The Inversion of Quasielastic Neutron Scattering Data from Differing Instruments

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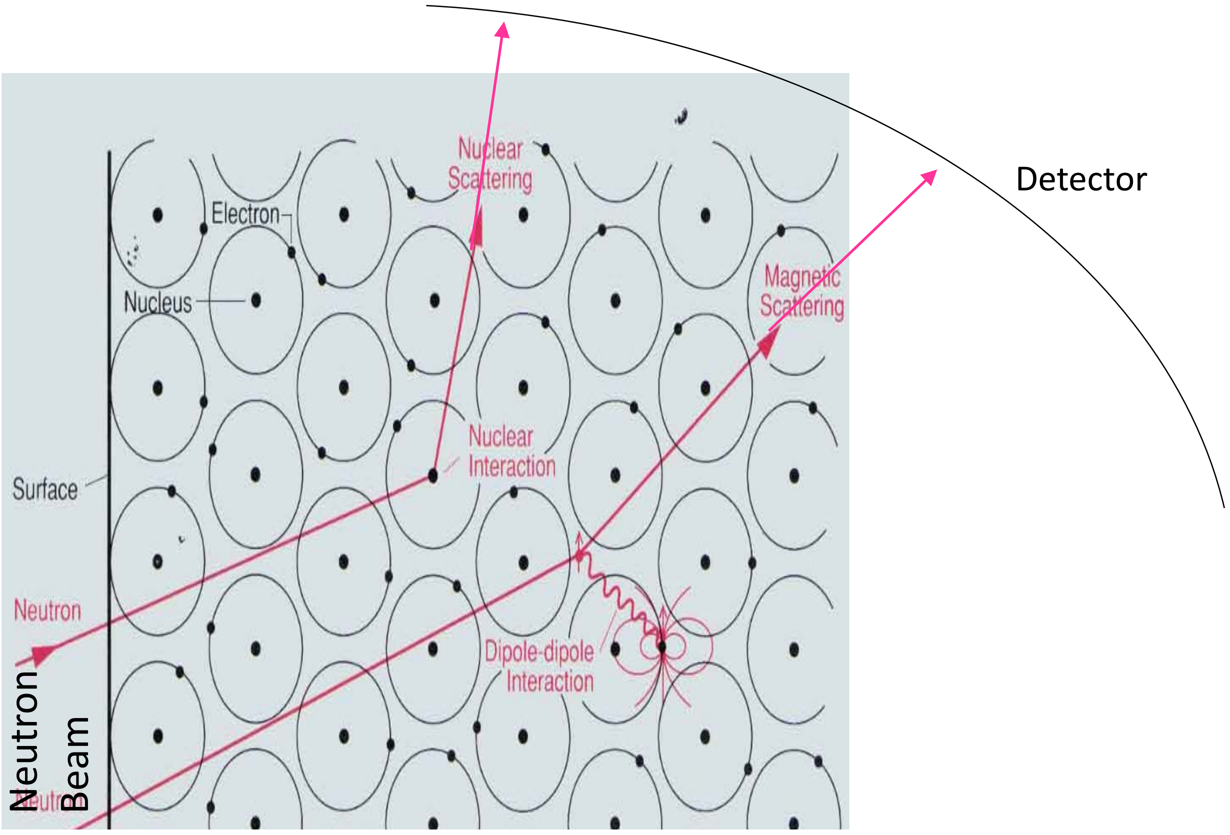
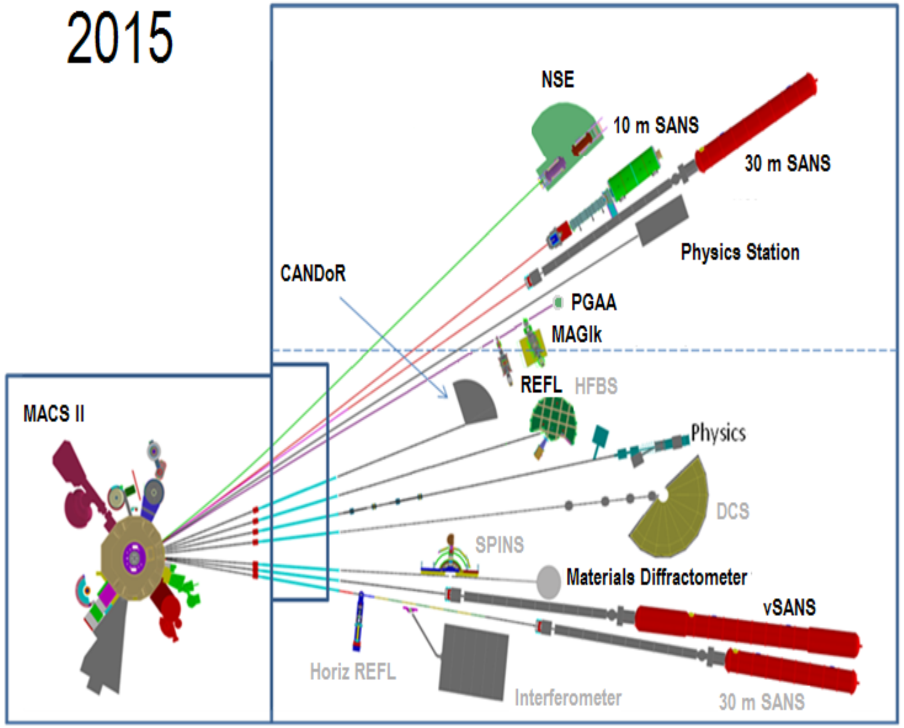
Overview:

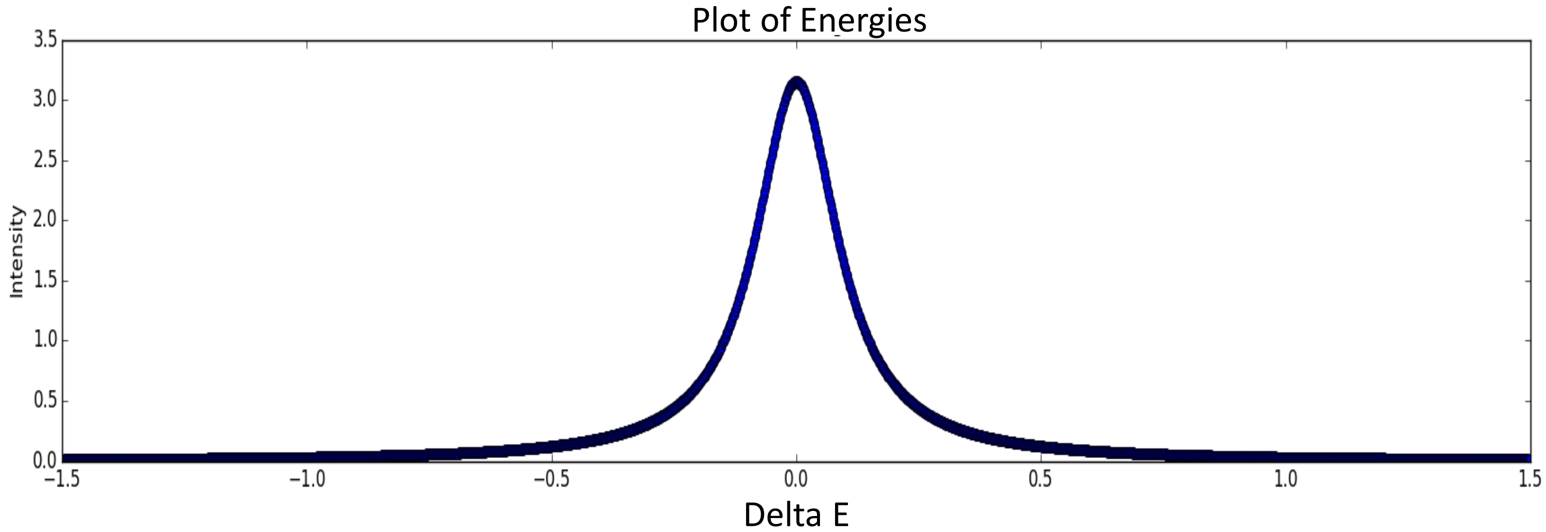
1. An Introduction to Cold Neutron Scattering and the Related Data
2. An Examination of the Current Data Needs Facing Users
3. A Summary of the Progress Towards a Solution
4. The Next Steps

Neutron scattering is a tool to study material dynamics through the interaction of neutrons with the material's atoms



