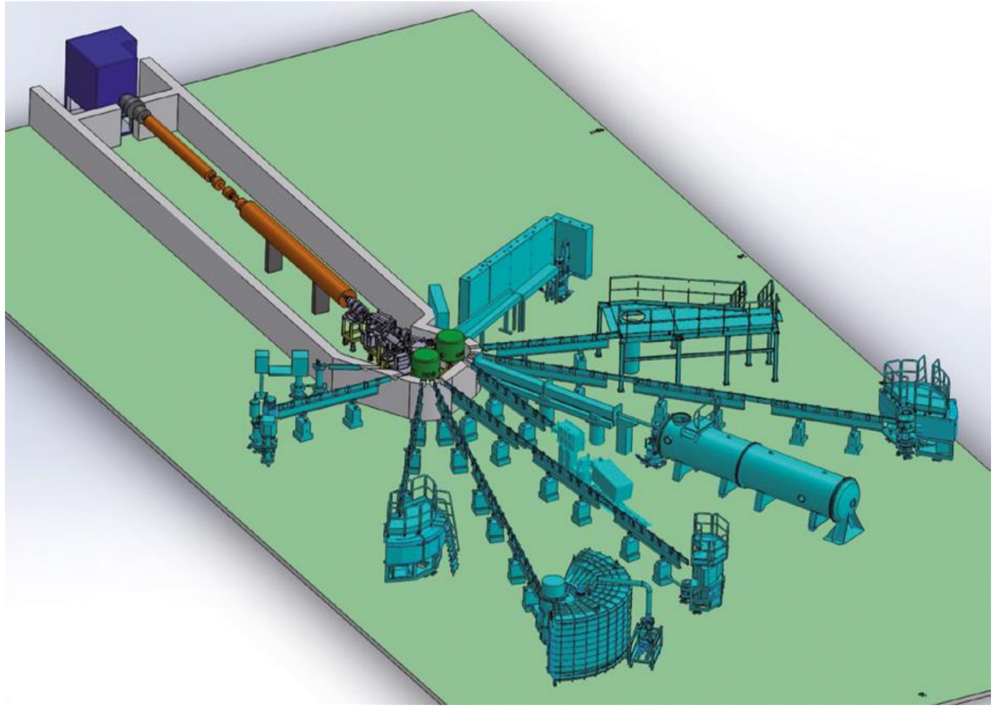
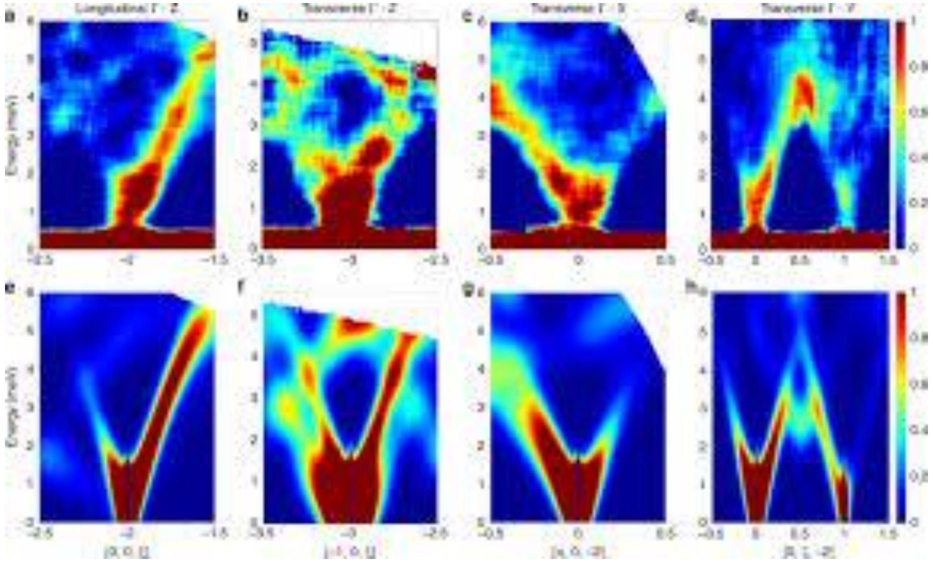
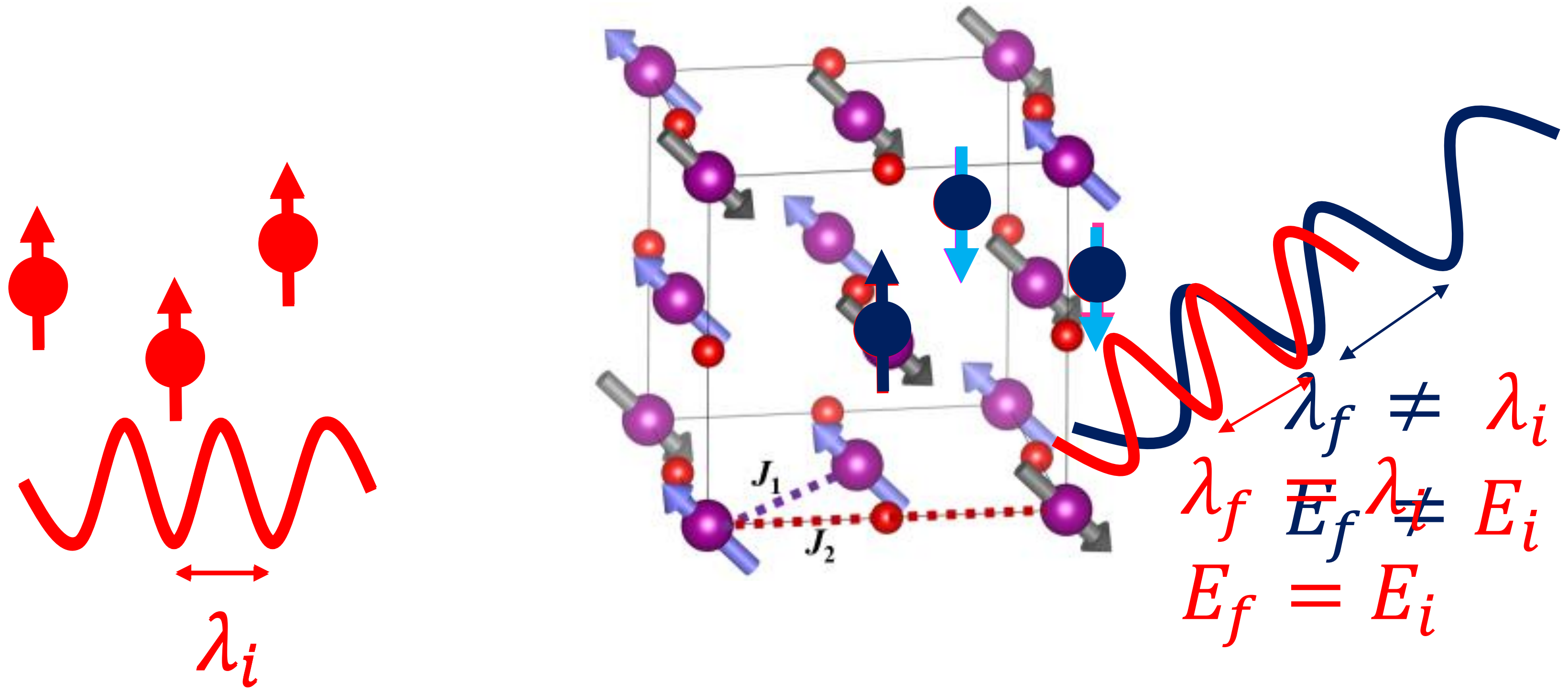
Quentin FAURE

Journées de la Diffusion Neutronique
Erquy – 10/2023

Spectroscopy : state of the art, and possibilities in HiCANS



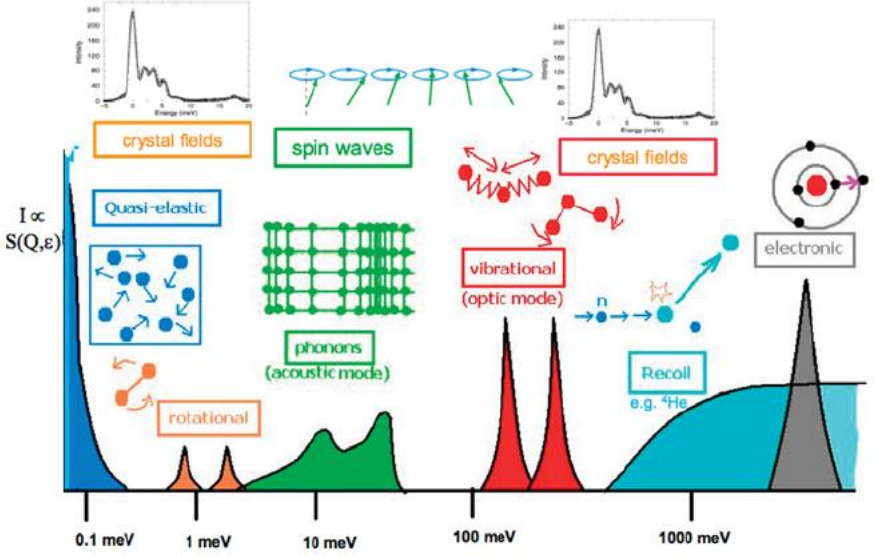


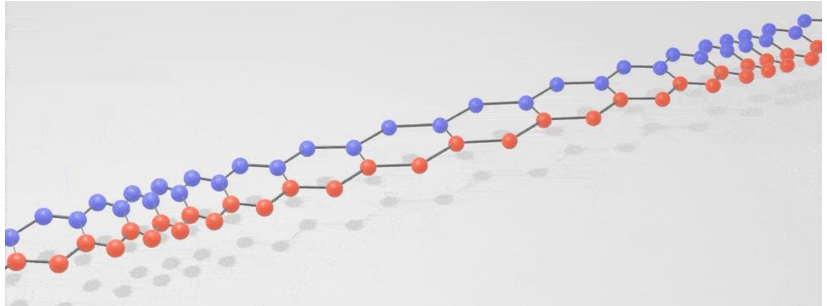


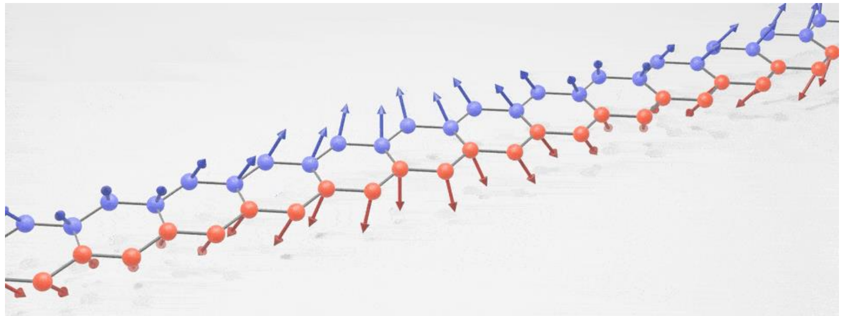
Neutron = particule neutre + S = ½ ⇔ ideal probe for condensed and soft matter physics

