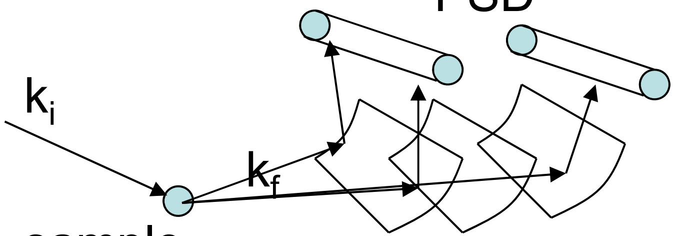
CAMEA

Felix Groitl, Jonas Okkels Birk, Marton Marko, Paul Freeman, Mads Bertelsen, Jacob Larsen, Fanni Juyrani, Christof Niedermayer, Kim Lefmann, Niels Bech Christensen,…



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Niels Bohr Institute

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

PNAS

Quantum dynamics and entanglement of spins on a square lattice

N. B. Christensen*†‡, H. M. Rønnow†§, D. F. McMorrow*¶‖, A. Harris
L. P. Regnault¶¶, and G. Aeppli¶

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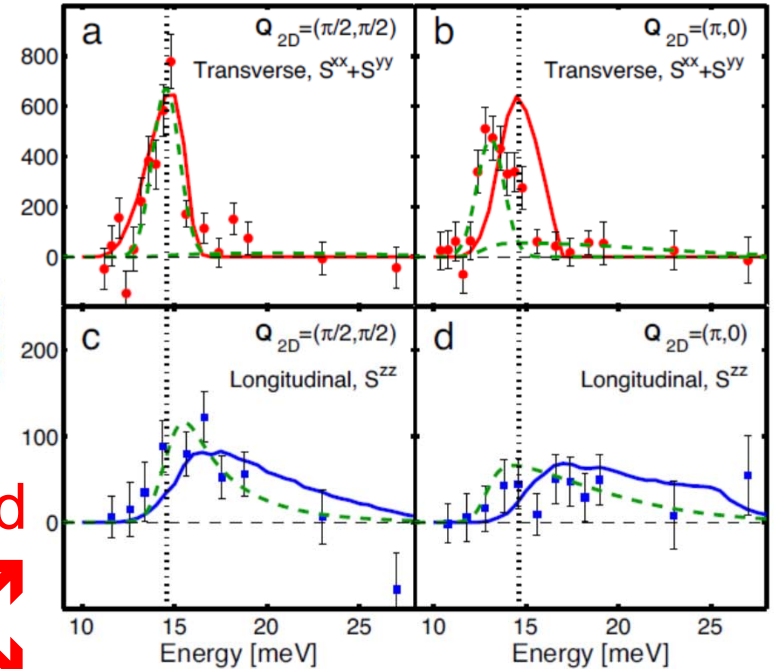
Scattering, ETH Zurich and Paul S… CH-5232 Villigen PSI, Switzerland; §L
Fédérale de Lausanne (EPFL), …erland; ¶London Centre for Nanotec
University College London, Lo… …ted Kingdom; ‖ISIS Facility, Rutherf
Kingdom; **Department of Ch… …rsity of Edinburgh, Edinburgh, EH9 3JJ, U
France; ‡‡Oxford Physics, Claren… …boratory, Parks Road, Oxford OX1 3PU, United K
1TL, United Kingdom; and ¶¶CEA, Grenoble, Département de Recherche Fondamentale

2007



Neutron spectroscopy statistically limited

$1\ cm^3$ for 1 week ↗

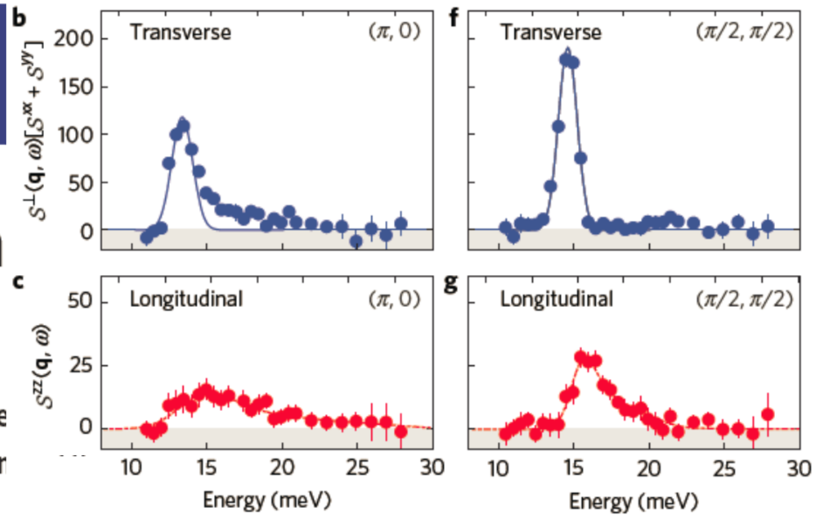
$3\ cm^3$ for 3 weeks ↘

nature physics
CEMBER 2014 | DOI: 10.1038/NPHYS3172

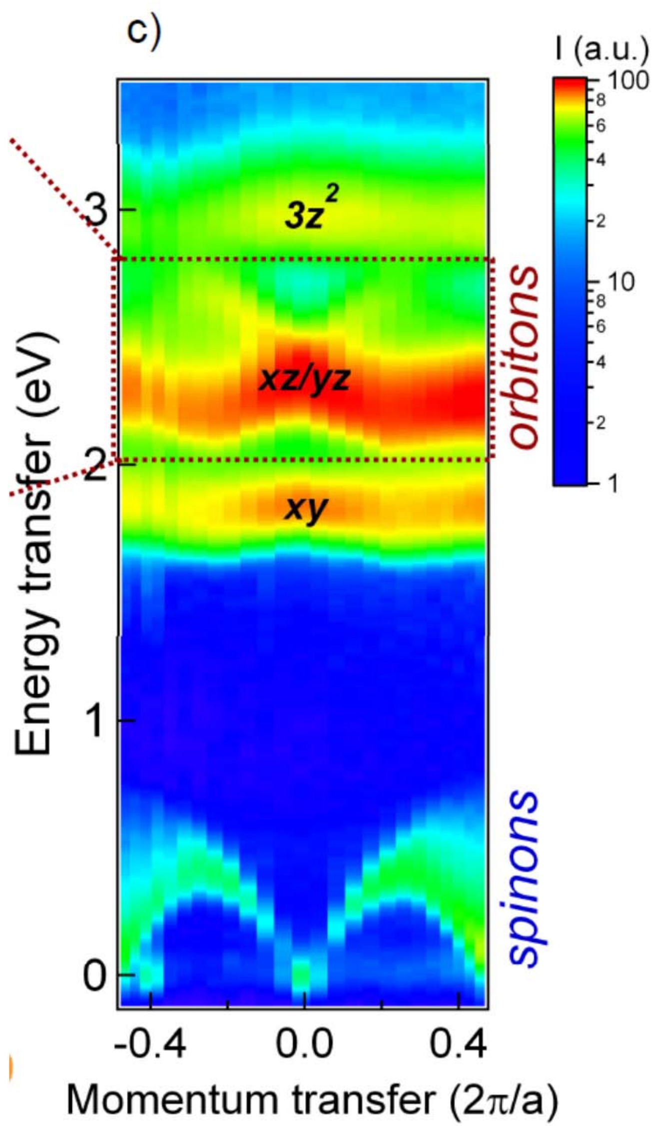
2014

Fractional excitations in the square-la quantum antiferromagnet

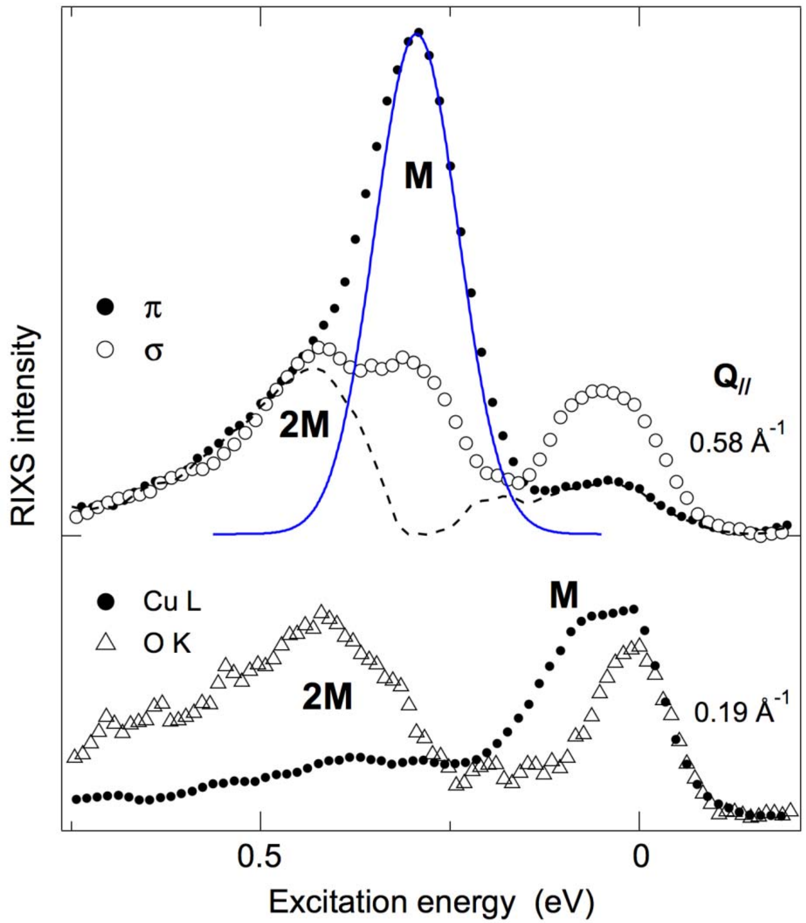
B. Dalla Piazza[1]*, M. Mourigal[1,2,3]*, N. B. Christensen[4,5], G. J. Nilsen[1,6], P. Tre
T. G. Perring[7], M. Enderle[2], D. F. McMorrow[8], D. A. Ivanov[9,10] and H. M. Rønr



Resonant Inelastic X-ray Scattering



Need better resolution and more quantitative scattering theory, but statistics is not a problem



Phonons vs. magnetic excitations

Phonons

$$\left(\frac{\partial^2\sigma}{\partial\Omega\partial E'}\right)_{phonon} \propto \frac{\sigma_{coh}}{4\pi}\frac{k_f}{k_i}\frac{(2\pi)^3}{v_0}\frac{1}{2M}\exp(-2W)x$$

$$\sum_s\sum_\tau \frac{(\vec{Q}\cdot\vec{e}_s)^2}{\omega_s}\left[(n(\omega_s)+1)\delta(\omega-\omega_s)\delta(\vec{Q}-\vec{q}-\vec{\tau})+n(\omega_s)\delta(\omega+\omega_s)\delta(\vec{Q}+\vec{q}-\vec{\tau})\right]$$

Increases with **Q**

Increases with T

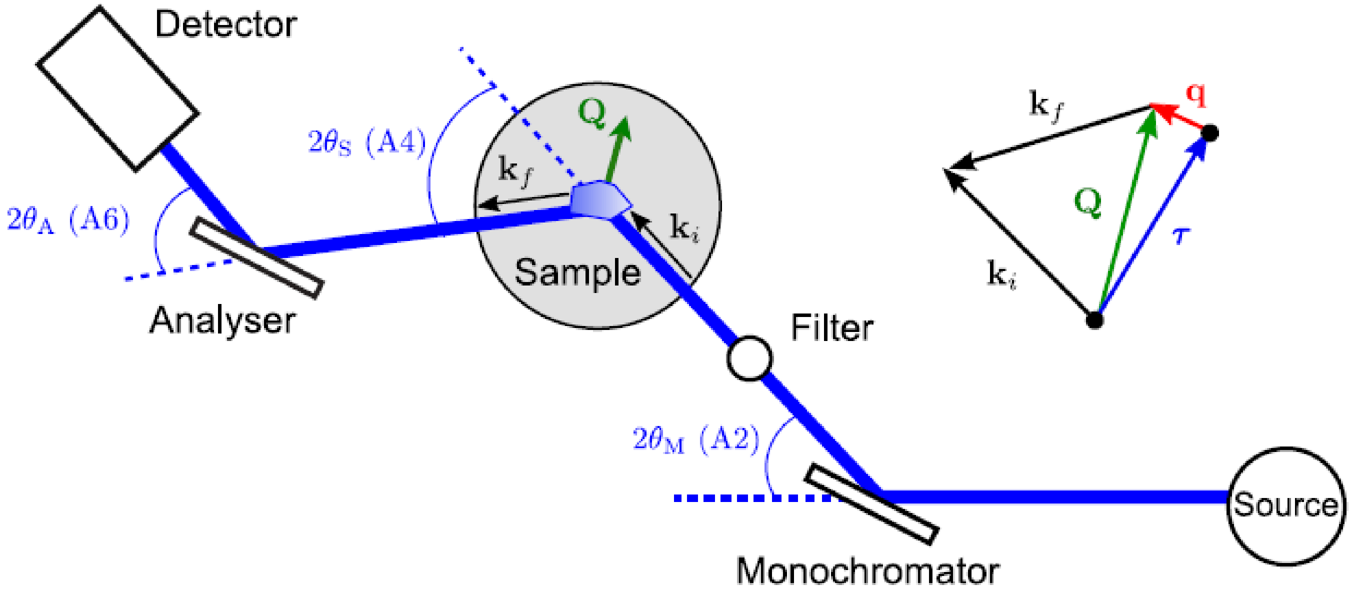
$$\left(\frac{\partial^2\sigma}{\partial\Omega\partial E'}\right)_{mag} \propto \frac{k_f}{k_i}\left\{\frac{1}{2}gF(\vec{Q})\right\}^2\sum_{\alpha\beta}\left(\delta_{\alpha\beta}-\hat{Q}_\alpha\hat{Q}_\beta\right)\sum_{ll'}\exp\left(i\vec{Q}\cdot(\vec{l}-\vec{l}')\right)\int\left\langle S_0^\alpha(0)S_l^\beta(t)\right\rangle\exp(-i\omega t)dt$$

Decreases with **Q**

Bose statistics for simple ordered systems (FM, AFM, etc.).
Spreads in **Q** and ħω at high T
Limited by sum-rules

