Monte-Carlo Neutron Simulation of Novel Neutron Intensity Modulated Spectrometer (NIMS)

NIST CENTER FOR NEUTRON RESEARCH

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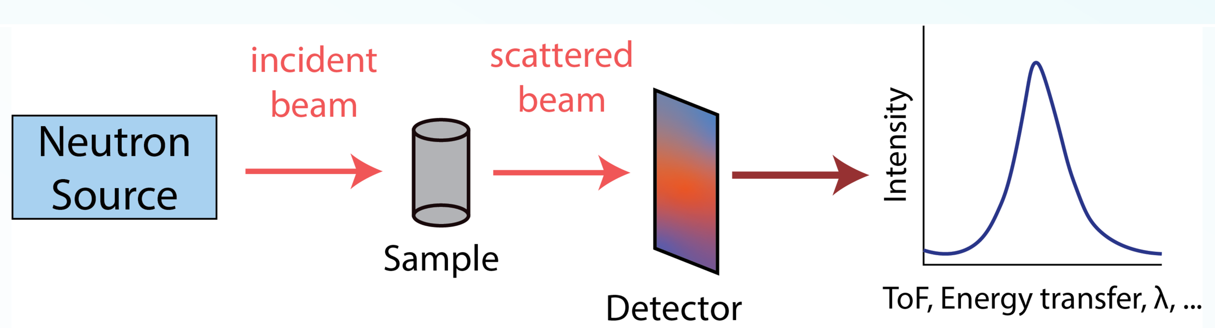
Abstract

McStas, a computational Monte Carlo neutron simulation tool, was used to virtually construct and test the viability of a novel chopper-based time-of-flight (ToF) neutron scattering instrument, named Neutron Intensity Modulated Spectrometer (NIMS). NIMS' Fourier-transform approach makes it compatible with a continuous source, circumventing the need for a pulsed monochromatic incident beam. The McStas simulation results indicate that NIMS is an appropriate instrument to probe dynamics over timescales up to 10^2 picoseconds.

Introduction

Neutrons are chargeless particles that can easily penetrate atomic electron clouds to interact with nuclei and magnetic inhomogeneities. Additionally, neutron wavelengths and energies are generally comparable to atomic scales. These properties make quasielastic neutron scattering (QENS) a very powerful method of probing the geometry and timescale of molecular, atomic, and spin motions.



One of the largest limitations of current QENS instruments is the loss of neutron flux from the typically prerequisite pulsation and monochromation of the incident beam.

The Neutron Intensity Modulated Spectrometer (NIMS) is a conceptual QENS instrument that would circumvent these limitations by using intensity-modulating chopper (IMC), Time of Flight (ToF), and Fourier-transform techniques.

