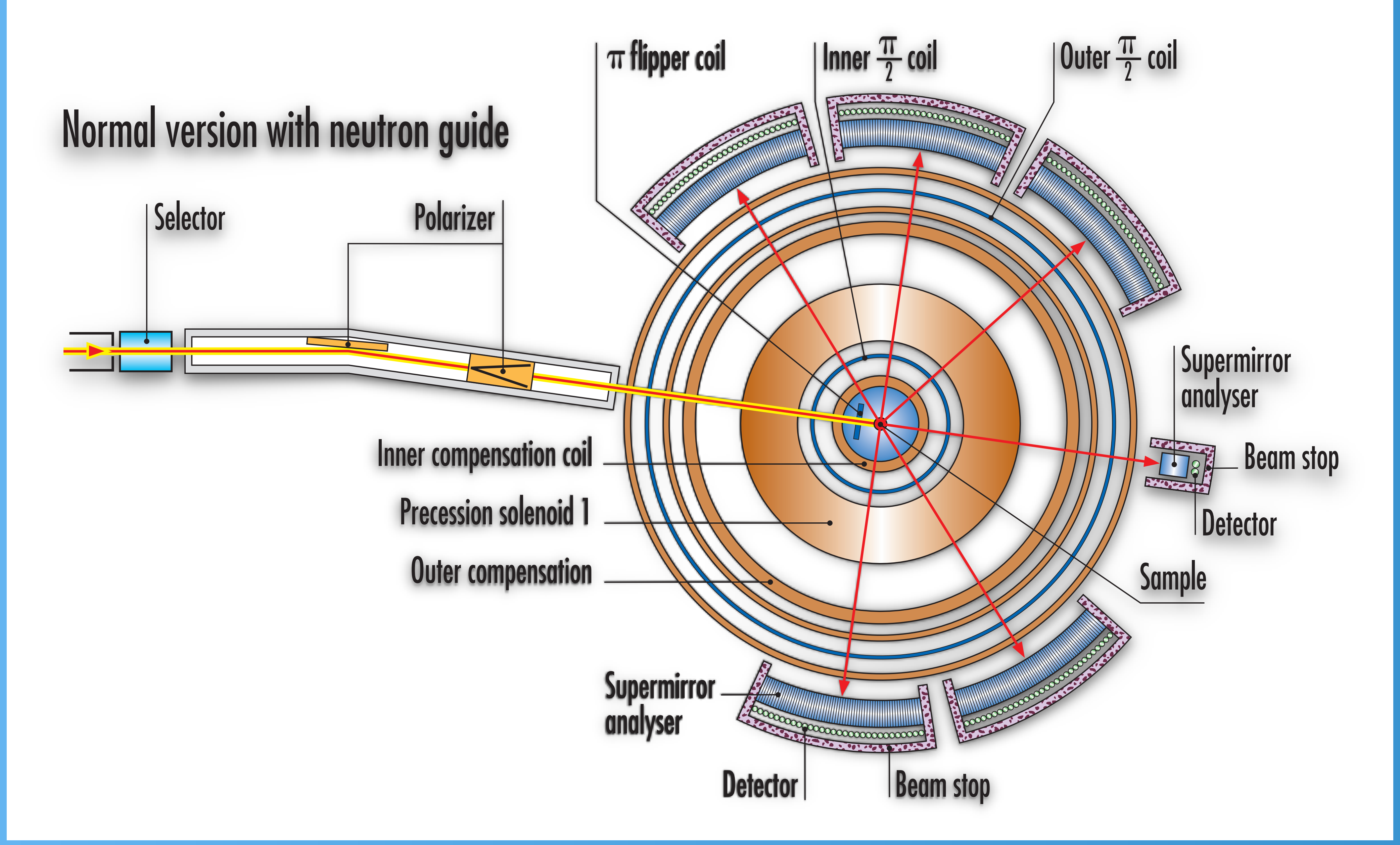
WASP advantages

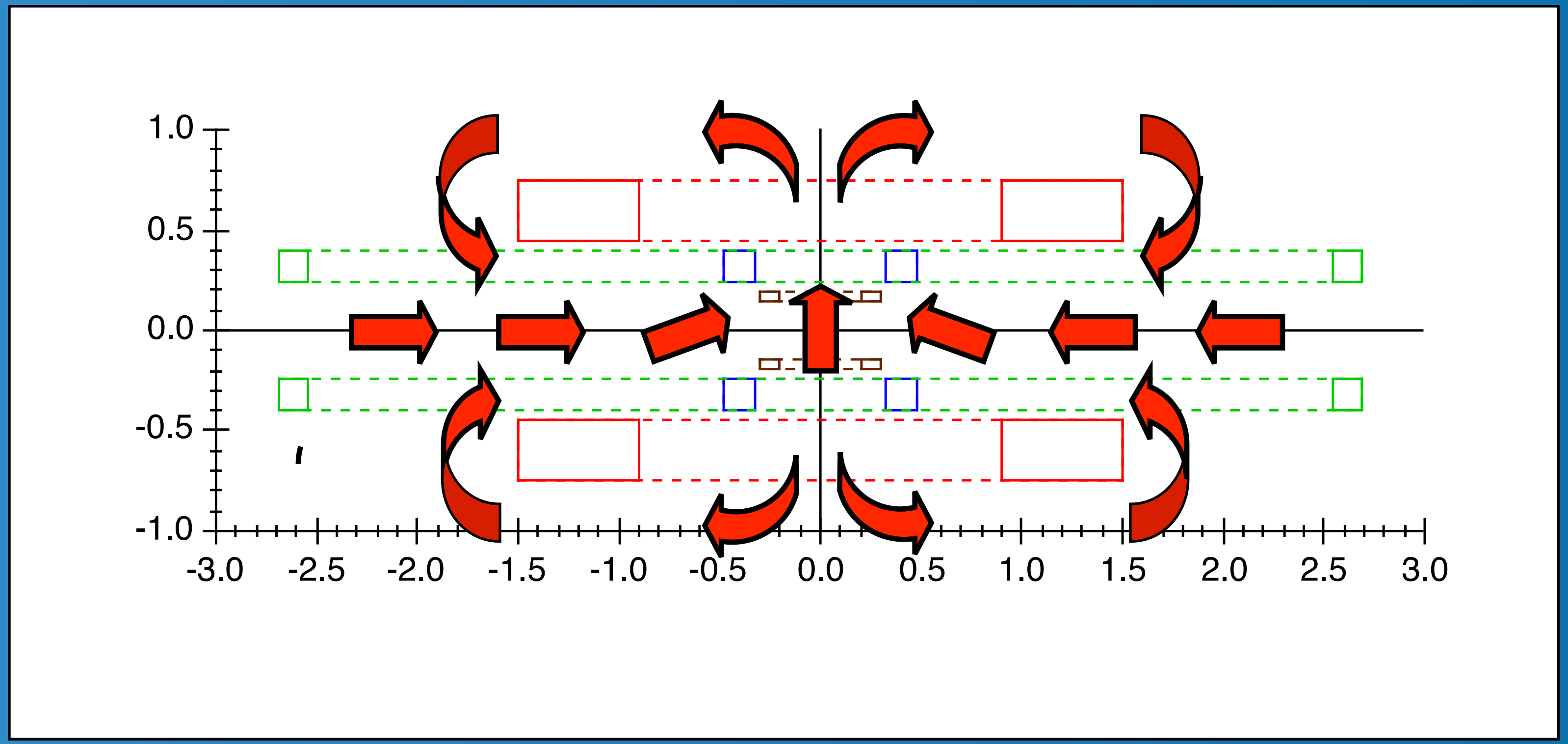


- ✓ High pixel intensity where overlaps with small angle NSE
- ✓ Wide Q-range less tuning, less scanning less overhead
- ✓ Kinetic studies at a pulsed source
- ✓ Usable as polarised diffractometer (D7)

- Wide Q-range : Sample environments are limited
- No ferromagnetic/intensity modulated echo
- Bigger footprint
- Construction cost (polarisers)

Wasp magnetic field layout (SPAN)