Elastic $(E_f = E_i)$
- Crystallographic structure
- Magnetic structure

Inelastic $(E_f \neq E_i)$
- Phonons
- Magnetic excitations

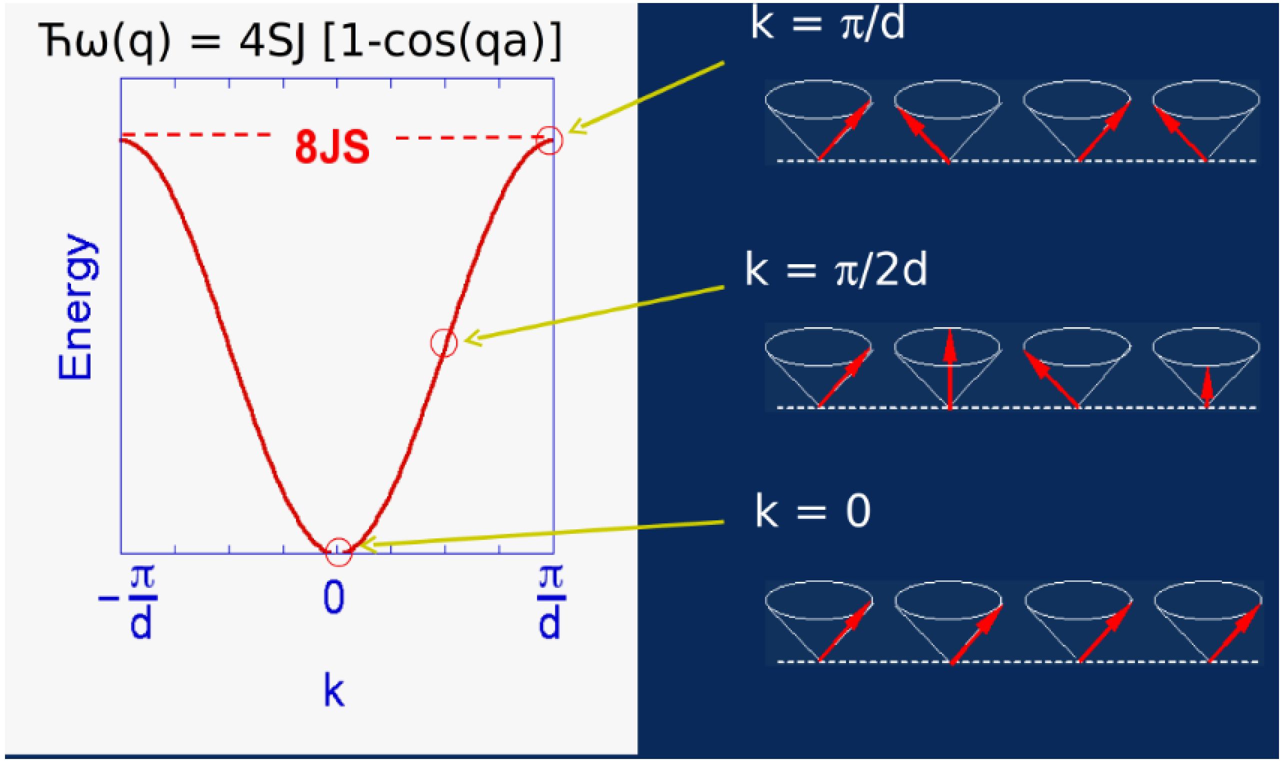






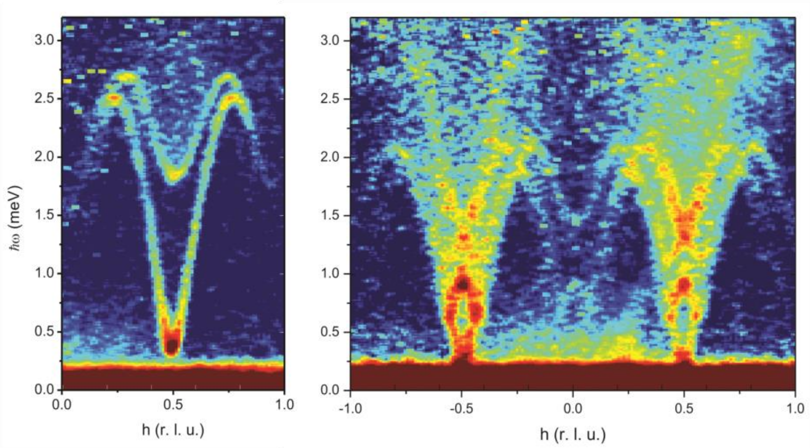
Inelastic ⇔ **Dynamics** $(E_f \neq E_i)$

“rigidity” of interactions

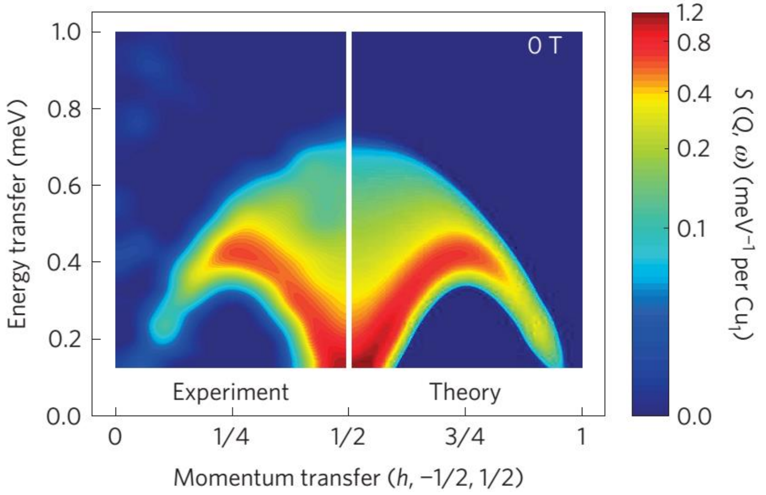


Inelastic Neutron Scattering (INS) nuclear & magnetic
→ **Excitations** (phonons …) (magnons, spinons …)

We measure $S(\vec{Q},\omega) =$ Double Fourier transform of the nuclear or spin correlation functions
→ dispersion curves, continuum of excitations, …



TLL dynamics Spin ladder DIMPY
Schmidiger et al, Phys. Rev. Lett. 111, 107202 (2013)

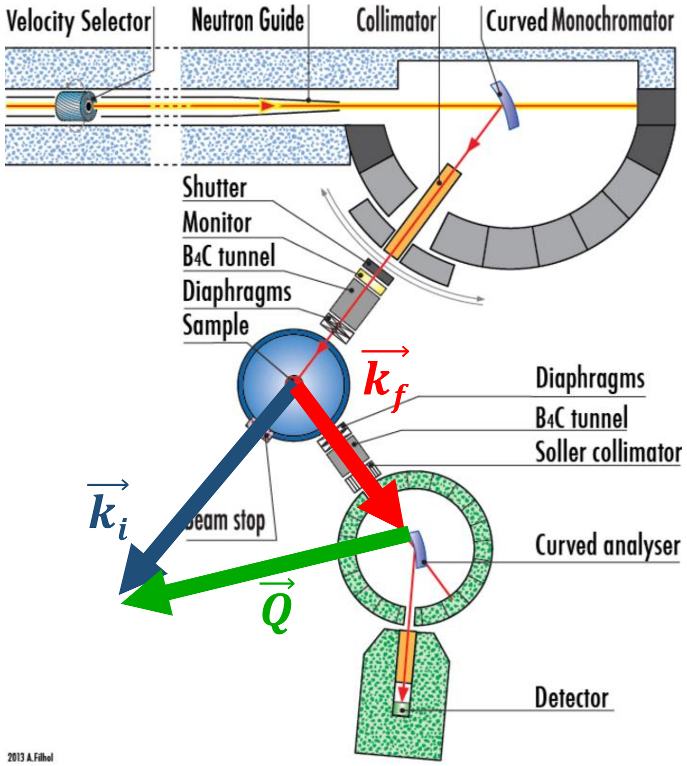


$CuSO_4 \bullet 5D_2O$
Mourigal *et al.*, Nat. Phys. **9**, 435 (2013)

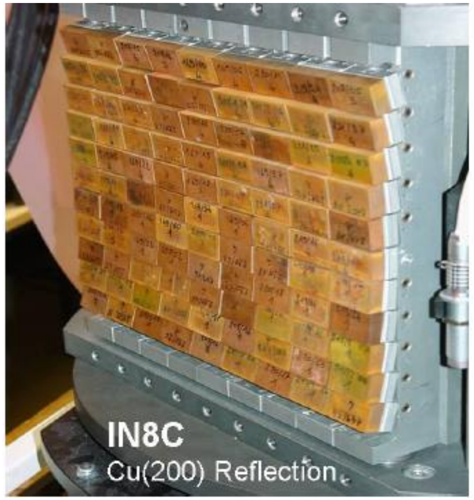
Neutrons scattering is the **most « natural »** way to probe **magnetic systems:**
« simple », versatile, high-energy resolution …

Indirect geometry : k_f fixed

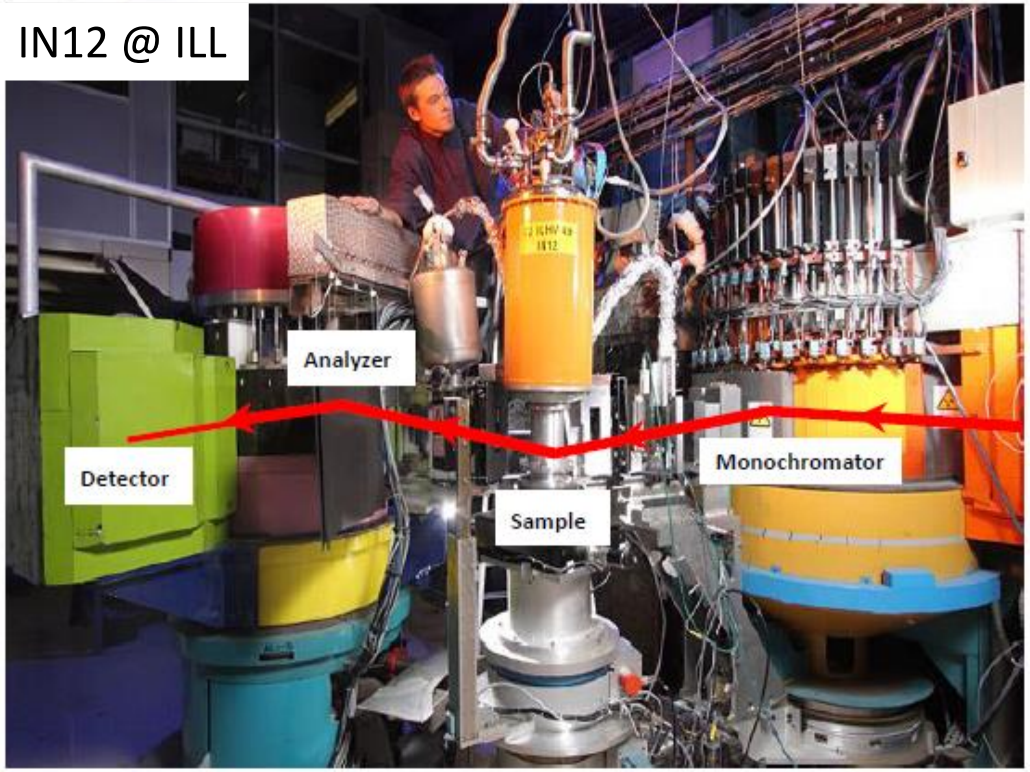
Triple-axis spectrometer (TAS)



$$\lambda = 2\, d \sin(\theta)$$
$$\lambda = 2\pi / |k|$$



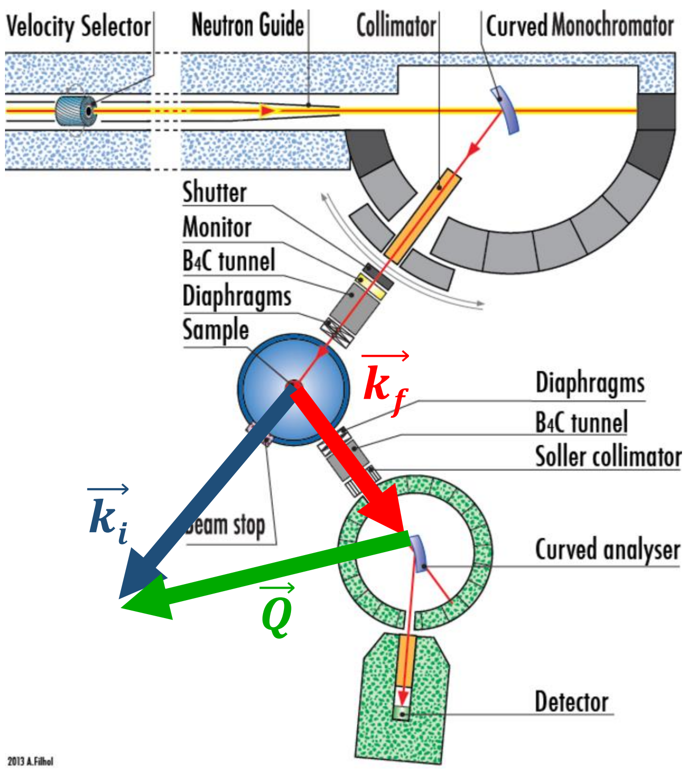
IN12 @ ILL



$$\Delta E = \frac{\hbar}{2m}\left(k_i^2 - k_f^2\right)$$

$$\vec{Q} = \vec{k_i} - \vec{k_f}$$

Indirect geometry : k_f fixed



$$\Delta E = \frac{\hbar}{2m}\left(k_i^2 - k_f^2\right)$$

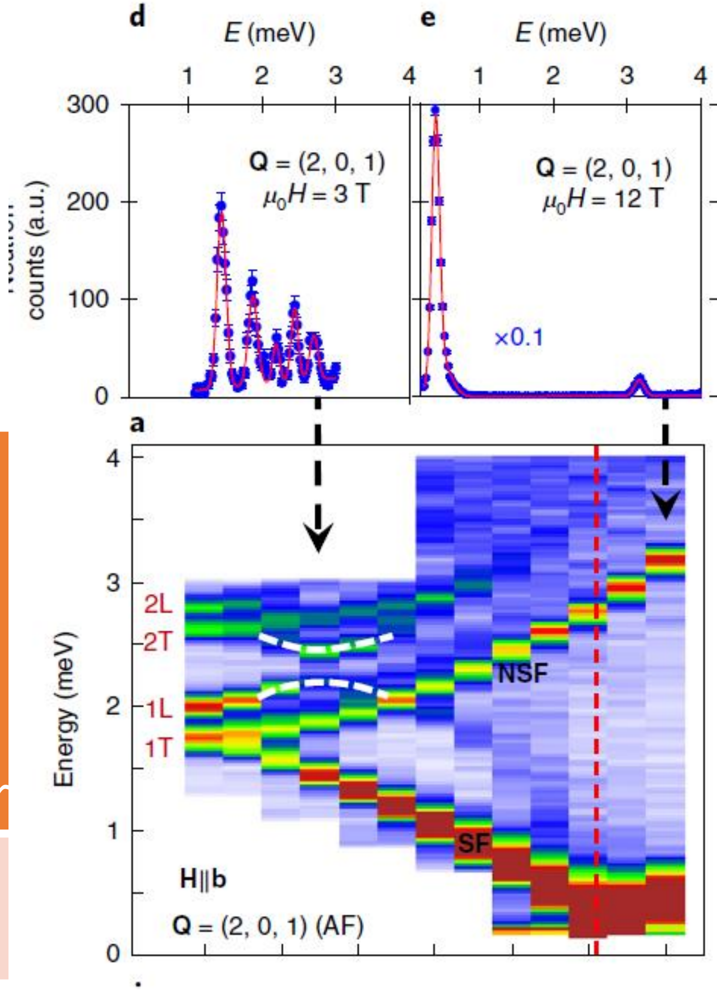
$$\vec{Q} = \vec{k_i} - \vec{k_f}$$

Triple-axis spectrometer (TAS)

