Prospects for future instrument developments

• • •

F. Mezei

EUROPEAN SPALLATION SOURCE

INSIS

Subjects

- Economy of useful neutron production

  - spallation → pulsed sources → short pulses → long pulses
- Multiplexing chopper systems to control pulse parameters

  - in TOF spectroscopy (RRM)

  -in diffraction, etc (WFM)
- Multiwavelength data collection
- Event recording (list mode)
- Asynchronous chopper systems
- Special choppers ("magic", selective, broad band)
- Beam modulation alternatives to pulse shaping
- Good use of more neutrons (?)

Neutron production economy: spallation

Fast neutrons produced / joule energy or heat:

Fission reactors:	~ 10^9	(in ~ 50 liter volume)
Spallation:	~ 10^{10}	(in ~ 2 liter volume)
Fusion:	~1.5×10^{10}	(in ~ 2 liter volume)
(but neutron slowing down efficiency reduced by ~20 times)		
Photo neutrons:	~ 10^9	(in ~ 0.01 liter volume)
Nuclear reaction (p, Be):	~ 10^8	(in ~ 0.001 liter volume)
Laser induced fusion:	~ 10^4	(in ~ 10^{-9} liter volume)

Spallation: most favorable energy efficiency for the foreseeable future

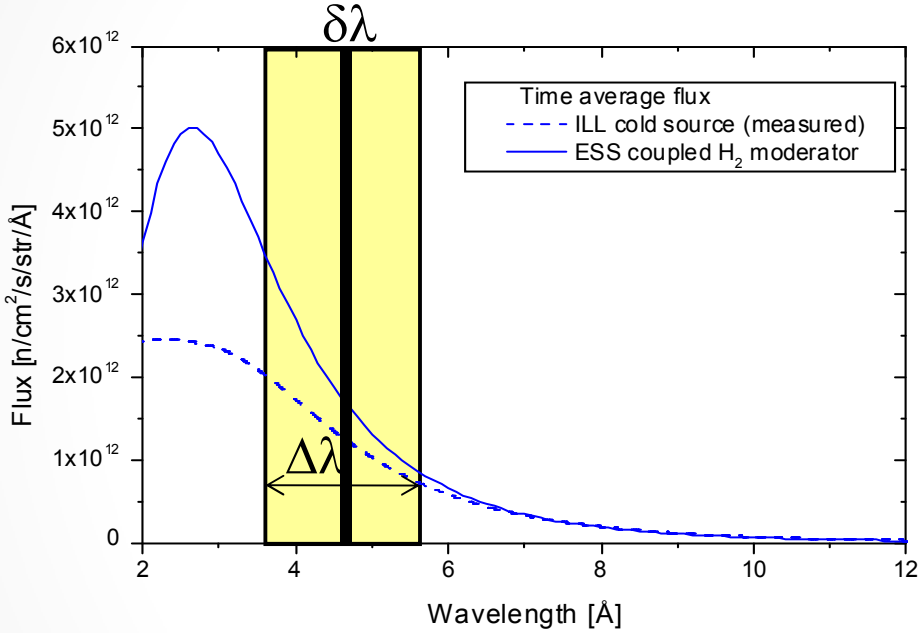
Price-to-pay: no accelerator was built for > 1.4 MW, fission reactors can be > 50 MW

Neutron production economy: pulsed sources

Monochromatization by

- wavelength selection (crystal)

- time-of-flight (TOF)



→ same flux at CW source

(Crystal) monochromator:

$\phi \propto \delta\lambda$

TOF monochromator:

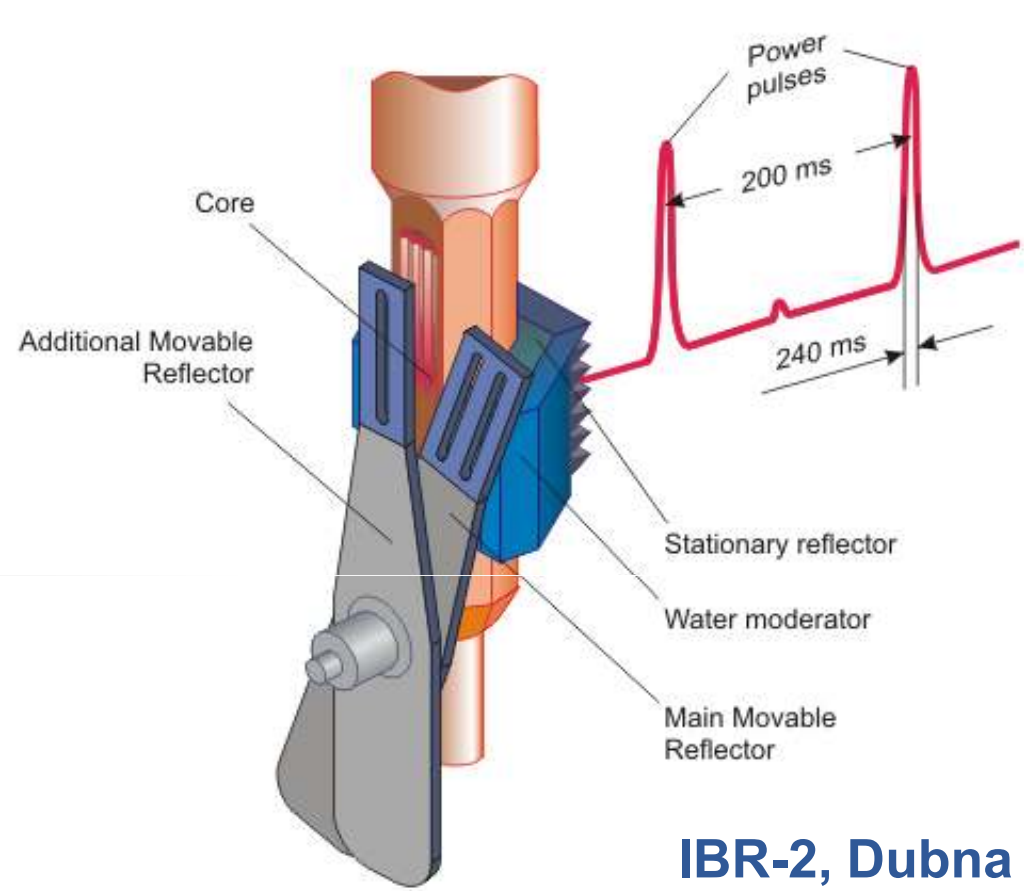
$\phi \propto \Delta\lambda(\delta t/T) = \delta\lambda$

↑

$\delta\lambda/\Delta\lambda$

TOF monochromatization: source only needs to be switched on for a short time, gain in economy ∝ 1/(pulsed source duty factor)

