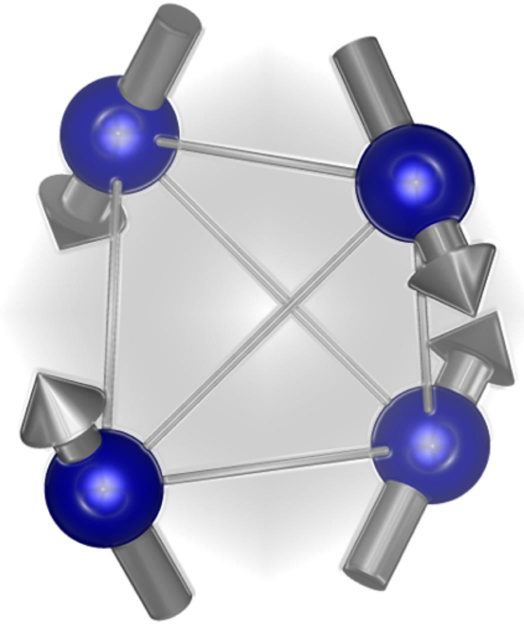
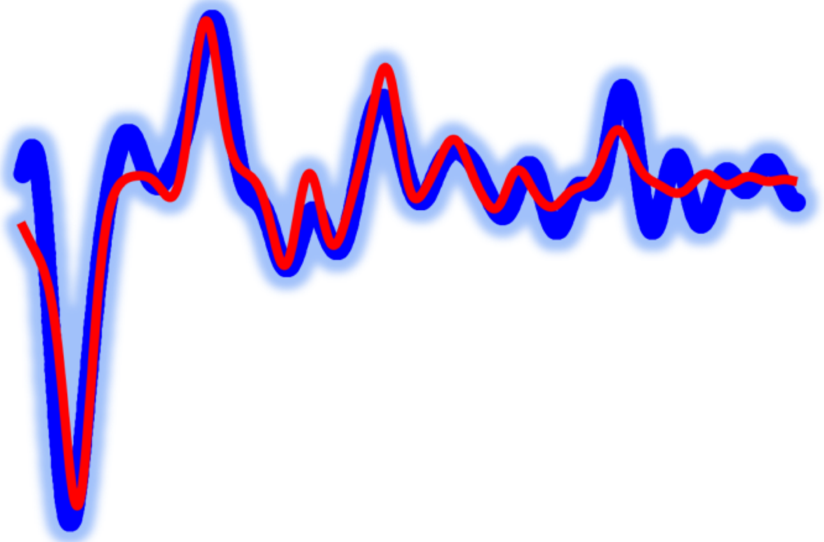
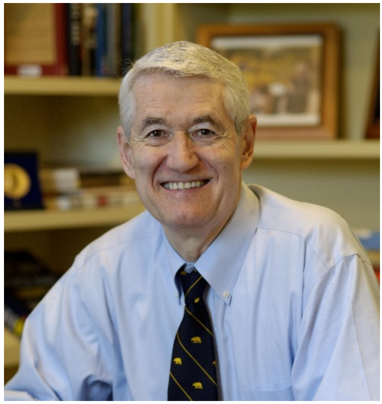
Taking a Spin with the Magnetic Pair Distribution Function





Benjamin A. Frandsen
Department of Physics and Astronomy,
Brigham Young University

Acknowledgments



Simon Billinge

Bob Birgeneau

COLUMBIA UNIVERSITY
IN THE CITY OF NEW YORK

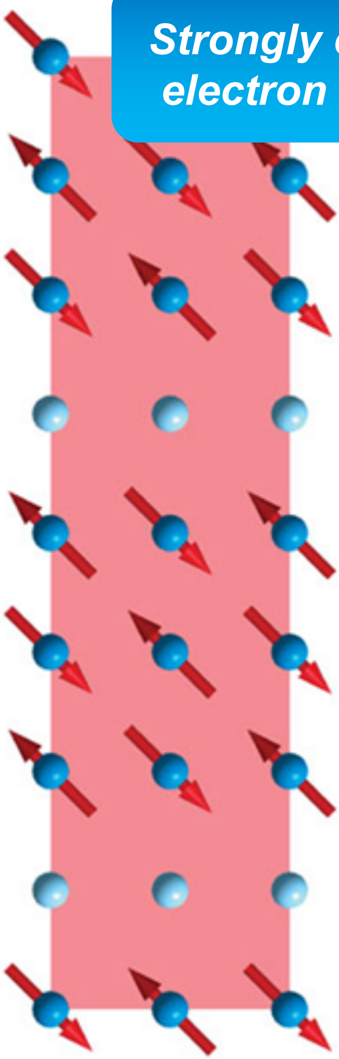
U.S. DEPARTMENT OF
ENERGY

NSF

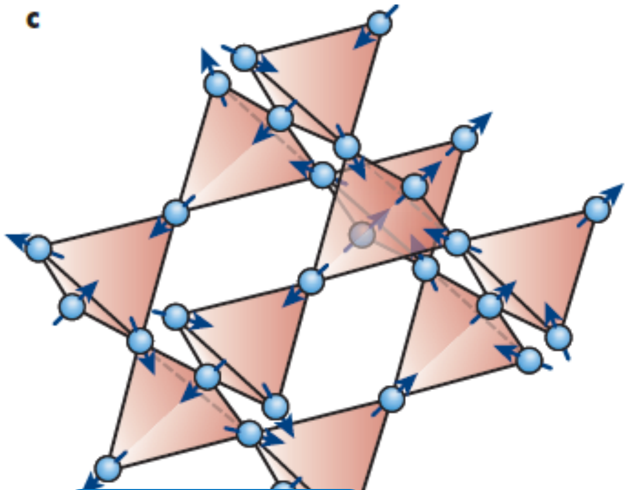
Outline

- Introduction to magnetic PDF analysis
- Building intuition: Calculated mPDFs from simple systems
- Putting it into practice: mPDF of MnO from two different instruments
- Application to a genuine short-range ordered magnet: $NaCaCo_2F_7$
- Sharing the love: diffpy.mpdf open-source software

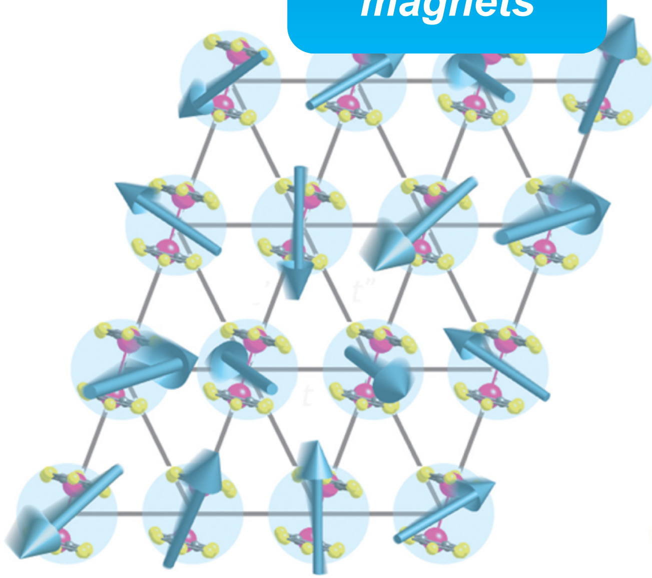
Short-range magnetic order: ubiquitous in modern magnetism



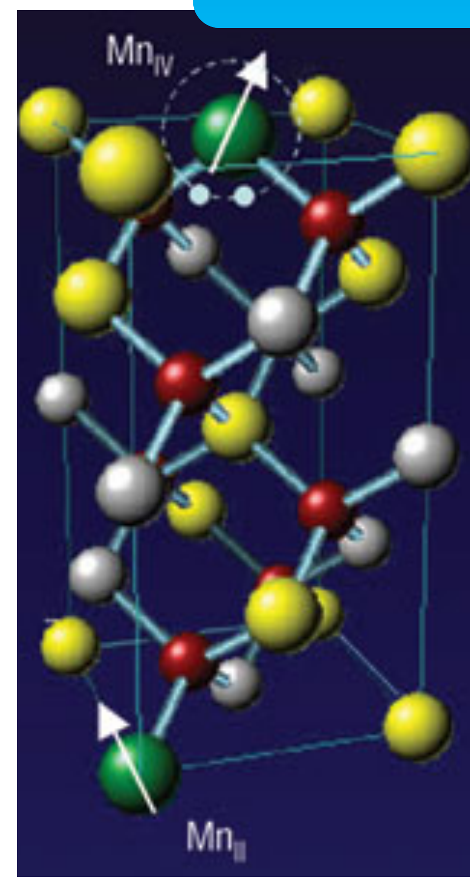
Strongly correlated electron materials



Frustrated magnets

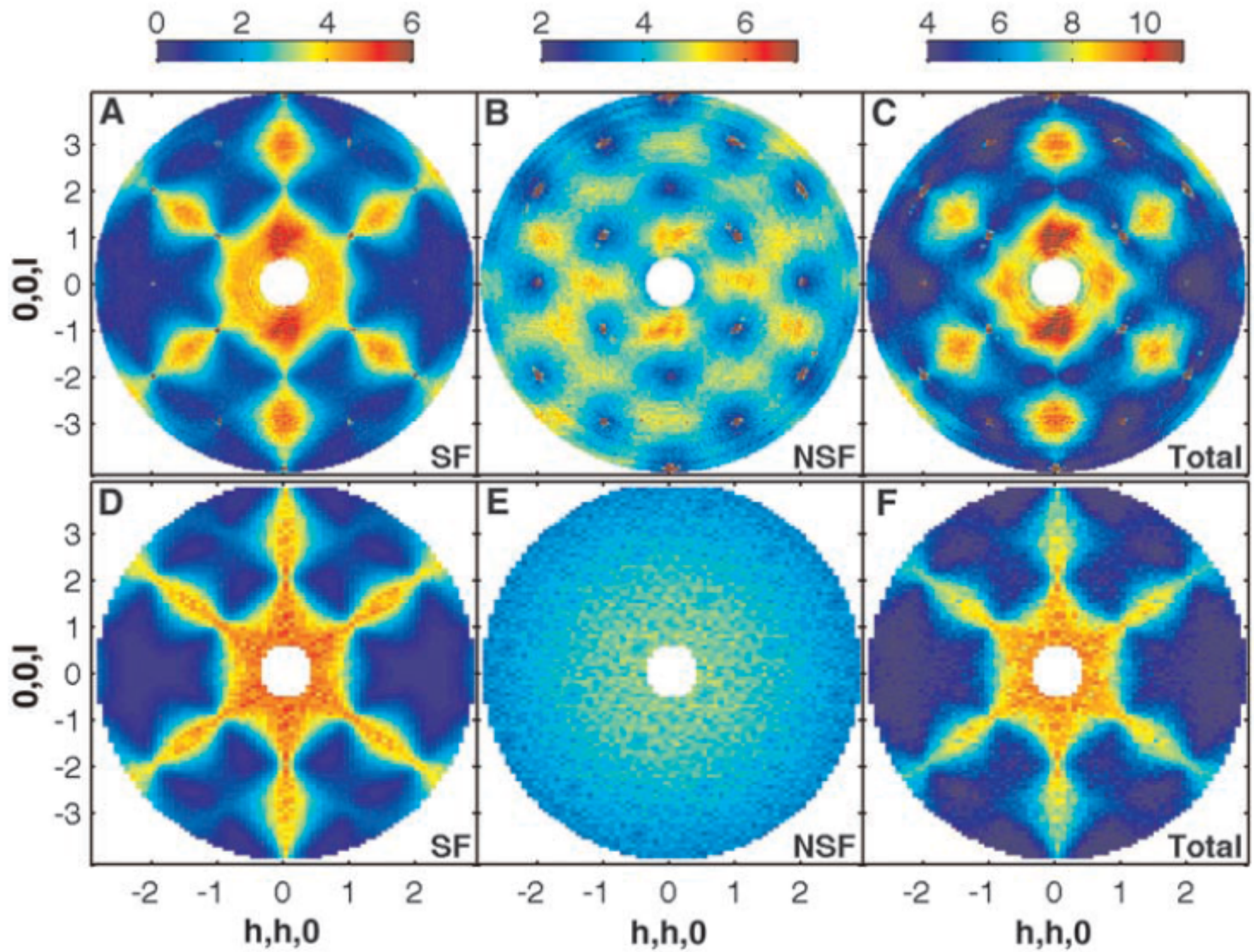


Dilute magnetic semiconductors



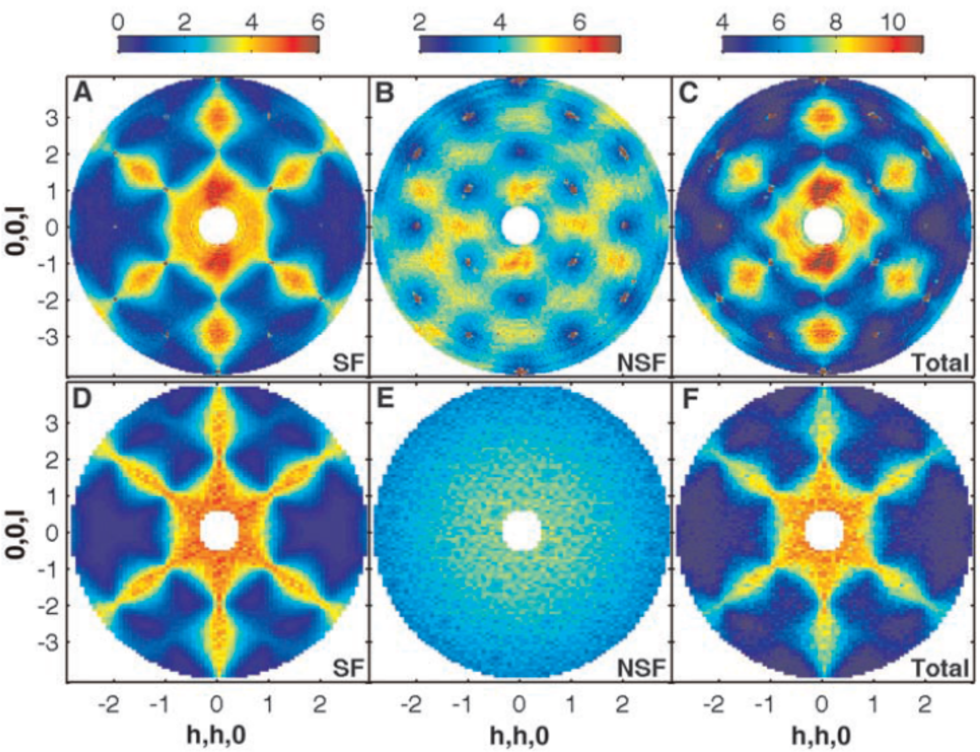
Many more examples!!

Neutron scattering from magnetic SRO

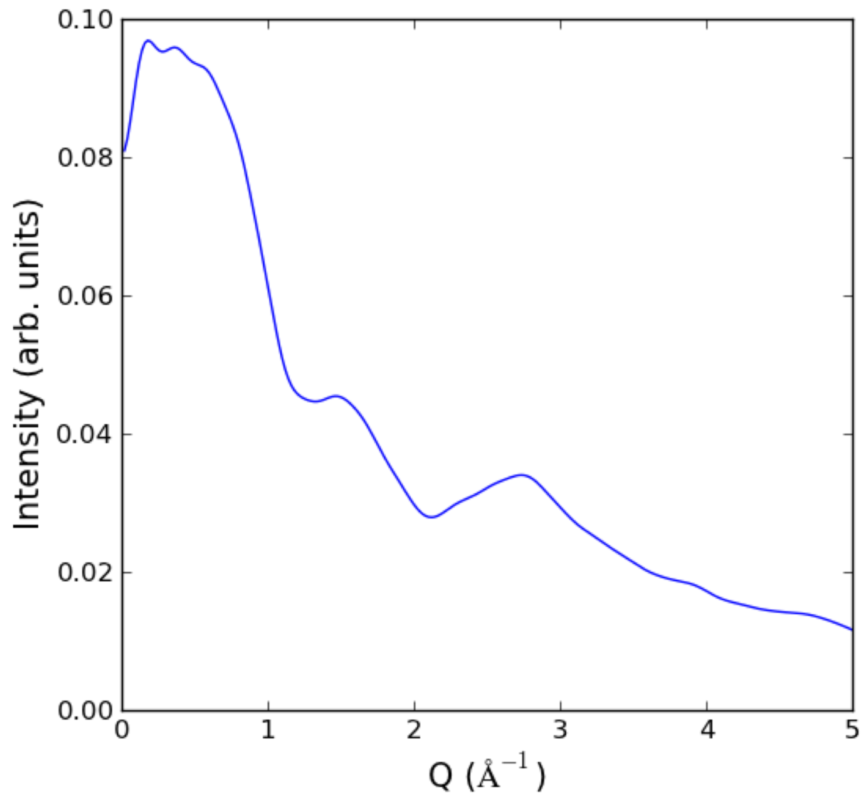


Fennel *et al*, Science **326** 415 (2009)

Neutron scattering from magnetic SRO

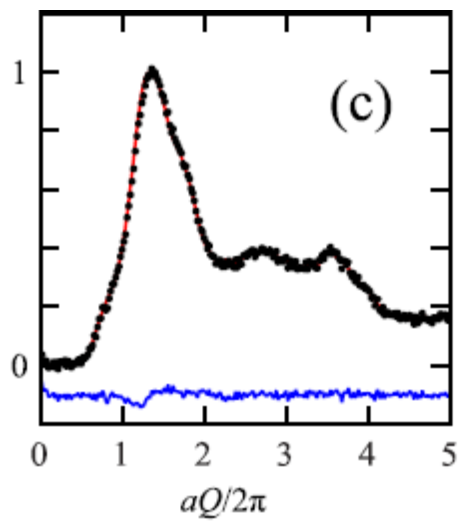


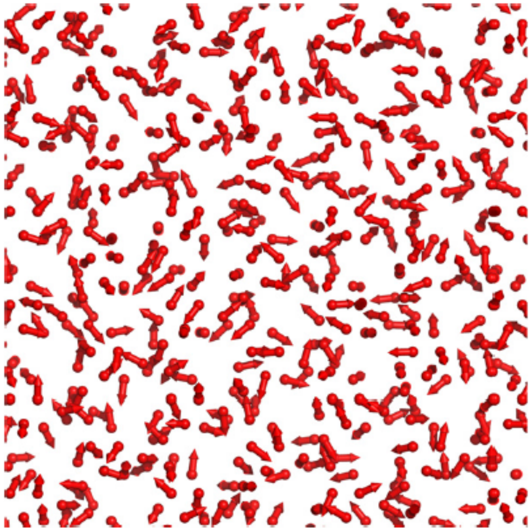
Fennel *et al*, Science **326** 415 (2009)



Previous work

- Model magnetic scattering in momentum space
  - Keen & McGreevy, J. Phys.: Cond. Matt. **3** 7383 (1991)
  - Stewart, Andersen, & Cywinski, *Phys. Rev. B* **78** 014428 (2008)
  - Paddison & Goodwin, PRL **108** 017204 (2012)
  - Paddison, Stewart, & Goodwin, JPCM **25** 454220 (2013)

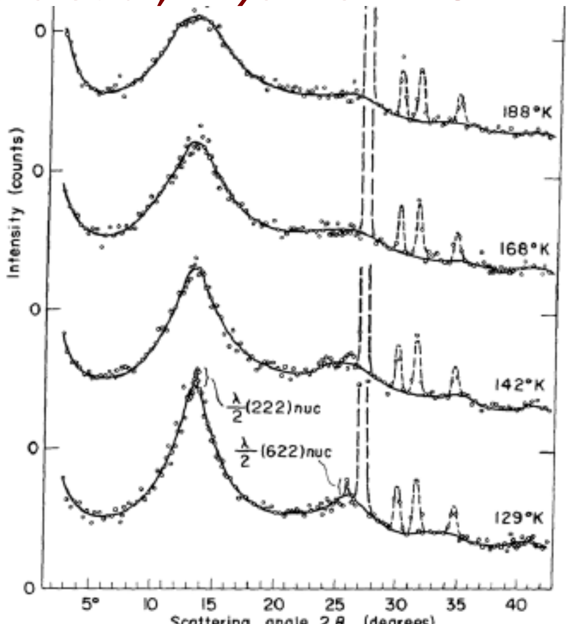




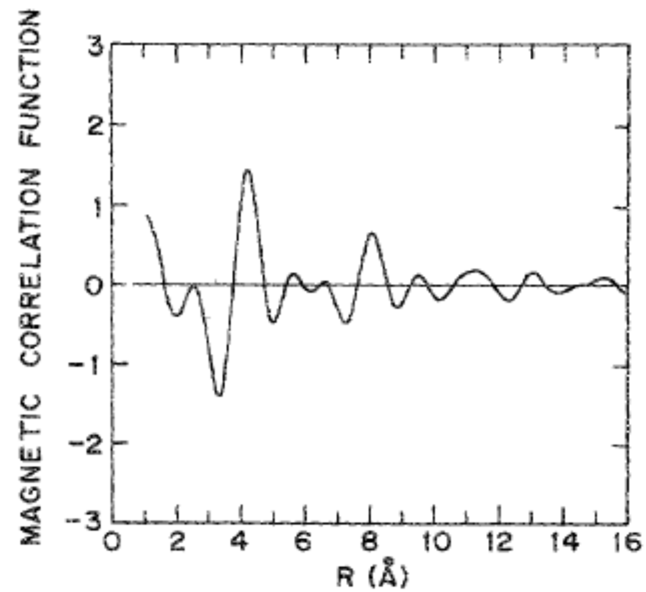
Paddison, Stewart, & Goodwin (2013)