Flux	$10^7 – 10^8$ n/s/cm²
Spatial angle	0.015 steradians
Energy transfer	single value

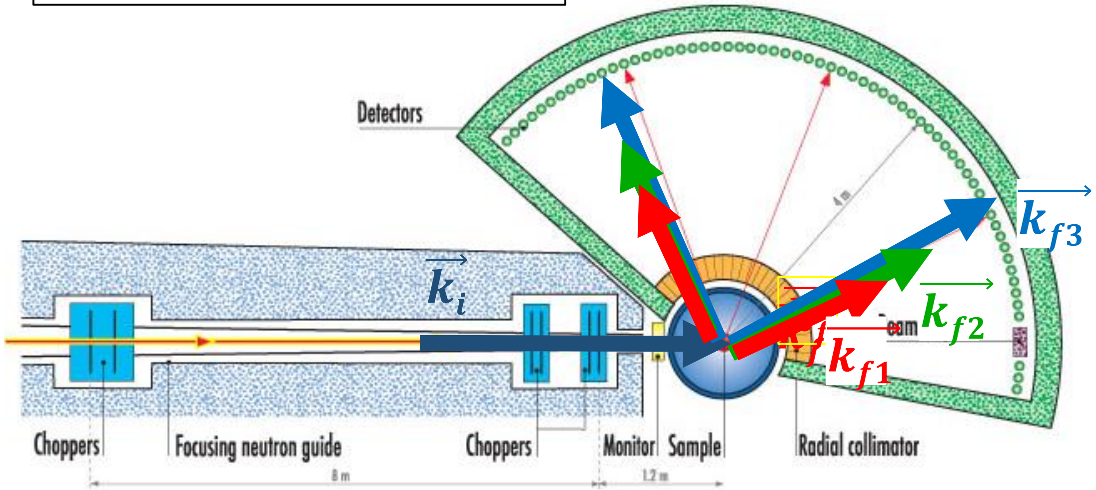
Pros	• High-flux (onto sample) • robust and simple measurements • Good for parametric studies (*Temperature, magnetic-field …*) • Polarized neutrons (cryopad …) • focus **onto** what you are looking for
Cons	focus **only** onto what you are looking for ⇔ no real mapping of S($\boldsymbol{Q}$, ω)

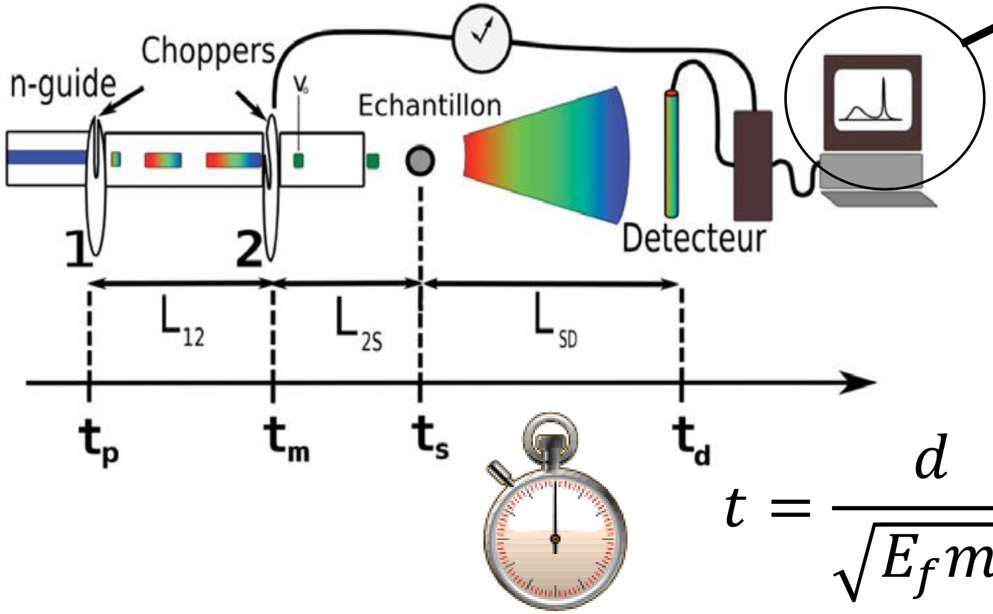
Natural with continuous source (reactor)



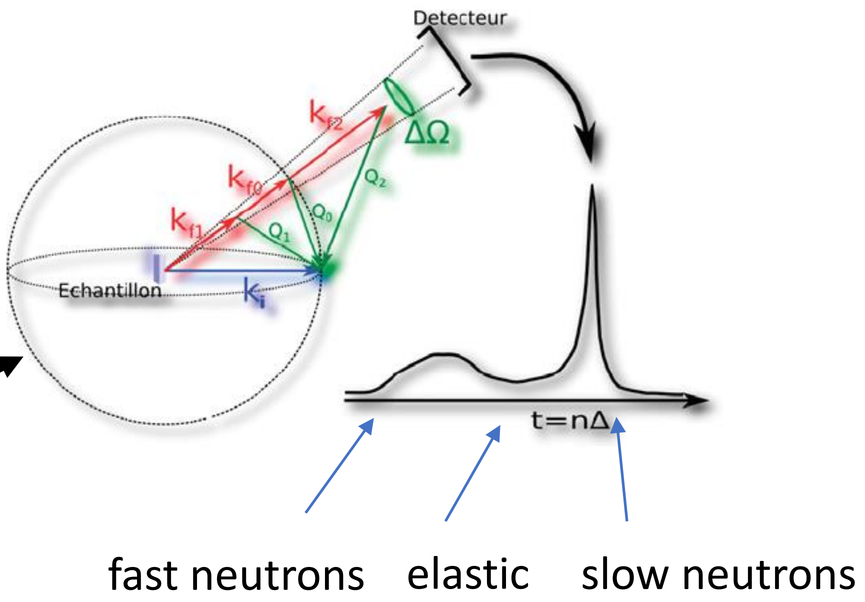
direct geometry : k_i fixed

Time of flight spectrometer (TOF)





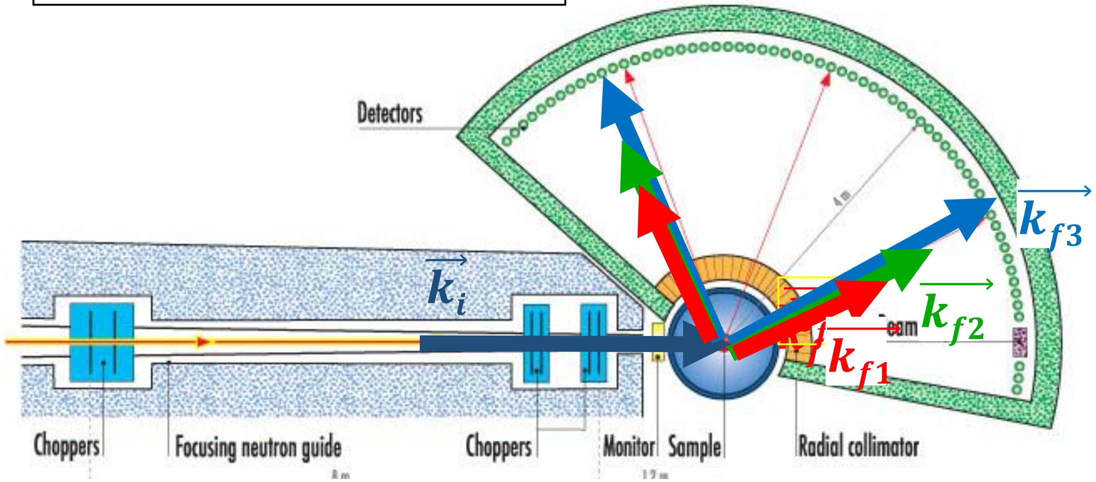
$$t = \frac{d}{\sqrt{E_f m_n}}$$

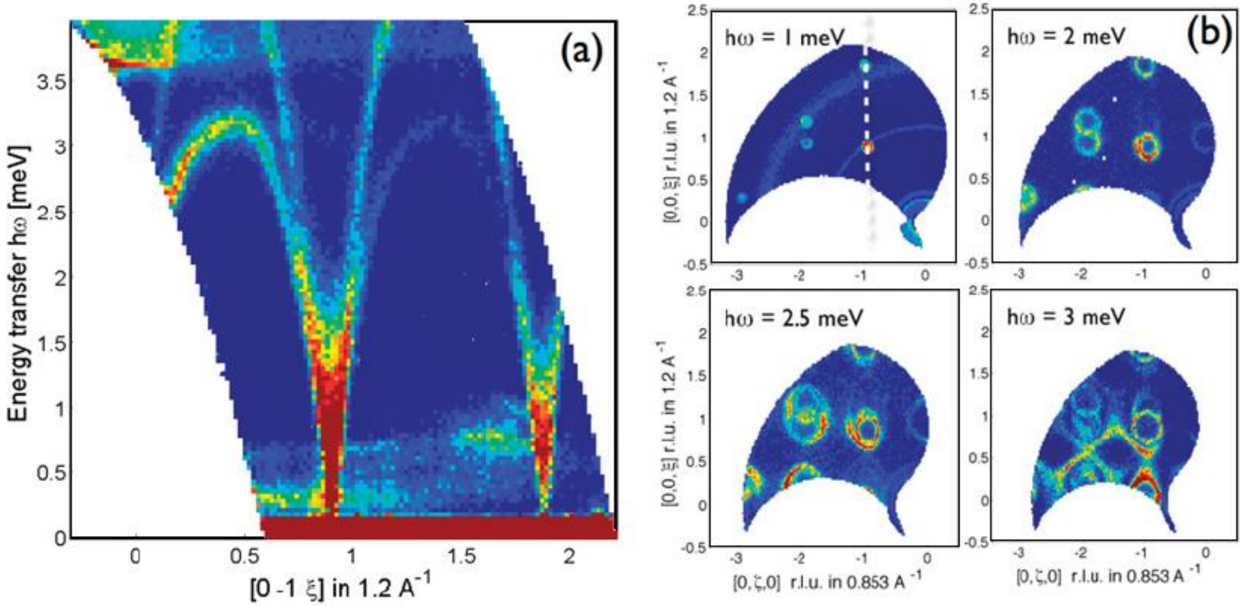


Historically very suitable for powders and soft matter

Now : for monocristals, need to rotate the sample by steps of 1 deg → quite fastidious and long direct geometry : k_i fixed

Time of flight spectrometer (TOF)





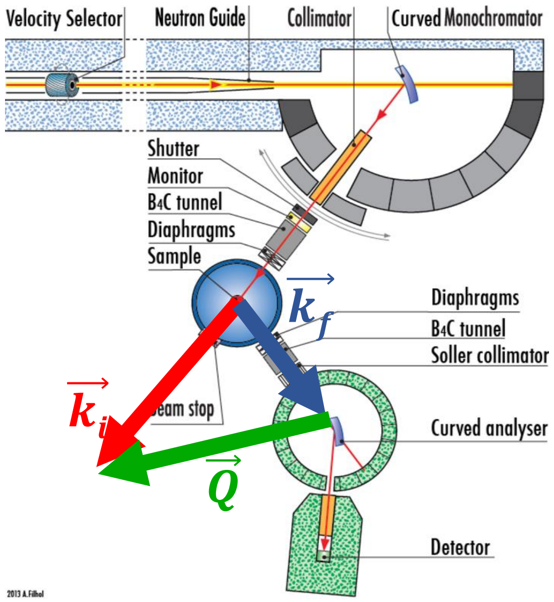
Flux	$10^4 – 10^6$ n/s/cm²
Spatial angle	π steradians
Energy transfer	Continuous