Neutron production economy: pulsed reactor



IBR-2, Dubna

Time average power:
2 MW

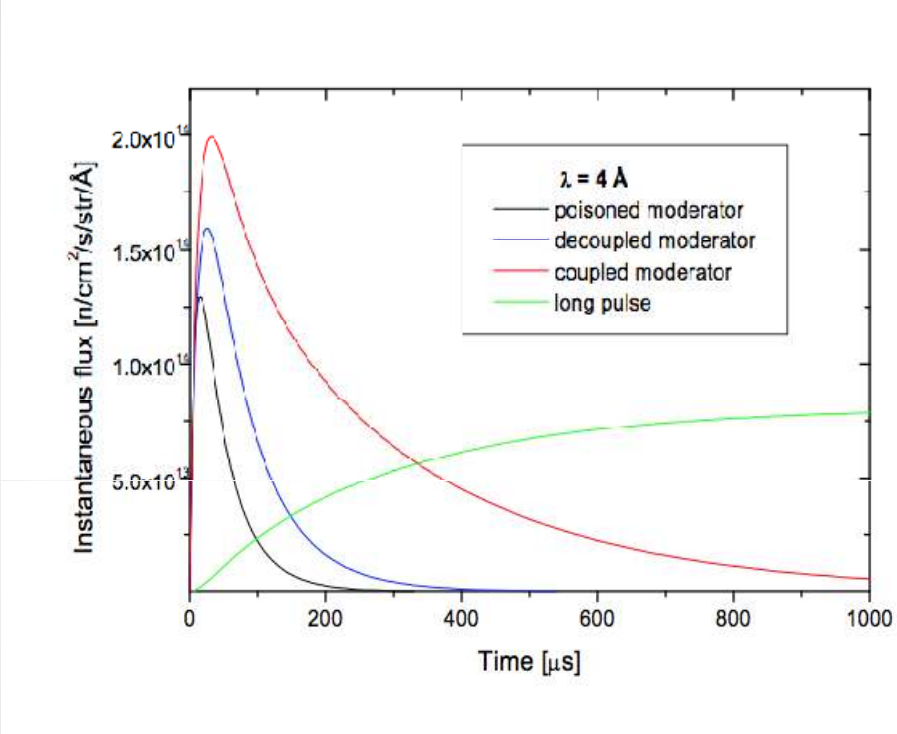
Peak power in pulse:
850 MW

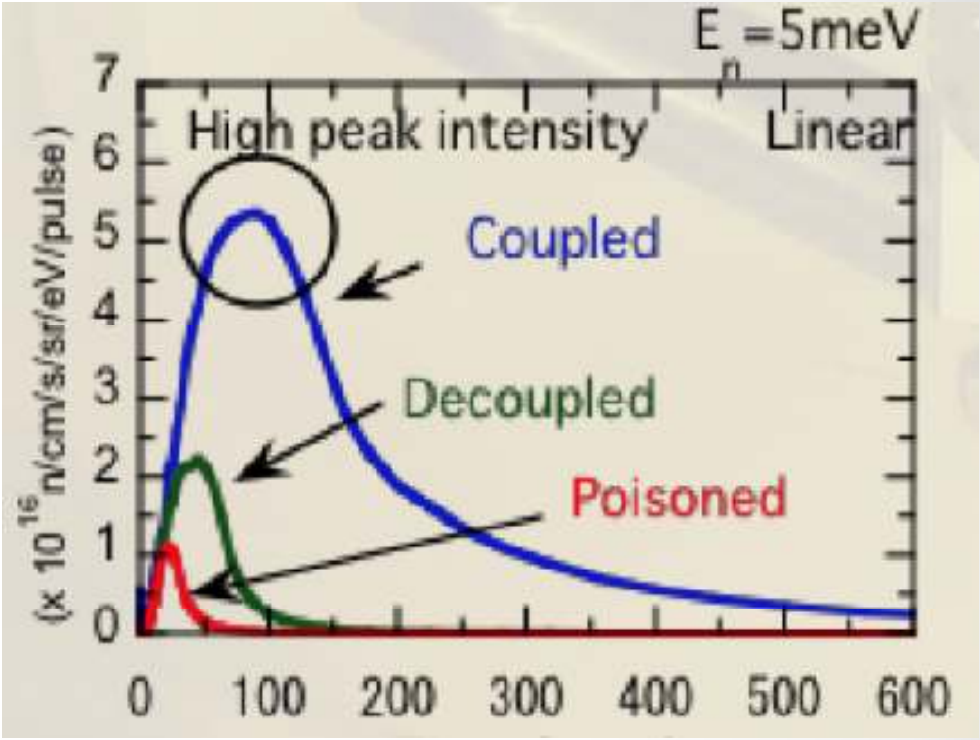
Great fuel economy!

Pulsed reactor source

Price-to-pay: fast neutron Pu reactor, technology limited in power

Neutron production economy: short pulses





Short pulse spallation sources

Price-to-pay:

a) pulse parameters imposed by the source design and/or fixed at each beam-line

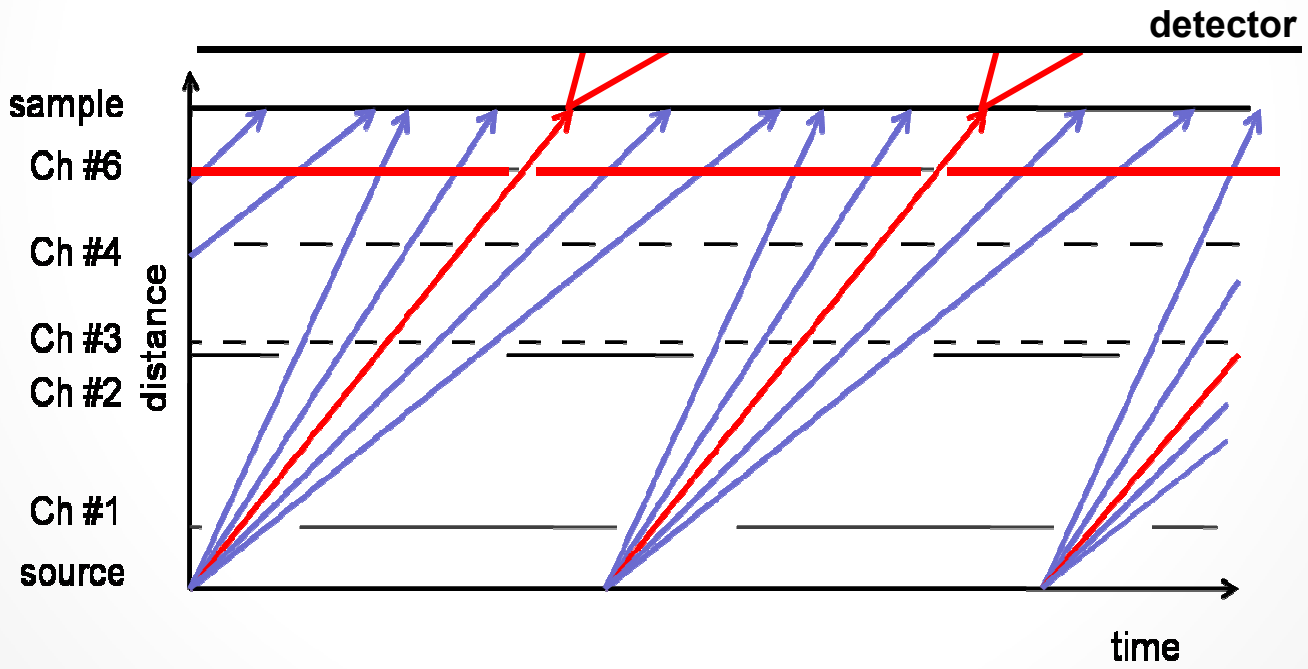
Multiplexing control of pulse frequency: RRM

Ideal pulse repetition rate (OK at CW source):

- 10 Hz (e.g. SANS)
- 600 Hz (e.g. thermal TOF spectroscopy)

Multiplexing:

fill in dead time by dissimilar sub-frames uses within one source frame



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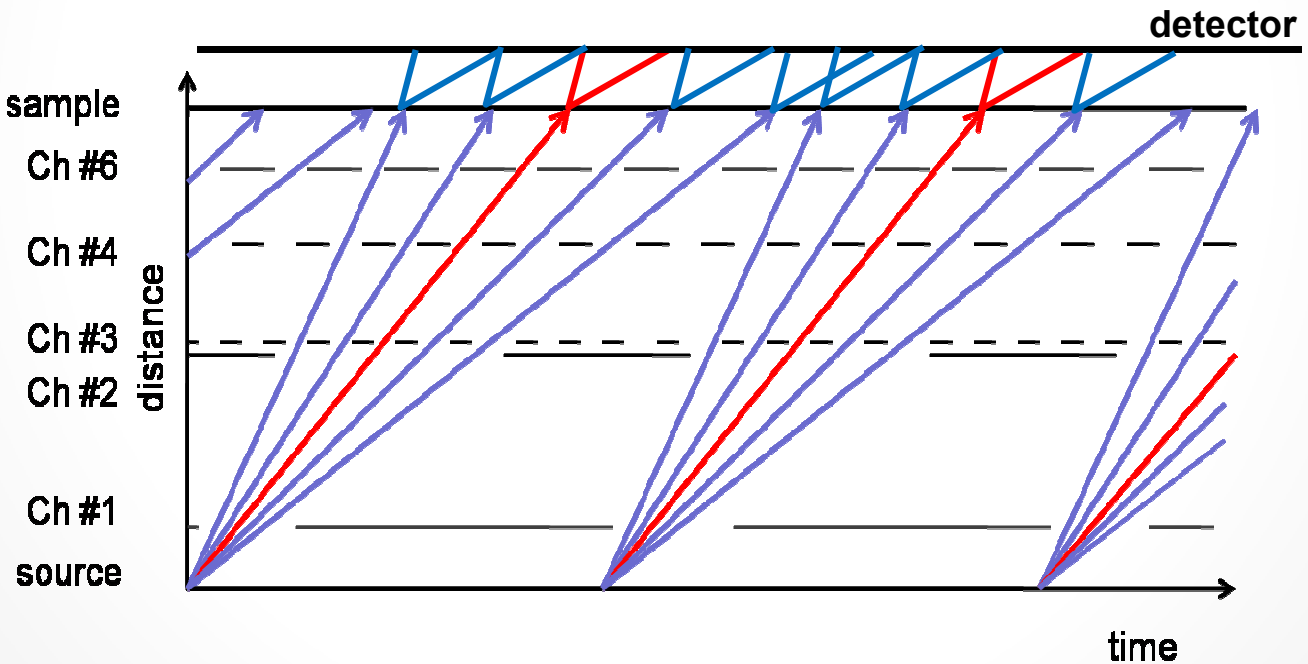
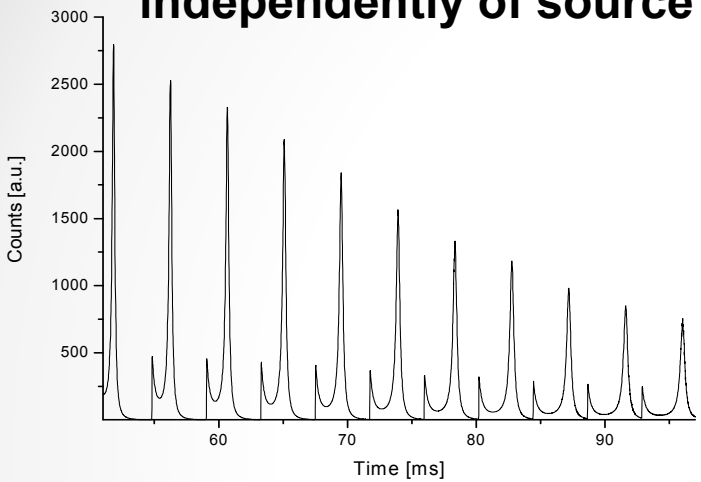
Repetition Rate Multiplication: (nearly) free choice of rep. rate on sample