Alternative approach in real space

- View and model magnetic correlations directly in real space
  - Blech & Averbach, *Physics* **1** 31 (1964)
  - Wu, Dmowski, Egami, & Chen, *J. Appl. Phys.* **61** 3219 (1987)
  - Greedan et al, *J. Appl. Phys.* **67** 5967 (1990)
  - Ehlers et al, *Phys. Rev. B* **81** 224405 (2010)



Blech & Averbach 1964



Wu et al 1987

Missing up until now: Analytical expression for the real-space magnetic pair distribution function

Derivation of the mPDF equations

Magnetic

Atomic

After CL Farrow & SJL Billinge, Acta A 65 (2009) 232

Derivation of the mPDF equations

Magnetic

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = (\gamma r_0)^2 \sum_{i,j} f_i(\boldsymbol{Q}) f_j^*(\boldsymbol{Q}) e^{i\boldsymbol{Q}\cdot(\mathbf{r}_i - \mathbf{r}_j)} \mathbf{S}_{\perp i} \cdot \mathbf{S}_{\perp j}$$

Atomic

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \sum_{i,j} f_i(\boldsymbol{Q}) f_j^*(\boldsymbol{Q}) e^{i\boldsymbol{Q}\cdot(\mathbf{r}_i - \mathbf{r}_j)}$$

After CL Farrow & SJL Billinge, Acta A 65 (2009) 232

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Orientational average:

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{2}{3} N S(S+1)(\gamma r_0)^2 f^2 +$$

$$(\gamma r_0)^2 f^2 \sum_{i \neq j} \left[A_{ij} \frac{\sin Q r_{ij}}{Q r_{ij}} + B_{ij} \left(\frac{\sin Q r_{ij}}{(Q r_{ij})^3} - \frac{\cos Q r_{ij}}{(Q r_{ij})^2} \right) \right]$$

$$A_{ij} = S_i^y S_j^y \qquad B_{ij} = 2 S_i^x S_j^x - S_i^y S_j^y$$

Atomic

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \sum_{i,j} f_i(\boldsymbol{Q}) f_j^*(\boldsymbol{Q}) e^{i\boldsymbol{Q}\cdot(\mathbf{r}_i - \mathbf{r}_j)}$$

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = N f^2 + f^2 \sum_{i \neq j} \frac{\sin Q r_{ij}}{Q r_{ij}}$$

After CL Farrow & SJL Billinge, Acta A 65 (2009) 232

Derivation of the mPDF equations

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Orientational average:

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{2}{3} N S(S+1)(\gamma r_0)^2 f^2 + (\gamma r_0)^2 f^2 \sum_{i \neq j} \left[A_{ij} \frac{\sin Q r_{ij}}{Q r_{ij}} + B_{ij} \left(\frac{\sin Q r_{ij}}{(Q r_{ij})^3} - \frac{\cos Q r_{ij}}{(Q r_{ij})^2} \right) \right]$$

$$A_{ij} = S_i^y S_j^y \qquad B_{ij} = 2 S_i^x S_j^x - S_i^y S_j^y$$

Normalize by form factor:

$$S(Q) = 1 + \frac{1}{N} \frac{3}{2S(S+1)} \sum_{i \neq j} \left[A_{ij} \frac{\sin Q r_{ij}}{Q r_{ij}} + B_{ij} \left(\frac{\sin Q r_{ij}}{(Q r_{ij})^3} - \frac{\cos Q r_{ij}}{(Q r_{ij})^2} \right) \right]$$

Atomic

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After CL Farrow & SJL Billinge, Acta A 65 (2009) 232

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Fourier transform:

$$f(r) = \frac{2}{\pi} \int_0^\infty Q \left(S(Q) - 1 \right) \sin Qr \mathrm{d}Q$$

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

Atomic

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \sum_{i,j} f_i(\boldsymbol{Q}) f_j^*(\boldsymbol{Q}) e^{i\boldsymbol{Q}\cdot(\mathbf{r}_i - \mathbf{r}_j)}$$

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = N f^2 + f^2 \sum_{i \neq j} \frac{\sin Q r_{ij}}{Q r_{ij}}$$

$$S(Q) = 1 + \frac{1}{N} \sum_{i \neq j} \frac{\sin Q r_{ij}}{Q r_{ij}}$$

$$f(r) = \frac{2}{\pi} \int_0^\infty Q \left(S(Q) - 1 \right) \sin Qr \mathrm{d}Q$$

$$= \frac{1}{N} \sum_{i \neq j} \frac{1}{r} \delta(r - r_{ij})$$

After CL Farrow & SJL Billinge, Acta A 65 (2009) 232

Effect of finite Q_{min} on Fourier transform

Atomic PDF:

$$
\begin{aligned}
G_{\text{nuc}}(r) &= 4\pi r\left[\rho(r) - \rho_0\right] \\
&= \frac{2}{\pi}\int_{Q_{\text{min}}}^{\infty} F_{\text{nuc}}(Q)\sin Qr\,\mathrm{d}Q \\
&\neq \frac{2}{\pi}\int_{0}^{\infty} F_{\text{nuc}}(Q)\sin Qr\,\mathrm{d}Q = 4\pi r\rho(r) = f_{\text{nuc}}(r)
\end{aligned}
$$

(see CL Farrow & SJL Billinge, Acta A 65 (2009) 232)

Magnetic PDF:

$$
\begin{aligned}
G_{\text{m}}(r) &= \frac{2}{\pi}\int_{Q_{\text{min}}}^{\infty} F(Q)\sin Qr\,\mathrm{d}Q \\
&= \frac{2}{\pi}\int_{0}^{\infty} F(Q)\sin Qr\,\mathrm{d}Q - \frac{2}{\pi}\int_{0}^{Q_{\text{min}}} F(Q)\sin Qr\,\mathrm{d}Q \\
&= f(r) - C\langle m\rangle r
\end{aligned}
$$

→ **Net magnetization**

- **Zero for antiferromagnets**
- **Nonzero for ferro/ferrimagnets**

A closer look

$$\frac{d\sigma}{d\Omega} = \frac{2}{3}NS(S+1)(\gamma r_0)^2 f^2 + (\gamma r_0)^2 f^2 \sum_{i \neq j} \left[A_{ij} \frac{\sin Q r_{ij}}{Q r_{ij}} + B_{ij} \left(\frac{\sin Q r_{ij}}{(Q r_{ij})^3} - \frac{\cos Q r_{ij}}{(Q r_{ij})^2} \right) \right]$$

Normalize by form factor,
Fourier transform

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

Peaks at spin separation distances,
overall 1/*r* envelope

Baseline term linear in r

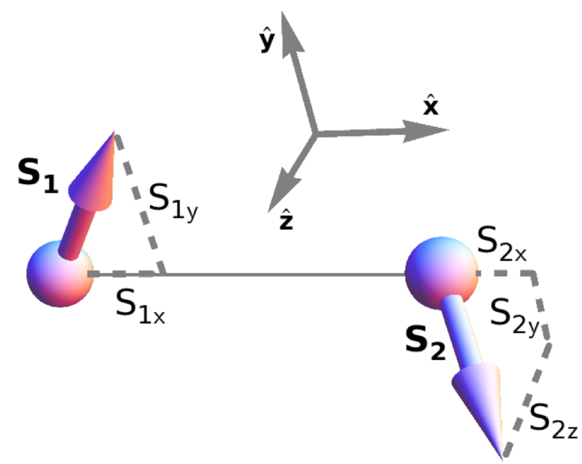
Sign and strength determined by
local spin correlations:

Transverse correlations
(peak height)

$$A_{ij} = S_i^y S_j^y$$

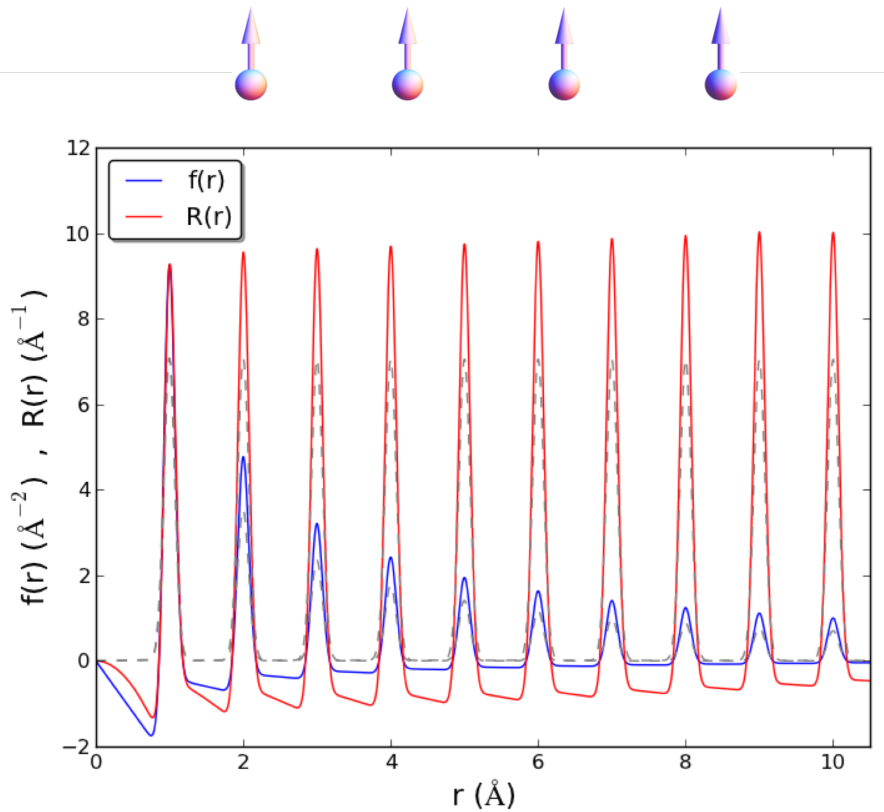
Transverse and longitudinal
correlations (baseline)

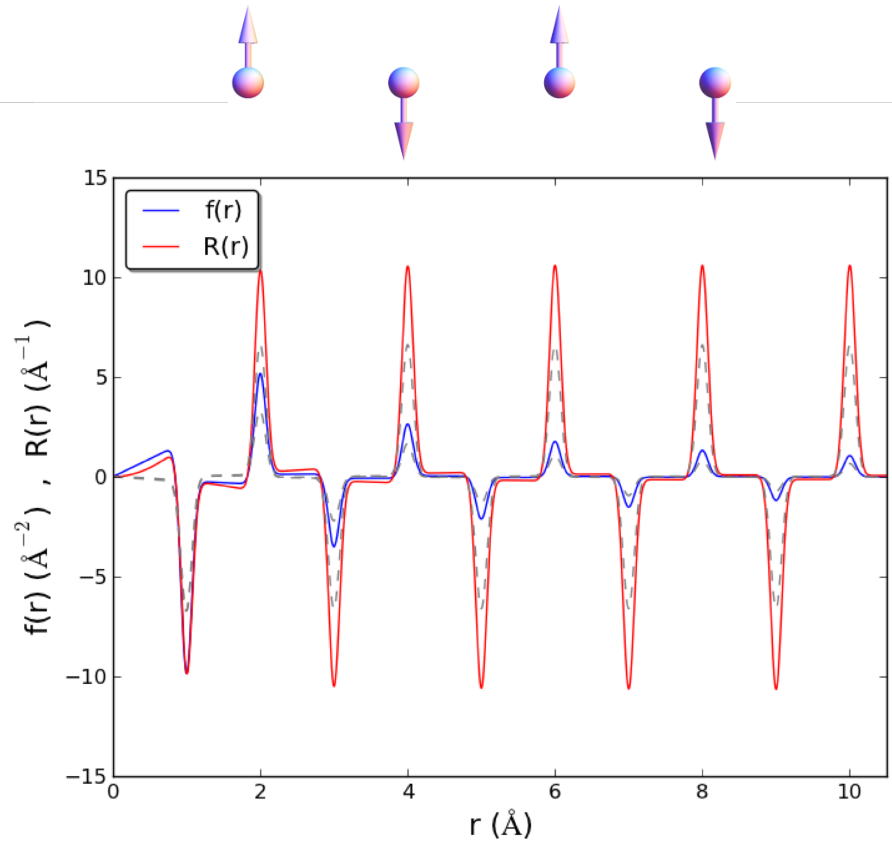
$$B_{ij} = 2 S_i^x S_j^x - S_i^y S_j^y$$