Pros	• Large covering ⇔ mapping of S($\boldsymbol{Q}$, ω) • Good resolution in $\boldsymbol{Q}$ and E
Cons	• parametric studies (single crystal) • Complex set of data; reduction complicated • Low-flux onto sample

Natural with pulsed source (ISIS, ESS …)

Triple-axis spectrometer (TAS)

indirect geometry
⇔ k_f fixed



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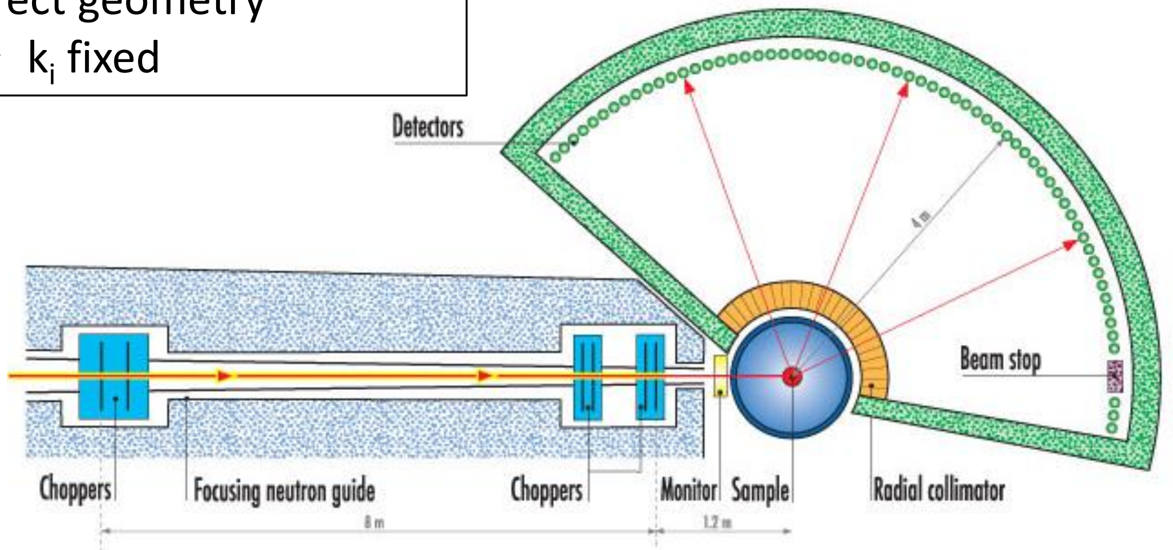
Time of flight spectrometer (TOF)

direct geometry
⇔ k_i fixed



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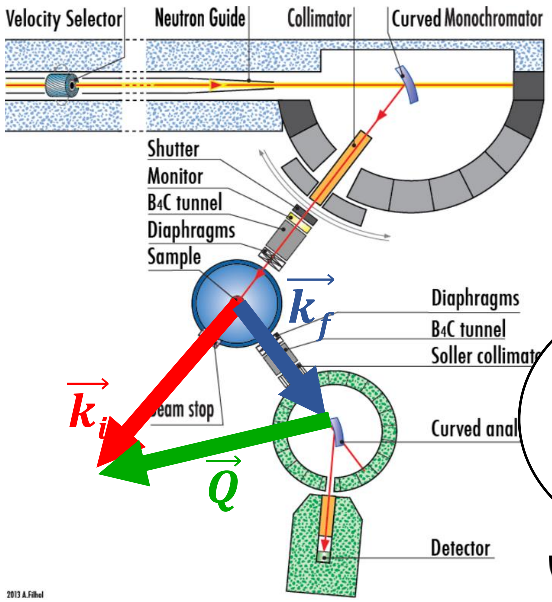

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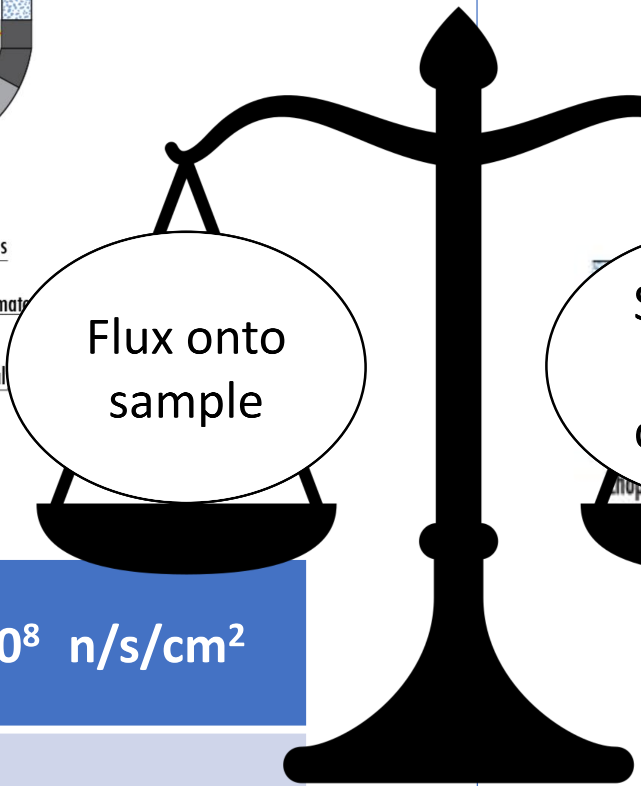

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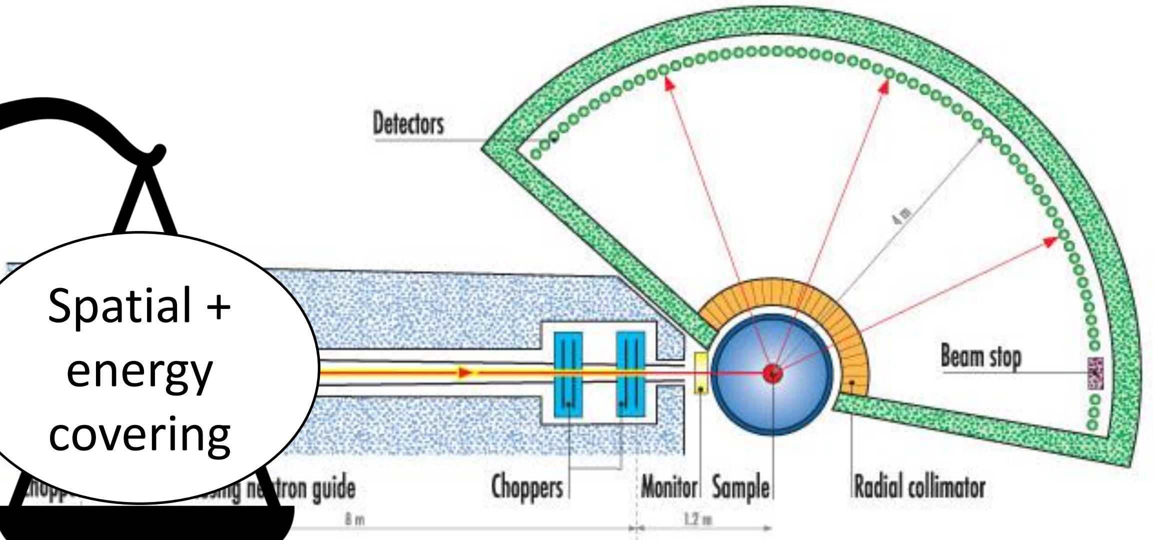

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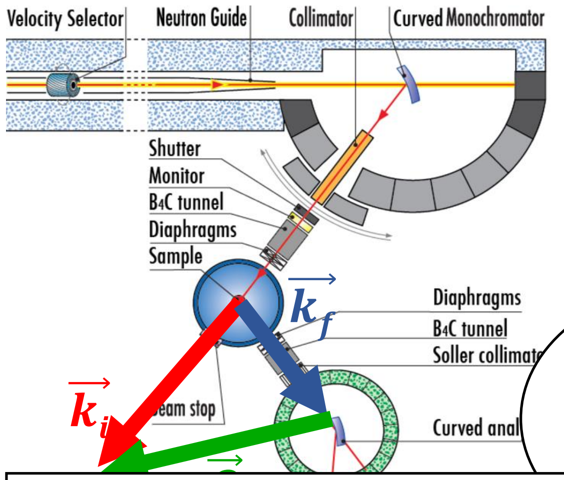
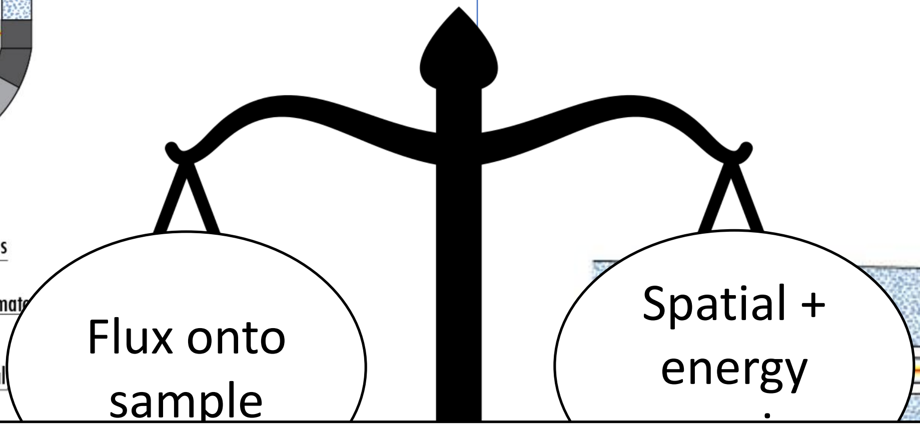
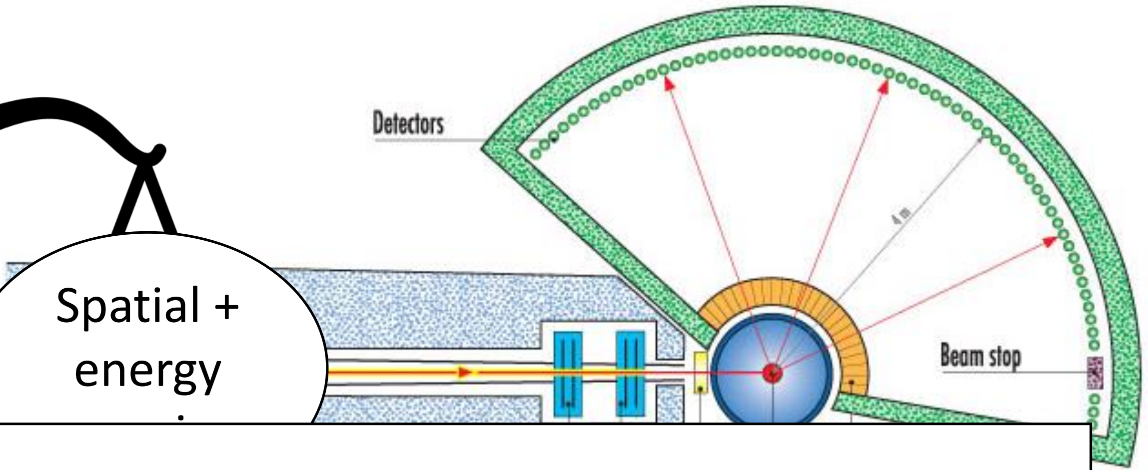


Time of flight spectrometer (TOF)

