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

Noah Sonfield

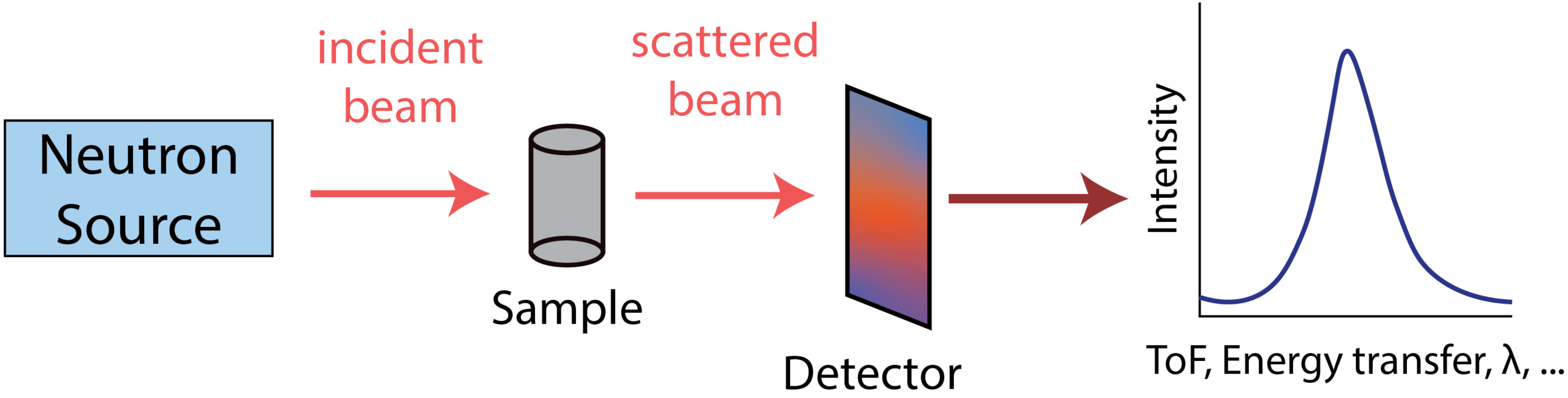
Bethesda-Chevy Chase High School

Mentors: Dr. Antonio Faraone, Dr. Leland Harriger

NIST CENTER FOR NEUTRON RESEARCH

NSF CHRNS CENTER FOR HIGH RESOLUTION NEUTRON SCATTERING NIST

Neutron Scattering

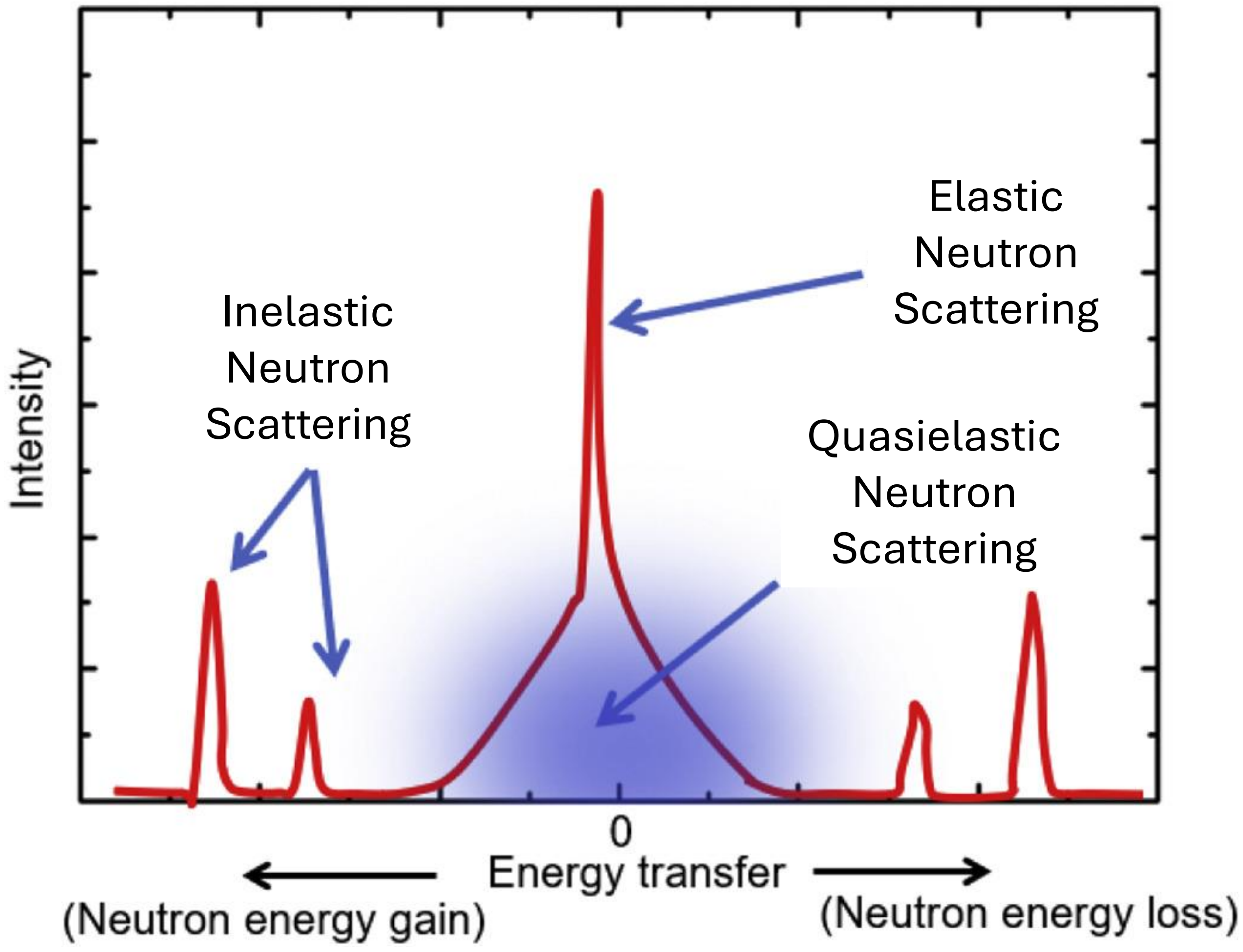


Neutron scattering is a powerful method of probing the geometry and timescale of molecular, atomic, and spin motions.

Quasielastic Neutron Scattering (QENS)

QENS → small exchange of energy between the neutron and the sample.

We can learn about the structure of the sample by determining how much energy was exchanged.



Current Instruments

Most current instruments measure the double differential scattering cross section:

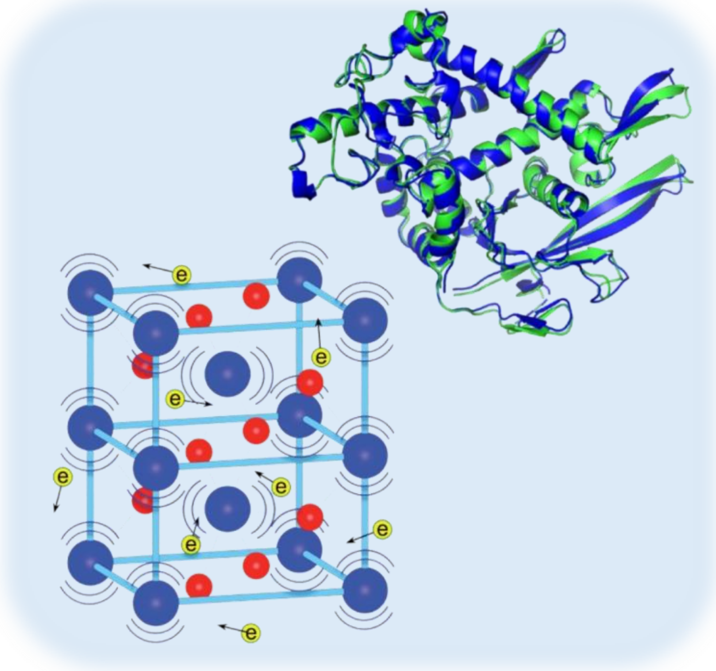
$$\frac{\delta^2 \sigma}{\delta \Omega \delta E}$$

Proportion of scattered neutrons

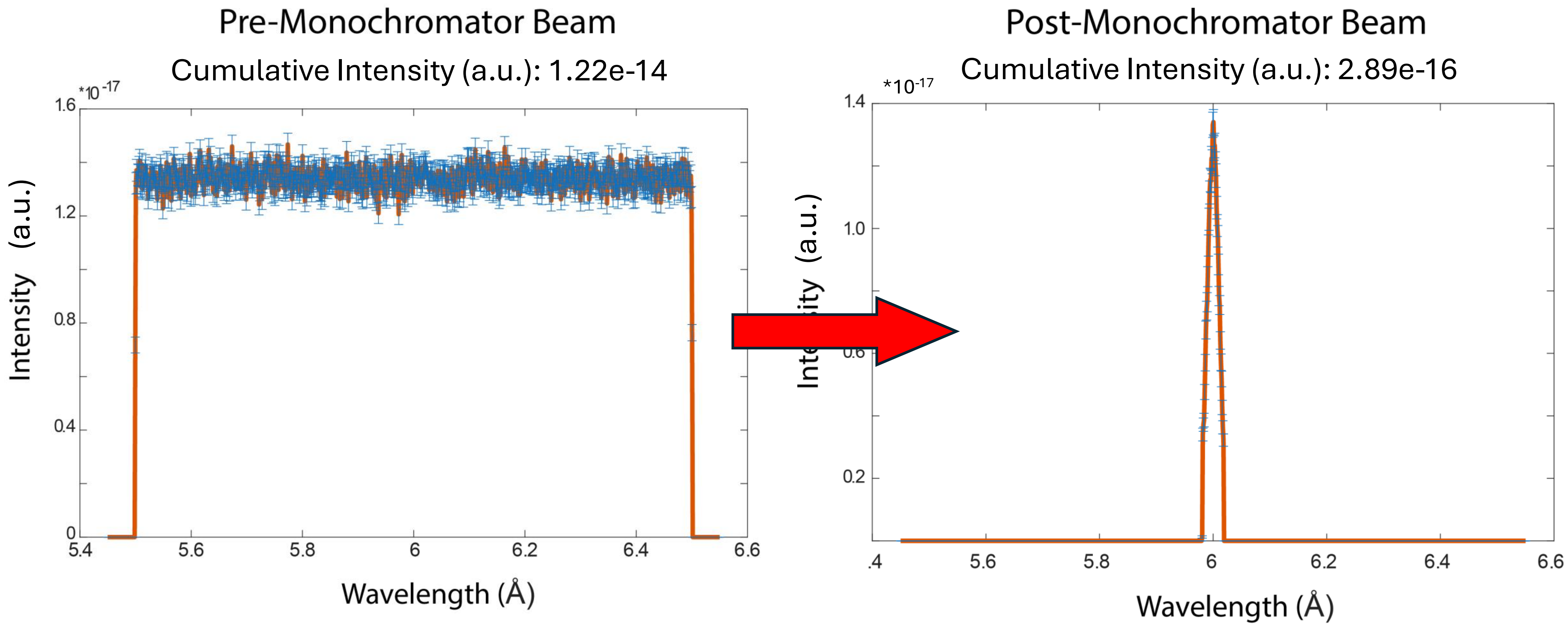
Per energy transfer

$E_{final} - E_{initial}$

Per solid angle

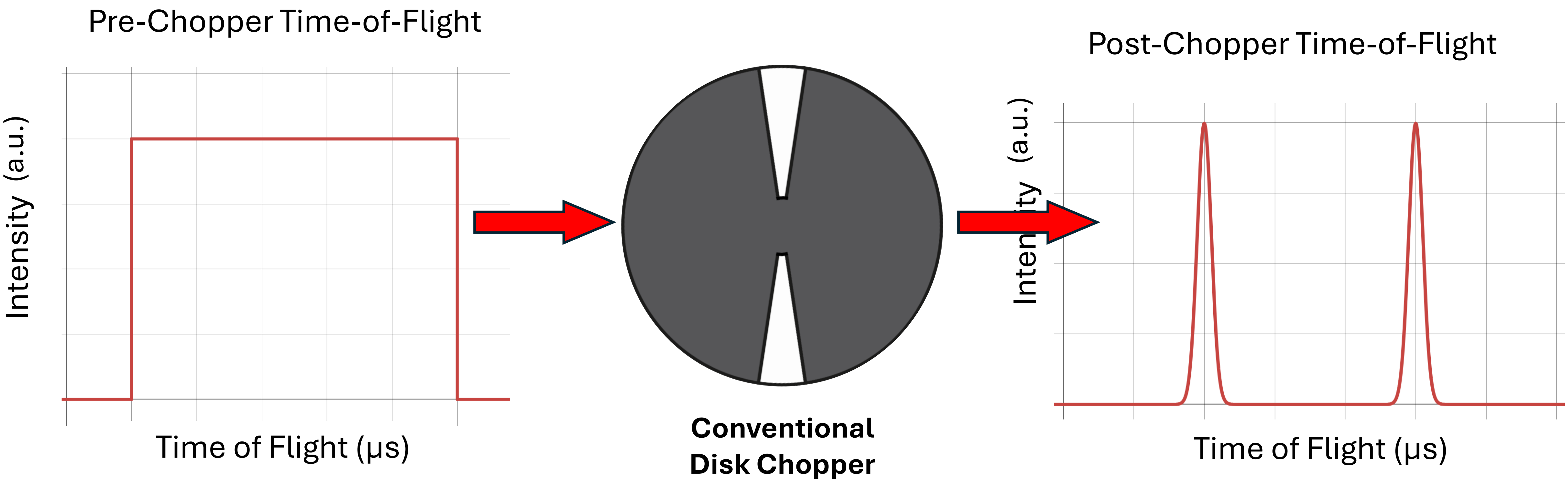


Need to monochromate the neutron beam to determine $E_{initial}$



Neutron Flux ↓↓↓ ☹

Need to pulse the beam to determine Time-of-Flight (ToF) → E_{final}



Neutron Flux ↓↓↓ ☹

Intermediate Scattering Function

Alternatively, we can obtain the exact same information by measuring the intermediate scattering function, I(Q,t).