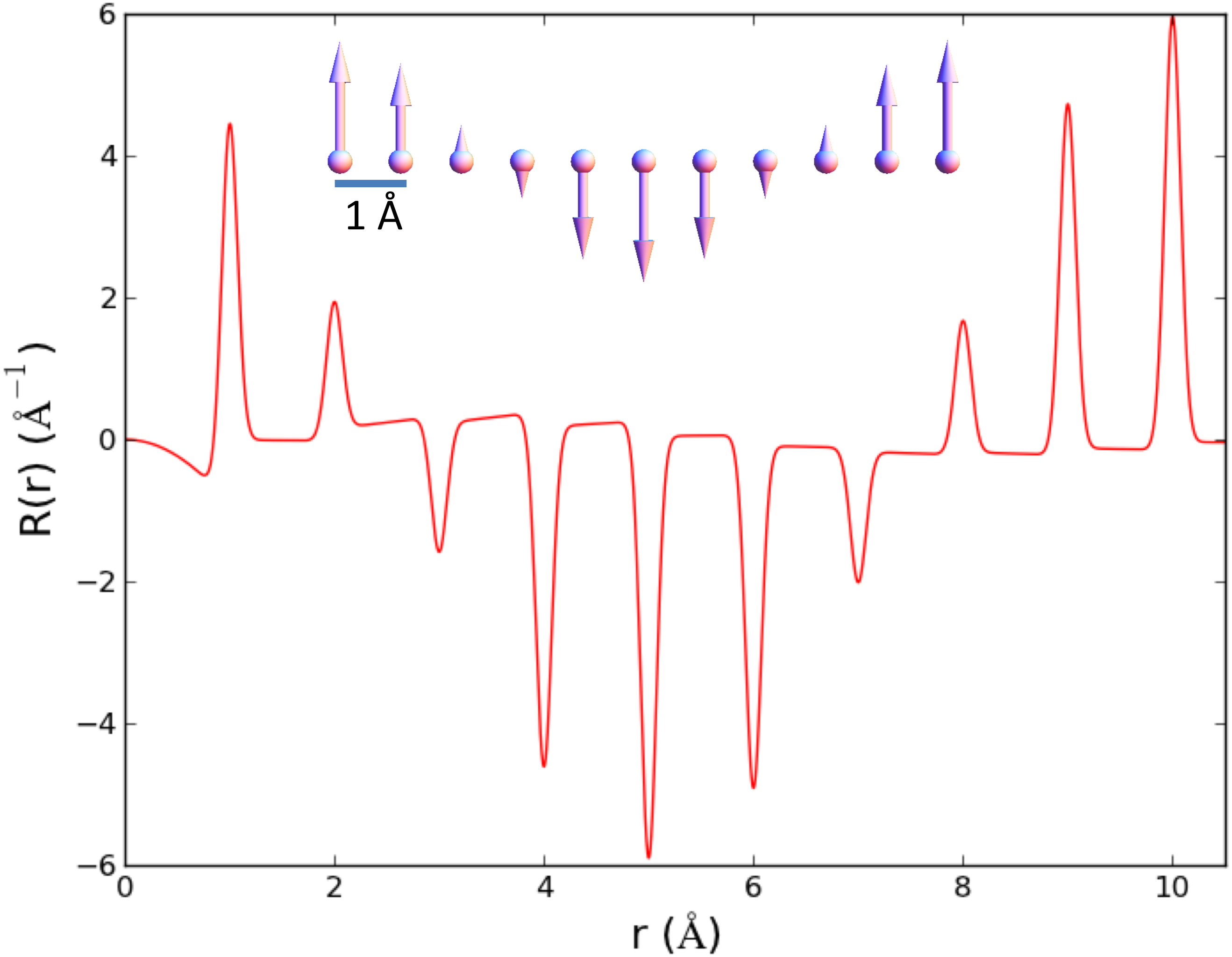
Example: One-dimensional chain

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

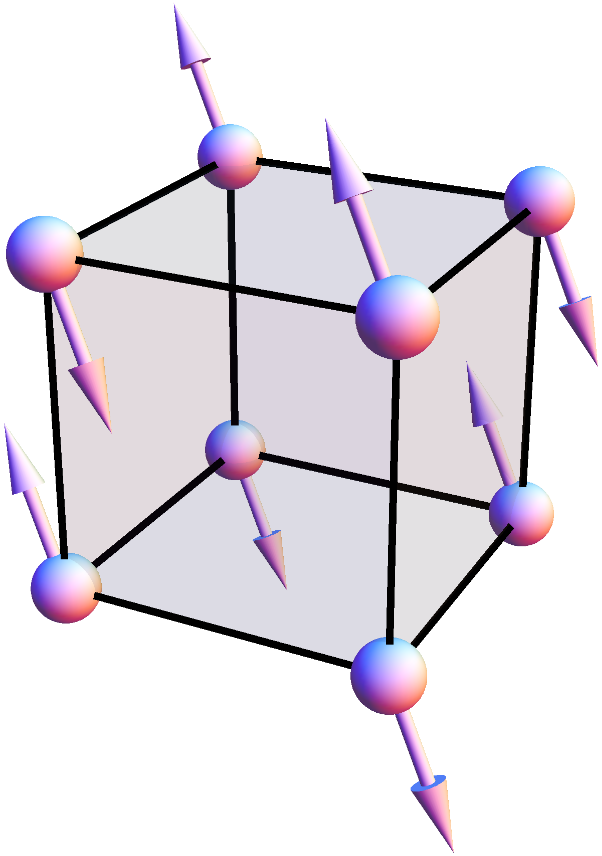


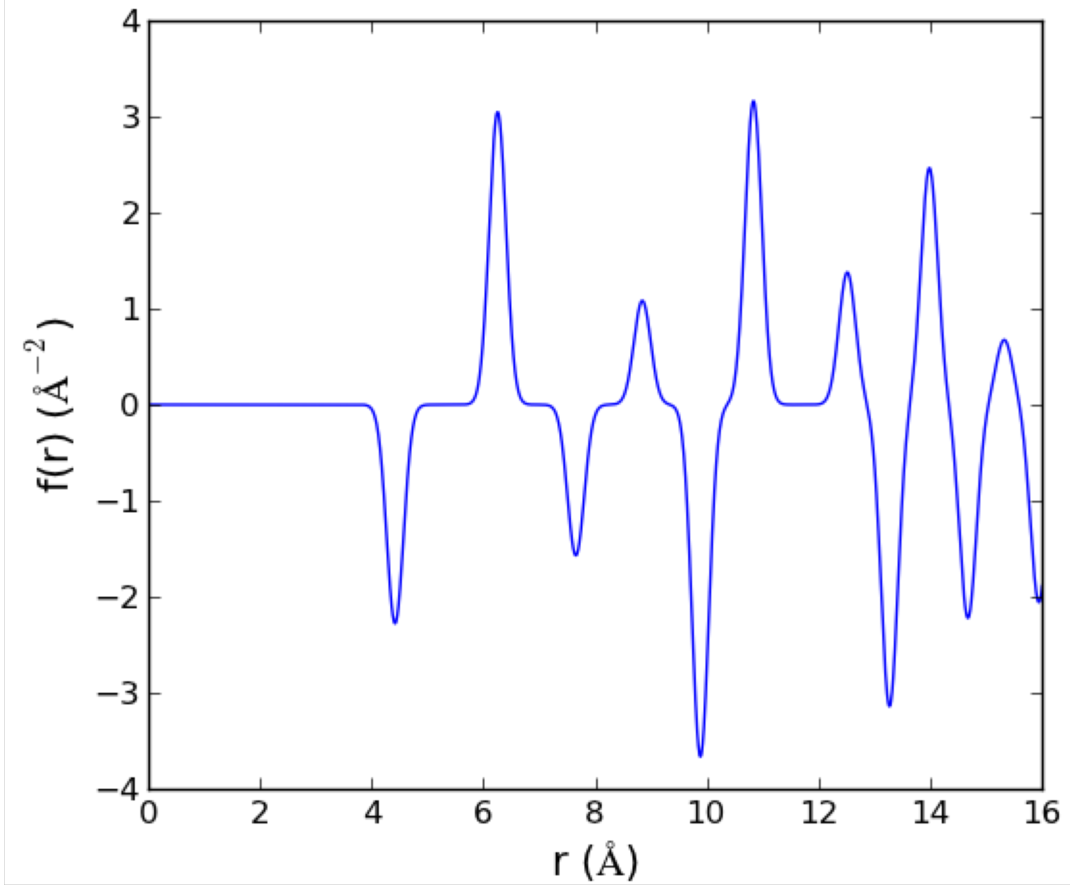


Example: One-dimensional SDW

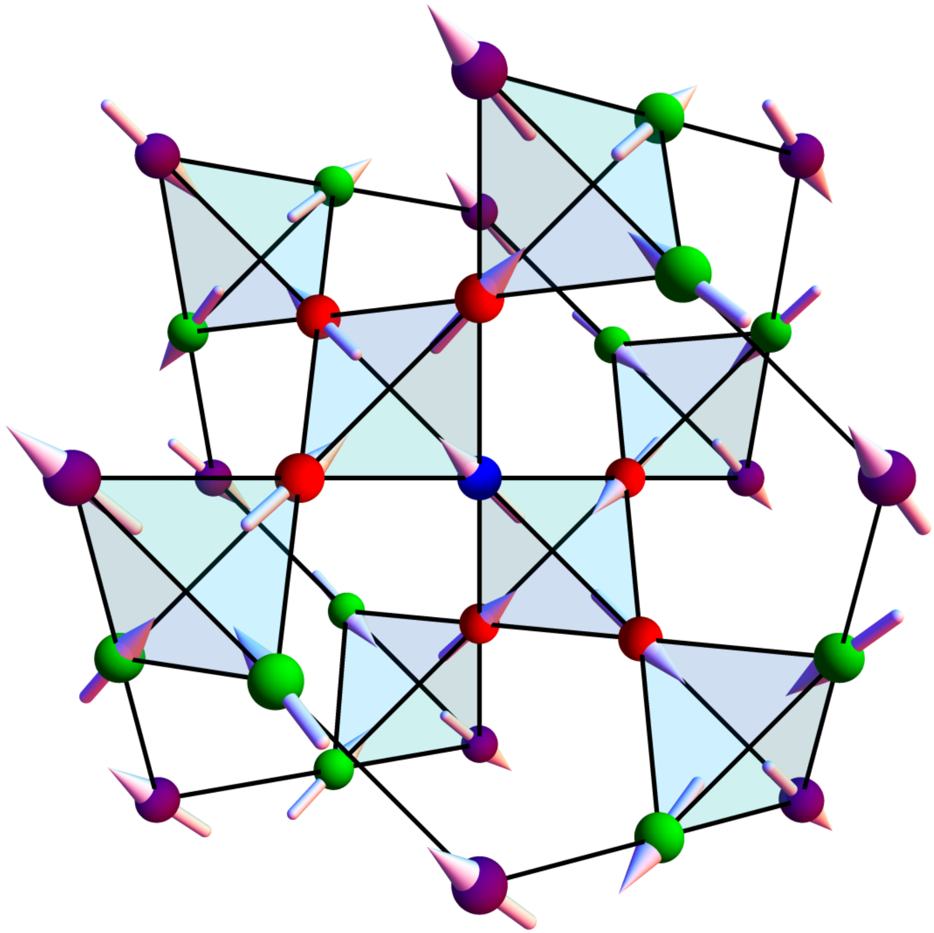


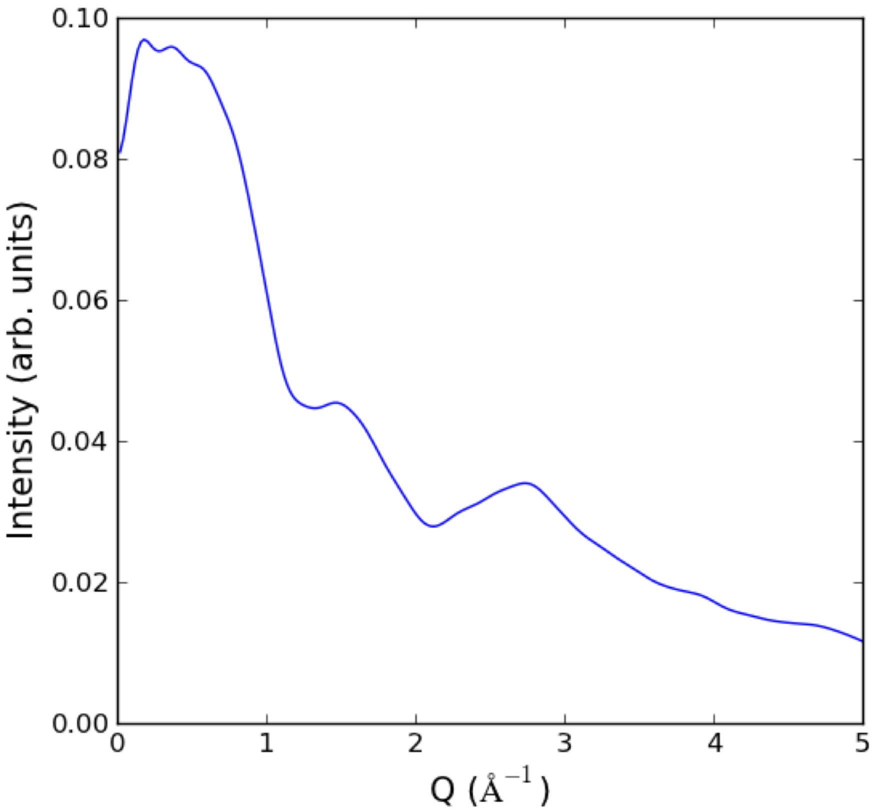
Example: Cubic antiferromagnet



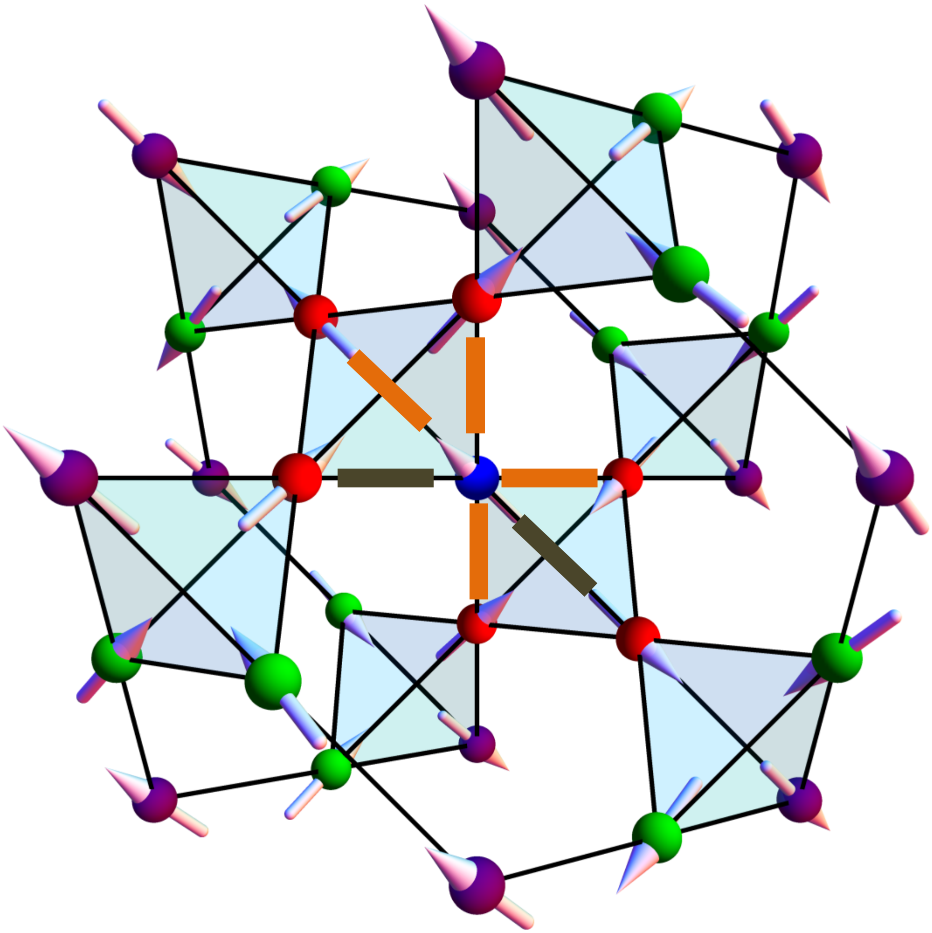


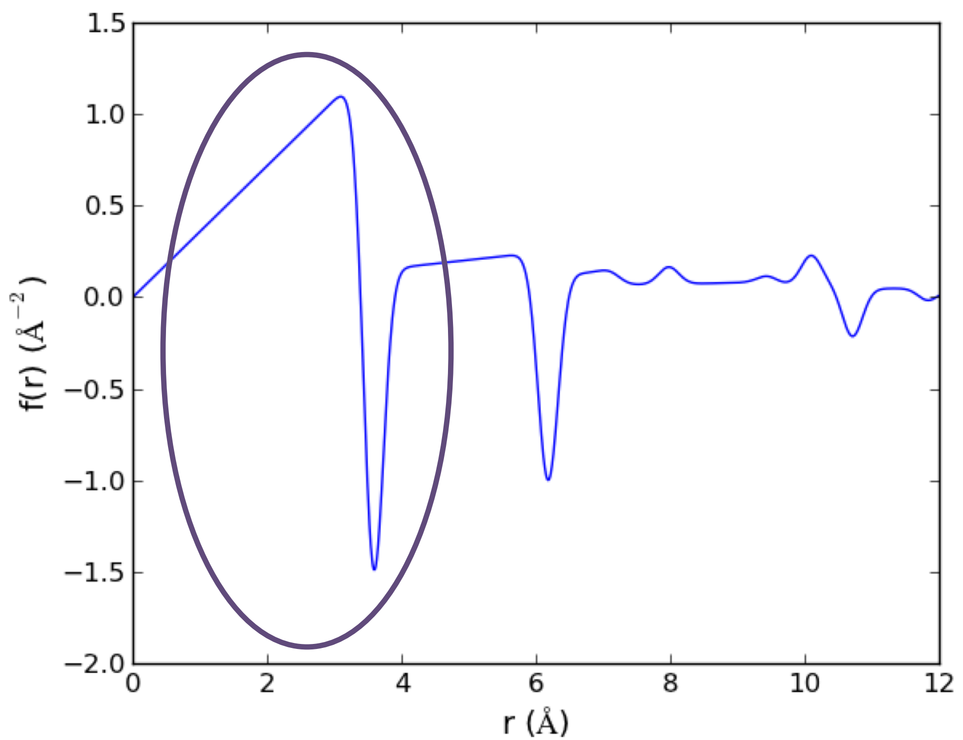
Spin ice





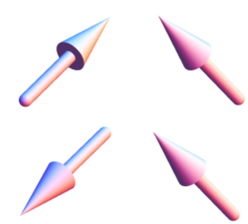
Spin ice



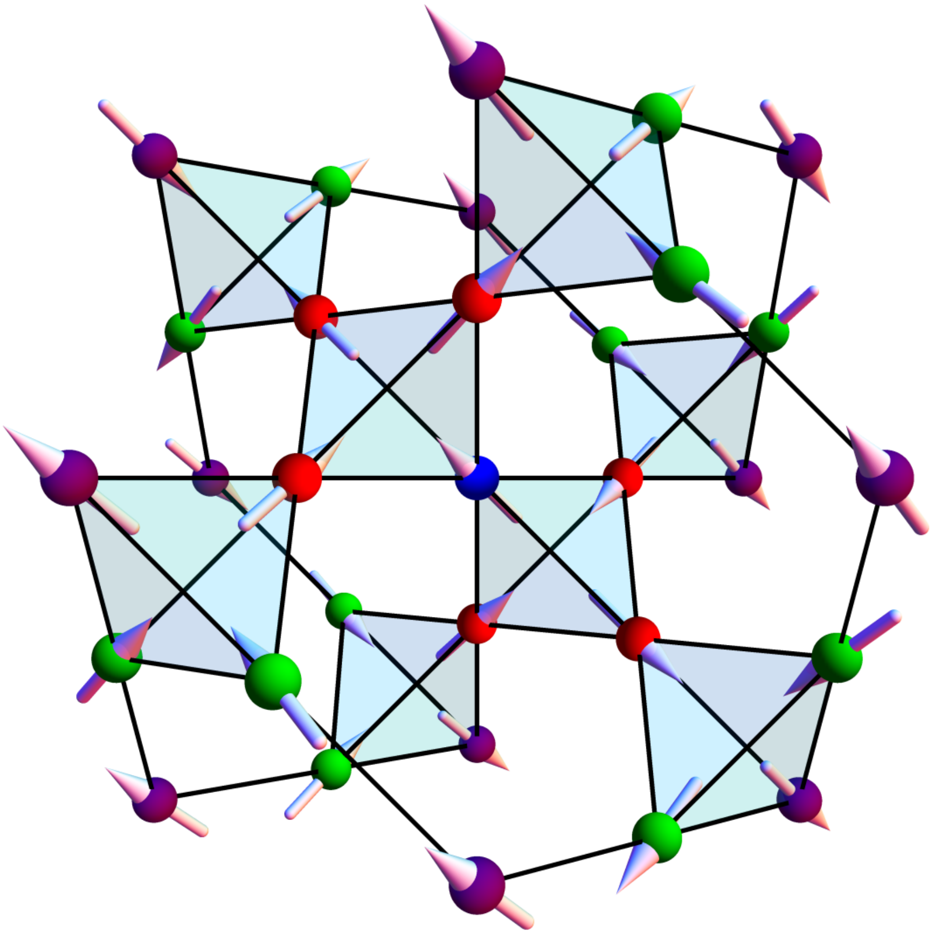


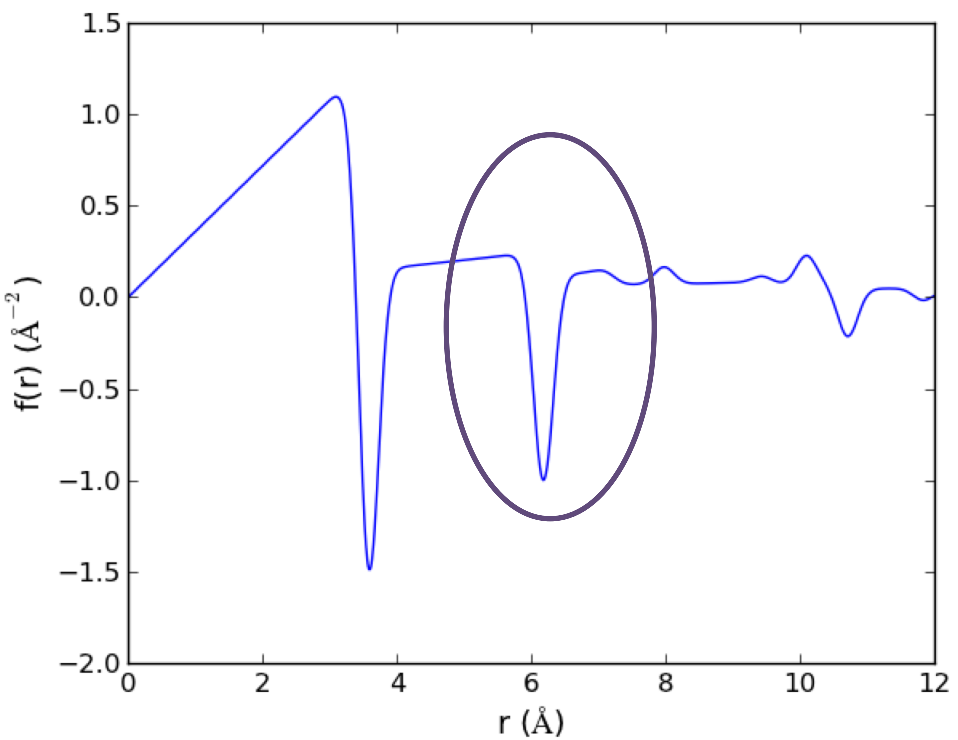
2 partners: positive peak, negative baseline

4 anti-partners: negative peak, positive baseline



Spin ice





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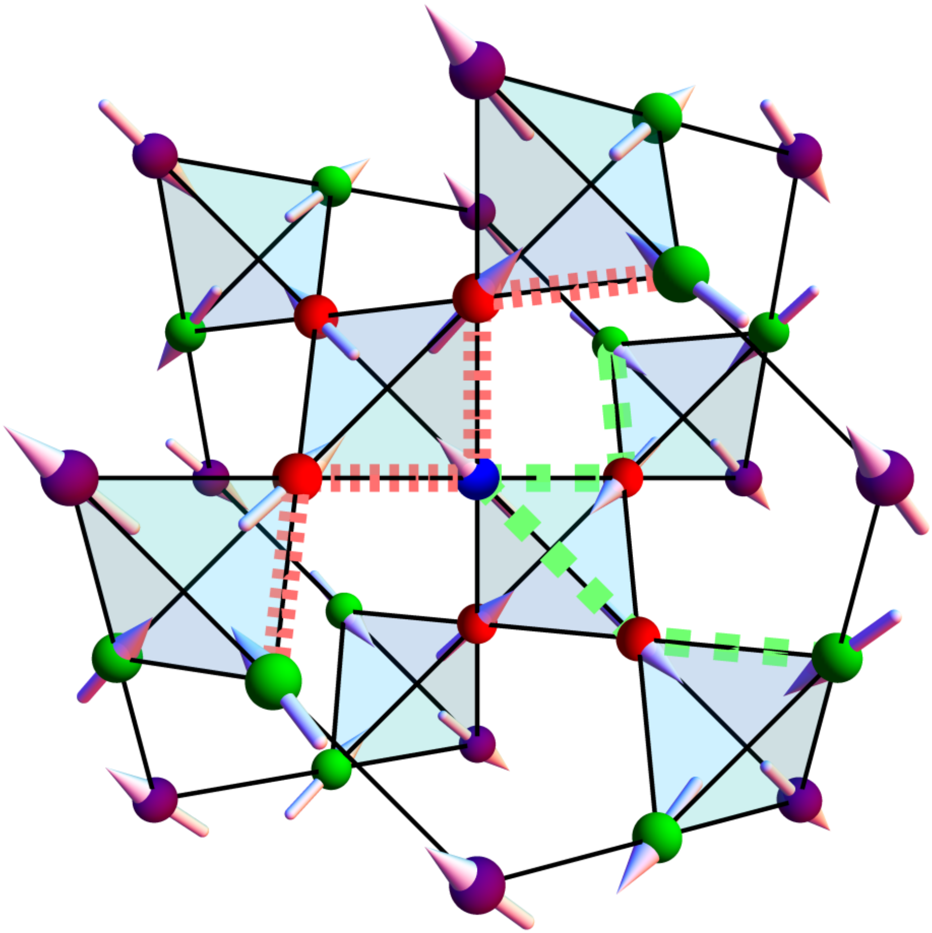