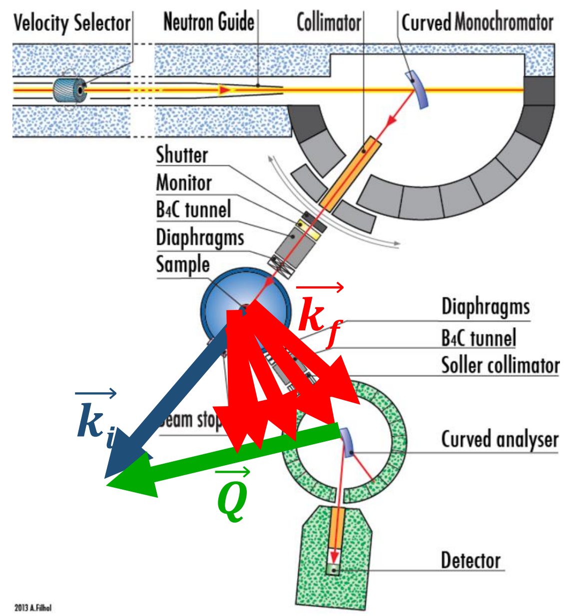


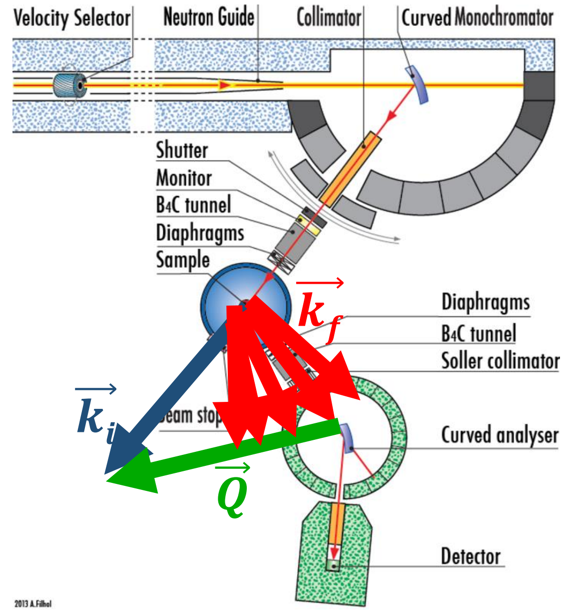


F	
Spati	
Energy	

Q1 : can **TAS be more efficient** ?
i.e. covering a larger volume of space and energy ?
➔ **MULTIPLEXING**

Q2: Can **TOF spectrometer be more efficient** ?
i.e. having higher flux onto sample ?
➔ **INDIRECT GEOMETRY (?).**


Velocity Selector
Neutron Guide
Collimator
Curved Monochromator
Shutter
Monitor
B4C tunnel
Diaphragms
Sample
Diaphragms
B4C tunnel
Soller collimator
Curved analyser
Detector
$\vec{k_f}$
$\vec{k_i}$
$\vec{Q}$
2013 A.Filhol



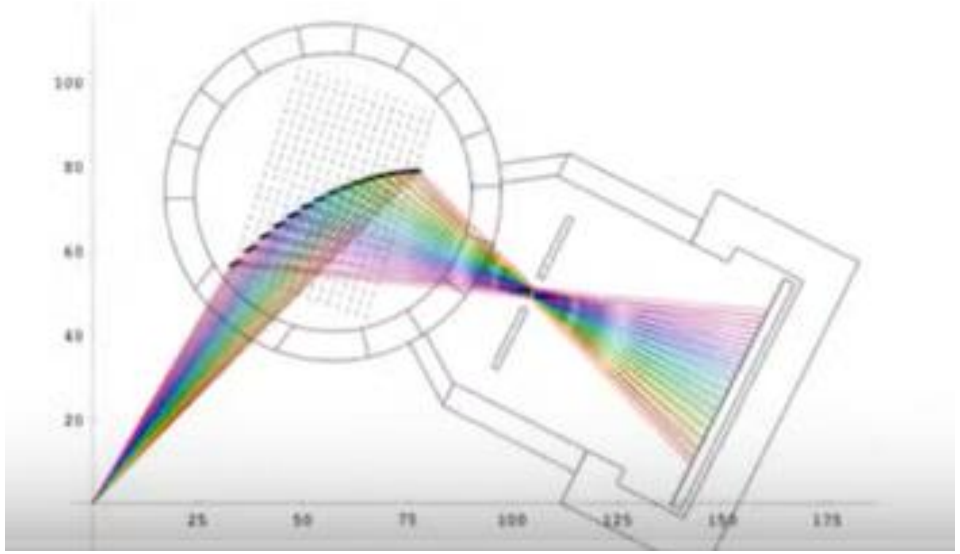
1st attempt for multiplexing

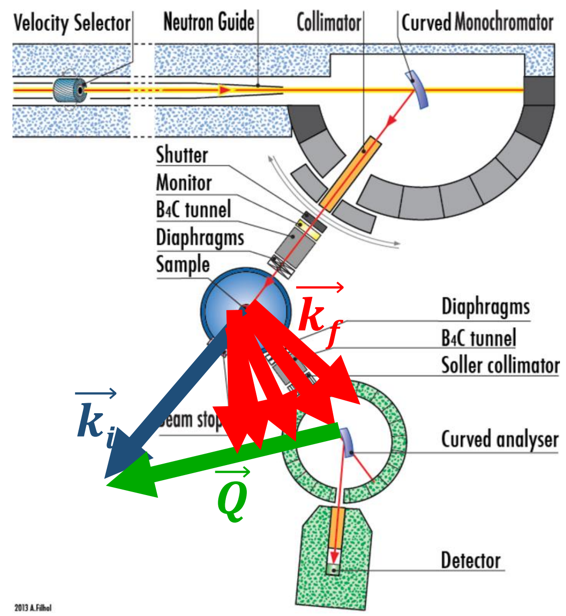
RITA-1, II, UFO …

Horizontal scattering

Prismatic effect

/ Rowland geometry

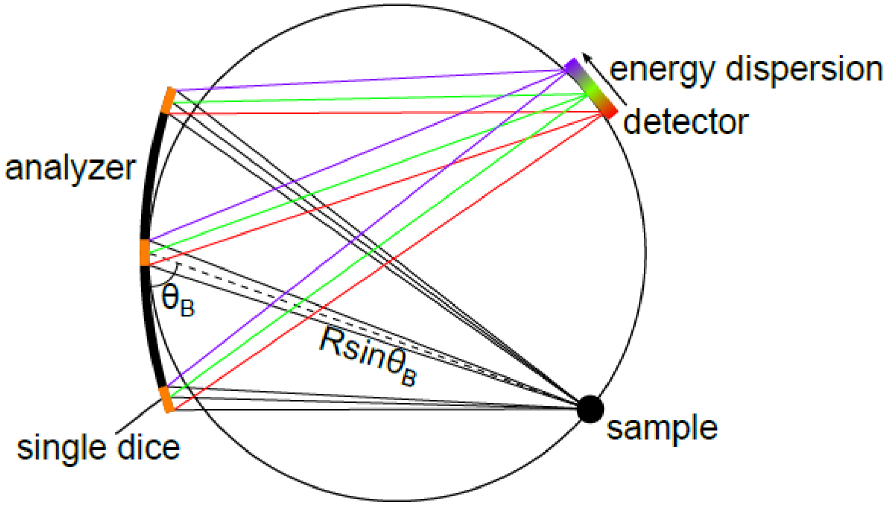


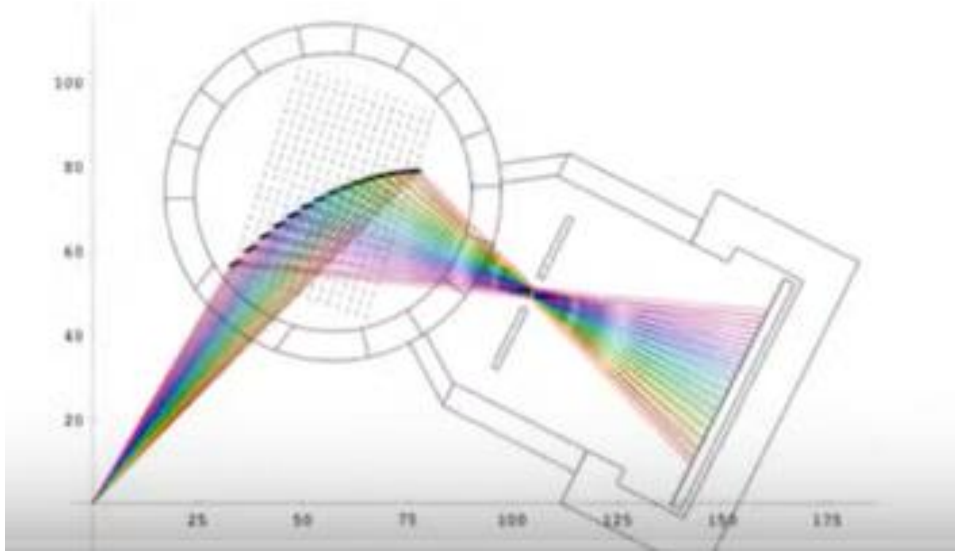


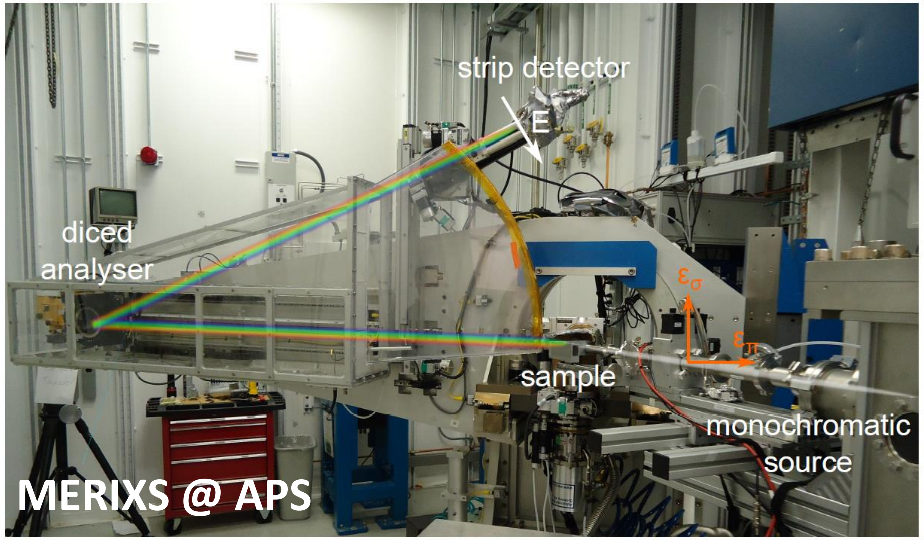
1st attempt for multiplexing

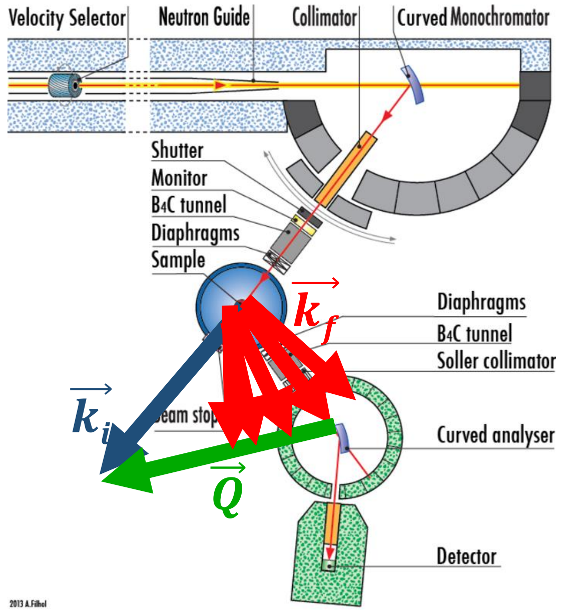
RITA-1, II, UFO …
Horizontal scattering
Prismatic effect
/ Rowland geometry

Prismatic effect / Rowland geometry
(very often used in X-ray spectroscopy)









