

Dynamic magnetic pair-density function (DymPDF) analysis

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Collaborators

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μ SR: Takashi U. Ito, Wataru Higemoto (JAEA)), Yasutomo Uemura (Columbia Univ.)

X-ray: Satoshi Tsutsui, Hiroshi Fukui, Taiushun Manjo (JASRI), Alfred Q.R. Baron (RIKEN)

Supercomputer FUGAKU: Kanako Yoshizawa, Yasuhiro Sunaga, Daisuke Matsuoka, Satoru Asami (RIST)

Samples: Yukio Yasui (Meiji Univ.), Jose Antonio Alonso (CSIC, ICMM)

Acknowledgments

Grants-in-Aid for Scientific Research (C) (**25K08263**, **22K04678**, 21K03478, and 19K12648) from the Japan Society for the Promotion of Science. Proposals 2024C0001(BL01), 2024A0053(S1), 2021C0001(BL01), 2020A0052 (BL01) (J-PARC), 2024A1156 (60524, BL35XU@SPRING-8). The samples were characterized using a magnetic properties measurement system at the CROSS user laboratory II.

Outline



1. Introduction

Fourier transform analysis of neutron scattering data

Pair Distribution Function (PDF)

Magnetic Pair Distribution Function (mPDF)

Dynamic Pair Density Function (DyPDF)

2. Dynamic magnetic Pair Density Function (DymPDF)

3. How to get DymPDF by 'Utsusemi'

4. How to simulate DymPDF by 'SpinW' and 'Utsusemi'

5. Summary



1. Introduction

Recent history of the Fourier transform analysis on neutron scattering

1990
Crystalline PDF

T. Egami,
Mater. Trans.
JIM **31**, 163–
176 (1990).

IPNS,
ANL
USA

1992
DyPDF

A. C. Hannon,
M. Arai, *et al.*,
J. Non-Cryst.
Solids
150, 239
(1992).

ISIS, RAL
UK

2014
mPDF

B. A. Frandsen,
X. Yang, S. J. L.
Billinge, *Acta*
Crystallogr.
Sect. A **70**, 3
(2014).

ILL
France

2022
DymPDF

K. Iida, K. Kodama, Y. Inamura,
M. Nakamura, L.-J. Chang,
S. Shamoto
Scientific Reports **12**: 20663
(2022).

J-PARC MLF
Japan

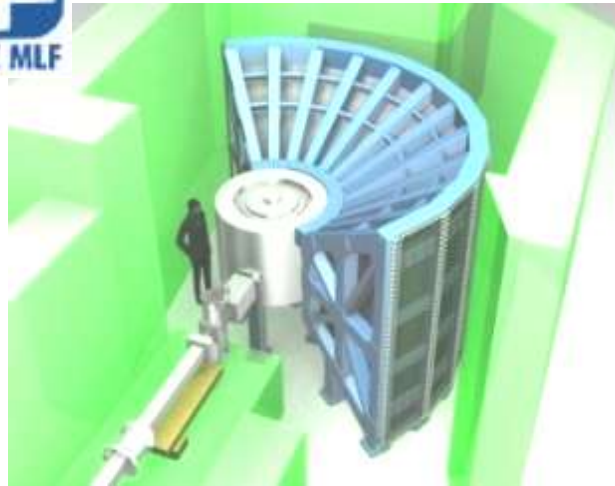
PDF : Pair Distribution (Density) Function

J-PARC : Japan Proton Accelerator Research Complex

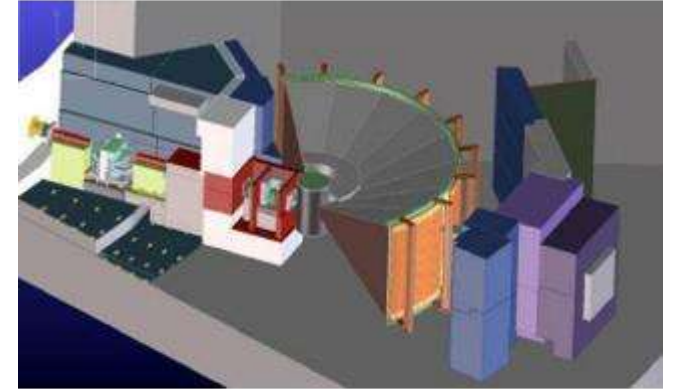
- Materials & Life Science Experimental Facility (MLF)



3



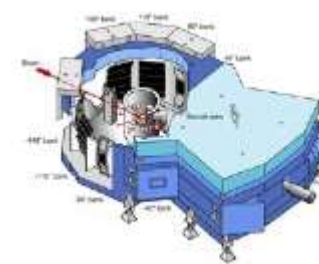
4SEASONS(BL01):
S/N=43.8



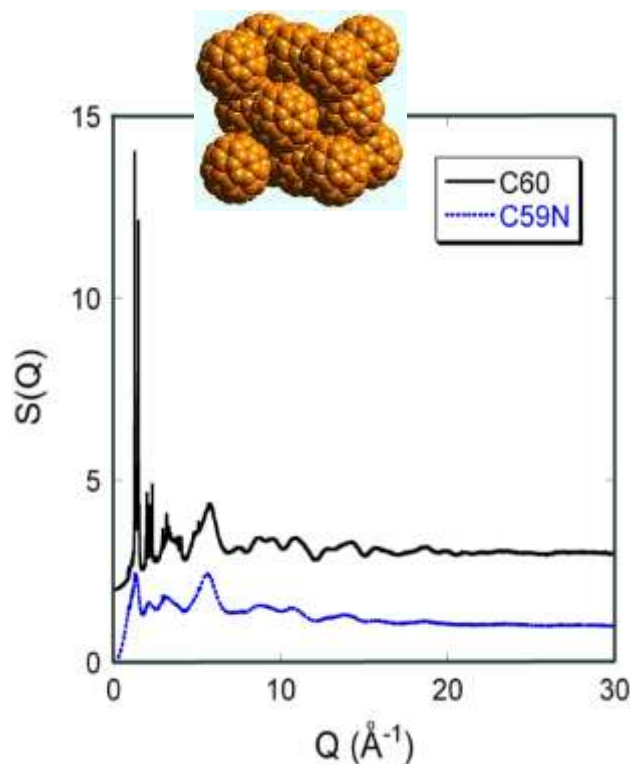
HRC(BL12):

Pair Distribution Function (PDF)

C60 Fullerene,
C59N Azafullerene



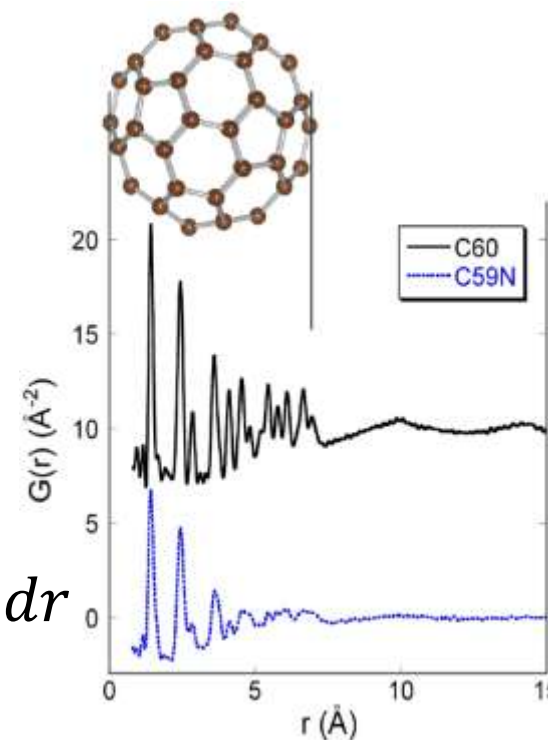
NPDF@Los Alamos



Fourier transform



$$G(r) = \frac{2}{\pi} \int_0^{\infty} Q[S(Q) - 1] \sin(Qr) dr$$



Scattering function

Atomic pair distribution function (PDF)

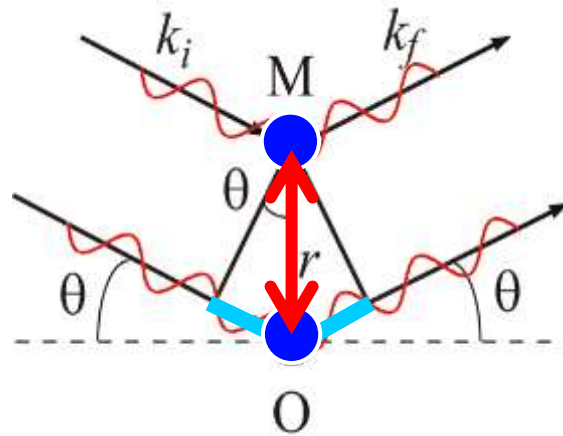
S. Shamoto, J. Phys. Soc. Jpn. **88**, 081008 (2019).

Pair Distribution Function (PDF)

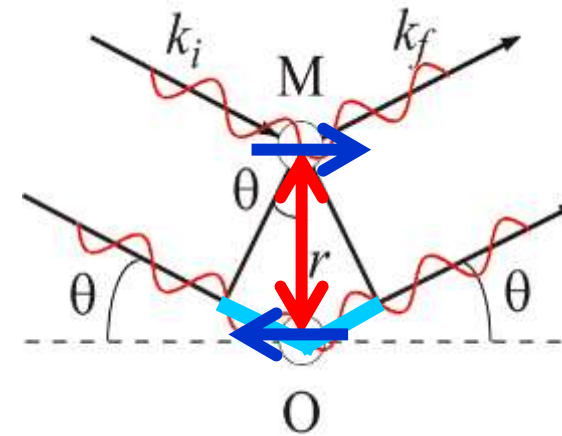
Elastic scattering by two atoms (O and M)

Sum of phase difference : $(k_f - k_i) \cdot r$

Bragg condition $(k_f - k_i) \cdot r = 2\pi n$



Atomic pair correlation



Spin pair correlation

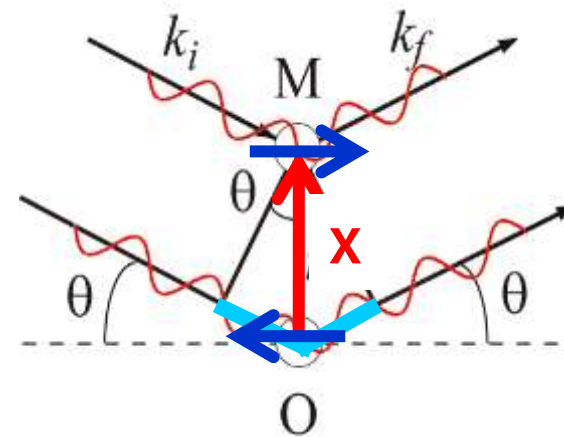
mPDF analysis

$$f(r) = \frac{2}{\pi} \int_0^\infty Q \left[\frac{I_m}{\frac{2}{3} N_s S(S+1) (\gamma r_0)^2 f_m^2(Q)} - 1 \right] \sin Qr \, dQ \quad (1)$$

$$= \frac{1}{N_s} \frac{3}{2S(S+1)} \sum_{i \neq j} \left[\frac{A_{ij}}{r} \delta(r - r_{ij}) + B_{ij} \frac{r}{r_{ij}^3} \Theta(r_{ij} - r) \right], \quad (2)$$