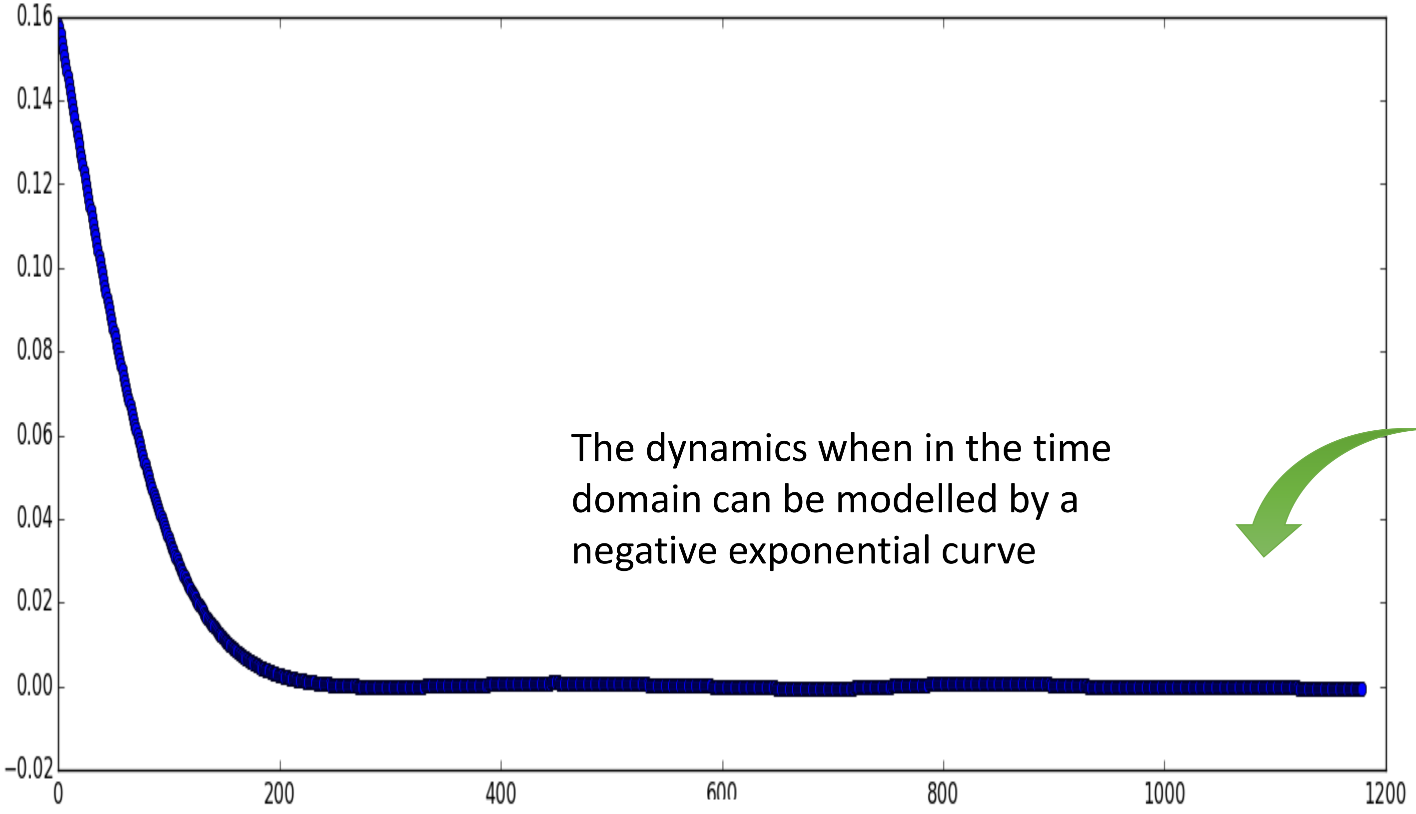
1. Pynn, Roger. *Scattering Interactions*. Digital image. *Neutron Scattering - A Primer*. N.p., n.d. Web. 03 Aug. 2015.





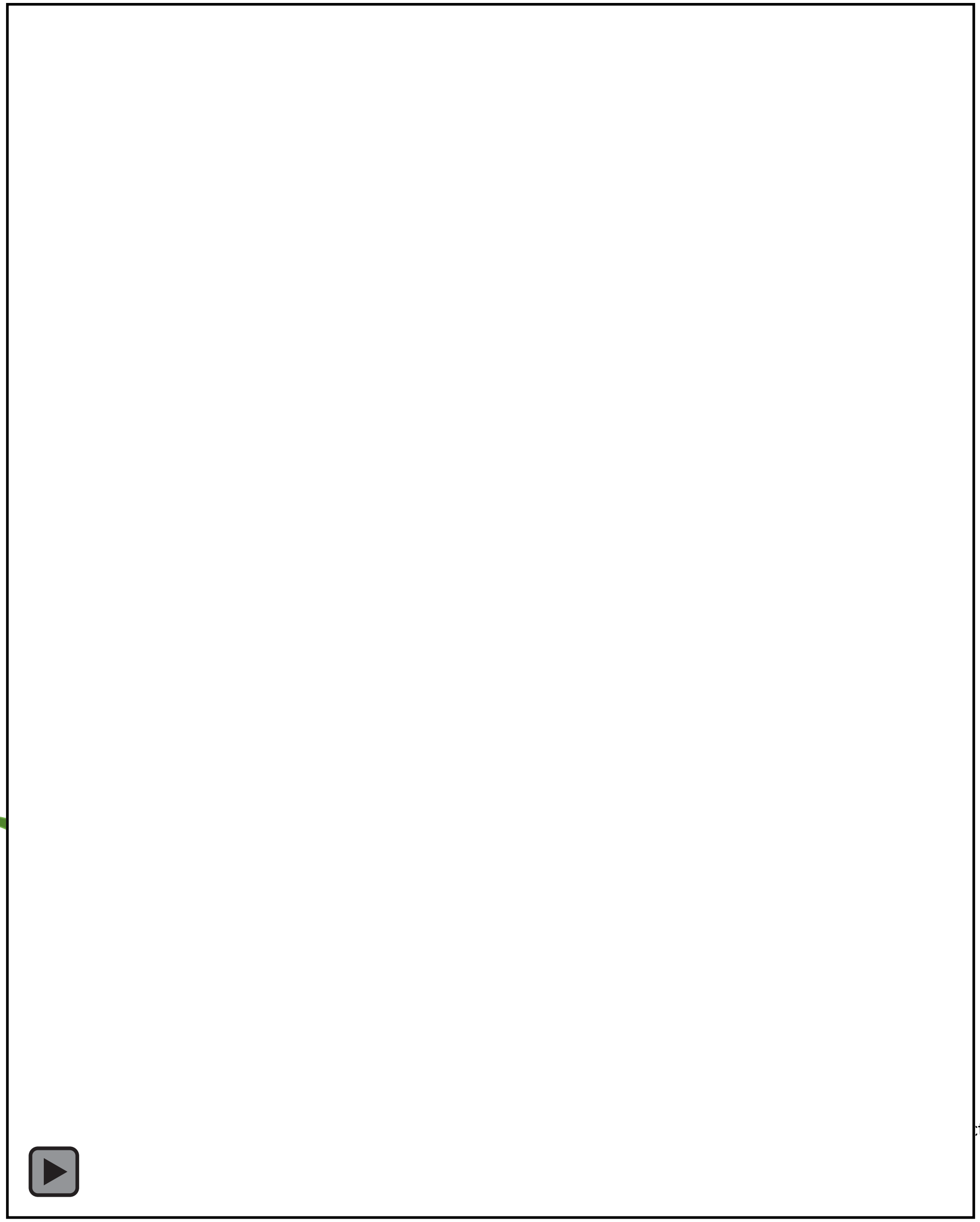
Material dynamics is the study of atom movement within a material