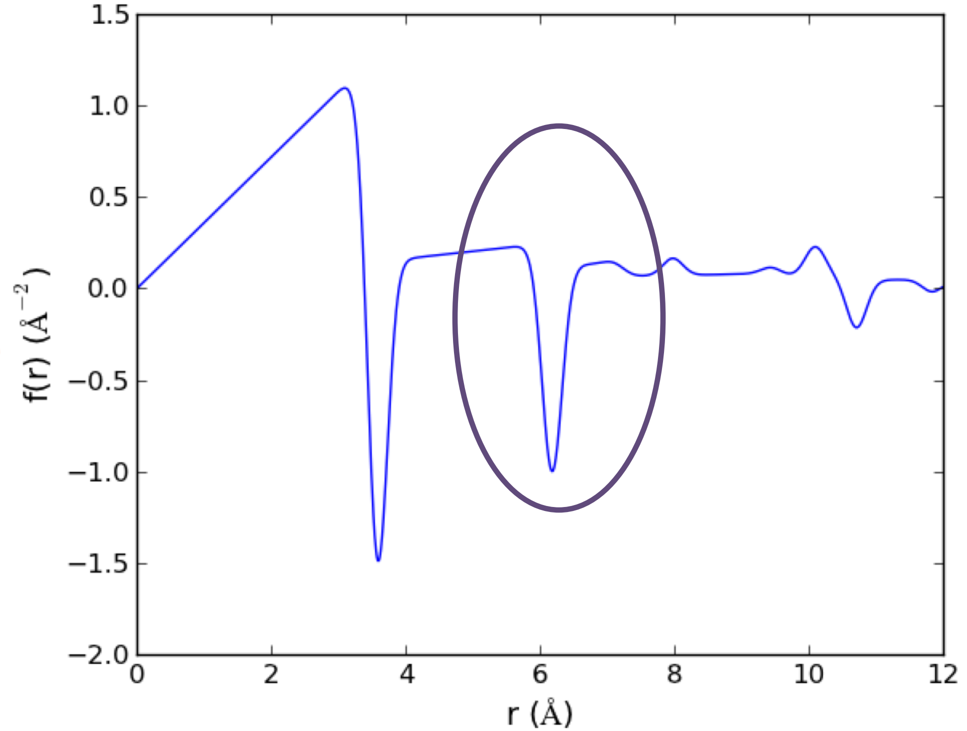

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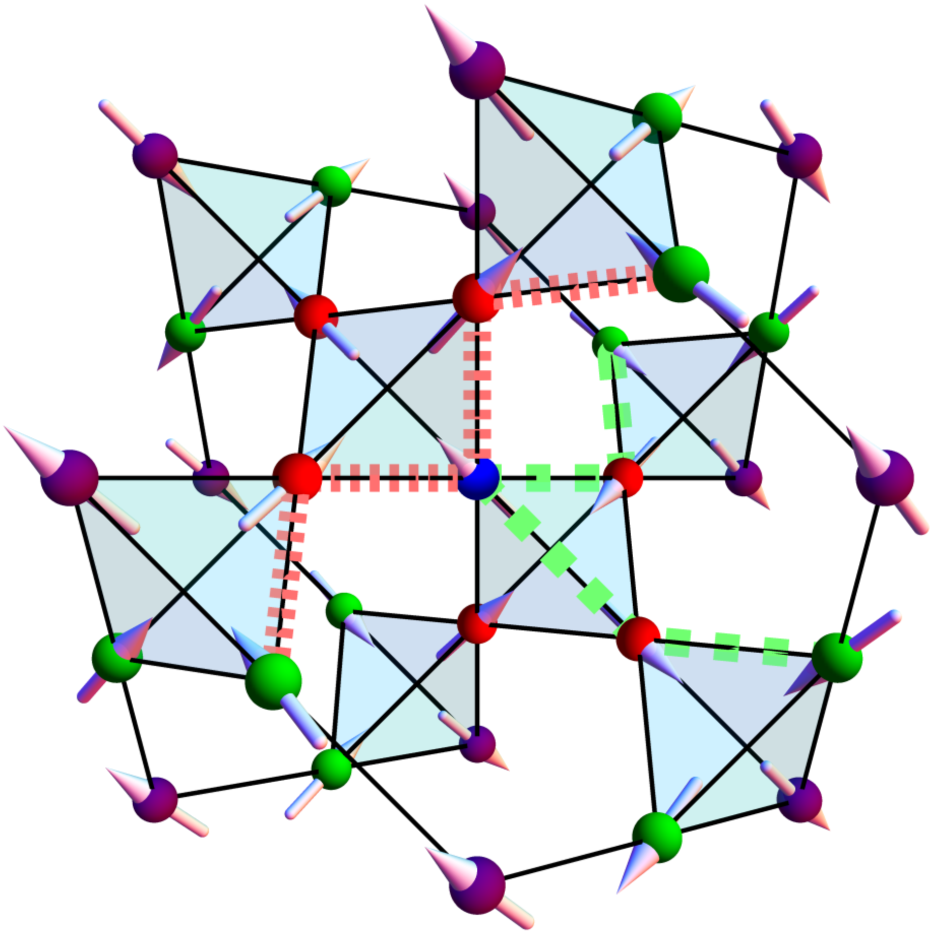
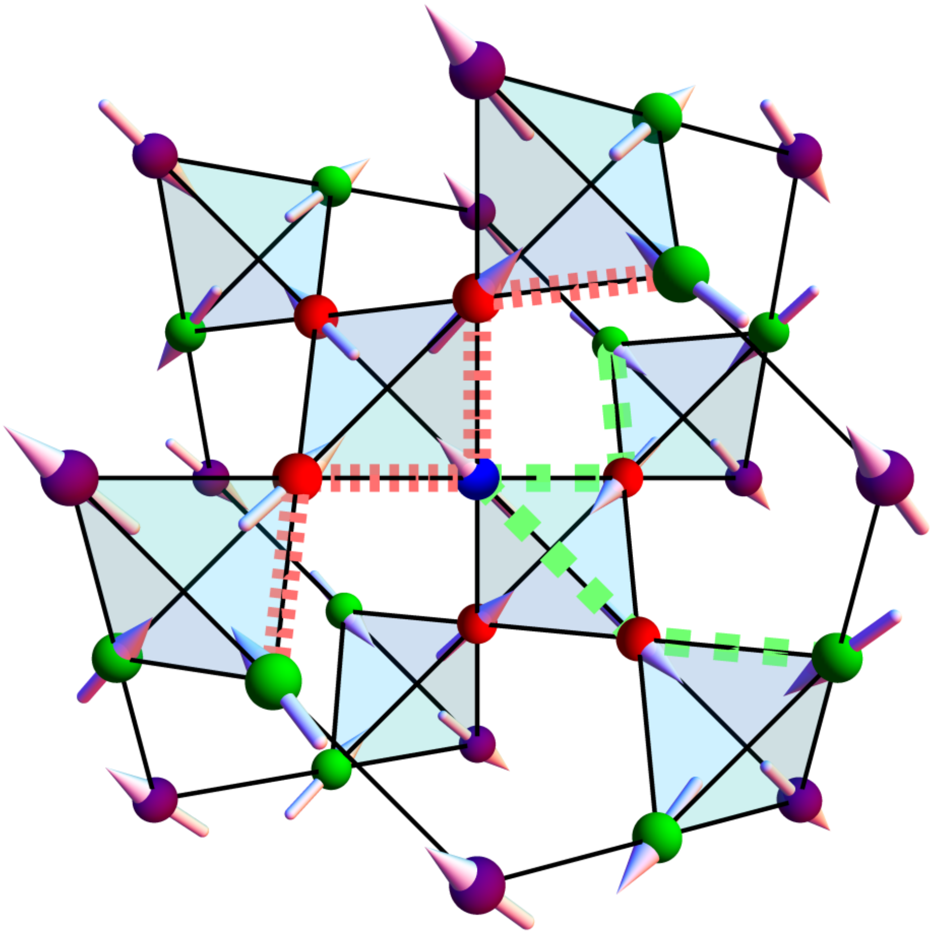


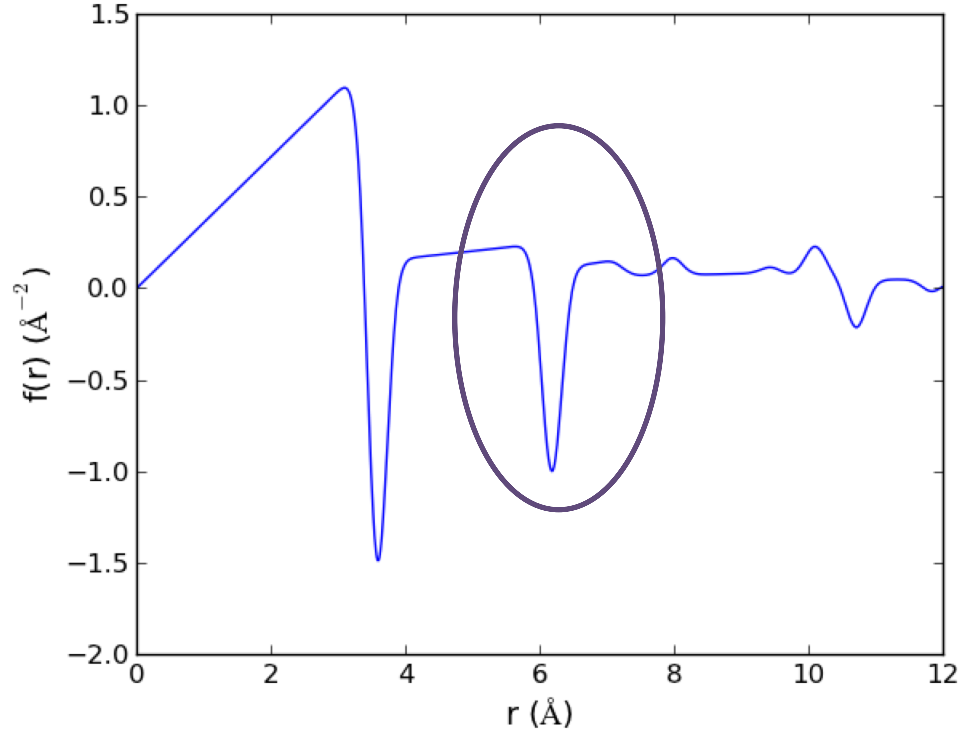
Types of 3-spin chains:
O-P-A, O-A-P: positive peak
O-P-P, O-A-A: negative peak

4 x 2 x 2 + 4x 1 x 2 + 2x 2 x 2 + 2 x 1 x 2
O-A-A O-A-P O-P-A O-P-P

36 possibilities:
16 O-P-A or O-A-P (positive peak)
20 O-A-A or O-P-P (negative peak)

Spin ice





3-spin chains:

O-P-A, O-A-P: positive peak

O-P-P, O-A-A: negative peak

36 possibilities:

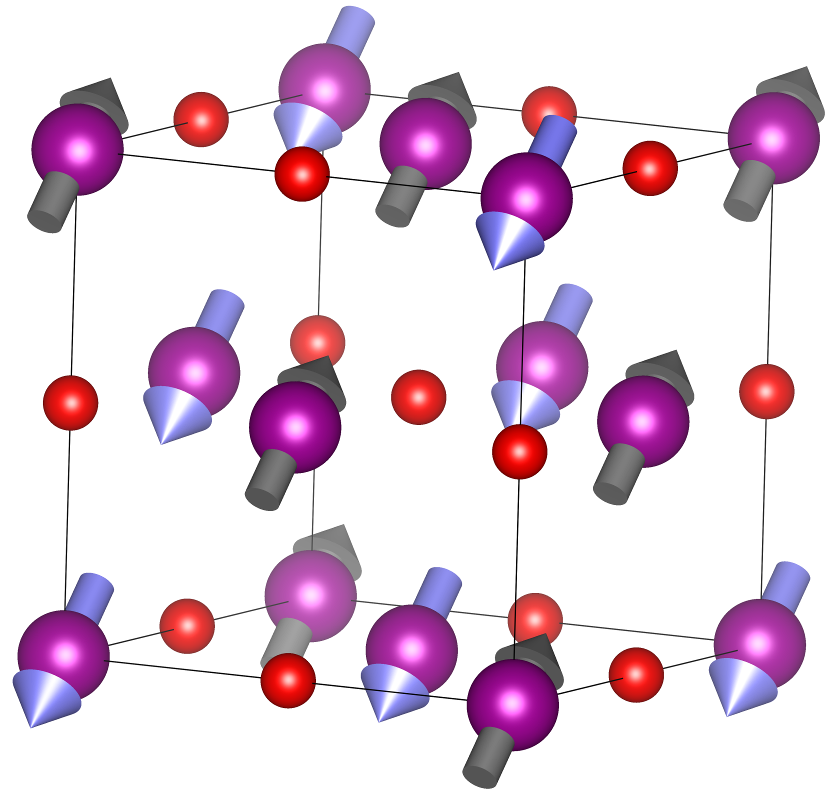
16 O-P-A or O-A-P (positive)

20 O-A-A or O-P-P (negative)

Obtaining the experimental mPDF

Test case: MnO

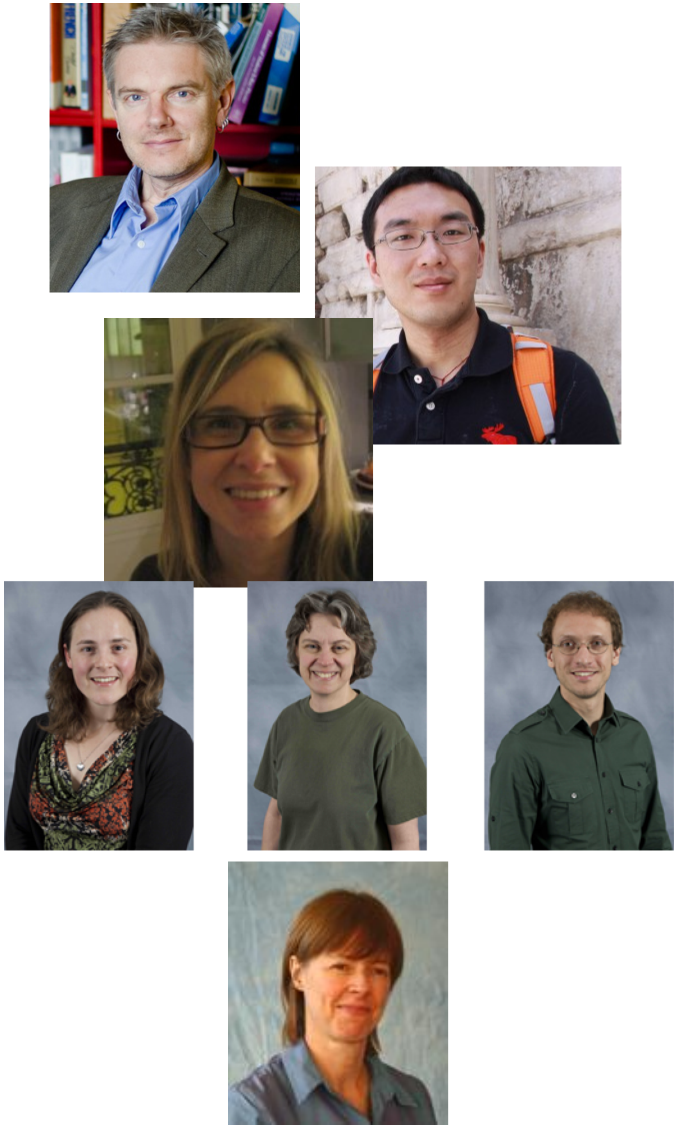
- T_N = 118 K
- Spins aligned within (111)-type sheets, anti-aligned between sheets
- Rhombohedral contraction along [111]
- First material to have its magnetic structure determined! (Schull et al 1951)



The challenge

- Accurately isolate the full magnetic scattering intensity over a sufficient Q-range
  – Polarized neutrons (i.e. xyz/10-pt polarization)
  – Fit to and subtract out nuclear structure
  – More sophisticated approaches: field-dependent measurements, combined x-ray/neutron, etc.
- Sequential/simultaneous nuclear and magnetic PDF analysis

mPDF analysis of MnO



Simon Billinge

Columbia University

Xiaohao Yang

Department of Applied Physics and Applied Mathematics, Columbia University

Michela Brunelli

Swiss Norwegian Beamlines, ESRF

Kate Page, Joan Siewenie,

& Graham King

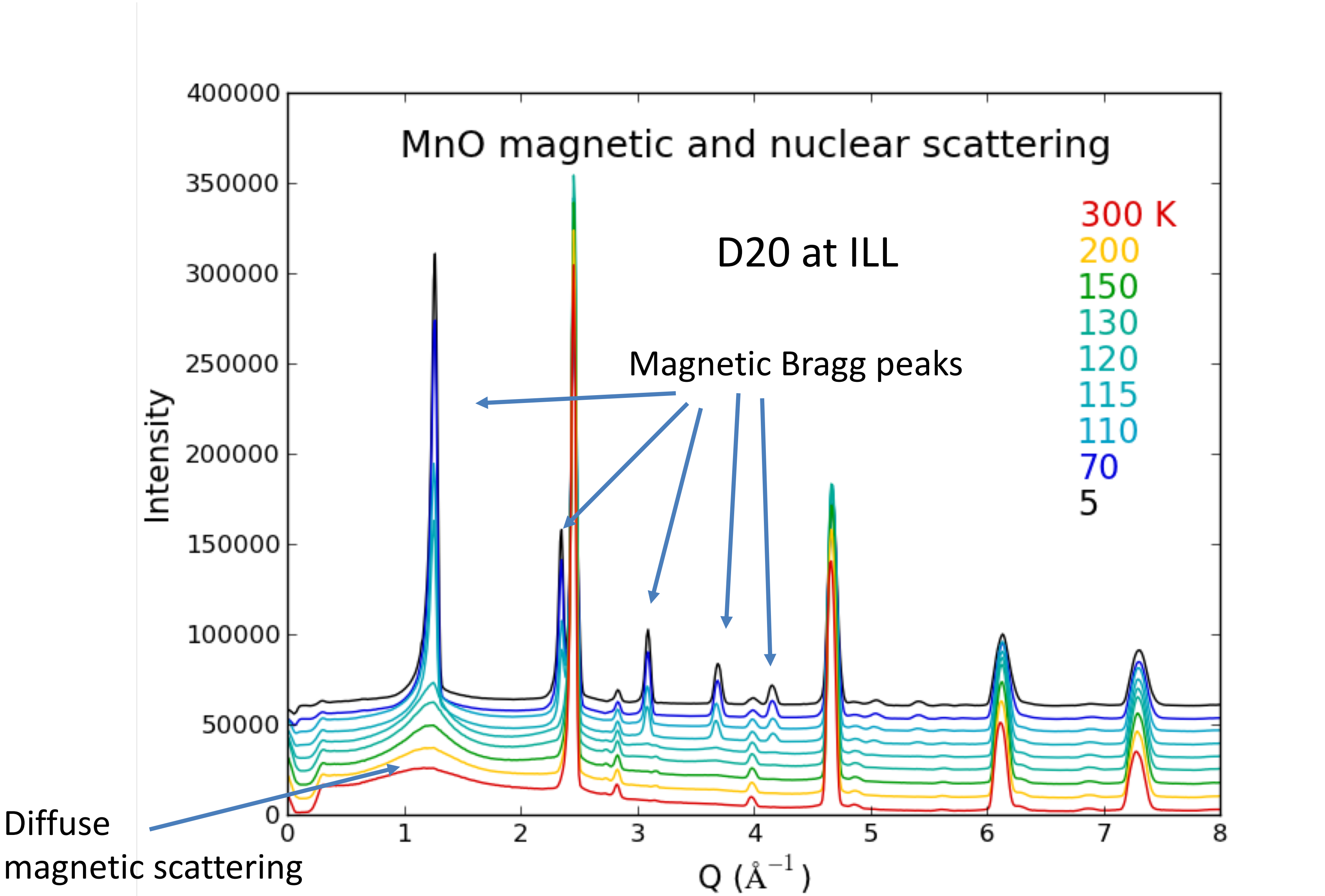
Lujan Center, Los Alamos National Laboratory