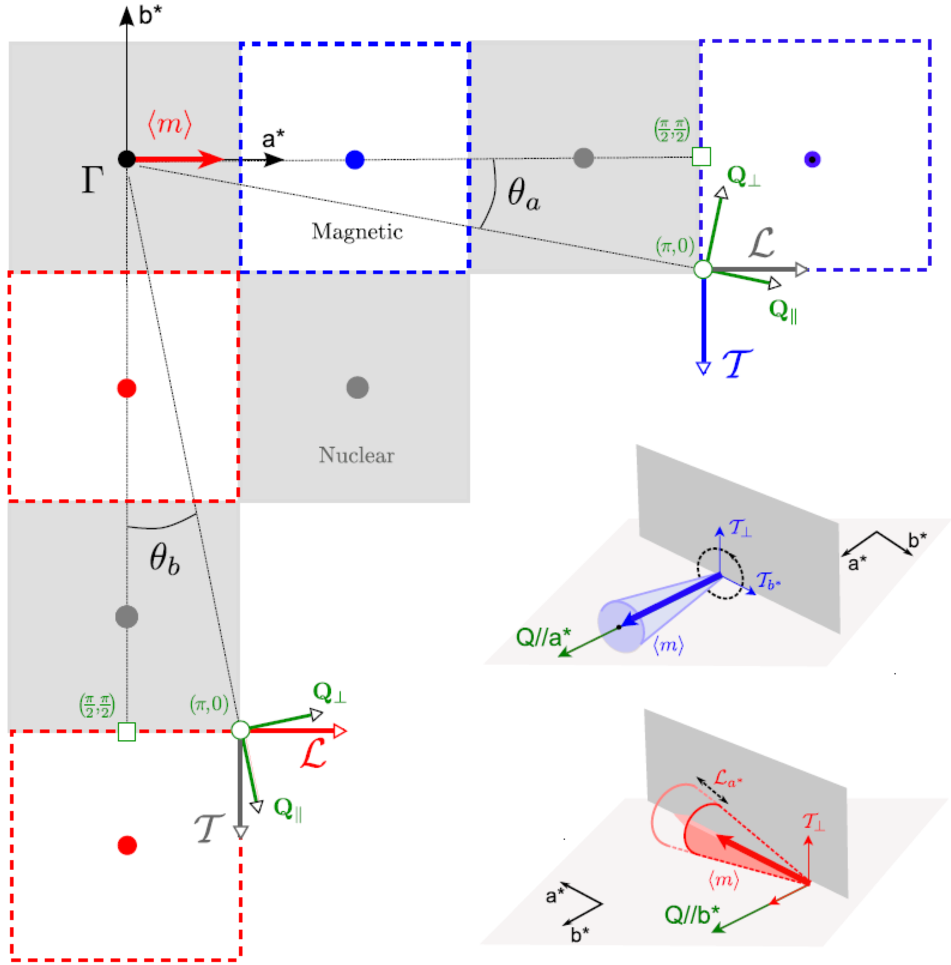
+ Neutron polarisation analysis

The 3 axes, and the scattering triangle



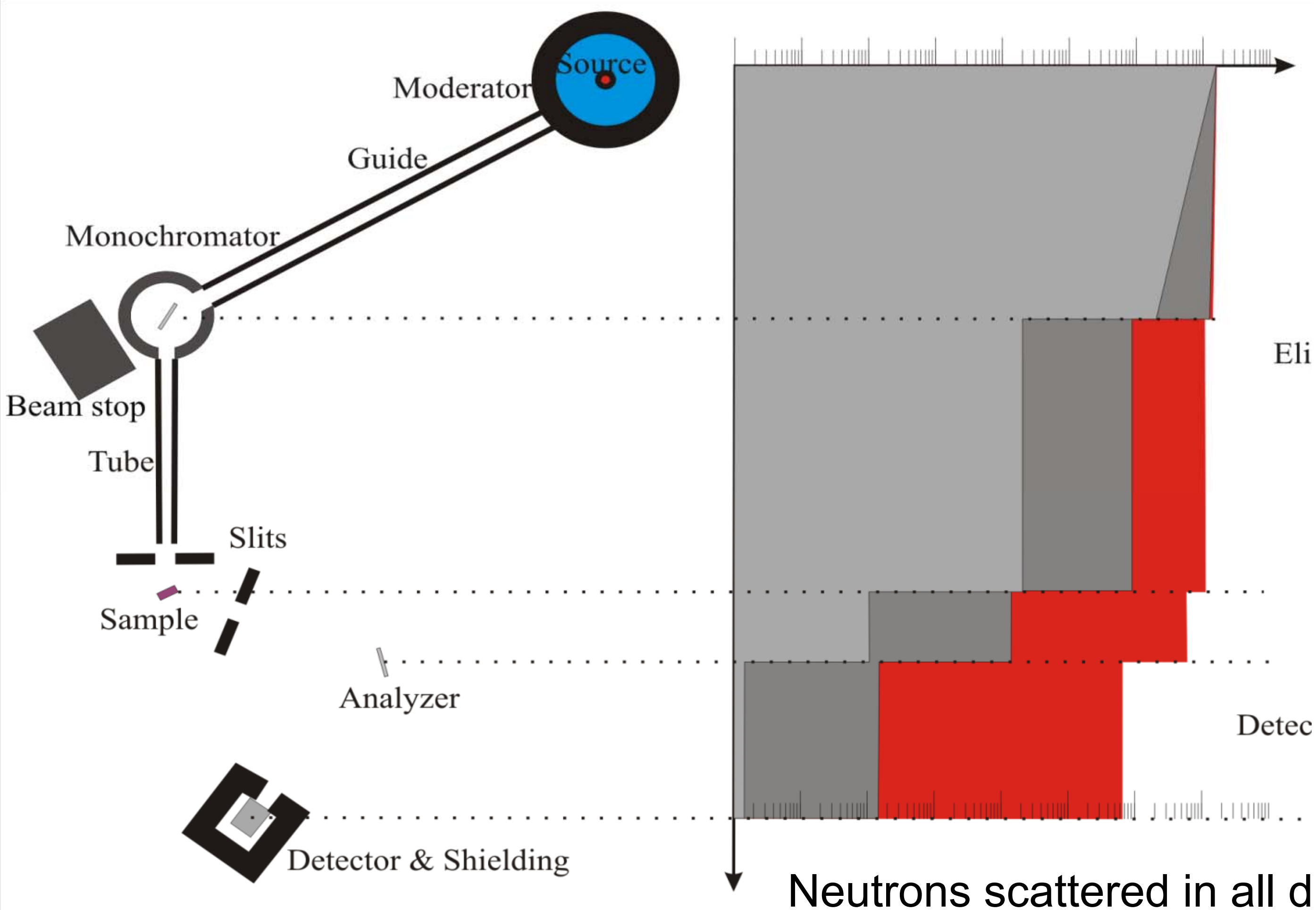
Advantage of flexibility

- Measure at cleverly chosen q-points
- With controlled neutron polarisation etc.
- Example ⇒
  – Geometry used to extract transverse and longitudinal magnetic spectra of CFTD



Inefficiency of a TAS

Source >10^{10}n/cm2 sec ⇒ 1 n/minute in detector



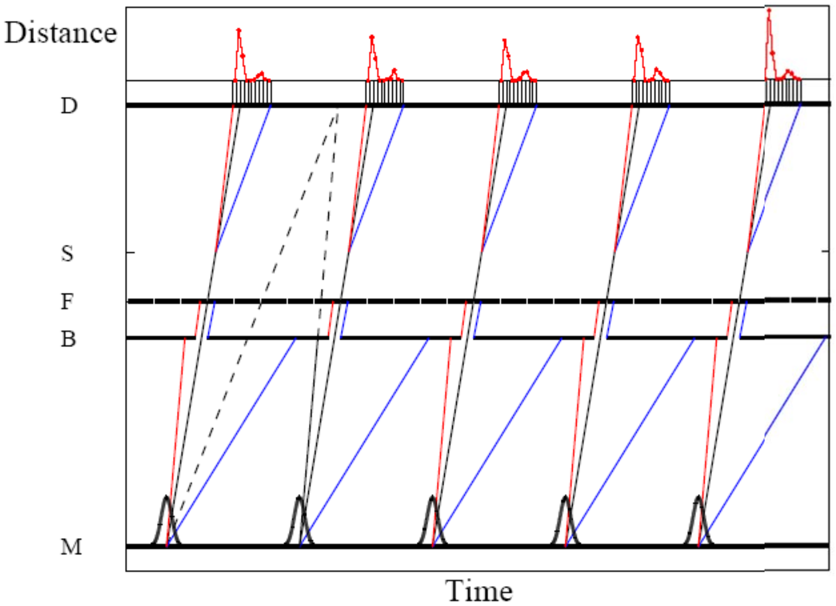
Neutrons scattered in all directions and all dE but we record only one direction and one dE

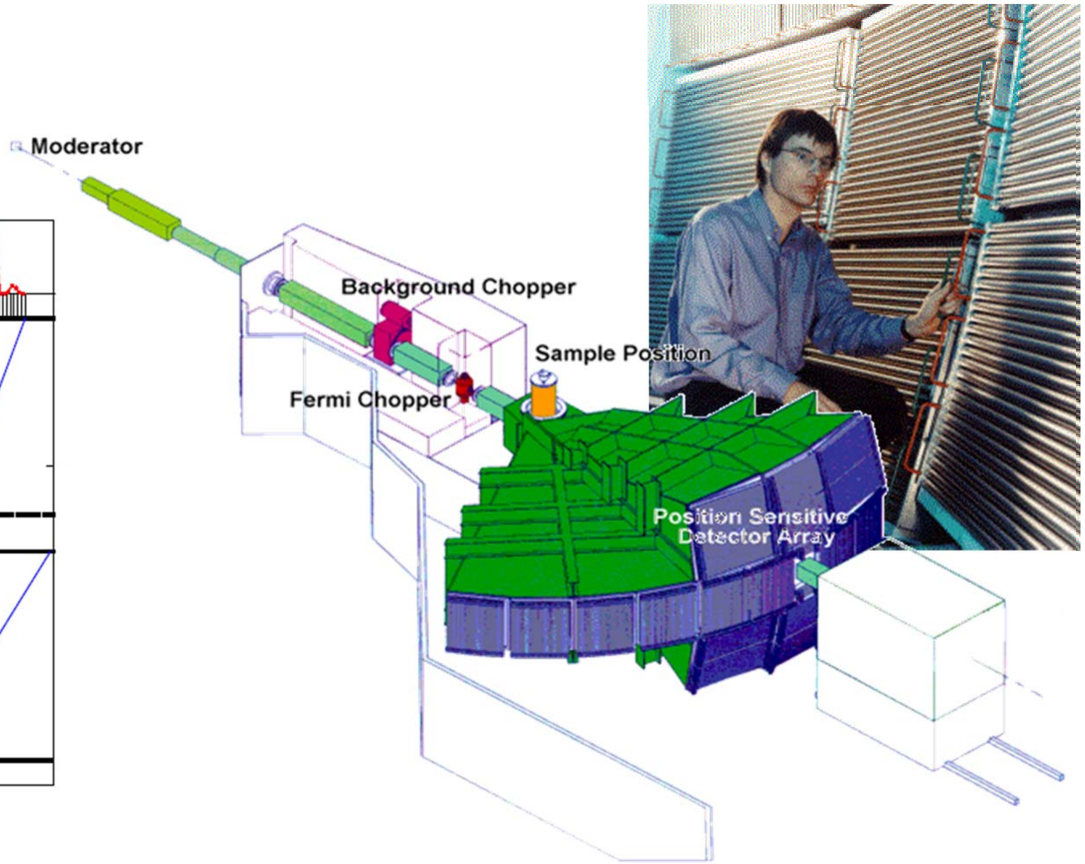
JO Birk

TOF: time-of-flight

Pulsed beam

known start time





Monochromatising chopper => E_i

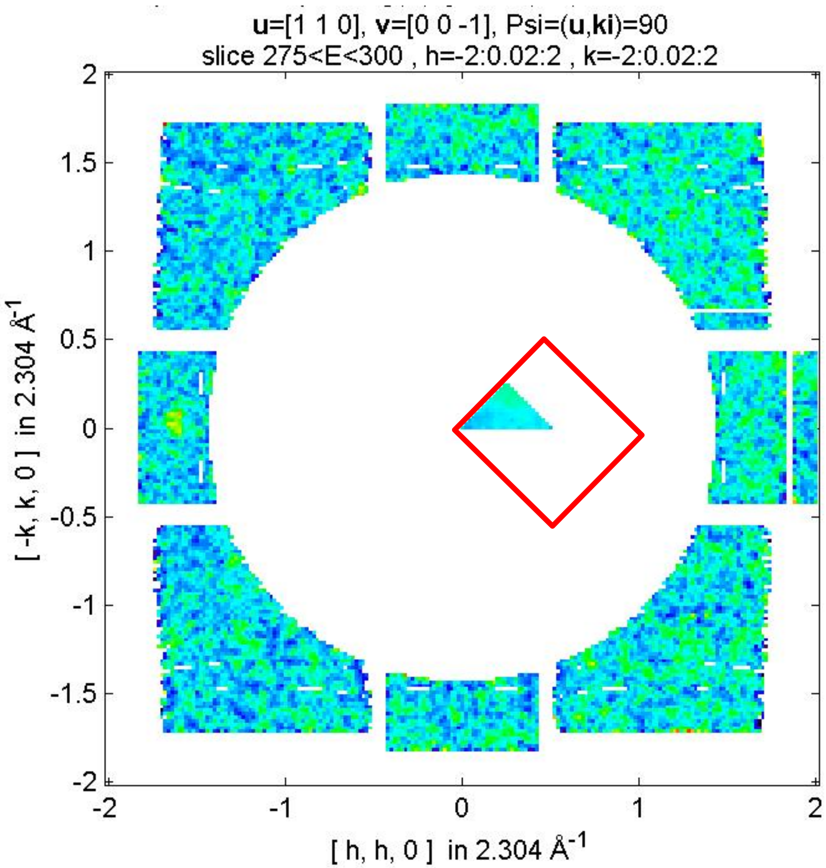
Time-of-flight => E_f

Advantage: nothing between sample and detector => easy large detector multiplexing

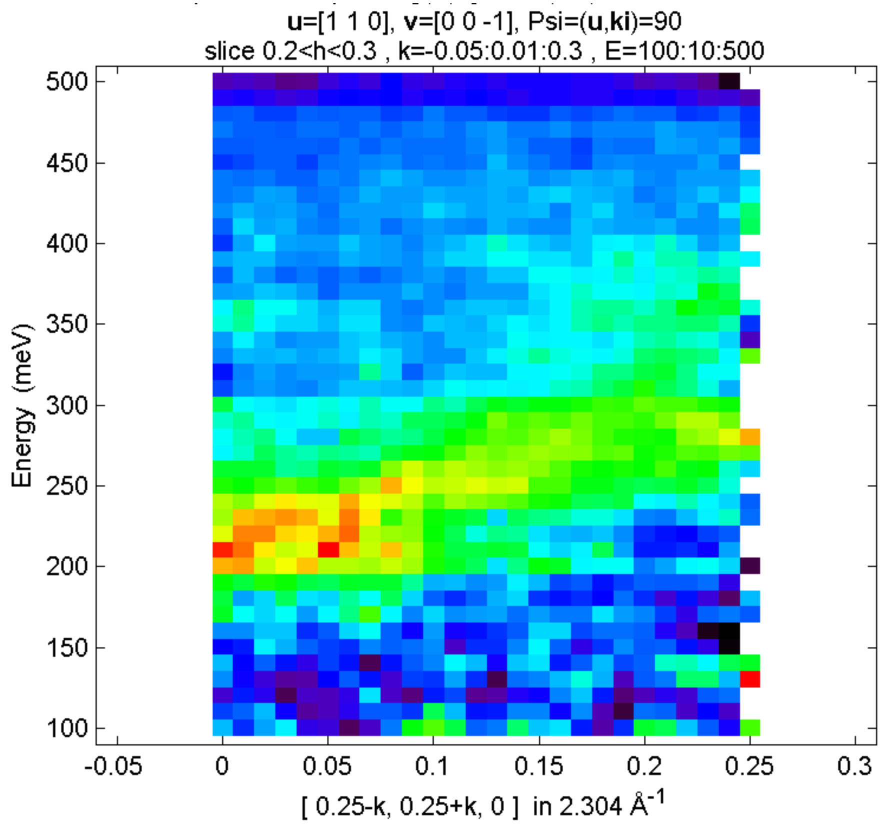
TOF – large detector + symmetry helps stats

$YBa_2Cu_3O_{6.9}$

16m^2 detector origami



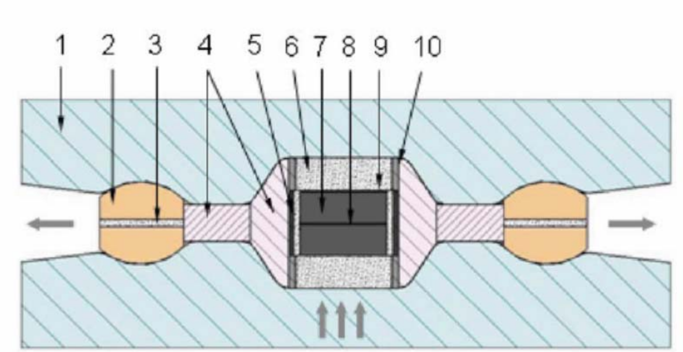
J_c ZB dispersion and (pi,0) intensity dip



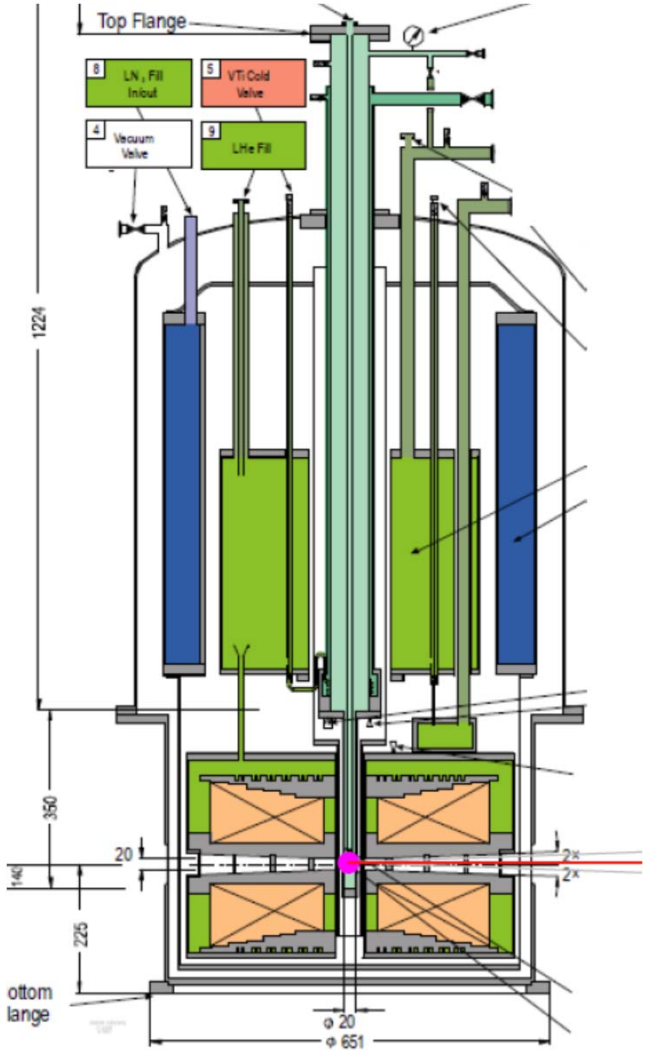
Hayden, Coldea, McMorrow and HMR

But, sample environments often narrow opening

- High-pressure anvil cells



- Split-coil high field magnets



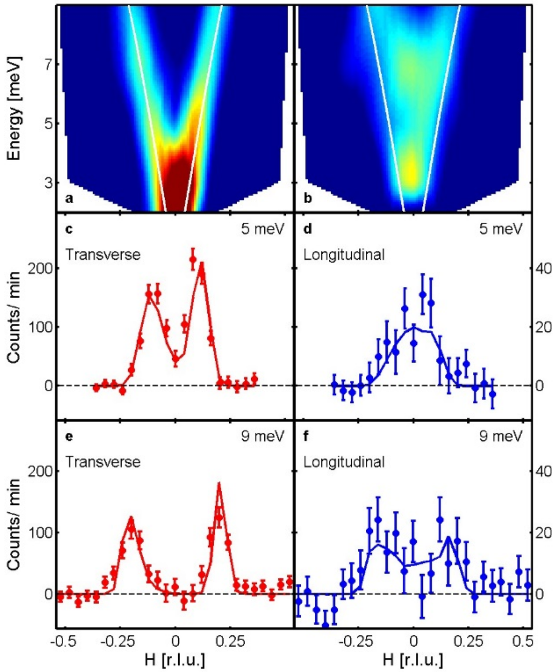
Direct TOF useful with extreme sample environment

Moreover, there is a background problem for dTOF and sample environment

Excitations: TAS v.s. dTOF ⇒ Multi-TAS

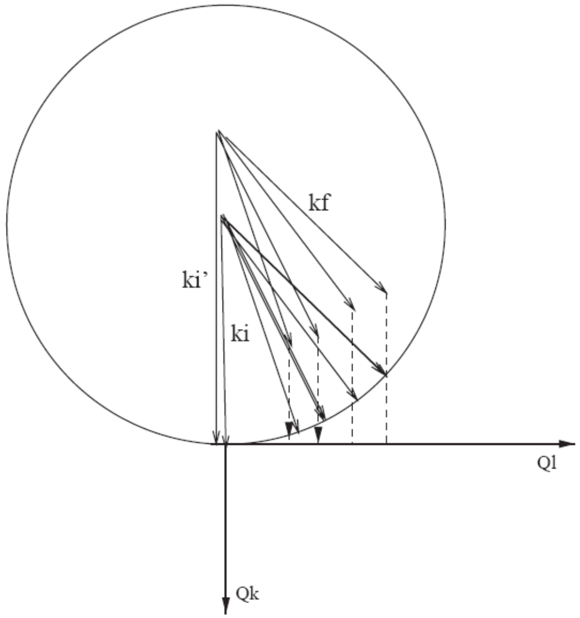
TAS

- Focus on <u>one</u> Point
- Intense
- Flexible
- Field, pressure etc.