Inverse Fourier Transform of Convoluted Data with Noise

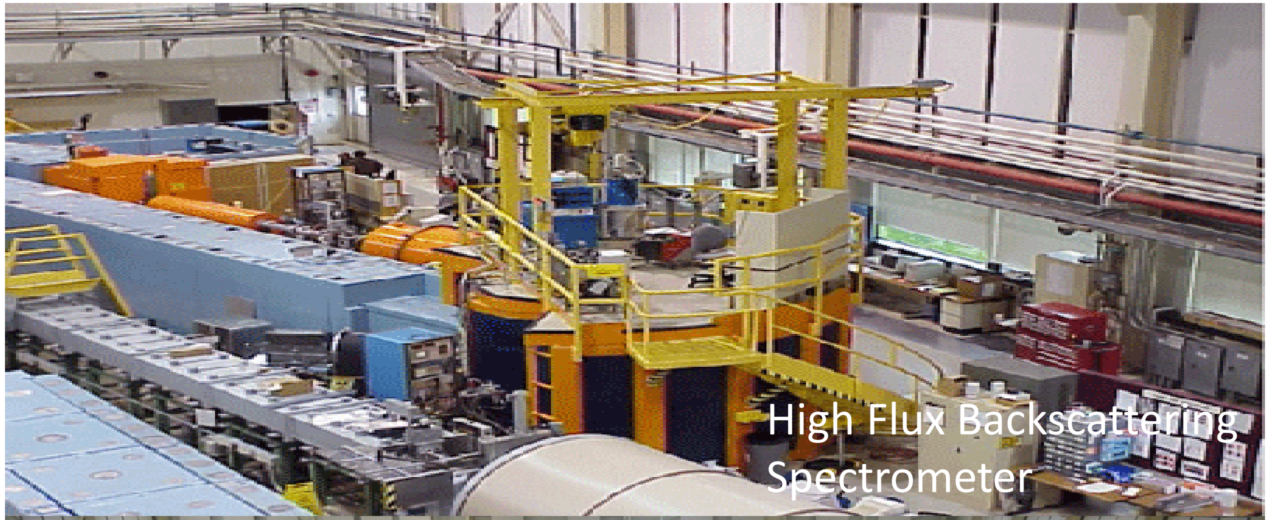


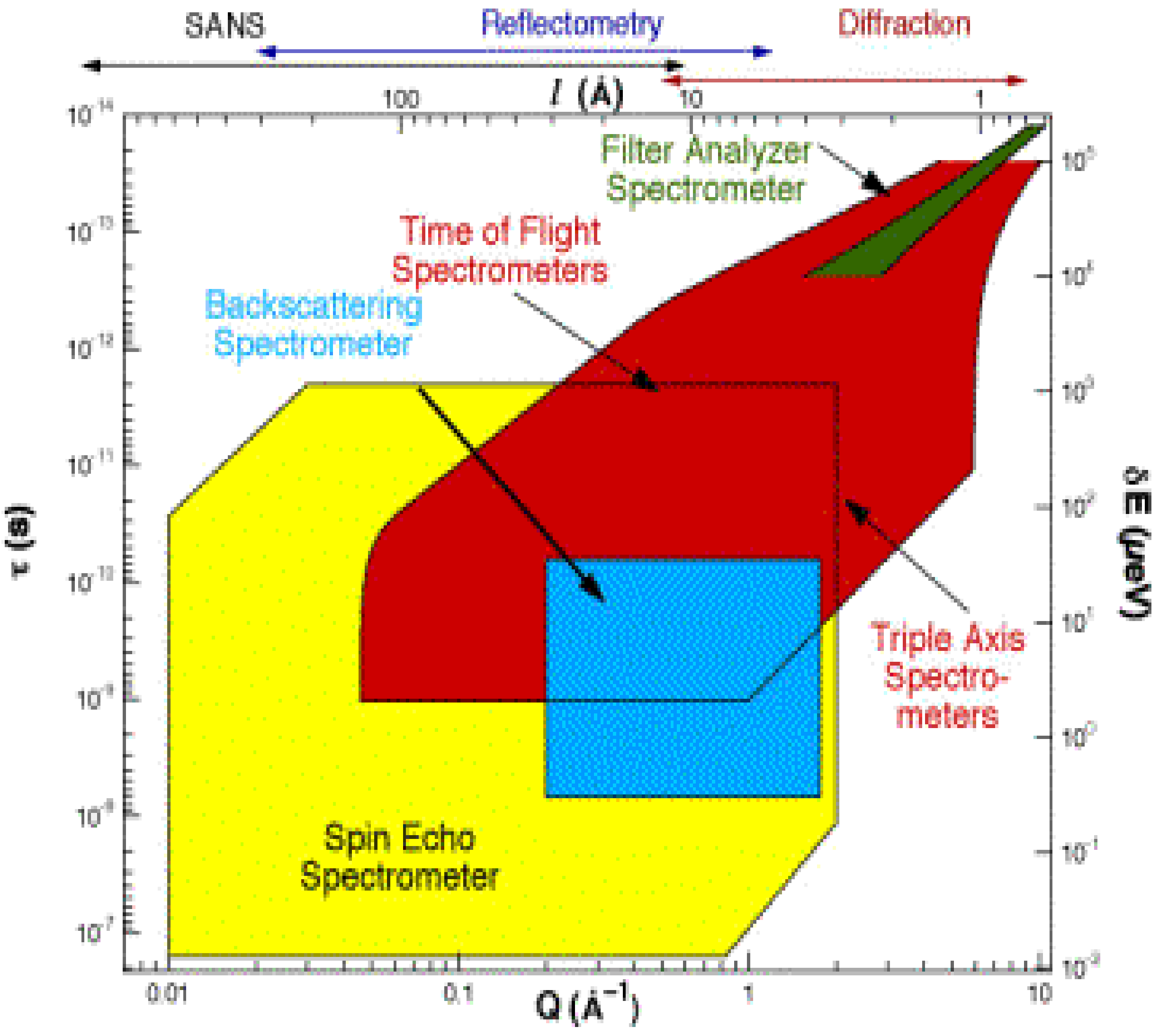
Time

The dynamics when in the time domain can be modelled by a negative exponential curve



Each cold neutron instrument's unique specifications allow for the study of different sections of the material's dynamics





The study of dynamics using neutron scattering has a variety of applications for both research and industry purposes

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Structure and Mobility of PEO/$LiClO_4$ Solid Polymer Electrolytes Filled with Al_2O_3 Nanoparticles

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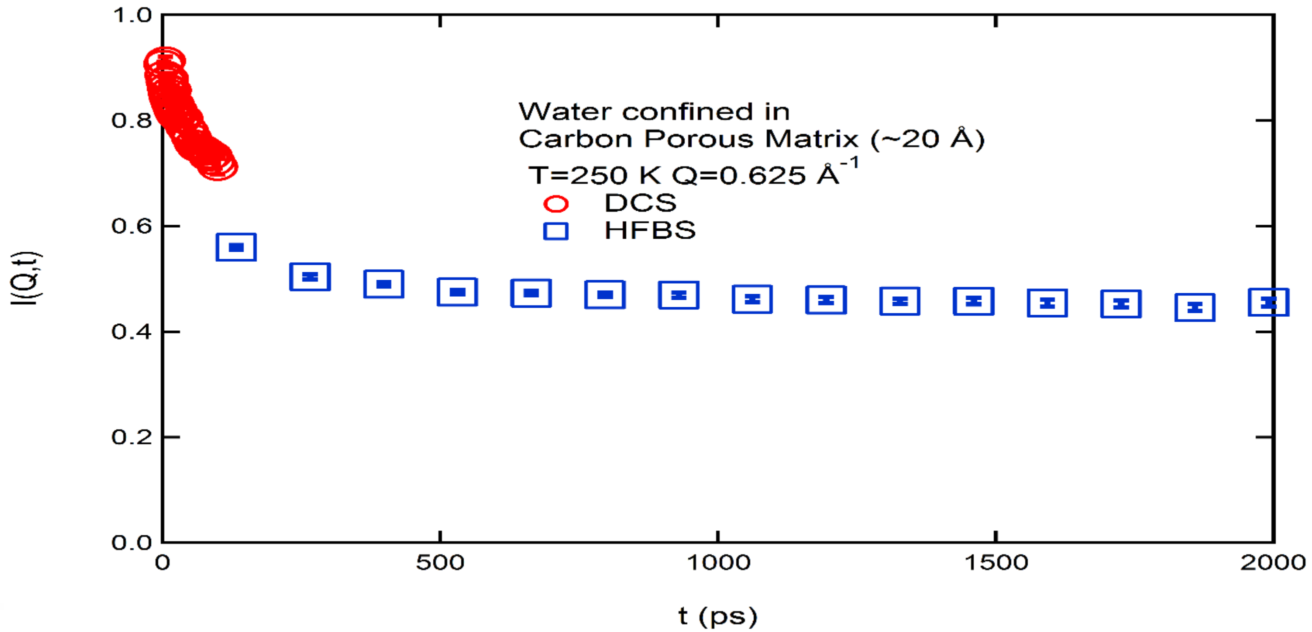
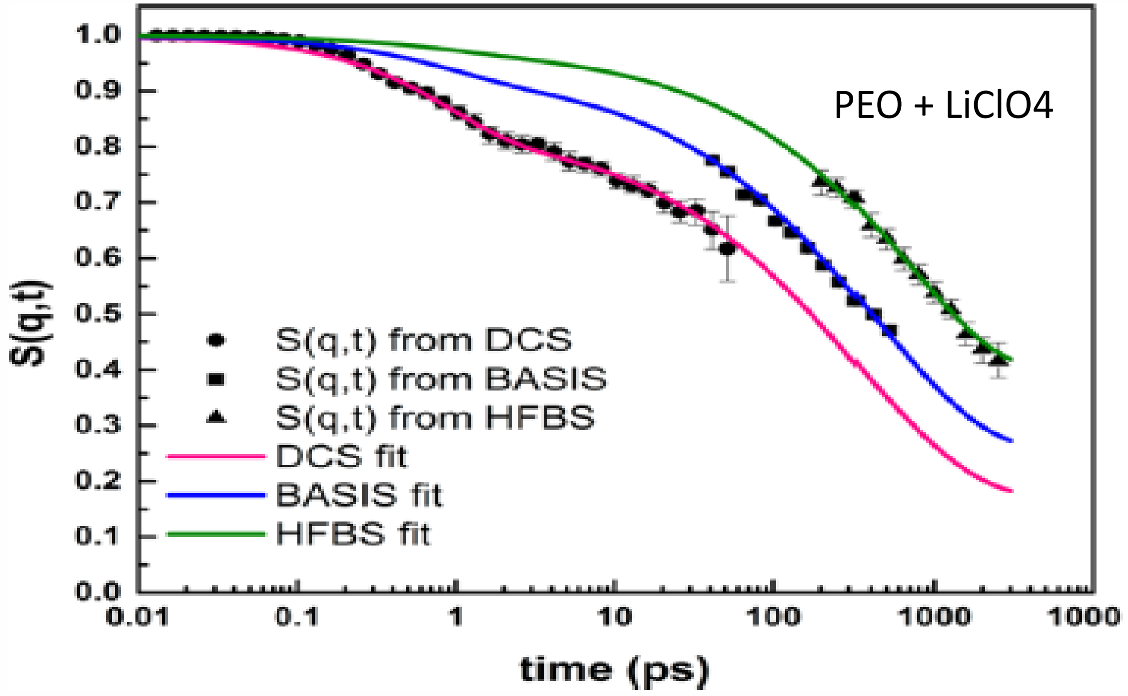
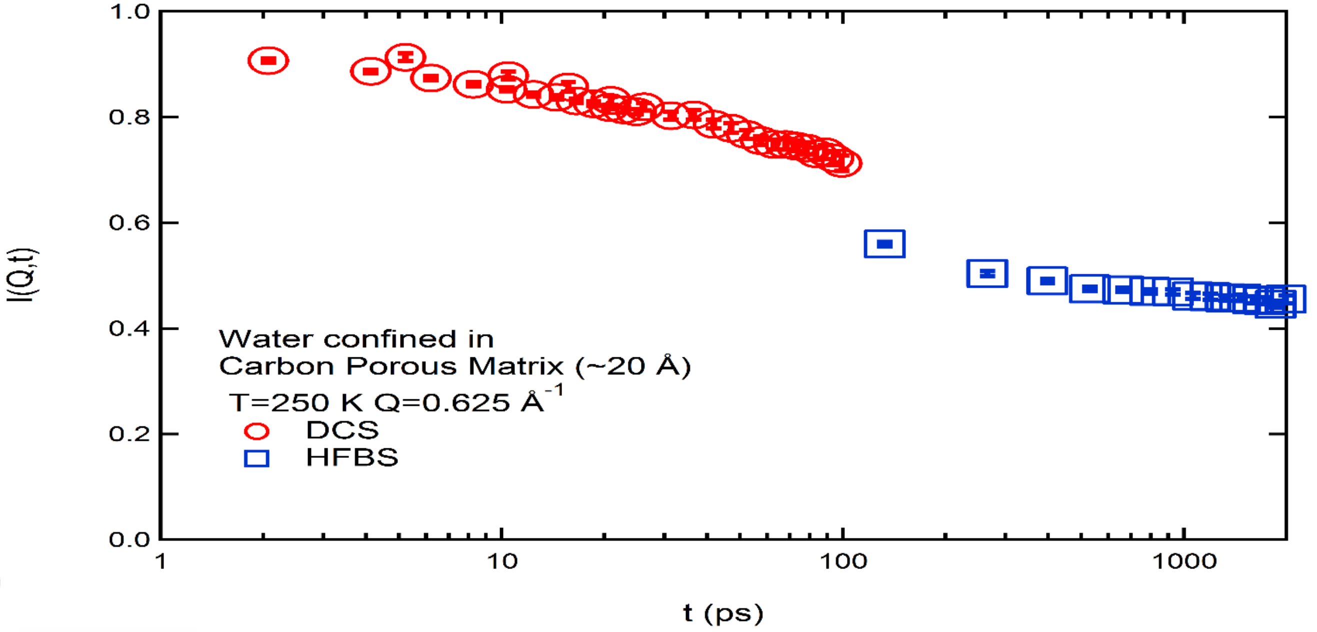
The mechanism for improved ionic conductivity in nanoparticle-filled solid polymer electrolytes containing polyethylene oxide [PEO], $LiClO_4$, and Al_2O_3 is investigated using differential scanning calorimetry [DSC], dielectric spectroscopy, small-angle neutron scattering [SANS], and quasi-elastic neutron scattering [QENS]. We measure samples with ether oxygen to lithium ratios ranging from 14:1 to 8:1 and Al_2O_3 nanoparticle concentrations ranging from 5 to 25 wt %. The T_g and pure PEO crystal fraction are unaffected by nanoparticle addition, and SANS reveals nanoparticle aggregation, with the extent of aggregation similar in all samples regardless of $LiClO_4$ or Al_2O_3 concentration. Despite the similarity between samples, nanoparticles improve conductivity at all temperatures, but only at the eutectic concentration (ether oxygen to lithium ratio of 10:1). Our QENS results indicate that a rotation is present in both filled and unfilled samples at all concentrations and is consistent with the rotation of $(PEO)_6$:$LiClO_4$, a channel-like structure that is more conductive than the amorphous equivalent. The rotation becomes more restricted in the presence of nanoparticles.