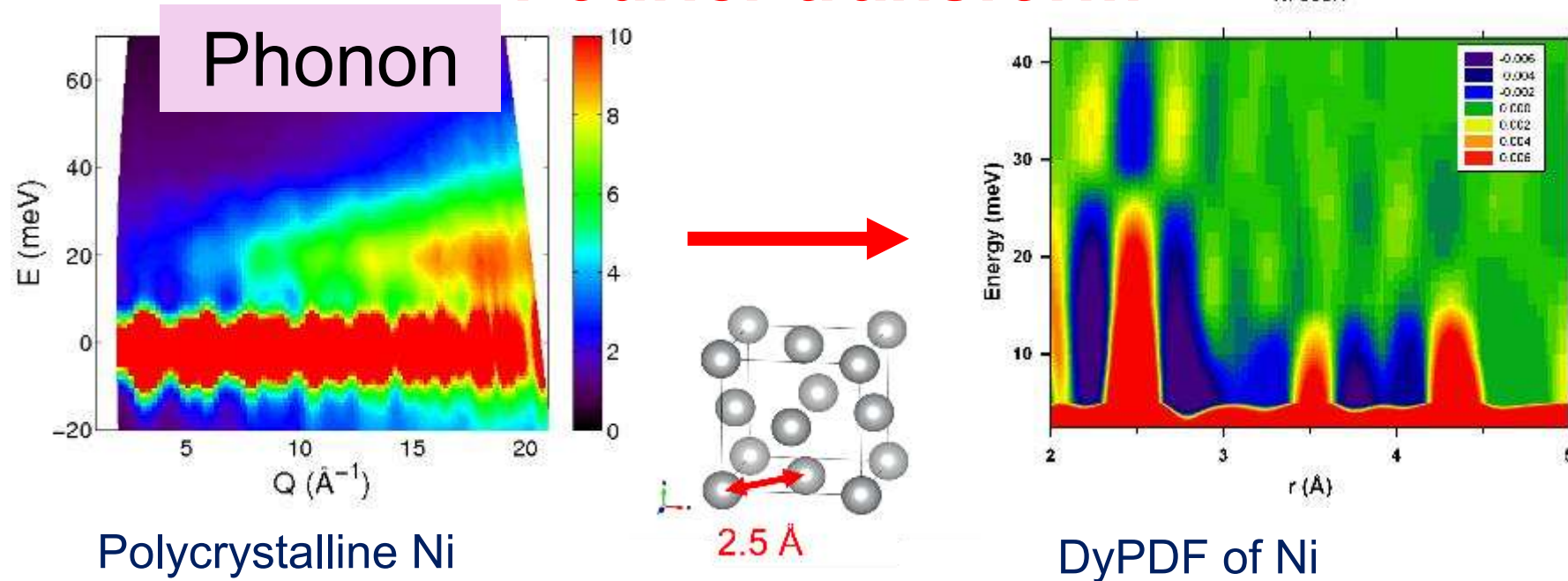
$$A_{ij} = \langle S_i^y \tilde{S}_j^y \rangle, \quad B_{ij} = 2 \langle S_i^x S_j^x \rangle - \langle S_i^y S_j^y \rangle$$

$$\hat{\mathbf{x}} = \frac{\mathbf{r}_j - \mathbf{r}_i}{|\mathbf{r}_j - \mathbf{r}_i|} \quad \hat{\mathbf{y}} = \frac{\mathbf{S}_i - \hat{\mathbf{x}}(\mathbf{S}_i \cdot \hat{\mathbf{x}})}{|\mathbf{S}_i - \hat{\mathbf{x}}(\mathbf{S}_i \cdot \hat{\mathbf{x}})|}$$



Dynamic Pair Density Function (DyPDF)

Fourier transform



Alex C. Hannon, Masatoshi Arai,
Roger N. Sinclair, Adrian C. Wright,
"A dynamic correlation function for
amorphous solids", Journal of Non-
Crystalline Solids, 150, 239 (1992)

Wojtek Dmowski et al. "Local
lattice dynamics and the origin of
the relaxor ferroelectric material."
Phys. Rev. Lett. 100, 137602
(2021).

Lattice component of the dynamic structure factor

$$\frac{S_L(Q, E)}{\langle 1 + n(E) \rangle} - 1 = \frac{(k_i/k_f)I(Q, E) - S_S(Q, E) - A_0}{S_S(Q, E)}$$

$$S_S(Q, E) = BQ^2 \exp(-Q^2 \langle u^2 \rangle / 3) \frac{\langle 1 + n(E) \rangle}{E}$$

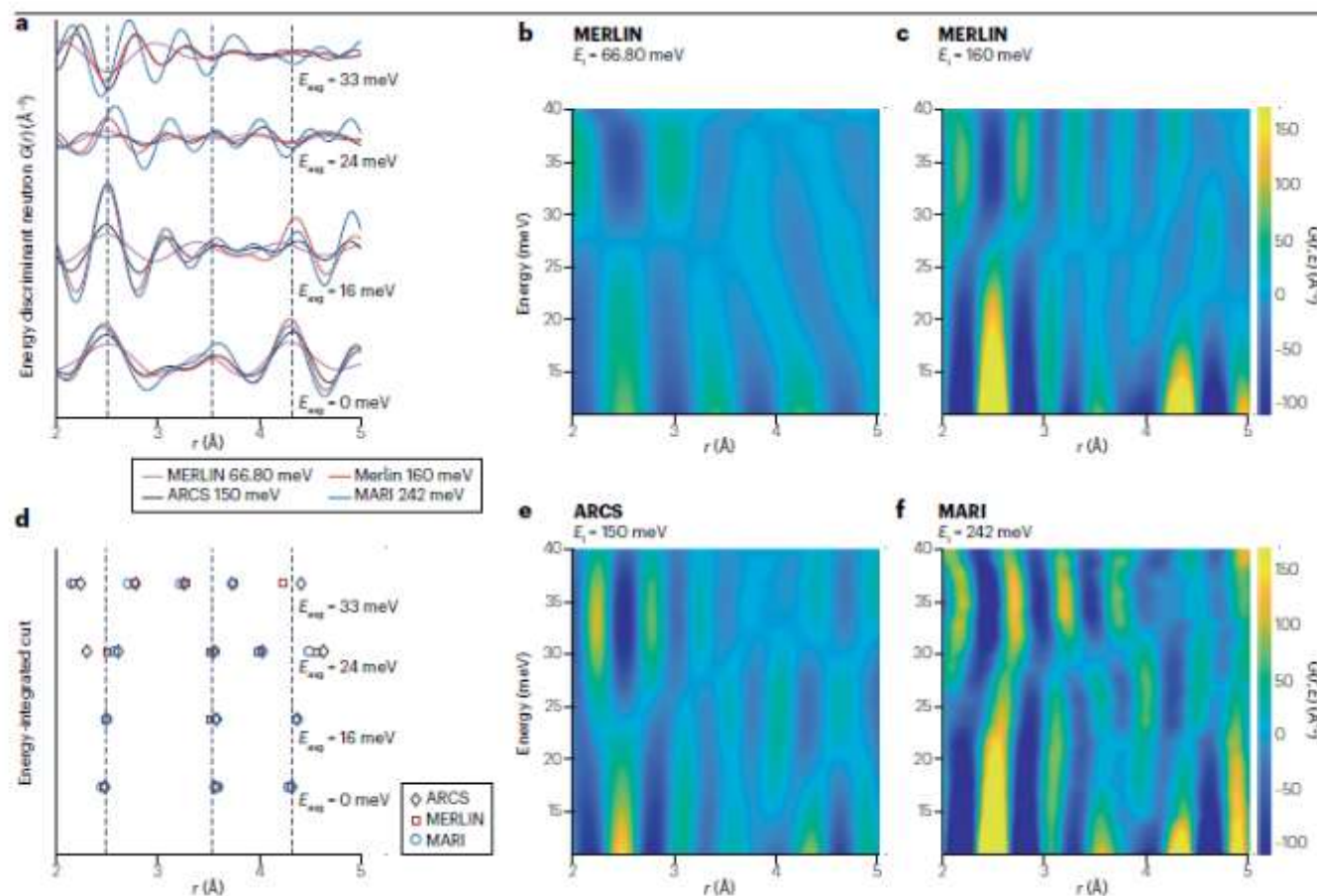
Alex C. Hannon, M. Arai et al., J. Non-Cryst. Solids 150, 239 (1992).

Lattice component of the dynamic pair-density function

$$D_L(r, E) = \frac{2}{\pi} \int_{Q_{min}}^{Q_{max}} Q \left[\frac{S_L(Q, E)}{\langle 1 + n(E) \rangle} - 1 \right] w(Q) \sin(Qr) dQ$$

Window function $w(Q) = \frac{Q_{max}}{\pi Q} \sin\left(\frac{\pi Q}{Q_{max}}\right)$

DyPDF, $D(r,E)$



Optimizing the dynamic pair distribution function method for inelastic neutron spectrometry

Kody A. Acosta, Helen C. Walker & Allyson M. Fry-Petit

Nature Reviews Physics **5**, 236–249 (2023). (Technical review)

<https://doi.org/10.1038/s42254-023-00564-5>

2. Dynamic magnetic Pair Density Function (DymPDF)

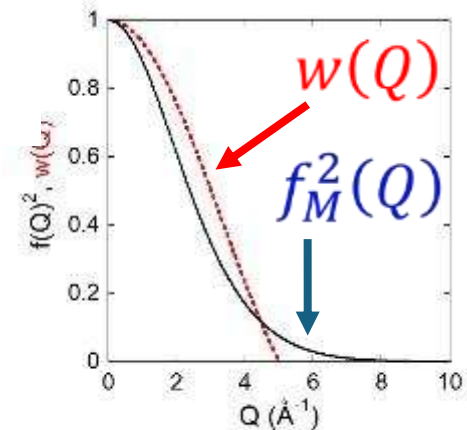
Magnetic component of the dynamic structure factor