Price-to-pay: multi wavelength data collection and evaluation

Practical Rep. Rate Multiplication

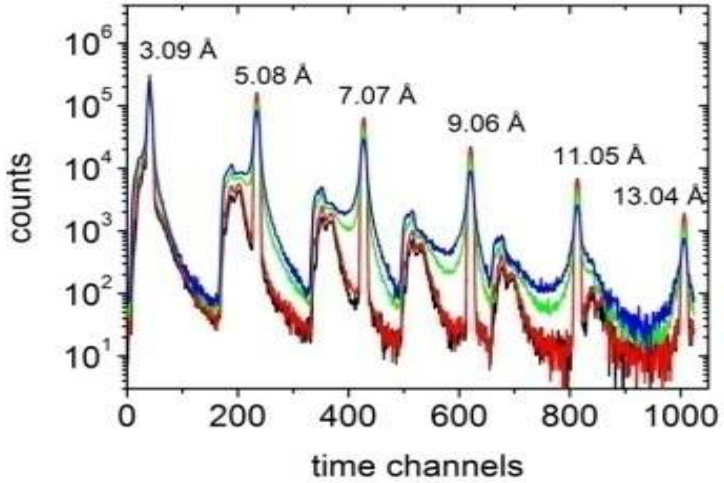
(Nearly) free choice of pulse repetition rate for TOF spectroscopy, (nearly) independently of source frequency: key to source design optimization



240 Hz data collection at 20 Hz source
Simulated data, IN500 project, Lujan Center

Optimized instrument length > 50 m

First experimental implementation: emulation of pulsed source operation at NEAT TOF spectrometer at HZB, Berlin

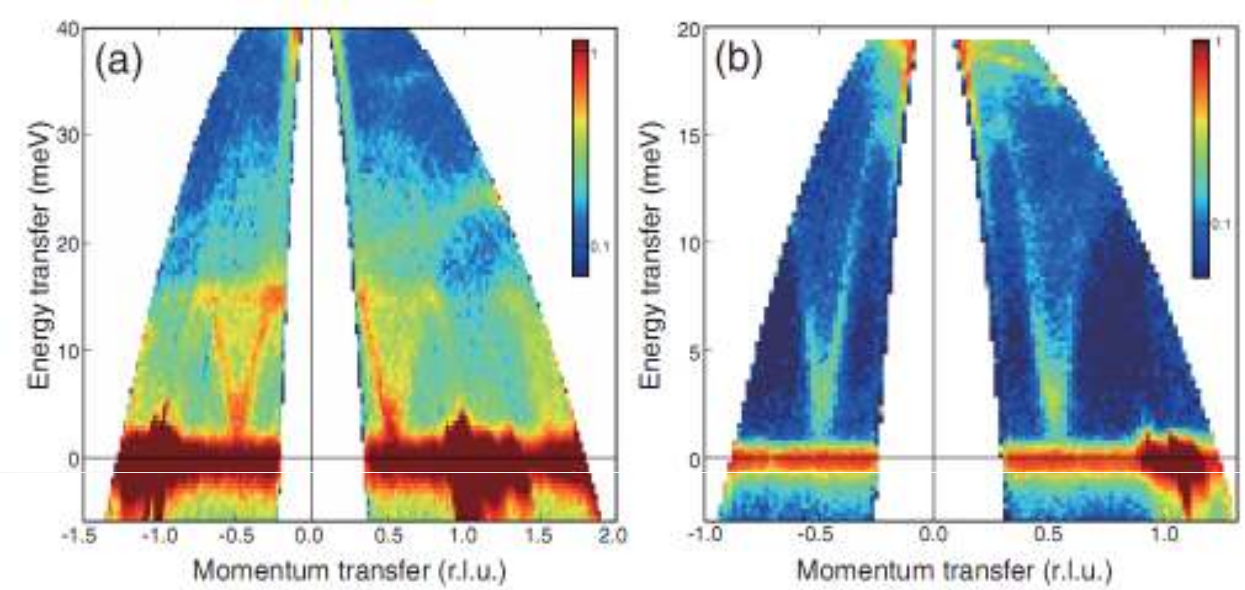


RRM chopper rules: $f_i = nf_S$ $f_iL_i = f_jL_j$
f_i, L_i "quantized"

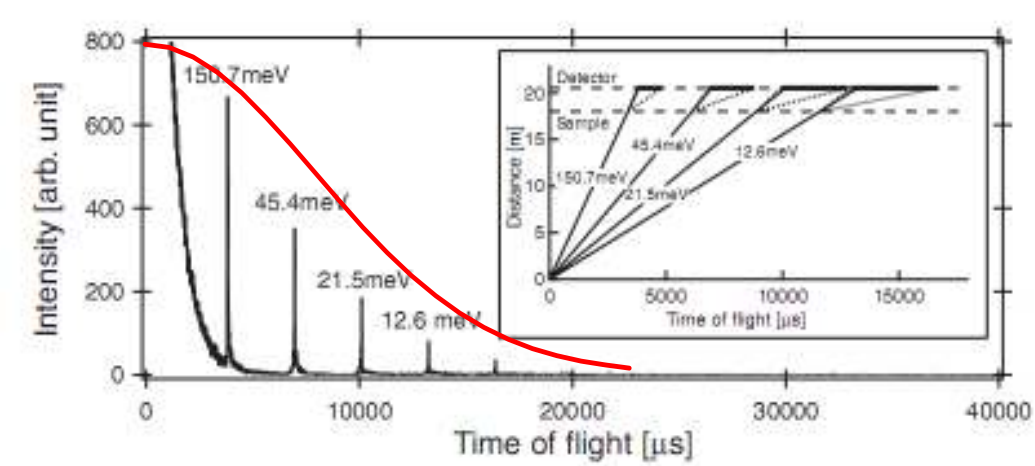
Evidence for significant, broad band simultaneous information over a broad range of incoming wavelengths

Practical Rep. Rate Multiplication

First RRM experimental data on a pulsed source instrument: 4-SAESONS



M. Nakamura, R. Kajimoto, Y. Inamura, F. Mizuno, M.Fujita, T. Yokoo, M. Arai, J. Phys. Soc. Jpn. 2009



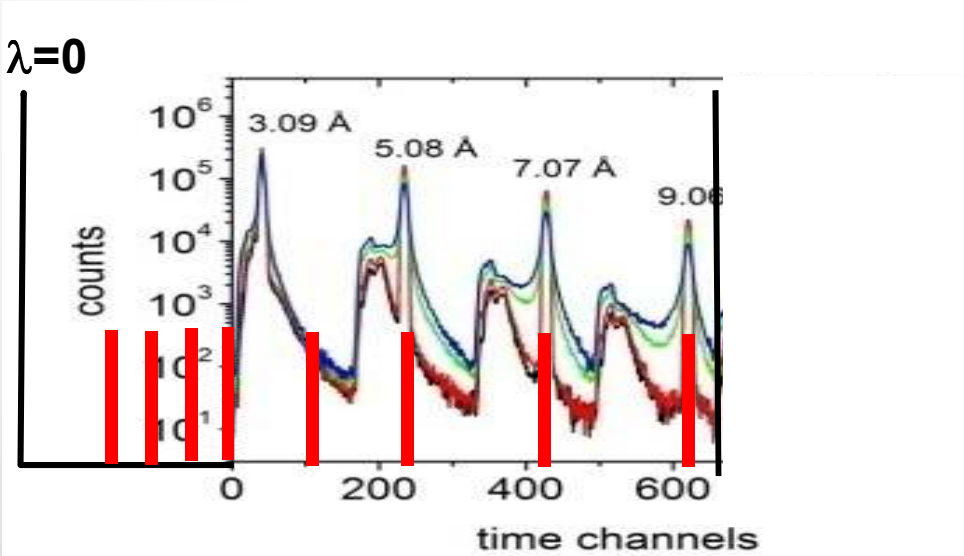
Simple implementation by transmission band of Fermi chopper (red line) and low source frequency (40 ms source repetition rate)

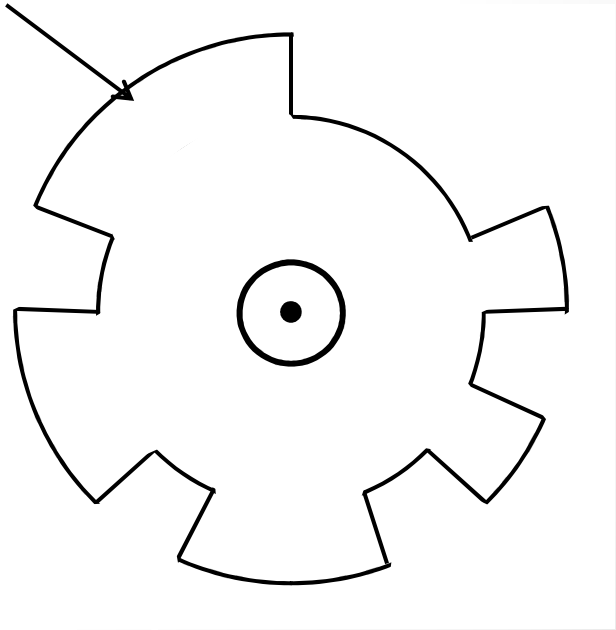
Practical Rep. Rate Multiplication

- **Broad band Fermi choppers:**
  short slit package (1-2 cm)
  (TOF Diffractom. EXED, HZB)

- **"Magic chopper": pulse length $\delta t \propto \lambda$**
  (J-PARC)

- **Selective pulse suppression:** by chopper synchronized to source frequency
  RRM frame length ΔT custom designed, e.g. $\propto \lambda$





Neutron production economy: short pulses

SNS (Oak Ridge, USA)

J-PARC (Tokai Japan)