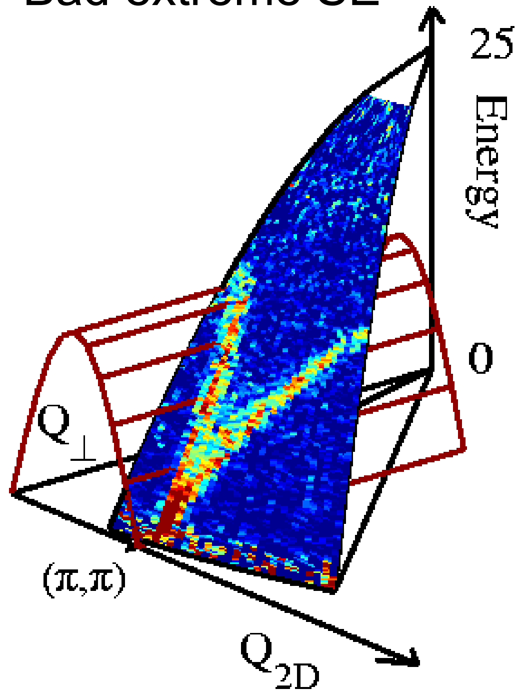
Multi-TAS

- a line in momentum-energy-space
- More Neutrons recorded than TAS
- More flexible than TOF



dTOF

- 2-3D manifold
- Overwiew – sees "everything"
- Less flexible
- Bad extreme SE



How to detect more neutrons with TAS

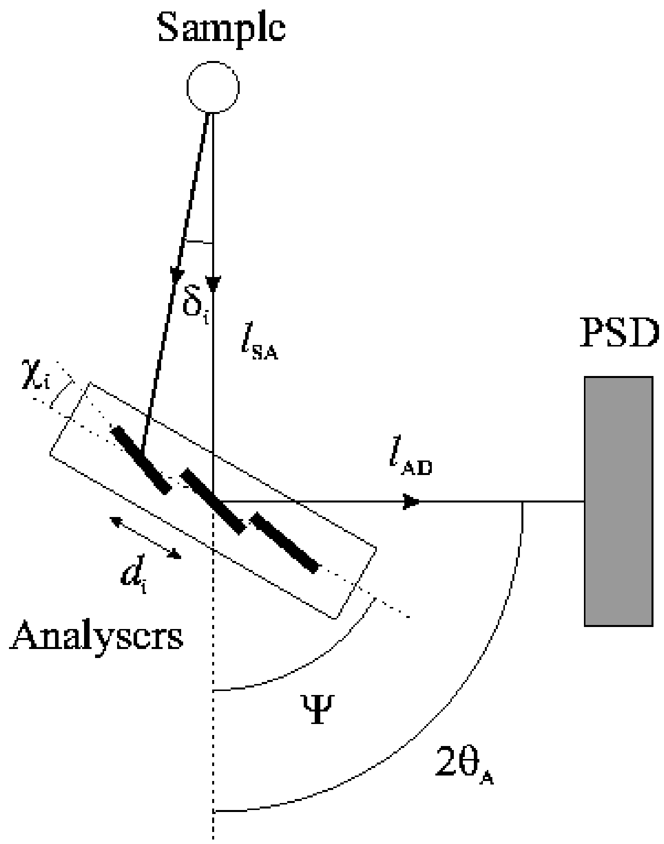
- Have bigger analyser
- # neutrons = analyser area
- But q-resolution width = analyser area
- So, have flexible analyser together with PSD

RITAs Re-Invented Triple Axis

Multi-blade analysers

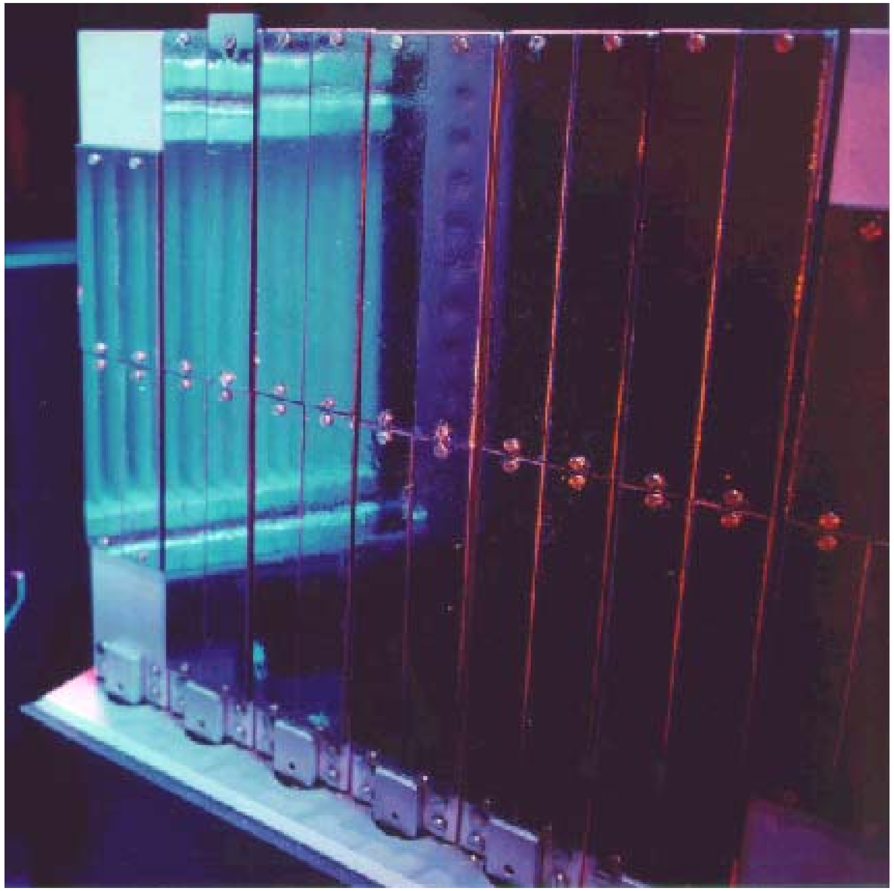
- Flexible focusing,
  resolution tuning,
  mapping

- By turning the block, we have some freedom in positioning the blades
- Each blade has its own little resolution ellipse in ($q_{||}$, $q_{\perp}$, E)
- "backwards compatible"



RITAs Re-Invented Triple Axis

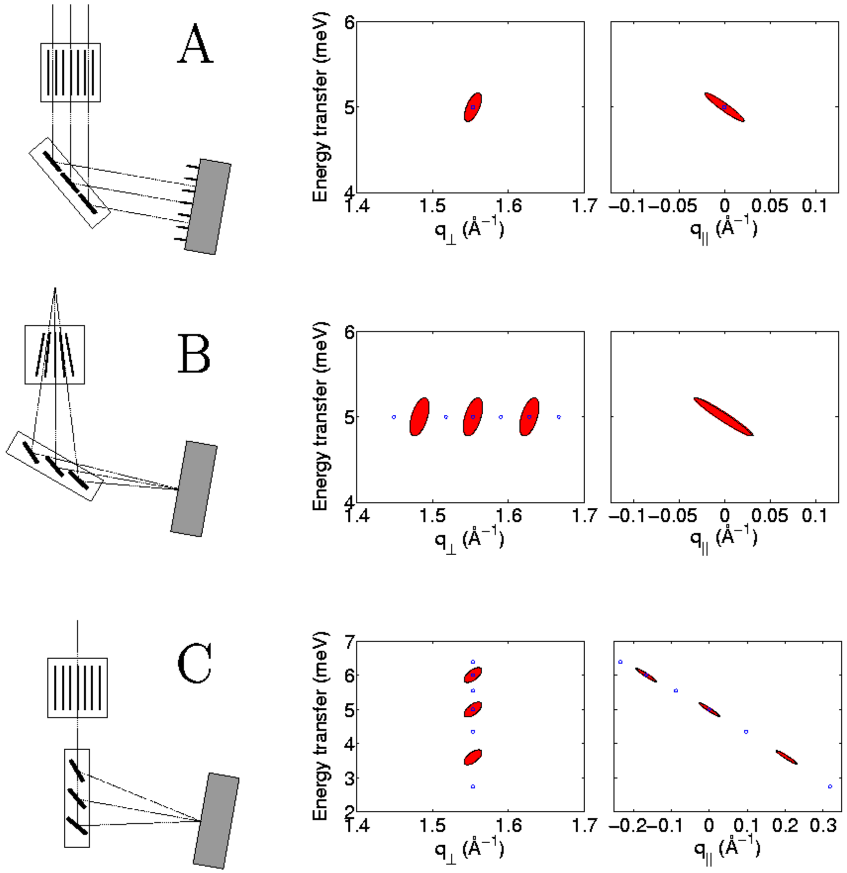
- Individual blades
- PSD detector



- The RITA philosophy re-think it all:
  - Focusing optics
  - Velocity selector
  - Filters:
    Be, BeO, Al_2O_3, …
  - Flexibility / customization

Focusing configurations

- A) Standard analyser, size of ellipse depends on collimation.
- B) Focusing in energy
- C) Focusing in $Q_\perp$
- Relaxing focal point on detector gives freedom in Q/E range
- Any combination possible

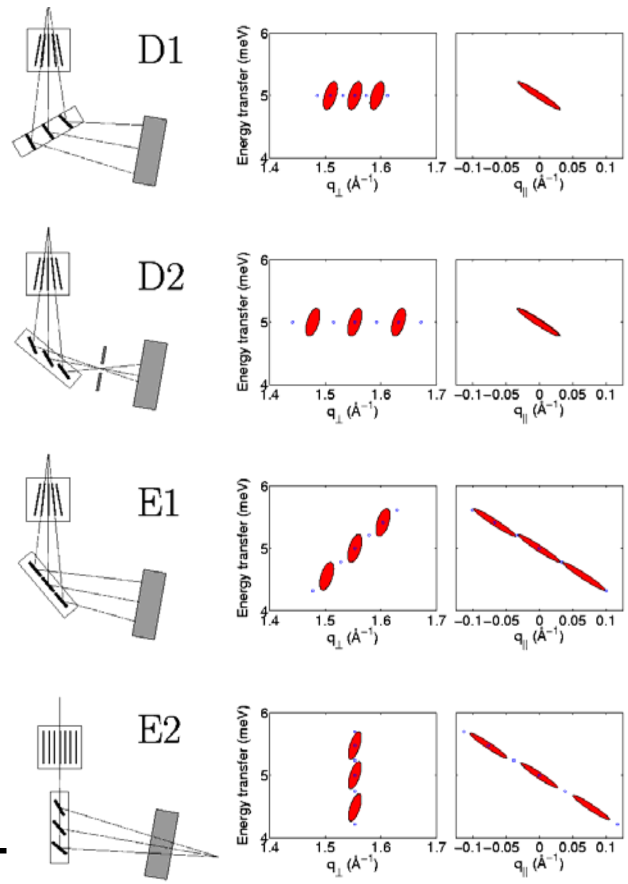


RITAs

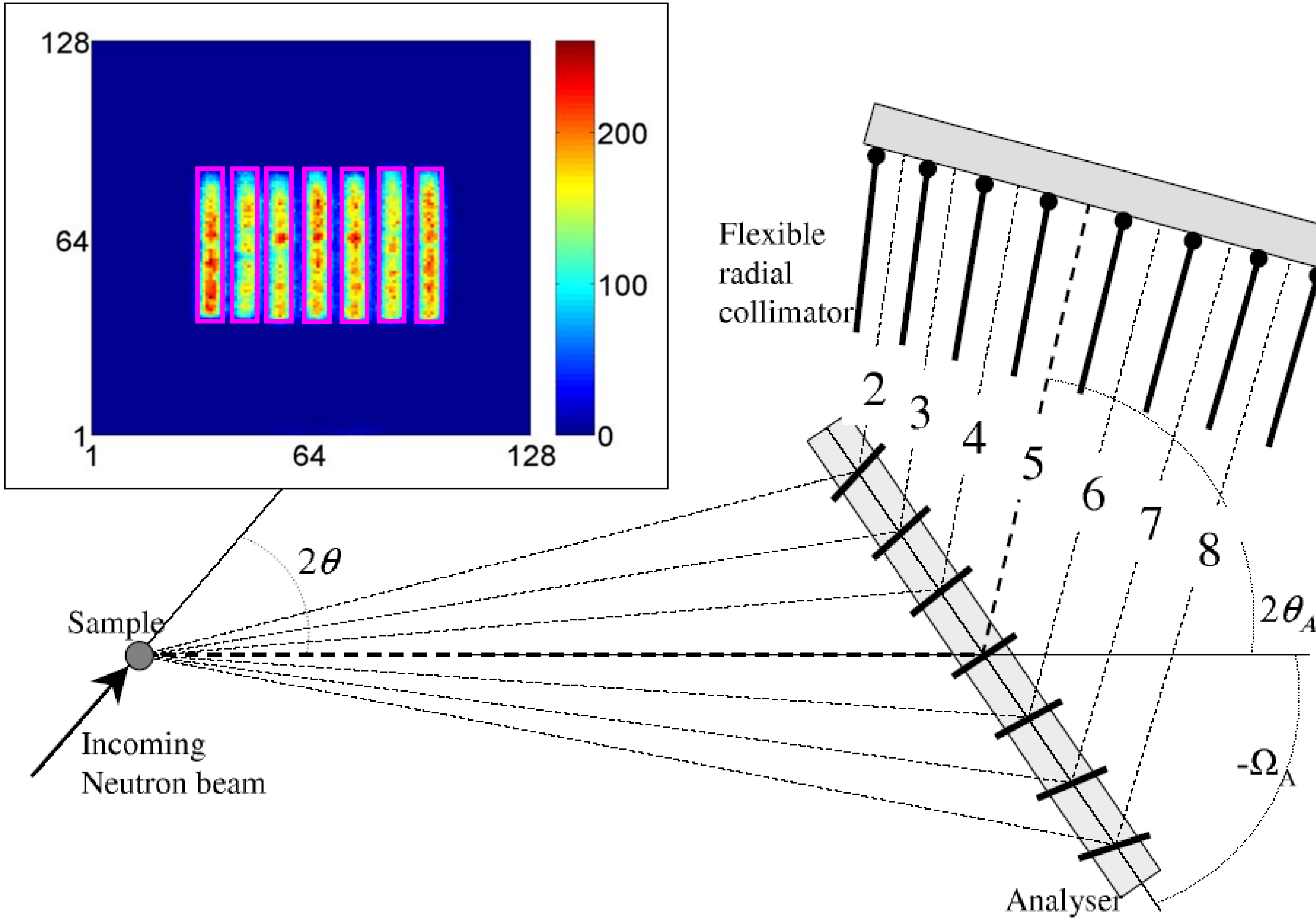
Mapping configurations

Distinguish blades on PSD

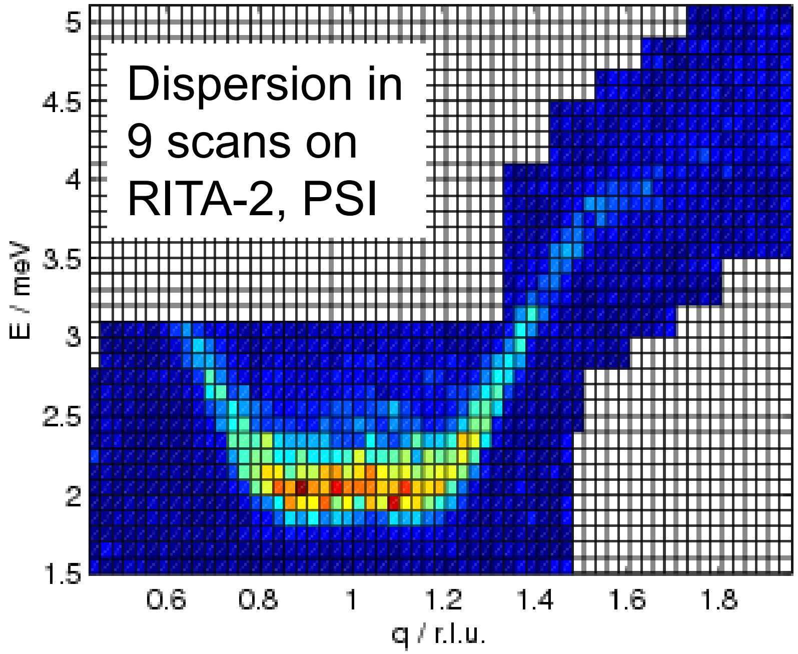
- D1) Multiplexing along Q
- D2) Wider version - requires longer analyser-detector arm
- E1) Flat analyser + 2 radial collimators (Broholm on SPINS)
- E2) Multiplexing along E, near-field for narrow E-spacing, far-field for broad E-spacing
- Almost any combination possible