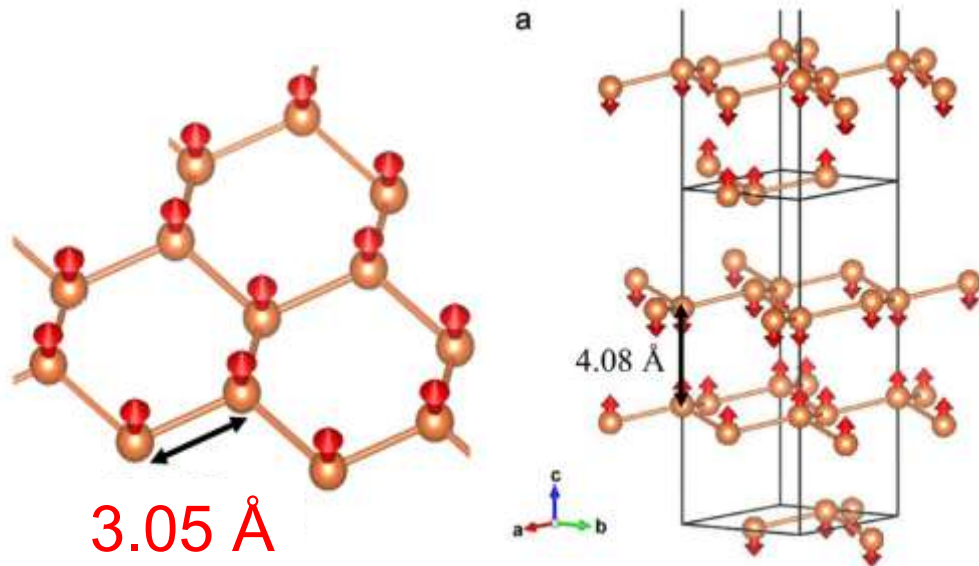
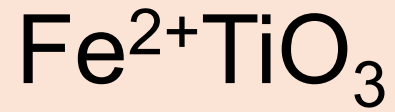
$$\frac{S_M(Q, E)}{\langle 1 + n(E) \rangle} - 1 = \frac{(k_i/k_f)I(Q, E) - A(Q - Q_{max})(Q + Q_{max}) - A_0}{\frac{2}{3} N_m g^2 S(S + 1) (\gamma r_0)^2 \langle 1 + n(E) \rangle f_M^2(Q)}$$

Magnetic component of the dynamic pair-density function

$$D_M(r, E) = \frac{2}{\pi} \int_{Q_{min}}^{Q_{max}} Q \left[\frac{S_M(Q, E)}{\langle 1 + n(E) \rangle} - 1 \right] w(Q) \sin(Qr) dQ$$

Window function $w(Q) = \frac{Q_{max}}{\pi Q} \sin\left(\frac{\pi Q}{Q_{max}}\right)$

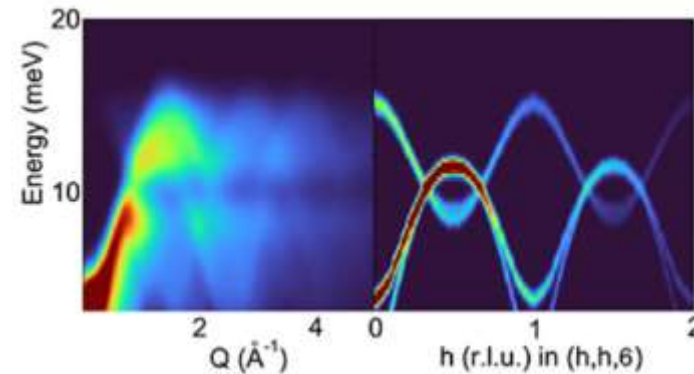




Crystal structure

$T_N = 59 \text{ K}$

**Spin-wave dispersion
(SpinW)**



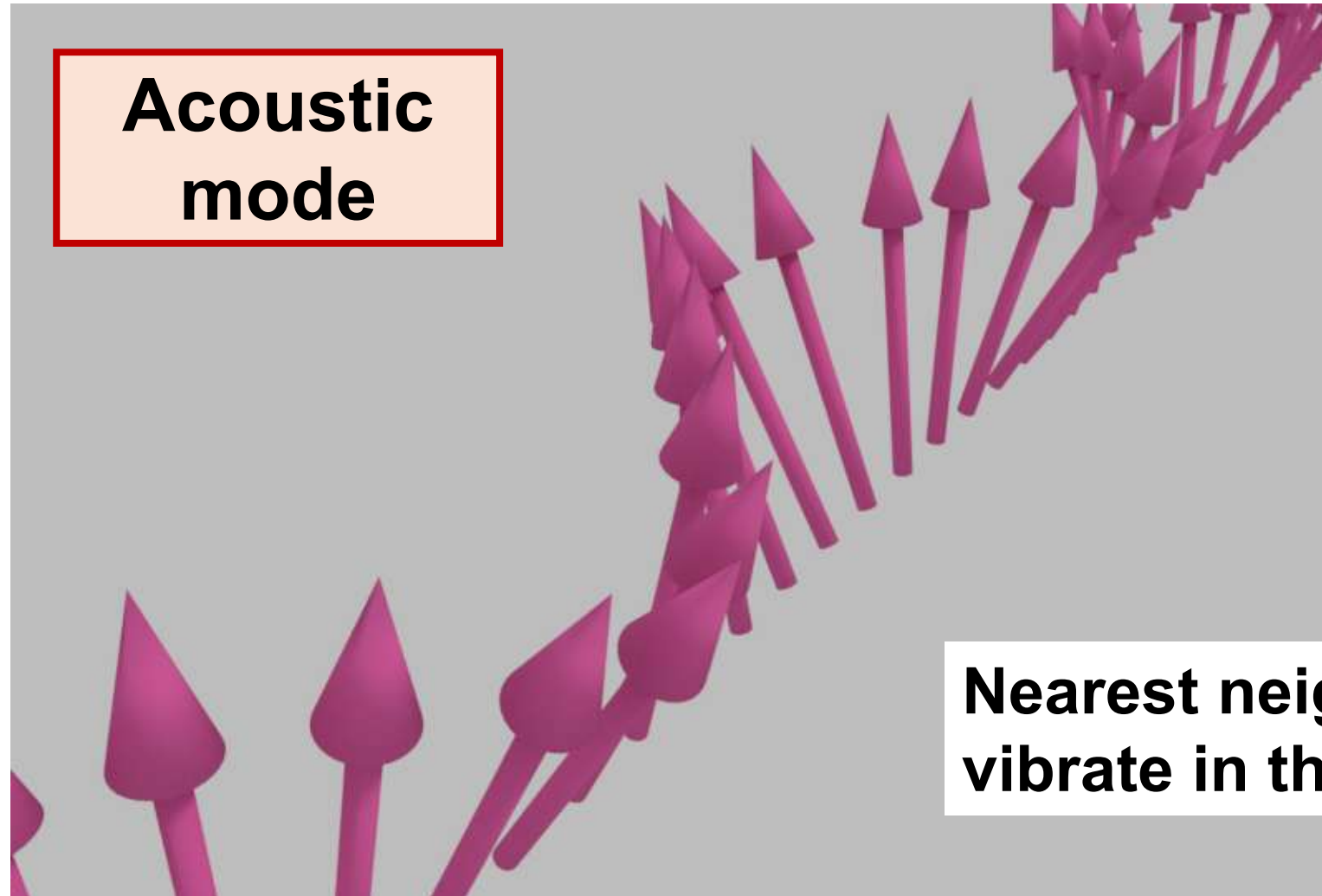
**Powder
average**

**Spin-wave
dispersion**

Spin

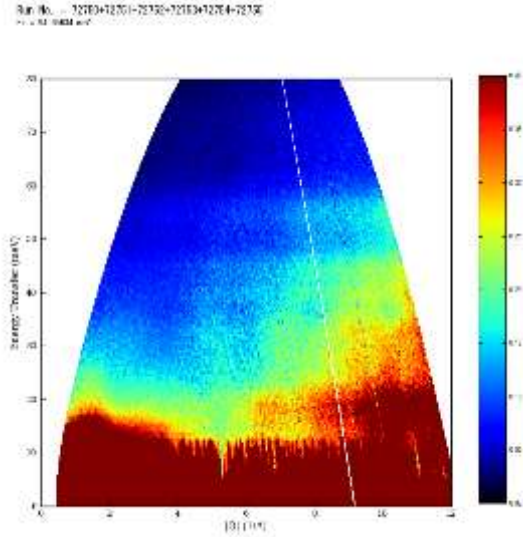
H. Kato, Y. Yamauchi et al., *J. Phys. C: Solid State Phys.* **19**, 6993 (1986).
S. Toth, and B. Lake, *J. Phys.: Condens. Matter* **27**, 166002 (2015).

Classical limit of spin dynamics

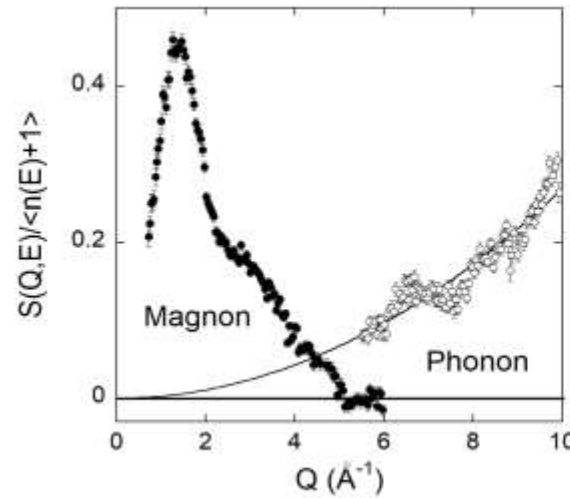


https://staff.aist.go.jp/v.zayets/spin3_68_heat.html

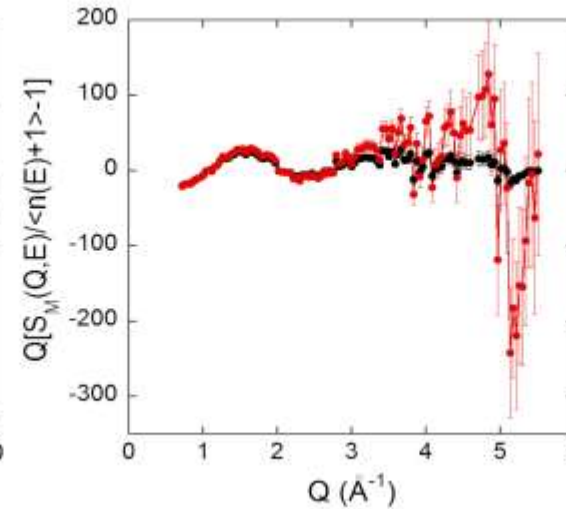
Separation of magnon from phonon



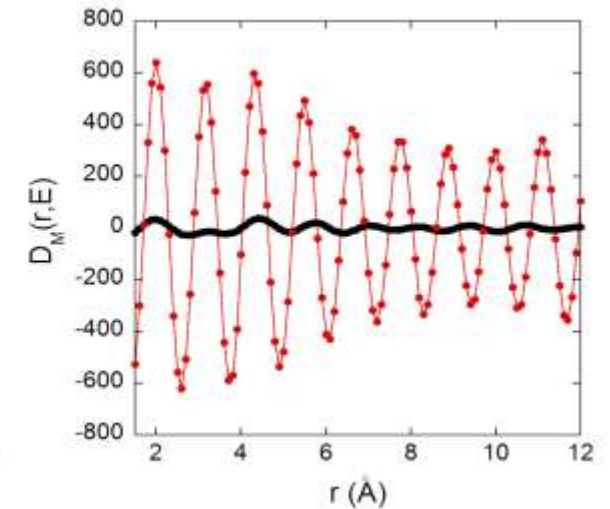
$$E_i = 95 \text{ meV}$$



$$E = 15 \text{ meV}$$



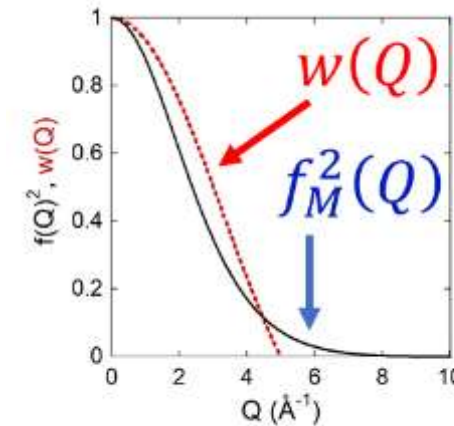
DymPDF



Hints:

$$\text{Fe}^{2+} gS = 4 \mu_B$$

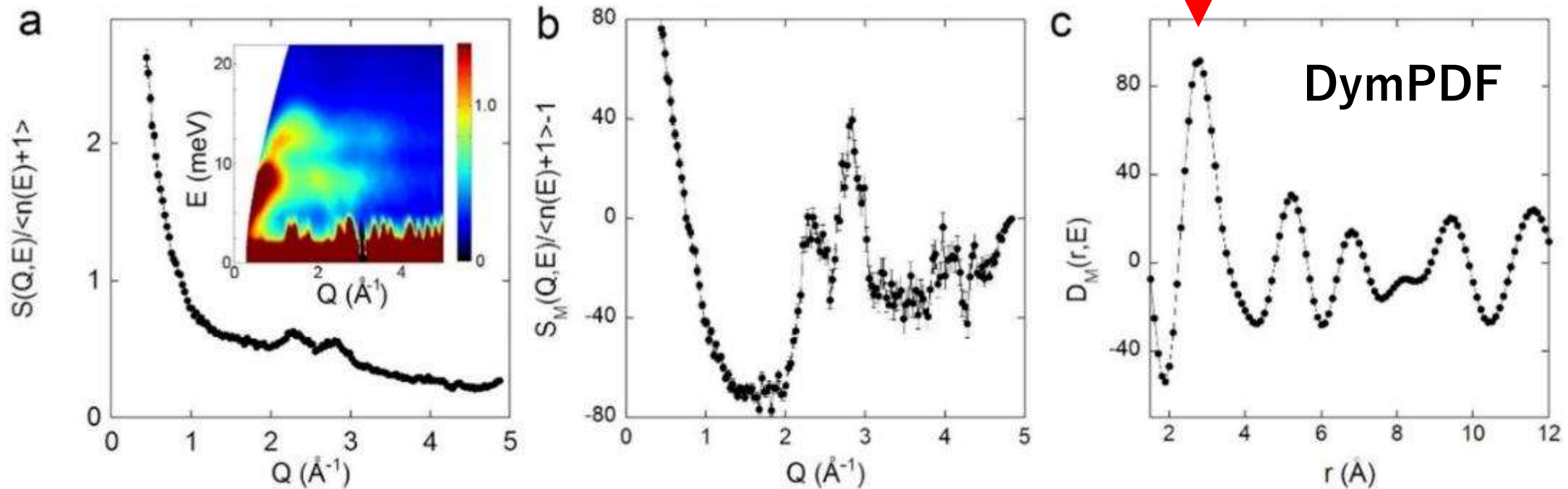
Fe	$b_c = 9.45 \text{ barn}$
Ti	$b_c = -3.37 \text{ barn}$
3O	$b_c = 5.805 \text{ barn}$



Window Function

Data Calculation Process of DymPDF

sliced at $E = 6$ meV ($T = 8$ K)
 $E_i = 46$ meV



$\times Q \rightarrow$ Fourier transform

Dynamic magnetic Structure Factor to DymPDF

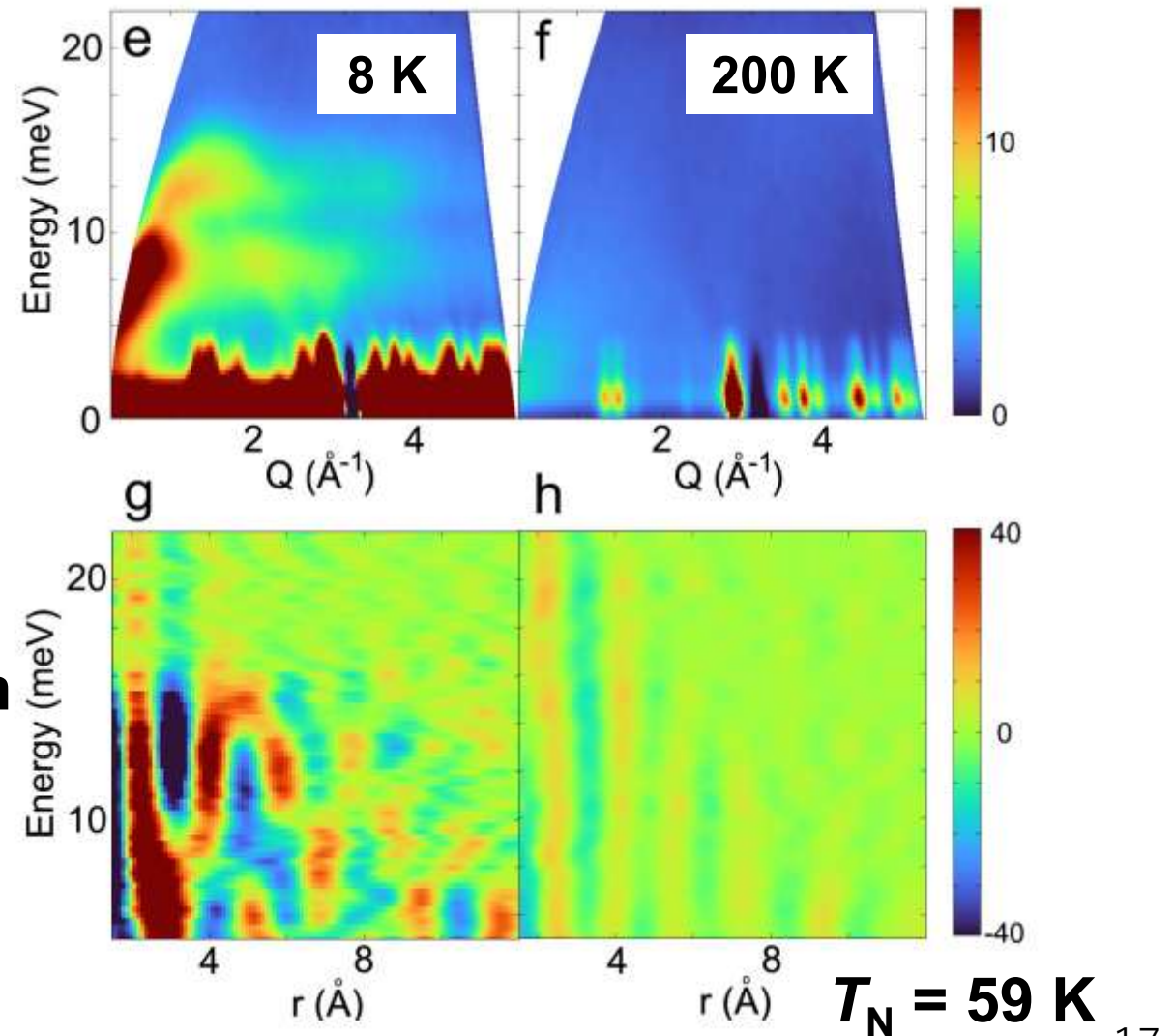
Dynamic magnetic Structure Factor



Fourier
transform

Dynamic magnetic Pair-Density Function
(DymPDF)

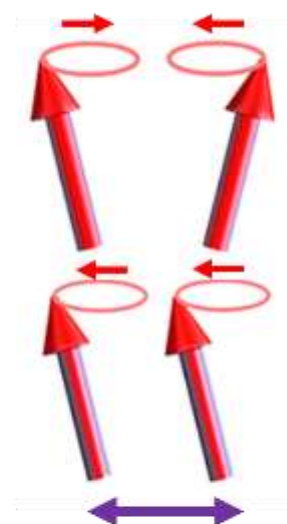
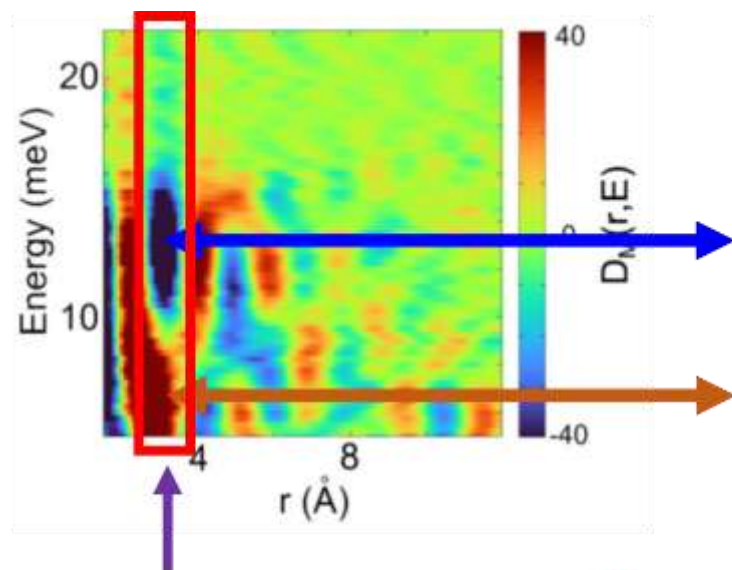
$\text{FeTiO}_3 : D_M(r, E)$



Observation of two spin fluctuation modes



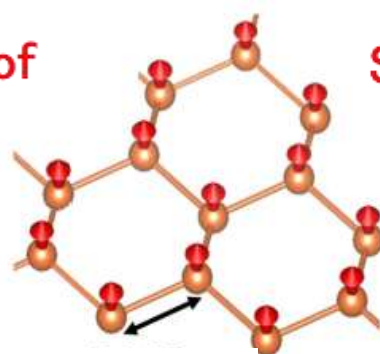
BL01
4SEASONS



Optical
mode

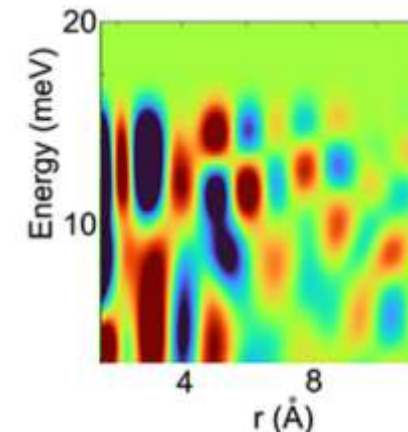
Acoustic
mode

Spin distance of
3.05 Å



3.05 Å

Spin distance of
3.05 Å



Simulation
(SpinW+Utsusemi)



3. How to get DymPDF by 'Utsusemi'



The screenshot shows the Utsusemi Portal Site, a web interface for neutron scattering. At the top, there's a header for 'J-PARC MLF' with the tagline 'Next to Meet@MLF'. A navigation bar includes links for 'Instruments', 'User Programs', 'Operation', 'Access', and 'Local Information'. A search bar is also present. Below the header, a pink banner reads 'Sample Shipment Before You Arrive'. The main content area features a 'Table of Contents' on the left with links to 'Utsusemi Portal Site', 'Installations', 'Documentations', 'Licence', 'Contact person', 'About Utsusemi', 'What Utsusemi can do', 'Many Beam Lines introduce Utsusemi', 'Developments', 'Origin of the name Utsusemi', and 'References'. The main content area has a large banner with the text '空蟬 UTSUSEMI FOR NEUTRON SCATTERING' and a cartoon character. Below the banner, the title 'Utsusemi Portal Site' is followed by a 'What's New' section listing updates: '2025.10.6 Update Installers' and '2025.7.22 Update Installers'. The 'Installations' section provides information about the installation and download of required files, with a link to the 'Portal for Utsusemi installation (Outer site)'. The 'Documentations' section is also visible.