$$\frac{\delta^2\sigma}{\delta\Omega\delta E}\frac{k_0}{Nk_1} = S(Q,E) = \frac{1}{2\pi}\int_{-\infty}^{\infty} I(Q,t)e^{(-iEt)}dt$$

Fourier Transform

Neutron Spin Echo

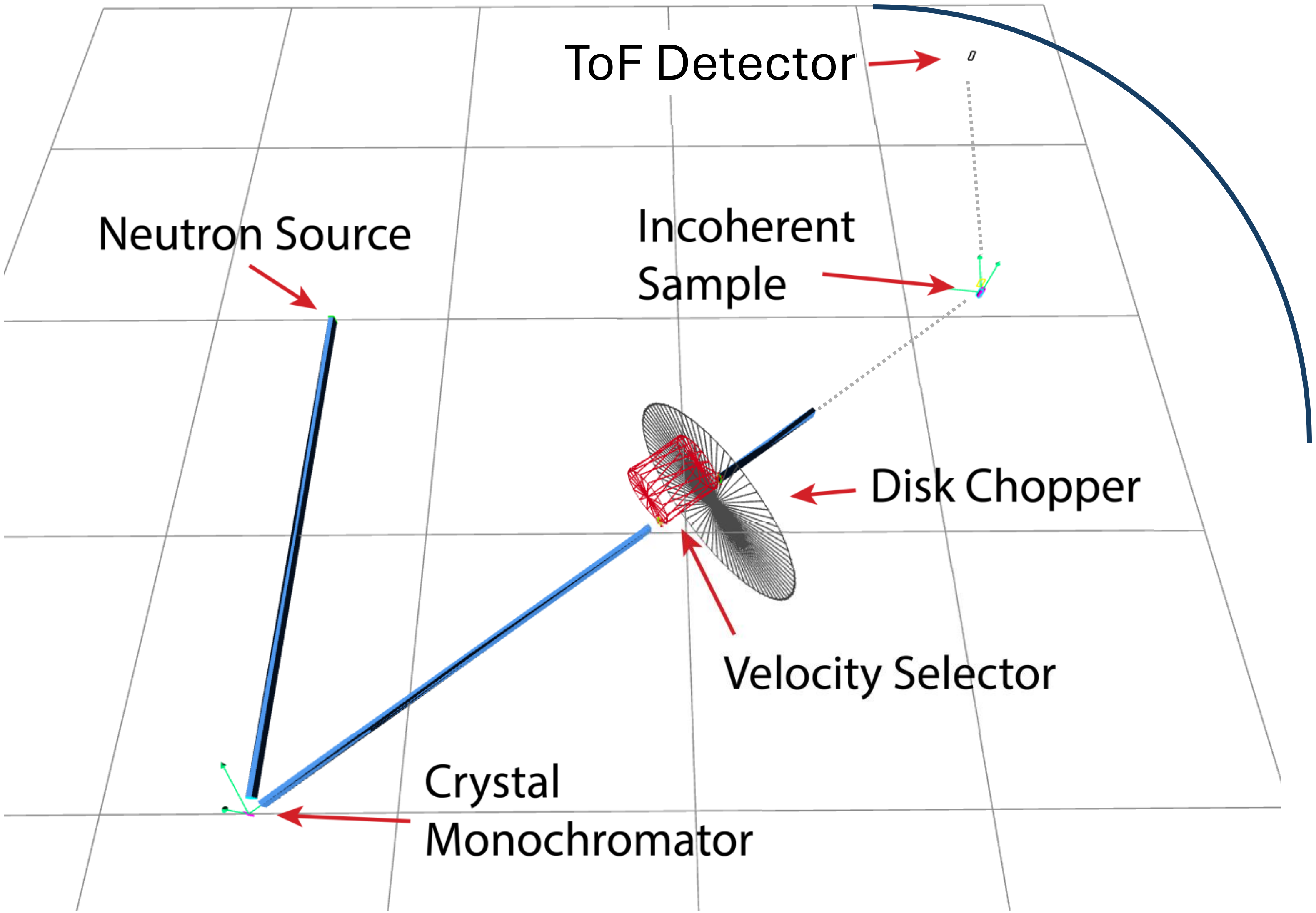
Pros:

- Can use polychromatic beam (neutron flux ↑↑↑ ☺)
- High energy resolution
- Can measure long timescales

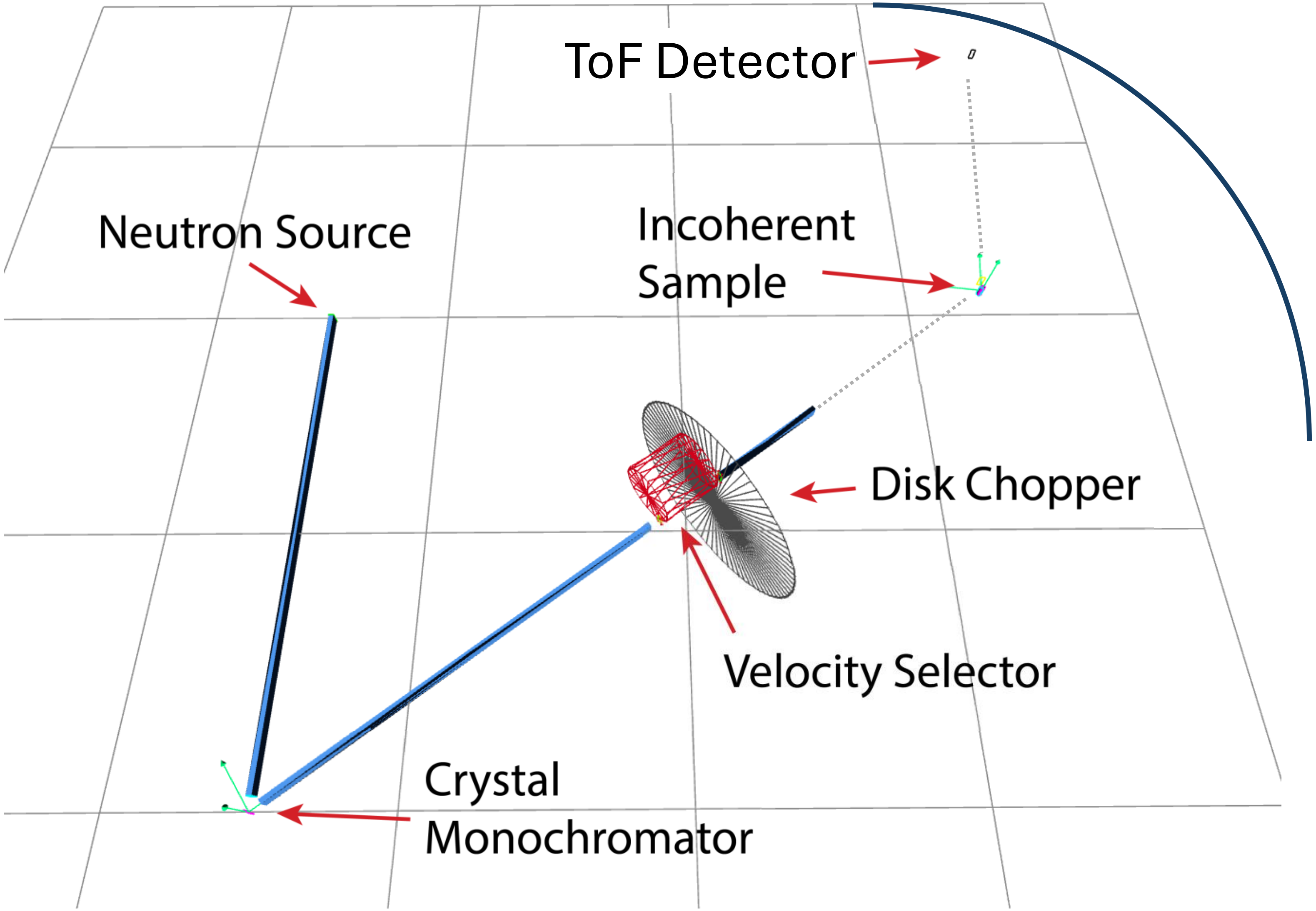
Cons:

- Small detector area
- Requires beam polarization (neutron flux ↓↓↓ ☹)

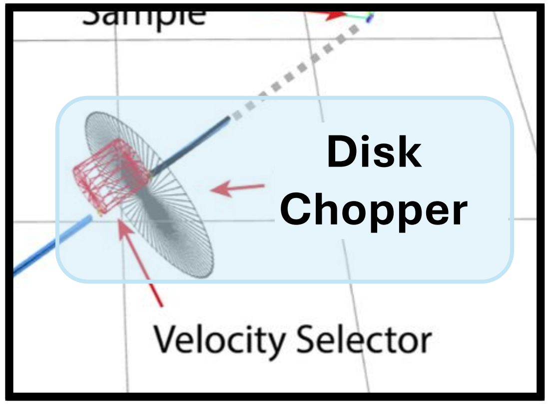
Neutron Intensity Modulated Spectrometer (NIMS)



Neutron Intensity Modulated Spectrometer (NIMS)