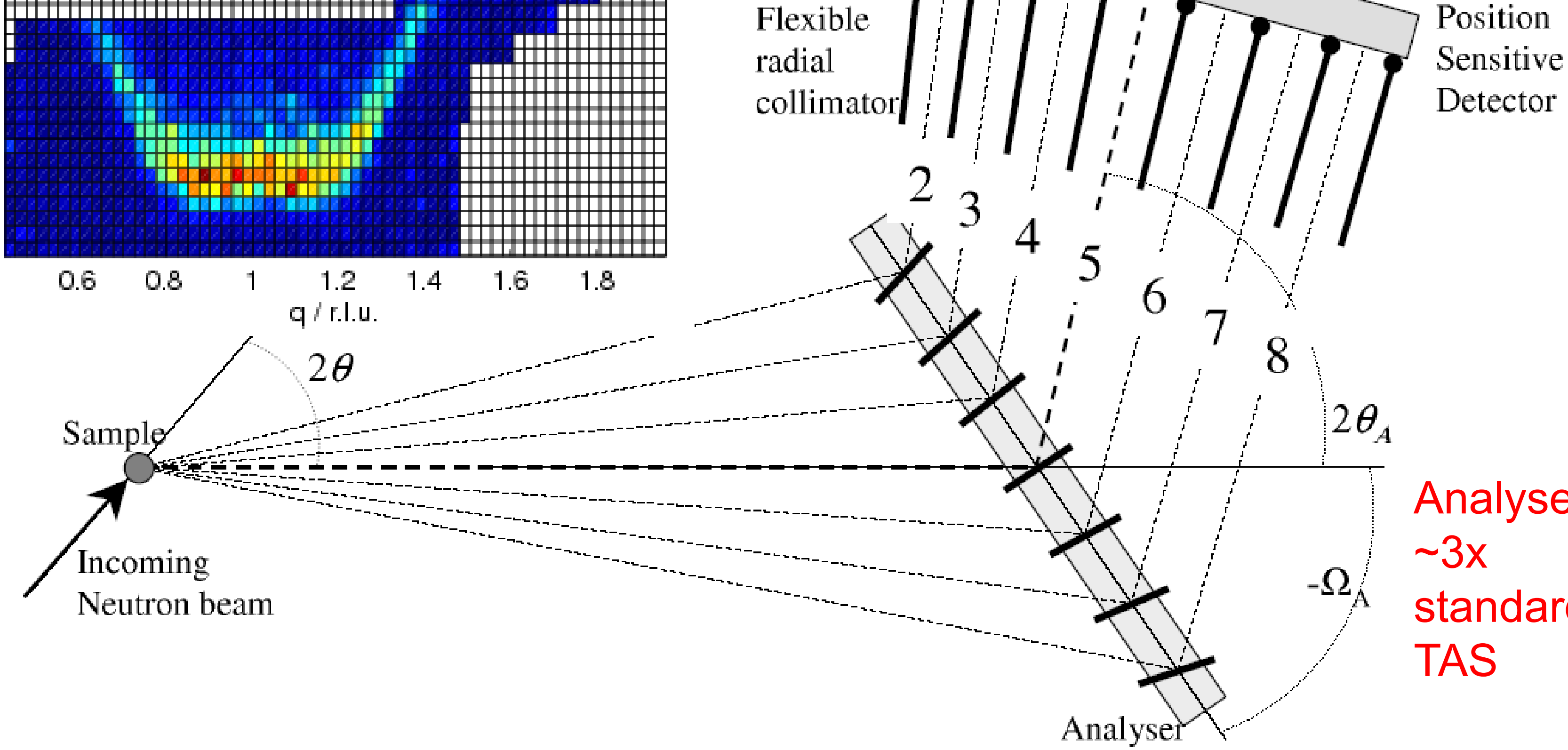


RITAs Monochromatic Imaging mode



RITAs Re-Invented Triple Axis





Analyser
~3x
standard
TAS

K Lefmann *et al*. Physica B **283** 343 (2000), CRH Bahl *et al*. NIMB **246** 452 (2006)

RITAs

But,…

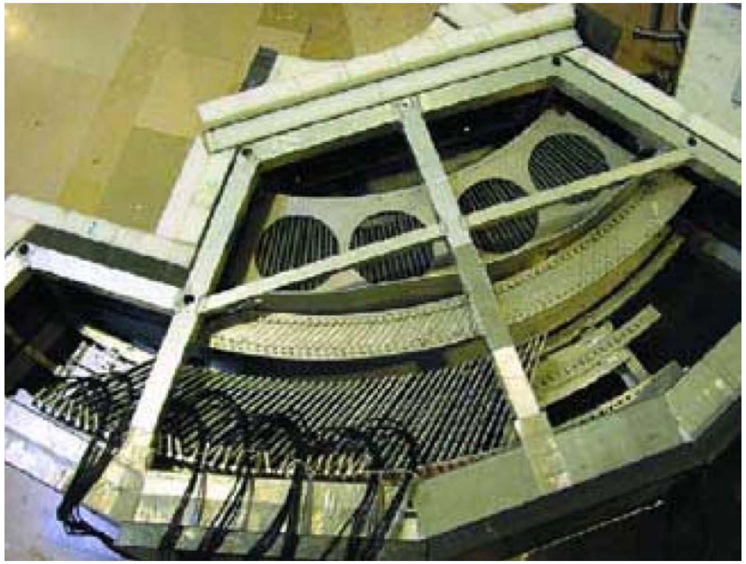
- In the end “only” 3 times normal TAS
- Too many modes and motors to keep track of
- Elastic tails due to short Ana-Det distance
- RITA concept was a “lung-fish”:

A great evolutionary step, but not an end result

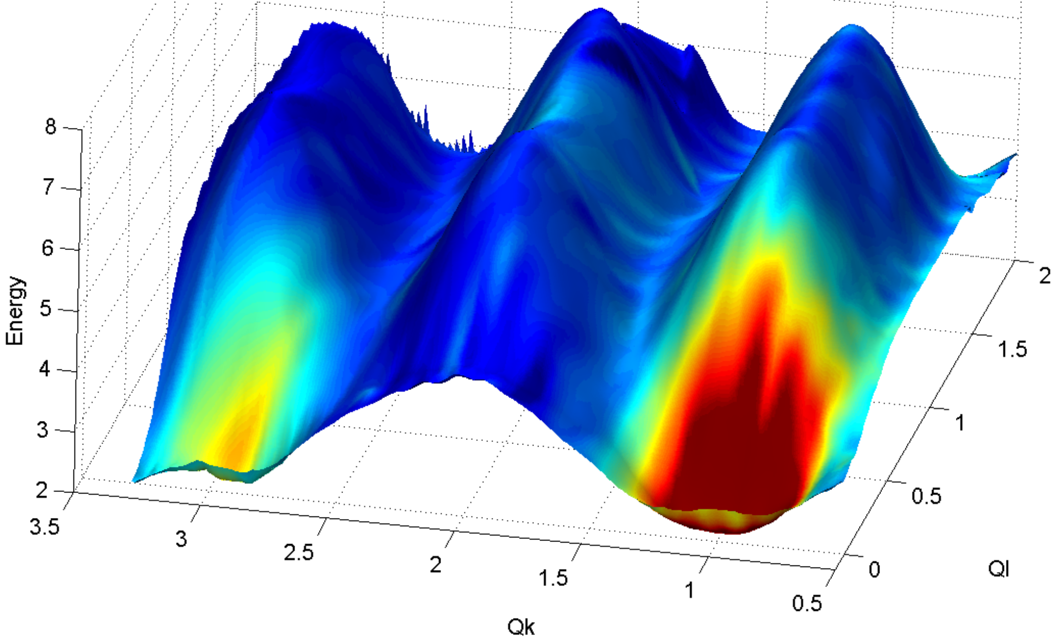
Multi-analyser-detector systems

– MAD Box:
– 47 x 0.33º detectors E_f = 30 meV

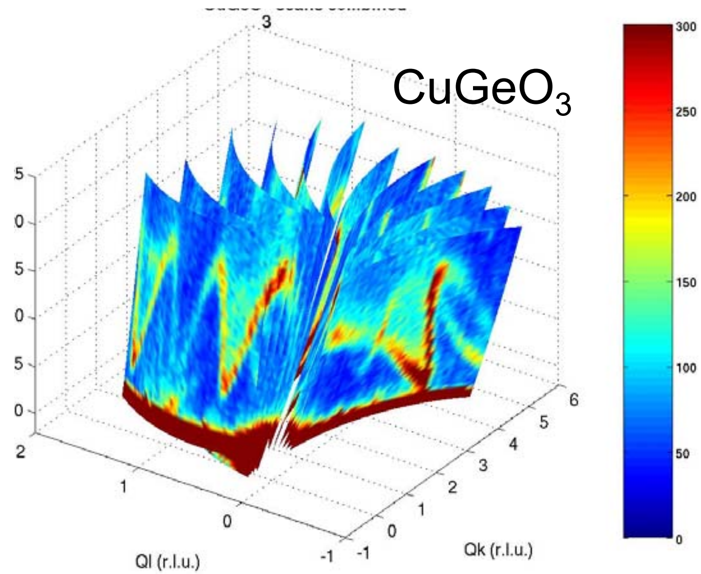
– Entire dispersion of 0.5cm^3 $LiNiPO_4$
  in 4h @ IN8+MAD
  20 scans ⇒ ~1000 (Q,E,Amp) Points



F Demmel *et al.* NIMA **530** 404 (2004)



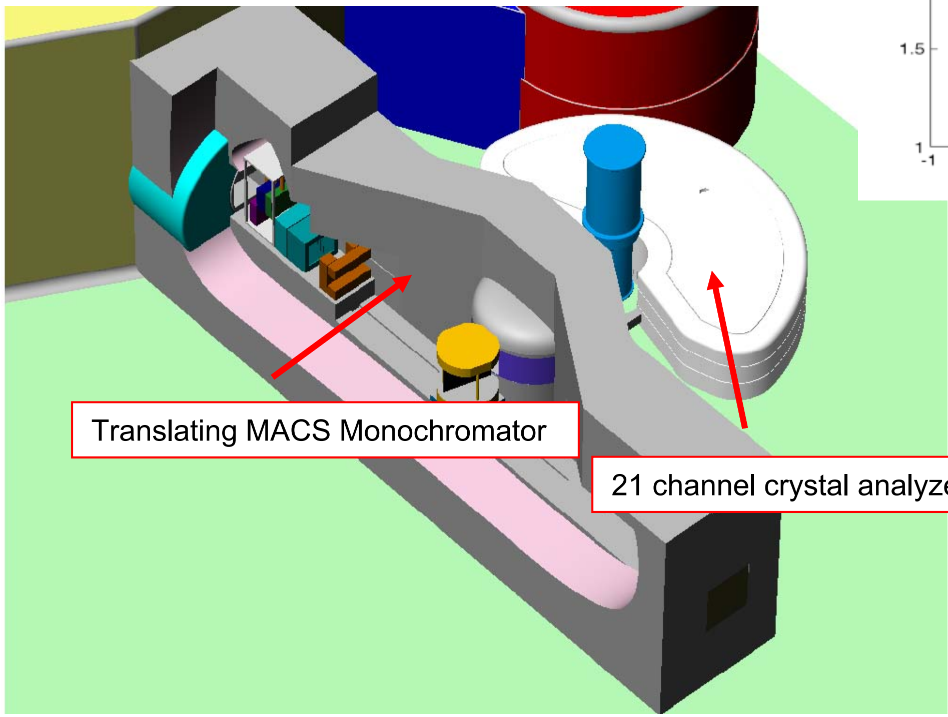
TBS Jensen *et al.* PRB **79** 092413 (2009)

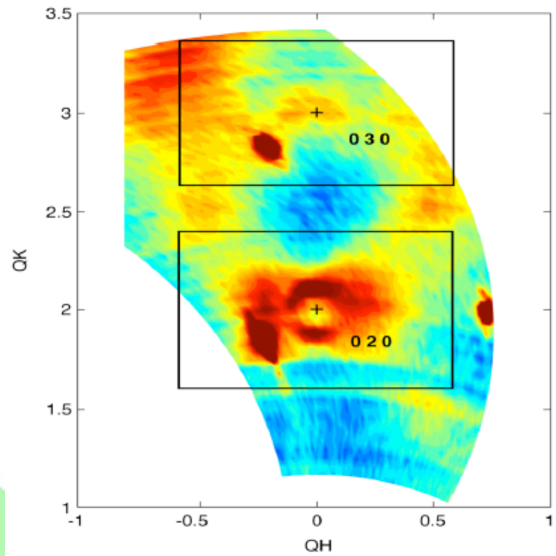


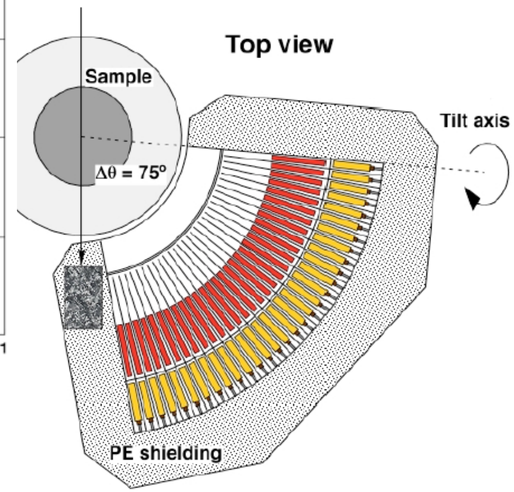
TAS multiplexing

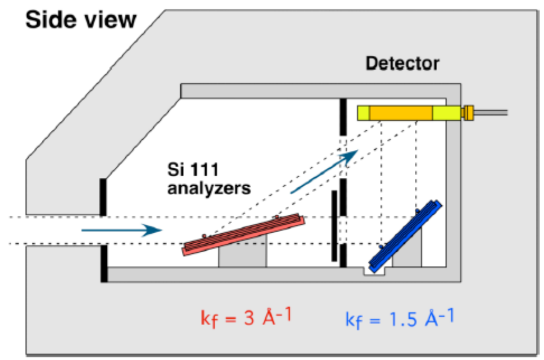
- MAD box (Demmel)
- Flat cone, ILL (Kulda)
- MACS, NIST (Broholm)
- …

20-40 analysers
But ~1/2 coverage
$\Rightarrow$ ~5x TAS
With much less
stats in pixels

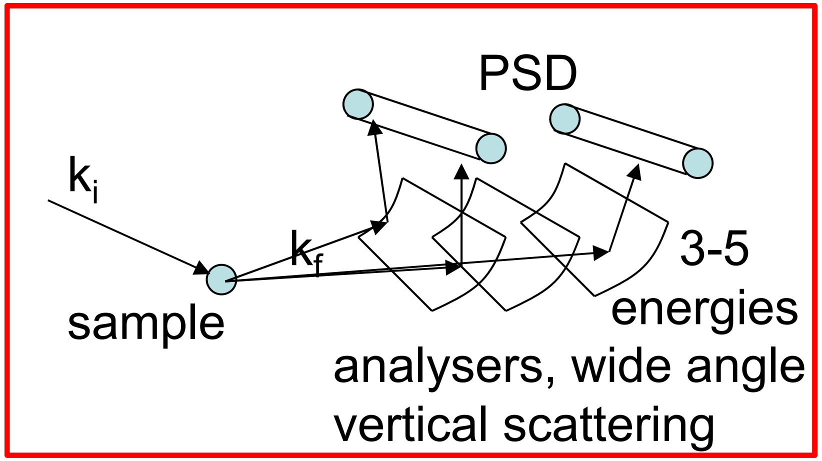








OK, so multiple q, but what about multiple energies?



Slide from 2004:

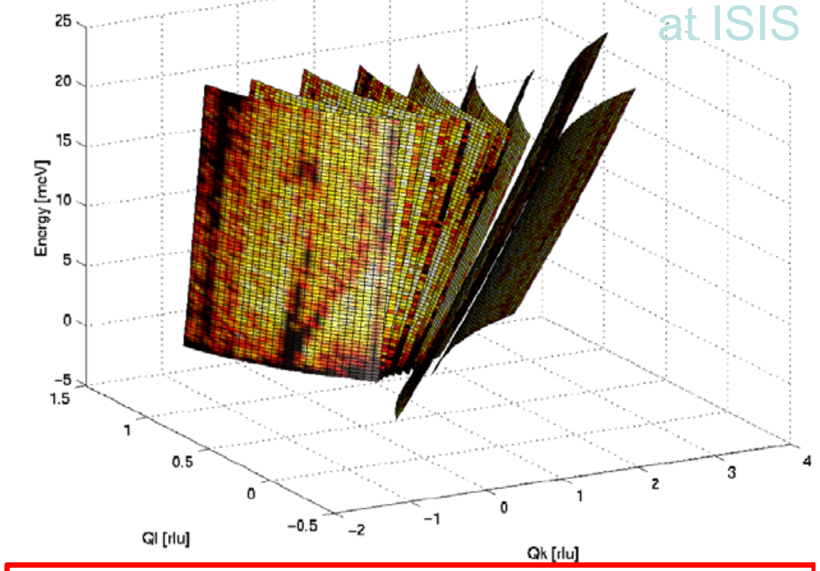
Phase 5: Analyser-detector system

EIGER

Analyser-detector backend(s)

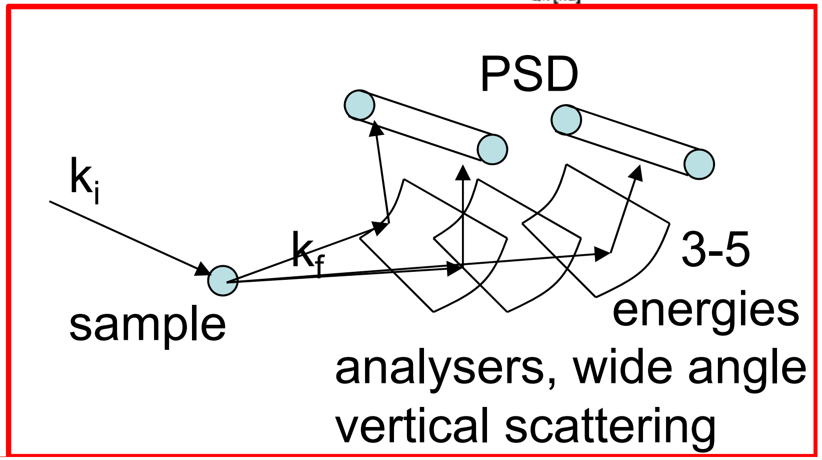
- PG in old Druchal housing
- ‘custom’ modes: Be-analyser…
- CAMEA: Continuous Angle Multiple Energy Analysis

IN3+32 detectors = MARI at ISIS



CAMEA:
no greek myth
Google ⇒

An amateur DJ !

