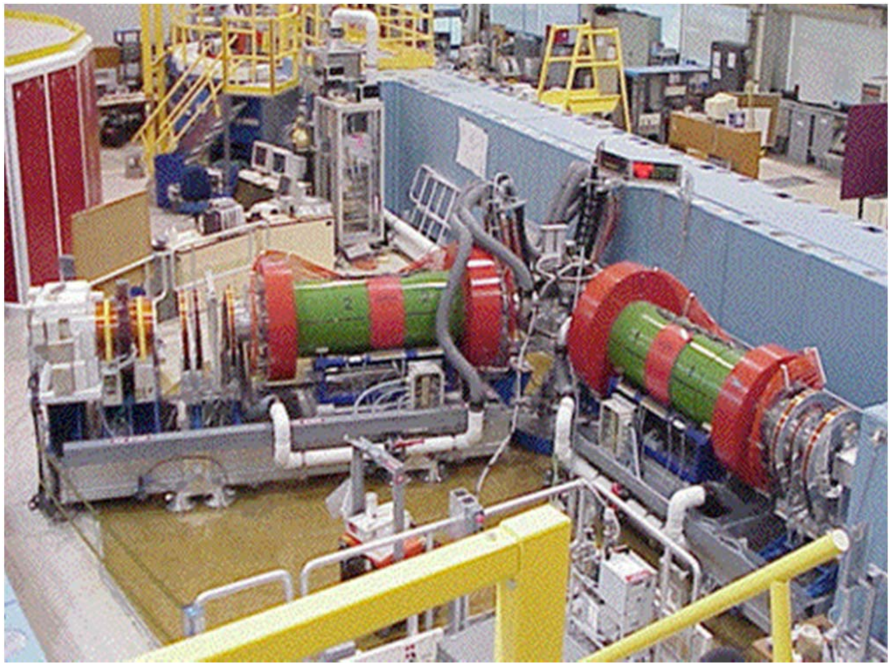
Neutron Spin Echo (NSE) Spectroscopy

Group A
NCNR Summer School
June 16th 2011

Outline

- Introduction
- Science background
- Instrument
- NSE Raw data
- Data analysis
- Conclusions



NSE facility at NIST Center for Neutron Research.

Why NSE?

- Study the dynamics of the material.
  - Coherent
  - Incoherent
- Measurements are made in space and time domain.
- Largest length and longest time scales.
- Maintain good signal intensity without losing resolution.

Neutron Spin Echo- Background

Neutron Spin Echo uses the velocity change of the neutrons to infer the energy transfer

Neutron Velocity selector → Neutron spin polarization → Magnetic field → sample → Magnetic field → detector

A large range of incident neutron energies (e.g. 10-20% spread) can be used in NSE

Velocity change of neutrons after scattering by a sample is measured by comparing the Larmor precession in known magnetic fields before and after the scattering.

NSE- high resolution and structural dynamic (motion of the macromolecules in nm and ns scale)

The experimental quantity measured is the polarization of the beam :

$$P_x = (\Delta J^{ph}, Q, t) = P_S(\Delta J^{ph}) \frac{\int S(Q,\omega)\cos[\omega, t]d\omega}{\int S(Q,\omega)d\omega} \; S(Q,\omega)$$

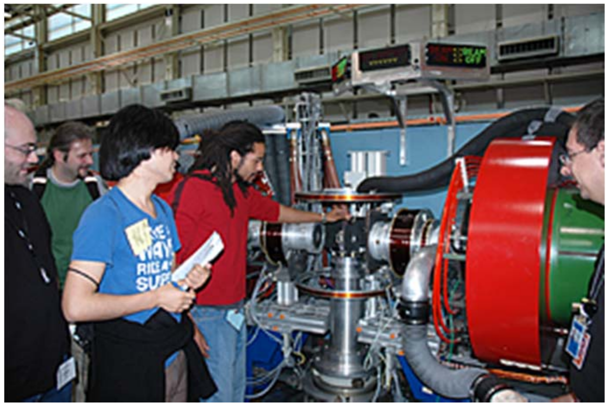
Through *P, one measures the Fourier Transform of the Dynamic Structure Factor*