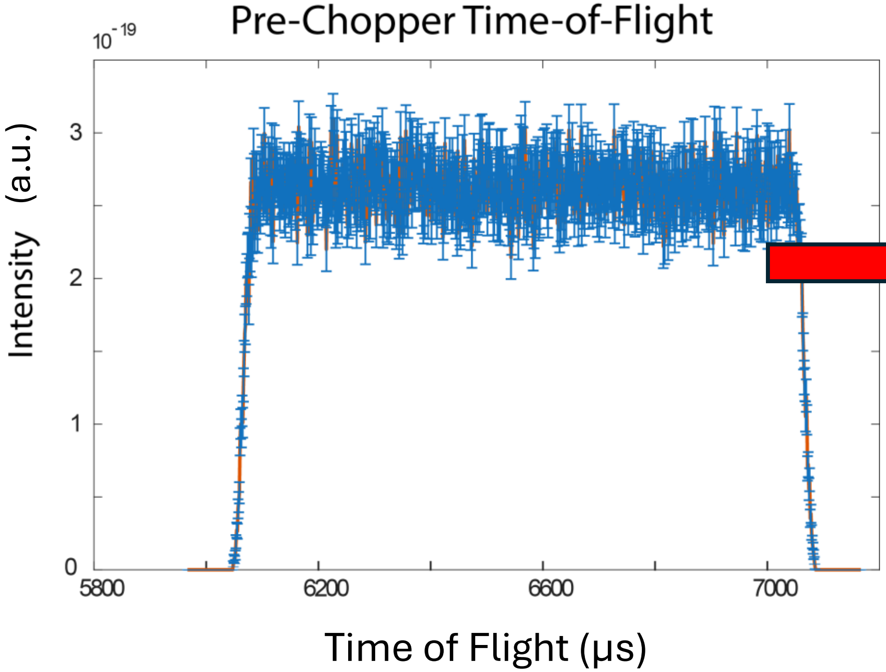


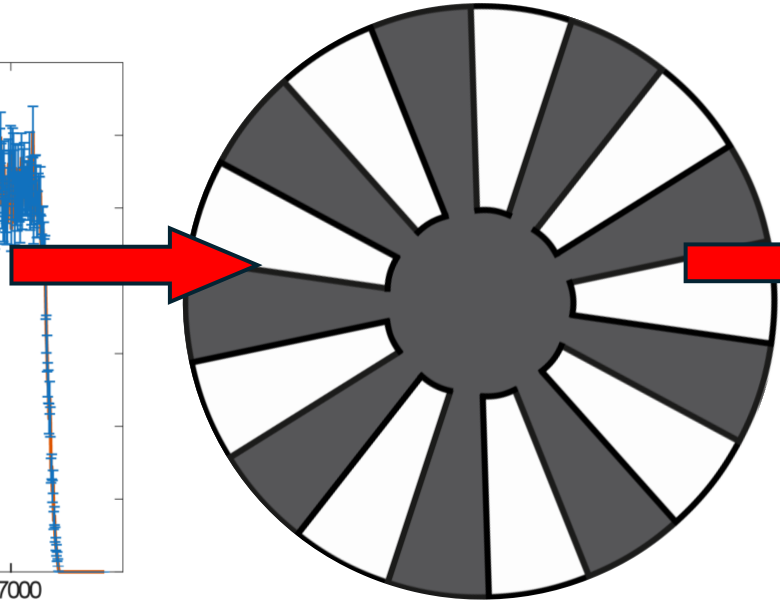
Disk Chopper

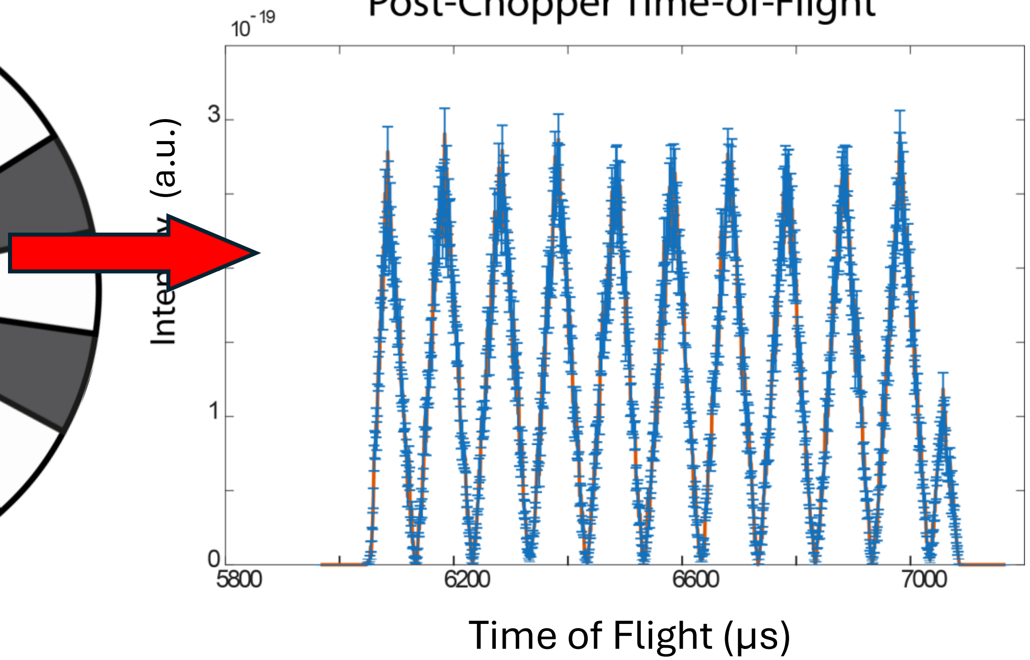


Rather than pulsing, the NIMS chopper creates a triangle wave profile.

Intensity-Modulating Chopper (IMC)

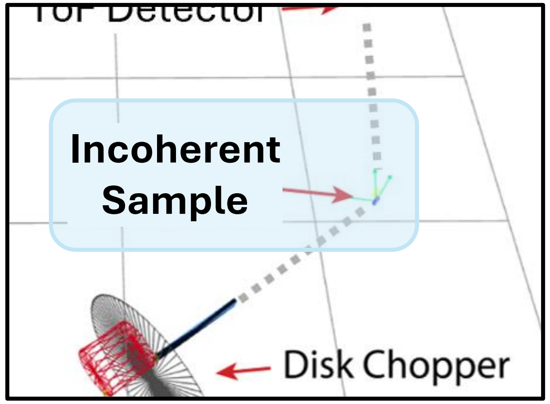


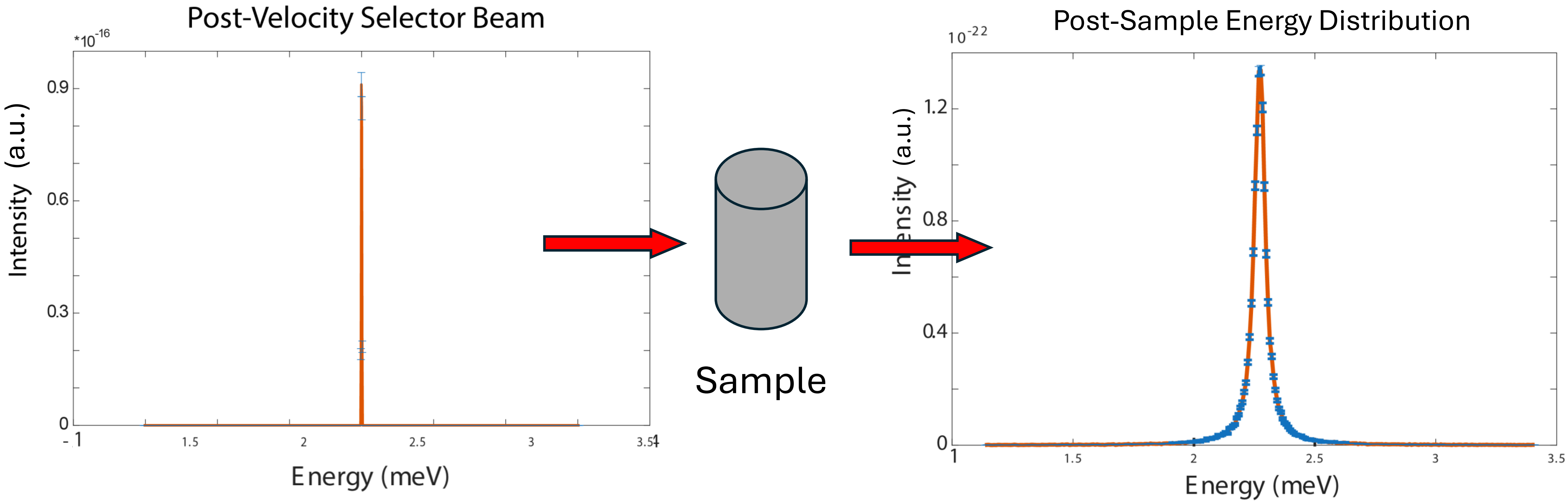




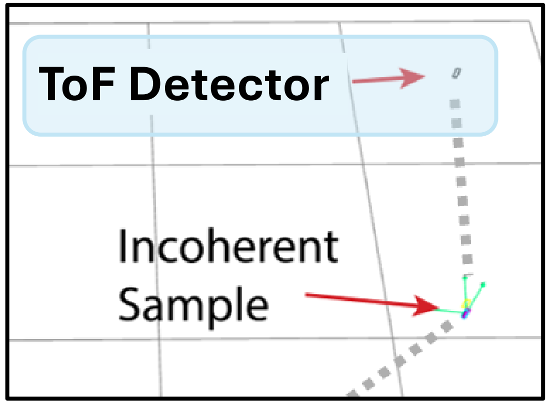
Scattering Sample

After quasielastic scattering, the neutrons' kinetic energies (velocities) are spread out.

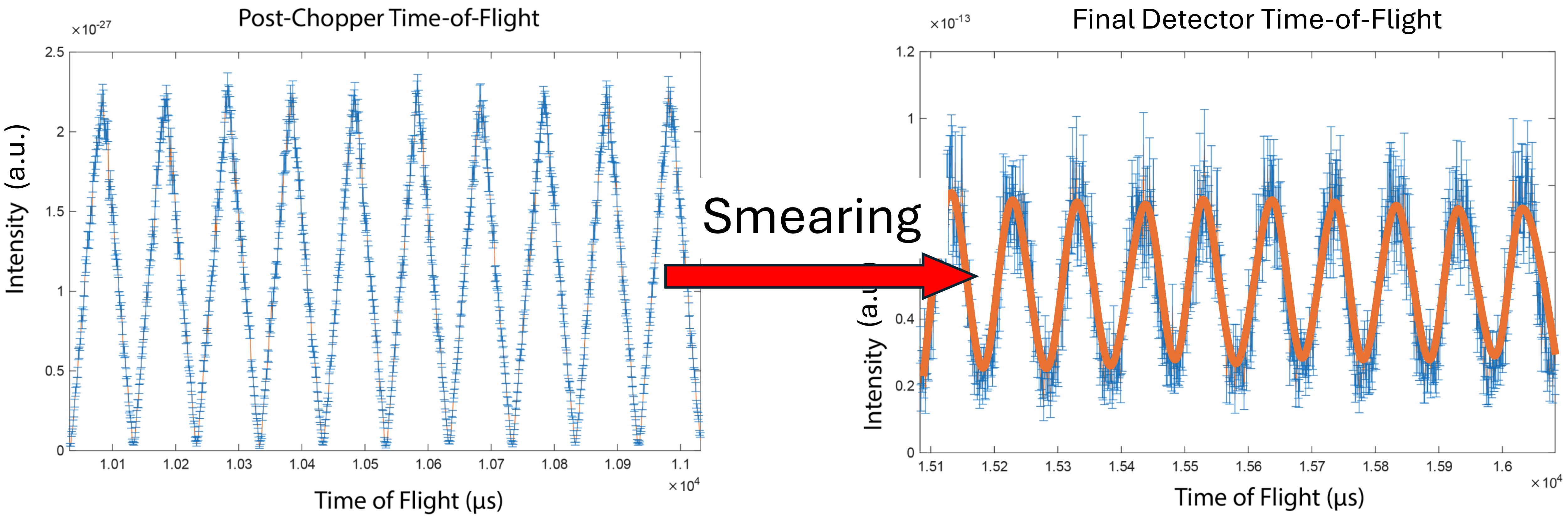




Final Detector

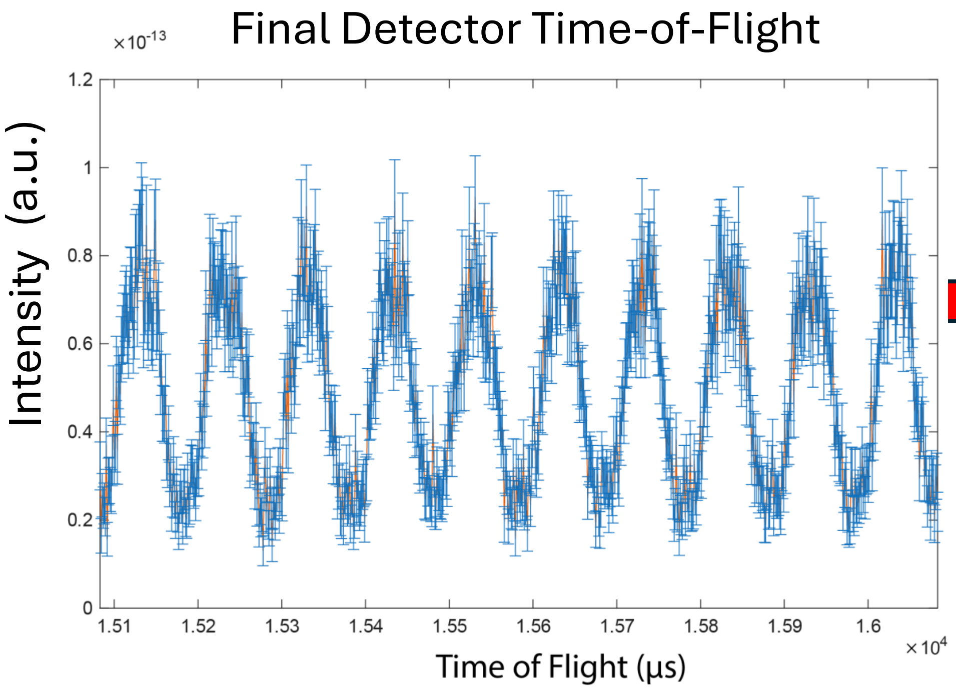


Differences in neutron velocities will smear the triangle wave shape over time.