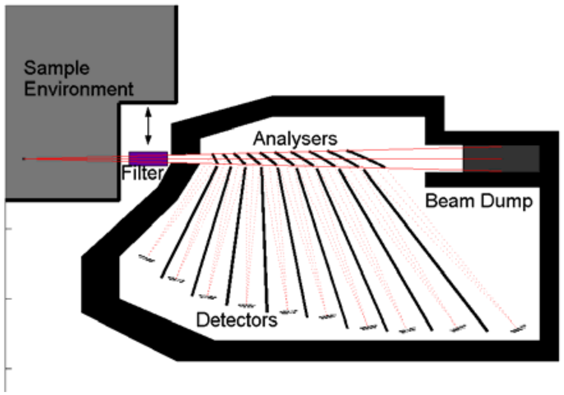


2004: CAMEA – a Seattle amateur DJ

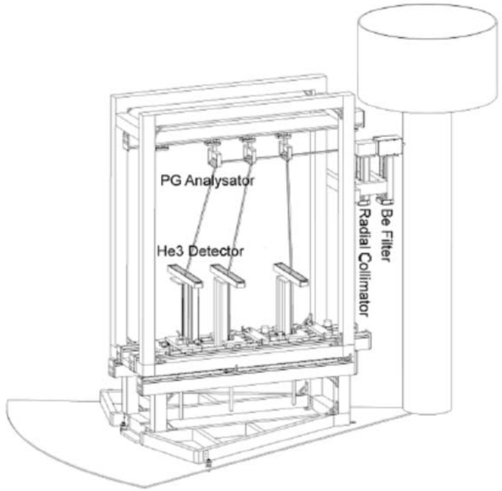
2014: CAMEA's Discography:

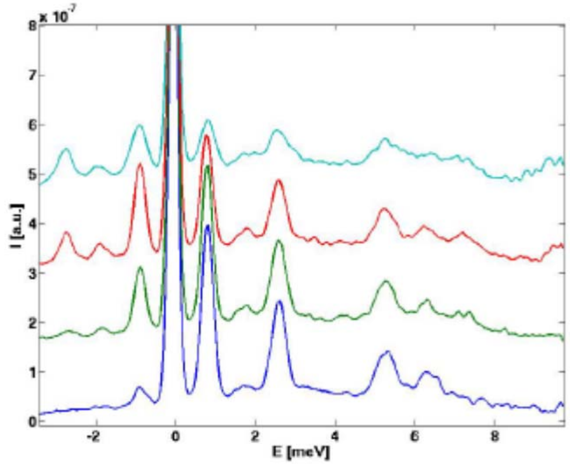
CAMEA

ESS Instrumnet

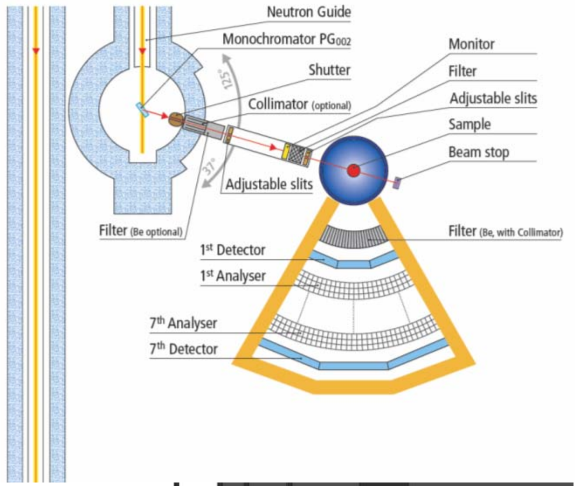


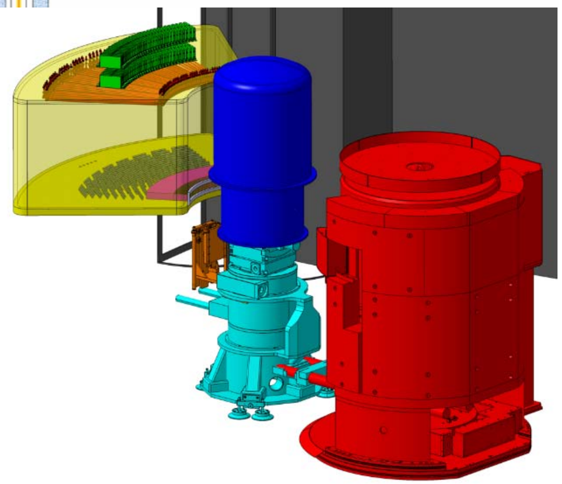
MARS prototype





PSI Instrument





Multiple Energies & Continuous Angle

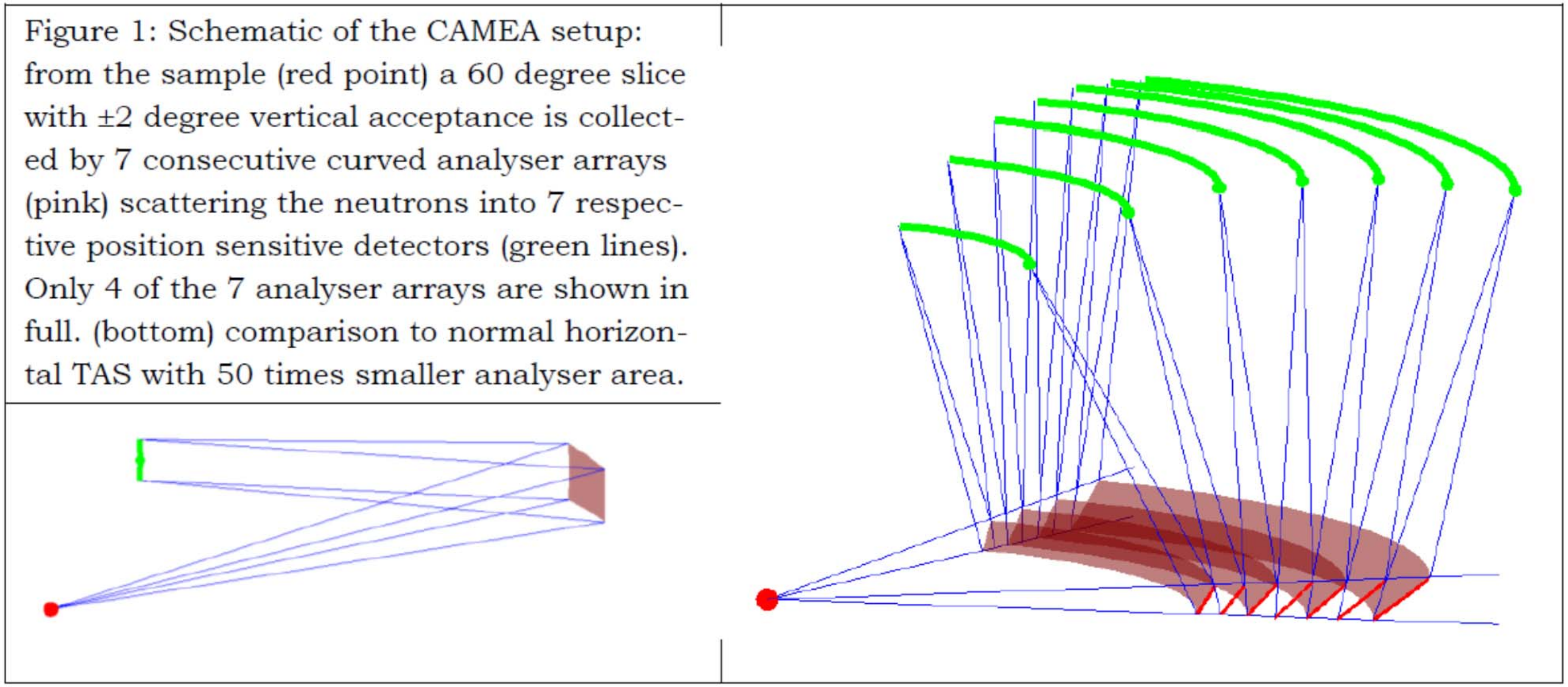
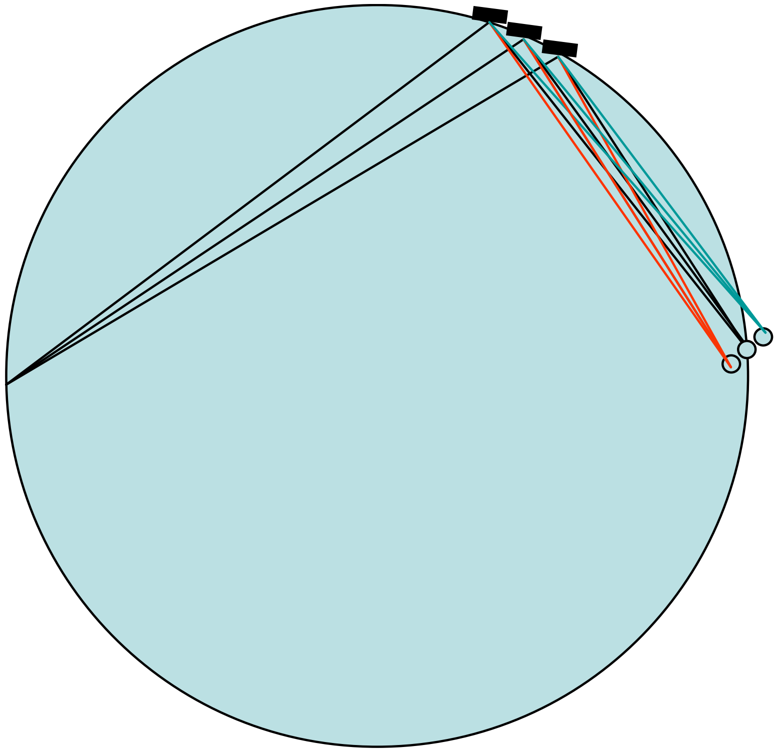


Figure 1: Schematic of the CAMEA setup: from the sample (red point) a 60 degree slice with ±2 degree vertical acceptance is collected by 7 consecutive curved analyser arrays (pink) scattering the neutrons into 7 respective position sensitive detectors (green lines). Only 4 of the 7 analyser arrays are shown in full. (bottom) comparison to normal horizontal TAS with 50 times smaller analyser area.

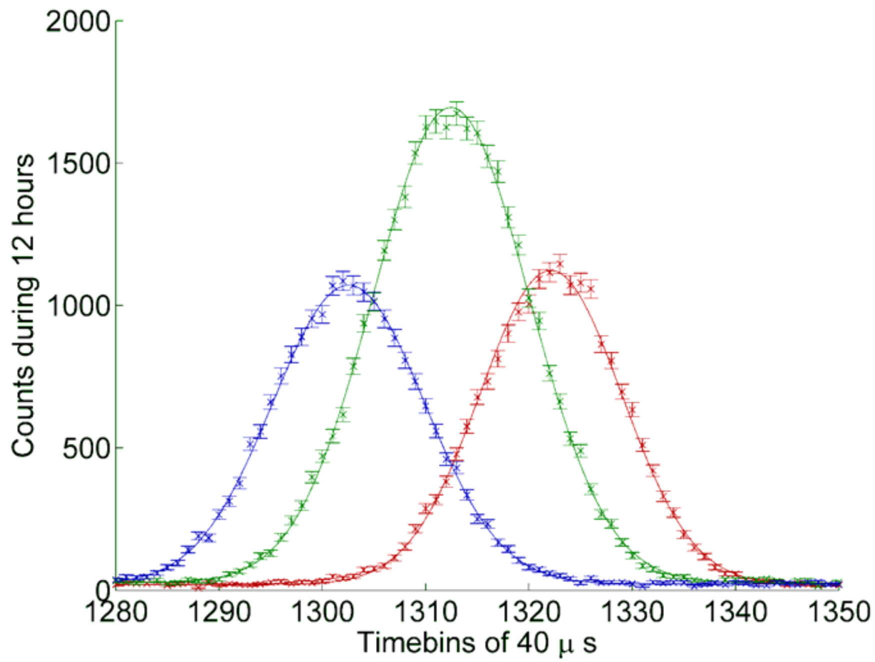
- Factor 50 more neutrons detected

$\Rightarrow$ Factor 50 better – <u>if</u> covered (q,E) useful

Prismatic Rowland analysers
Better E_f resolution at no flux cost !

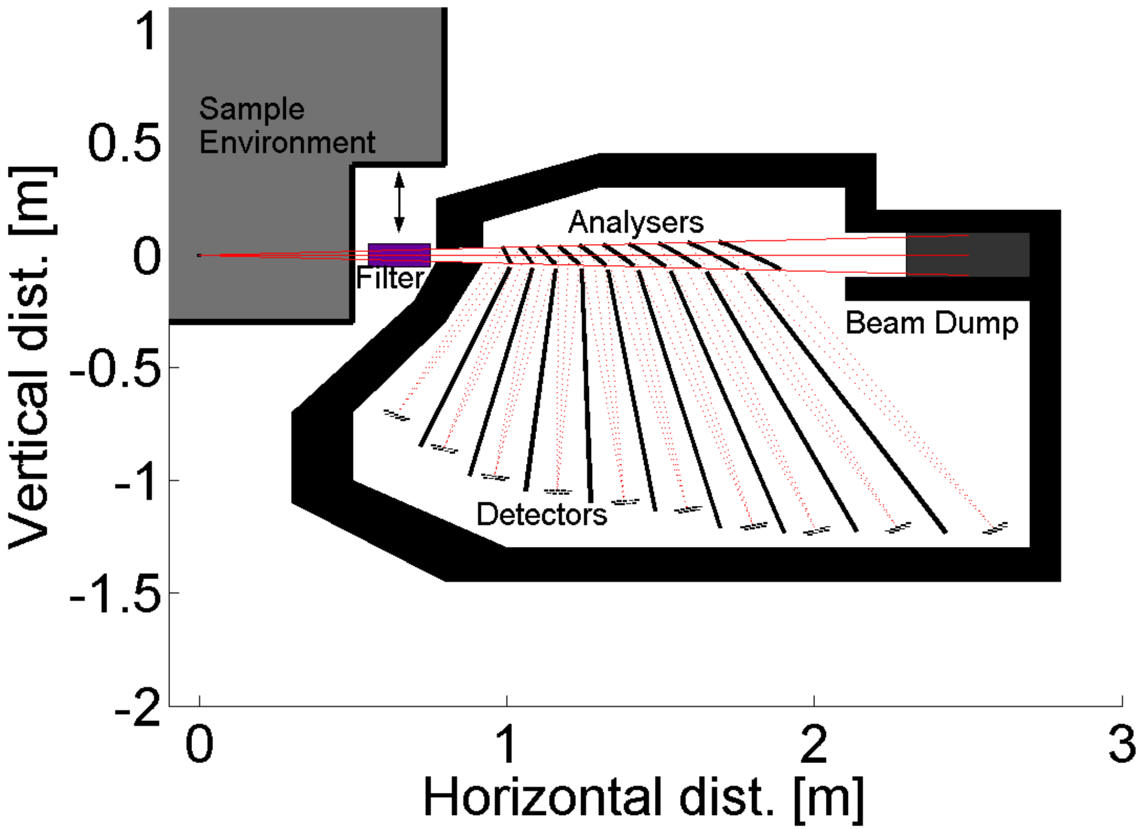


- Distance collimation ⇒ 50% better resolution than standard TAS
- Multiple energies for each analyser
- Adjacent detectors record different energies ⇒ 2.7x neutrons



J.O. Birk et al., Review of Scientific Instruments, 85 (2014)

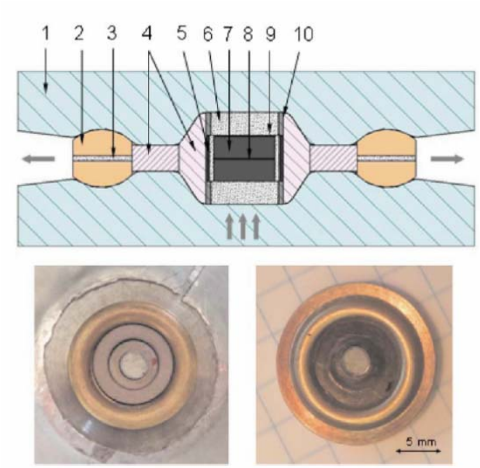
Concept:
Multiple energies * multiple detectors

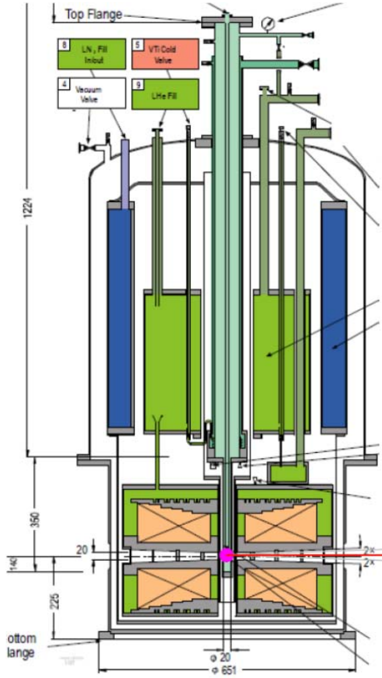


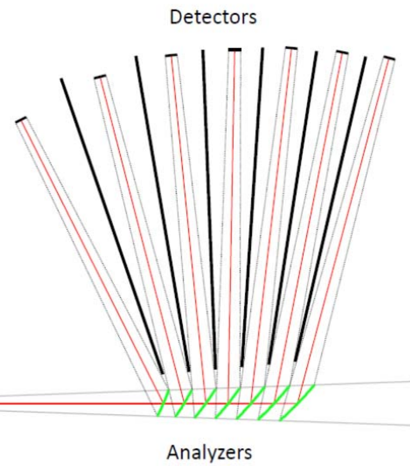
- A conventional analyser selects 1-2% energy band, discards rest
- CAMEA:
  - 8-10 consecutive analysers
  - Energies per analyser
  - Total 24-60 energies
  - Covers ~30% of scattered energy range

Extreme sample environments

- Data focused on single scattering plane
- Ideal for extreme environments



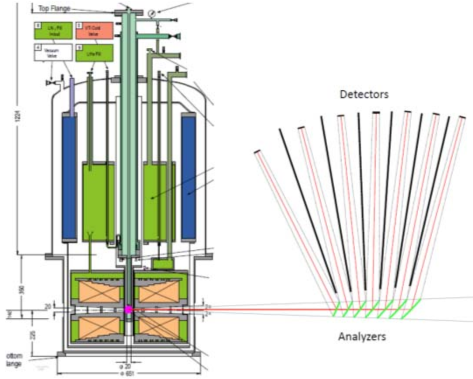




- High-pressure anvil cells
- Split-coil high field magnets

- But, CAMEA competitive for “all” experiments on small samples, parametric studies, time resolved etc.