Water confined in Carbon Porous Matrix

The curves resulting from measurements on separate instruments should be consistent with each other

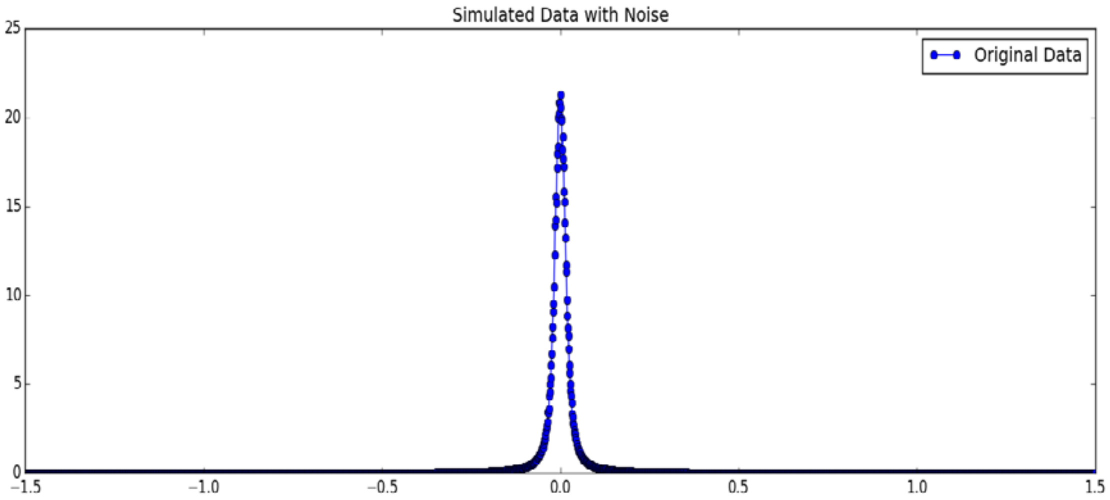




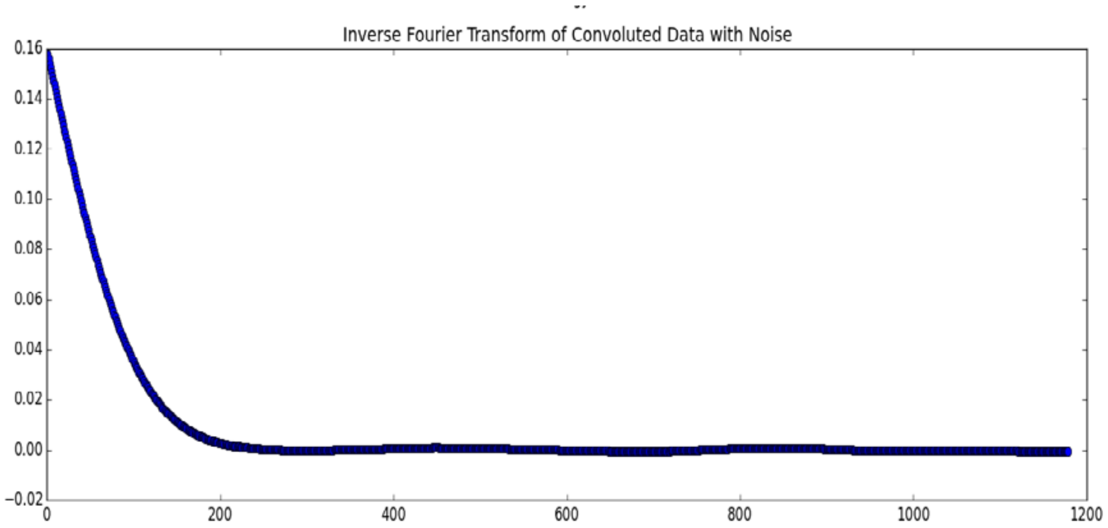


3. Ganapatibhotla, Lalitha and Janna Maranas. "Structure and Mobility of PEO/LiClO4 Solid Polymer Electrolytes Filled with Al2O3 Nanoparticles." *The Journal of Physical Chemistry*. Web. 31 July 2015.

The Inverse Fourier Transform converts the data into a form suitable for directly visualizing the dynamics