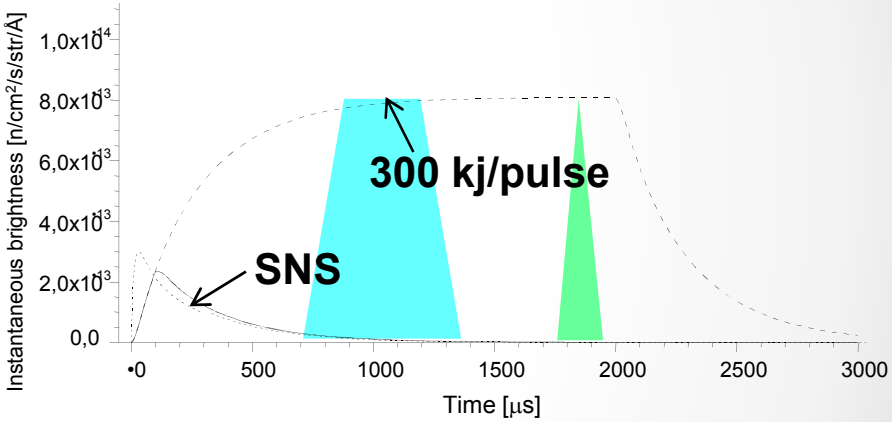
b) Instantaneous power on target sets early limit on power

1 MW at 60 Hz, i.e. 17 kj in ~1 μs pulses: **17 x**
→ ~ 300 bar pressure wave

Neutron production economy: long pulses

Cost equivalent linear accelerator alone can produce at 60 bar pressure wave

- more neutrons pulse
- higher peak flux



Long pulse sources: more neutrons, higher peak flux at same costs

Price-to-pay:

- must implement neutron pulse shaping chopper systems

- fringe benefit: regaining full individual control on pulse parameters (as CW sources)

Neutronic performance: "peak flux theorem"

In neutron scattering work for a neutron source with sufficiently long source pulses the peak flux alone matters, independently of any reasonable source time structure (continuous or pulsed)

Neutronic performance: "peak flux theorem"

For an arbitrary source repetition rate f one will choose the instrument length L so that to assure the desired band $\Delta\lambda$:

$$L = A\,\Delta\lambda^{-1} f^{-1}$$

(A=3956 Åm/s). With this L the pulse length t for the required resolution $\delta\lambda$ has to be

$$t = A^{-1} L\,\delta\lambda = f^{-1}(\delta\lambda/\Delta\lambda)$$

Can be as much as 10 % of f^{-1}=T

The neutron flux on the sample will be given in terms of the peak source brightness function $\Phi_P(\lambda)$, beam divergence $\delta\Omega$ and the efficiency factor of the beam delivery system η

$$\varphi = \eta\,\delta\Omega\, t\, f \int \Phi_P(\lambda)\, d\lambda = \eta\,\delta\Omega\,(\delta\lambda/\Delta\lambda) \int \Phi_P(\lambda)\, d\lambda\,,$$

Independent of f!

The integral is over the wavelength band $\Delta\lambda = \lambda_{max} - \lambda_{min}$. There must be no dead time between pulses: multiplexing mandatory

Neutronic performance: "peak flux theorem"

What is "sufficiently long pulse t_{min}"?

- **Irradiation work: ∞**
- **Single (Q,ω) experiments (D3, TAS?): ∞**
- **SANS, NSE: 2 – 4 ms**
- **Reflectometry: 0.5 – 2 ms**
- **Single Xtal diffraction: 100 – 500 μs**
- **Powder diffraction: 5 – 500 μs**
- **Cold neutron spectroscopy: 50 – 2000 μs**
- **Thermal neutron spectroscopy: 20 – 600 μs**
- **Hot neutron spectroscopy: 10 – 300 μs**
- **Electronvolt spectroscopy: 1 – 10 μs**

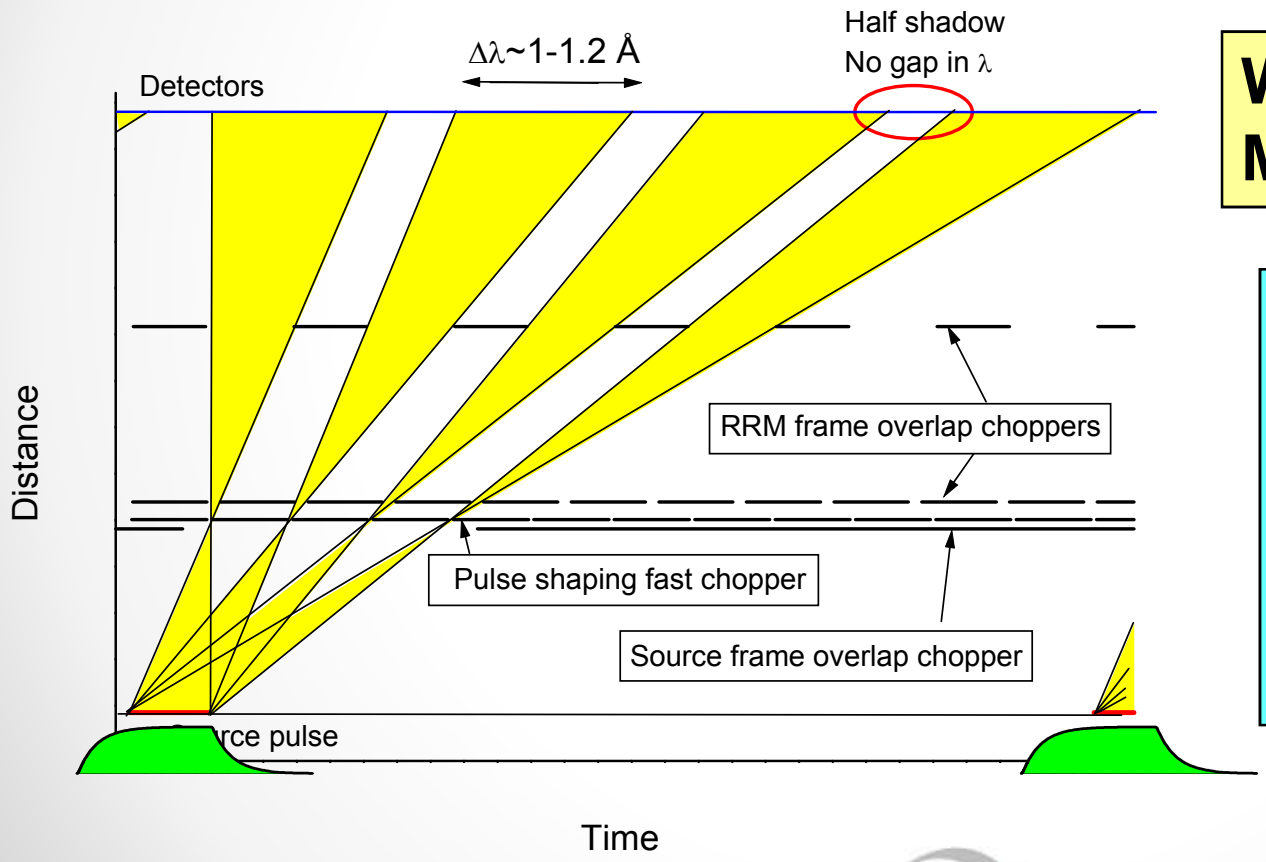
Rough estimate: $t_{min}/T \sim \delta\lambda/\lambda$

Pulse shaping not always required (blue numbers).

Multiplexing control of pulse length: WFM

All-round pulse shaping tool for diffraction and inverted geometry spectroscopy at long pulse sources:

Multiplexing chopper system: **(nearly) invisible for the user**

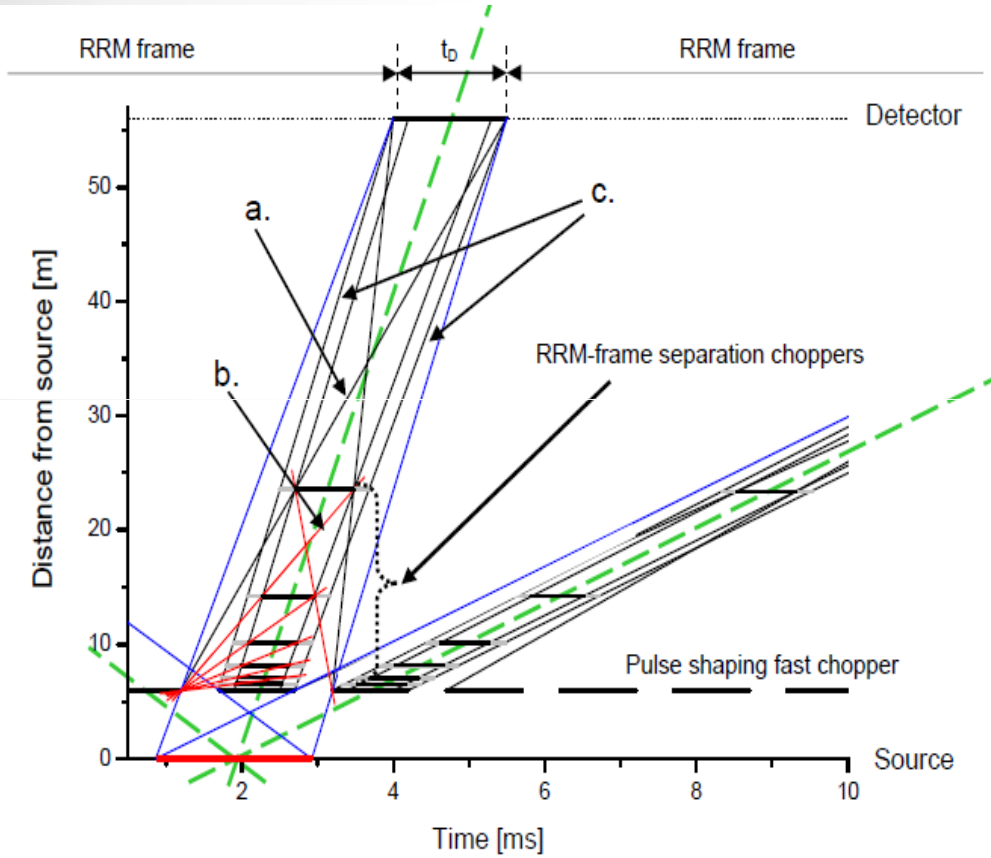


Wavelength Frame Multiplication

One to one relation between time at sample and chopper opening.