Science case: magnetic fields



- 30% of TAS experiments use magnetic fields
  - Need instrument optimized for magnetic fields

Instrument (Neutron Source/institution)	Overload*	Magnetic fields (%)	Pressure (%)	1 K < (%)	Polarized Neutrons (%)	Furnace (%)
RITA-II, TASP (PSI)	2.5	33.9	4.3	19.2	N/a	
PANDA (FRM-II)	2.7	30	5	20	N/a	
LET (ISIS)#					Commissioning	
IN14 (ILL)	2.5	30-40	< 5	60	20-25	
IN12 (JCNS@ILL)	2.6	23.5	-	27.5	9.8	3.9
Osiris (ISIS)**	2	40		40	Planned	
FLEX (HZB)	1.53	56.3		19.9	Commissioning	

P. Freeman et al., EPJ Web of Conferences, 83 (2015)

- Currently few experiments under pressure
  - Need more flux, higher count rate and optimized instrument to unlock new science
- Sub-optimal instruments built around huge magnet (25T Berlin project) or huge pressure apparatus (Planet@J-parc) often too compromised, can only work for some experiments

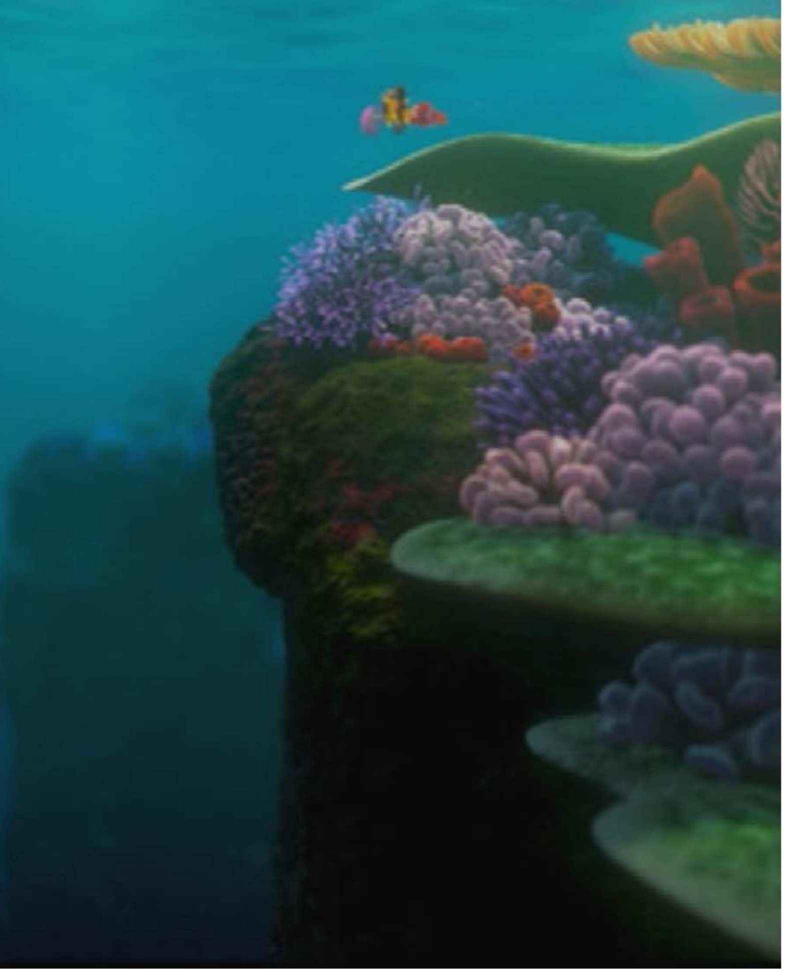
Scientific case:
Finding a plastic T_c>50K superconductor

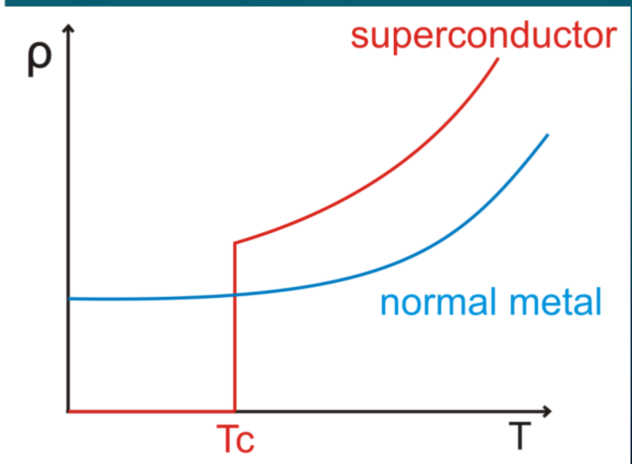
Discovering superconductors:

How to know $\rho(T)$ is close to a drop-off ?

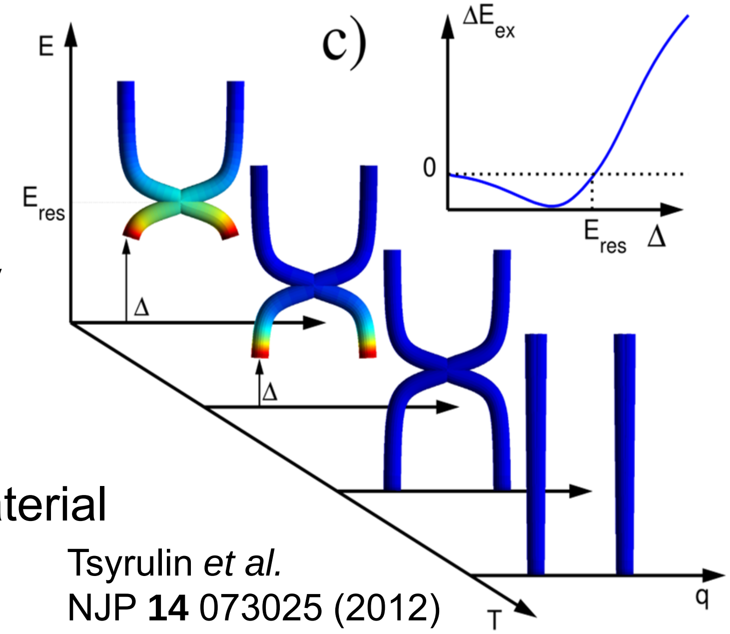
High-Tc superconductors are poor metals !

Need guiding hypothesis





Quest for new superconductors:



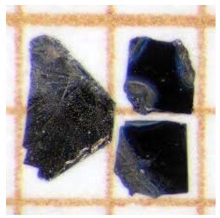
a conjecture:

- ⌛ necessary condition for superconductivity
- Search for materials with IC fluctuations
  - and mobile charges. IC spectrum makes material susceptible to competing spin/charge order

Tsyrulin *et al.* NJP **14** 073025 (2012)

Scalapino and White PRB **58** 8222 (1998)

- When finding a new material class
  - E_{hg} sets upper limit for Tc~5.3 E_{hg} achievable, and hence whether more exploration within this class is fruitful



- “random blind walk” in the table of elements ⇒ slow at best
- ⌛ - conjecture: we may go in wrong direction, but we will get there fast !
- Need instrument to screen for ⌛ in (<1mm^3) novel samples ⇒ CAMEA

European Flag ship projects

Human Brain Project

- Objective: simulate the human brain Budget: 1.19 B€

GRAPHENE FLAGSHIP

- Objective: future graphene technology Budget: 1.05 B€

European Superconductor Search

- Objective: widely applicable superconductor Budget: 2.12 B€

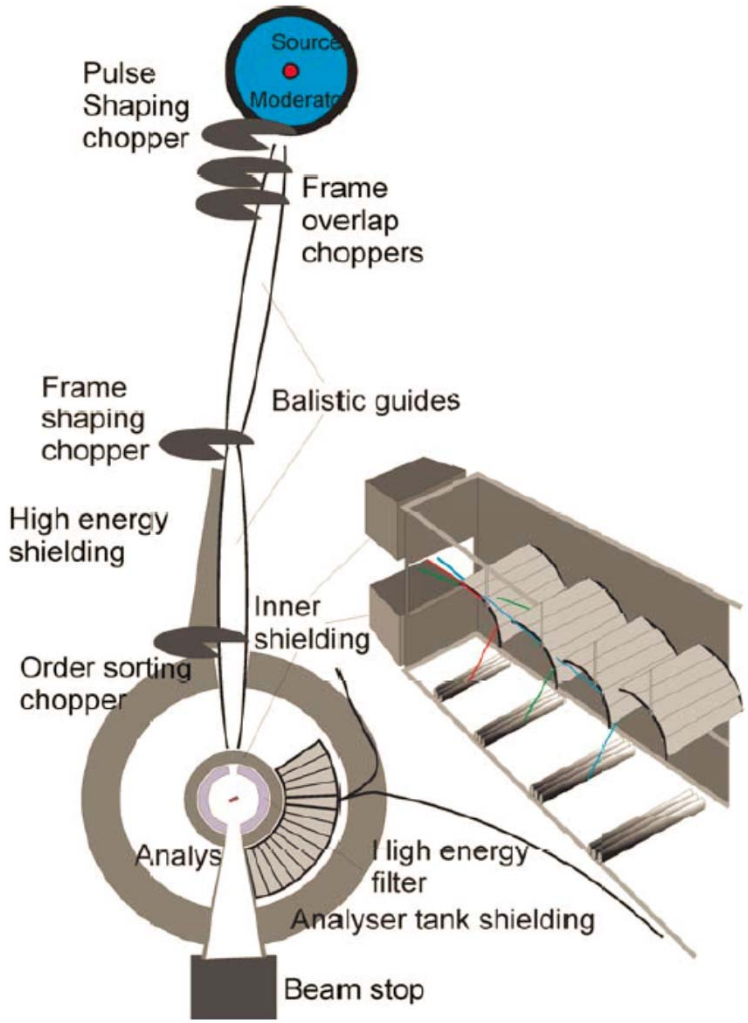
A room temperature superconductor is arguably worth 2 b€

Science case (dreaming aside)

- Materials discovery:
  - Small samples: new synthesis methods, INS as iterative analytic tool
- Correlated electrons:
  - High field & pressures: tune crystalline and electronic structures
- Magnetism:
  - High fields: new fundamental states
- Functional materials:
  - parametric and μs to s time-dependent studies: catalysts, batteries, multiferroics, thermoelectrics…
- Planetary science:
  - High pressure & temperature: confined water, H-diffusion, sound modes…
- Soft-condensed matter and life-science:
  - Small samples, weak signals, sample environments

CAMEA-ESS

- Inverse time of flight spectrometer
- Vertically scattering analyzers.
- Multiple analyzers behind each other select several energies.
- E_f=2-32meV
- Energy resolution as cold TOF, better than cold TAS
- Can use full ESS long pulse, shaping $\Rightarrow$ better res
- Optimized for small sample size 1cm^3 down to <1mm^3
- High field (25T), high pressure (300kbar)



Performance numbers:

- Energy range: E_i=1-80meV, E_f=2.5-32meV
- Resolution: 0.8% - 4.2% tunable
- Angular range: 3-135° resolution 0.5-1.5° tunable
- Flux: 1.8×10^{10} n/cm^2/s for 1.7Å λ-band full 2.8ms pulse
  1.5×10^{9} n/cm^2/s for 1% E-res and 0.5° angle-res
- Background: $<5 \times 10^{-5}$ (compared to vanadium, data from prototype)
- Time resolution: 20μs
- Magnetic fields: 20-25T split-coil magnet
- Pressure: 30GPa in 5mm^3, 10GPa in 40mm^3 } T=2-2000K
- Field + pressure: 10T + 10GPa in 5mm^3

Gain factors

CAMEA ±1° vertical, ±0.75° horizontal,1.8 x 10^{10} ncm^{-1} s^{-1} centered on 3 Å

Instrument	CAMEA Flux Gain	CAMEA Analyser ±1.4° Solid Angle Gain[§]	CAMEA Gain Factor
IN14 with Flatcone	105	27.7	2910
PANDA with Flatcone[*]	947	27.7	26200
THALES with Flatcone[#]	[illegible]	[illegible]	1410
MACS[+]	[illegible]	17.8	640
OSIRIS	[illegible]	7.7	4270
IRIS	1500	8.4	12600
PRISMA	>20[Ξ]	82.4	>1650

Spectroscopy possible from <1mm^3 crystals

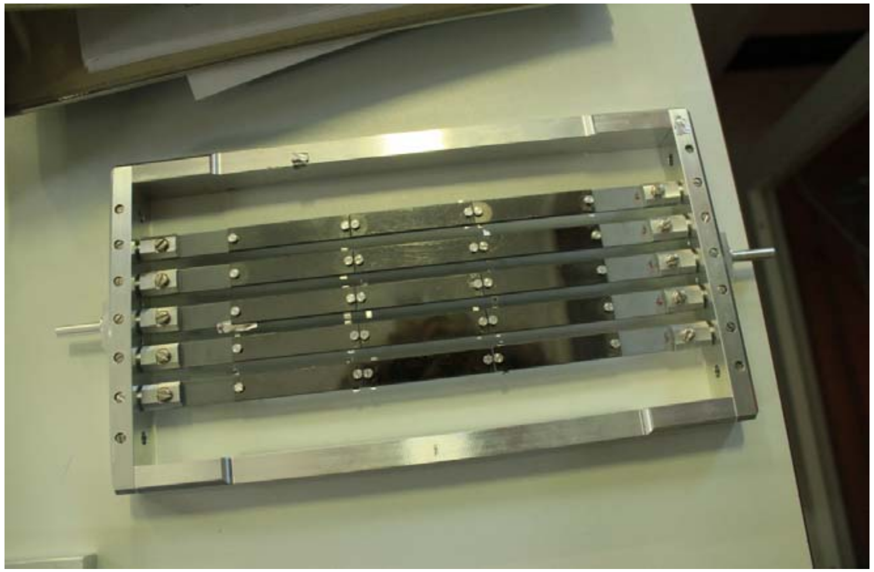
[§]The full multiplied gain factor is only applicable for cases where the entire coverage of S(q,ϖ) is scientifically relevant. The solid angle gain includes a comparison of the total analyser coverage of CAMEA corrected for transmission efficiency of the CAMEA analysers, conservatively estimate as a total gain factor of 7.1 for the 10 analysers.

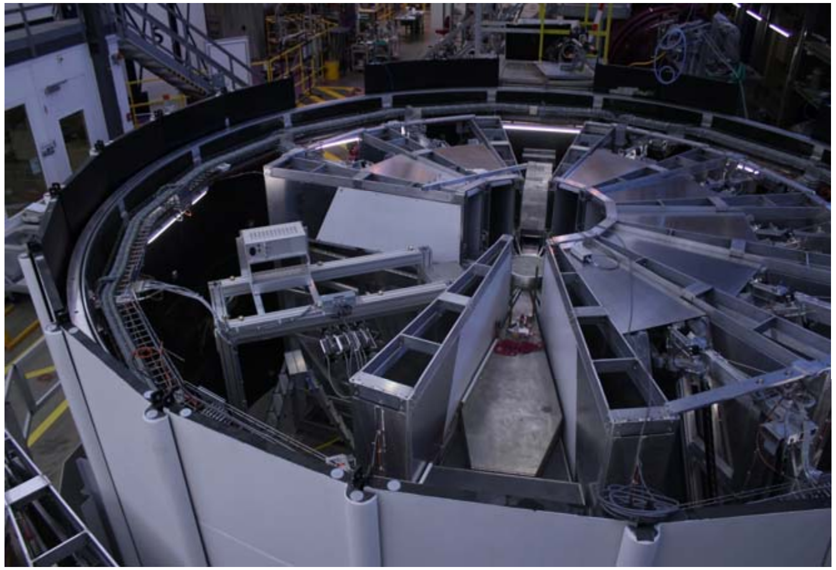
Gain factors are like tequila – should be taken with a handful of salt !