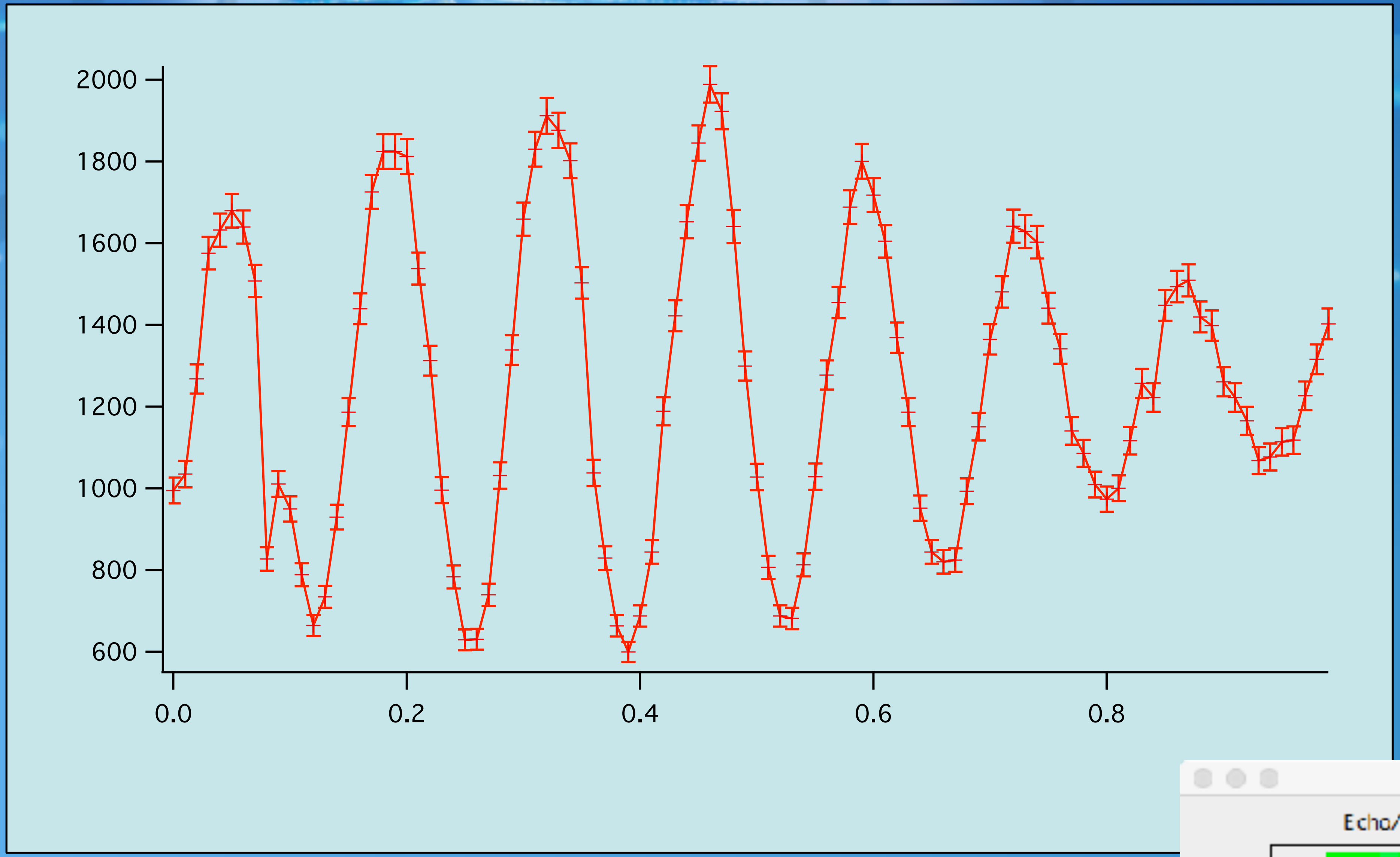




Analysers (D7)

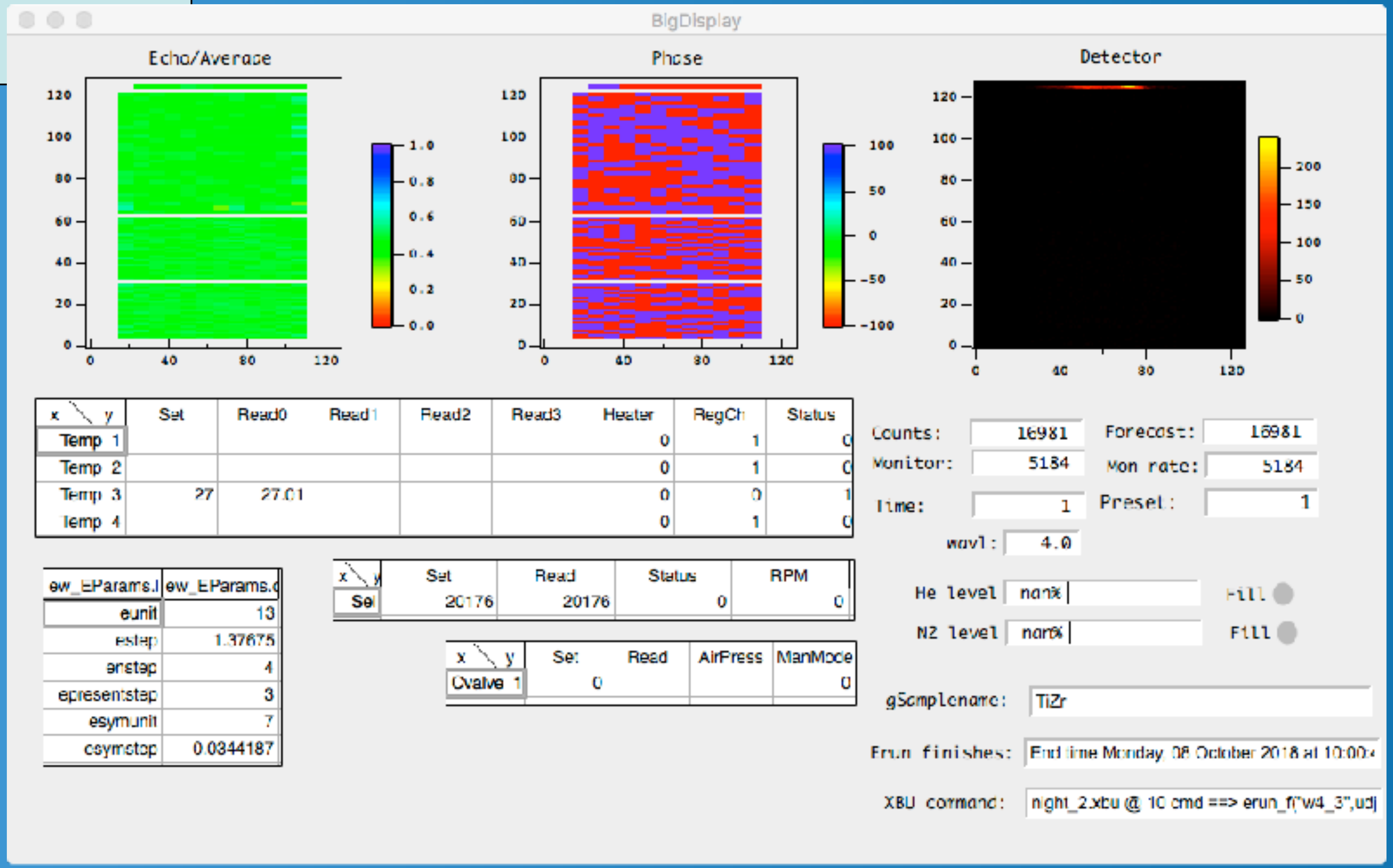
- 5 years mirror production 240m² coating
- 90 casettes 3300 mirrors for 90 degrees
- Permanent magnet produced field