Pulse shaping chopper repetition time: ~ useful source pulse length (0.8 – 2 ms → 500 – 1250 Hz)

Multiplexing control of pulse length: WFM



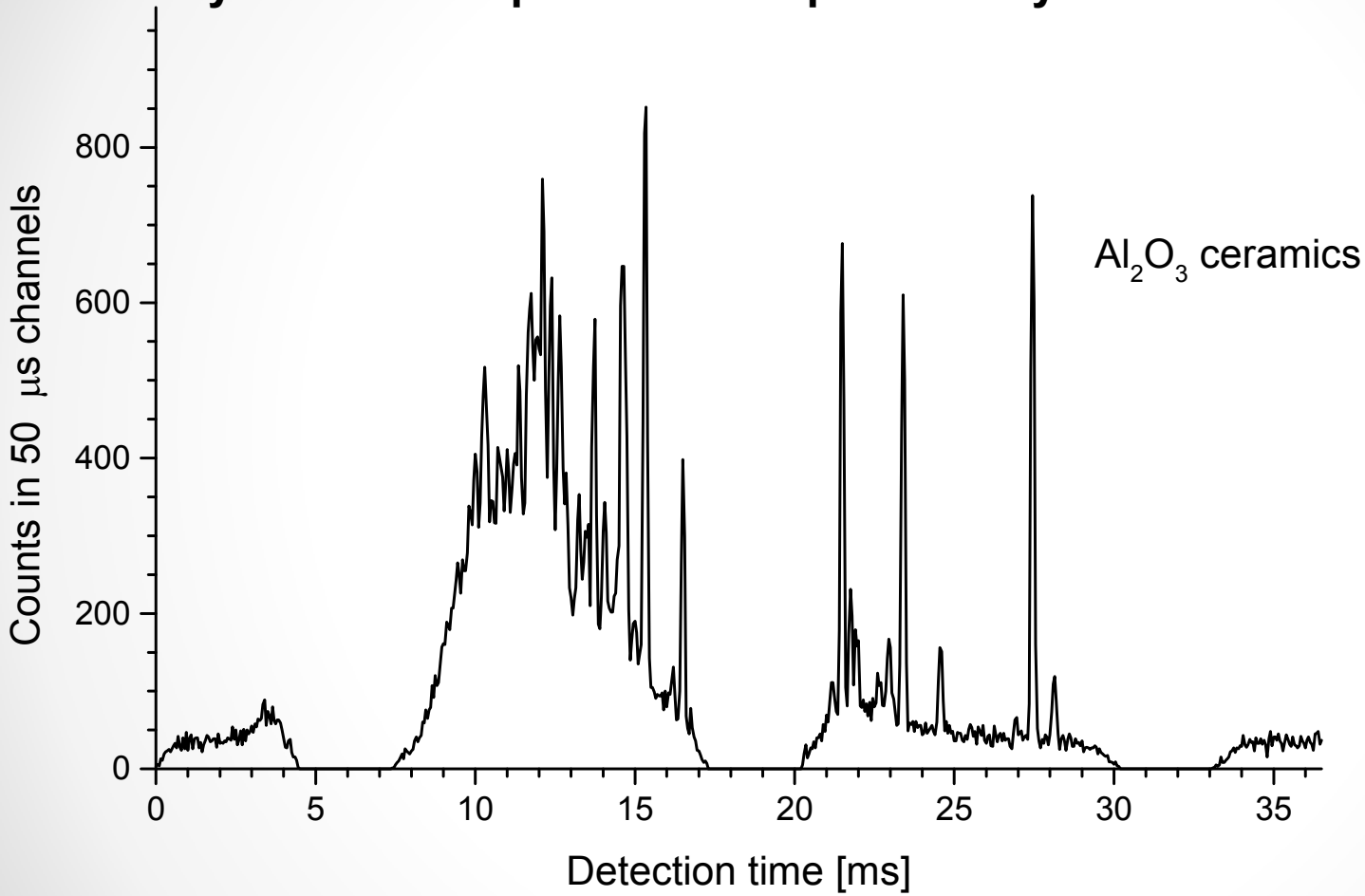
Design principles of chopper system for WFM (RRM) pulse shaping:

Turns a LP source into an ideal short pulse source with > 90 % efficiency (some dead time) for ~ 1 M€ extra cost for choppers per beam line

First implementation in full scale instrument: DNA (J-PARC), L=40 m, 3 RRM-frame choppers 0.7 ms collection time for short coupled cold moderator pulses (N. Takahashi, et al. 2010)

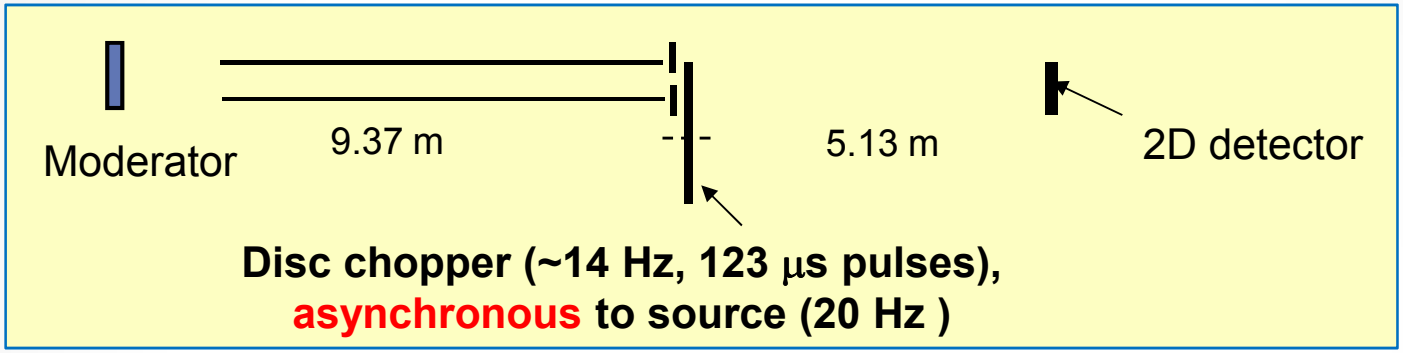
Practical Wavelength Frame Multiplication

Spectrum as a function of time of detection: synchronous operation
Asynchronous operation also possible by event recording ("list mode")



Key tool for multiplexing: event recording

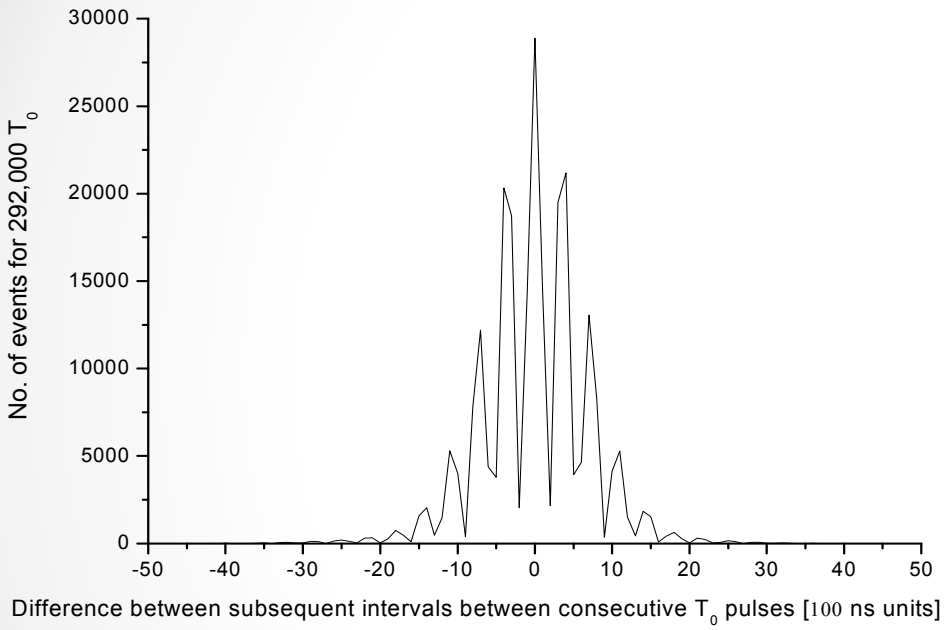
Event recording ("list mode") data acquisition: return to Galileo's fundamentals: experiment = as it happened