CAMEA @ ESS

Step by step:

- Mounted and tested at MARS@PSI
  - Flux is 1·10-4 of the proposed ESS instrument
  - Background-to-vanadium ratio is 1·10-4 in air (mostly electronic)
- Back-end: 3 1.5x15 cm2 PG-analyzers, 9 detectors
  - 2% of the proposed CAMEA back-end

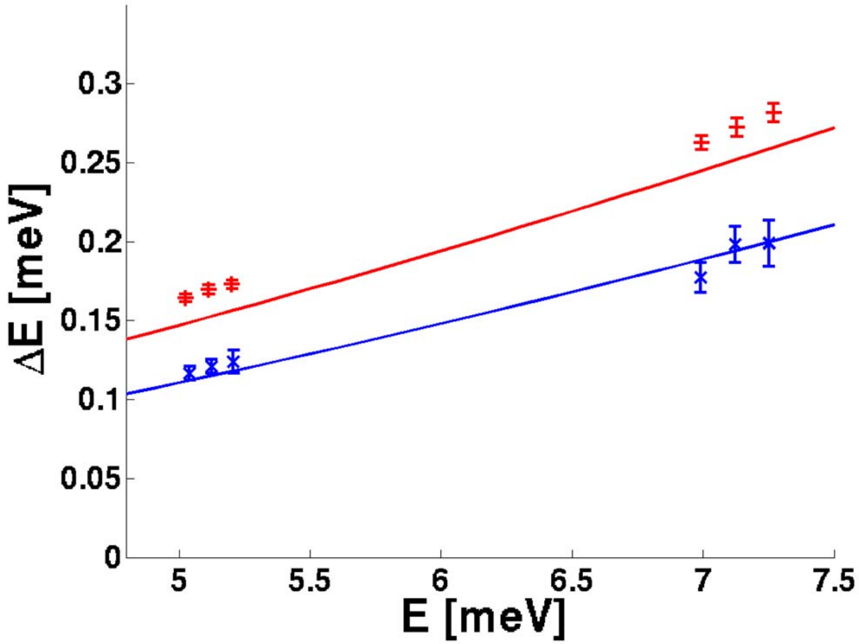


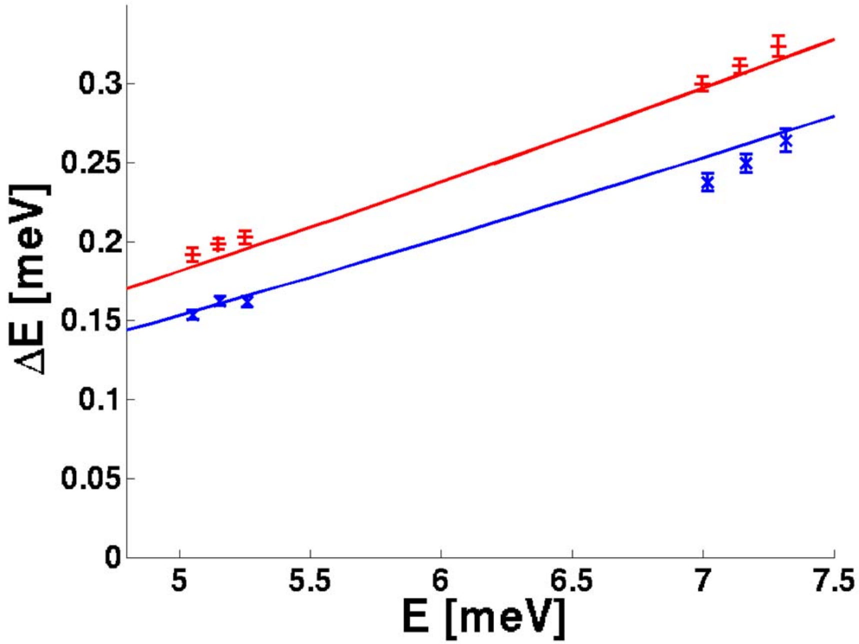


CAMEA-prototype

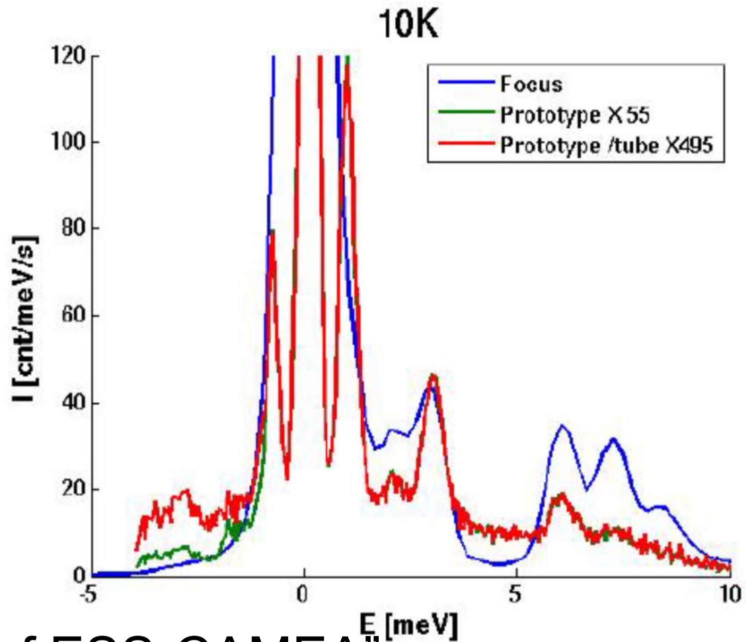
Results match calculations

- 1cm sample:
  - As typical TAS
  - 20% more for full pulse
  - 20% less for shaped pulse
- 3cm sample
  - Wider resolution
  - But still acceptable
  - Non-spherical samples OK

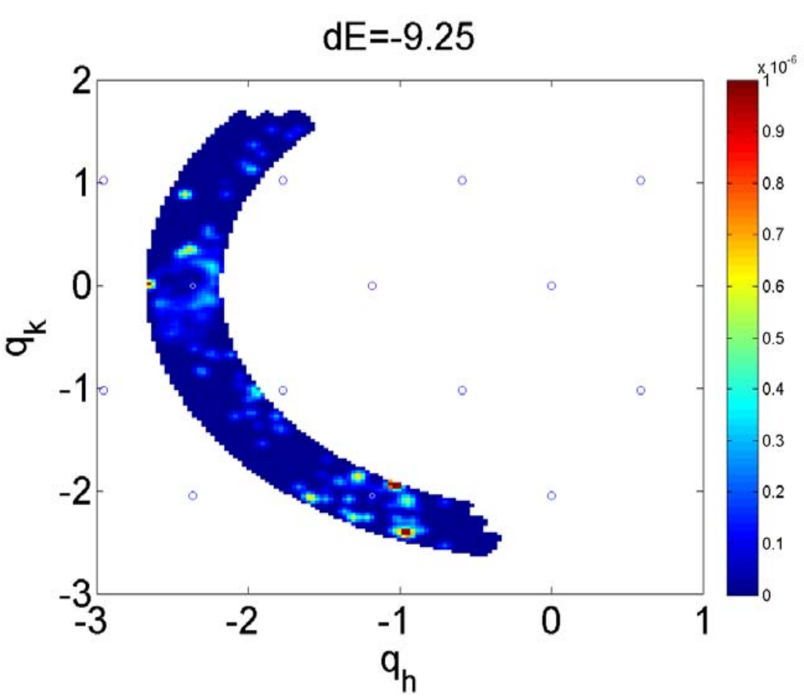


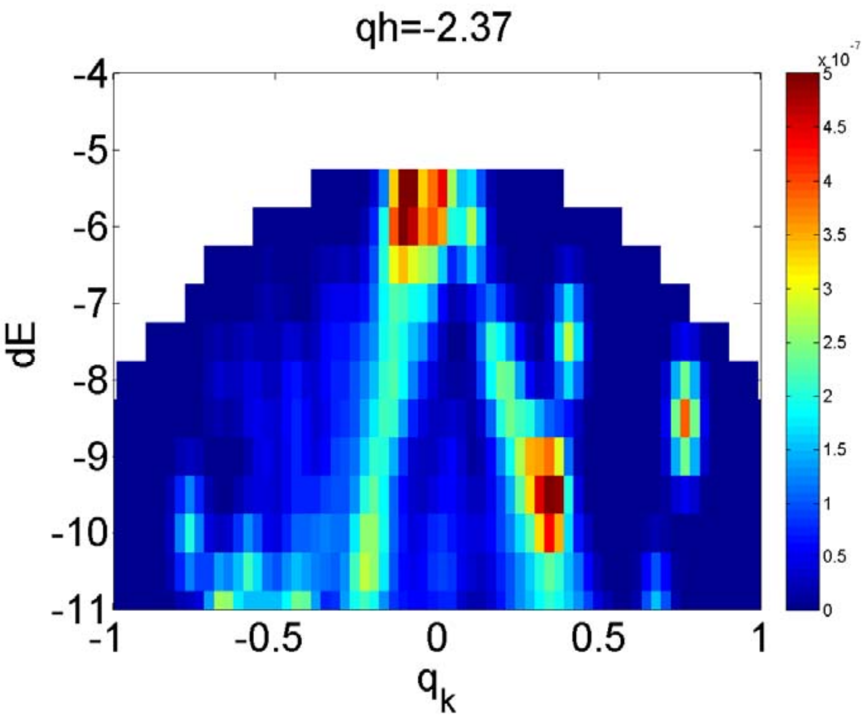


Prototype, test exp.



- Test experiments:
  - a) Crystal field ex. in LiHoF4
    - 3 hours per data set
  - b) Magnons in YMnO3
    - 24 h in total; crystal rotation scan
    - Data corrsponds to 8 seconds at “2% of ESS-CAMEA”

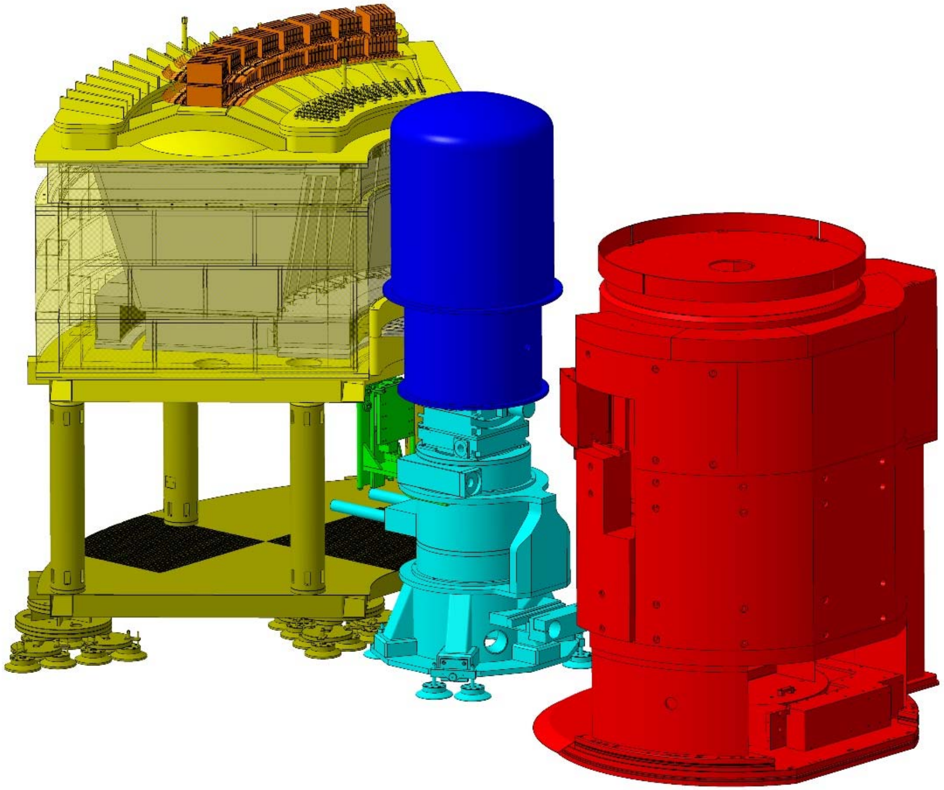




CAMEA @ PSI

Joint PSI-EPFL instrument

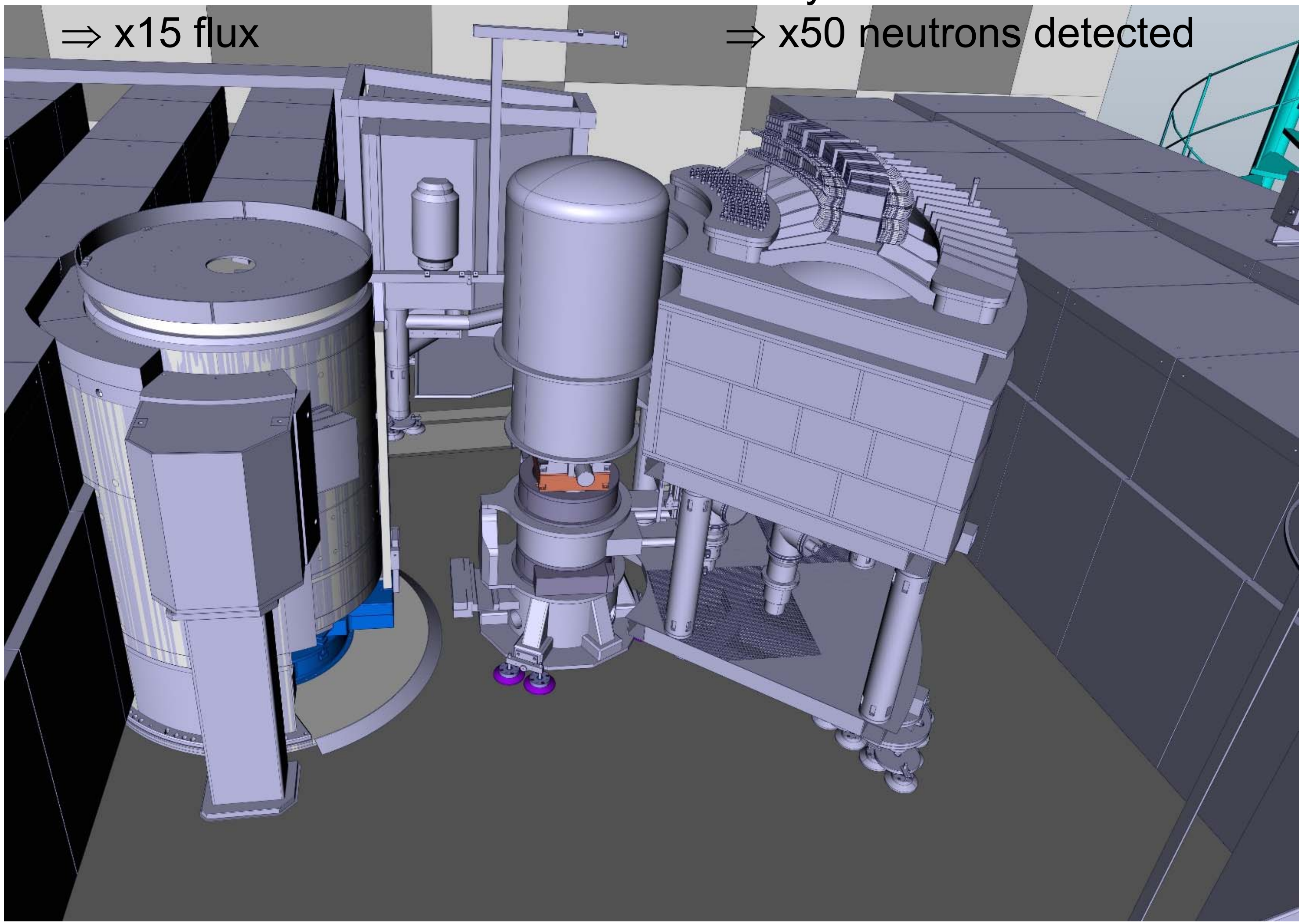
- ~60° Angular coverage
- 8 Energies (3.2 – 5 meV) => ~0.5 m^2 HOPG (0.02 m^2 @ RITA-II)
- ~100 PSD detectors