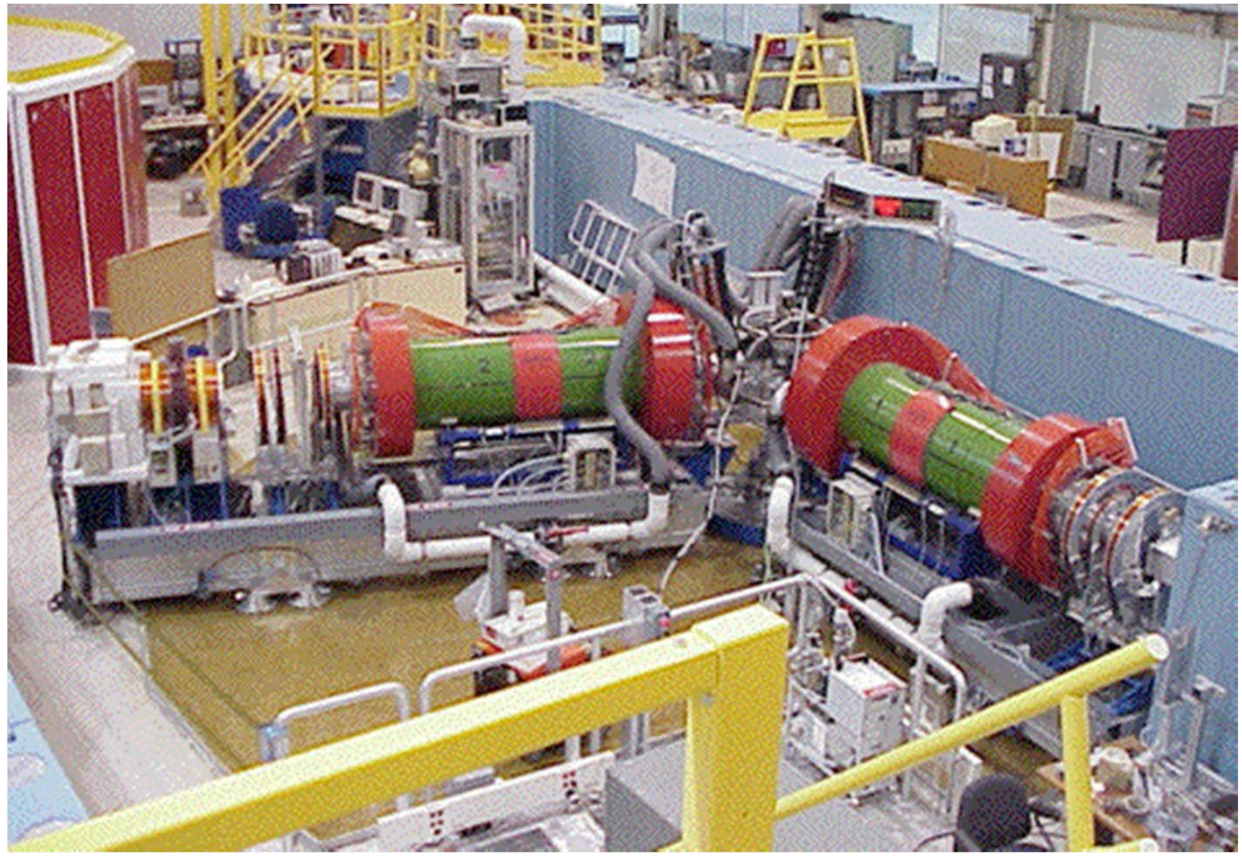
Why NSE?

Because the width of the incoming neutron beam is larger than the energy transfer resulting from scattering, the result is a marginalization of the relationship between resolution and intensity.

- One can mesure dynamic events takin place on a timescale of .01 to 100 ns.
- One can get dynamic information about the mciro and macro structure because of the length scale for taking data, Å.