Methodology

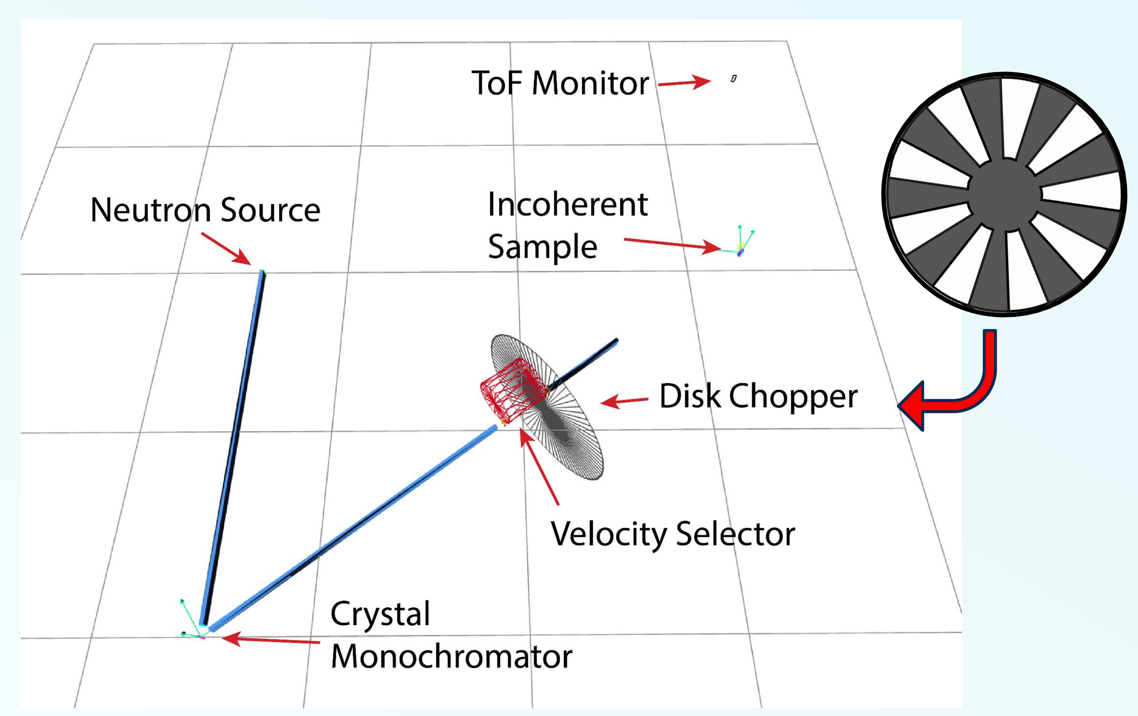
McStas is a computational program that utilizes Monte-Carlo methods and ray tracing to simulate neutron scattering.

For this project, I used McStas to virtually construct and simulate multiple variations of the conceptual NIMS instrument. The results outputted by McStas allow us to validate and optimize the conceptual NIMS instrument in non-ideal conditions.

Instrument Frameworks

Setup A: Monochromatic Single-Chopper NIMS

A flat crystal monochromator is used to monochromate the incident beam. A singular disk chopper with equal slits and covers is then used to create a triangle-wave transmission profile. Since the incident beam is not pulsated, neutron flux is not as severely reduced.