M. Russina, F. Mezei, T. Kozloski, P. Lewis, S. Pentilla, J. Fuzi, E. David, G. Messing, ICANS-XVI, 2003

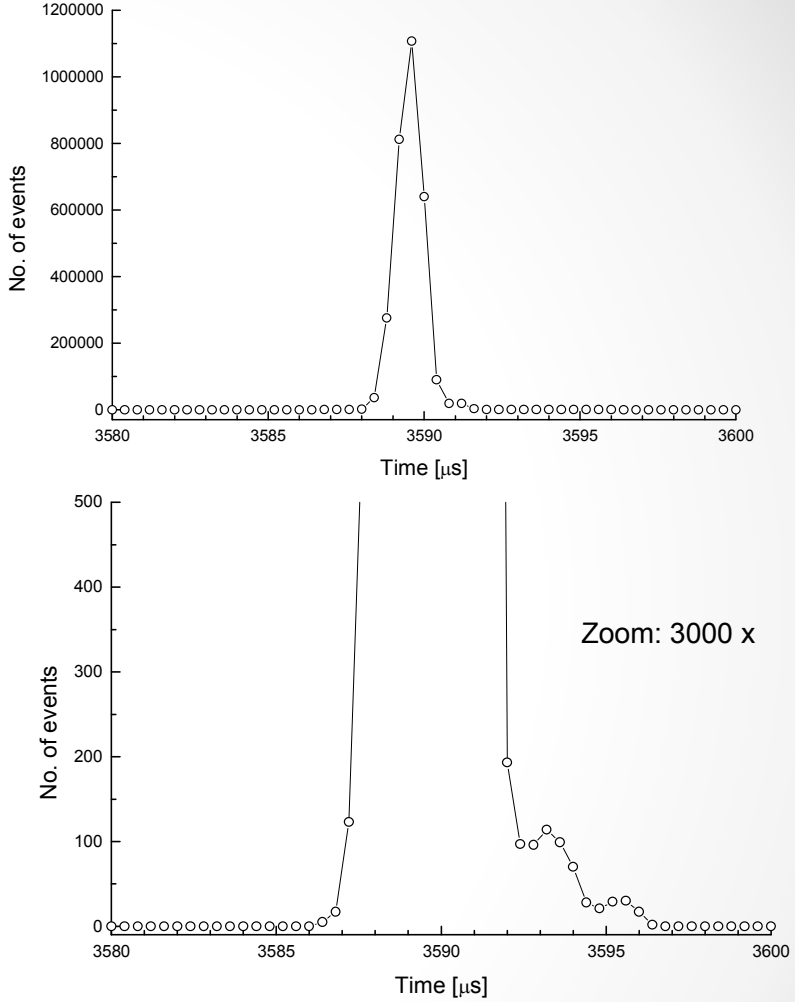
List mode data:
00004E75 00020000
0000573E 02000000
000062E5 00040000
000078F2 02000000
000088EE 00080000
00008EDF 08000000
0000C386 00080000
0000FE1F 00080000

Key tool for multiplexing: event recording



Jumps between subsequent T_0 time signal intervals (Lujan Center):

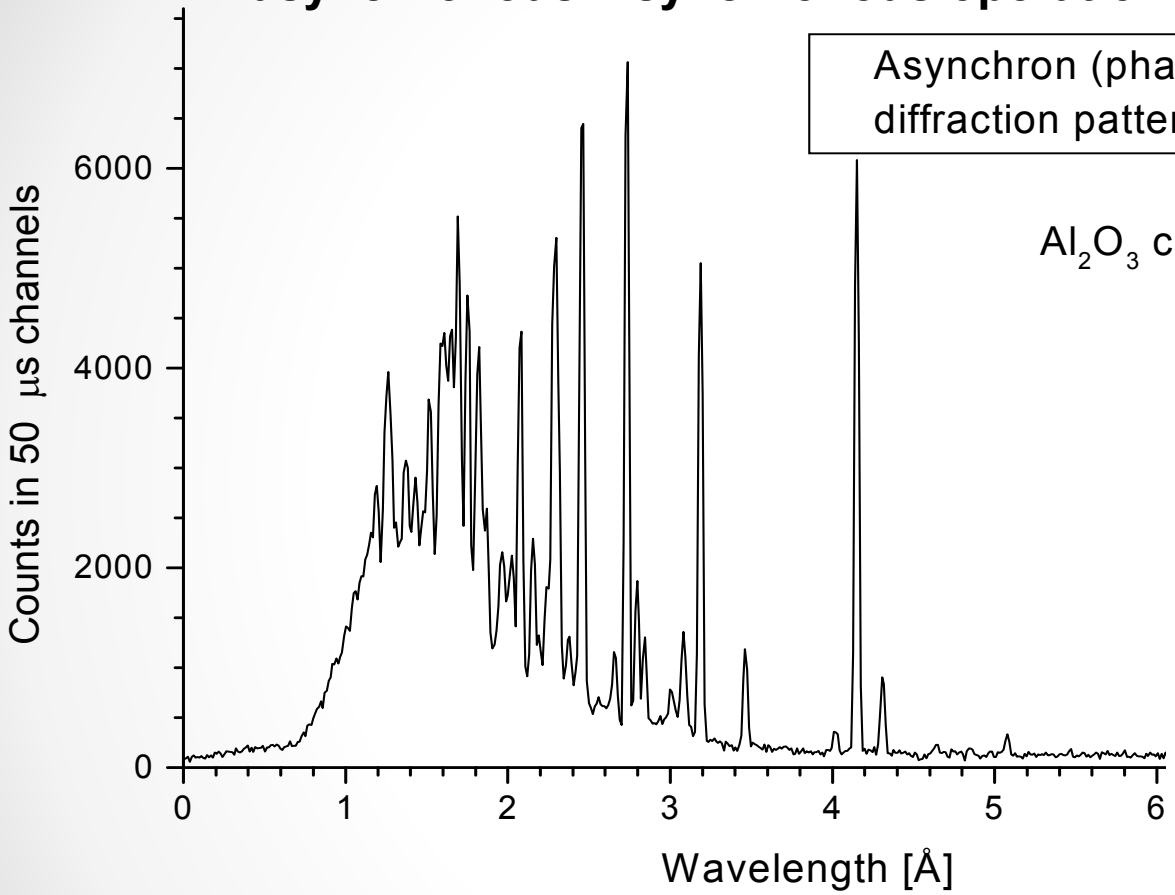
- **uncontrolled error for higher frames**
- **choppers have no chance to follow on short term**



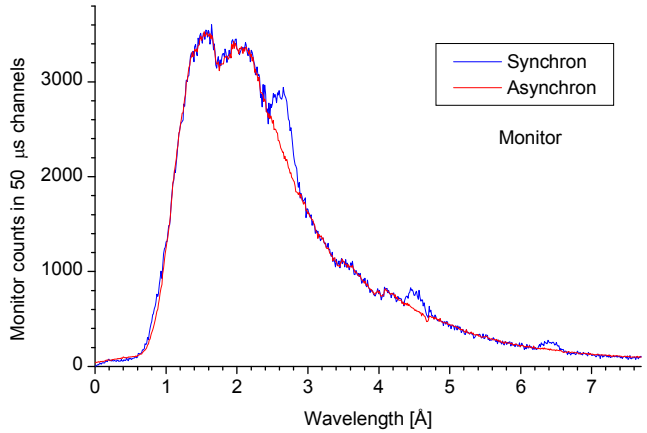
Timing stability between the master and a slave chopper (BNC)

Multiplexing control of pulse length: WFM

Spectrum as a function of neutron flight time:
asynchronous = synchronous operation (normalized by monitor)



Monitor spectra:

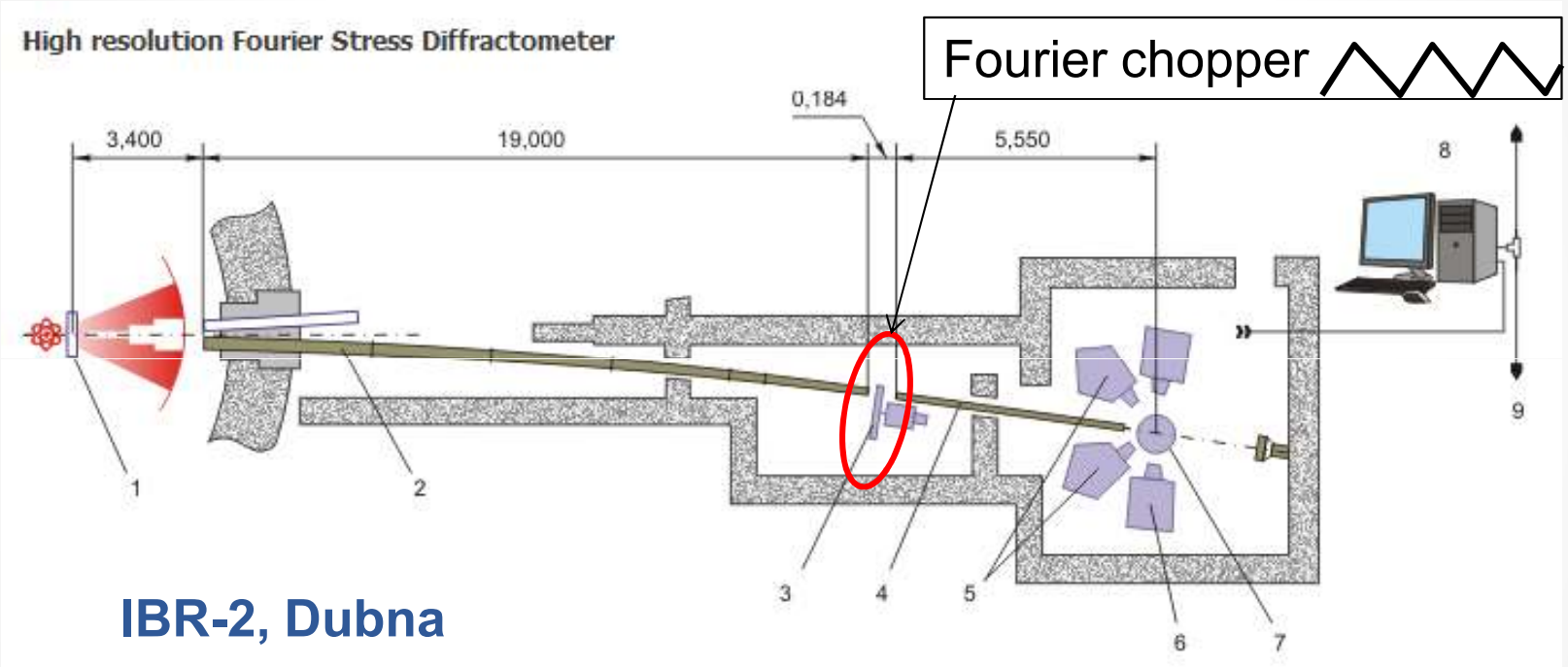


Price-to-pay: choppers for pulse shaping and sub-frame overlap
→ Fringe benefits: ideal shaped short pulses with dial up length, multiplexing invisible and verified, single pulse work possible