Julie Staunton

Department of Physics,

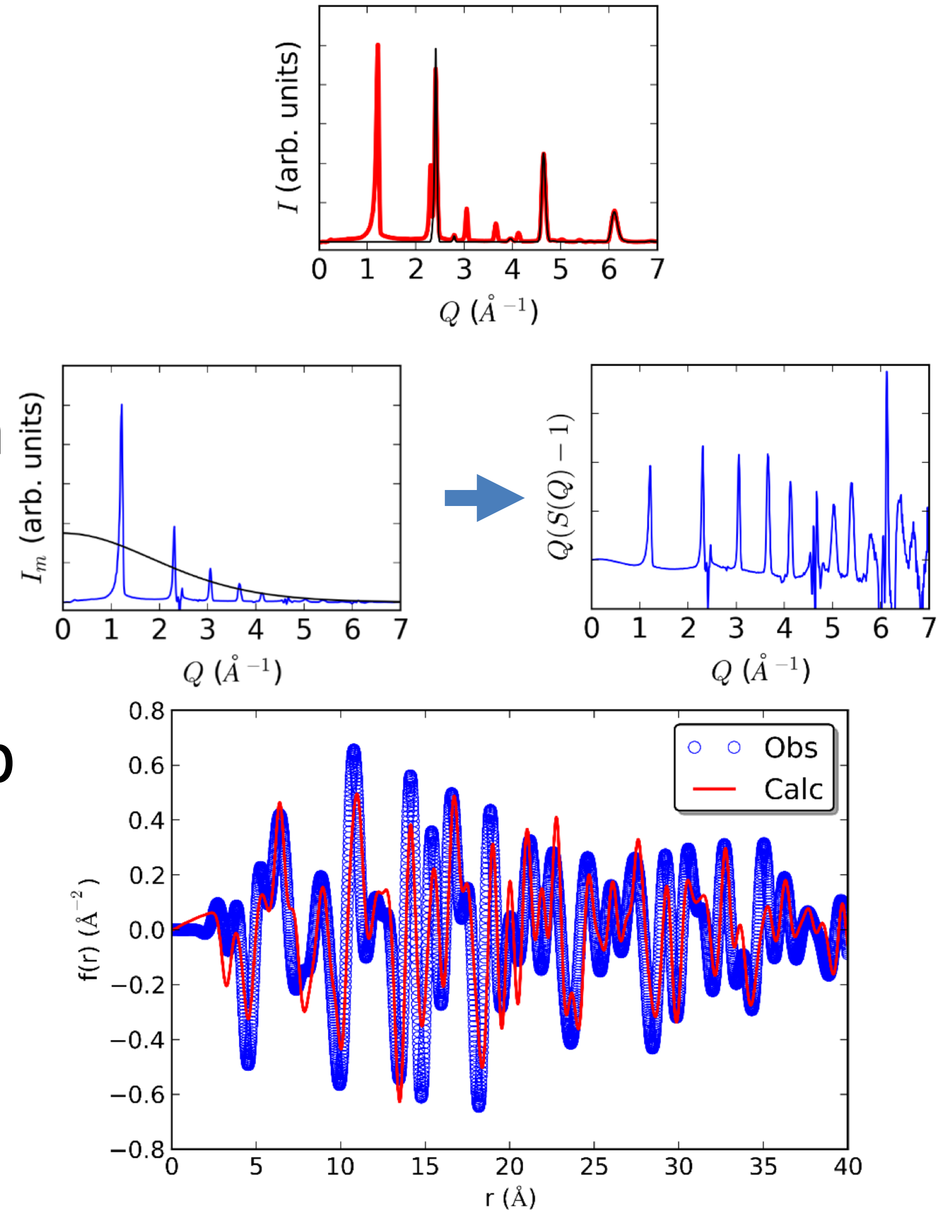
University of Warwick

Conventional neutron scattering from MnO



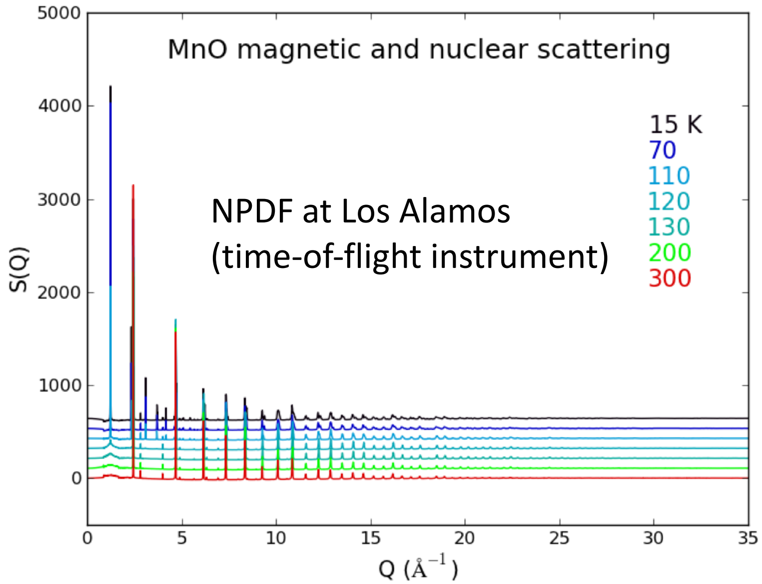
Obtaining the experimental mPDF

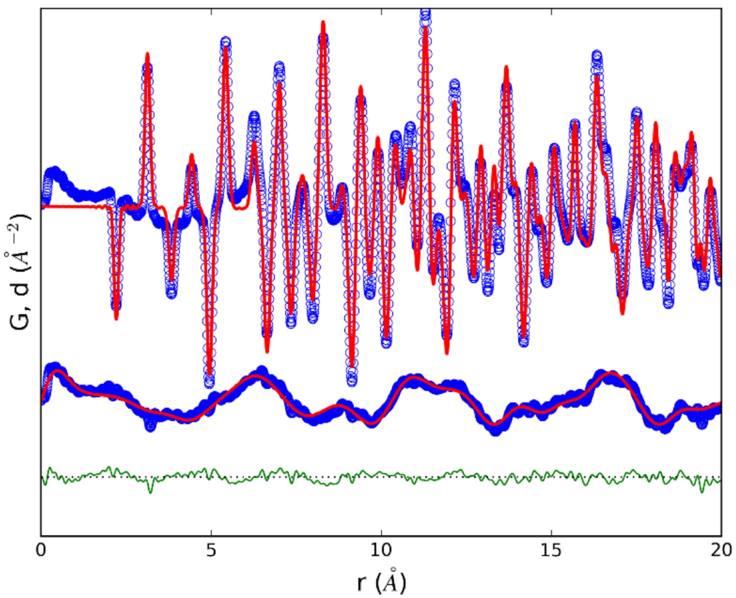
- Fit to and subtract out the nuclear Bragg peaks
- Normalize by the magnetic form factor
- Fourier transform to obtain the real-space mPDF
- Quite noisy due to amplification of small errors in normalization step
- Sufficient to verify mPDF equations and encourage future developments
- Is there another way?



Simultaneous atomic and magnetic PDF

- Perform neutron total scattering experiment just like usual atomic PDF
- Process data according to standard atomic PDF protocols
- Result: additive combination of the usual atomic PDF and the (unnormalized) mPDF
- Model the atomic and magnetic PDFs together





Total PDF: nuclear PDF + mPDF

$$G_{tot}(r) = \mathcal{F}\left[Q(S_{tot}(Q) - 1)\right]$$

$$S_{tot}(Q) - 1 = \frac{I_{tot}}{N\langle b\rangle^2} - \frac{\langle b^2\rangle}{\langle b\rangle^2}$$

$$I_{tot} = I_n + I_m$$

$$G_{tot}(r) = \mathcal{F}\left[Q\left(\frac{I_n}{N\langle b\rangle^2} - \frac{\langle b^2\rangle}{\langle b\rangle^2}\right)\right] + \mathcal{F}\left[Q\frac{I_m}{N\langle b\rangle^2}\right]$$

$$= G_n(r) \qquad + \qquad \boxed{d(r)}/N\langle b\rangle^2$$

d(r): "unnormalized" mPDF

$$d(r) = \mathcal{F}\left[QI_m(Q)\right]$$

cf.

$$f(r) \sim \mathcal{F}\left[Q\left(\frac{I_m(Q)}{f^2(Q)} - 1\right)\right]$$

Properly normalized mPDF

$$d(r) = f(r) * S(r) - \sqrt{2\pi}\frac{\mathrm{d}S}{\mathrm{d}r}$$

$$S(r) = s(r) * s(r) = \int \mathrm{d}r' s(r') s(r - r')$$

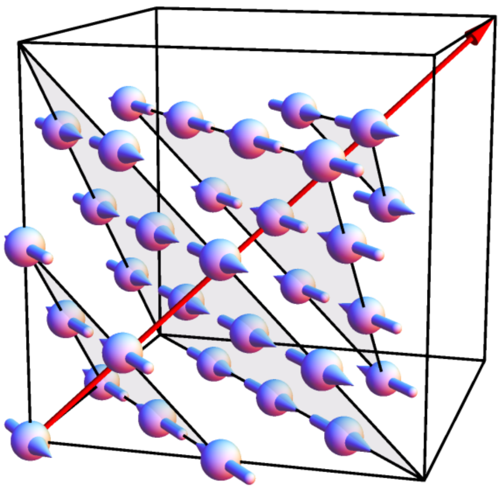
Related to real-space extent of magnetic moment

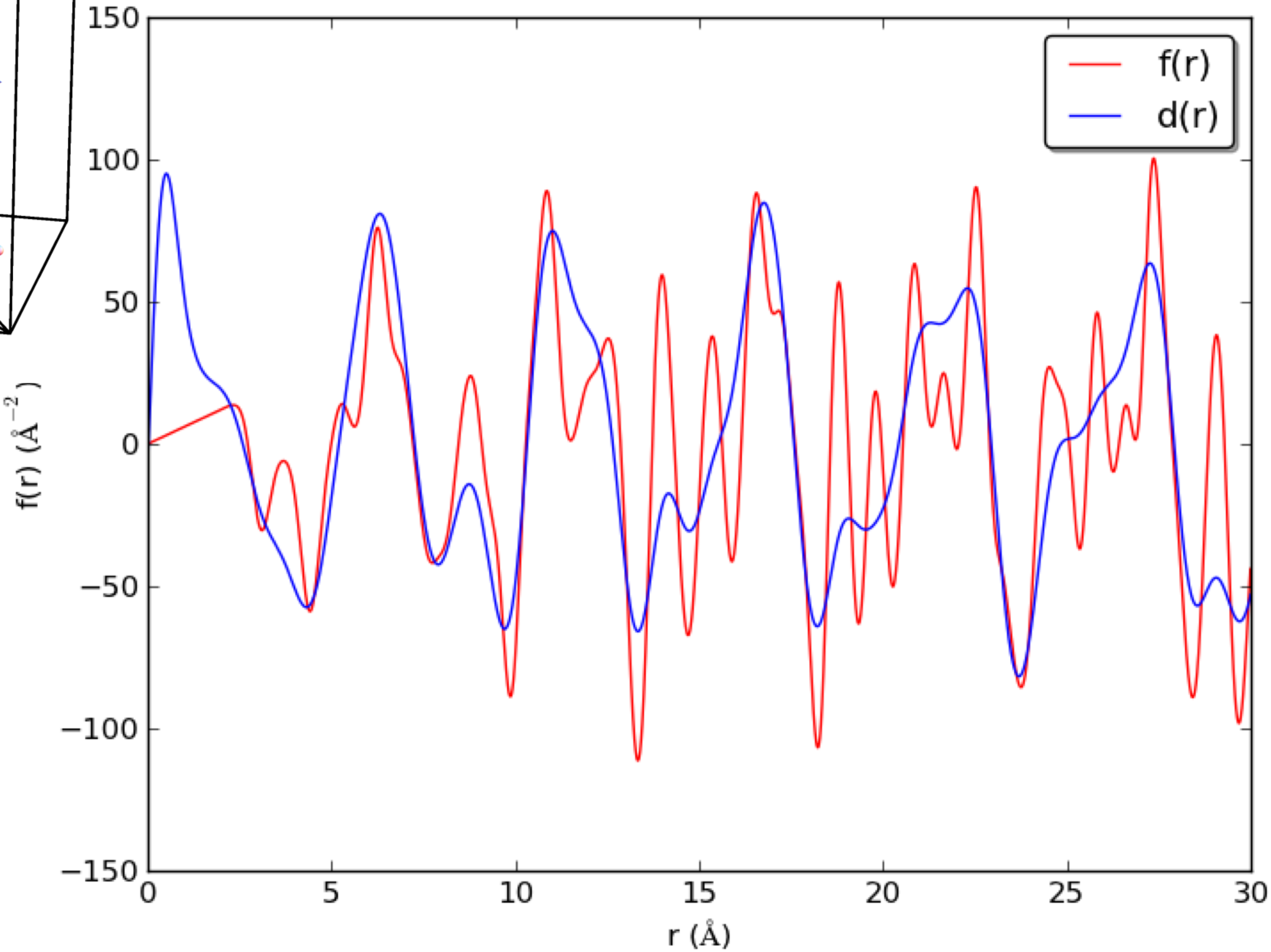
$$s(r) = \mathcal{F}\left[f(Q)\right] = \int \mathrm{d}Q \exp iQr\, f(Q)$$

Magnetic form factor

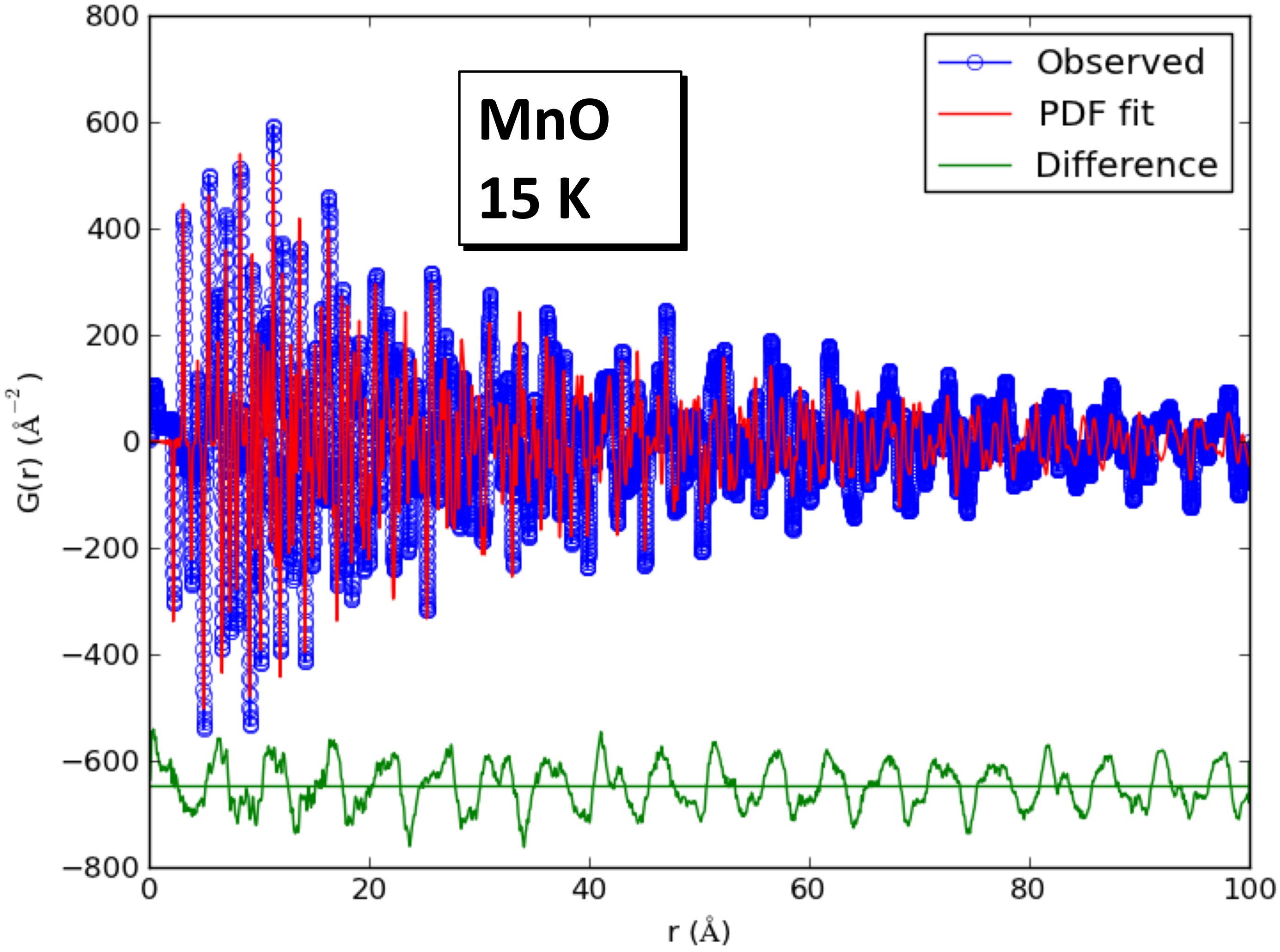
For details: Frandsen & Billinge, Acta A **71** 325 (2015)

“Unnormalized” mPDF: MnO

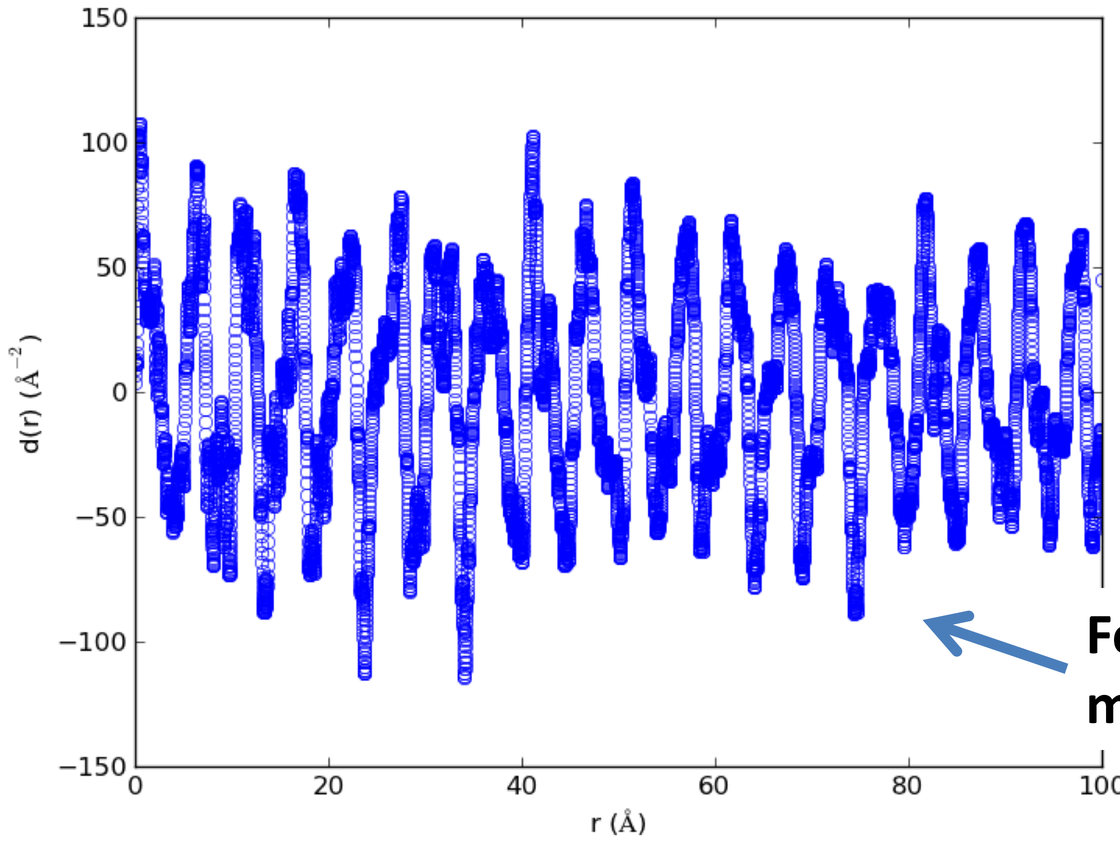




Atomic PDF fits

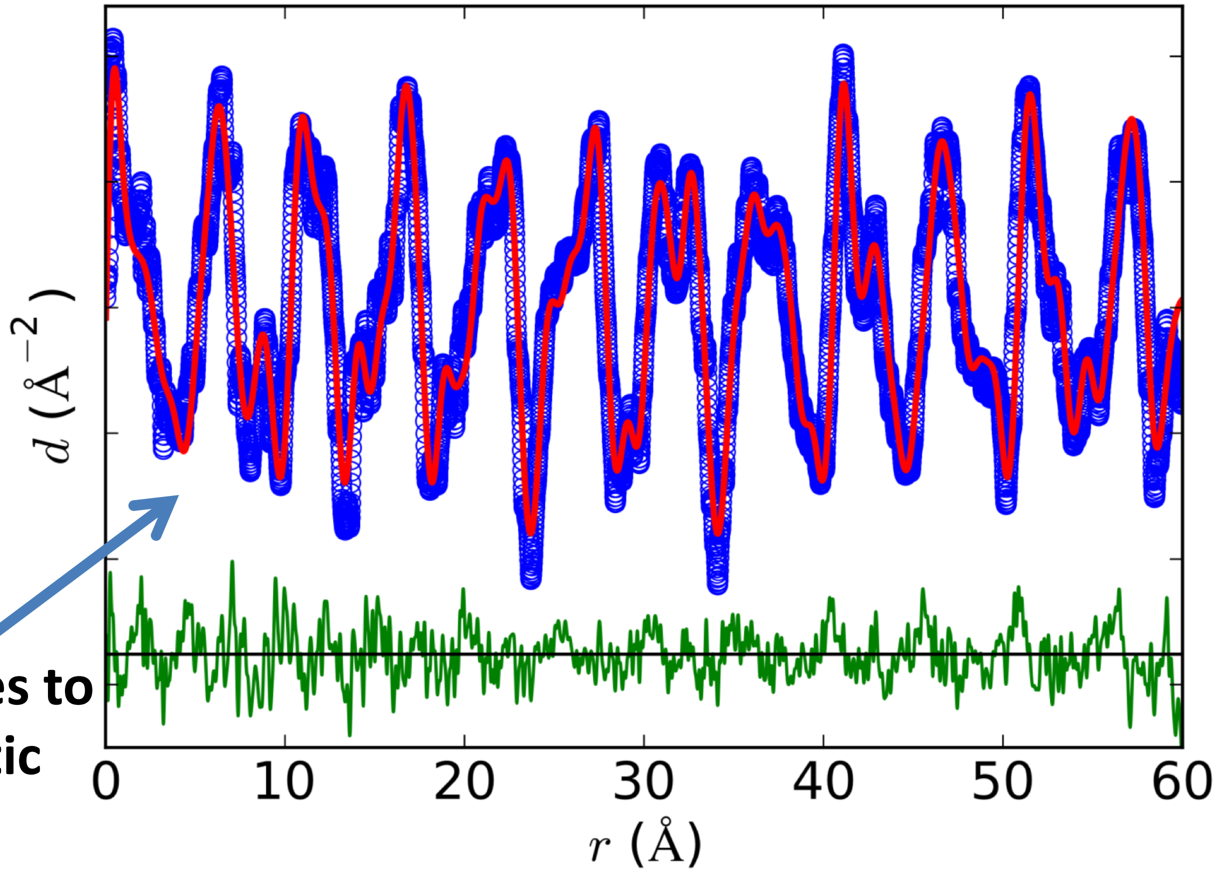


Atomic PDF fit: difference curve



Fourier transformed magnetic signal d(r)