Neutron spin-echo - Instrument Introduction





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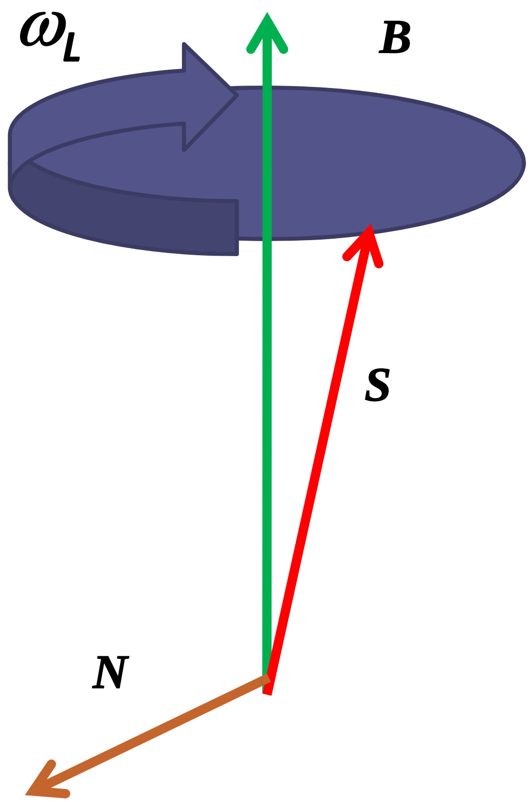
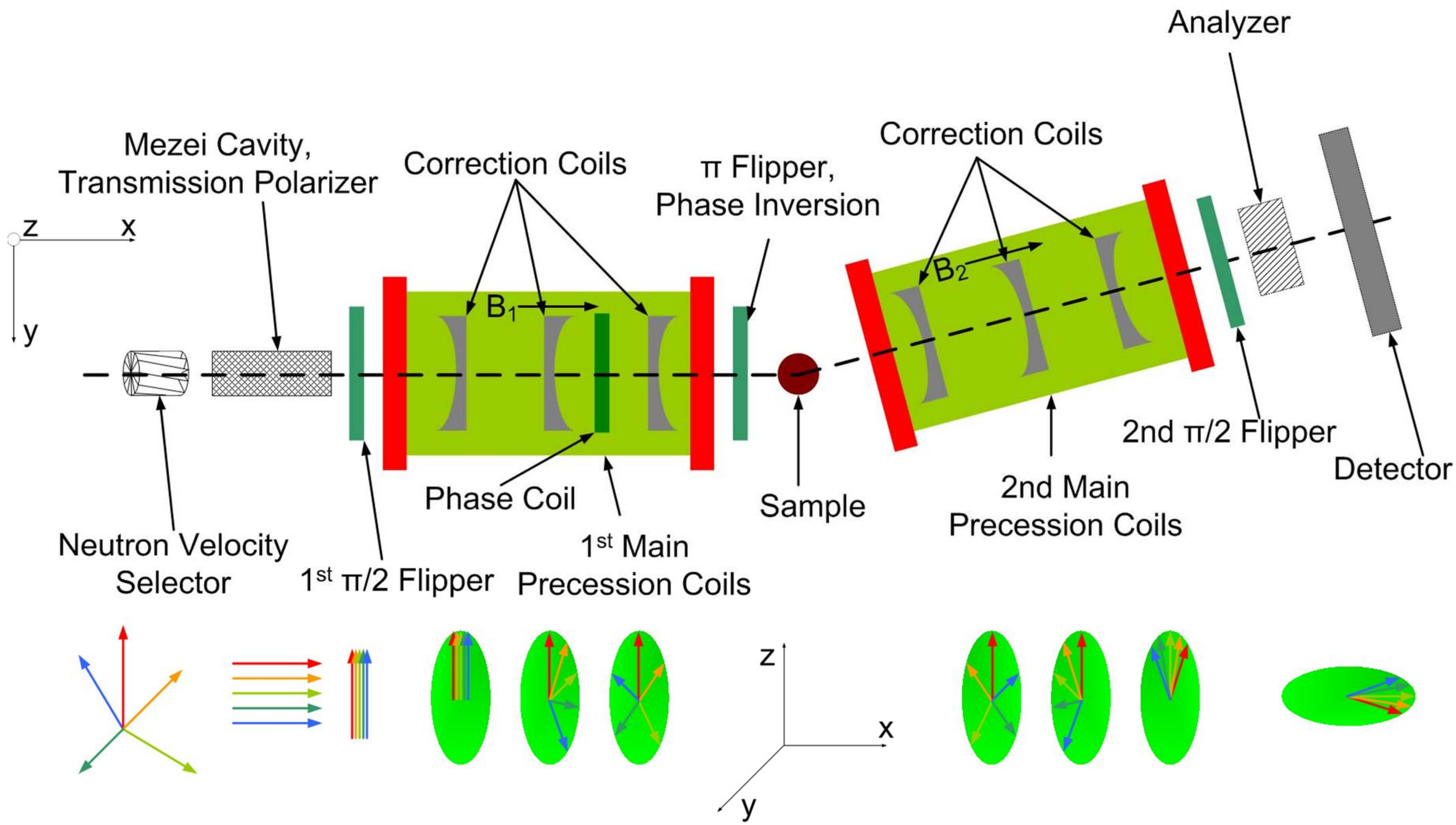
Neutron Precession in Magnetic Field