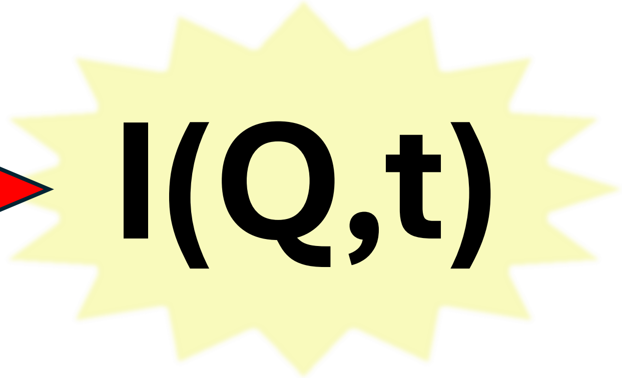


Data Analysis

We can measure the Fourier components of the ToF smear to obtain the Intermediate Scattering Function, I(Q,t).



Fancy Math



Single-Chopper Setup - Review

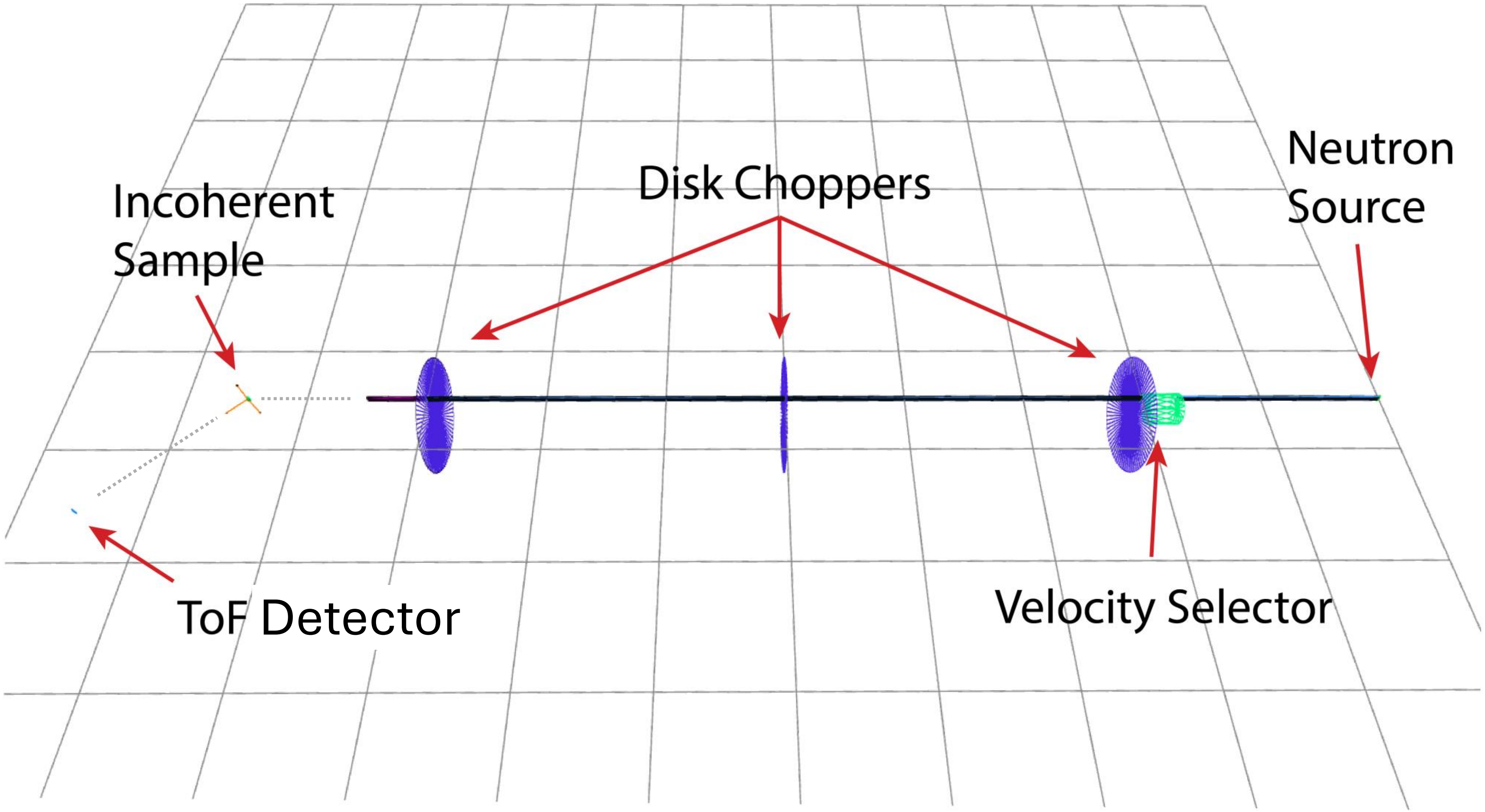
Pros

- Intensity modulating instead of pulsing (neutron flux ↑↑ ☺)
- Wide detector range
- No polarization or magnets needed (neutron flux ↑↑ ☺)

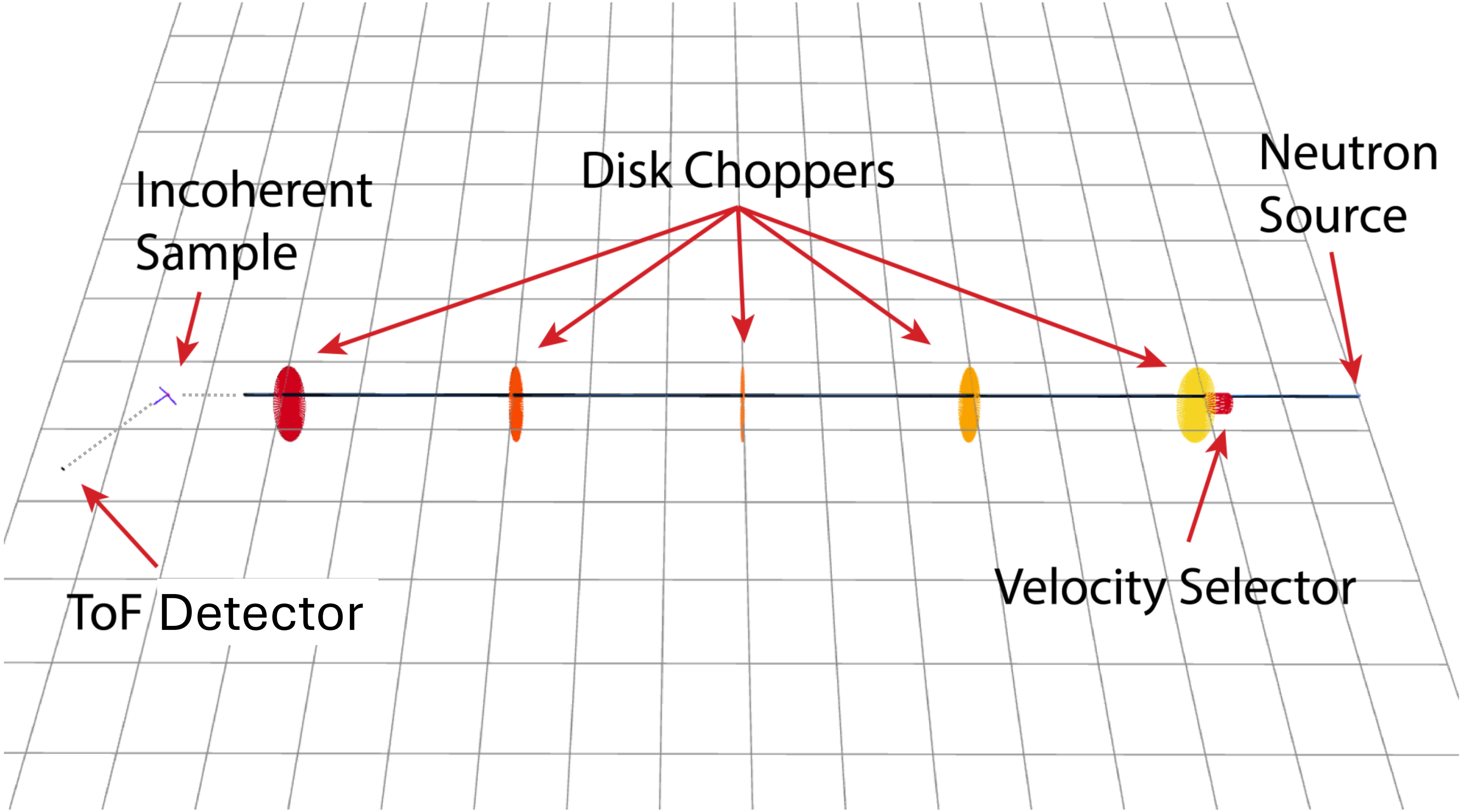
Cons

- We don't know ΔE (but we don't care)
- Still have to monochromate the beam (neutron flux ↓↓ ☹)