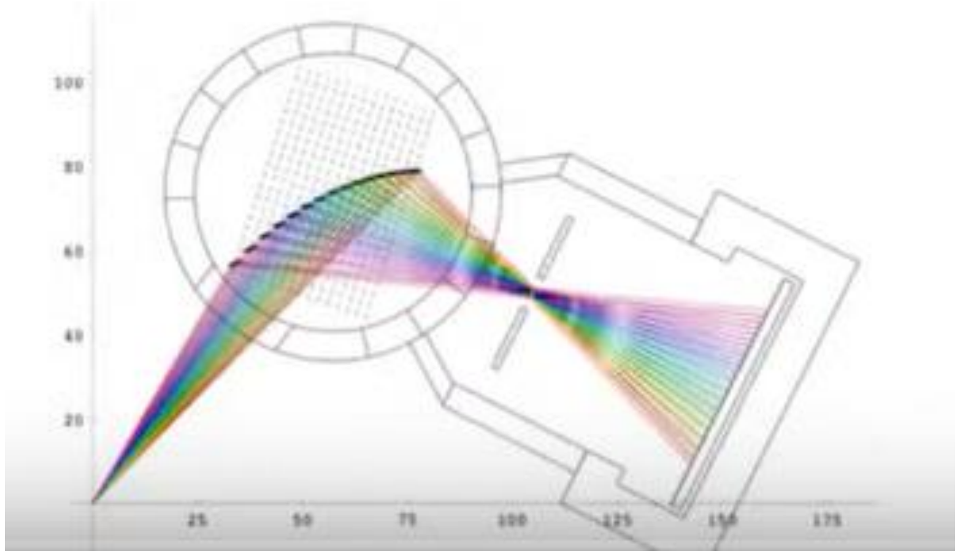
1st attempt for multiplexing

RITA-1, II, UFO …

Horizontal scattering

Prismatic effect

/ Rowland geometry

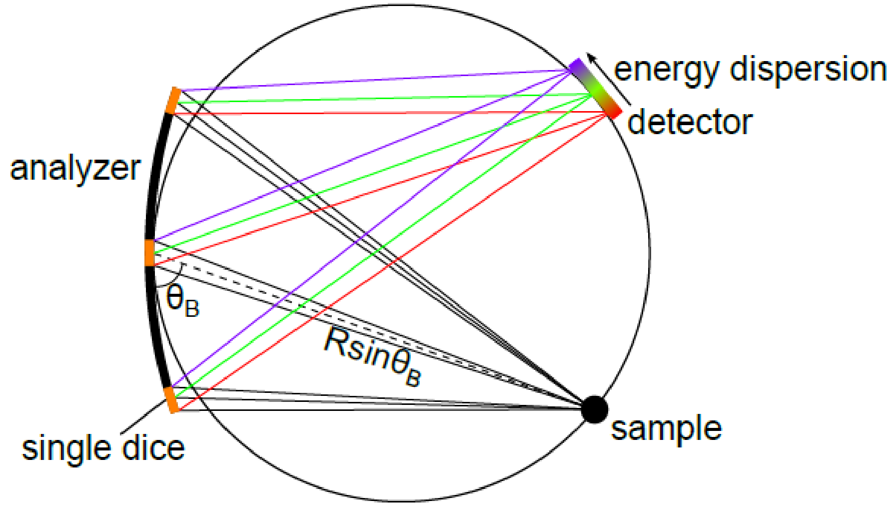


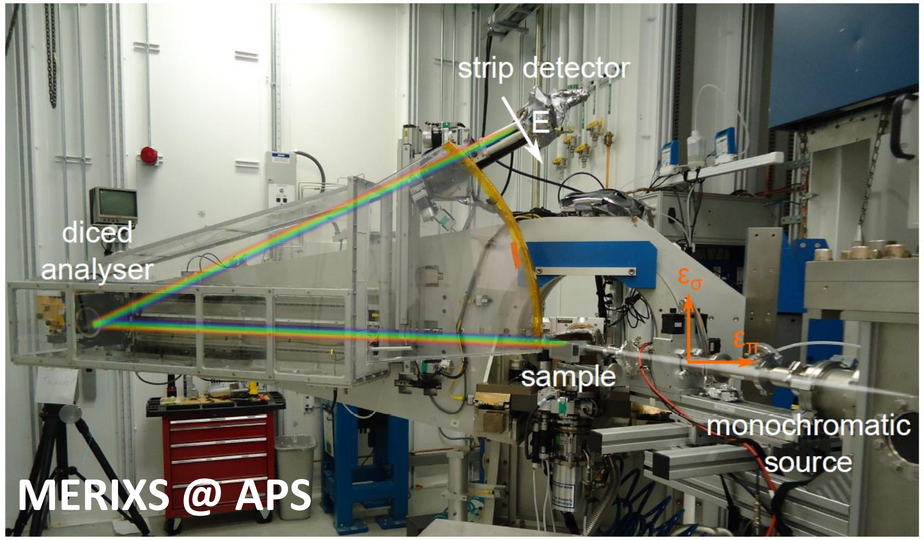
Problem :

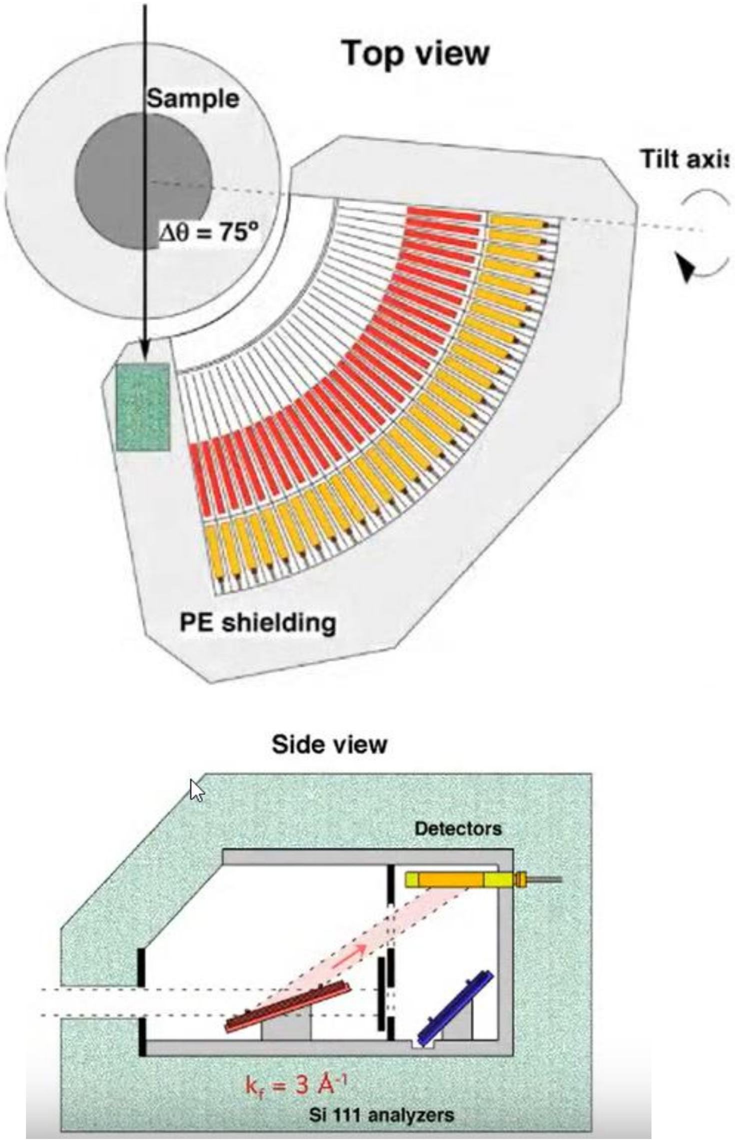
cross-talking …

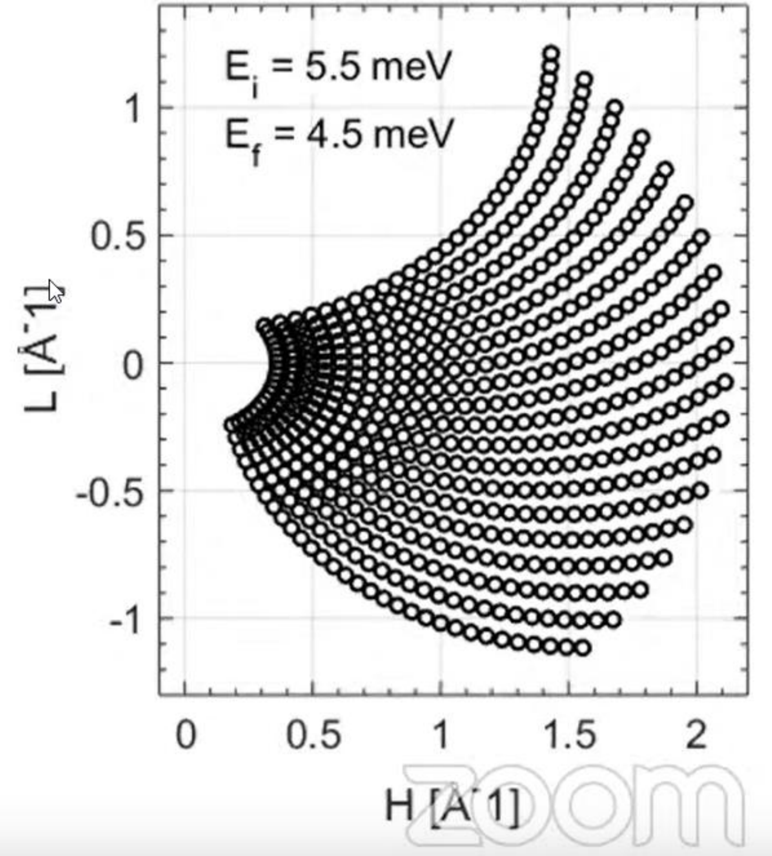
Prismatic effect / Rowland geometry

(very often used in X-ray spectroscopy)



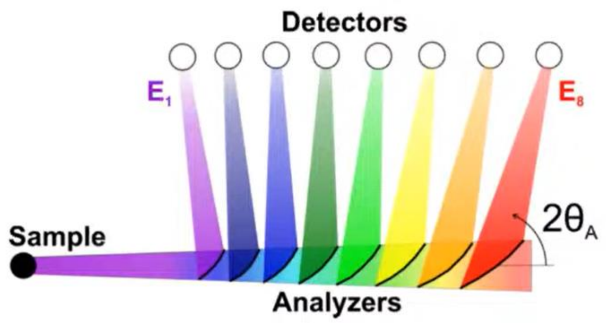


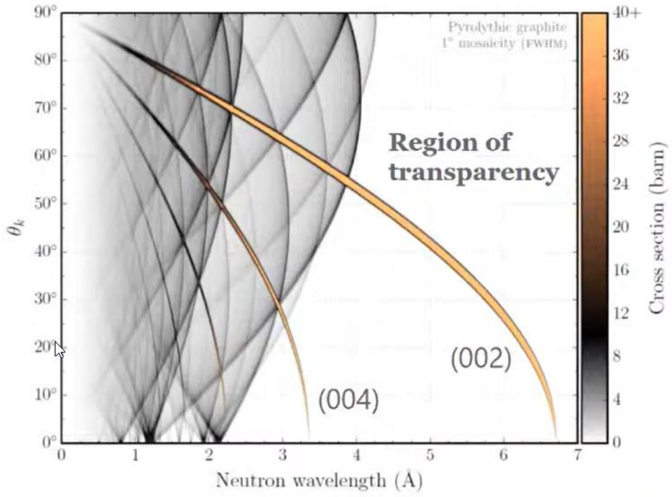


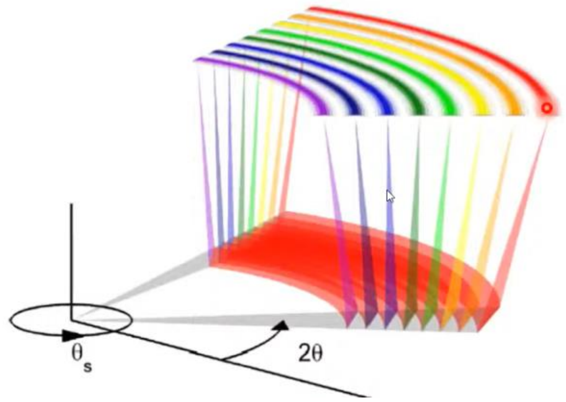


Vertical scattering
Transportable, tiltable

CAMEA @ PSI

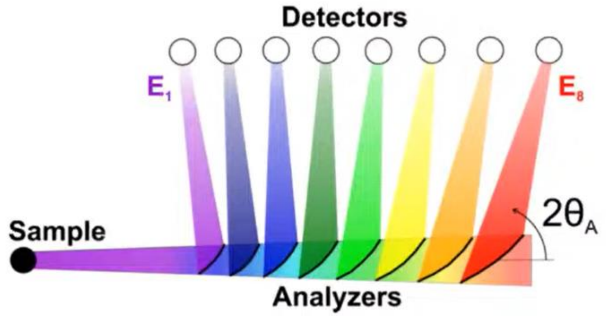

Detectors
E1
E8
Sample
2θA
Analyzers

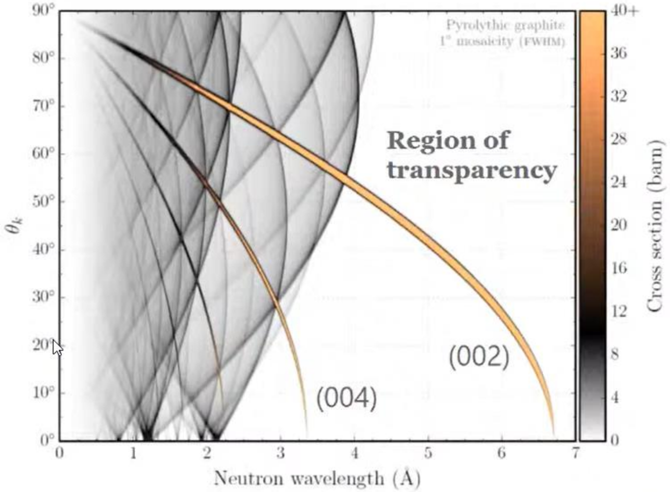

Pyrolythic graphite
1° mosaicity (FWHM)
Region of transparency
(002)
(004)
Neutron wavelength (Å)
Cross section (barn)