$$\vec{N} = \vec{S} \times \vec{B}$$

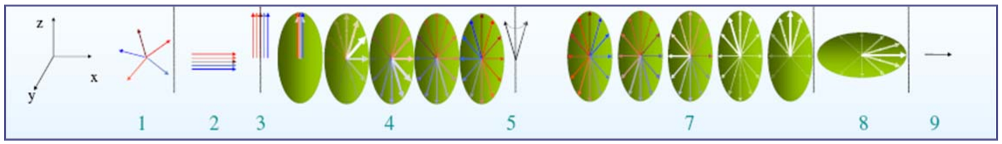
$$\omega_L = \gamma B$$

$$\frac{d\vec{S}}{dt} = \vec{S} \times \vec{\omega_L}$$

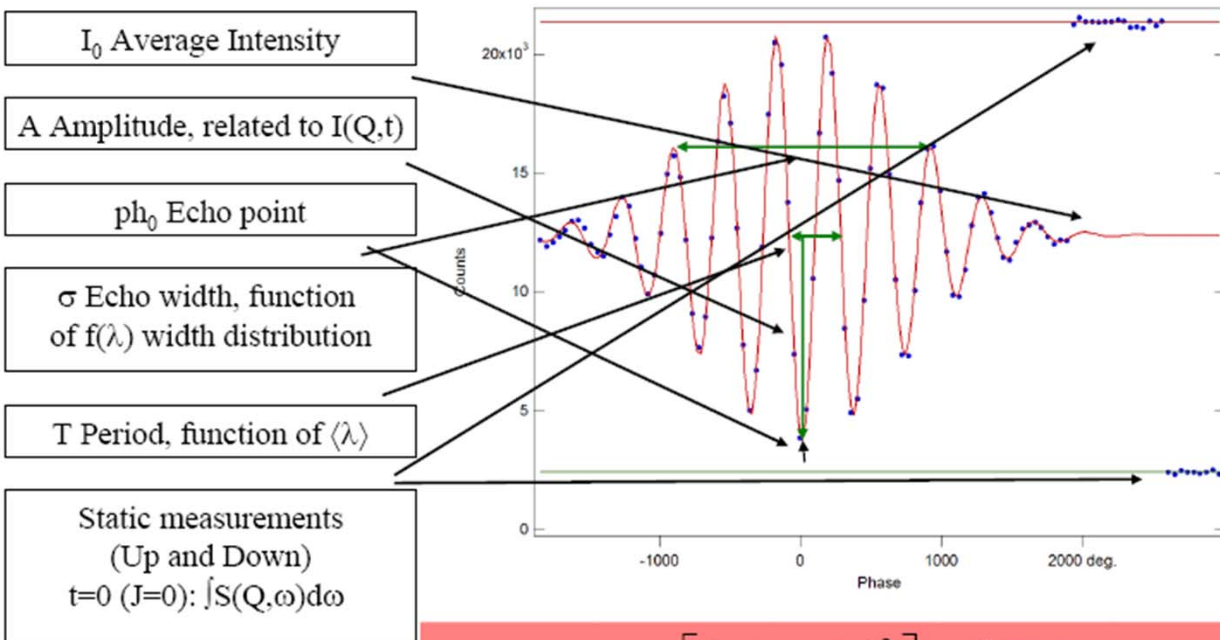

Analyzer
Mezei Cavity,
Transmission Polarizer
Correction Coils
π Flipper,
Phase Inversion
Correction Coils
z
x
y
B1
B2
Phase Coil
Sample
2nd π/2 Flipper
Detector
2nd Main
Precession Coils
Neutron Velocity
Selector
1st π/2 Flipper
1st Main
Precession Coils
z
x
y

RAW DATA

What do we obtain after a measurement?



NSE measure Polarization vs Phase and Fourier time



$$I^p = I_0 + A\exp\left[\frac{(ph - ph_0)^2}{2\sigma^2}\right]\cos\left[\frac{360}{T}(ph - ph_0)\right]$$

RAW DATA

What do we obtain after a measurement?

Physical information about the sample is all in the Amplitude

$$\frac{I(Q,t)}{I(Q)} \propto \frac{2A}{Up - Dwn}$$

3 Samples are necessary:

Resolution (Carbopack)

Blank (Solvent...)

Sample (System to study)