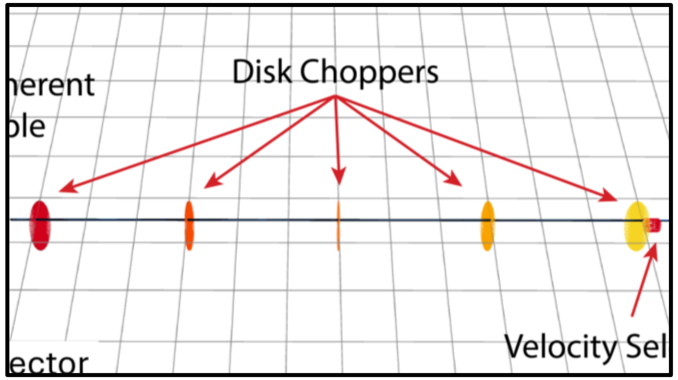
3-Chopper Instrument Configuration



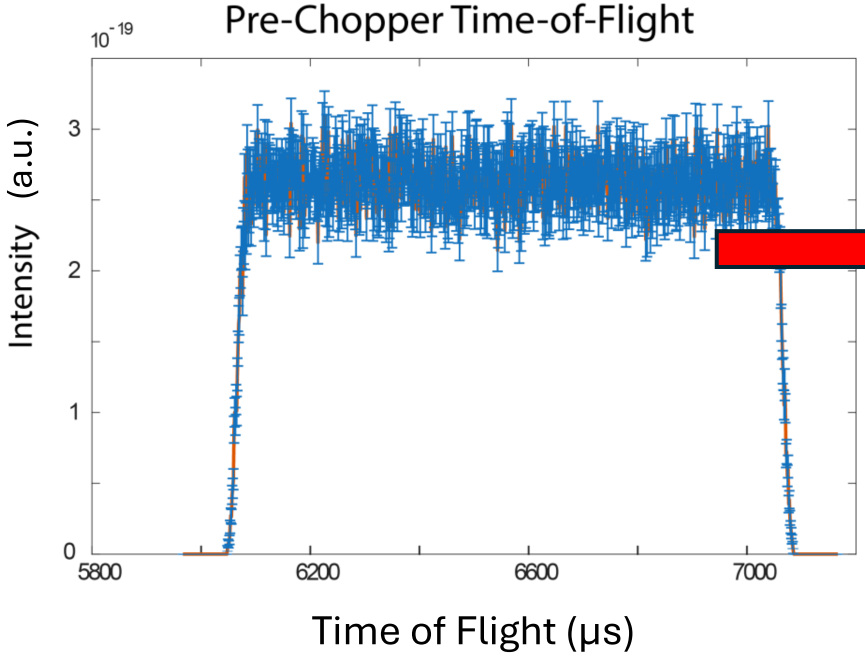
5-Chopper Instrument Configuration



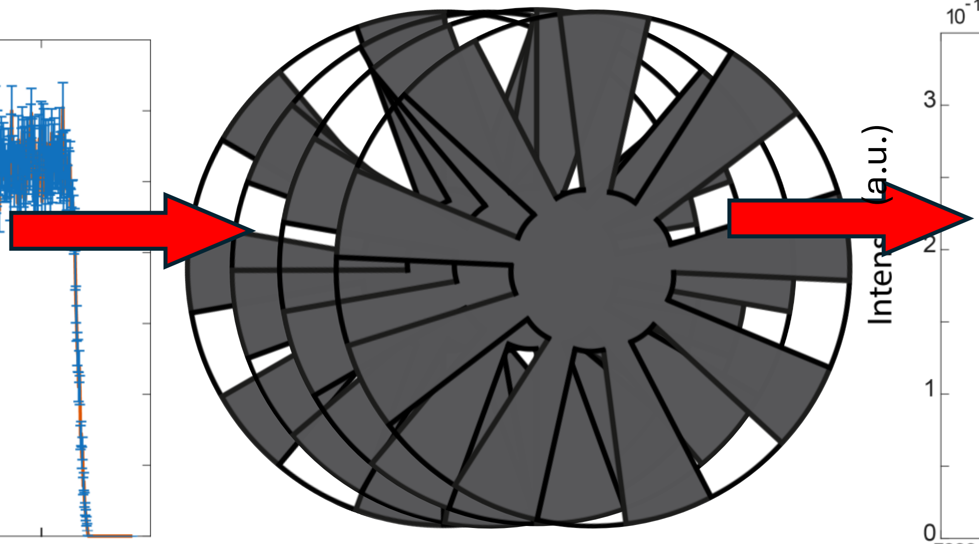
Multi Disk Choppers

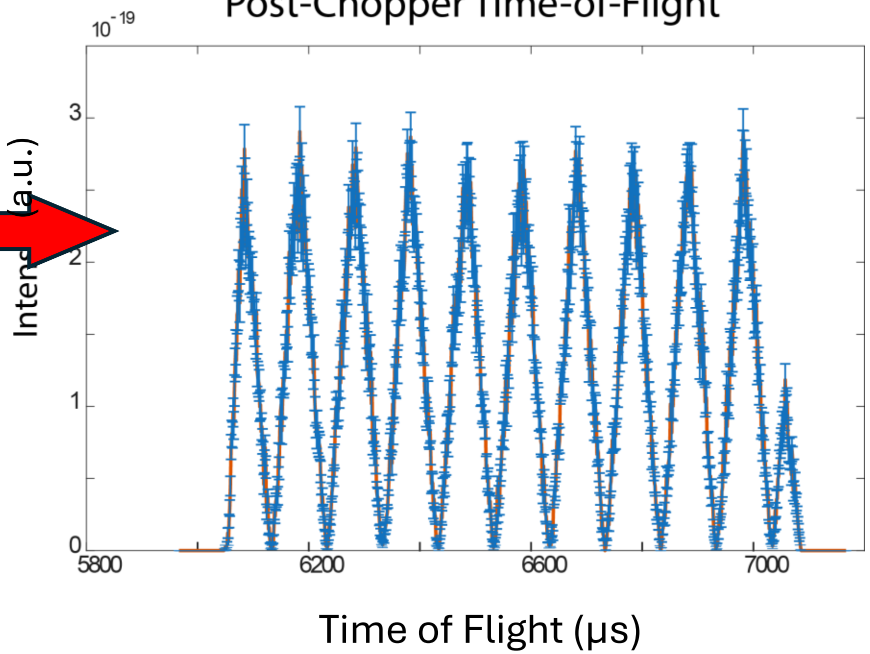


The multi-chopper setups still create the triangle-wave profile.

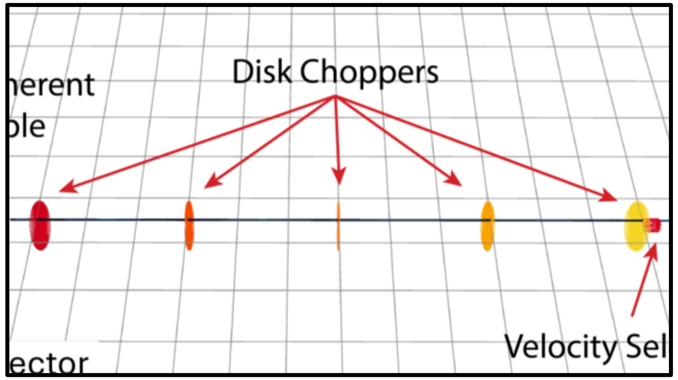


Intensity-Modulating Choppers



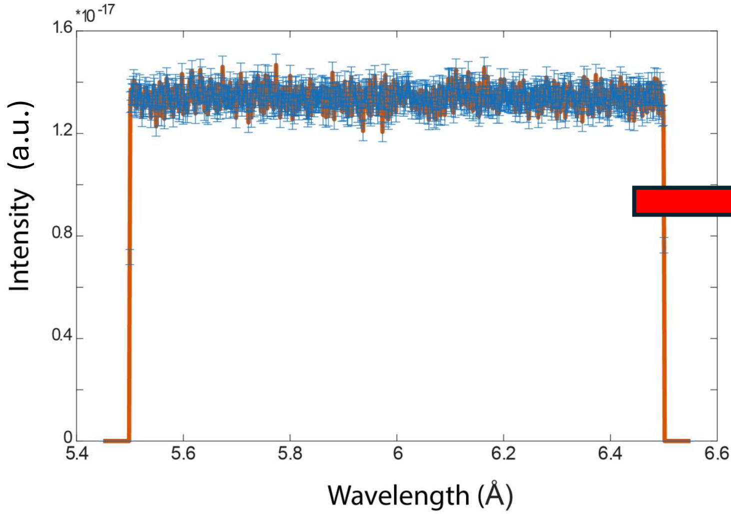


Multi Disk Choppers

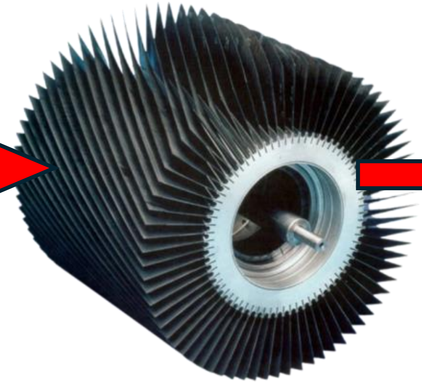


Instead of monochromating the beam, we use the disk choppers to modulate the wavelengths.

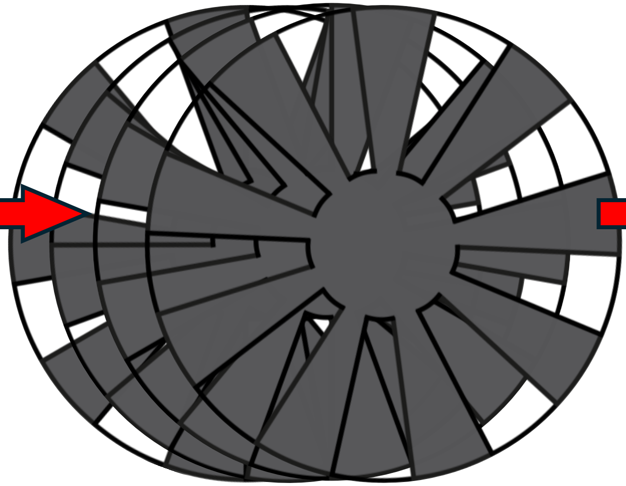
Initial Beam

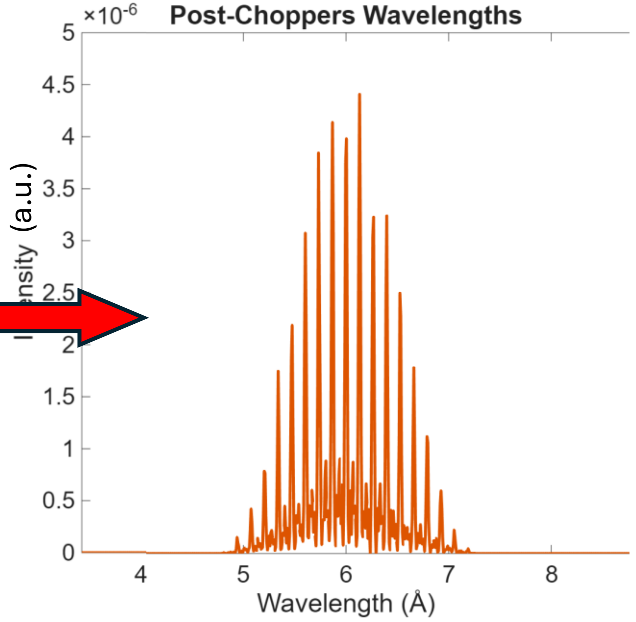


Velocity Selector



Intensity-Modulating Choppers

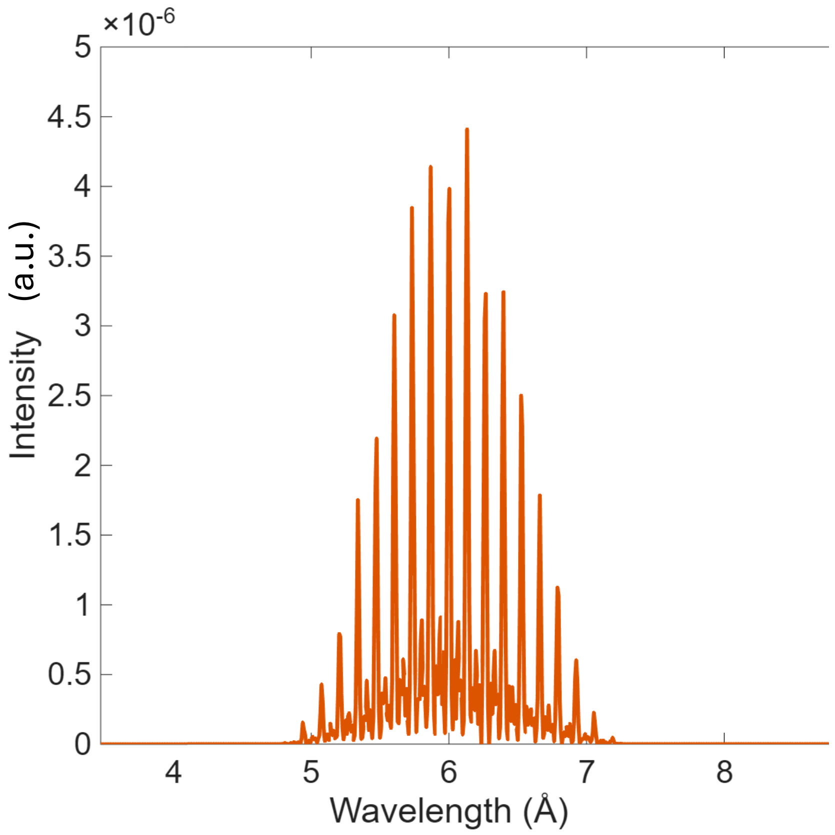




Multi Disk Choppers

More wavelengths → **more flux**!!

Modulated Beam



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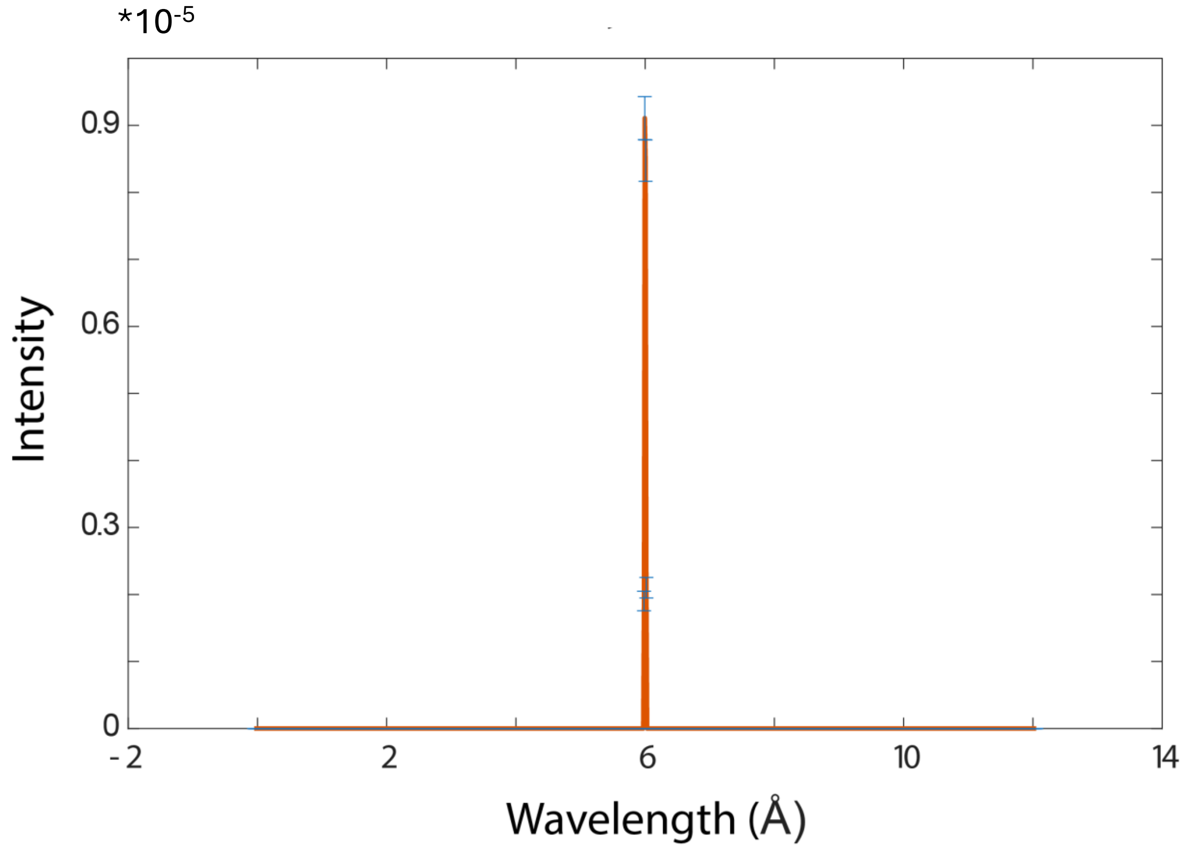
Monochromated Beam