First Results

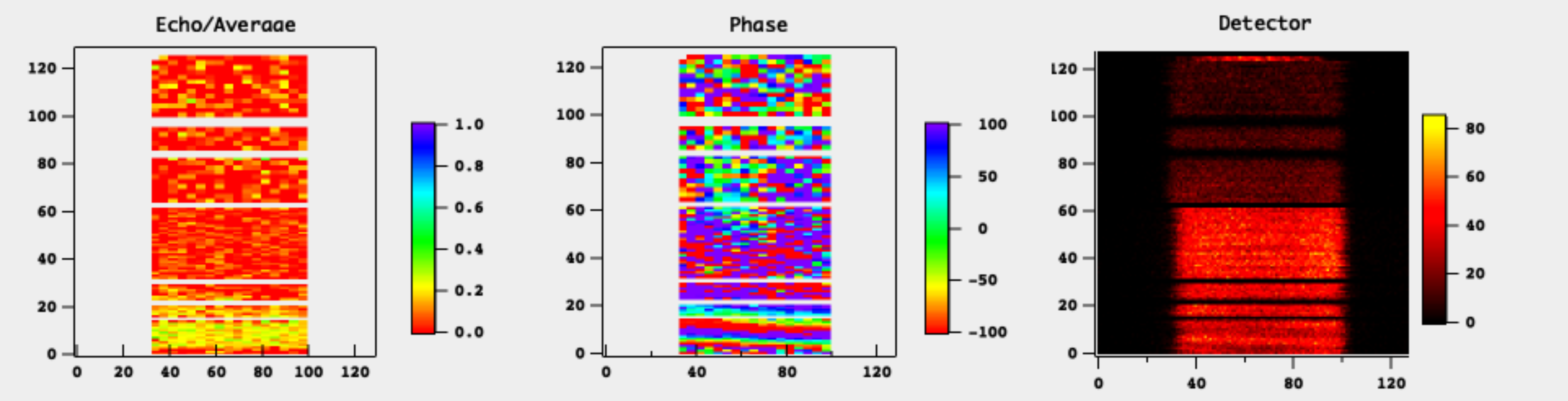


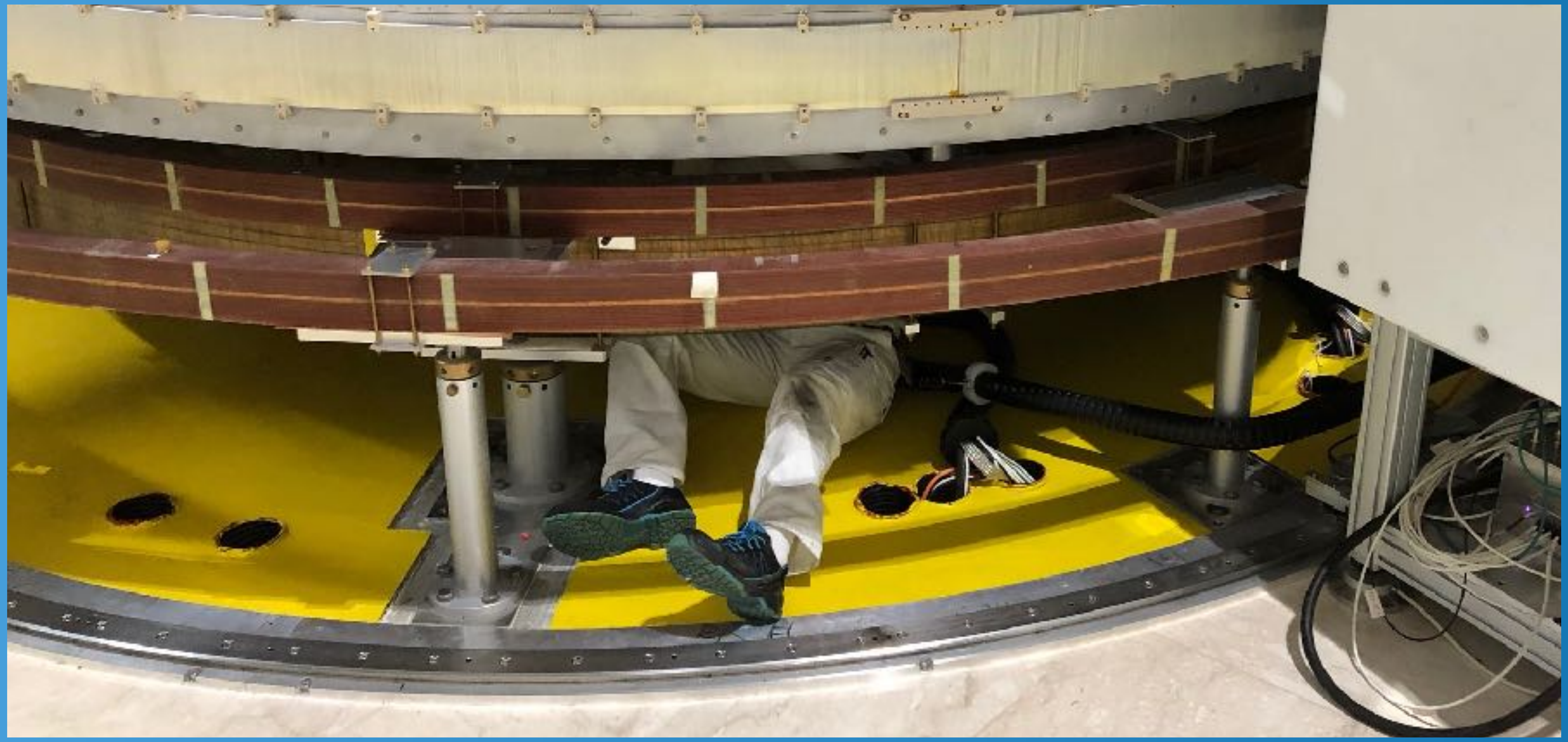
Security file signed 3/10/2018
(limited to 1/5 intensity)
First echo 4/10/2018