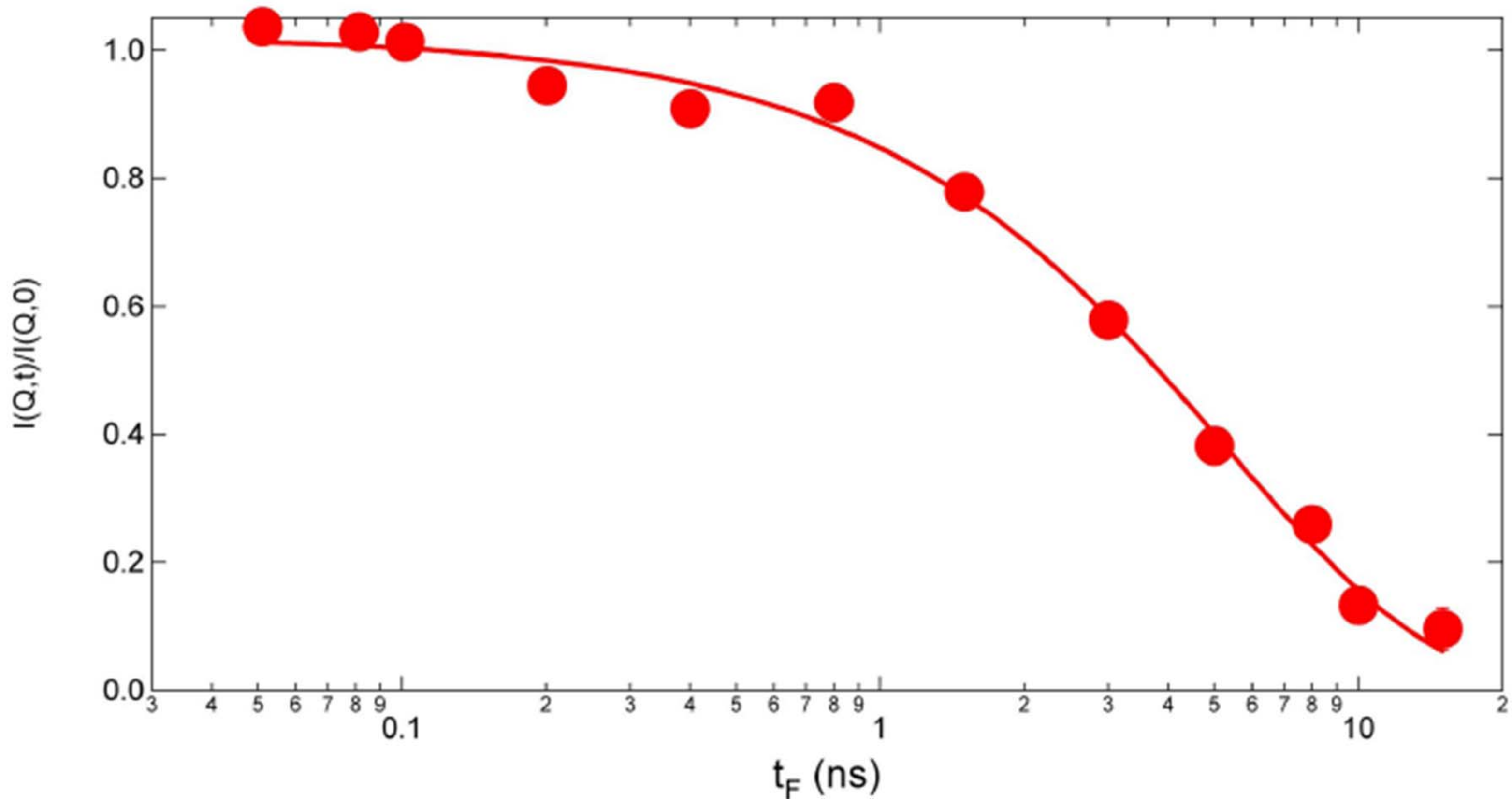
Normalization

$$\frac{I(Q,t)}{I(Q,0)} = \frac{2A/(Up - Dwn)}{2A^R/(Up^R - Dwn^R)}$$

$$\frac{I(Q,t)}{I(Q)} = \frac{2\left[A - (1-\phi)\frac{T}{T^{BKG}} A^{BKG}\right] \Big/ \left[(Up - Dwn) - (1-\phi)\frac{T}{T^{BKG}}\left(Up^{BKG} - Dwn^{BKG}\right)\right]}{2A^R/(Up^R - Dwn^R)}$$

RAW DATA

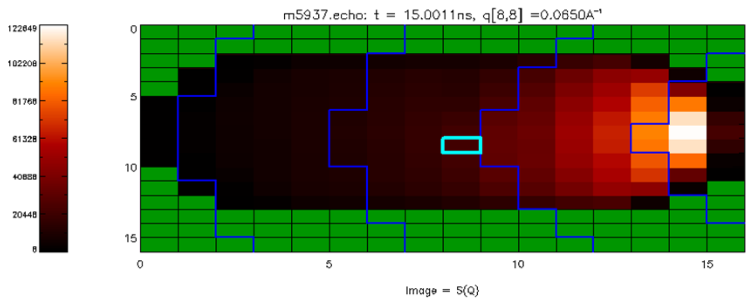
What do we obtain after a measurement?