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- Documentations
- Licence
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- About Utsusemi
 - What Utsusemi can do
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 - Origin of the name Utsusemi
 - References

Proposal Application

- Proposal Application
- Proposal Review Process

Instruments

- Neutron + Muon Sources
- Instruments
 - List of Instruments
 - Maps of Experimental Halls
- Laboratory / User Facilities
- Sample Environment
- Software

Utsusemi Portal Site

What's New

- 2025.10.6 Update Installers
- 2025.7.22 Update Installers

Installations

Information about Utsusemi Installation and download of required files is contained on the Installation Portal Site below.

- Portal for Utsusemi installation (Outer site)

In this site, you can find installer files (the binary installer for Windows and macOS, the debian package for Ubuntu Linux) and the installation manuals.

Documentations

Utsusemi

<https://mlfinfo.jp/groups/comp/en/utsusemi.html>

Utsusemi Installation

Windows 11, MacOS, Unix (Ubuntu)

Utsusemi Installation
1.0 documentation

Search

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空欄ダウンロードポータル
Portal for Utsusemi installation
Dockerによるインストール

Utsusemi Installation
1.0 documentation

Portal for Utsusemi installation

To Japanese Page: [空欄ダウンロードポータル](#)

Authors: Y. Inamura

Last Updated: Nov 11, 2025

In this site, there are links to files and documents for Utsusemi installation on various operation systems.

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 - [Documents](#)
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[macOS](#)

[Linux](#)

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- [Other Ubuntu Linux](#)
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- [AlmaLinux 9](#)

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Utsusemi Installation
1.0 documentation

Search

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Portal for Utsusemi installation
Dockerによるインストール

Utsusemi Installation
1.0 documentation

Available Windows

Available Windows for installation

CPU architecture	version
Intel / AMD (64bit)	11 and 10
ARM	Not Available yet

Documents

- [Quick Installation Guide of Utsusemi for Windows](#)

Download links

Download links for Windows Binary Installers

Type	Python Ver	Download Link
All-in-one	3.13.5 inside	4.0.251011_PY313(all-in-one)
Minimum (PY313)	3.13.x required	4.0.251011_PY313(minimum)
Minimum (PY312)	3.12.x required	4.0.251011_PY312(minimum)
Minimum (PY311)	3.11.x required	4.0.251011_PY311(minimum)

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[macOS](#)

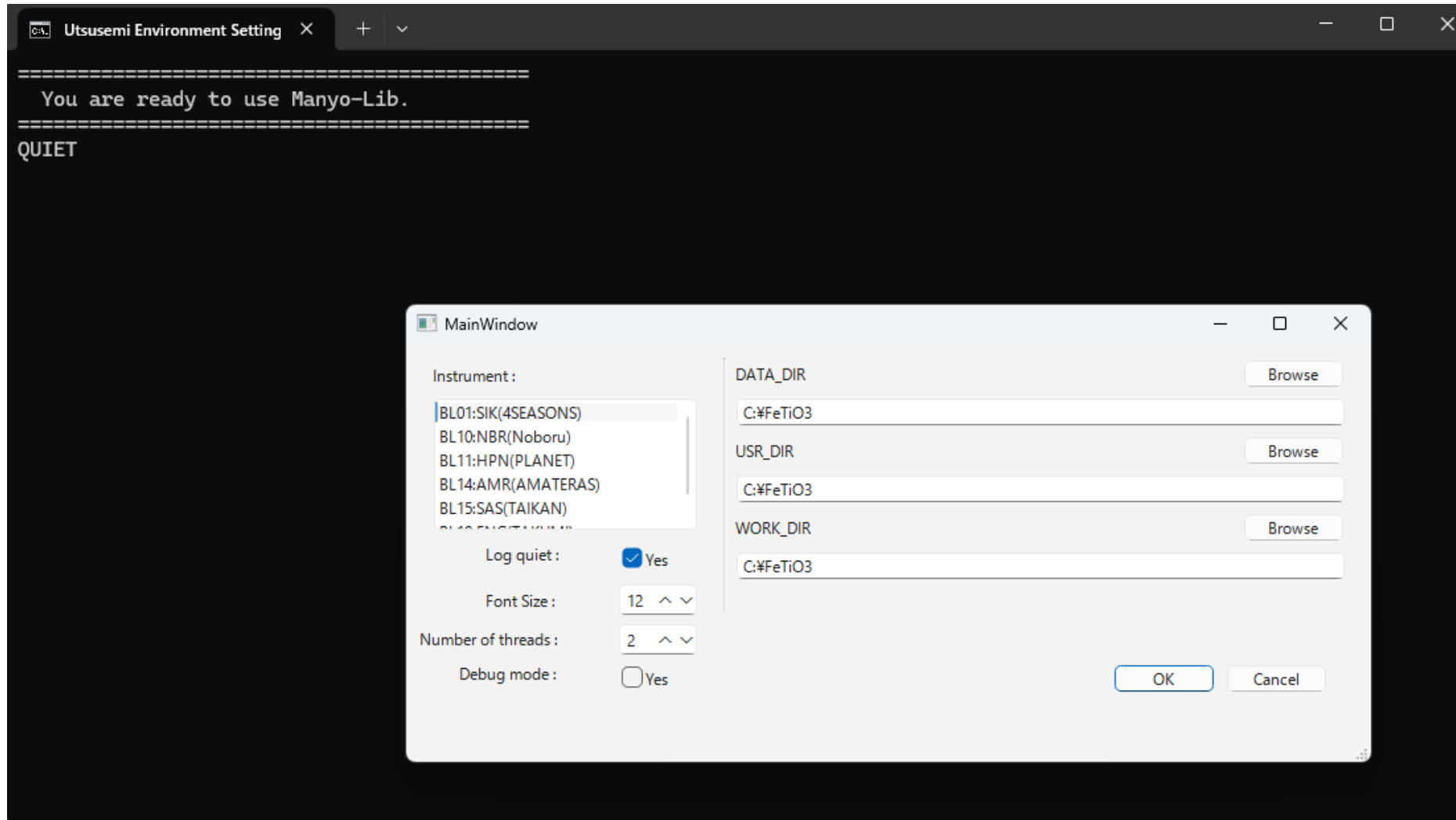
[Linux](#)

- [Debian Packages for Ubuntu 22.04/24.04](#)
- [Other Ubuntu Linux](#)
- [CentOS 7](#)
- [AlmaLinux 8 or RockyLinux 8](#)
- [AlmaLinux 9](#)

[Appendix](#)

- [Version number confirmation](#)

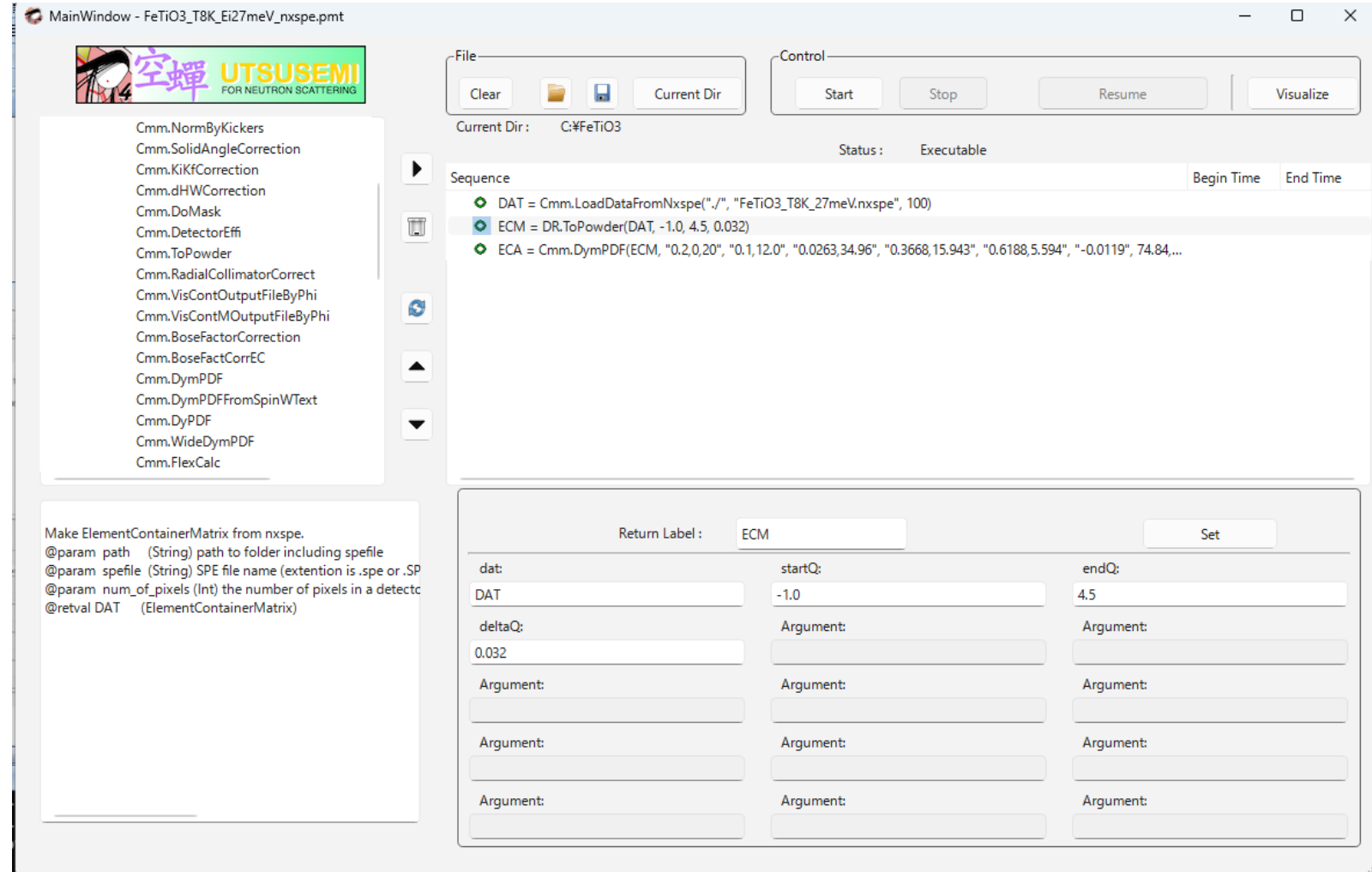
After installation of 'Utsusemi.4.0.251011.PY313.x86_64.msi' 'Utsusemi Environment Settings'