Full intensity authorised, echo in all detectors 10/2018



Tuning





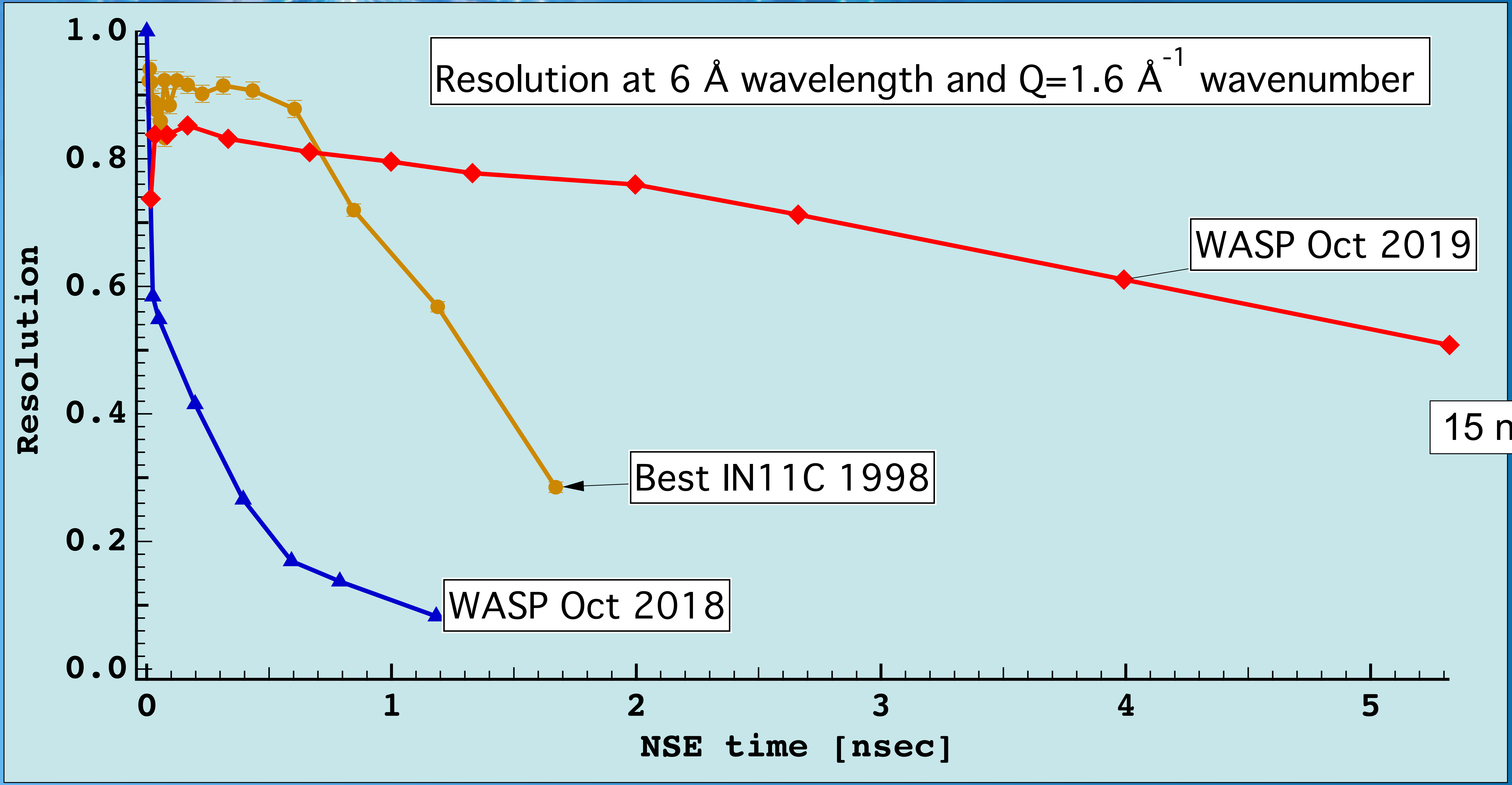
3x

Mechanical

Magnetic

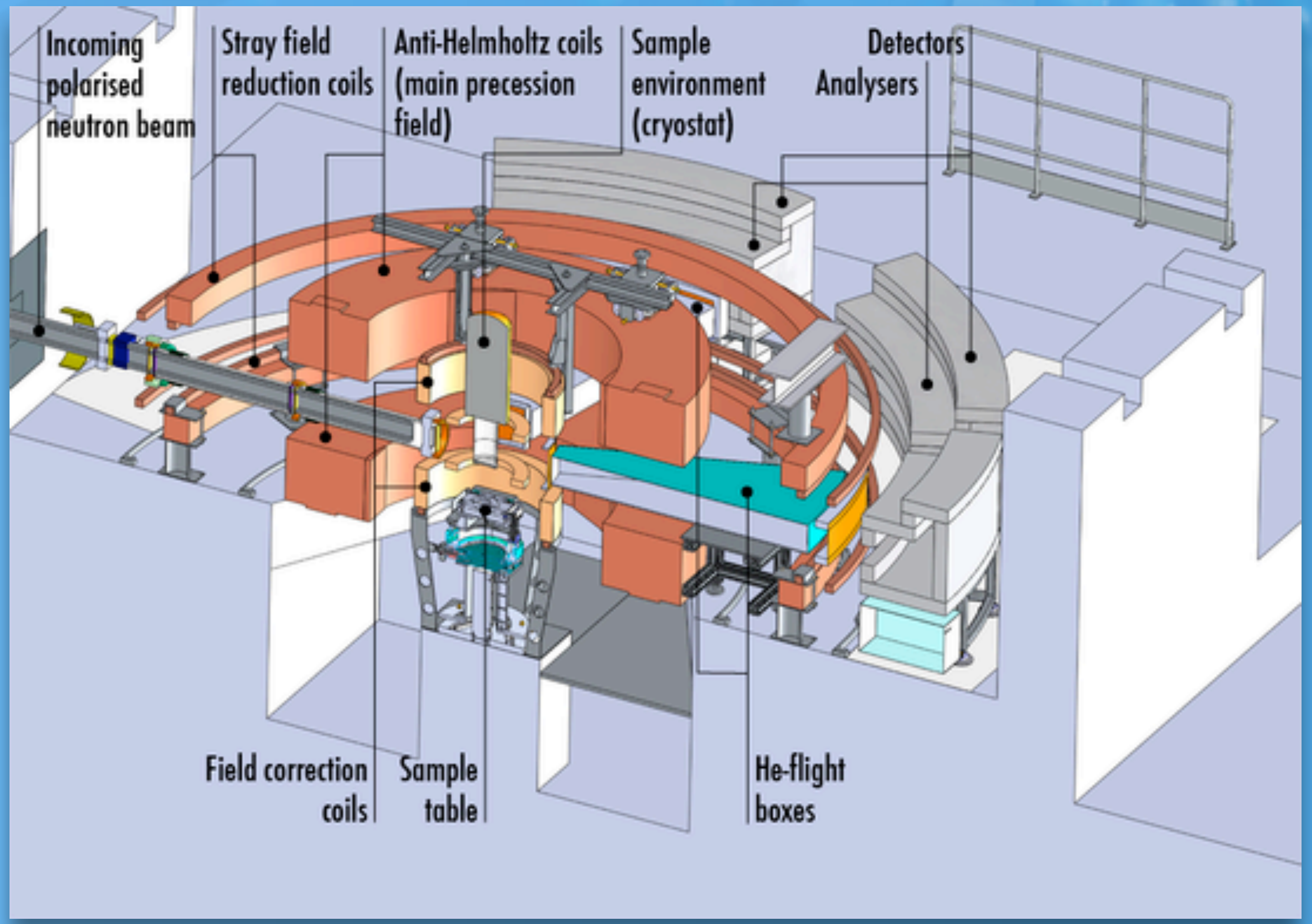
Neutrons

Resolution



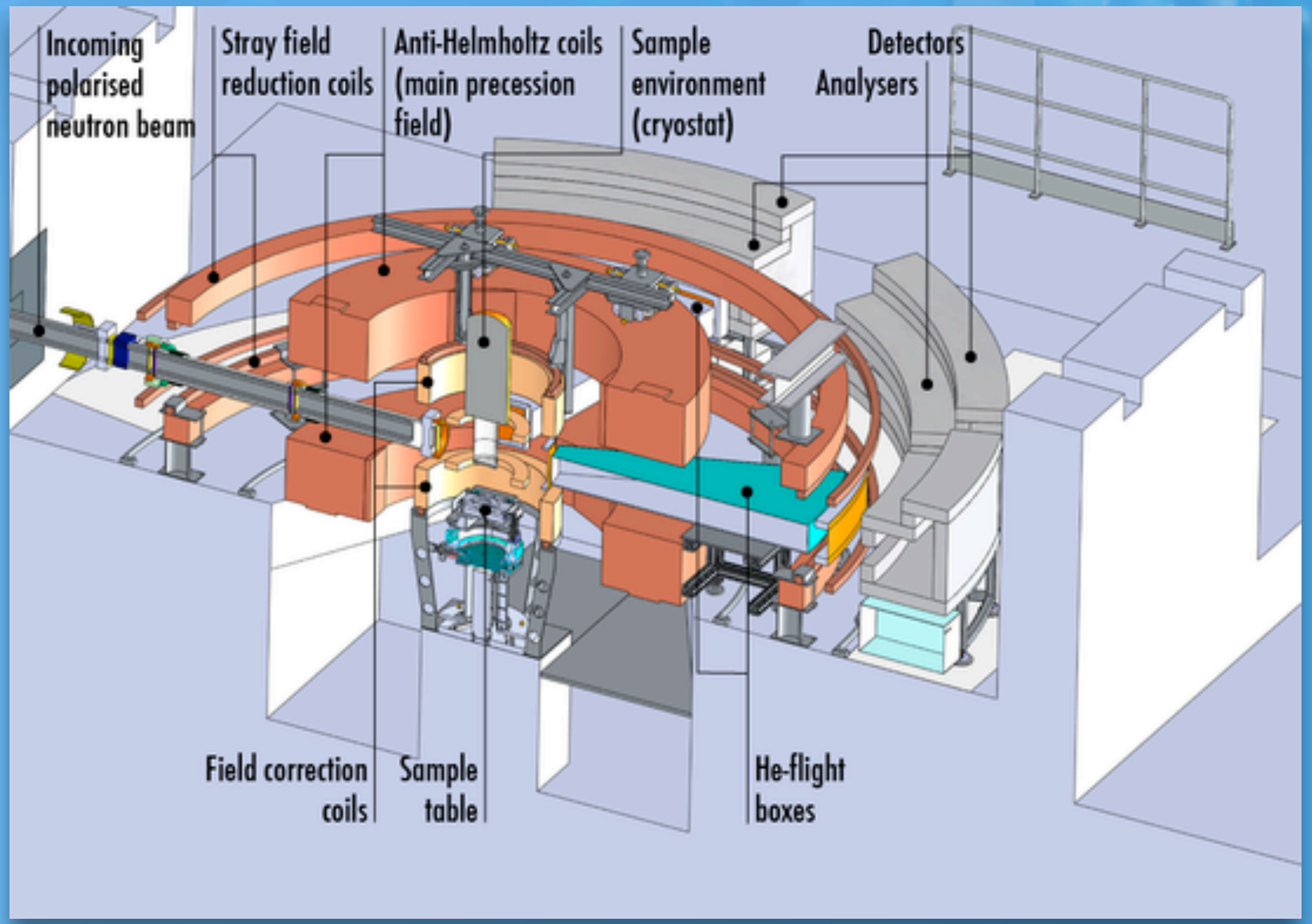
15 ns in 2023?

WASP specs



- dynamic range 0.2 ps - 100 ns
- 0.05 - 4 Å^{-1}
- 3-14 Å wavelength
- signal = 500x IN11A
- ~ 50 t Cu
- ~ 0.6 MW max power, 50 kW average power

WASP specs



First draft of proposal 2001

Proposal to instrument subcommittee 2005

Coil manufacturing 2015

Polarisation tests Apr 2018

First echo 4 October 2018

First users end of ~~2019~~ 2020

- dynamic range 0.2 ps - 10~~0~~ ns
- 0.05 - 4 Å^{-1}
- 3-14 Å wavelength
- signal = 500x IN11A
- ~ 50 t Cu
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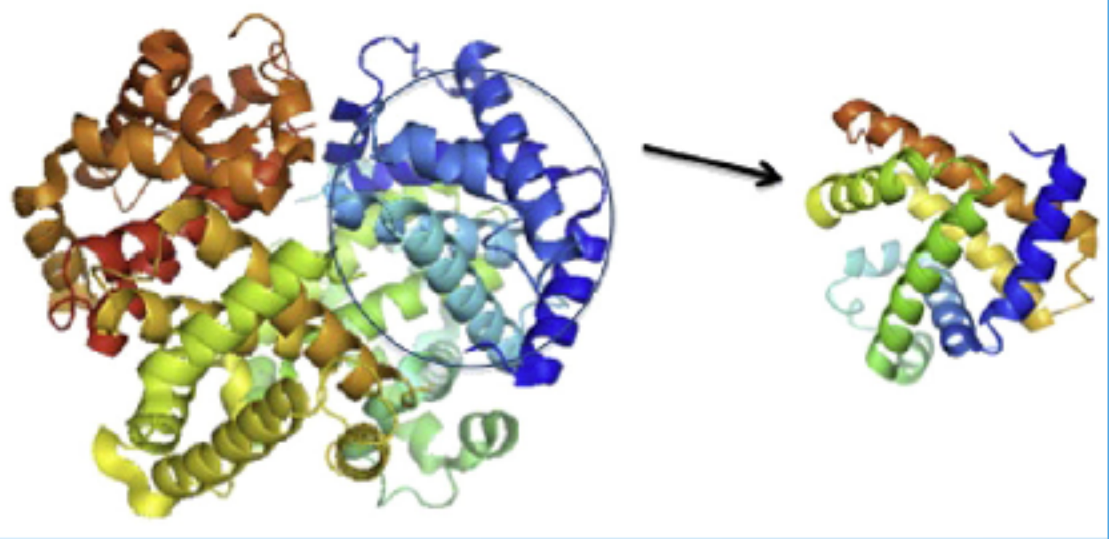
Scientific Case for WASP