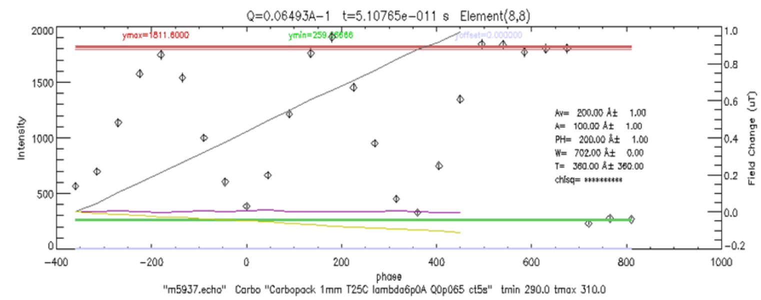


RAW DATA

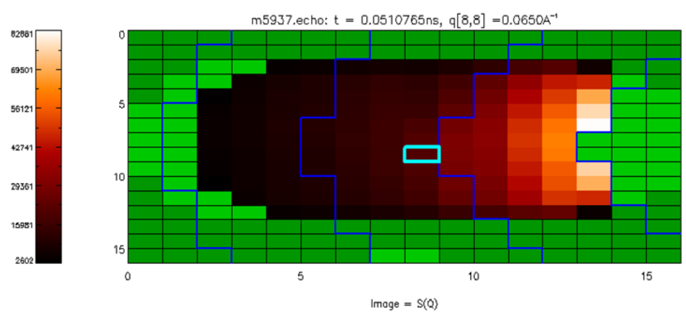
2D Detector Resolution

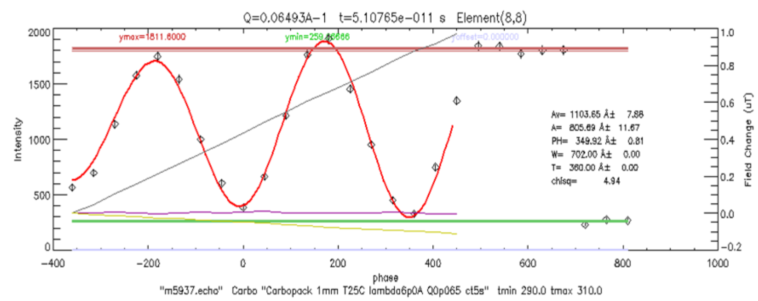
The echoes at each detector pixel have to be fitted individually.