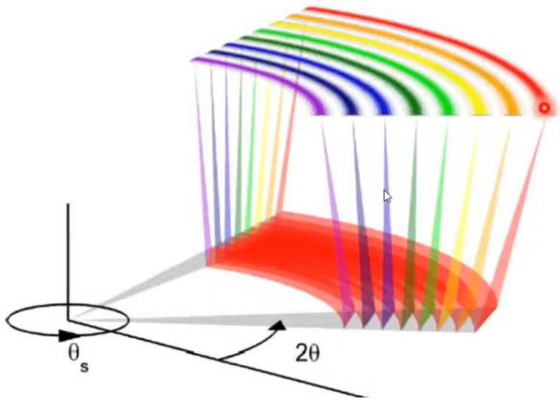

θs
2θ


CAMEA

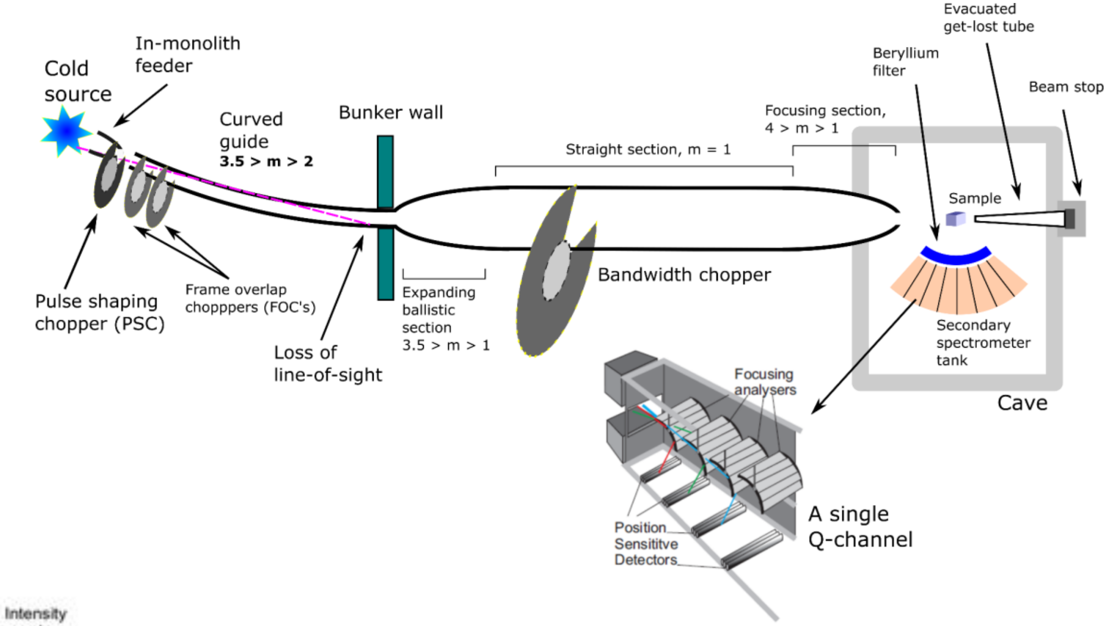
CAMEA @ PSI

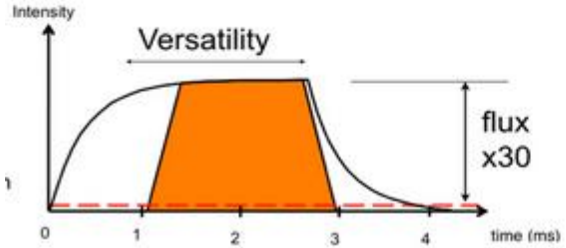


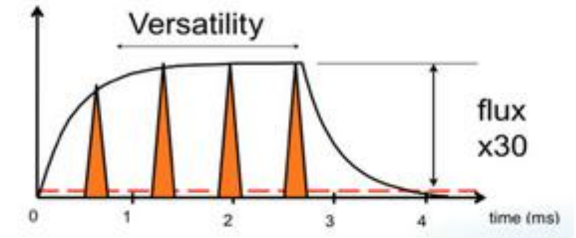




BIFROST @ ESS … the beast !

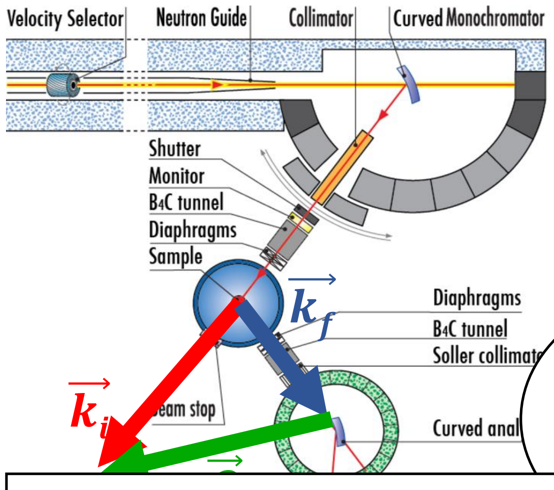


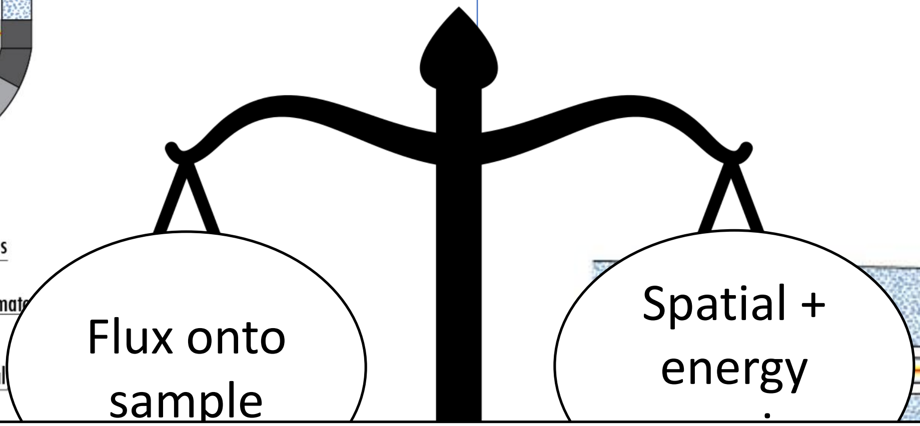




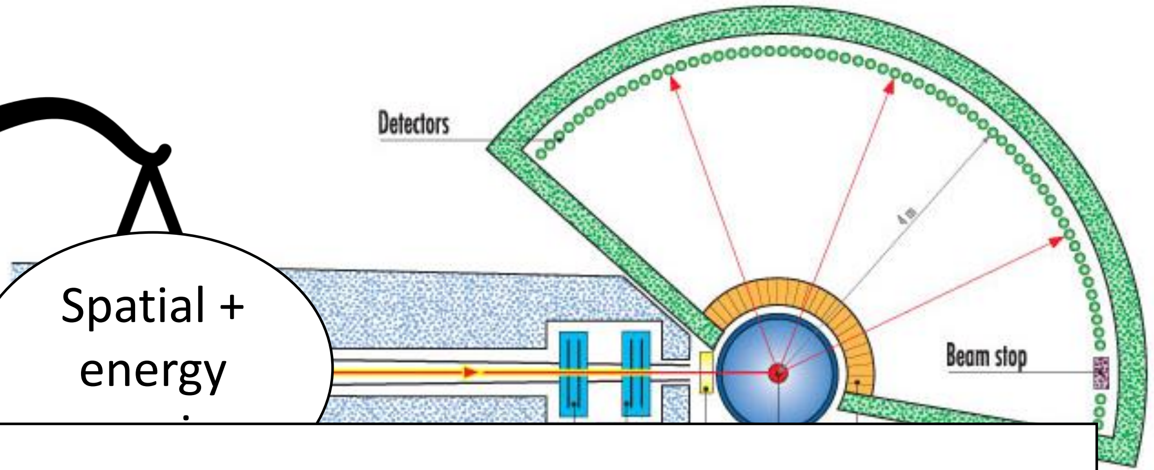
Polychromatic incoming beam : possibility to manipulate the pulse
+
Multiplexing

Triple-axis spectrometer (TAS)





Time of flight spectrometer (TOF)

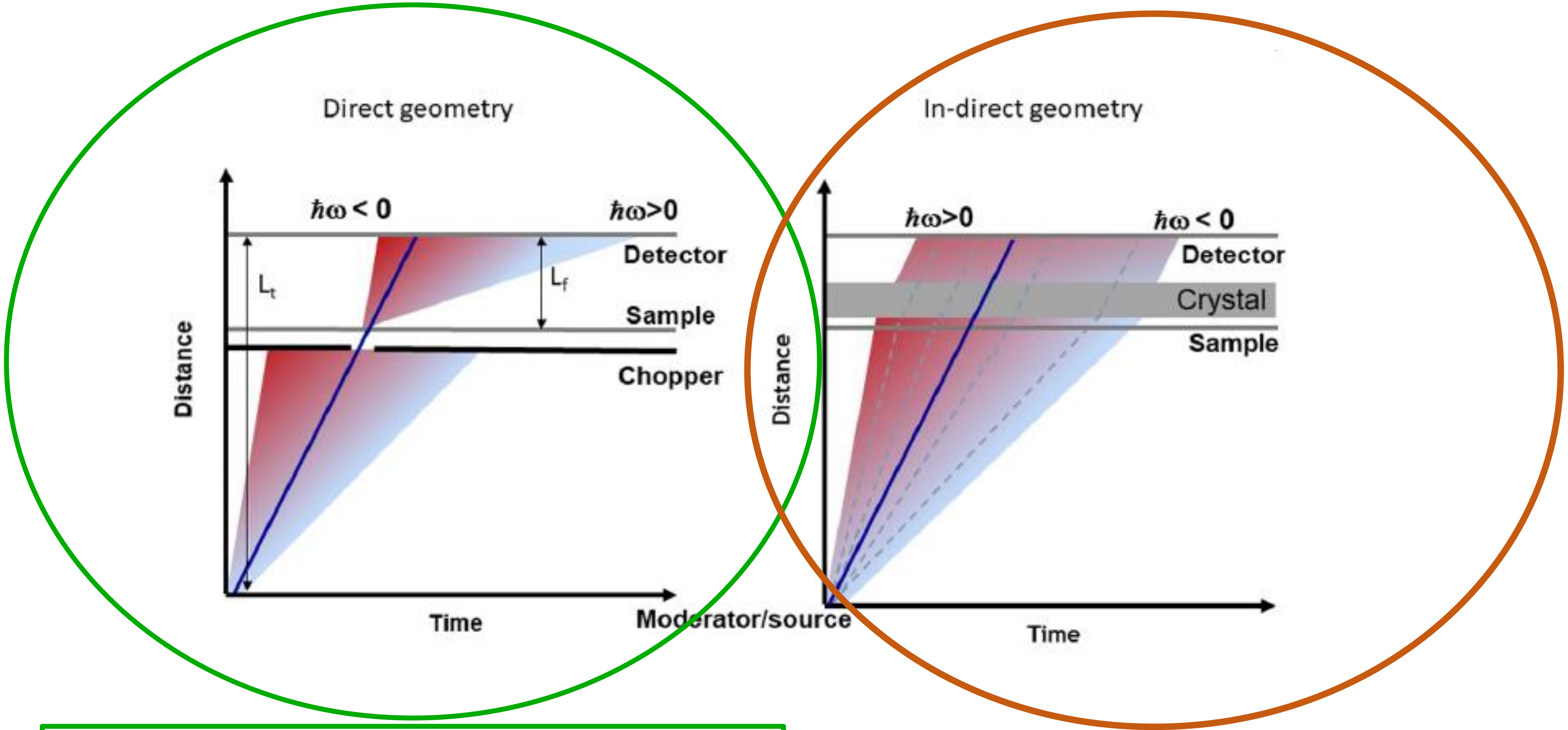


Spati

Energy

Q1 : can **TAS be more efficient** ?
i.e. covering a larger volume of space and energy ? ✓
➔ **MULTIPLEXING**