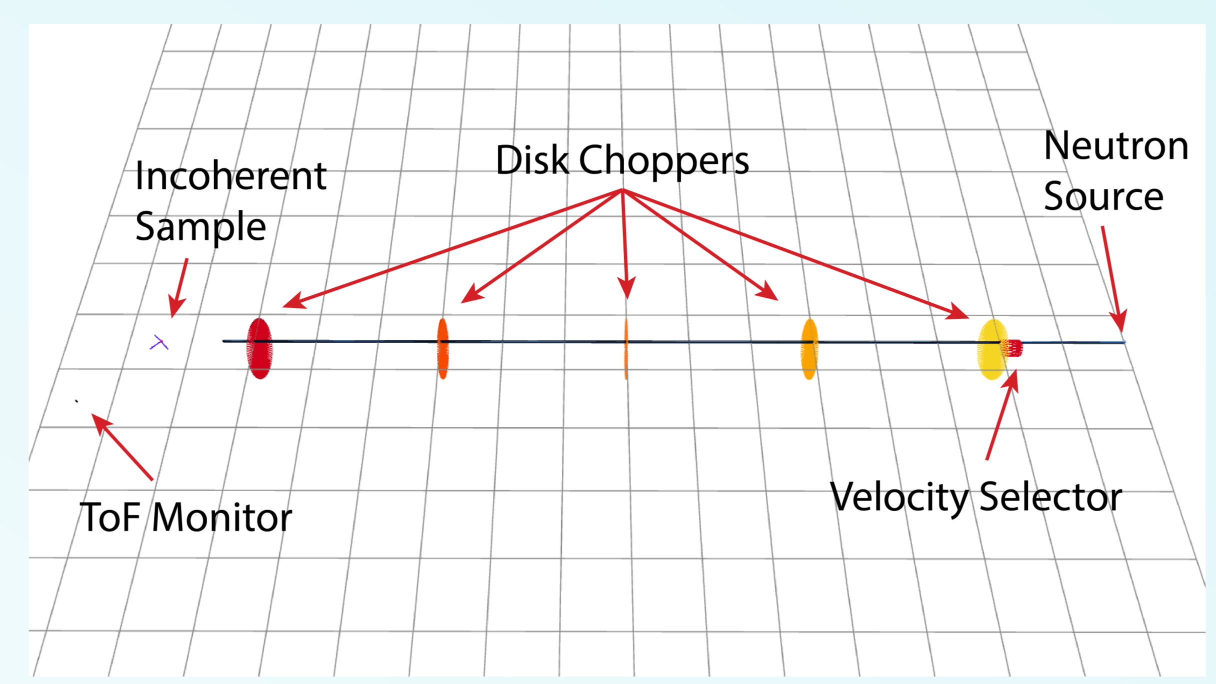


Following scattering, differences in neutron velocities will smear the triangular profile over time. By measuring the Fourier components of this smear, we can obtain the Fourier transform of the dynamic structure factor, S(Q,E).

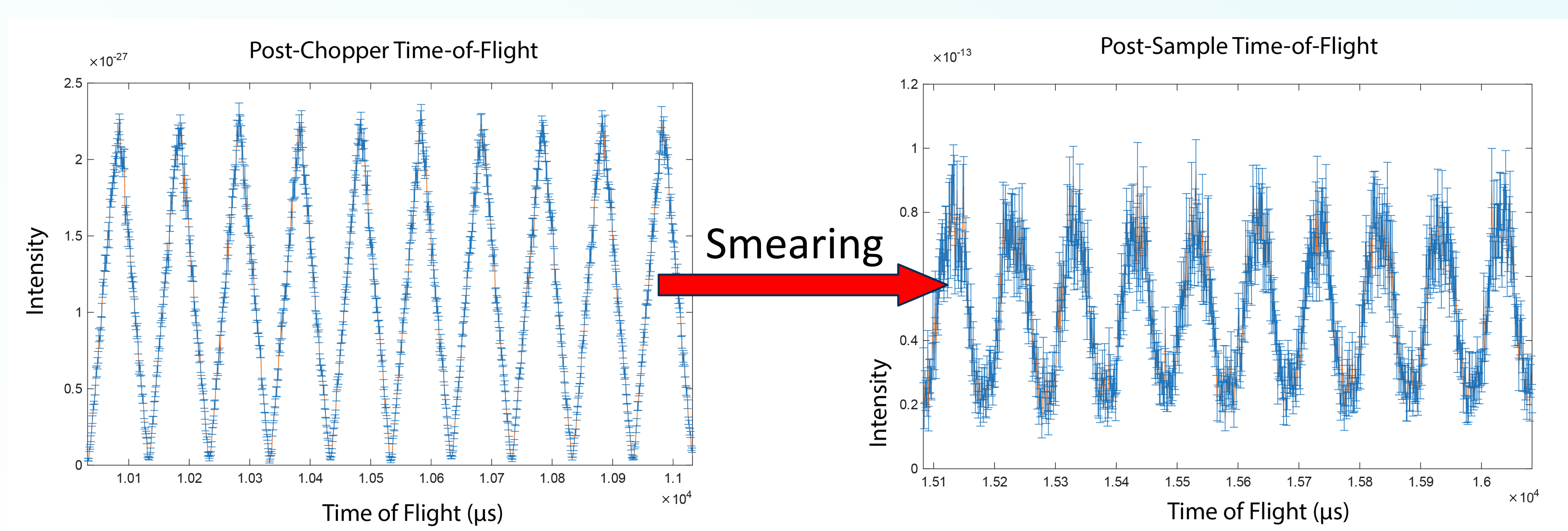
Setup B. Polychromatic Multi-Chopper NIMS

Rather than monochromating the incident beam, multiple choppers can be used to selectively transmit desired wavelengths from a polychromatic beam, increasing neutron flux compared to the single-chopper setup.