NOT for coherent simple diffusion

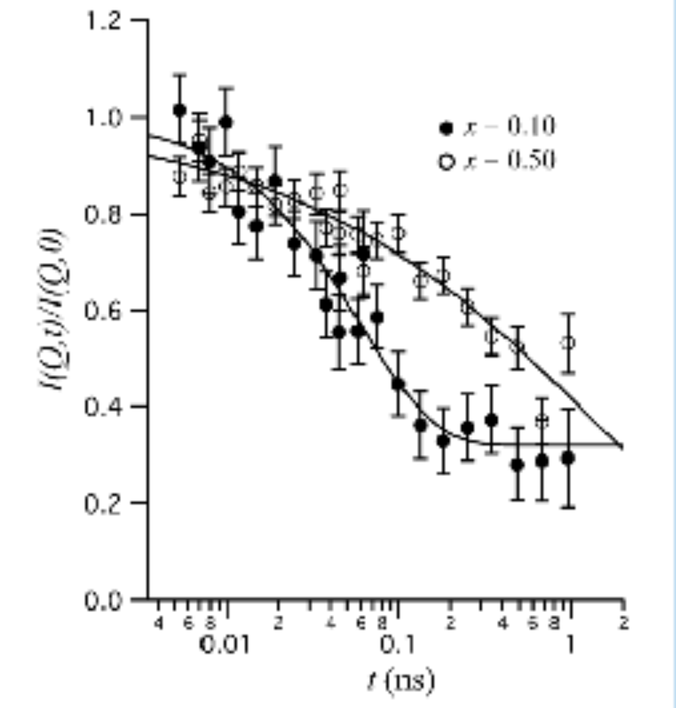
Functionality of Biomolecules



Hemoglobin Activity (incoherent)

J. Lal et al.,
J. Mol. Biol. **397**, 423 (2010)

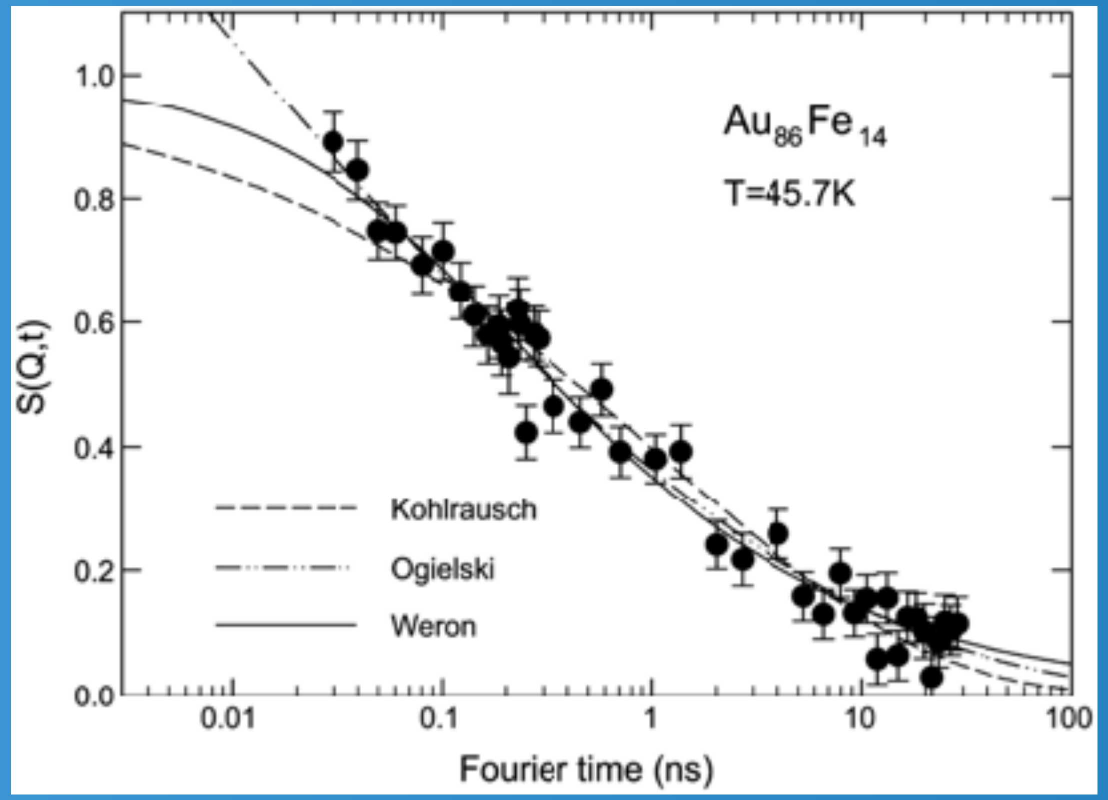
Energy Materials Incoherent Scattering



Proton Conductors

M. Karlsson et al.,
J. Phys. Chem. C **114**, 3292 (2010)

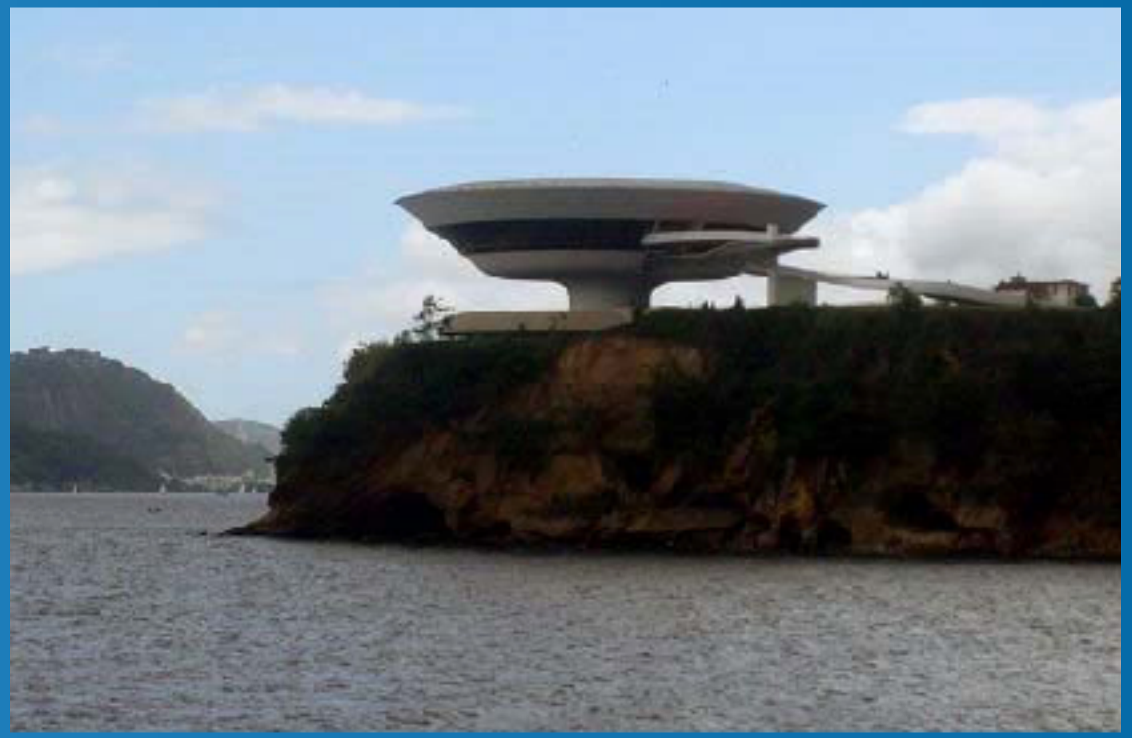
Glass Transition



Relaxation Function Test on Spin Glasses

R.M. Pickup et al.,
PRL **102**, 097202 (2009)