Methodology

McStas

- Design/construct instrument
- Simulate instrument operation
- Output raw detector data (# counts)

MATLAB

- Import raw data
- Validate McStas functionality
- Extract I(Q,t), signal to noise, error bars
- Plot processed data

McStas

```
DEFINE INSTRUMENT Example(Param1=1, string Param2="two", ...)

COMPONENT A = Source(Parameters...)
AT (0, 0, 0) ABSOLUTE

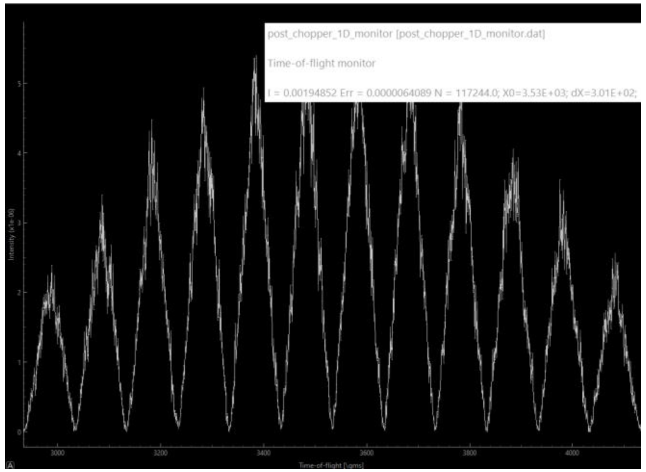
COMPONENT B = Guide(Parameters...)
AT (0, 0, 1) RELATIVE A

COMPONENT C = DiskChopper(Parameters...)
AT (0, 0, 1) RELATIVE B

COMPONENT D = TOF_monitor(Parameters, filename="Tof.dat")
AT (0, 0, Param1) RELATIVE PREVIOUS
```

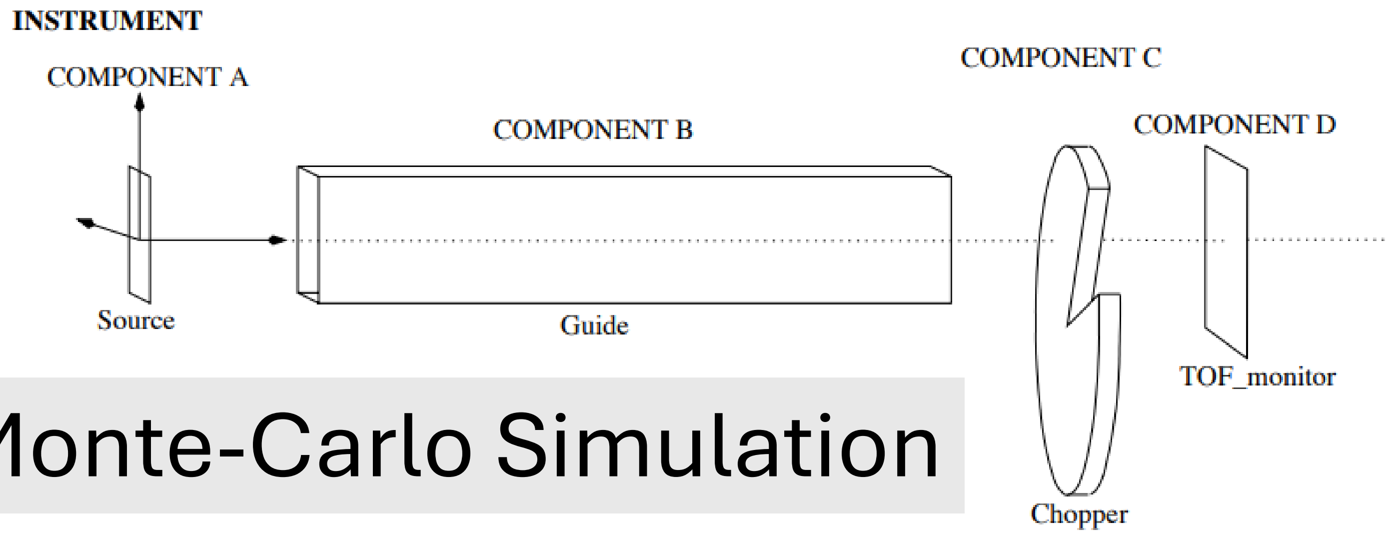
Code

Detector Data




```
File    Edit    View

# Format: McCode with text headers
# URL: http://www.mccode.org
# Creator: McStas 3.5.1 - Sep. 16, 2024
# Instrument: IMS_old.instr
# Ncount: 1000000
# Trace: no
# Gravitation: no
# Seed: 330562425
# Directory: C:\Users\nos\Downloads\1C_old\IMS_old_20250730_112119
# Param: detector_angle=45
# Param: chopper_period=100
# Param: sample_gamma=0
# Param: num_peirods=10
# Param: source_divergence=1e-007
# Param: source_lambda_d=1e-007
# Date: Wed Jul 30 11:21:21 2025 (1753888881)
# type: array_1d(1000)
# Source: IMS (IMS_old.instr)
# component: final_1D_monitor
# position: 1.0253 0 4.5253
# title: Time-of-flight monitor
# Ncount: 1000000
# filename: final_1D_monitor.dat
# statistics: X0=8001.74; dX=287.477;
# signal: Min=0; Max=3.79078e-031; Mean=1.44767e-031;
# values: 1.44767e-028 2.78499e-031 280587
# xvar: t
# yvar: (I,I_err)
# xlabel: Time-of-flight [\gms]
# ylabel: Intensity
# xlimits: 7483.35 8683.35
# variables: t I I_err N
7517.551408 2.749725063e-033 1.052309863e-033 7
7518.751408 1.551167098e-032 2.567503772e-033 41
7519.951408 3.05305467e-032 3.61357006e-033 78
7521.151408 5.809486828e-032 5.206276898e-033 137
7522.351408 8.235832239e-032 6.230491493e-033 190
7523.551408 1.181900492e-031 7.79414698e-033 246
7524.751408 1.337256592e-031 8.315109881e-033 279
7525.951408 1.735281828e-031 9.549325632e-033 348
```



Monte-Carlo Simulation

Matlab

Math!!

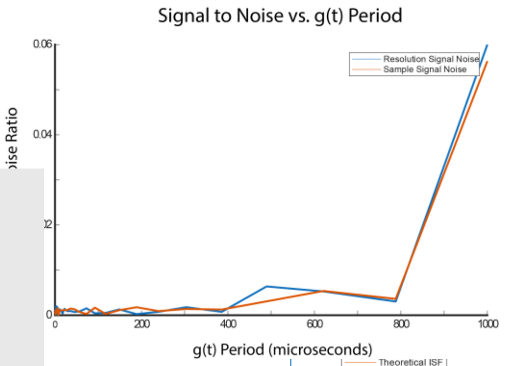
$$\frac{F(\boldsymbol{Q},t_F)}{S(\boldsymbol{Q})} = \frac{a_n^{sample}(\Omega)}{a_n^{res}(\Omega)}\frac{g_0^{res}(\Omega)}{g_0^{sample}(\Omega)} = \frac{b_n^{sample}(\Omega)}{b_n^{res}(\Omega)}\frac{g_0^{res}(\Omega)}{g_0^{sample}(\Omega)}$$

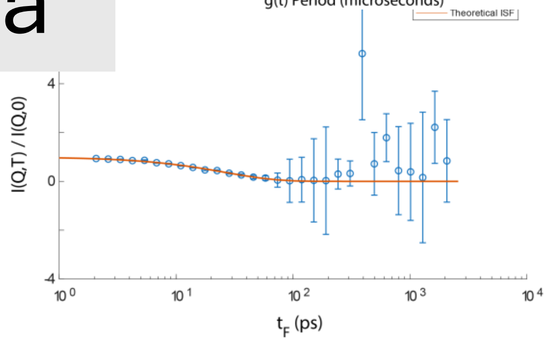
$$= \frac{g_0^{res}(\Omega)}{g_0^{sample}(\Omega)}\frac{\int_0^T I_D^{sample}(\Omega,t)\cos\left(2\pi\frac{n}{T}t\right)dt}{\int_0^T I_D^{res}(\Omega,t)\cos\left(2\pi\frac{n}{T}t\right)dt}$$

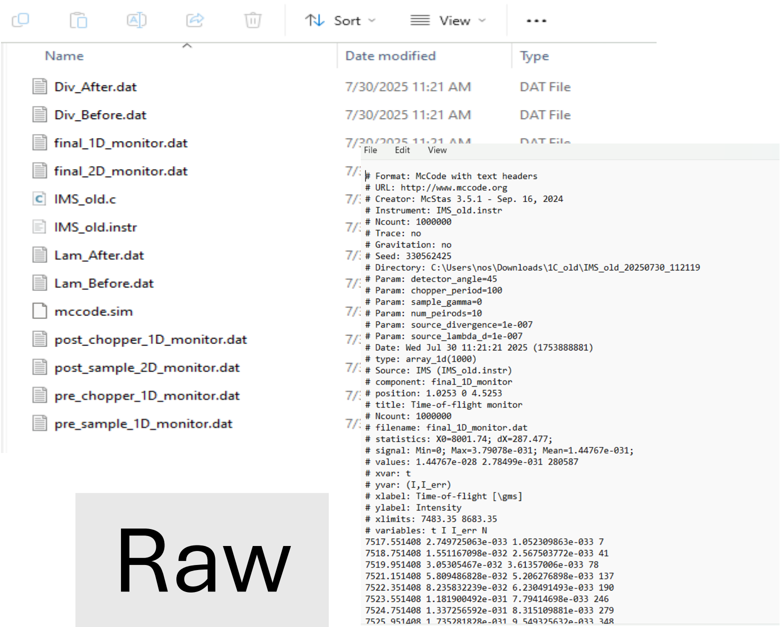
$$= \frac{g_0^{res}(\Omega)}{g_0^{sample}(\Omega)}\frac{\int_0^T I_D^{sample}(\Omega,t)\sin\left(2\pi\frac{n}{T}t\right)dt}{\int_0^T I_D^{res}(\Omega,t)\sin\left(2\pi\frac{n}{T}t\right)dt}$$

$$= \frac{g_0^{res}(\Omega)}{g_0^{sample}(\Omega)}\frac{\sqrt{[a_n^{sample}(\Omega)]^2+[b_n^{sample}(\Omega)]^2}}{\sqrt{[a_n^{res}(\Omega)]^2+[b_n^{res}(\Omega)]^2}}$$