Five identical choppers as before are spaced evenly apart, their phases adjusted to allow only the desired wavelength to perfectly transmit.

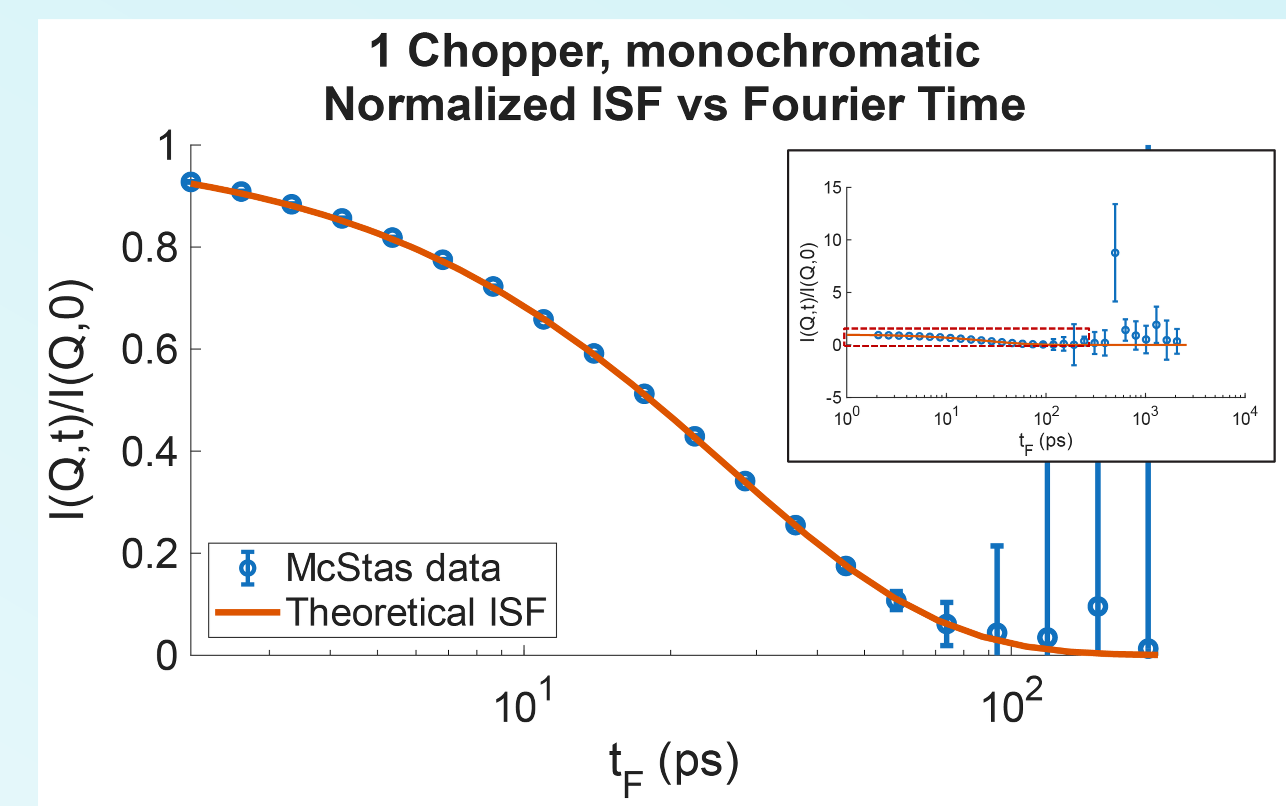


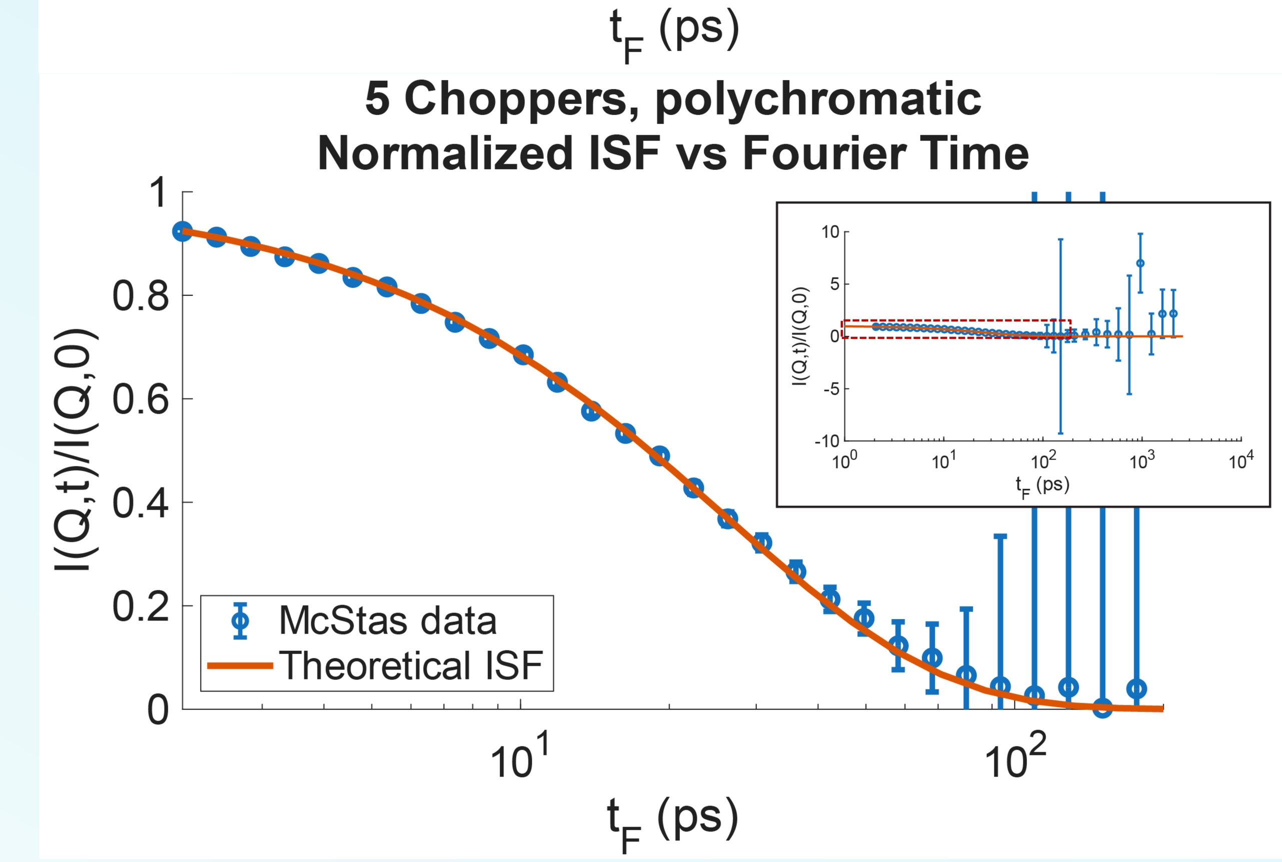
The same method as before of obtaining the Fourier transform of S(Q,E) is used.



Results & Conclusion

Below is the Fourier-transformed S(Q,E) data outputted by the McStas simulations, overlayed with theoretical equations calculated by assuming perfect conditions (i.e., perfectly monochromatic, perfectly columnated, negligible chopper geometry).





The agreement up to 10^2 ps indicates that both variations of NIMS are realistically appropriate to probe timescales of molecular, atomic, and spin motions of up to 10^2 picoseconds, corresponding to ≈10μeV energy resolution.