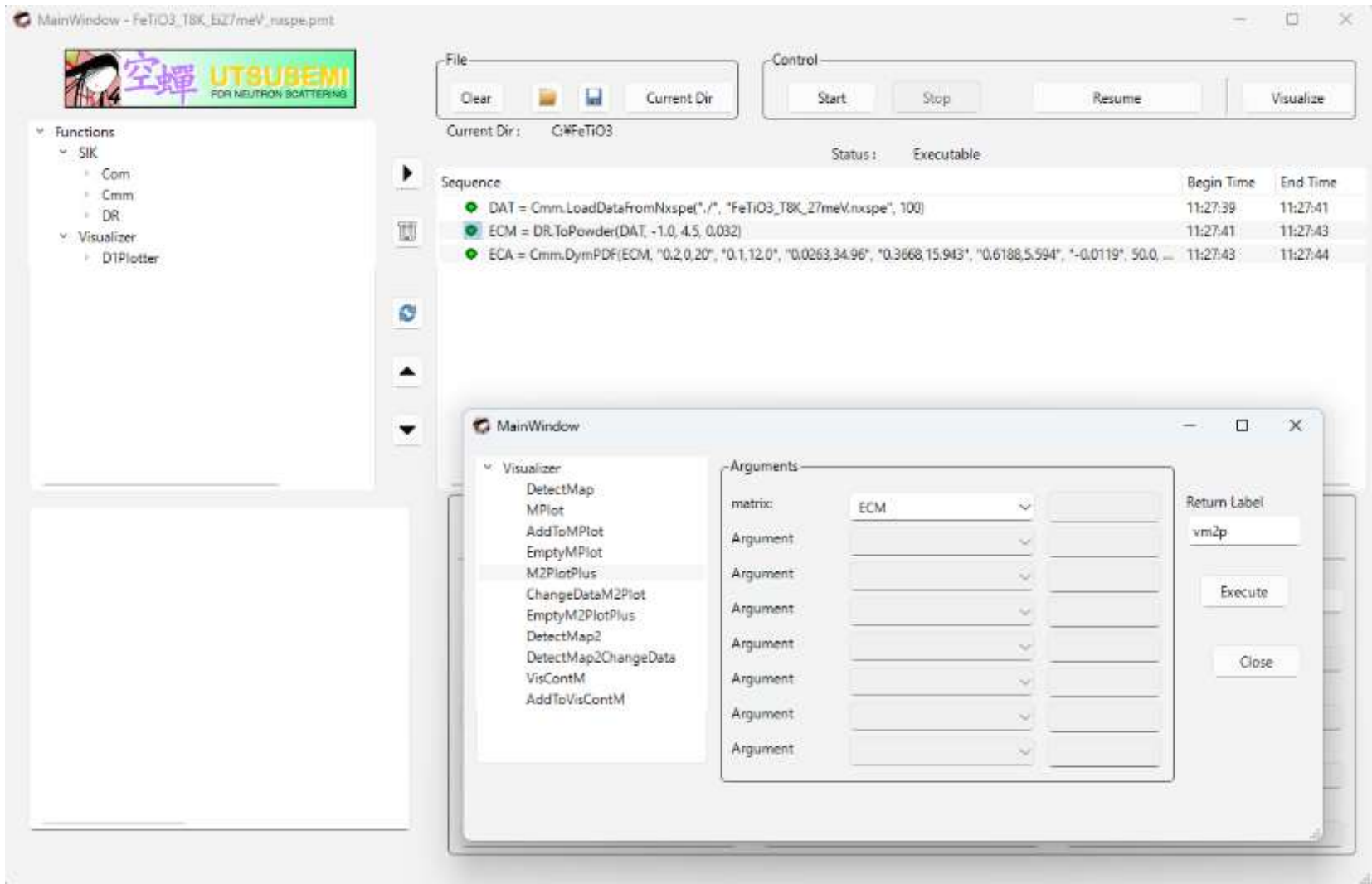
Nxspe file

**‘Sequence Editor’, Functions, SIK,
DAT=Cmm.LoadDataFromNxspe
ECM=DR.ToPowder
ECA=Cmm.DymPDF**

**Available data formats:
SPE, Nxspe, Dump,
Srlz, ManyoBinary,
NeXus**

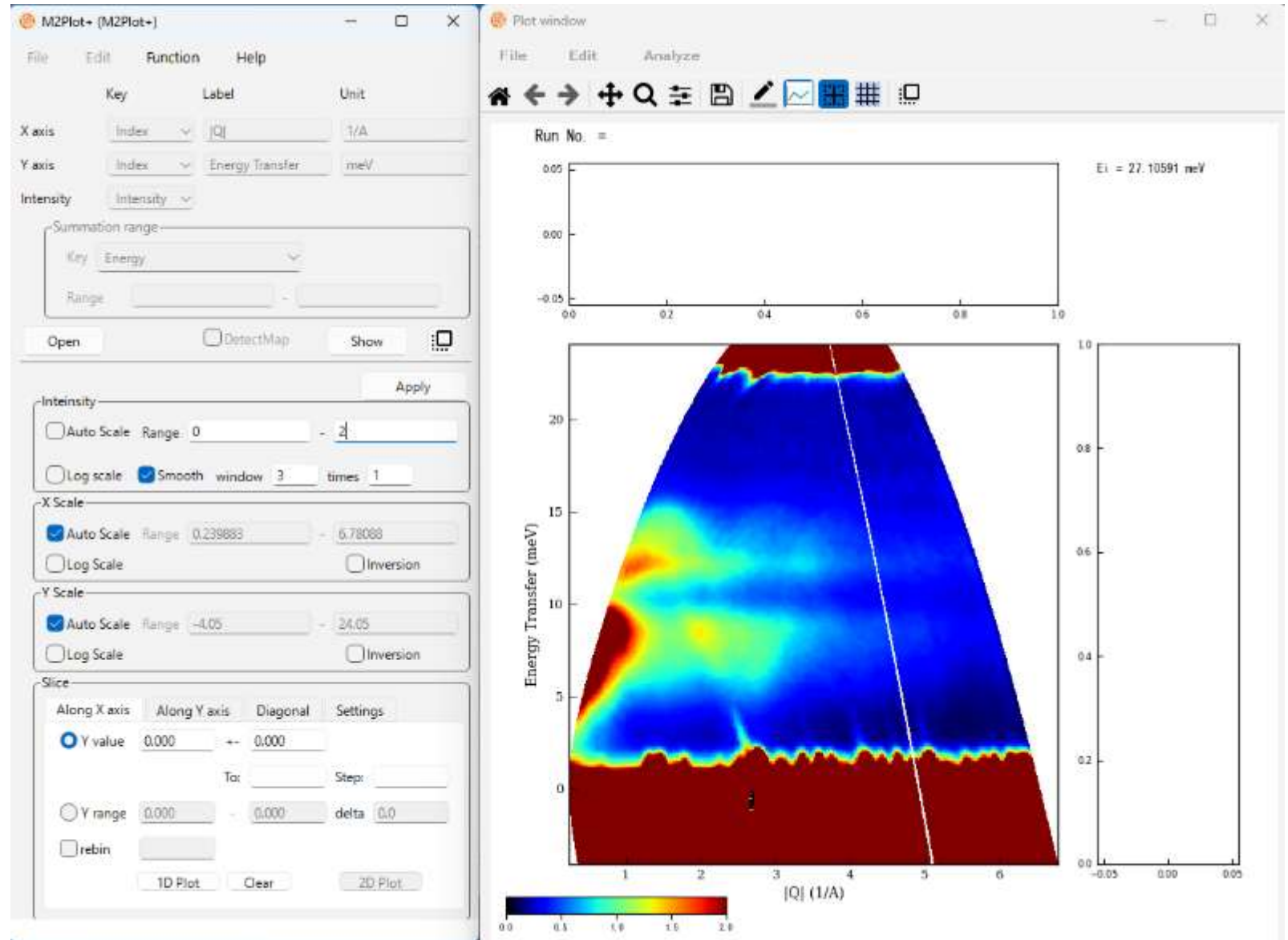


‘Sequence Editor’
Start
Visualize M2PlotPlus
matrix **ECM**
Return Label vm2p
Execute