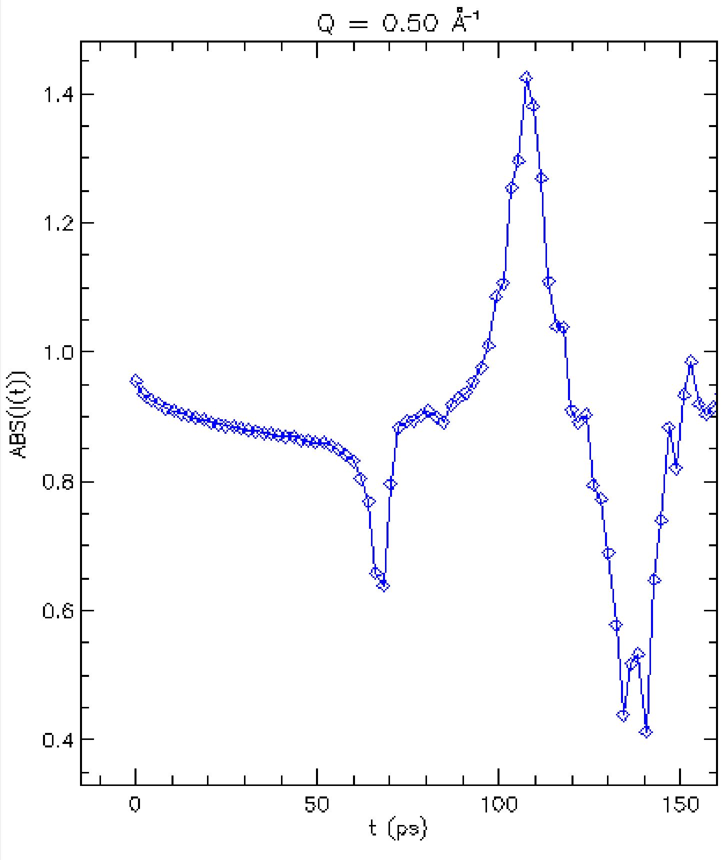
Energy



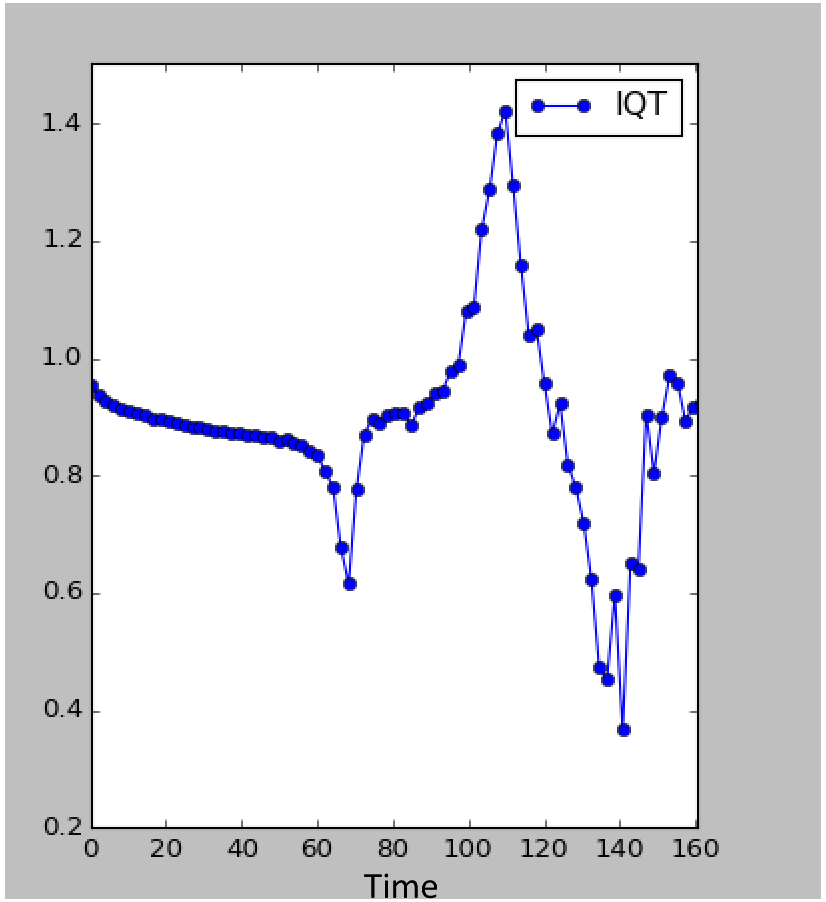
Time

The current processing algorithms contained within DAVE were used to test the new way of processing data.

From DAVE:



From my program:



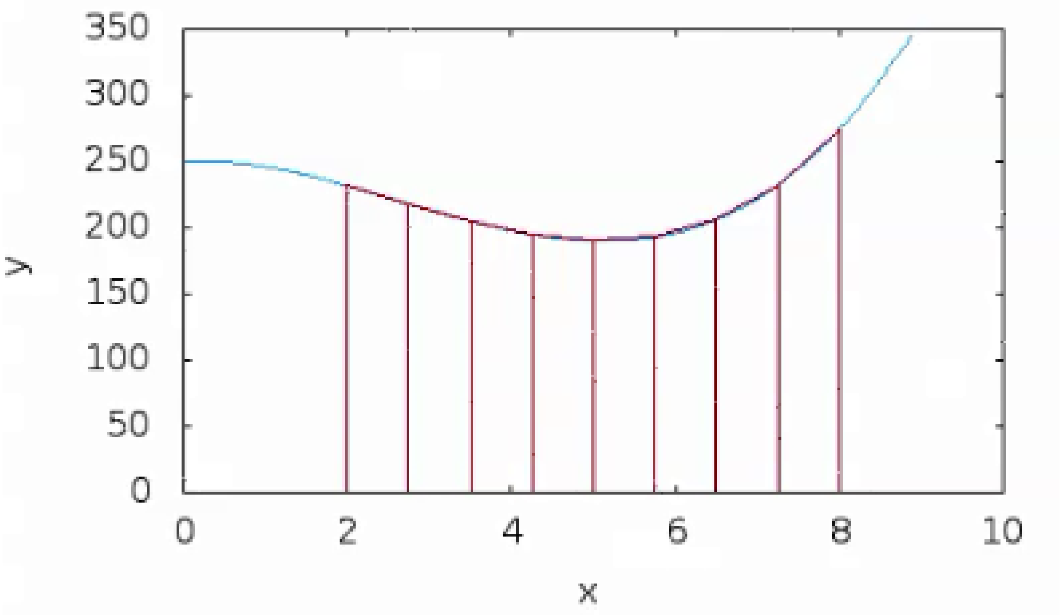
The primary difference between DAVE and the code used for this project is the treatment of the Inverse Fourier Transform

Continuous Inverse Fourier Transform:

$$f(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} F(\omega)e^{i\omega t}d\omega$$

&

Trapezoidal Rule:



VS.

Discrete Inverse Fourier Transform:

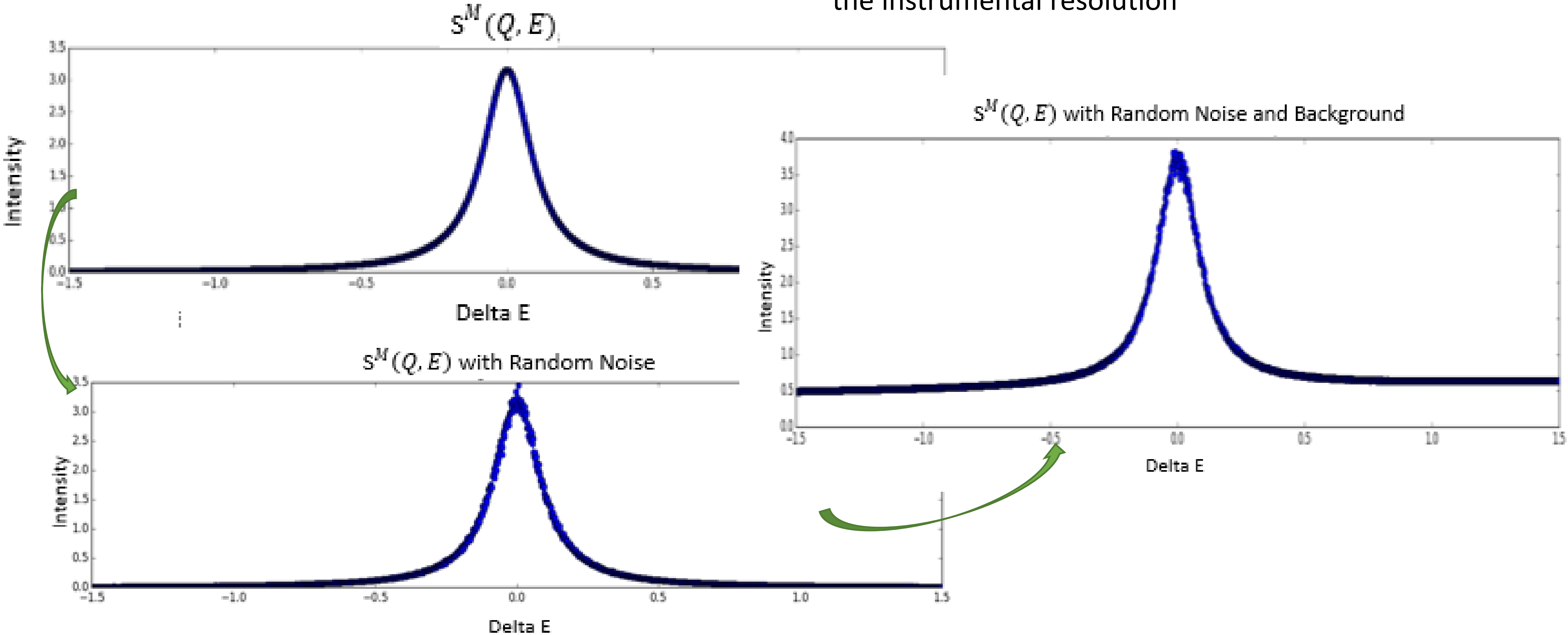
$$x_n = \frac{1}{N}\sum_{k=0}^{N-1} X_k \cdot e^{i2\pi kn/N}, \quad n \in \mathbb{Z}$$