Final Data





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7519.951408 3.05305467e-032 3.61357006e-033 78
7521.151408 5.809486828e-032 5.206276898e-033 137
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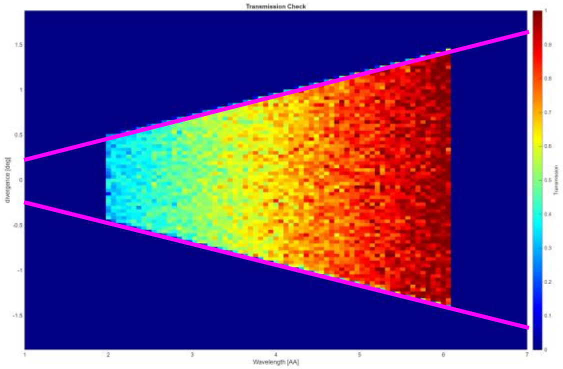
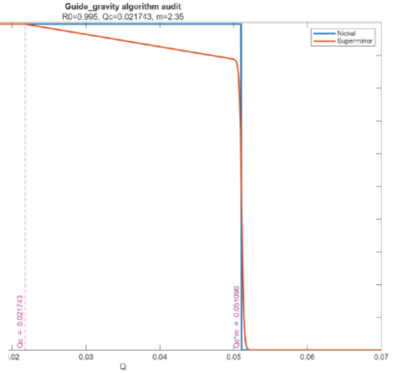
7524.751408 1.337256592e-031 8.315109881e-033 279
7525.951408 1.735281828e-031 9.549325632e-033 348
```

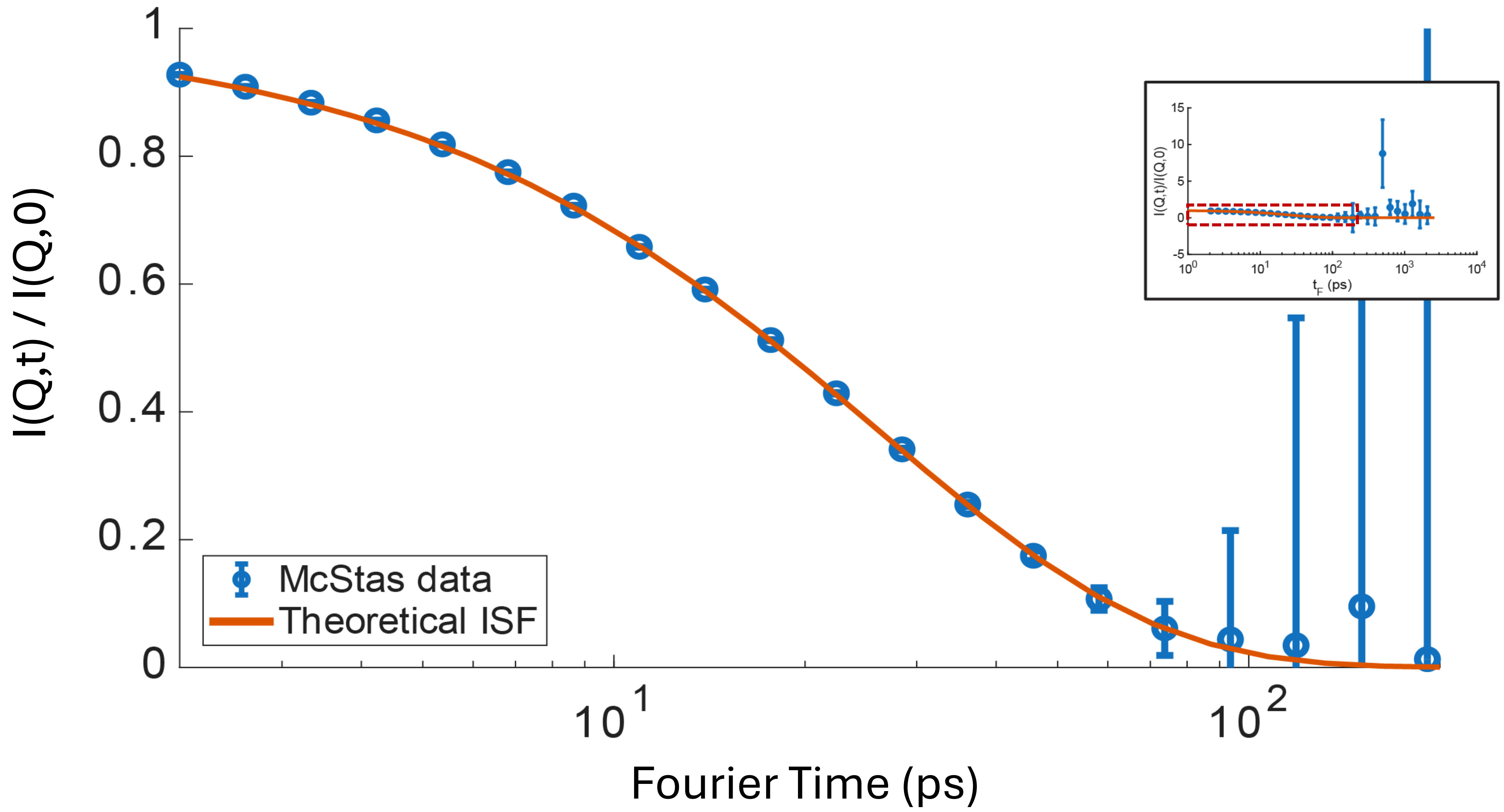
Raw Data

McStas Validation





1 Chopper, monochromatic
Normalized ISF vs. Fourier Time



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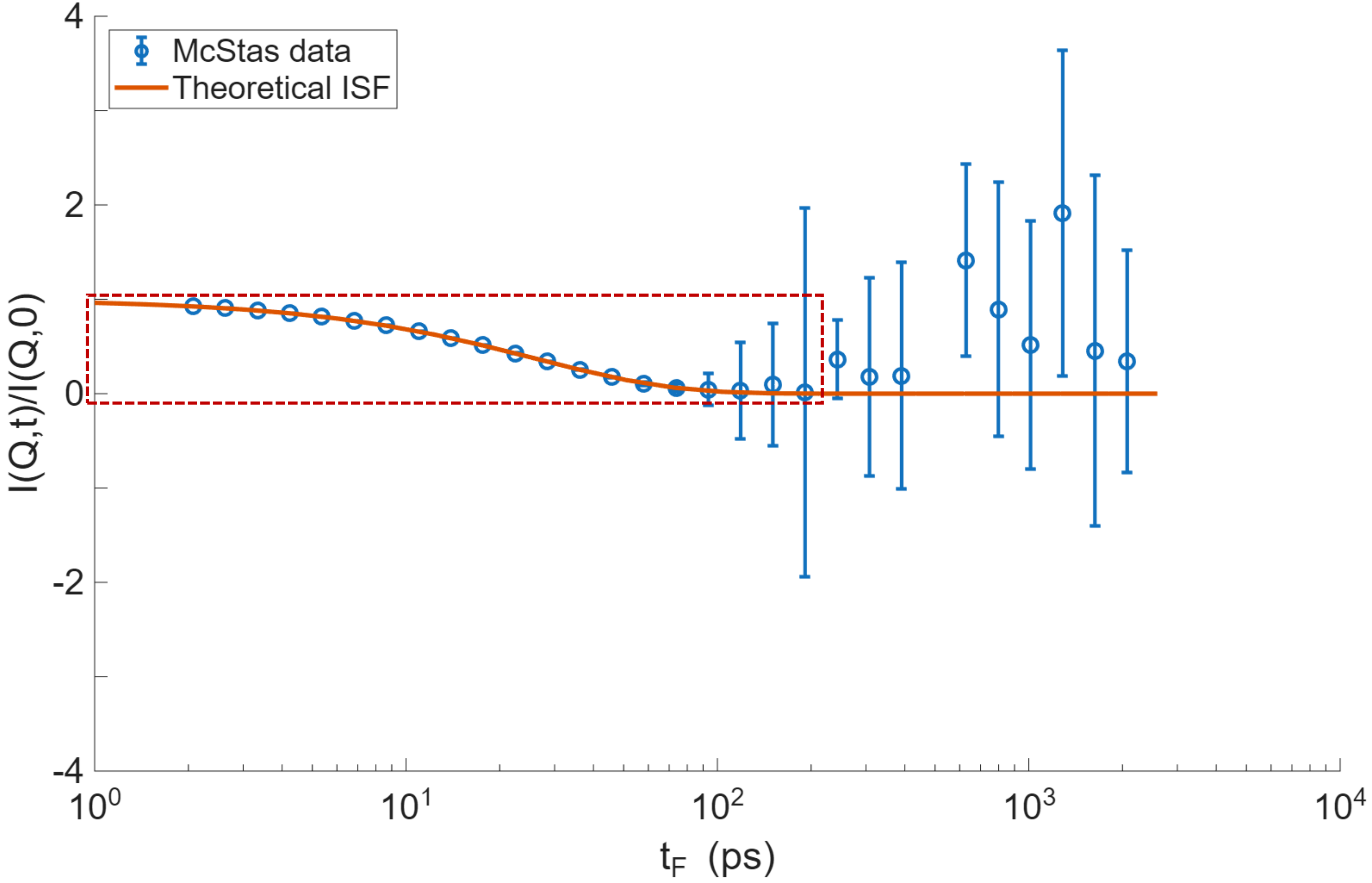
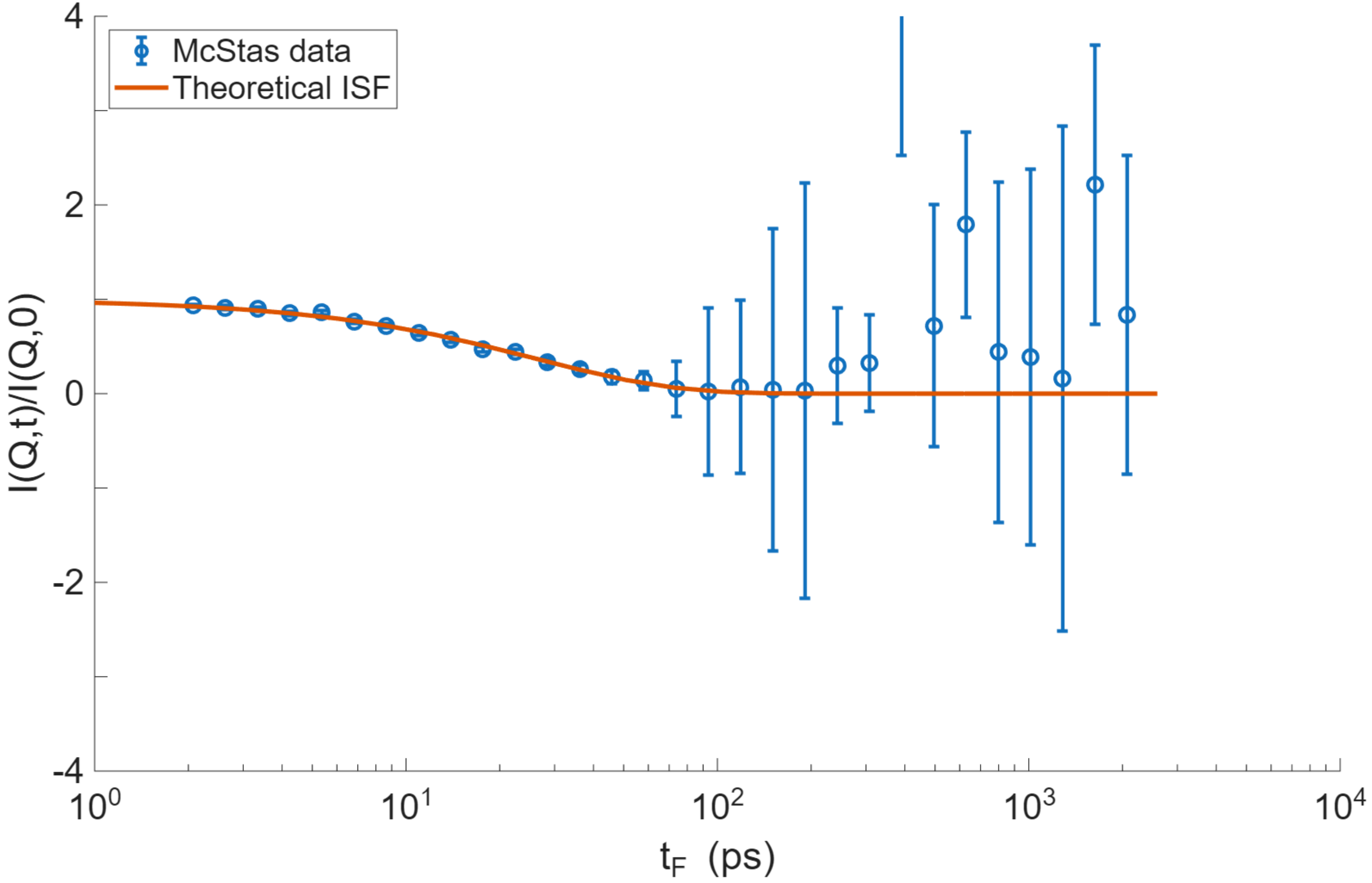
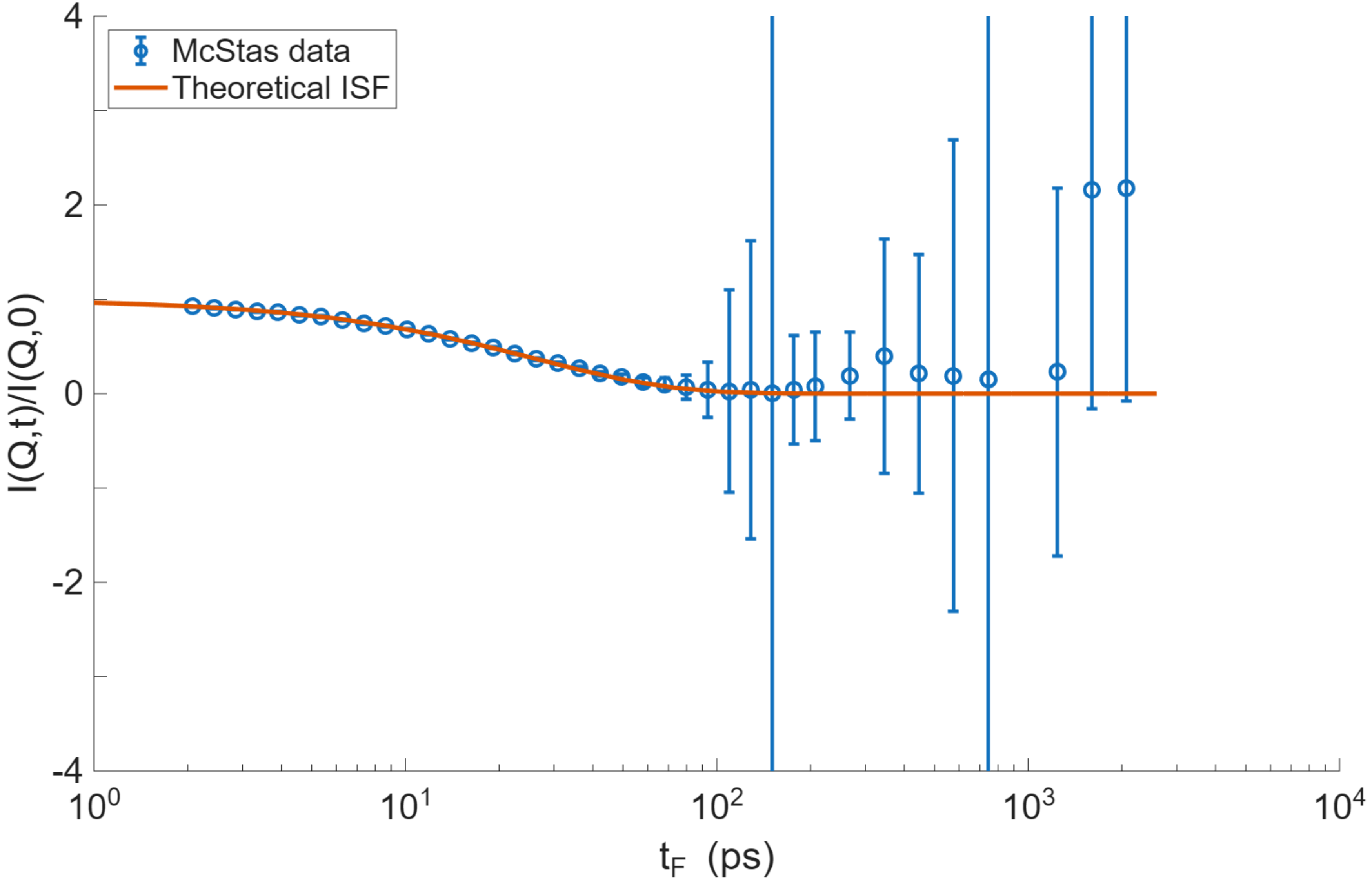
Normalized ISF vs. Fourier Time



3 Choppers, polychromatic
Normalized ISF vs. Fourier Time

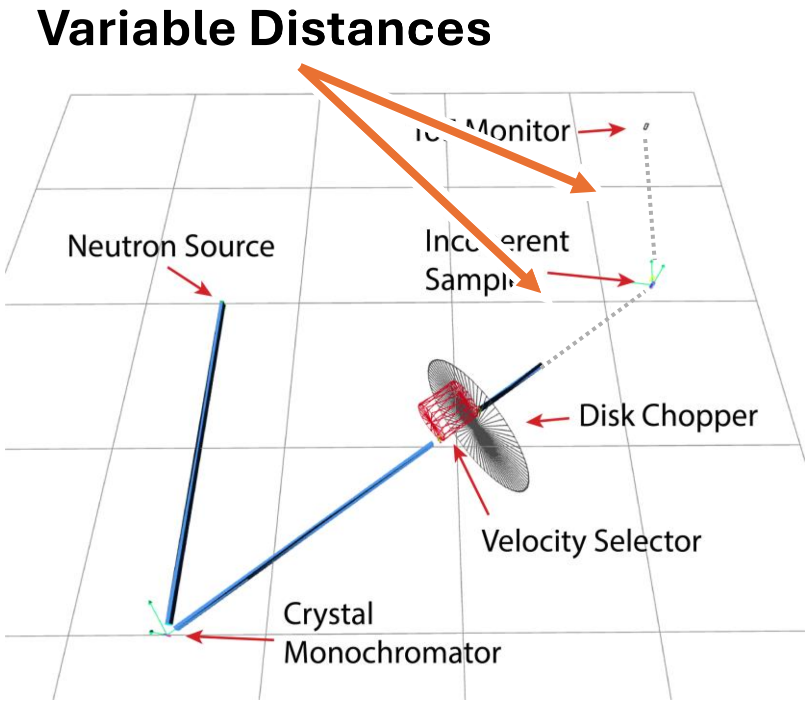


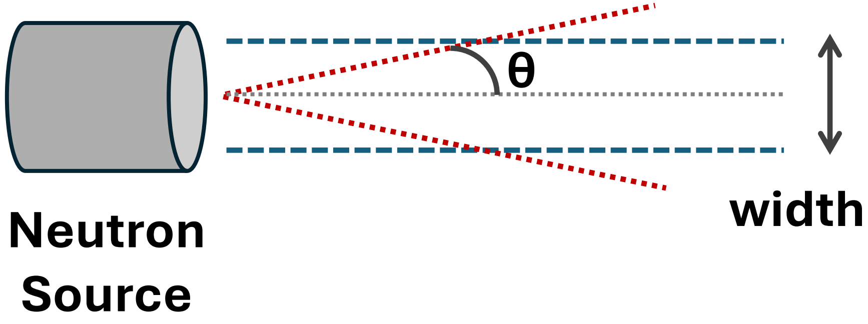
5 Choppers, polychromatic
Normalized ISF vs. Fourier Time



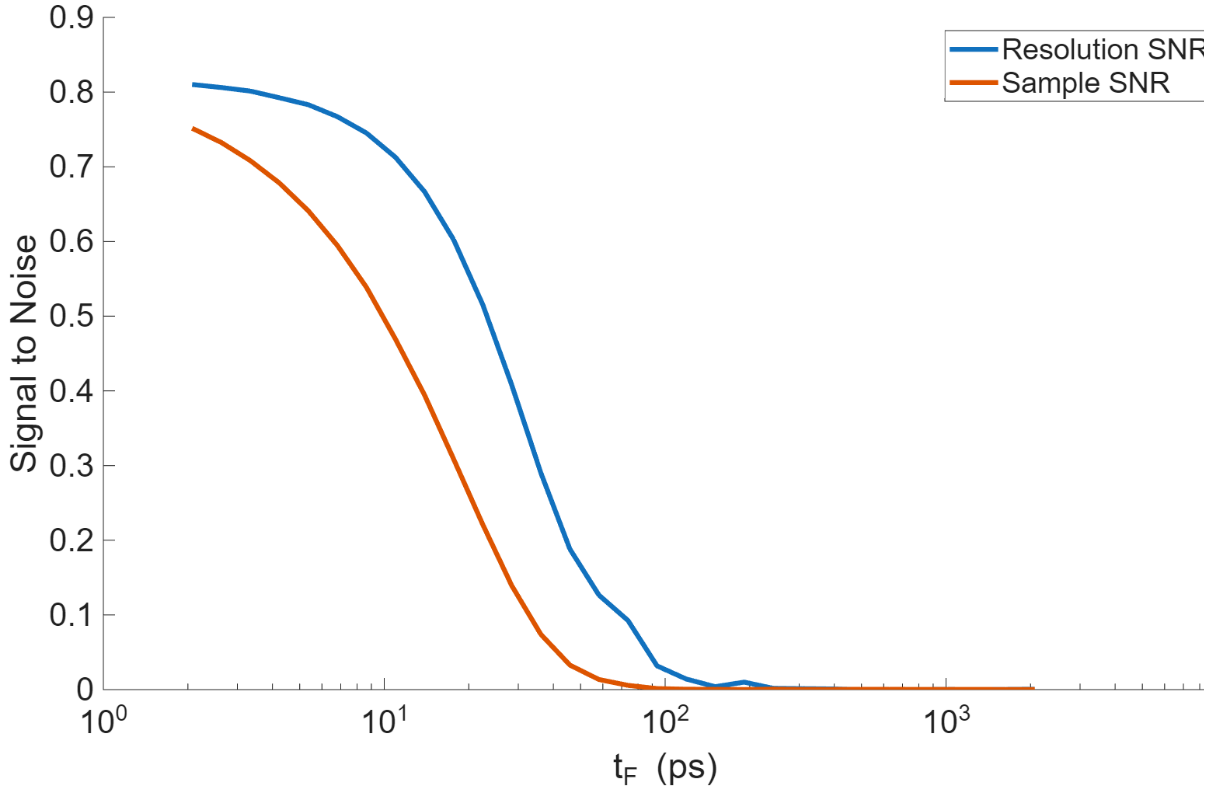
Next Steps

- Optimize instrument parameters