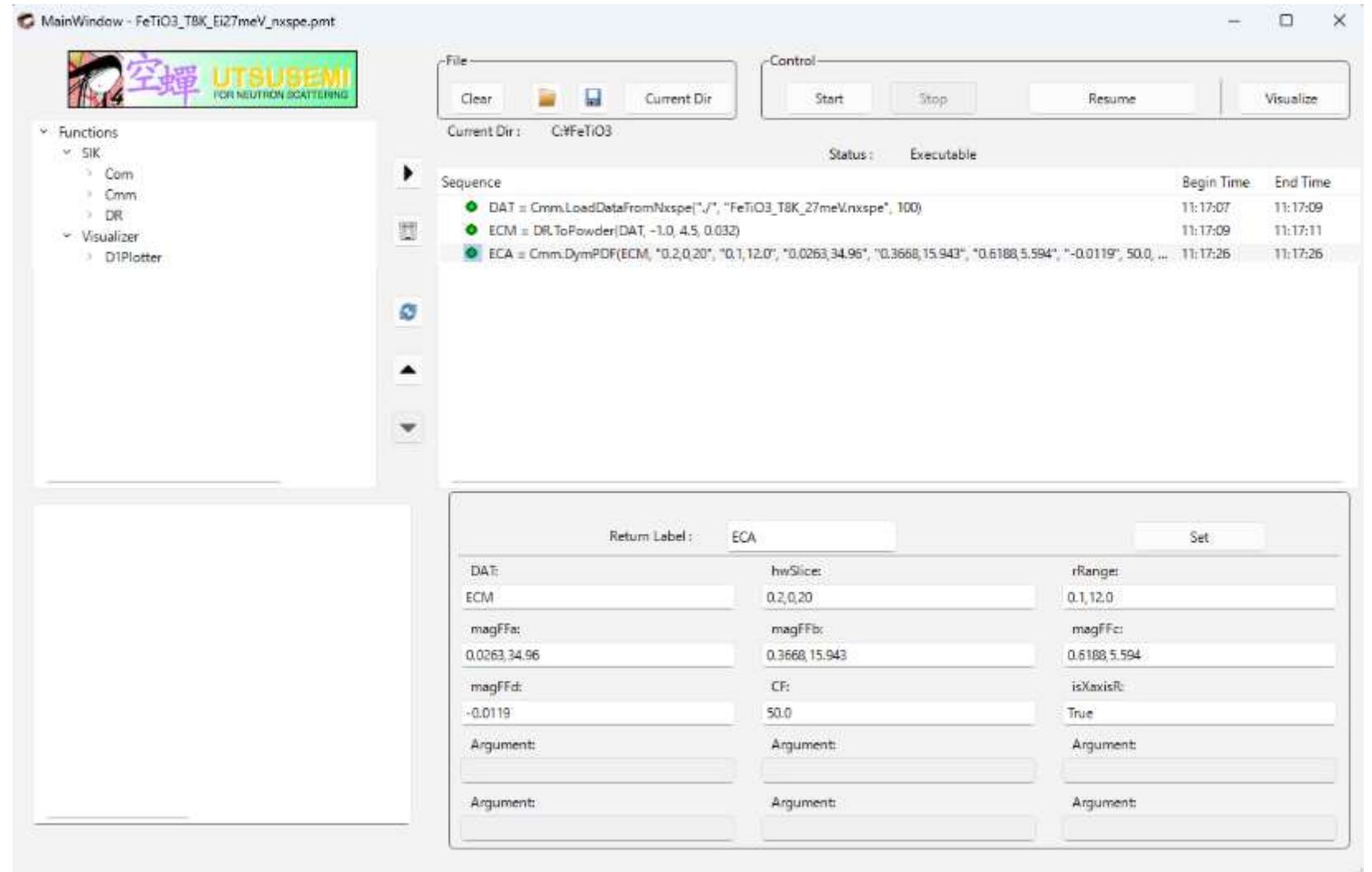
‘Sequence Editor’ M2Plot+

Dynamic structure
factor $S(Q,E)$



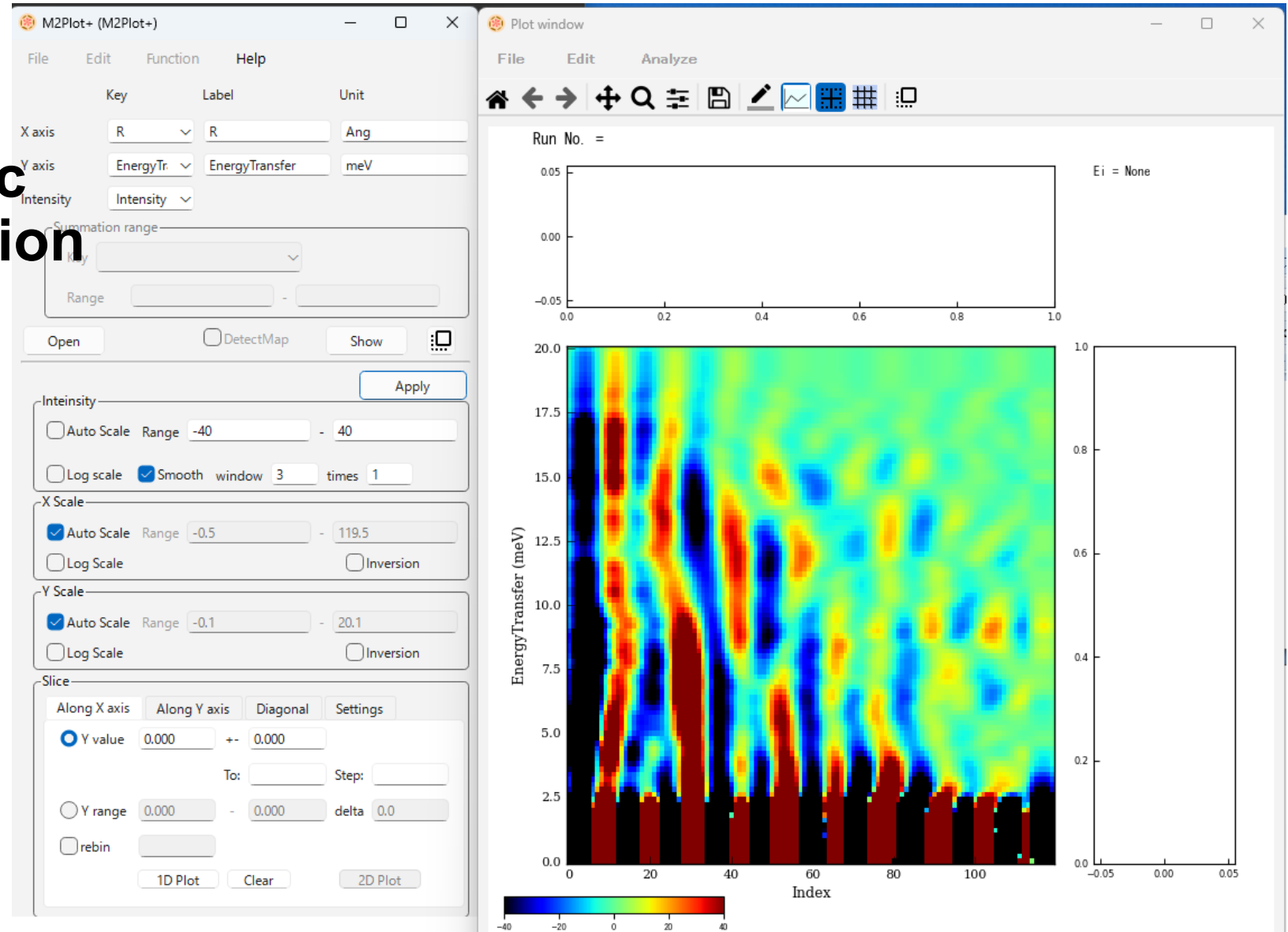
‘Sequence Editor’

Visualize M2PlotPlus
matrix **ECA**
Return Label vm2p
Execute



‘Sequence Editor’ M2Plot+

Dynamic magnetic
pair density function
 $D_M(r,E)$



4. How to simulate DymPDF by 'SpinW' and 'Utsusemi'

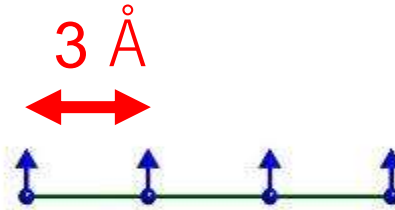
DymPDF SpinW simulation (MATLAB)

Simple model magnets: $S = 1$, $J_a = -1$ meV

1D chain Ferromagnet

Spin 

$$H = \sum_{i,j} J_{ij} S_i S_j = J_a (S_i S_{i-1} + S_i S_{i+1})$$

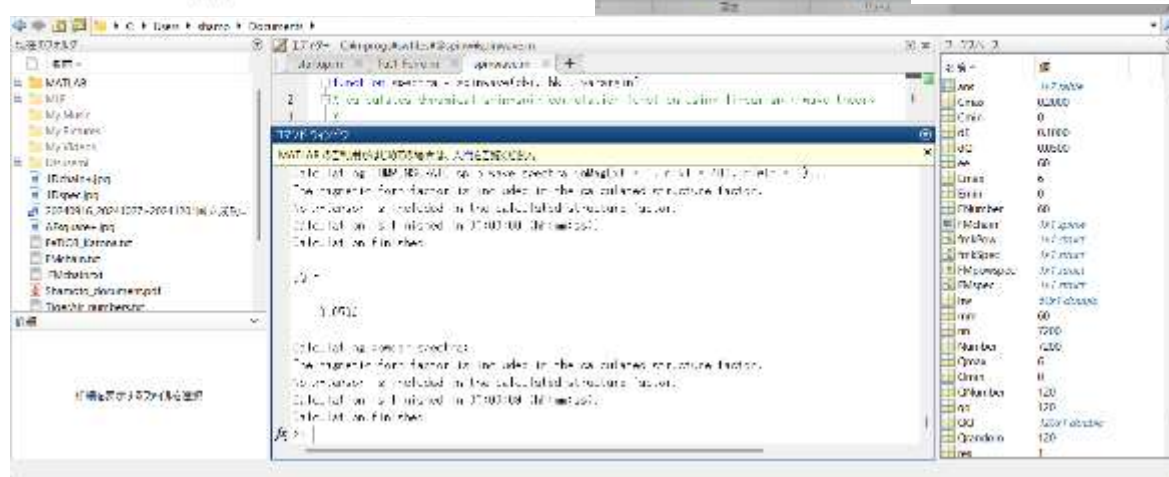
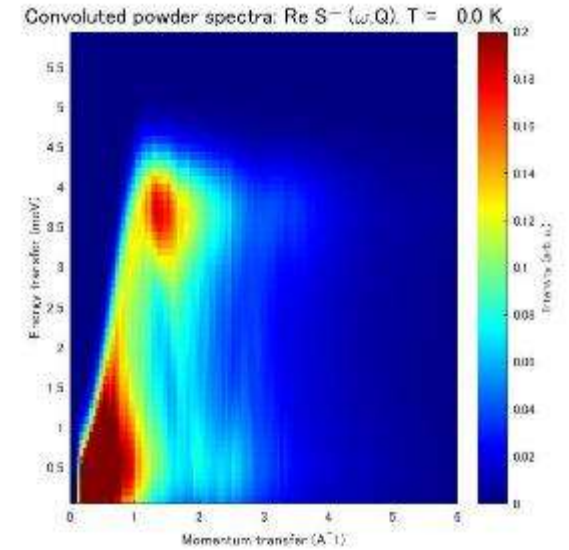
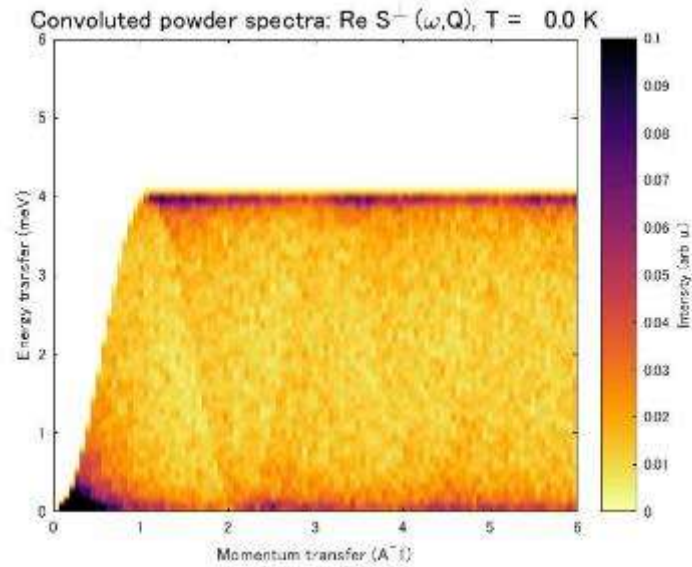
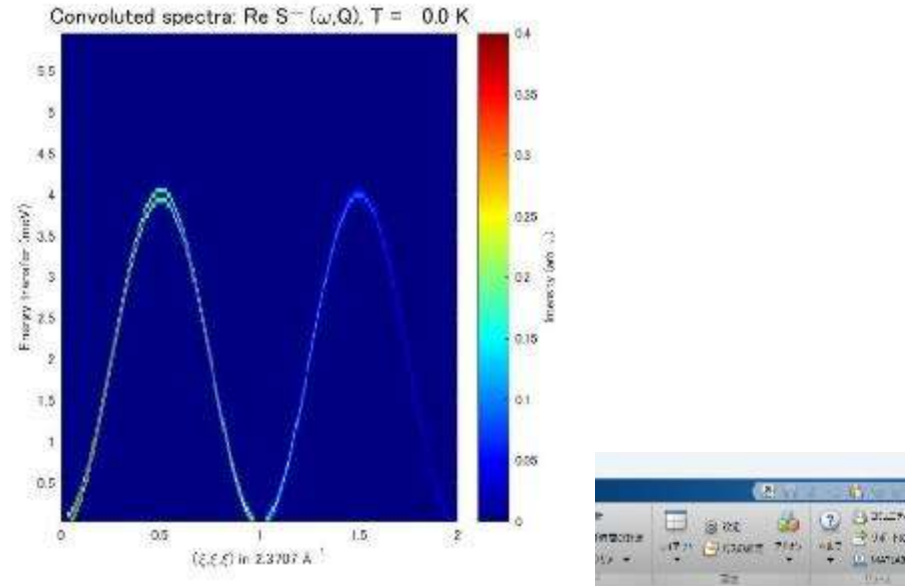