Liquids at the Nanometer Scale, Confinements

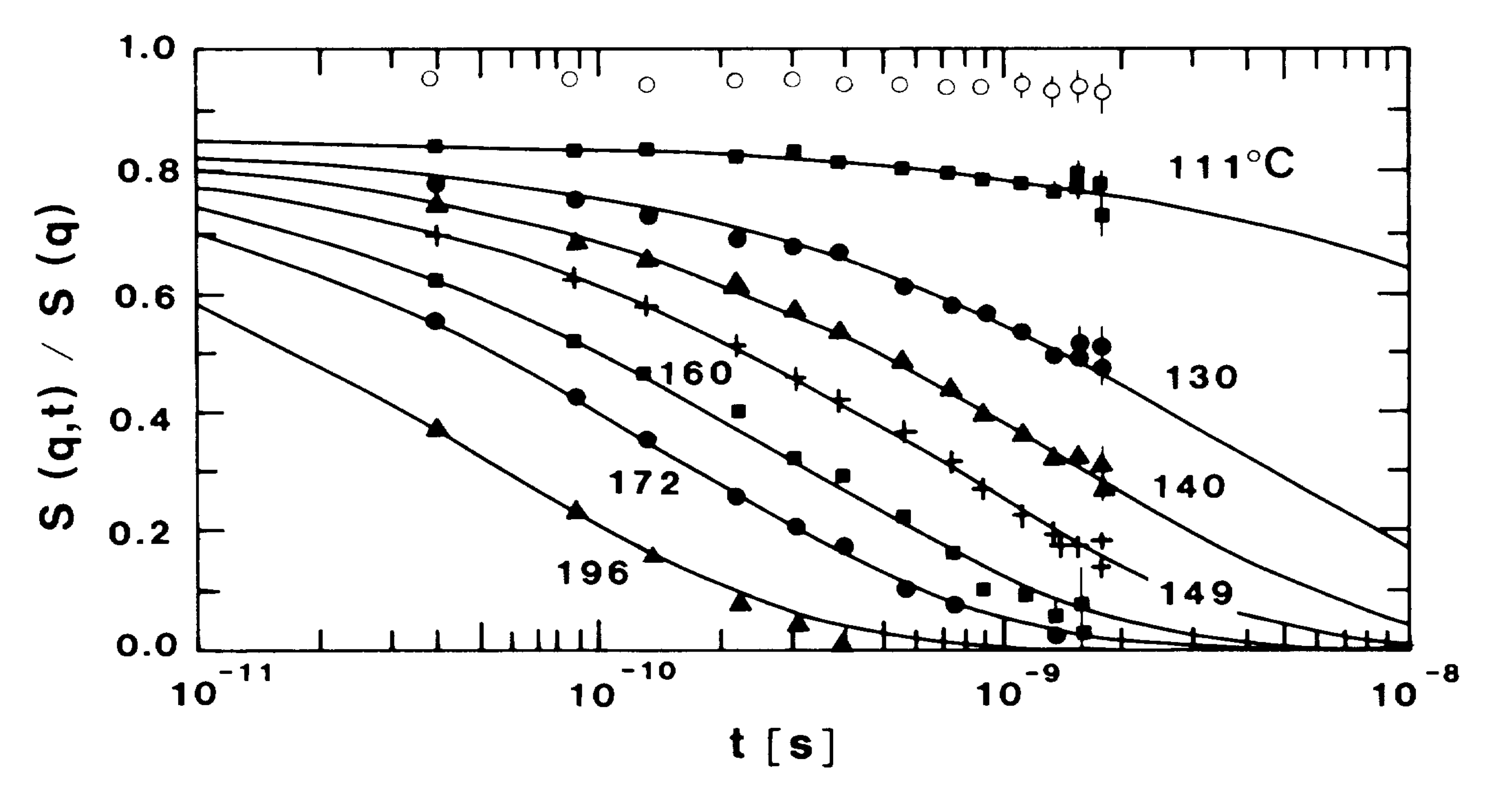


Water mobility in concrete

H. Bordallo et al., ACS Applied Materials & Interfaces **1**, 2154 (2009)

Courtesy of P Fouquet

CKN comparison

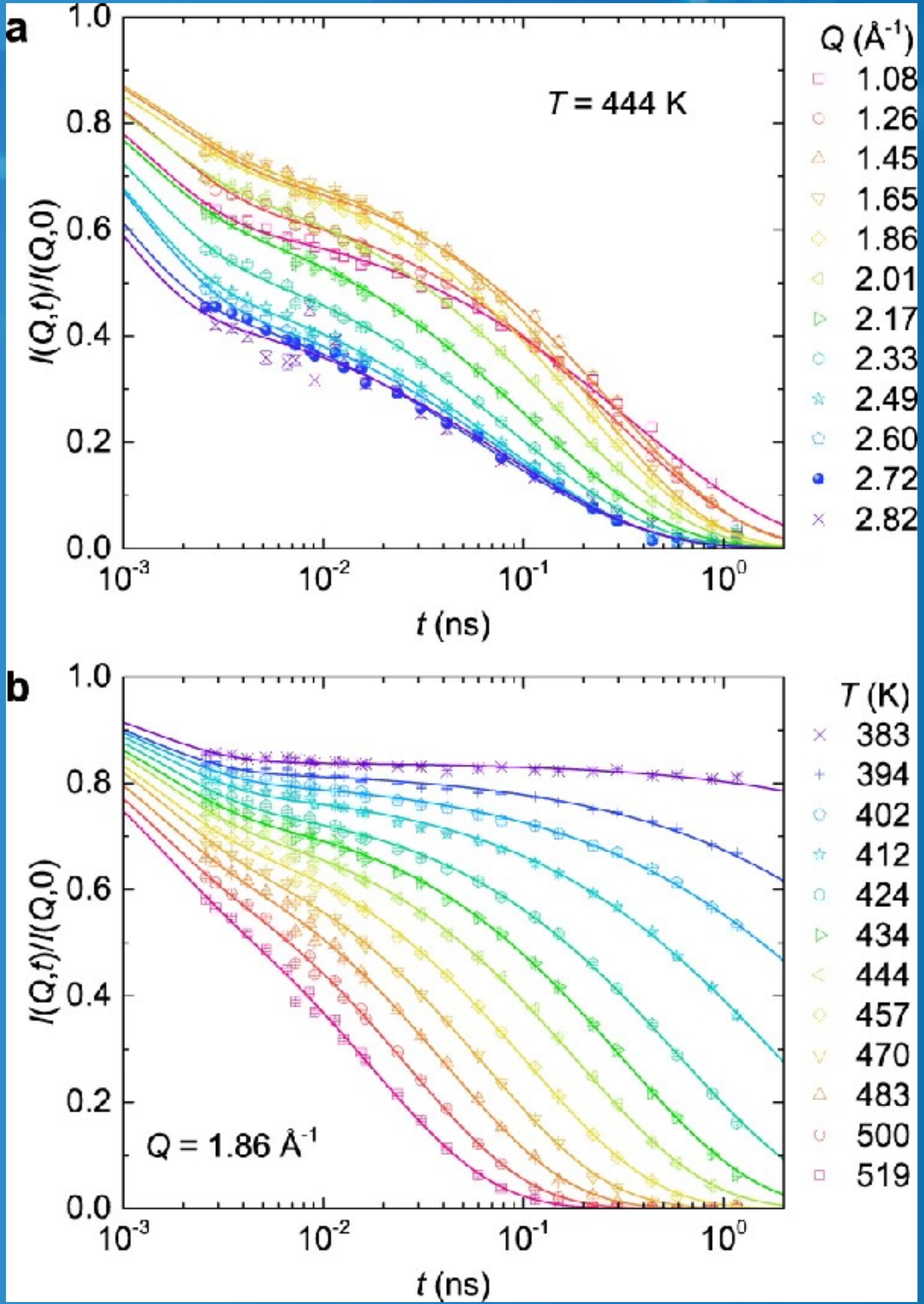


Neutron spin echo study of dynamic correlations near the liquid-glass transition

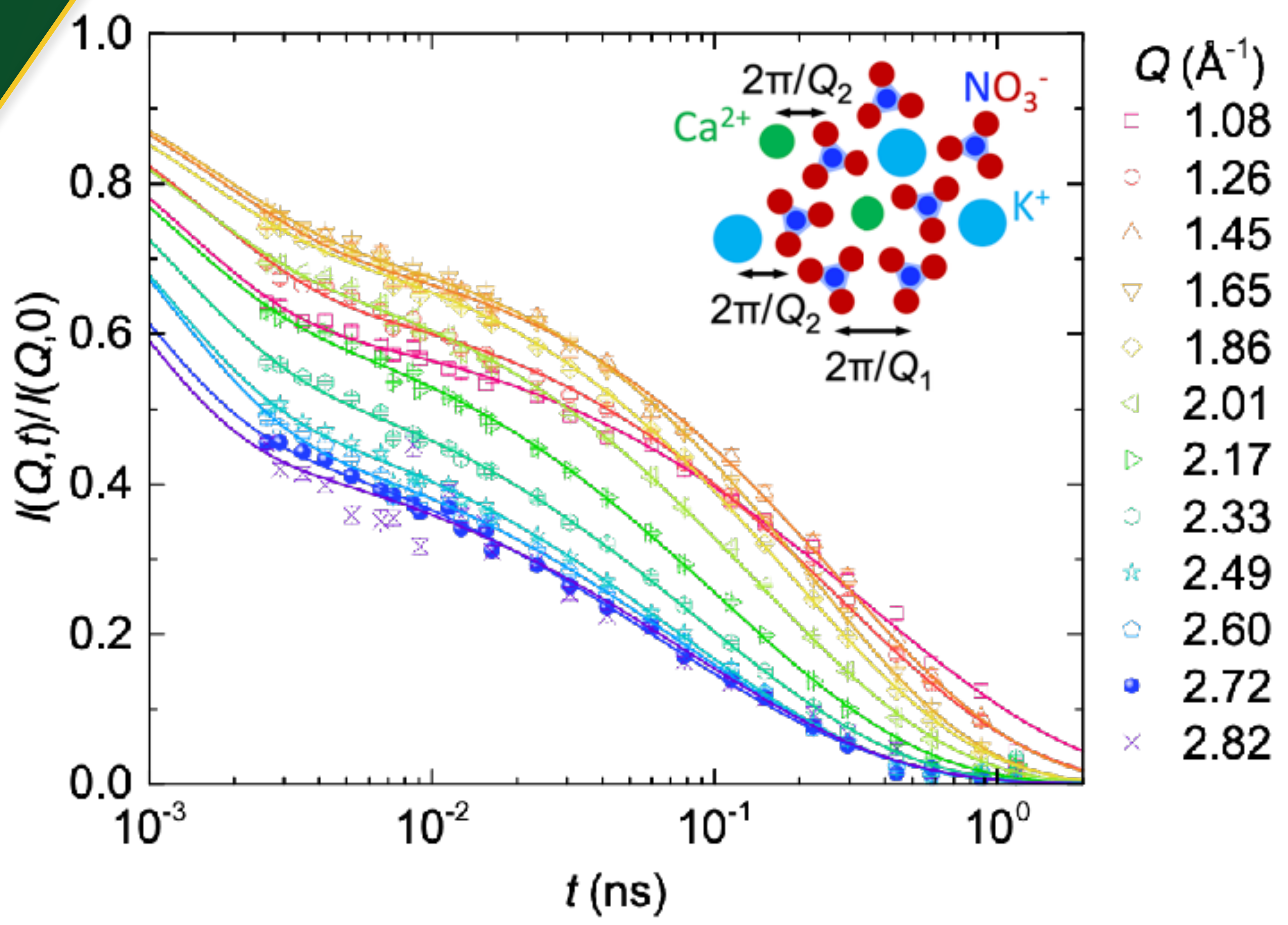
F. Mezei, W. Knaak, and B. Farago
Phys. Rev. Lett. 58, 571 – IN11. 1987.

Q-dependent collective relaxation dynamics of glass-forming liquid $Ca_{0.4}K_{0.6}(NO_3)_{1.4}$ investigated by wide-angle neutron spin-echo

P. Luo, Y. Zhai, P. Falus, V. García Sakai, M. Hartl, M. Kofu, K. Nakajima, A. Faraone, Y Z. Nature Communications, 13, 2092 (2022). DOI: 10.1038/s41467-022-29778-4
WASP 2022



New insight into the collective relaxation dynamics of glass-forming liquid revealed by wide-angle neutron spin echo



Wide-angle neutron spin echo measurement of a model fragile liquid $Ca_{0.4}K_{0.6}(NO_3)_{1.4}$ (CKN) at T=444 K at various wavevectors (Q). The inset is an illustration of CKN structure.

P. Luo, Y. Zhai, P. Falus, V. García Sakai, M. Hartl, M. Kofu, K. Nakajima, A. Faraone, **Y Z**. *Nature Communications*, 13, 2092 (2022). DOI: 10.1038/s41467-022-29778-4