Beam modulation alternatives

Alternatives to pulse shaping monochromatization:

- beam modulation (Fourier = Larmor, statistical,….)

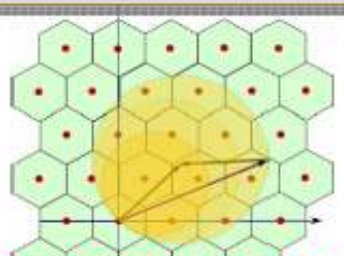


Beam modulation alternatives

Project Corelli (ANL – SNS)

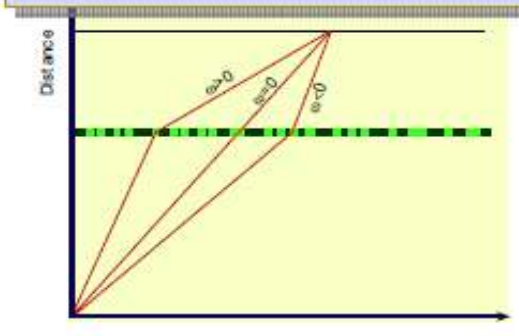
Cross Correlation Spectrometer

TOF Laue Diffractometer



Very efficient for large momentum coverage

Statistical Chopper



Energy discrimination

Intensity at detector when beam transmission is modulated in time by M(t)

$$I(t_0,t)=\int_0^{T_S} M(\tau-t_0)S(t,\tau)d\tau+B(t)$$

The scattering law can by reconstructed through the cross correlation

$$C(t,t_1)\equiv\frac{1}{T_S}\int_0^{T_S} M(t_1-t_0)I(t_0,t)dt_0$$
$$=c_1\cdot S(t,t_1)+c_2\cdot B(t)$$

if M(t) obeys

$$A^{MM}(\tau)\equiv\frac{1}{T_S}\int_0^{T_S} M(t)M(t-\tau)dt=c_1\cdot\delta(\tau)+c_2$$

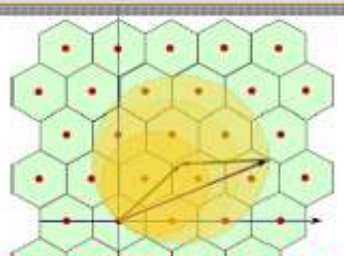
L. Pal *et al*, *Neutron Inelastic Scattring*, p. 407 (Vienna, 1968)
R. Von Jan & R. Scherm, Nucl. Inst. Meth. **80**, 69 (1970)
P. Pellionicz *et al*, Nucl. Inst. Meth. **92**, 125 (1971)
W. Matthes, *Neutron Inelastic Scattering*, p. 773 (Vienna, 1972)
R. K. Crawford *et al*, ICANS-IX (1986)
L. D. Cussen *et al*, Nucl. Inst. Meth. A**314**, 155 (1992)

Beam modulation alternatives

Project Corelli (ANL – SNS)

Cross Correlation Spect

TOF Laue Diffractometer



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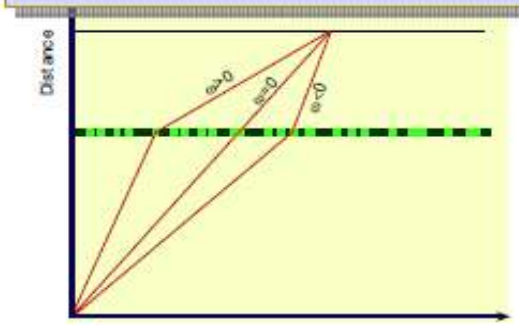

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Beam modulation alternative

Advantageous for large features in the scattering signal and in case of very high background / weak signal

I_{sc} = total scattering without monochromatization
ρ = scattering fraction of interest

	Signal	*Noise*
Monochromatization:	$\rho I_{sc}\delta\lambda/\lambda$	$(\rho I_{sc}\delta\lambda/\lambda + I_{BG})^{1/2}$
Beam modulation:	$\rho I_{sc}1/2$	$(I_{sc}1/2+ I_{BG})^{1/2}$

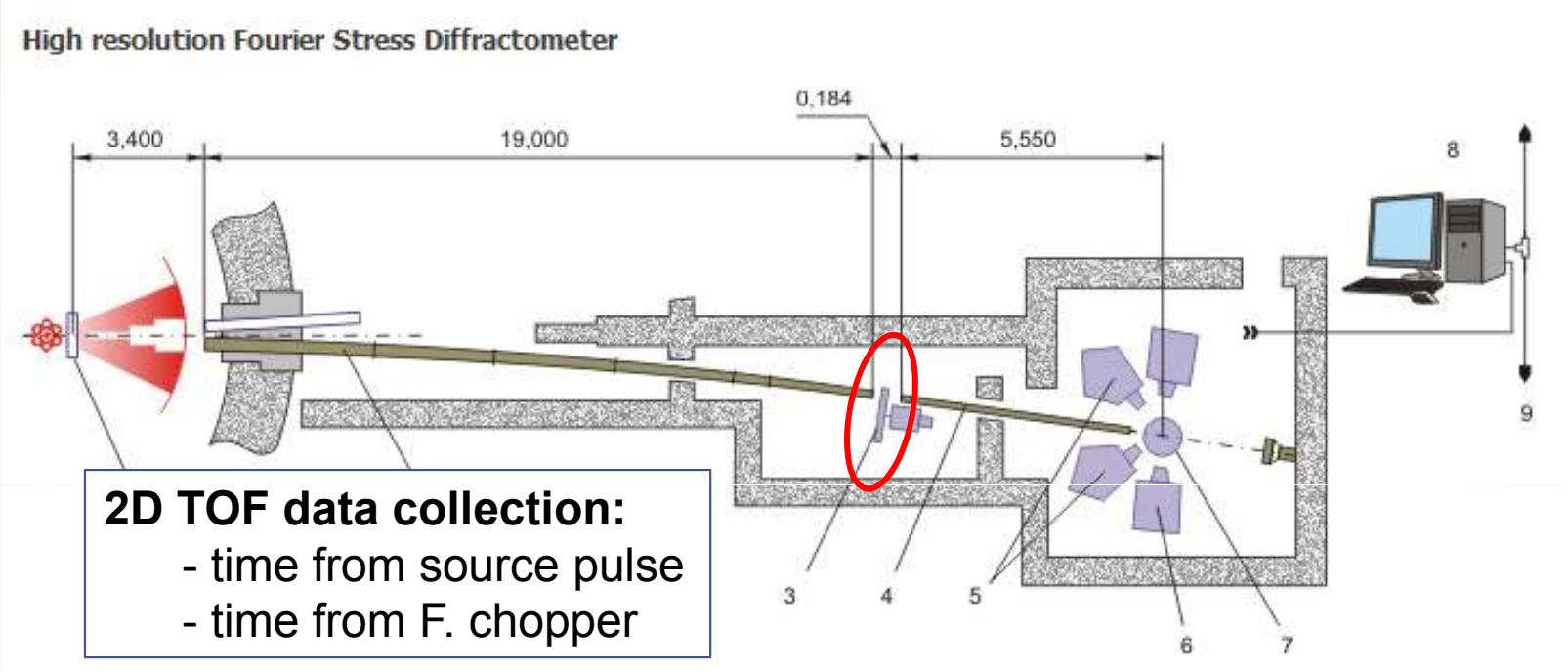
Gain in relative error:

a) I_{BG} is negligible:	$(\rho\ \lambda/2\delta\lambda)^{1/2}$	(e.g. NSE)
b) I_{BG} is dominant:	$\lambda/2\delta\lambda$	(Skjöld vs. ILL)

Simplest and cheapest way to refine wavelength resolution

Price-to-pay: reduced signal for low intensity feutures *within the TOF selected part* of spectrum, a potential for pulsed sources