Atomic PDF fit: difference curve

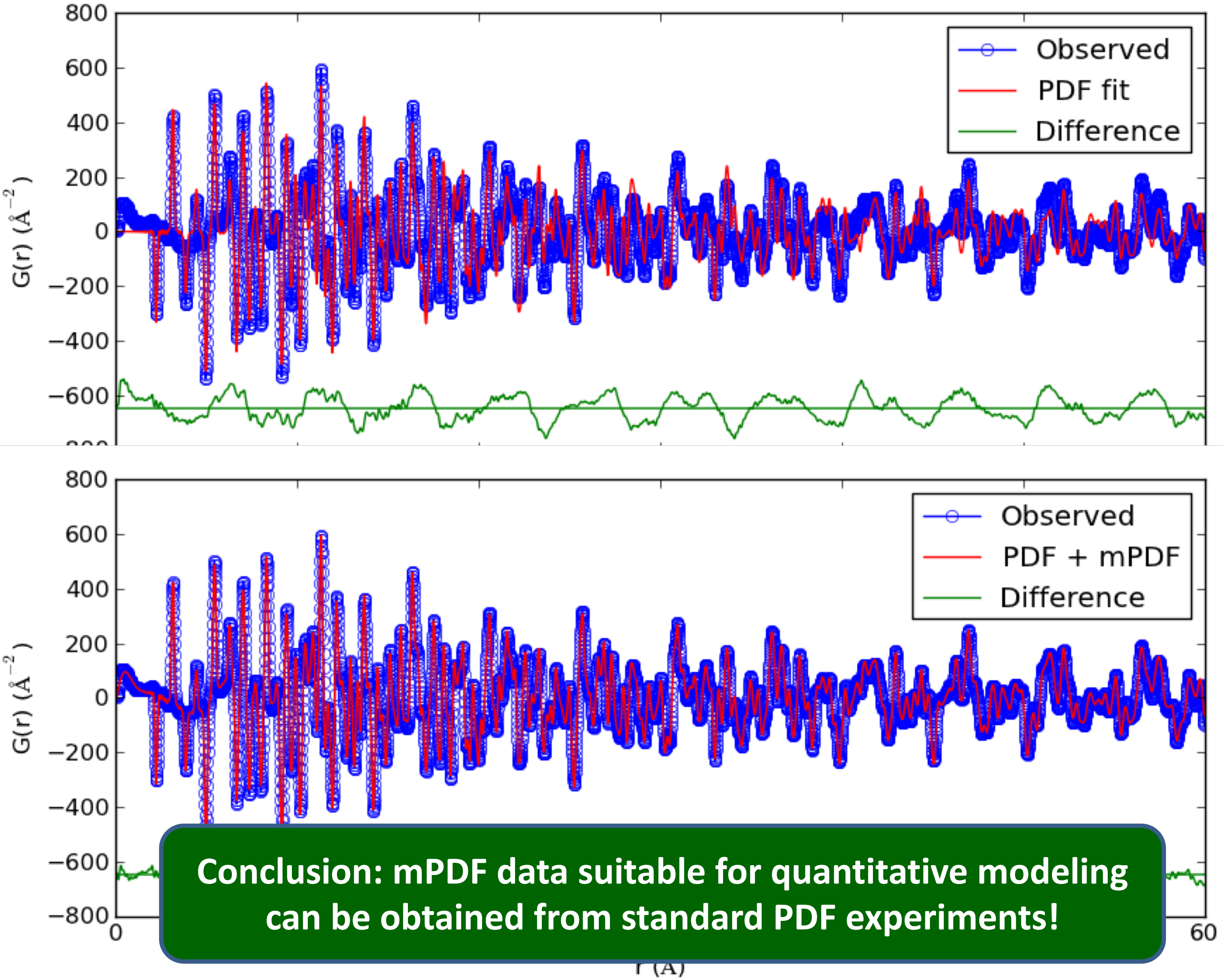


Robustly refines to known magnetic structure

$$G_{\mathrm{tot}}(r) = G_{\mathrm{n}}(r) + d(r)/N_{\mathrm{a}}\langle b\rangle^2$$

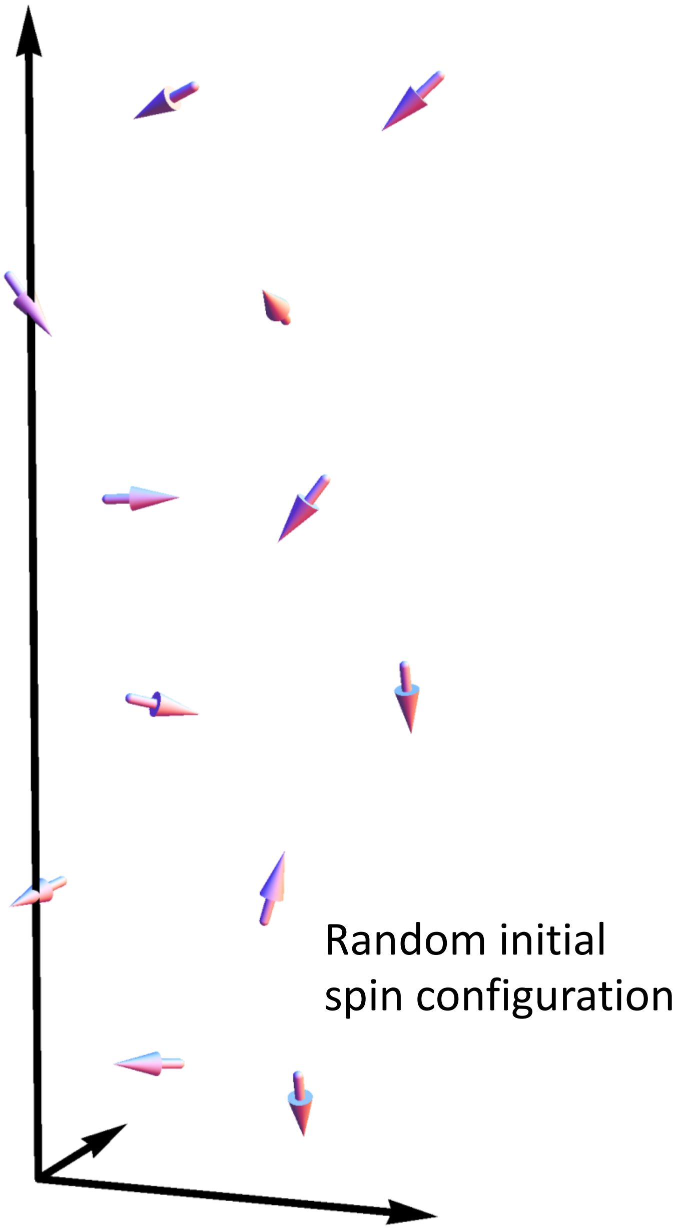
$$d(r) = C_1 \times f(r) * S(r) + C_2 \times \frac{\mathrm{d}S}{\mathrm{d}r}$$

Including the mPDF contribution

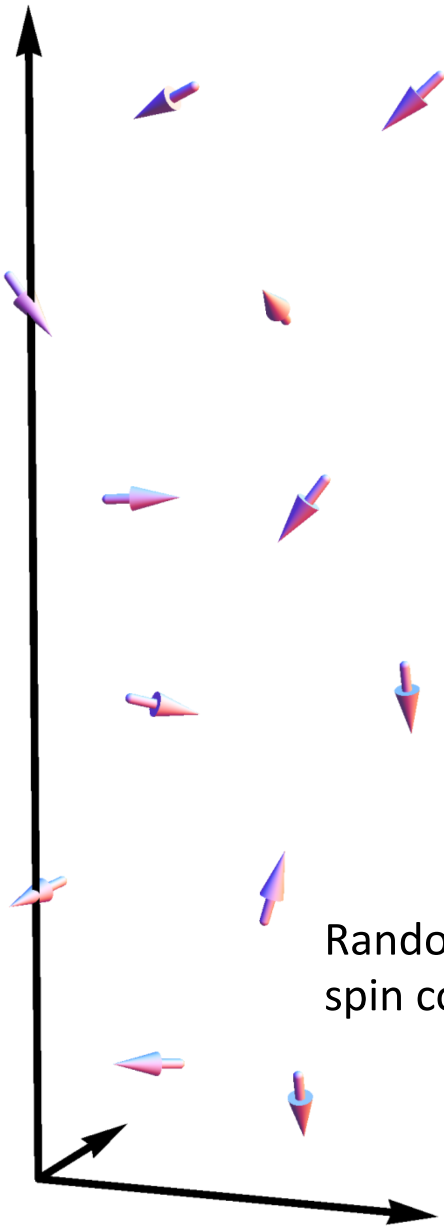


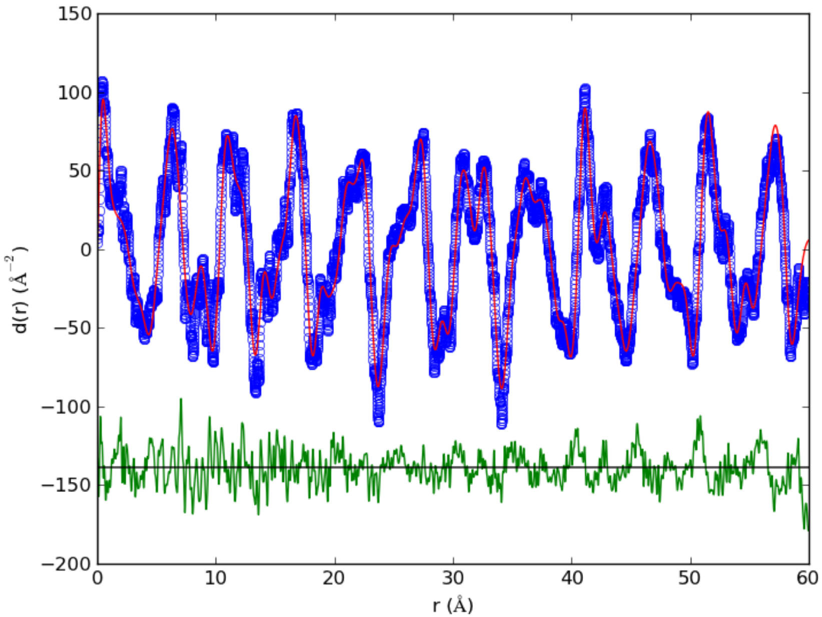
Conclusion: mPDF data suitable for quantitative modeling can be obtained from standard PDF experiments!

Ab initio magnetic structure solution



Ab initio magnetic structure solution

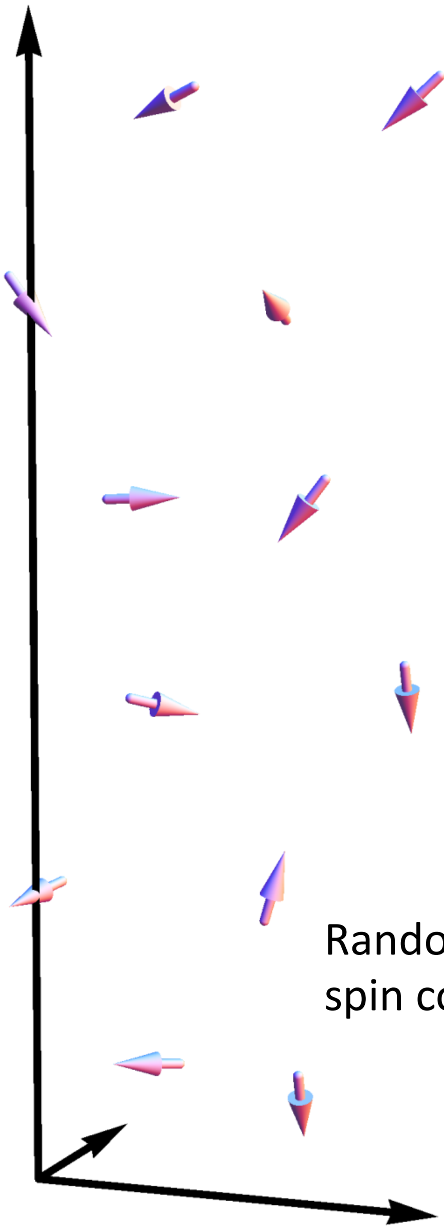


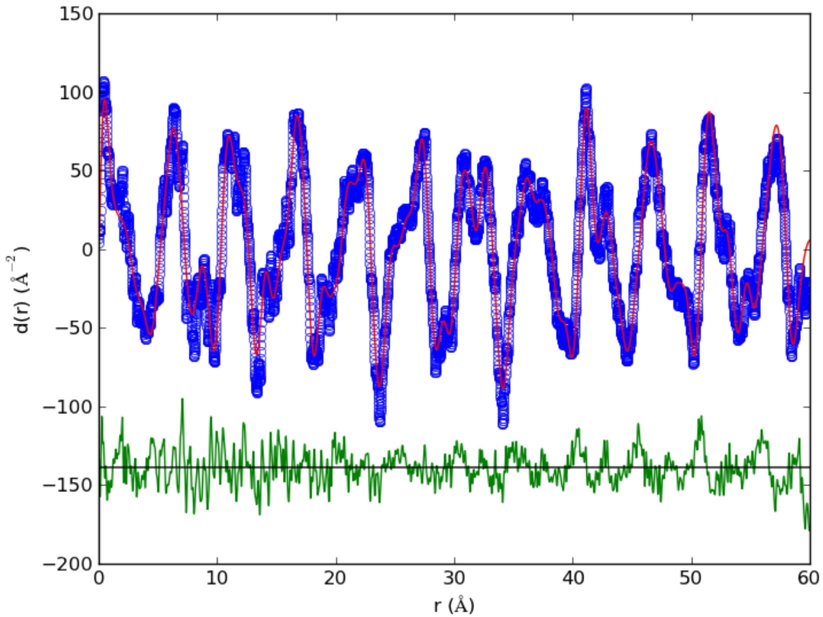


Refine all spins independently against experimental data

Random initial spin configuration

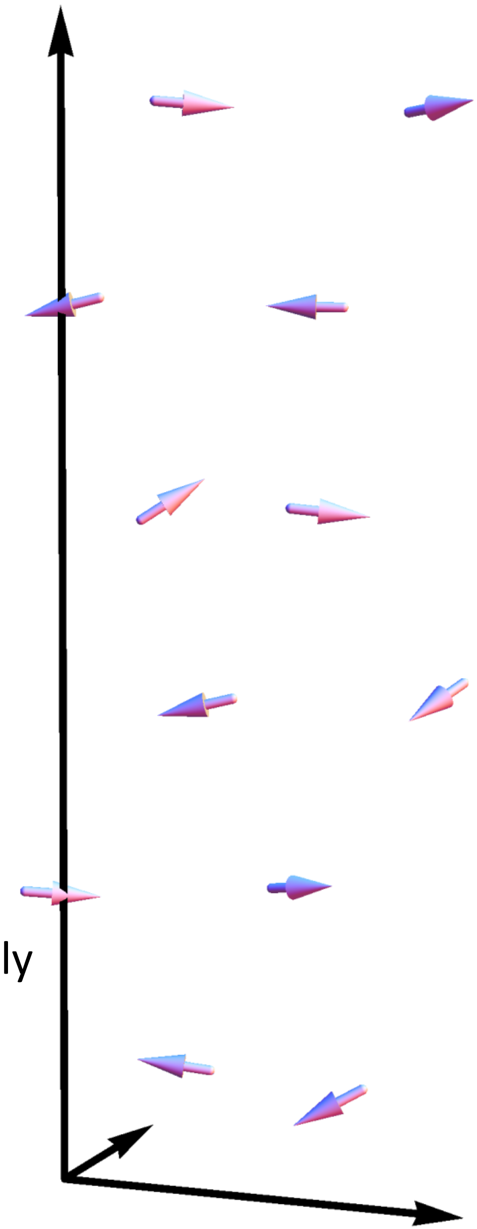
Ab initio magnetic structure solution





Refine all spins independently against experimental data

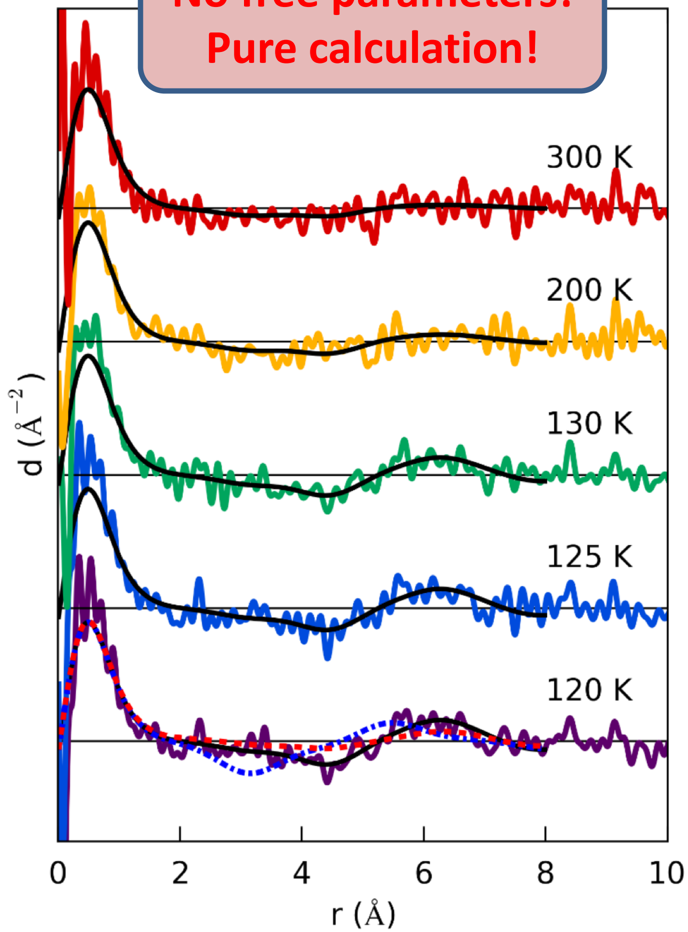
Random initial spin configuration



Correct AF arrangement quickly produced

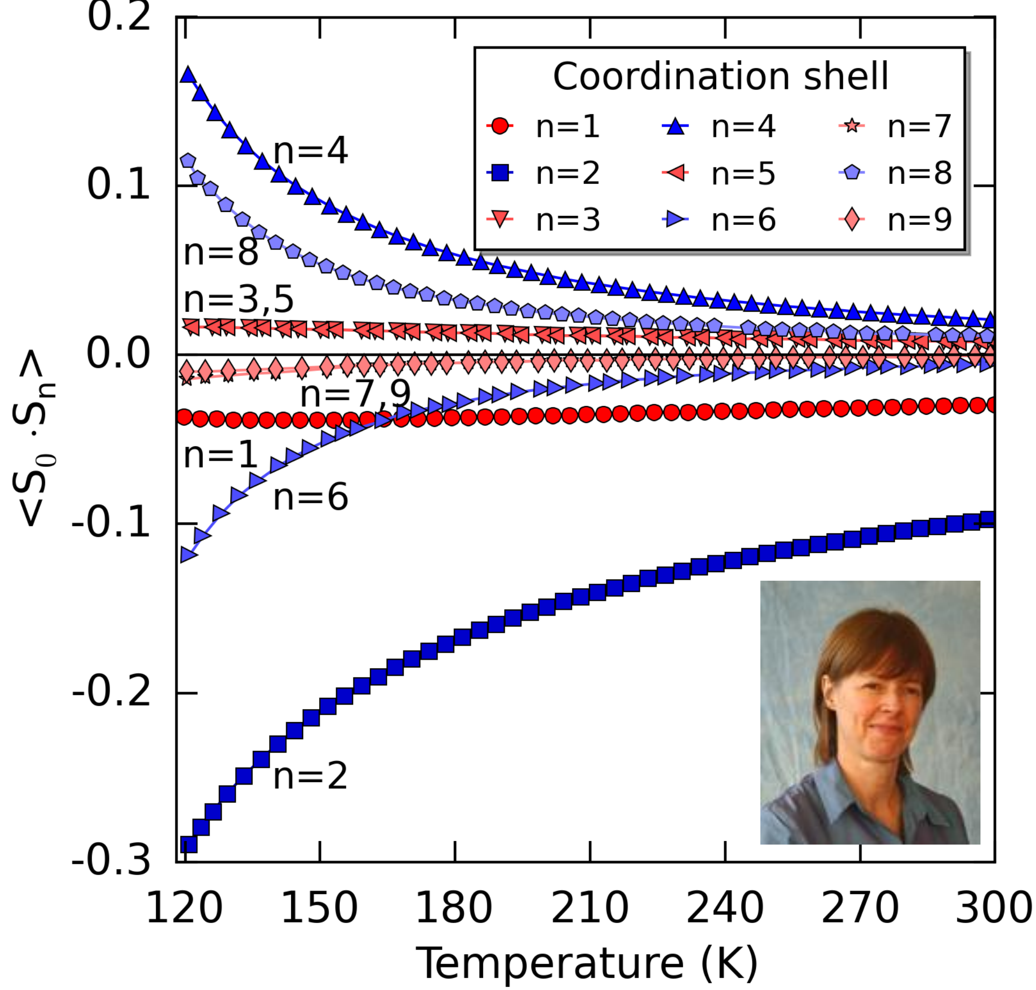
mPDF from MnO in paramagnetic phase

No free parameters!
Pure calculation!