&

The Fast Fourier Transform

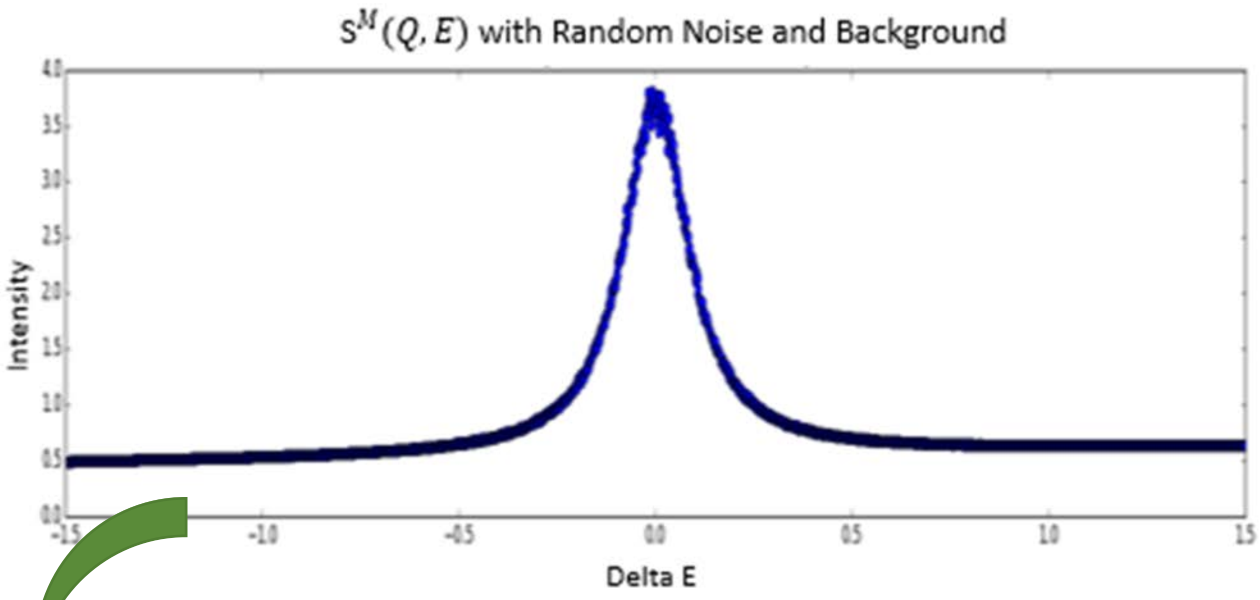
Using code, simulated data mimic the real data in order to investigate the reasoning behind the mismatched curves

$S^M(Q,E)$ is the convolution of a material dynamics and the instrumental resolution

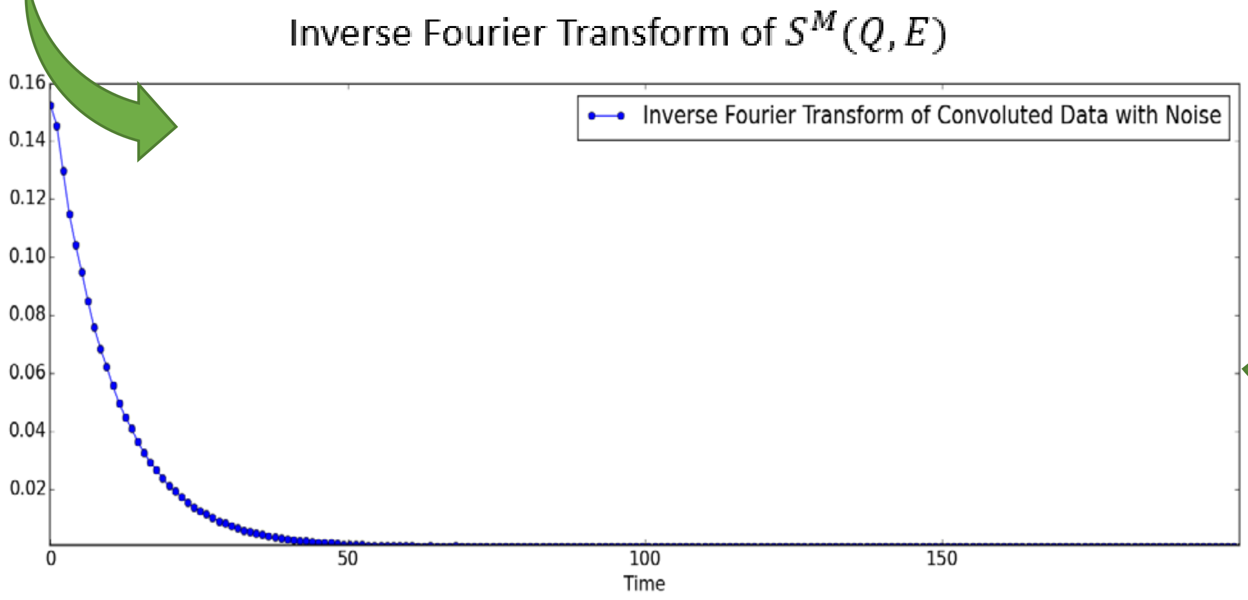


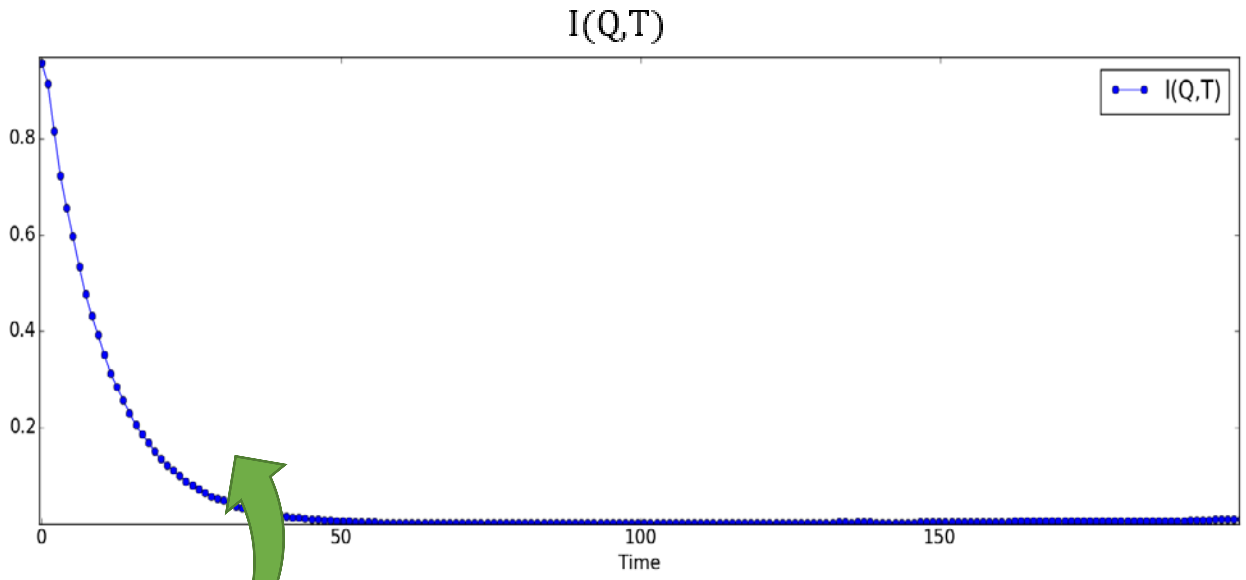
$S^M(Q, E)$ is the convolution of a material dynamics and the instrumental resolution