  - Distances between components
  - Sample / beam sizes
  - Divergence
  - Δλ/λ (incident wavelength spread)
- Figure out Signal to Noise ratio

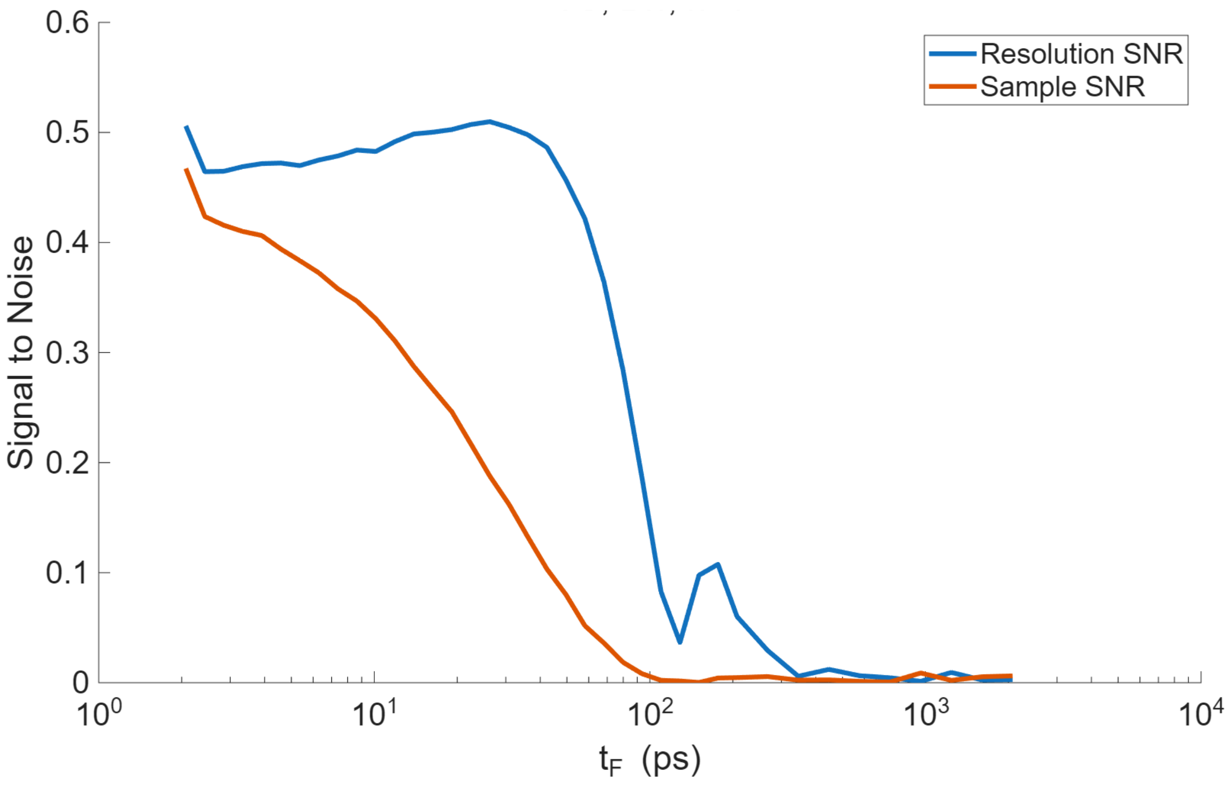




Signal to Noise Ratio vs. Fourier Time



1-Chopper Setup



5-Chopper Setup

Special Thanks!

Mentors: **Leland Harriger, Antonio Faraone**

SHIP Directors: **Julie Borchers, Leland Harriger**

NIST, NCNR, SHIP, CHRNS

CENTER FOR NEUTRON RESEARCH

CHRNS CENTER FOR HIGH RESOLUTION NEUTRON SCATTERING

Image References

Center for High Resolution Neutron Scattering | NIST. (2017, April 25). NIST. https://www.nist.gov/ncnr/chrns

Zhao, K., Zhang, P., Xue, S., Han, S., Müller, H. S., Xiao, Y., Hu, Y., Hao, L., Mei, L., & Li, Q. (2021). Quasi-elastic neutron scattering (QENS) and its application for investigating the hydration of cement-based materials: State-of-the-art. *Materials Characterization*, *172*, 110890. https://doi.org/10.1016/j.matchar.2021.110890

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