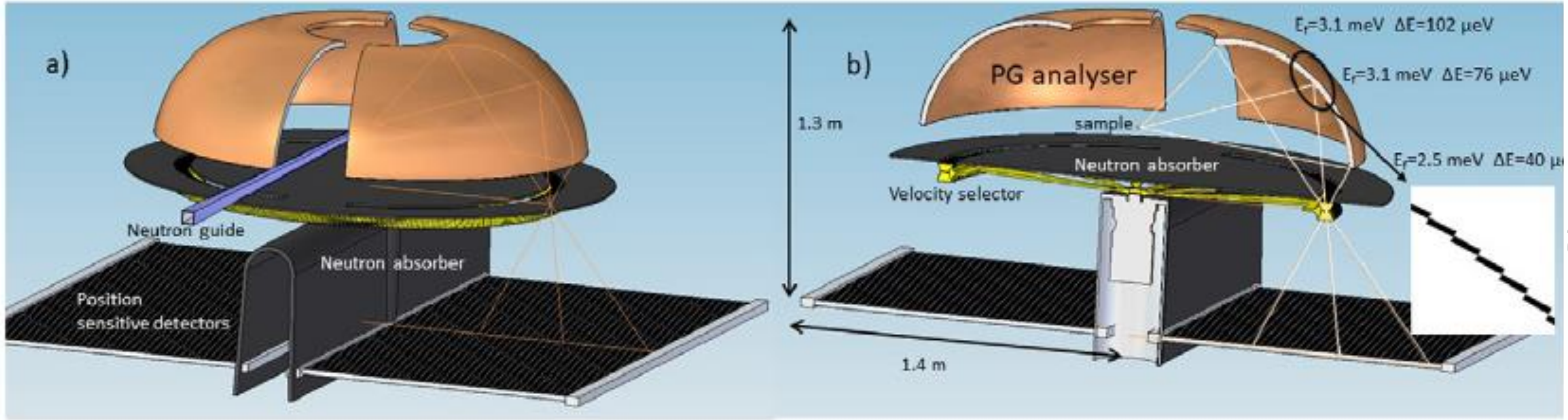
Q2: Can **TOF spectrometer be more efficient** ?
i.e. having higher flux onto sample ?
➔ **INDIRECT GEOMETRY (?).**

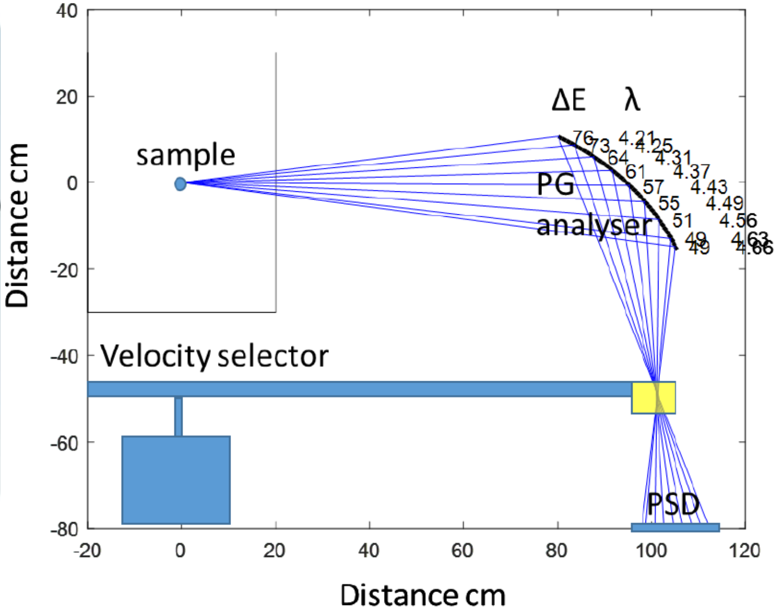


The usual one : IN5, SHARP(+), LET, FOCUS …

?

Energy resolution depends of the **overall instrument length** (guide + spectrometer) rather than just the secondary spectrometer



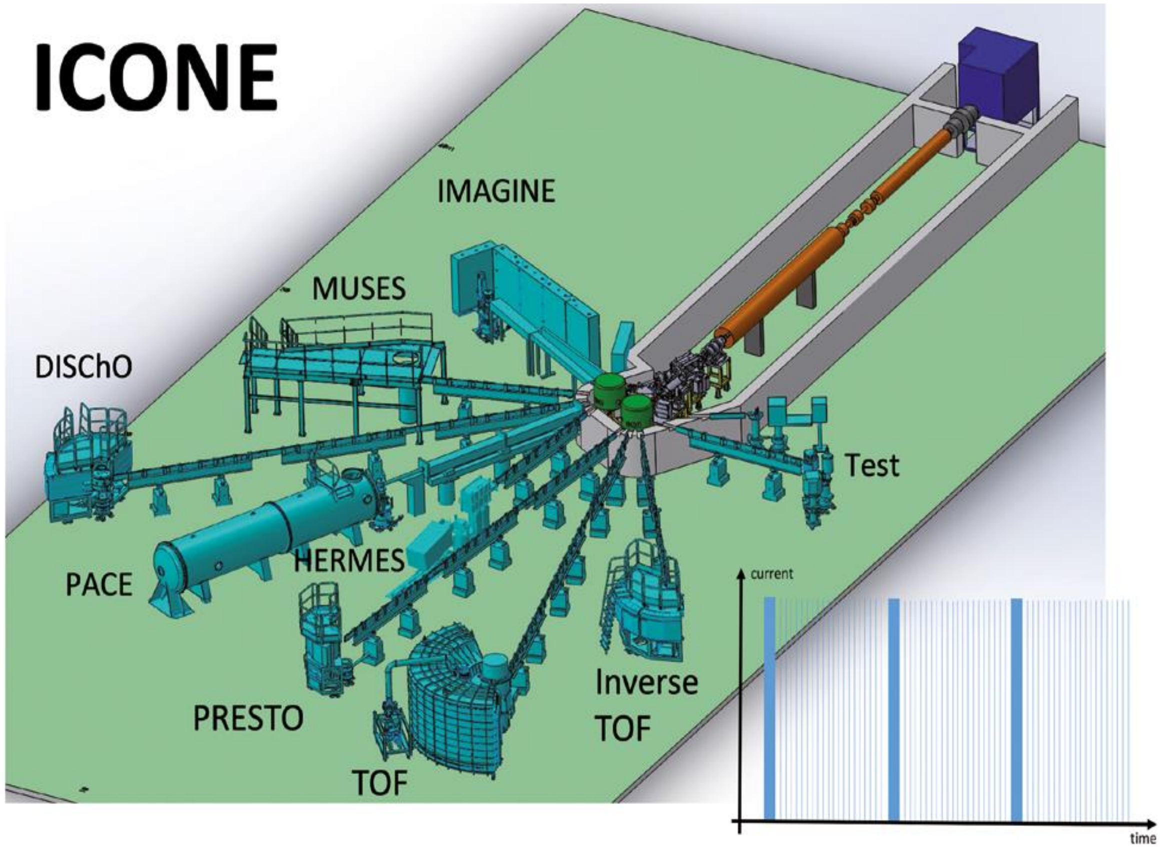


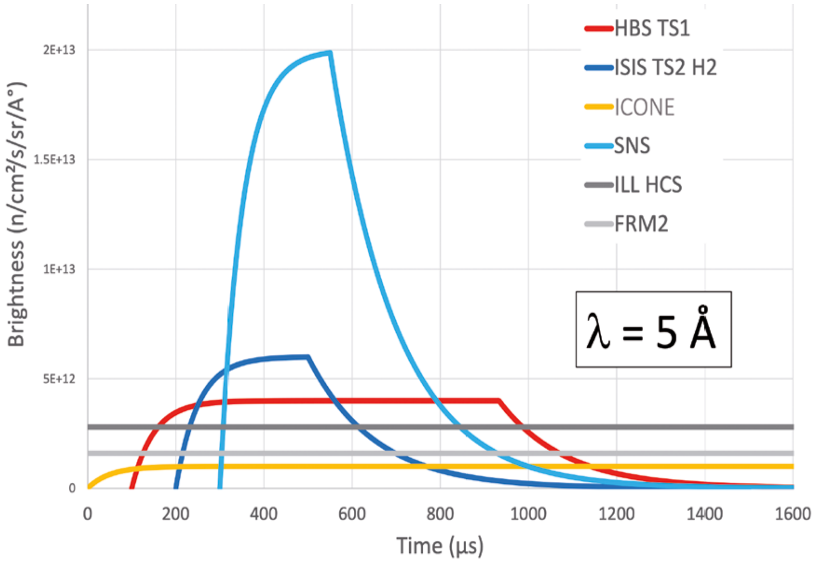
Prismatic effect + ≃ 2 π stéradian covering + compact

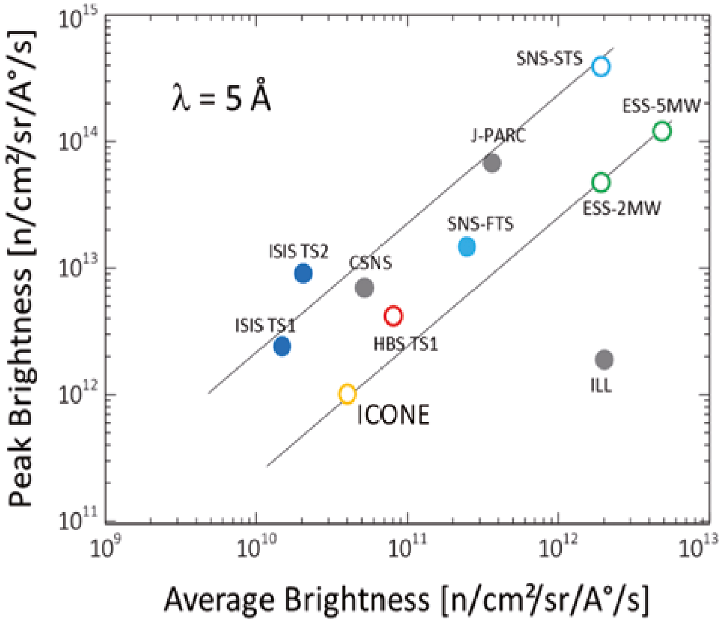
indirect geometry:

- the second spectrometer is compact
  - → **94 L** vs **8000 L** for LET
  - → cheaper (less ^{3}H detector)

- 30 to 75 more flux onto sample vs LET
  - → possibility for parametric studies (?) in TOF mode


ICONE
IMAGINE
MUSES
DISChO
Test
PACE
HERMES
PRESTO
Inverse
TOF
TOF
current
time


HBS TS1
ISIS TS2 H2
ICONE
SNS
ILL HCS
FRM2
λ = 5 Å
Brightness (n/cm²/s/sr/A°)
Time (µs)

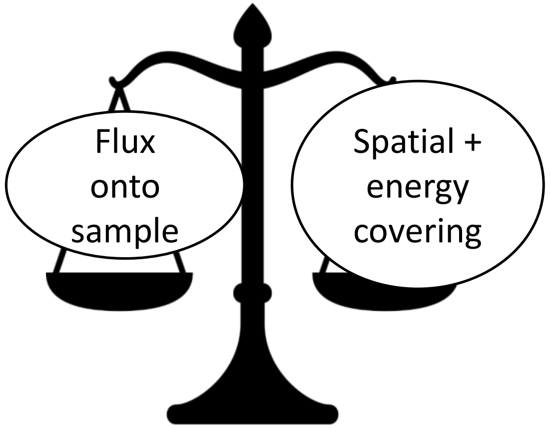

λ = 5 Å
SNS-STS
ESS-5MW
J-PARC
ESS-2MW
SNS-FTS
ISIS TS2
CSNS
ISIS TS1
HBS TS1
ICONE
ILL
Peak Brightness [n/cm²/sr/A°/s]
Average Brightness [n/cm²/sr/A°/s]

TAS McSTAS Simulation (@Xavier)

Compare flux onto sample with actual sources

Which spectrometer for ICONE (?)

Flux vs info



Multiplexing ? @ BIFROST bis
TOF ? @ MUSHROOM / SHARP+

For who ?

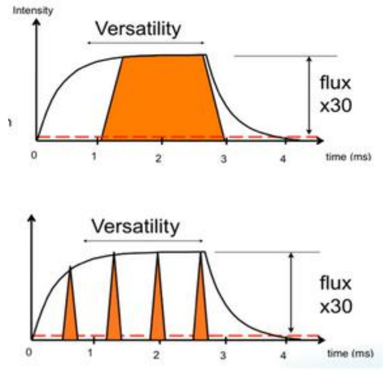
versatility (@SHARP+) VS very specific

SFN questionnary

Brainstorming

Spectrometer ?

Long pulse (2 ms)



What to do with it ?

- ESS type : flexible but complex
- ILL type (short pulse using choppers) : less flexible but we know what we do

Polychromatic beam ⇔
Indirect geometry might be more adapted

@ MUSHROOM
@ BIFROST

Cost (ideally = 10 M€)

Indirect geometry ⇔ 2nd spectrometer compact = less ^{3}H detector but need more sophisticated guide
@ BIFROST = 150 m of guide → ideally we should do 40 m (~1/4 of BIFROST)