$I(Q, T)$ is the function describing the material dynamics



Take the Inverse Fourier Transform

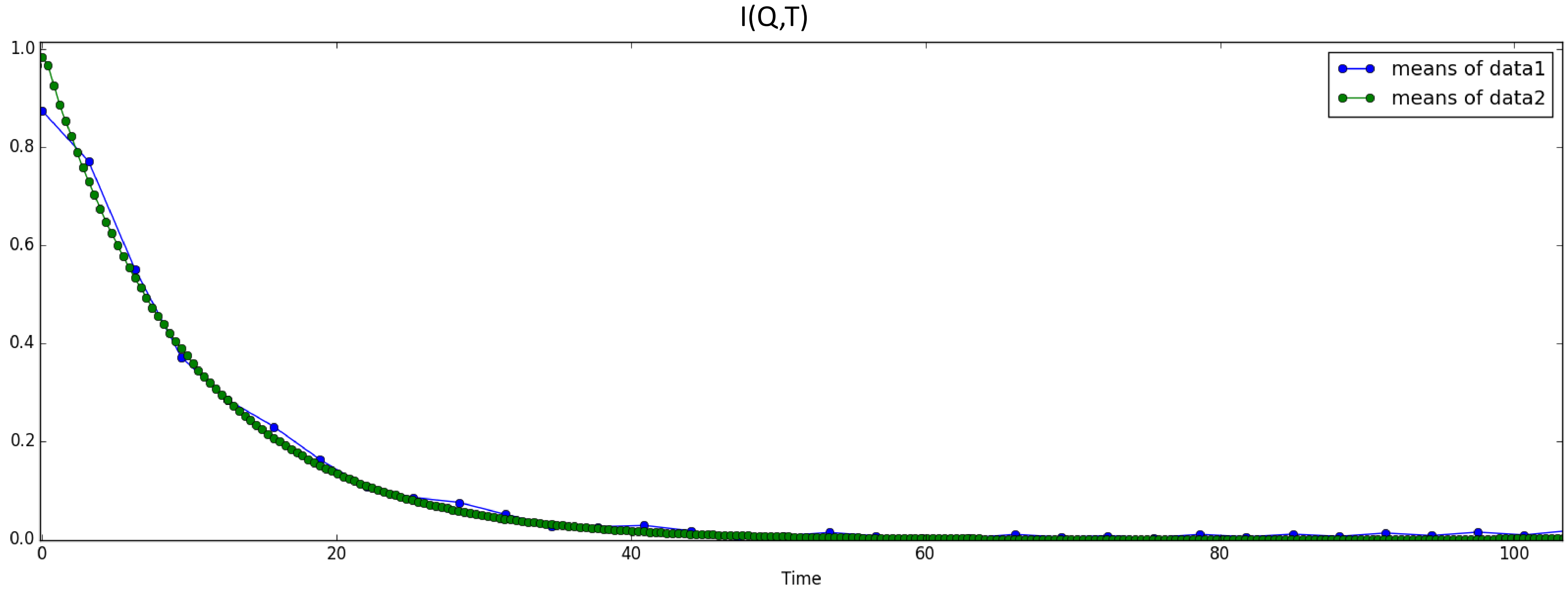




Divide by the Resolution

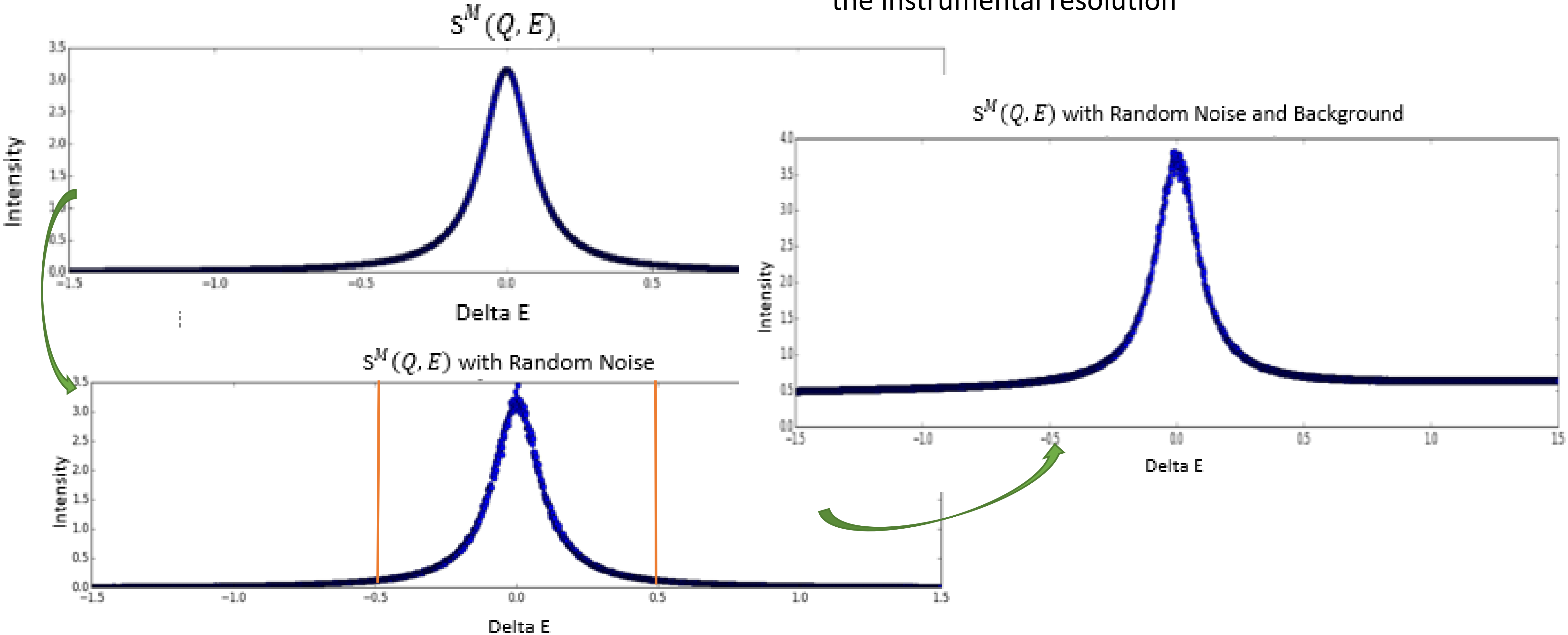
Through the manipulation of simulated data, the potential for additional unforeseen instrumental effects was tested

1. Cutoff decreases the peak and increases oscillation



Using code, simulated data mimic the real data in order to investigate the reasoning behind the mismatched curves

$S^M(Q, E)$ is the convolution of a material dynamics and the instrumental resolution



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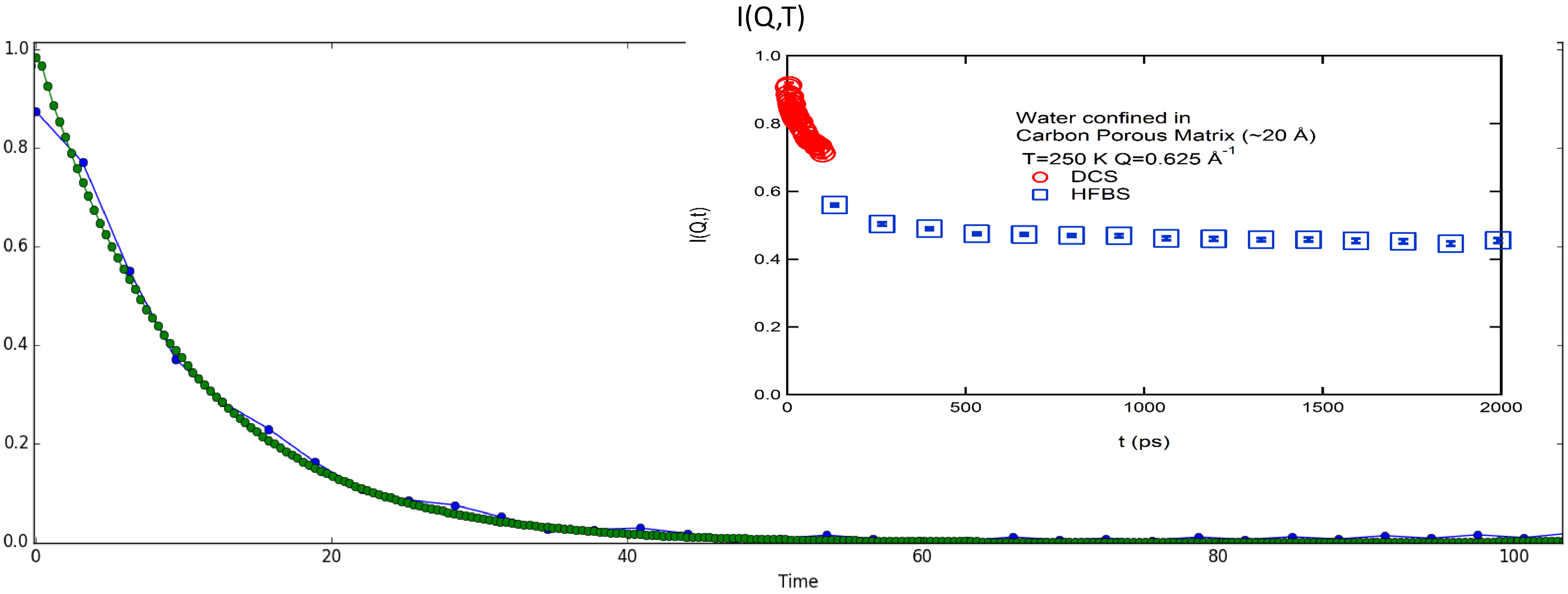
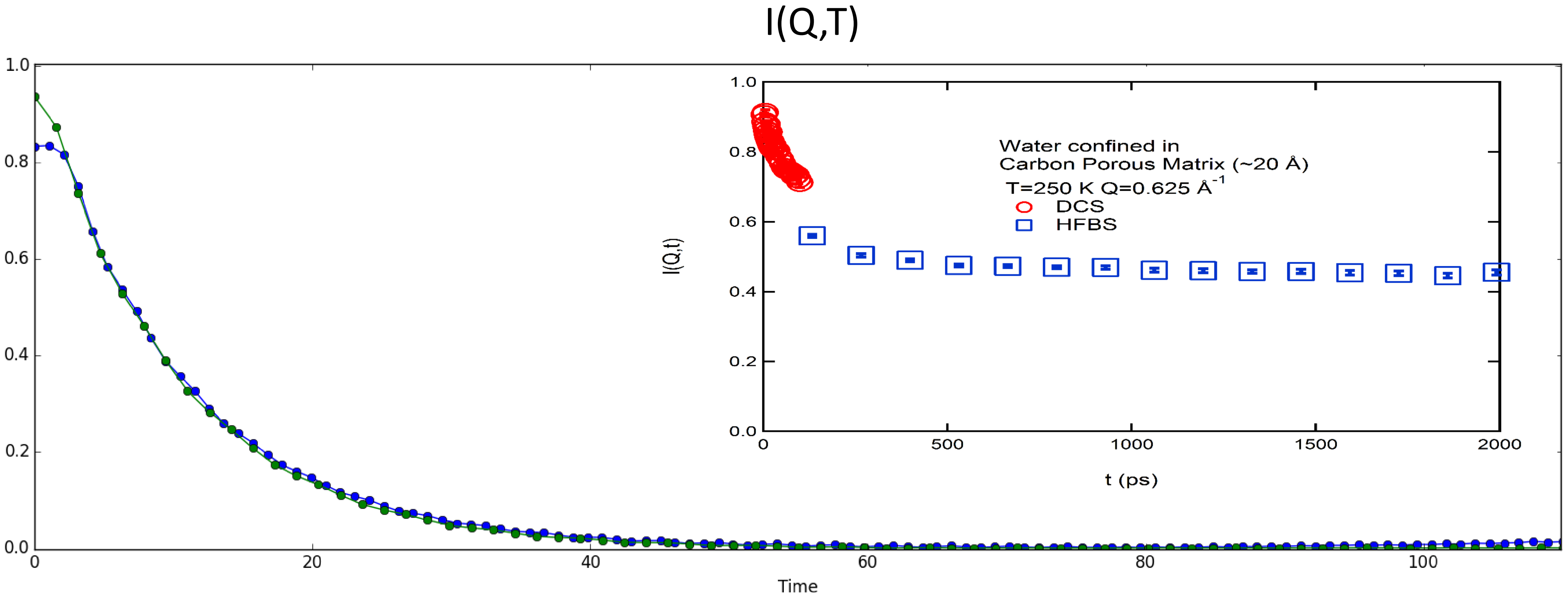
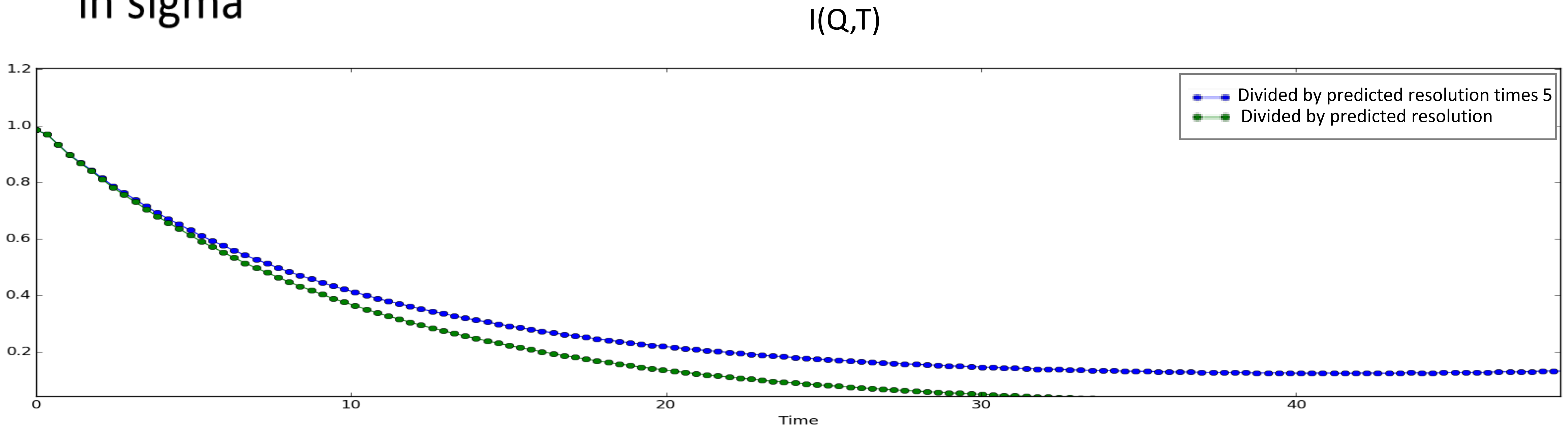
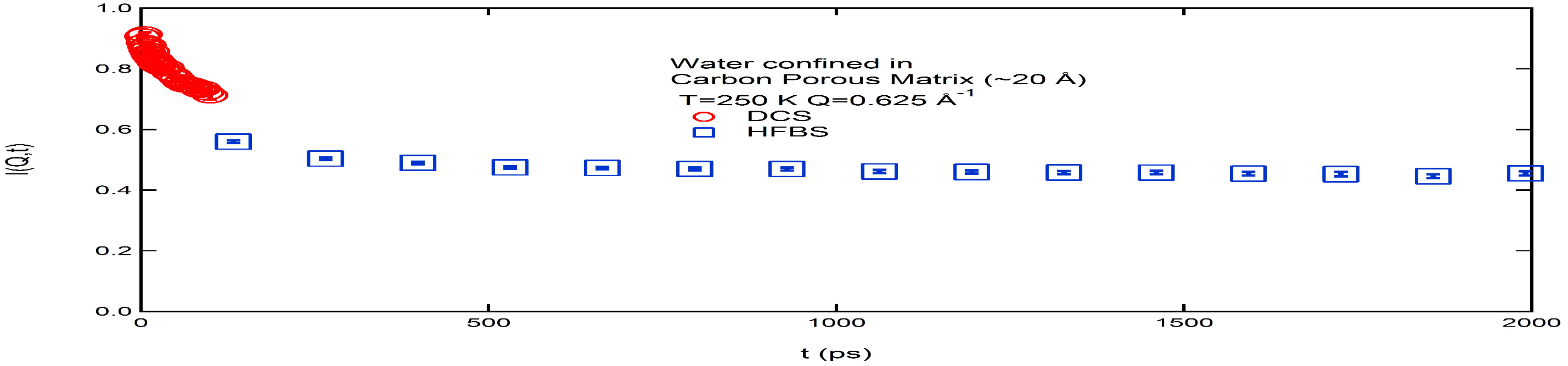