Weak intensity data pixel could be masked

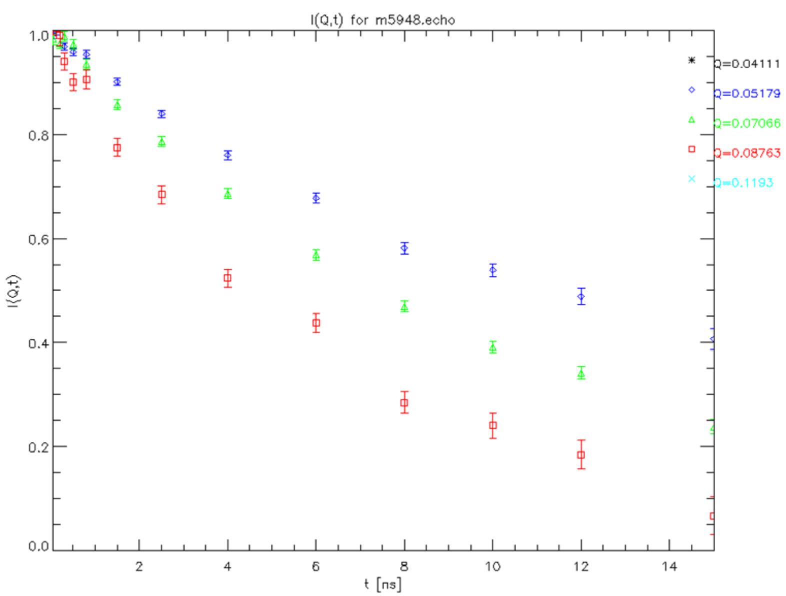




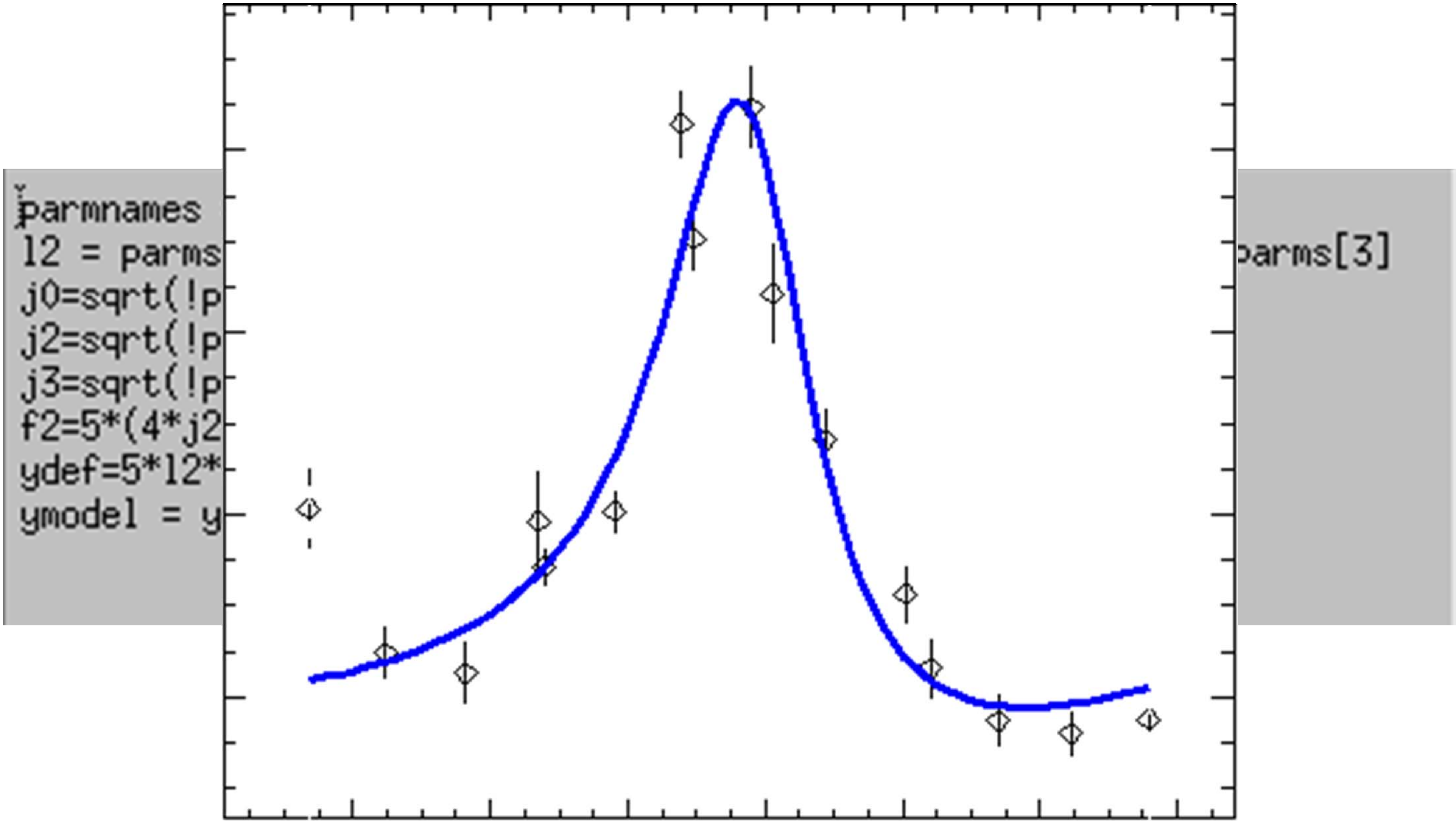
RAW DATA

The Intermediate Scattering function values are calculated pixel by pixel and averaged

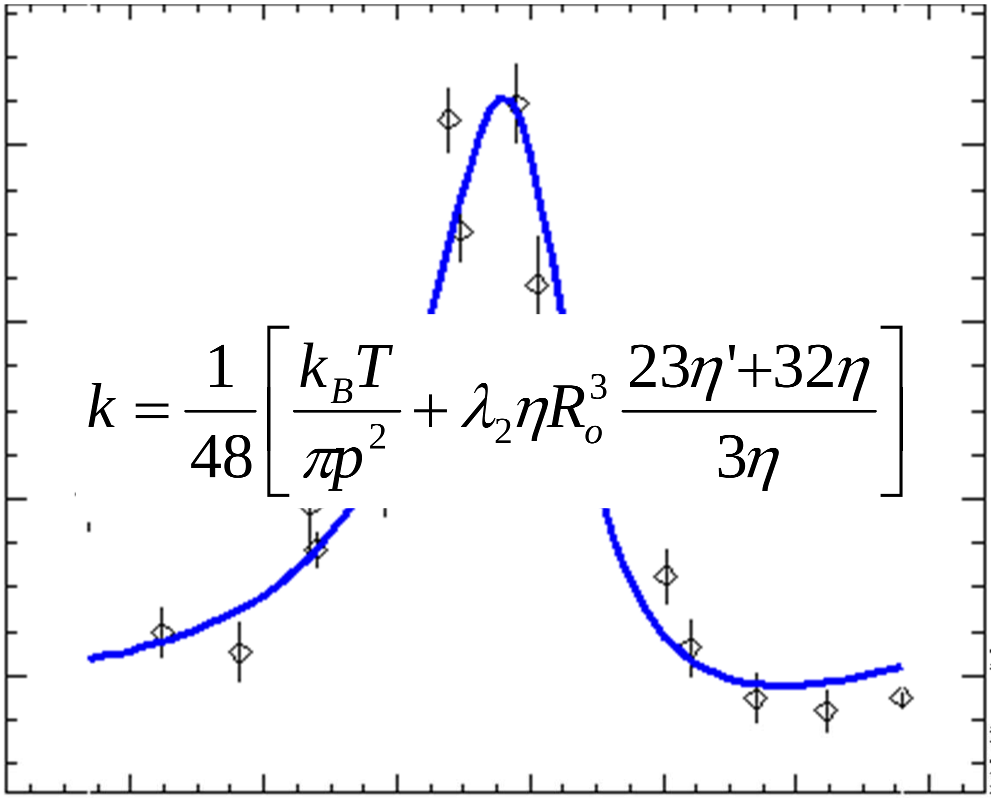
At the end of the reduction process the I(Q,t) contains information about the sample.