Superexchange dominates over direct exchange

Frandsen et al, PRL **116** 197204 (2016)



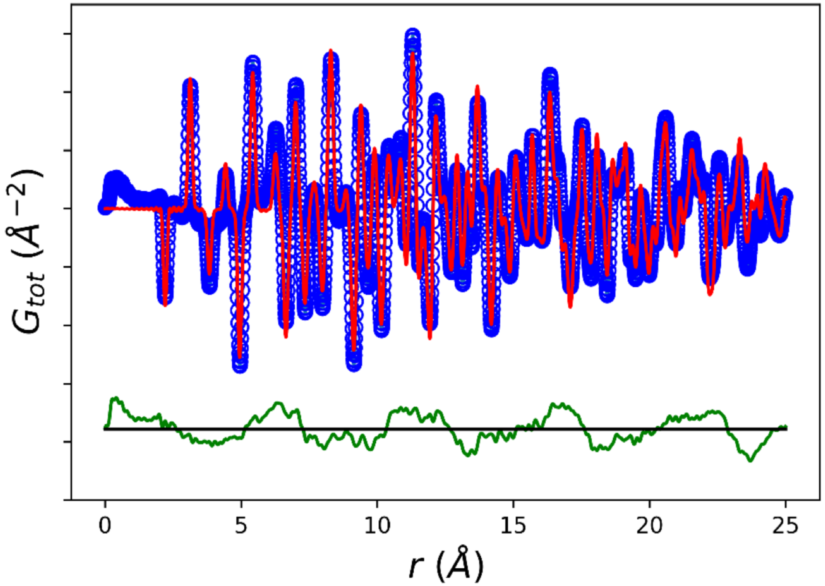
Density functional theory (SIC-LSDA/DLM approach), with Julie Staunton at U. Warwick

Summary of methods to obtain the mPDF

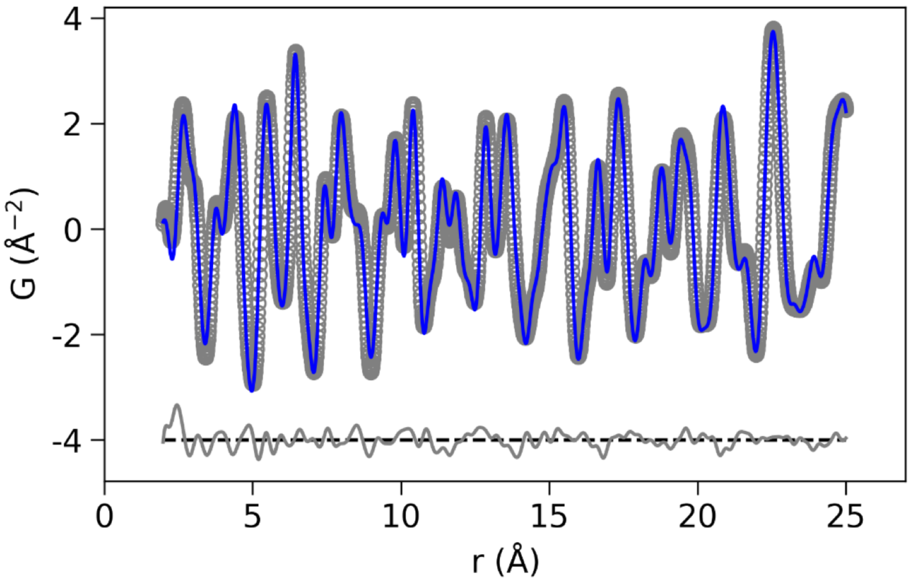
- Separate magnetic/nuclear scattering in reciprocal space and do proper normalization
  - Potential for high-resolution mPDF data
  - Data must be treated carefully
  - Should be developed further!
- Perform standard PDF experiment and get nuclear and (unnormalized) magnetic PDFs together
  - Easy and practical; no special effort required!
  - Lower real-space resolution
  - Easiest entry-point for PDF practitioners looking to do mPDF analysis

Handling sub-optimal mPDF data

- What if the mPDF is much smaller than the nuclear PDF?
- What if your model for the atomic structure is of limited quality?



MnO



$NaCaCo_2F_7$

Relative scales of magnetic/atomic PDFs

Ratio of mPDF scale factor to nuclear PDF scale factor:

$$\frac{N_s}{N_a}\frac{\frac{2}{3}(\frac{\gamma r_0}{2})^2(gJ)^2}{2\pi\langle b\rangle^2}$$

MnO

- N_s/N_a = 1/2
- <b> is quite small due to negative scattering length of Mn
- Very large mPDF signal!

$NaCaCo_2F_7$:

- N_s/N_a = 2/11
- <b> is much larger
- Greatly reduced mPDF signal

(Side note: This gives us a way to determine the ordered moment from mPDF measurements!)

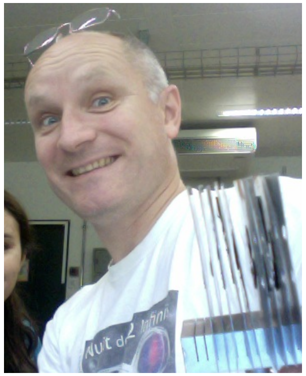
mPDF Analysis of $NaCaCo_2F_7$

Kate Ross

Bob Cava

Jason Krizan

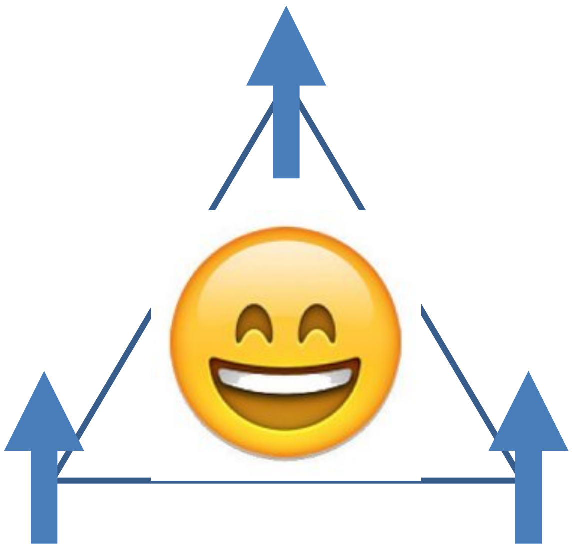
Andrew Wildes



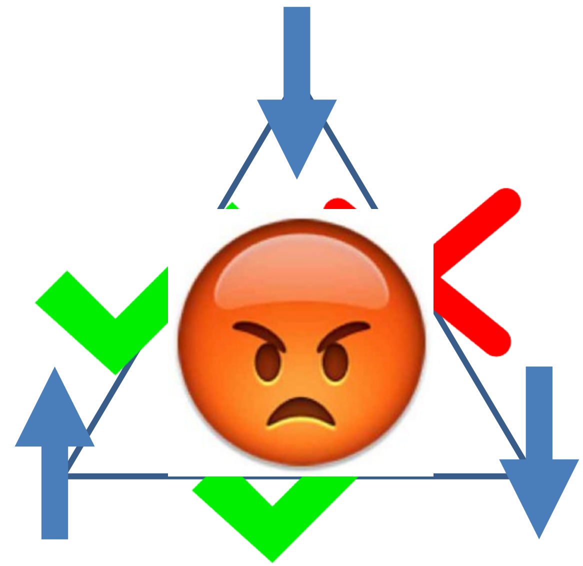
Gøran Nilsen

Gemoetrically Frustrated Magnets

Spins on a triangular lattice

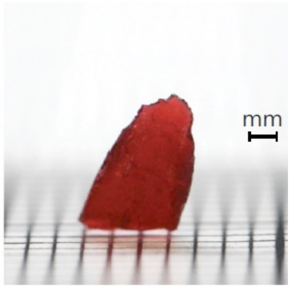


Case 1:
Ferromagnetic interactions



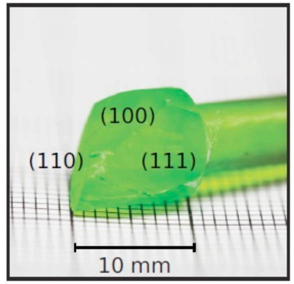
Case 2:
Antiferromagnetic interactions

Transition Metal Fluoride Pyrochlores



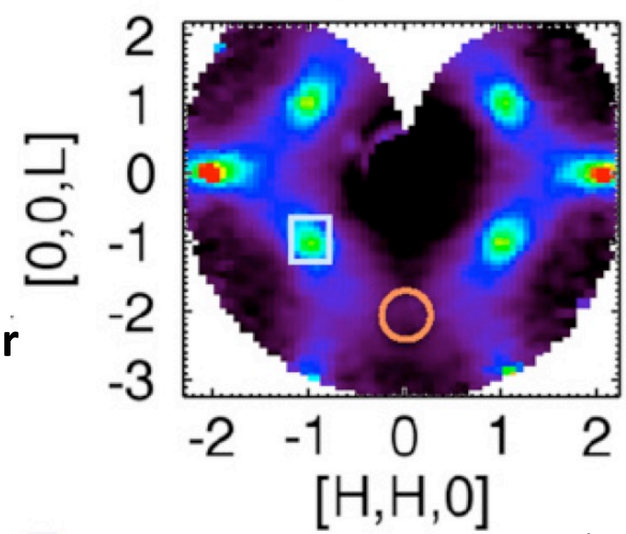
$NaCaCo_2F_7$

$NaSrCo_2F_7$

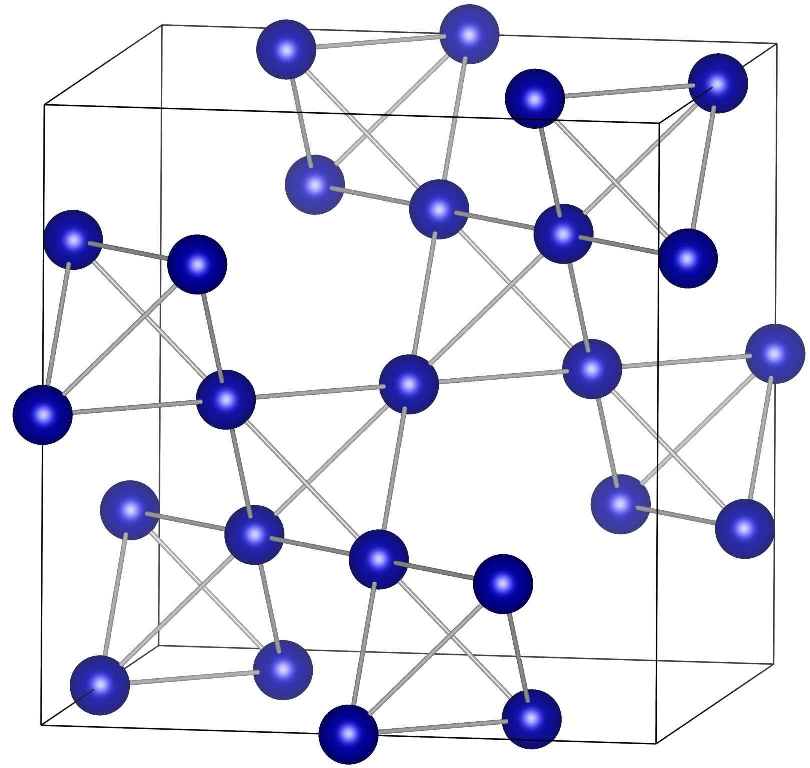


$NaCaNi_2F_7$

Co compounds: Spins freeze into short-range order below 5 K, remain correlated at higher temperatures



Ross et al, PRB 93, 014433 (2016)

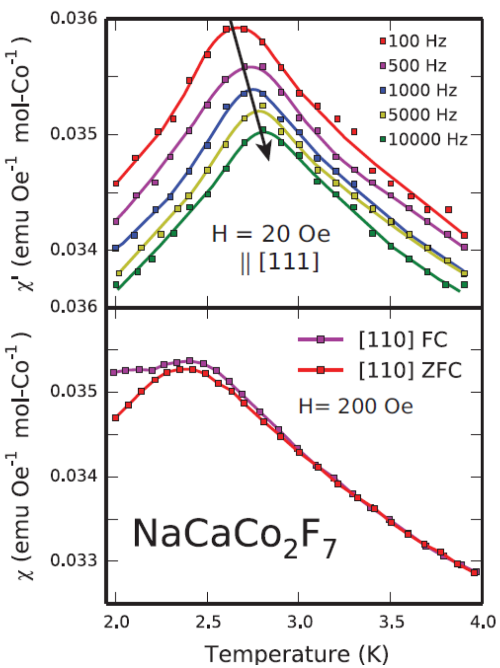


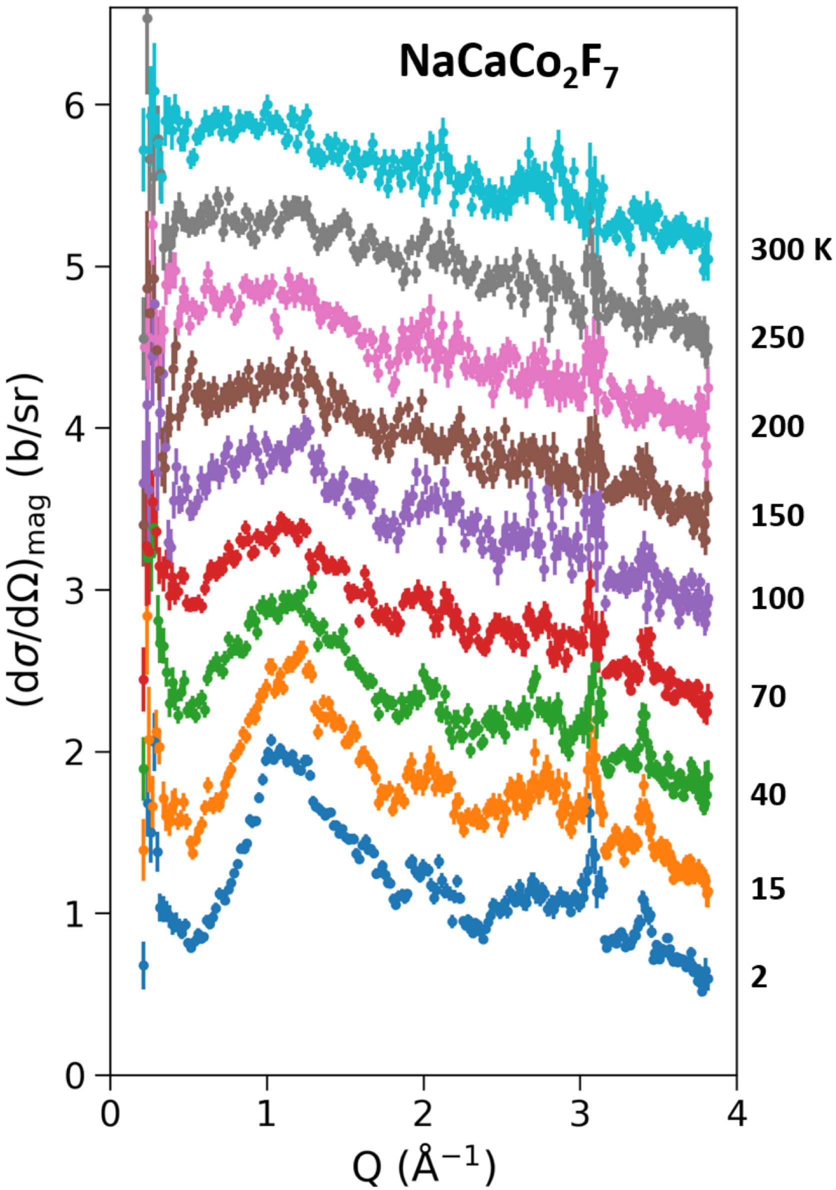
Pyrochlore network: Corner-sharing tetrahedra, HIGHLY FRUSTRATED!

What is the nature of the short-range magnetic correlations?

$NaCaCo_2F_7$

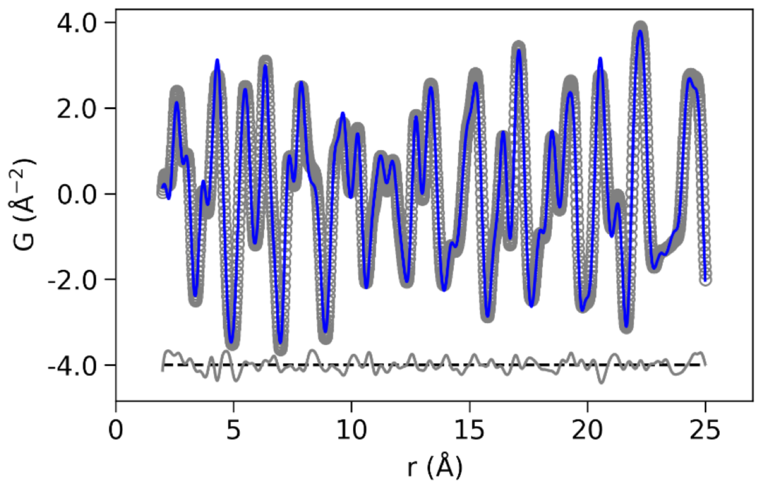
- Magnetic Co^{2+} ions on the highly frustrated pyrochlore lattice
- Short-range magnetic correlations freeze below ~3 K
- Promising material for extending studies of frustrated magnetism to strongly correlated 3*d* atoms



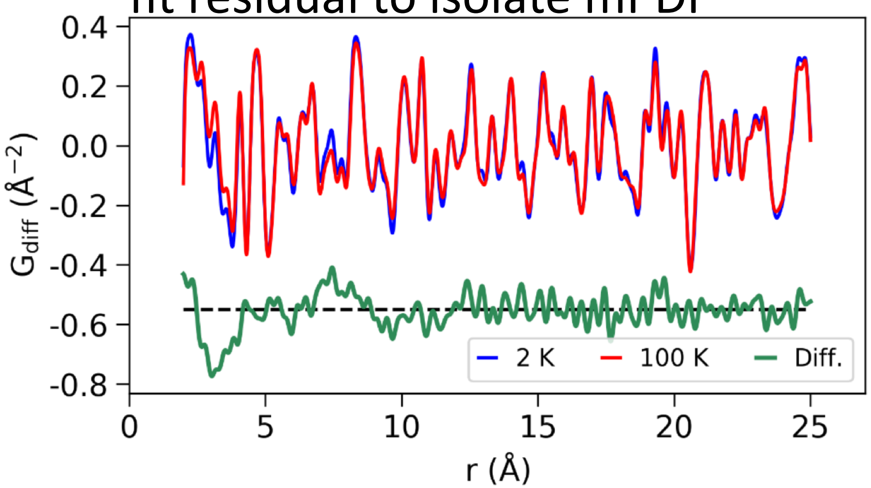


Obtaining the mPDF for $NaCaCo_2F_7$

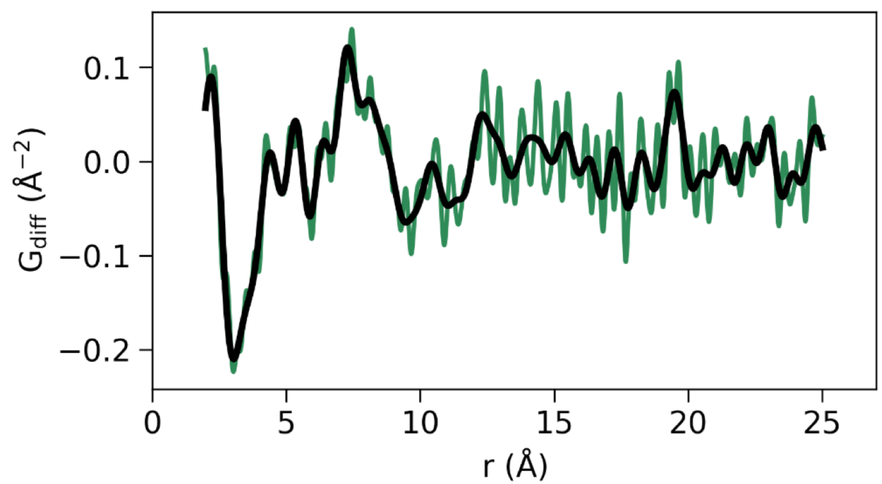
1. Perform standard PDF measurement on NOMAD, collecting atomic and magnetic PDFs together



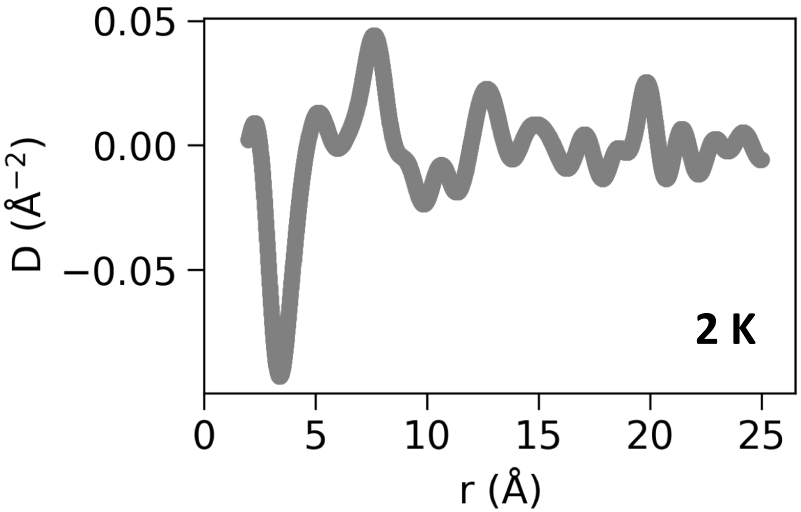
2. Refine the atomic structure, subtract high-temperature atomic fit residual from low-temperature fit residual to isolate mPDF