2. Background again decreases the peak and increases oscillation



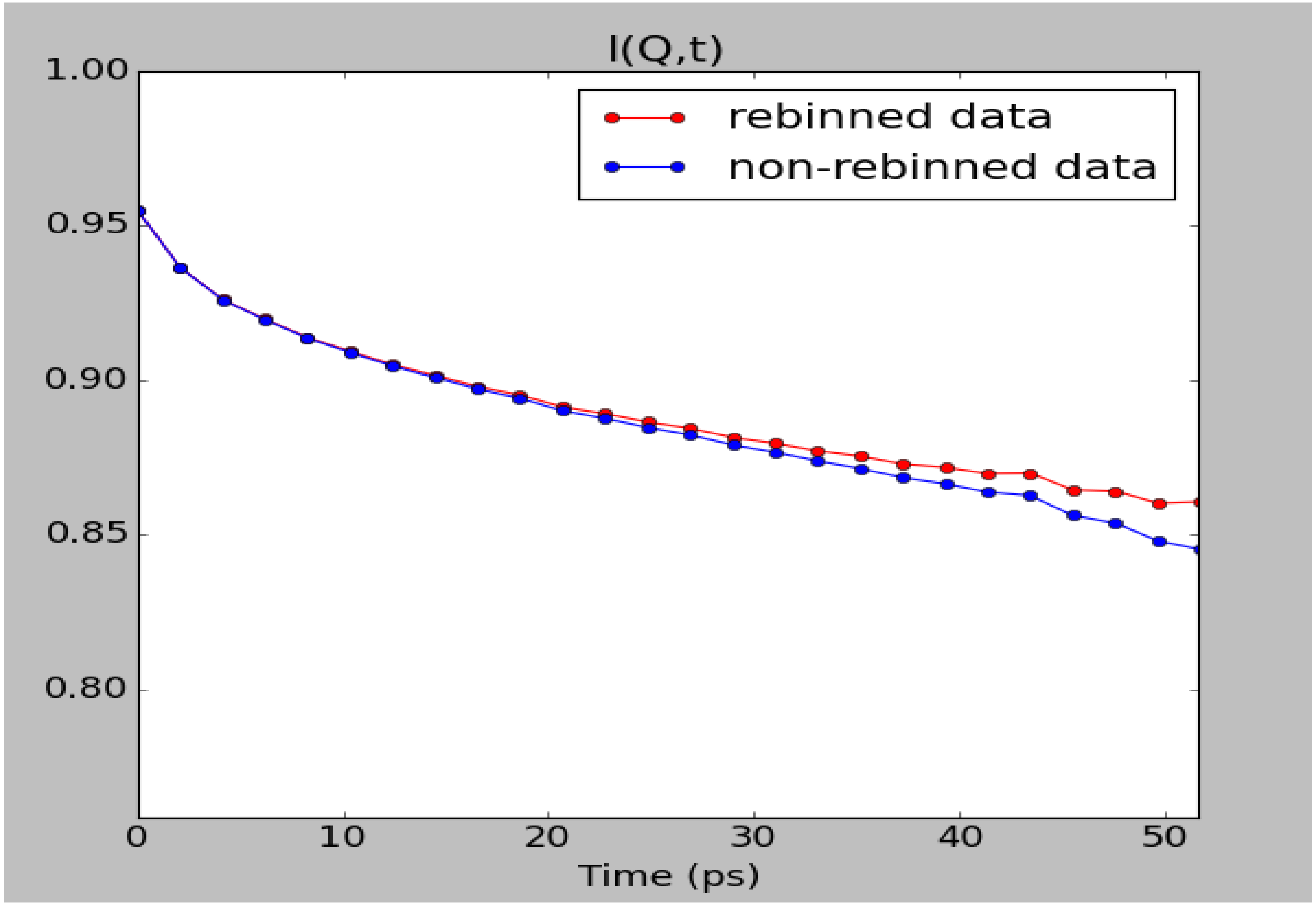
3. Resolution creates an offset, but there must be a significant change in sigma





The lack of rebinning is leading to initially surprising results.

The Fast Fourier Transform
vs.
Trapezoidal Rule



Further investigation into this problem needs to be done particularly into the results of the non-rebinned data

Next Steps:

Artificial Data	**Real Data**
Asymmetry in the Errors	Add in Error Bars
Smoothing	Investigate the non-rebinned data

Thank You

- Antonio Faraone
- Paul Kienzle
- Julie Borchers
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- NSF

NIST Center for Neutron Research

CHRNS
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