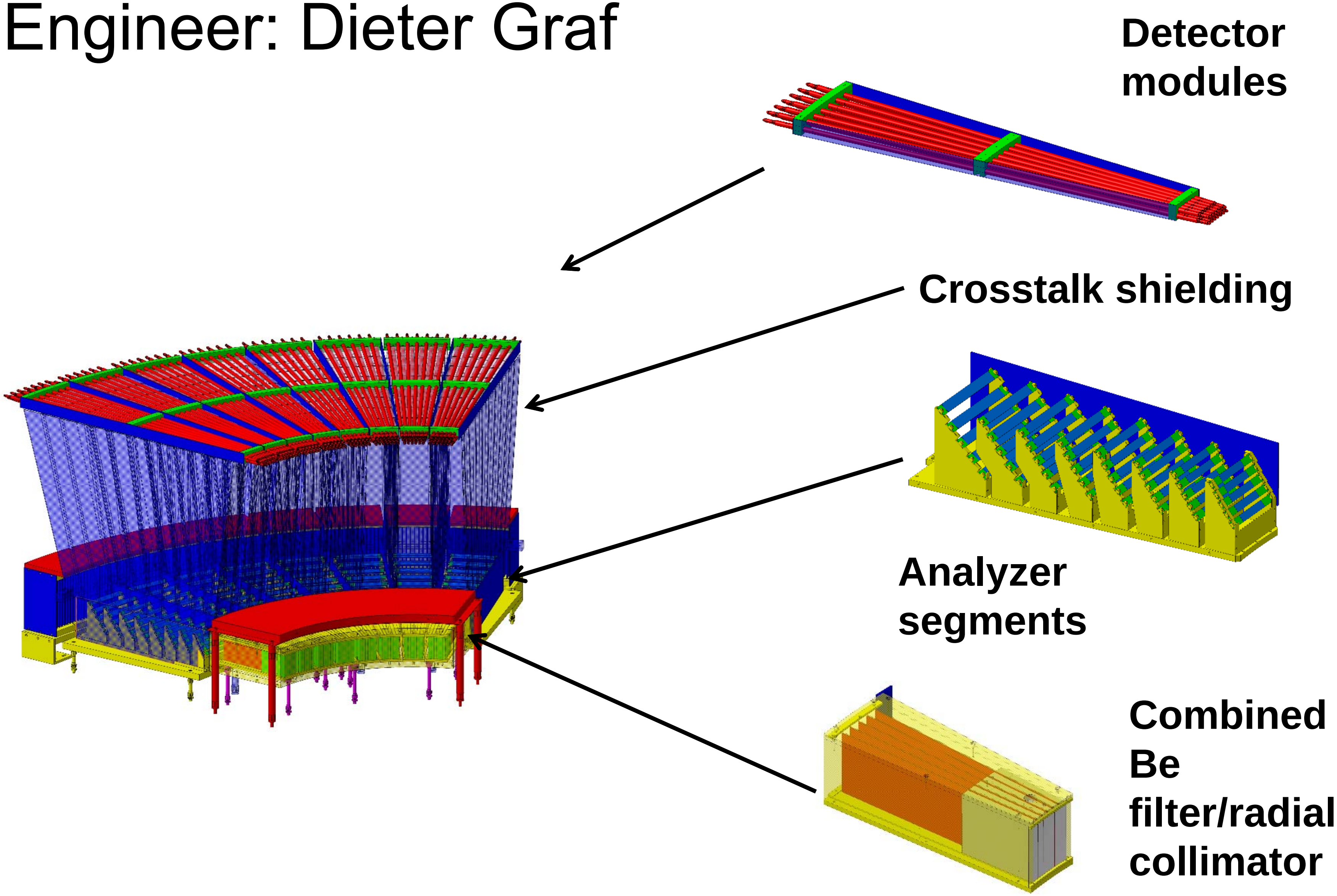
On cold neutron monochromator RITA-2

Stage 2:
New guide &
monochromator
⇒ x15 flux

Stage 1:
CAMEA
analyser-detector
⇒ x50 neutrons detected

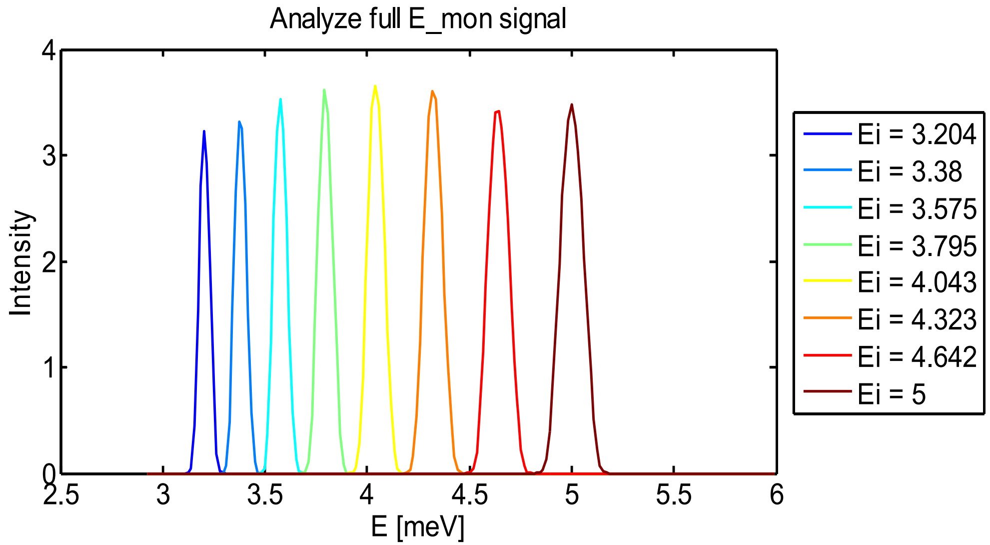


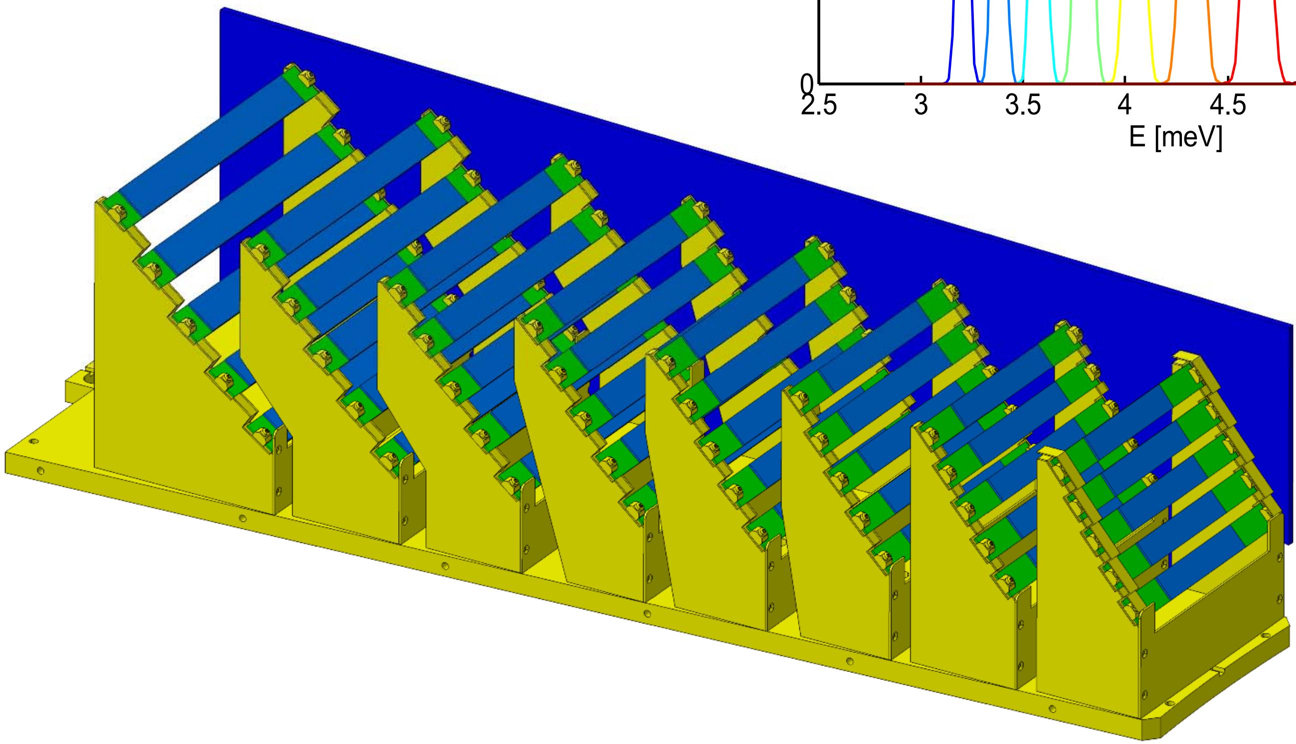
- Scientist: Felix Groitl
- Engineer: Dieter Graf



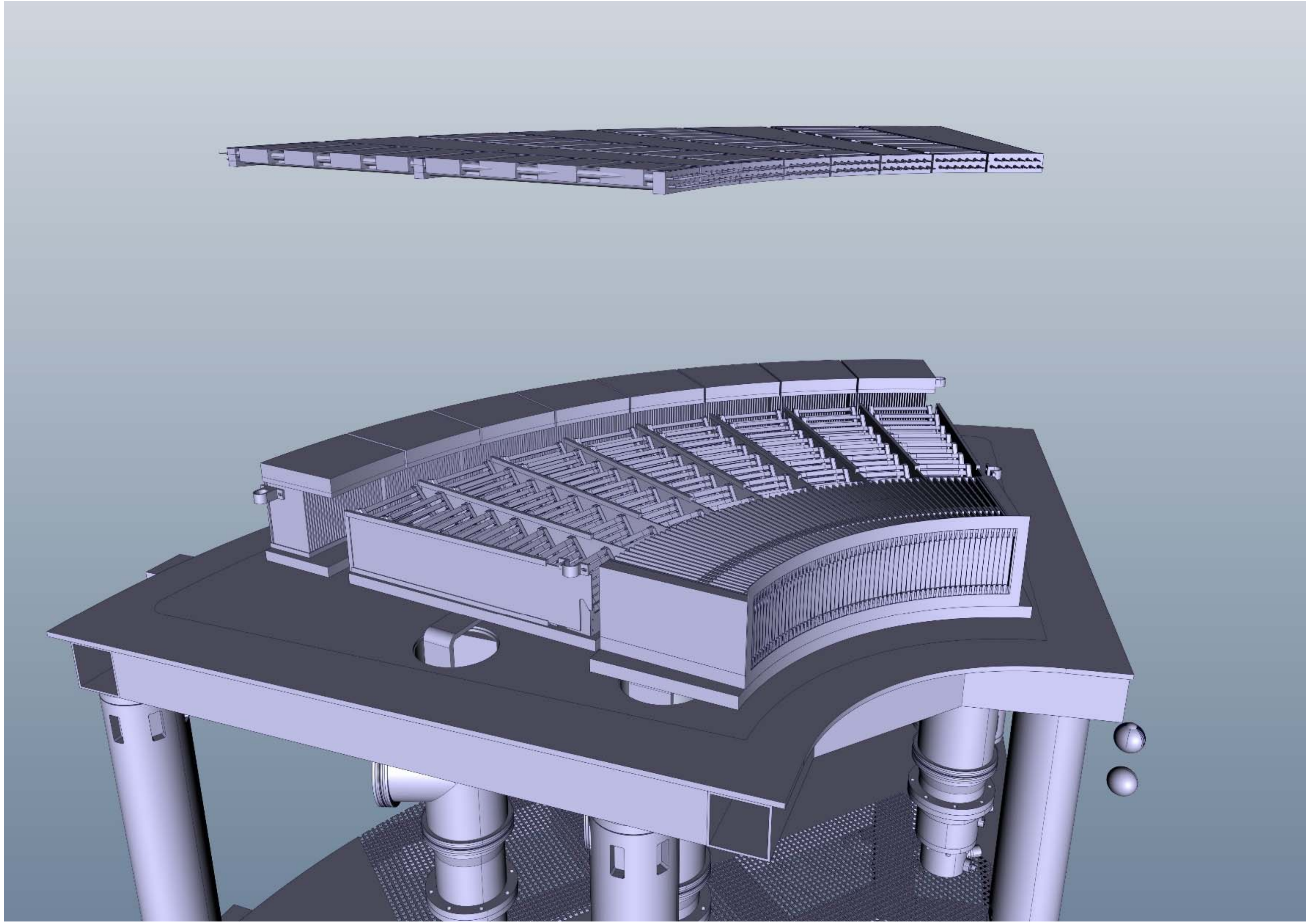
8 prismatic analysers (24 energies)

Closely stacked 3.2 to 5 meV



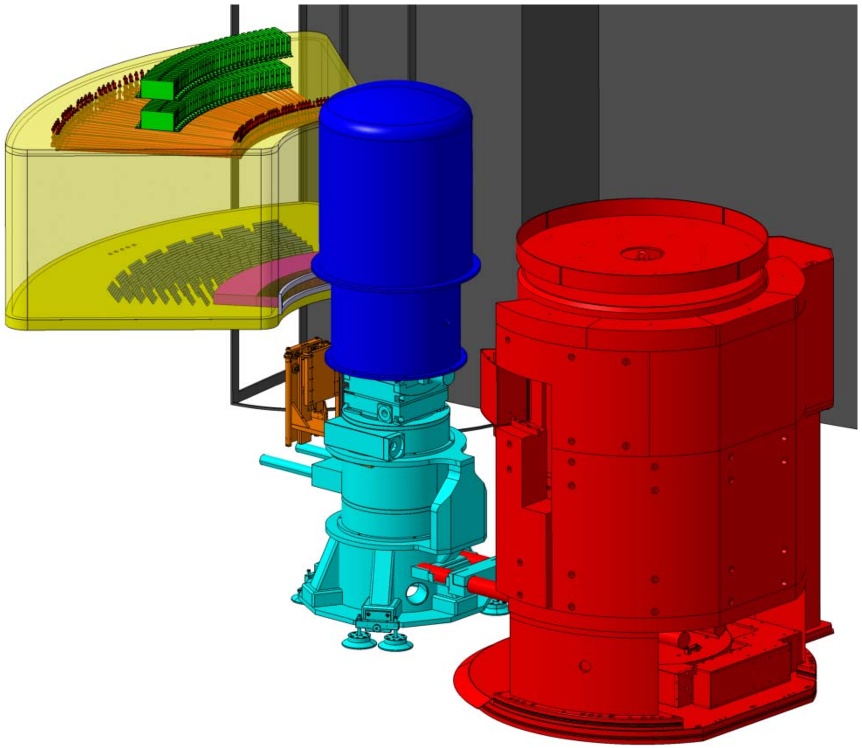


8 “cake pieces” ⇒ 60° scattering angle



PSI-CAMEA

- Joint EPFL-PSI instrument on cold PG monochromator
- Status: Engineering design
- Construction 2015-2016, Commissioning 2017



Wahl Neutronics Geometrie/Optimierung, Test der Kühlung (Prototyp)

04/2014

Konstruktion, Technische Zeichnungen

04/2015

Beschaffung, Fertigung, Qualitätskontrolle, Montage

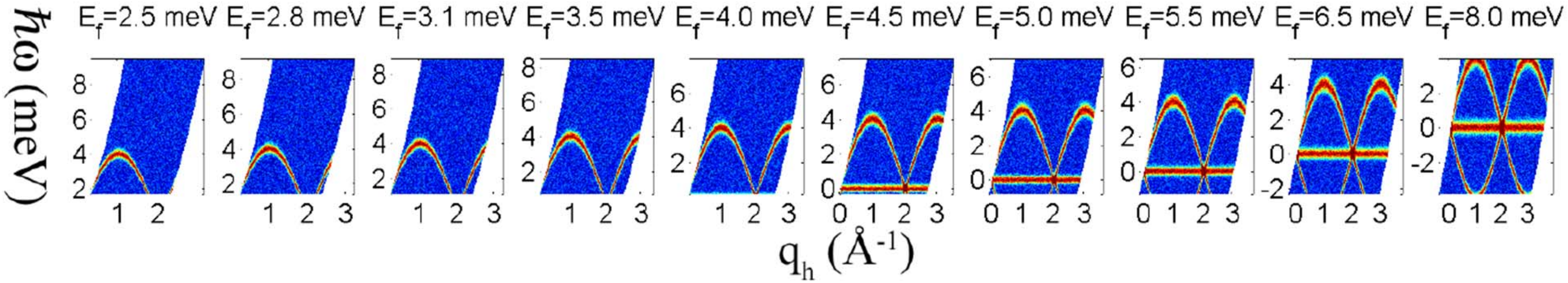
03/2016

Justage, Implementation, Kalibrationsmessungen

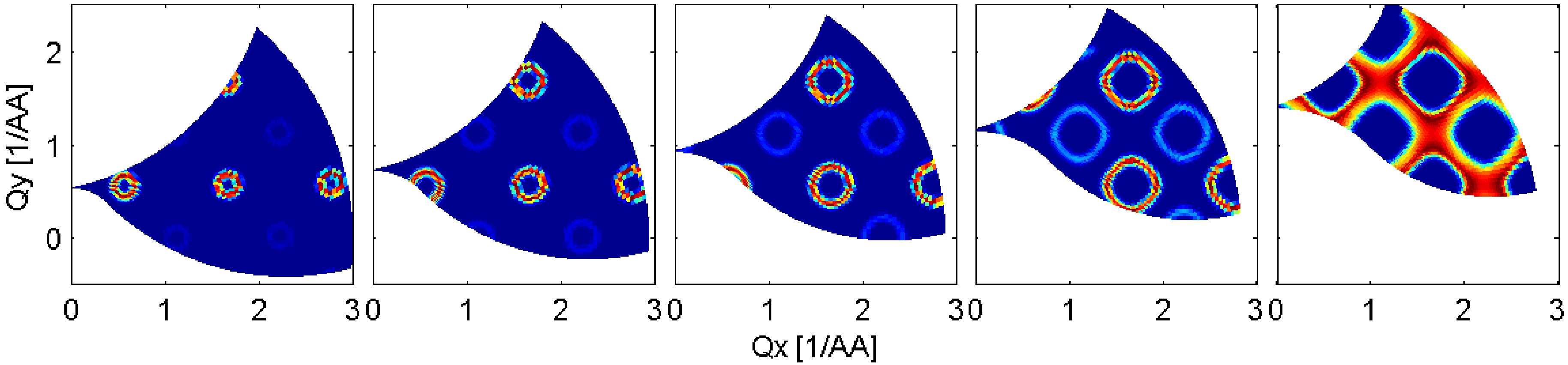
08/2016

CAMEA: best possible "in-plane spectrometer"

- iTOF-CAMEA @ ESS: dispersions in one acquisition



- TAS-CAMEA @ PSI: Q-maps in one rotation scan



CAMEA From all of us to all of you