Neutron facilities at the ILL, NCNR, and J-PARC were used.

Scientific Achievement

The collective relaxation dynamics over the full range of the microscopic structural length scales have been characterized by employing the recently developed wide-angle neutron spin-echo (WASP) spectroscopy.

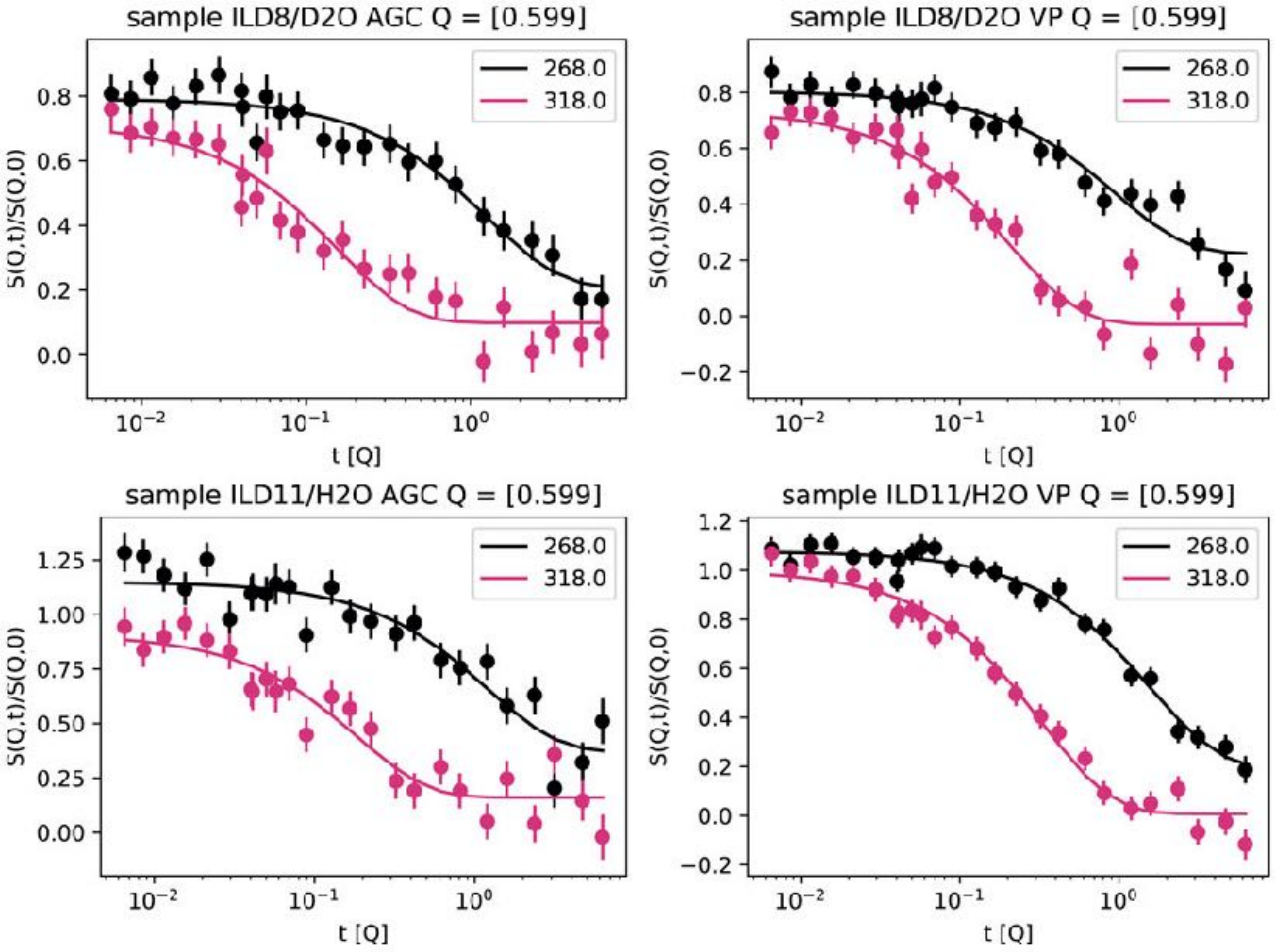
Significance and Impact

A change in the dominant relaxation mechanisms was found in liquid $Ca_{0.4}K_{0.6}(NO_3)_{1.4}$ (CKN) at the length scale of 2.6 Å, below which the relaxation process exhibits a temperature independent distribution and more Arrhenius-like behavior, revealing new insight into the collective dynamics in glass-forming liquids – a key to understand the universality of liquid state physics.

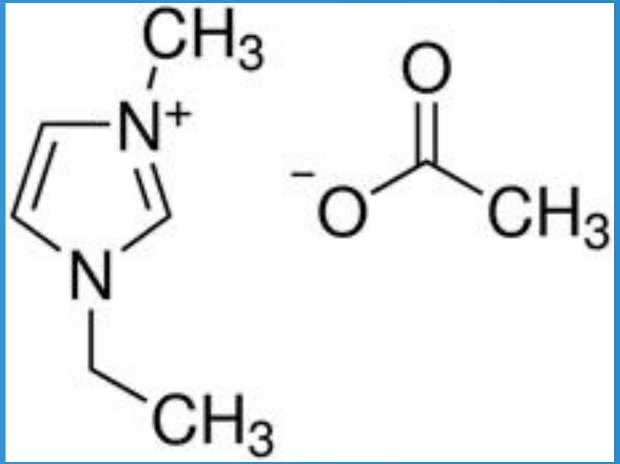
Research Details

- CKN sample was prepared by mixing high-purity $Ca(NO_3)_2$•$4H_2O$ and KNO_3 and then drying the mixture in vacuum above the melting point.
- Intermediate scattering functions of liquid CKN at various temperatures from 383 K to 519 K, and in the Q-range from 1.08 $Å^{-1}$ to 2.82 $Å^{-1}$ were measured on WASP at the ILL.