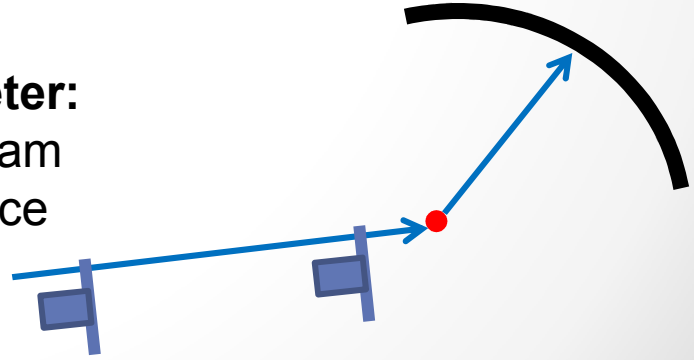
Beam modulation alternative



2D TOF data collection:
- time from source pulse
- time from F. chopper

Maier-Leibnitz's total S(q,ω) spectrometer:
2 statistical choppers → 25 % of white beam
- 2D TOF data collection at CW source
- 3D TOF data at pulsed source

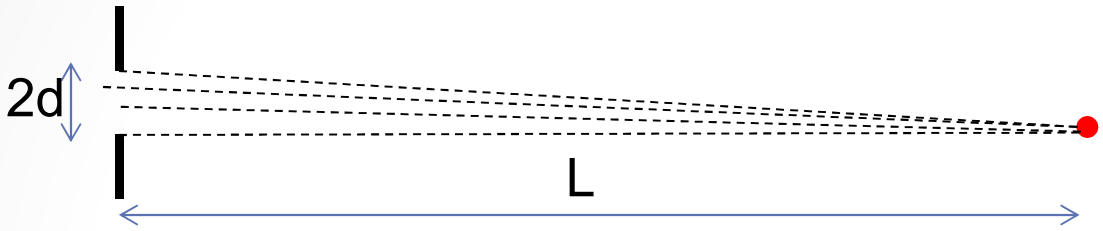
Cf. Fourier NMR,…
(E. Fahri, ,,,)



What neutrons do in the instruments?

Neutron behavior in parctical scattering experiments:

a) **Propagate as classical particles** in the instruments,…



Path differences ~ $d^2/2L >> \lambda_{neutron}$ → **particle** (e.g. 1 μm for d=0.5 cm, L=10 m)
Different from light, some X-ray cases….

b) **Propagate as waves** when scattering on atoms:
path differences ~ λ

Calculating neutron trajectories as waves: possible, but of no use (like calculating Apollo flights by the Schrödinger equation). E.g. multiple scattering inside a sample: particle → wave (1st scattering) → particle → (2nd scattering) →

Simulations codes are correct!

What neutrons do in the instruments?

Good use of simulations: together with

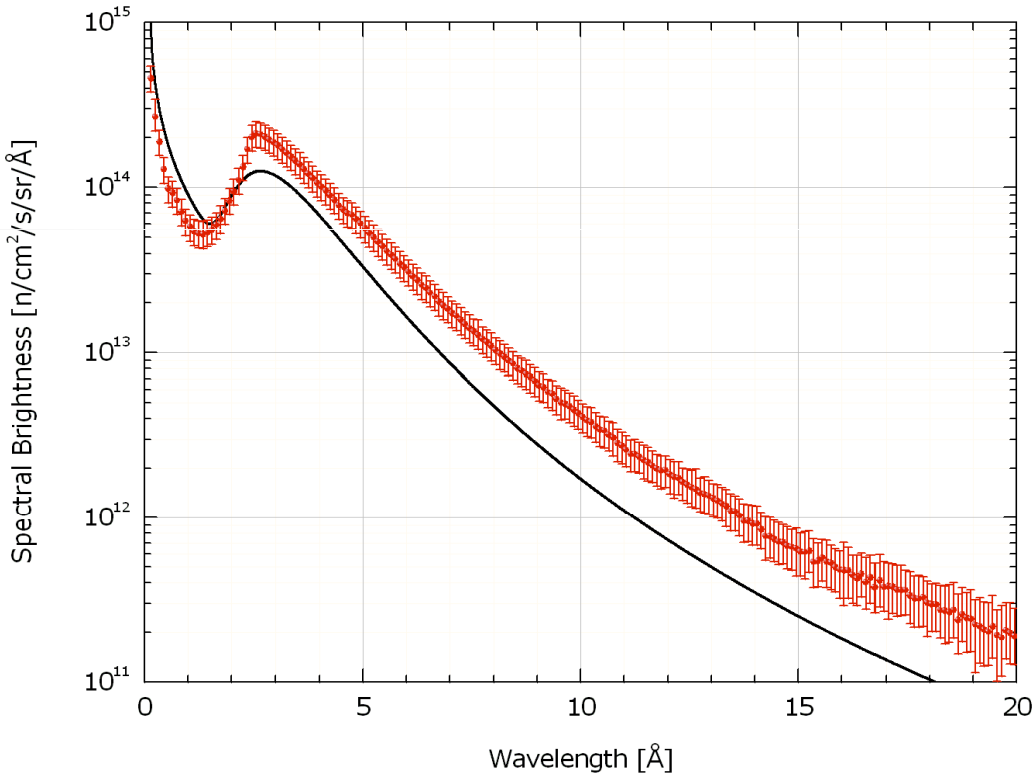
-"analytical understanding" (E. P. Wigner)

-"back-of-the-envelop calculations" (P. Radaelli)

ESS cold moderator performance & baseline

TSDU Baseline Change 1 (7)

Prepared by	No.		
Luca Zanini, Group Leader for Neutronics	TS.Baseline.V2.002		
Approved by	Date	Rev	Reference Baseline:
Ferenc Mezei, Head of Target Division	2012-06-18		V2.0 (EDMS:1166507)



LINE.V2.CHANGE.002

modification:

erator are described in Ref. [1].
ı of wavelength and time:

Conclusion

A back-of-the-envelop calculation

Total scattered count rate in $\delta E \sim 100\ \mu eV$ quasielastic resolution
TOF spectroscopy at ESS for sample availably in quantity

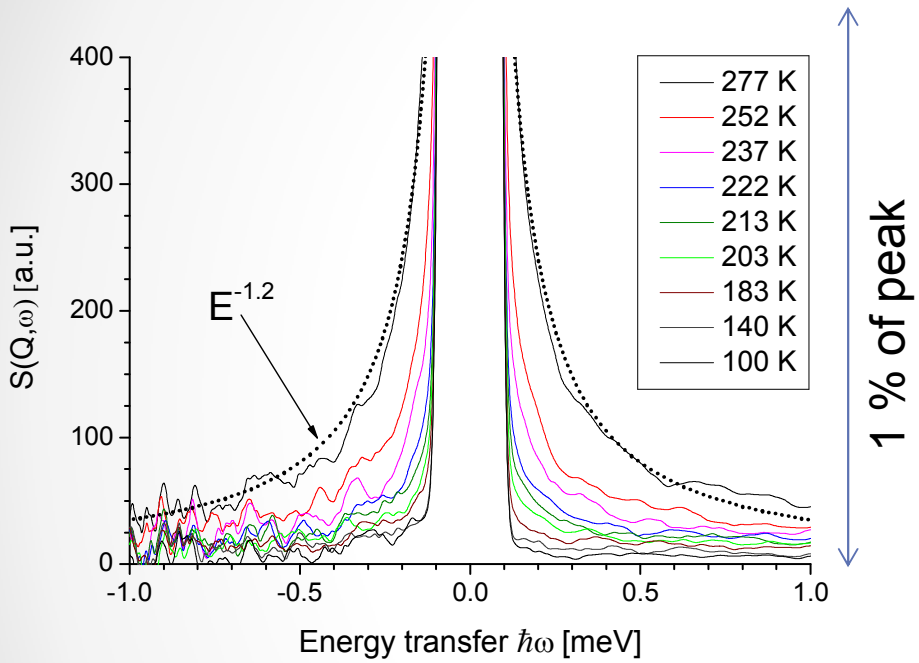
Moderator brightness (at λ = 4Å):	10^{14} n/cm^2/s/str/Å
Sample area:	10 cm^2
Beam divergence (ballistic guide $\pm 3\theta_{Ni}$)	0.0018 str
Ballistic guide phase space transmission (150 m):	80 %
Incoming wavelength resolution:	0.03 Å
Pulse length of chopper before sample (L_{SD} = 4 m):	30 μs
Repetition Rate Multiplication factor:	12
Source pulses per s:	14
Detector solid angle:	1.3 π !!
Detector efficiency, incl. losses in spectrometer:	60%
Sample total scattering probability:	10 %

$$\eta \phi_{mod}\, \delta\lambda_{in}\, \delta\Omega_{in}\, F\, n\, \delta t\, p_{SC}\, \delta\Omega_{det} \rightarrow \mathbf{4.25 \times 10^6\ counts/s}$$

For total scattering spectrometer: 10^9 c/s

Conclusion

NEAT 2008 data (HZB): protein dynamics



NEAT upgrade project (x40)
HZB vs. new source ESS (x300):

4 h scans → will be made in 1 s !!☺

Sample environment?
Data evaluation?
Use medium flux sources for "large" samples / effects!

"Neutrons are intensity limited" will no longer be true for samples in > cm^3 quantities and sizable scattering effects.

Learn from life sciences how to study huge and one by one poorly understood data sets: look for systematics in the "raw" pictures

To find more:

Multiplexing chopper systems:
M. Russina, F. Mezei, G. Kali, Journal of Physics, conference series, 340 (2012) 012018

Fourier diffraction:
http://flnp.jinr.ru/150/ , http://flnp.jinr.ru/250/

Correlation spectroscopy:
See page 25 and Corelli web site @ SNS

Event recording:
www.ante.hu

Thank you…

…and have fun!