$$E(k) = 2J_a S (1 - \cos ka)$$



The SpinW software package is based on the linear spin-wave theory with the Holstein–Primakoff approximation.

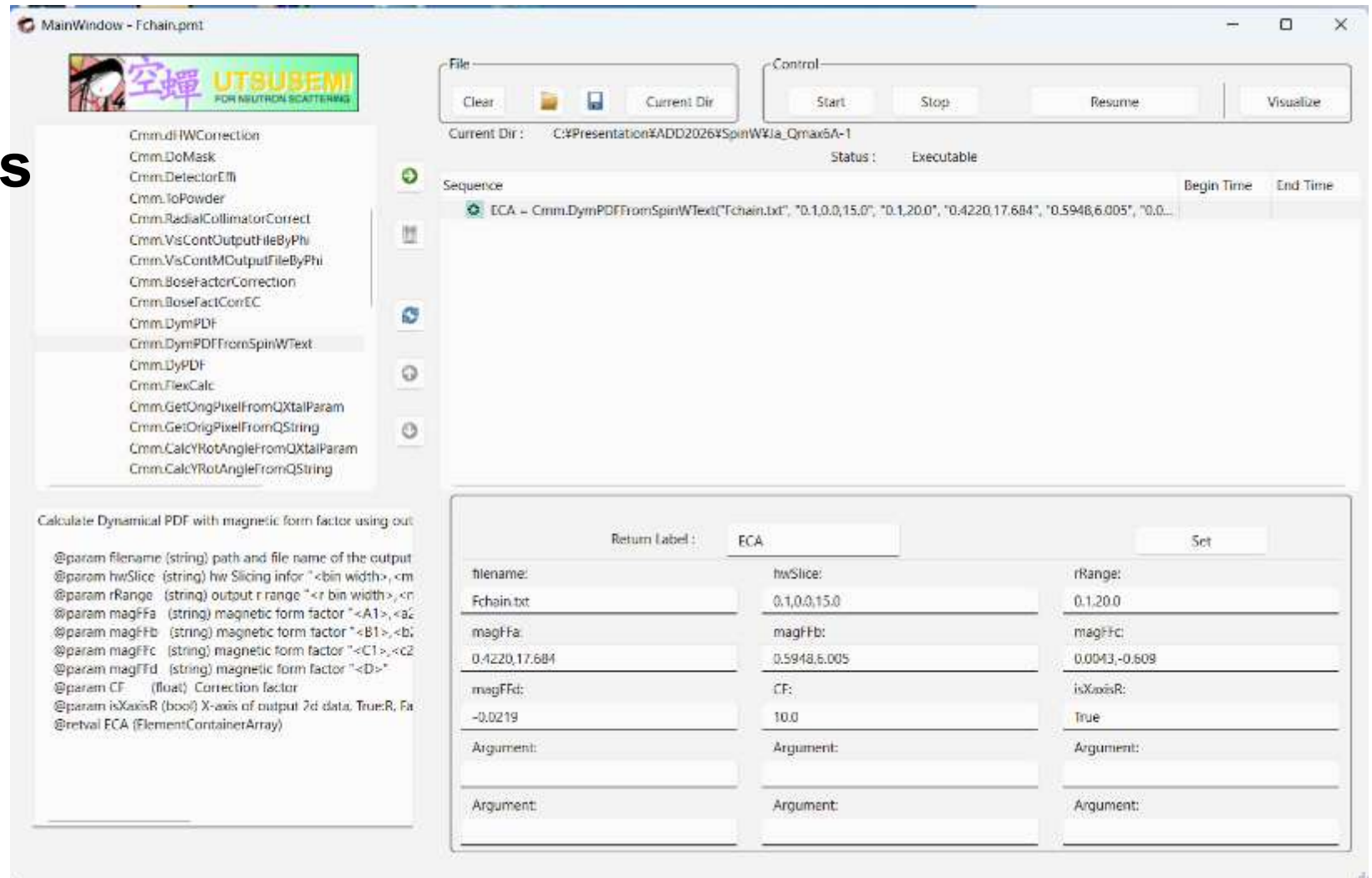
Tutorial 1 in SpinW homepage “Spin wave spectrum of the Heisenberg ferromagnetic nearest-neighbor spin chain”



<https://spinw.org/tutorials/>

‘Sequence Editor’, Functions, SIK, ECA=Cmm.DymPDFFromSpinWText

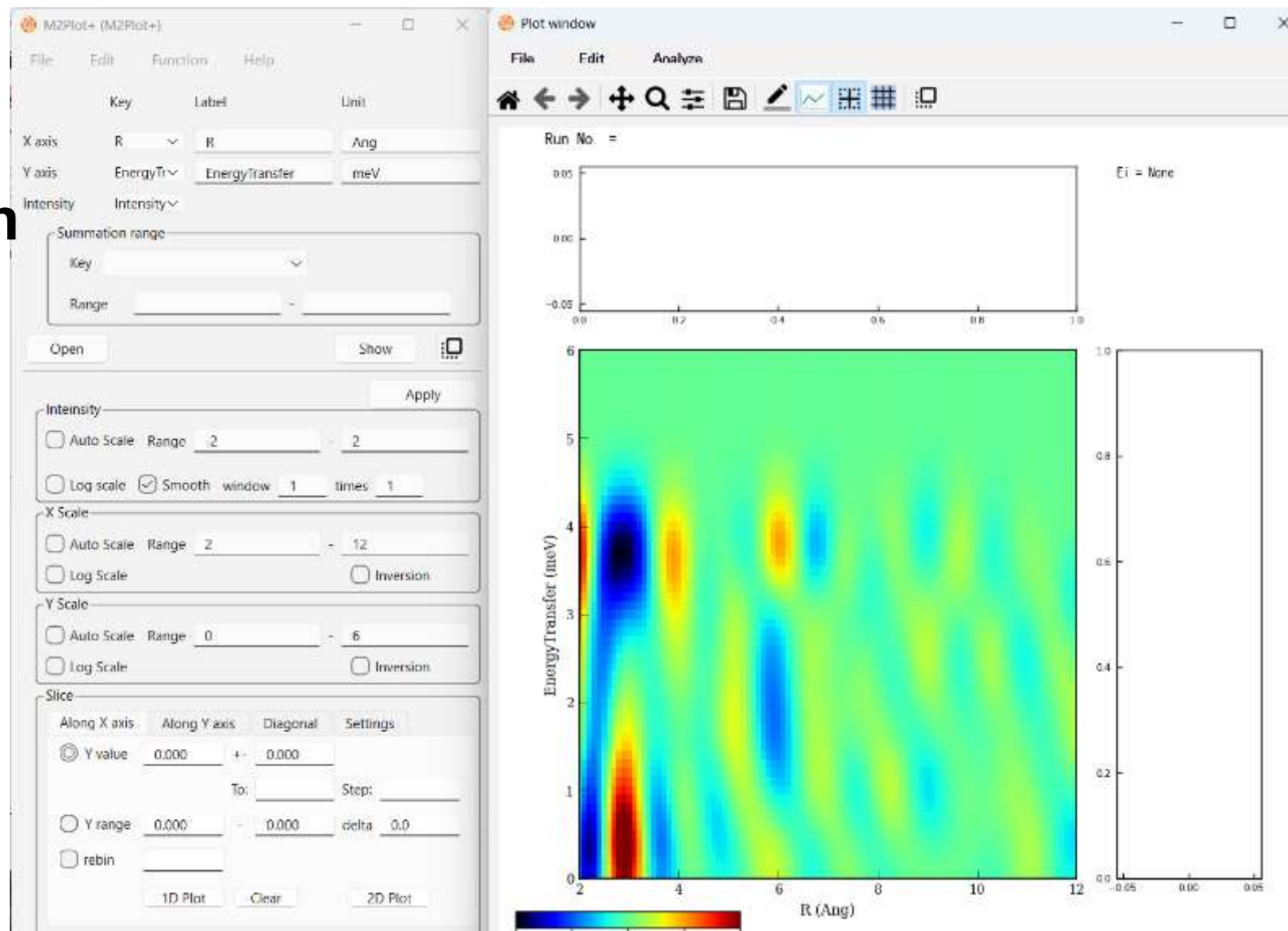
‘Sequence Editor’
Start
Visualize M2PlotPlus
matrix **ECA**
Return Label vm2p
Execute



‘Sequence Editor’

M2Plot+

Dynamic magnetic
pair density function
 $D_M(r,E)$



5. Summary

1990
Crystalline PDF
IPNS, ANL USA

PDFgetN

Billinge, S. J. L.
<https://www.diffpy.org/products/pdfgetx.html>

PDFFIT

Proffen Th. and
Billinge, S. J. L.
<https://www.xray.cz/ecm-cd/soft/xray/general/discus/discus/pdfit.html>

1992
DyPDF
ISIS, RAL UK

**DyPDF
(Utsusemi)**

<https://mlfinfo.jp/groups/comp/en/utsusemi.html>

2024 CROSS technical
development program

2014
mPDF
ILL France

mPDF

Billinge, S. J. L.
<https://mpdf.github.io/>

mPDF

Billinge, S. J. L.
<https://mpdf.github.io/>

2022
DymPDF
J-PARC MLF Japan

**DymPDF
(Utsusemi)**

<https://mlfinfo.jp/groups/comp/en/utsusemi.html>

2021 CROSS technical
development program

SpinW+Utsusemi

<https://spinw.org/>