Ionic Liquid (EmimAc)-Water Mixture Confined in Nanoporous Glass Matrices Studied With High-Resolution Neutron Spectroscopy



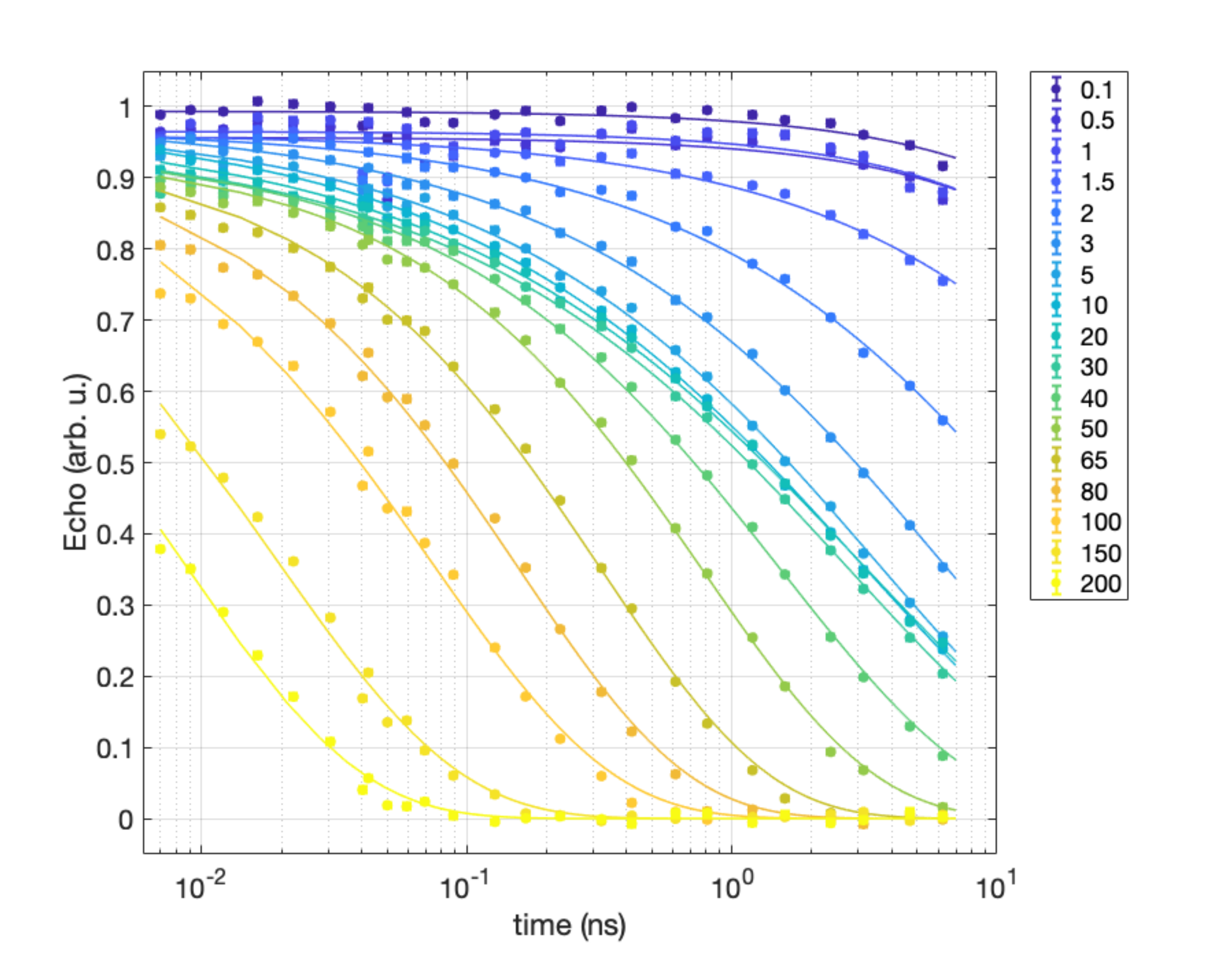
H. Frielinghaus, M. Fomina, D. Hayward, P. S. Dubey, S. Jaksch, P. Falus, P. Fouquet, L. Fruhner and O. Holderer



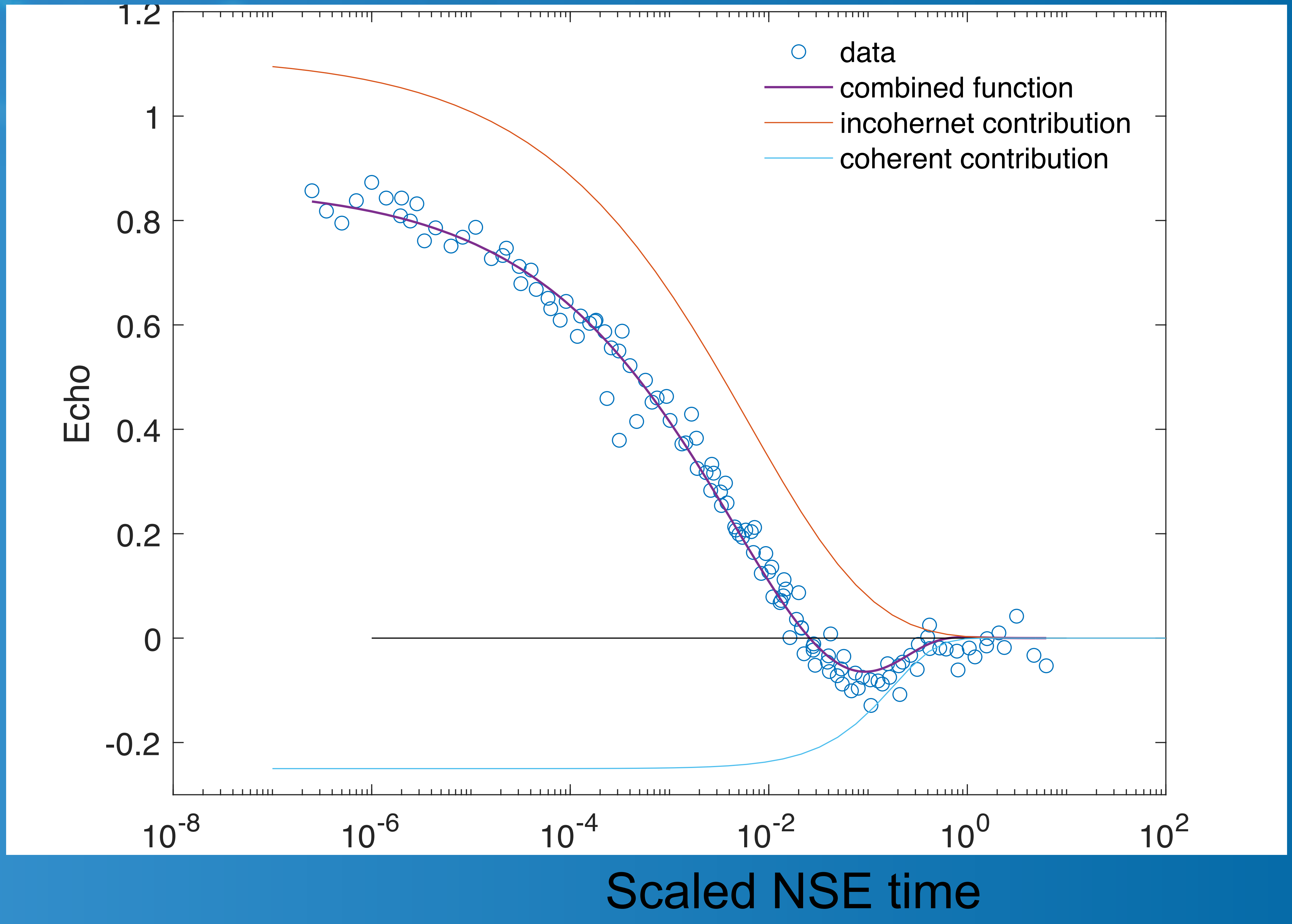
Front. Phys., 21 April 2022
Sec. Physical Chemistry and Chemical Physics
https://doi.org/10.3389/fphy.2022.872616

More examples

Doped HoTiO spin glass



Diluted ionic liquid electrolyte



J. Phys. Chem. C (2022), 126, 38, 16262–16271

Conclusion/ Homework

- Wasp sees things we have never seen before, apply for ILL beamtime ! (Result in hours not a week)

- Need higher resolution than time of flight or backscattering ? Need more intensity at high Qs than small angle NSE ? Apply for beam time !

- ESS has no Neutron Spin Echo, lobby for one !

Thank you !