Data Analysis



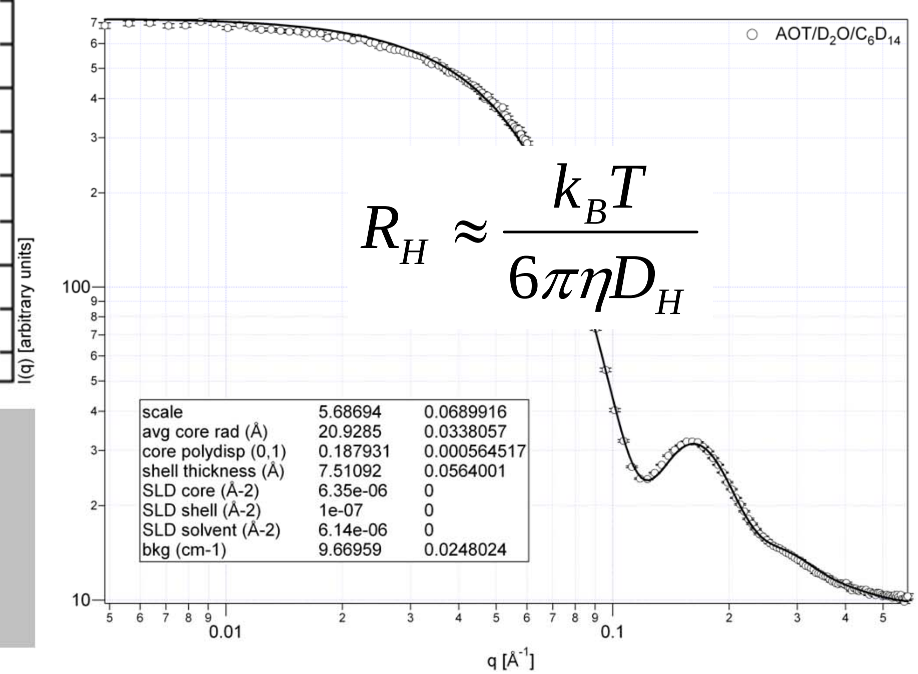
Complementary Data



$$k = \frac{1}{48}\left[\frac{k_B T}{\pi p^2} + \lambda_2 \eta R_o^3 \frac{23\eta' + 32\eta}{3\eta}\right]$$

```
#0: 12: 9.075e+07 +/- 4.461e+06
#1: radius: 2.677e+01 +/- 1.342e-01
#2: amp2: 1.176e-02 +/- 1.696e-03
#3: Dtr: 1.789e+10 +/- 1.212e+08
```

scale	5.68694	0.0689916
avg core rad (Å)	20.9285	0.0338057
core polydisp (0,1)	0.187931	0.000564517
shell thickness (Å)	7.51092	0.0564001
SLD core (Å-2)	6.35e-06	0
SLD shell (Å-2)	1e-07	0
SLD solvent (Å-2)	6.14e-06	0
bkg (cm-1)	9.66959	0.0248024



$$R_H \approx \frac{k_B T}{6\pi\eta D_H}$$

Take Home Message

- Pro's
  - Good energy resolution despite large range of incident neutron energies
  - Dynamics ranging from ps to ns
    - Insight into many types of dynamics
  - NSE data measure in time domain allowing simpler analysis
- Con's
  - Neutron/Time intensive
  - Must have a good sample and characterize it well
  - Must have theoretical support
    - Data analysis is sensitive to model