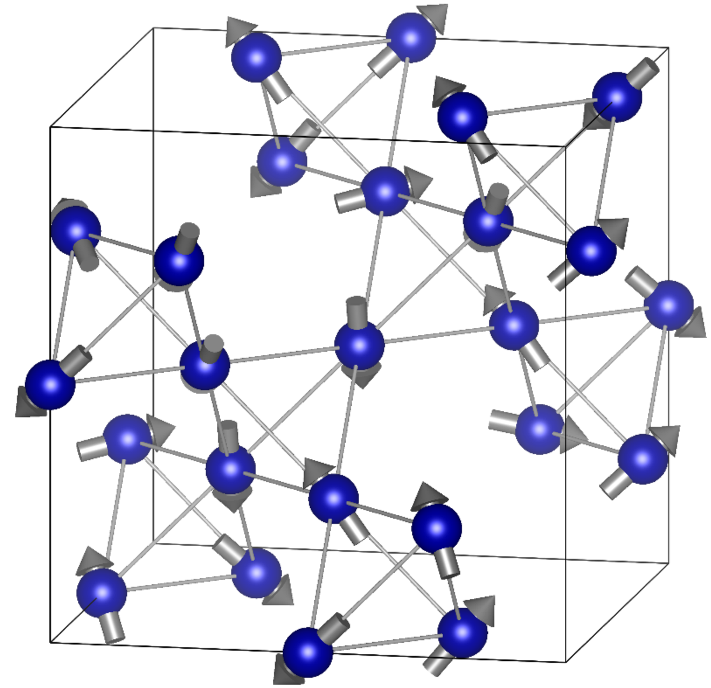


3. Remove high-frequency components that cannot arise from magnetic scattering



Magnetic PDF analysis of $NaCaCo_2F_7$

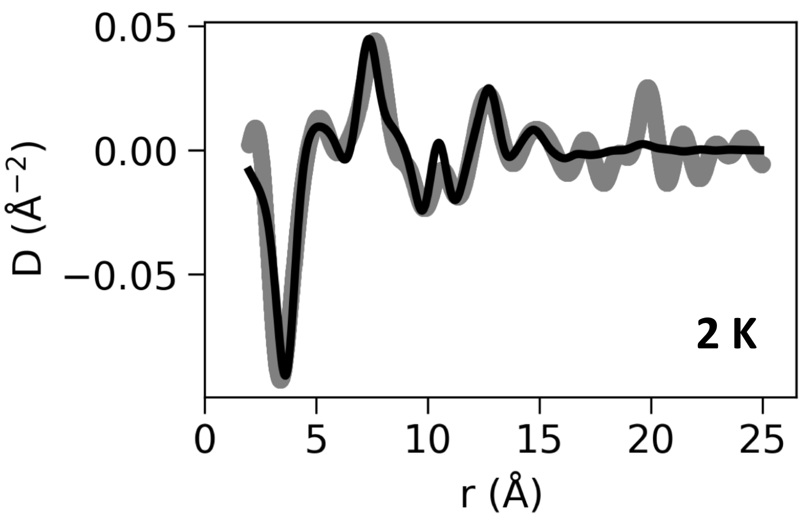




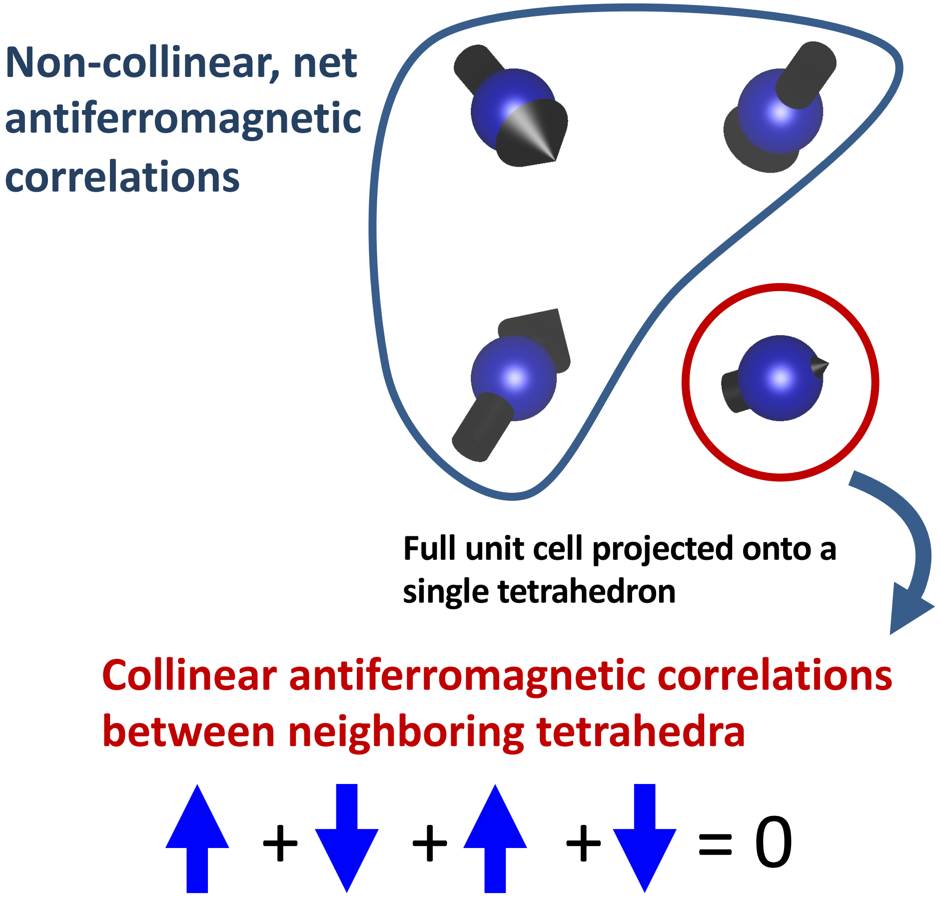
Modeling Attempt #1: Start with randomly oriented spins on each site and refine each independently, with scale factor and correlation length

Frandsen et al, *Phys. Rev. Mater.* **1**, 074412 (2017)

Magnetic PDF analysis of $NaCaCo_2F_7$

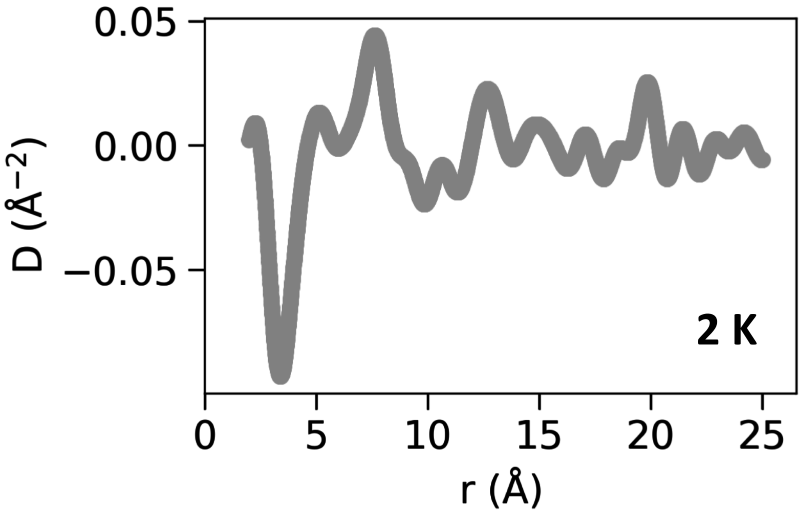


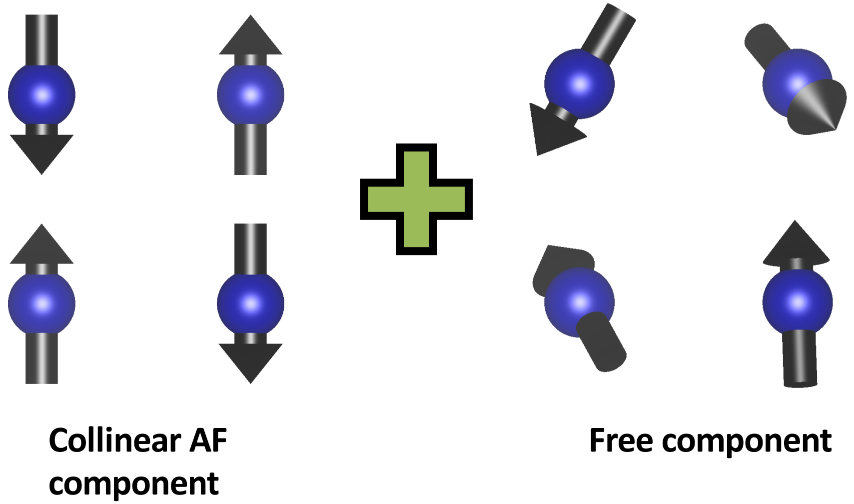
Modeling Attempt #1: Start with randomly oriented spins on each site and refine each independently, with scale factor and correlation length



Frandsen et al, *Phys. Rev. Mater.* **1**, 074412 (2017)

Magnetic PDF analysis of $NaCaCo_2F_7$

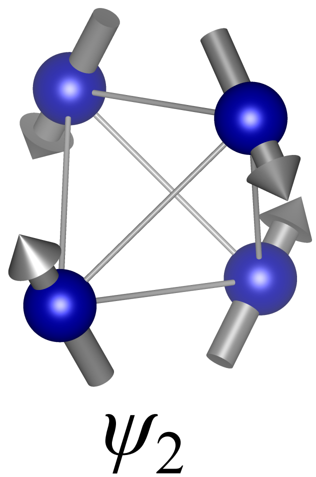




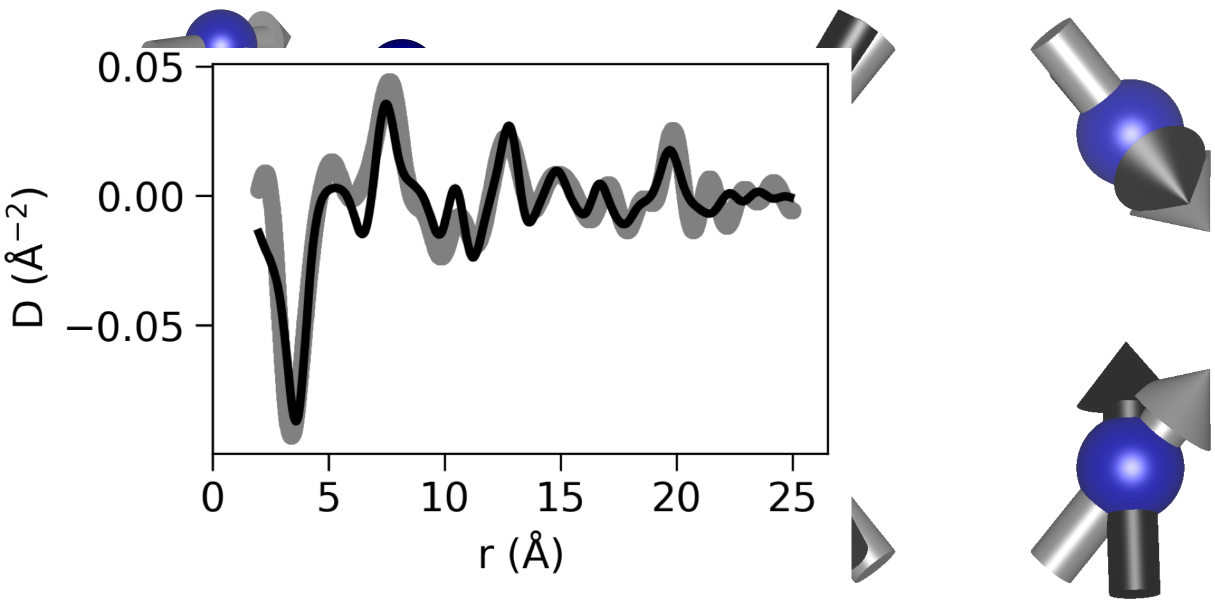
Modeling Attempt #2: Same as #1, but with an additional collinear antiferromagnetic component

Success!

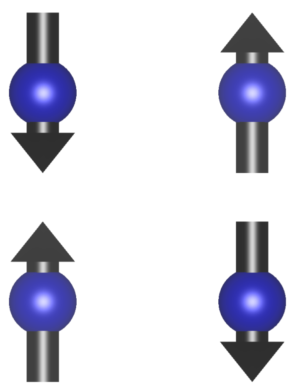
Significance of the refined spin directions



Expected conf
presence of LC



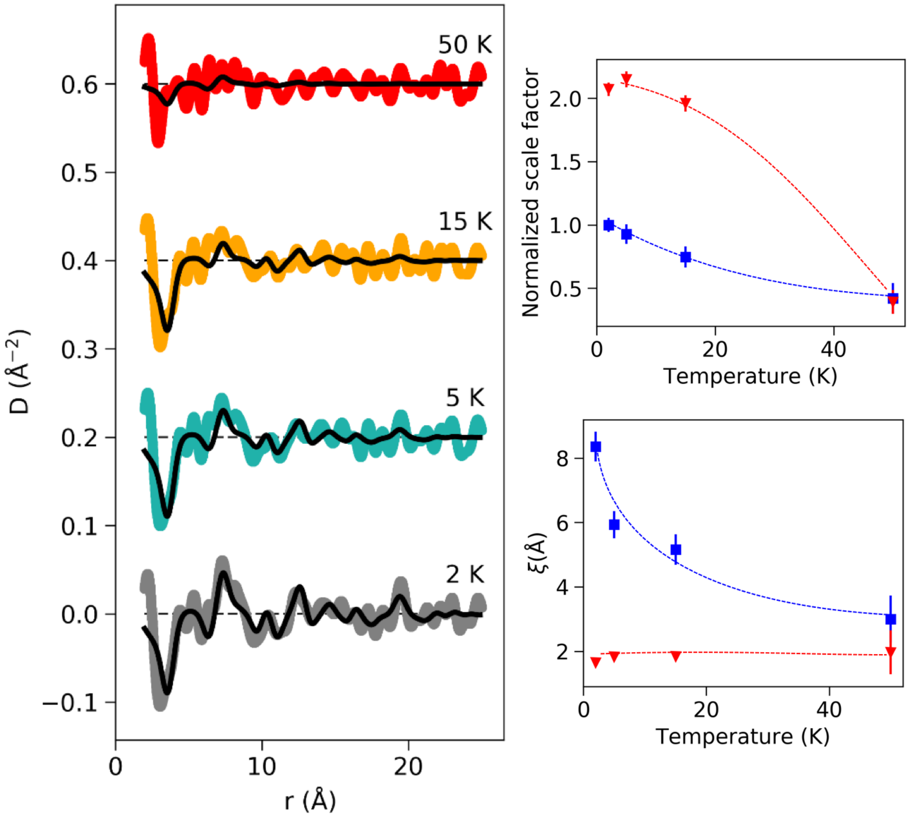
Refined spins closely match linear combination of ψ_2 and ψ_3; fit with either BV nearly as good. Correlation length ≈ 1 nm.



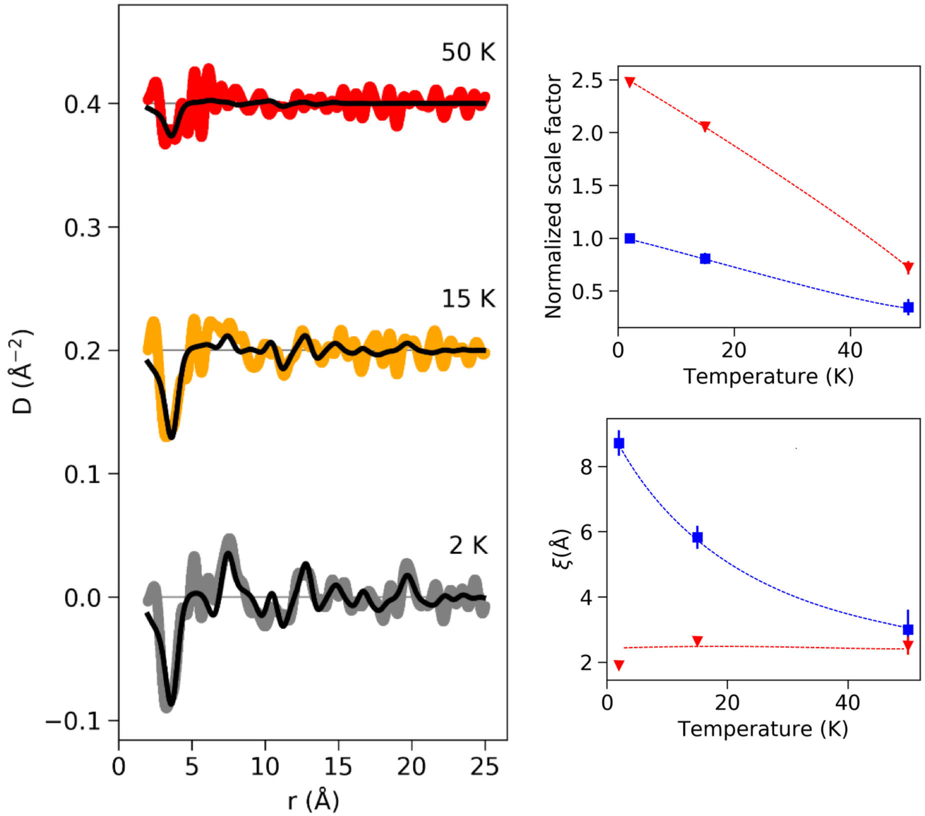
Collinear AF component: low-energy (< 10 meV) excitations observed from single-crystal INS; ξ ≈ 4 Å

Temperature Dependent mPDF analysis

$NaCaCo_2F_7$



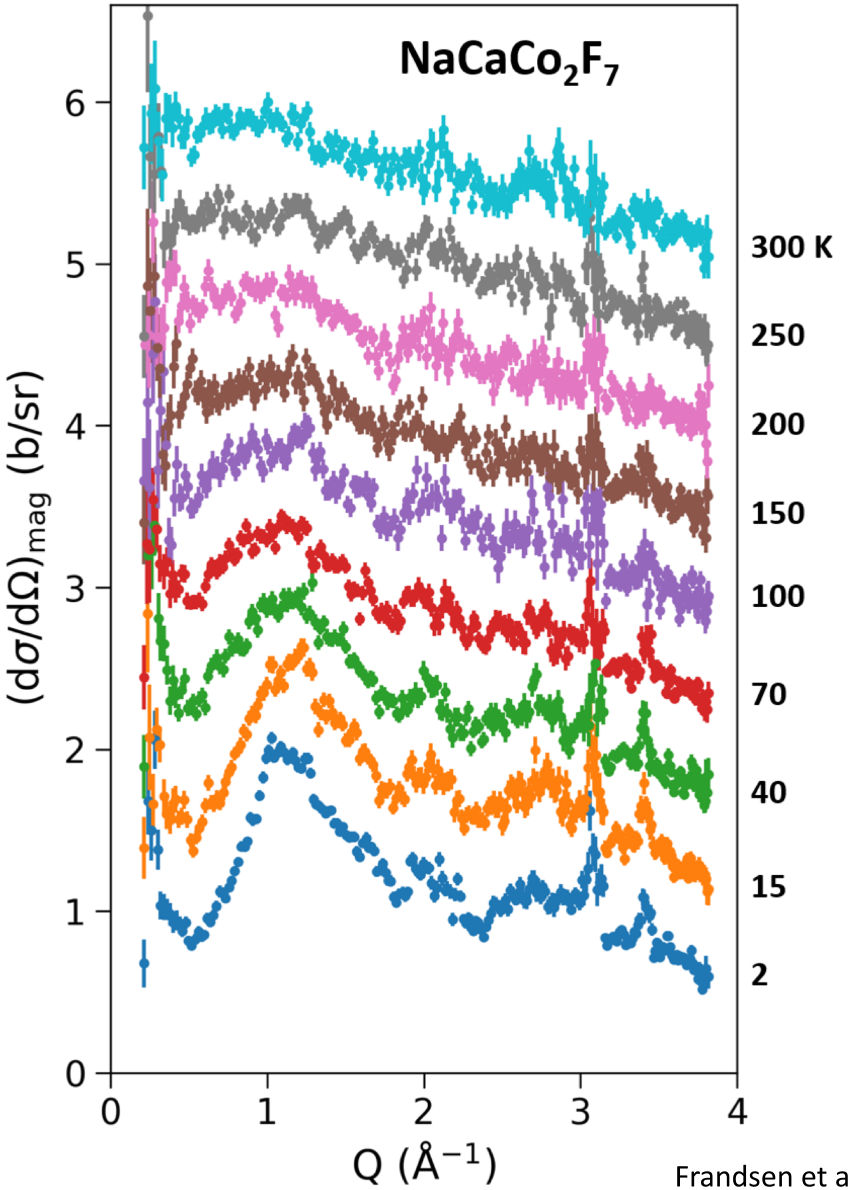
$NaSrCo_2F_7$



Correlations persist to unusually high temperatures!

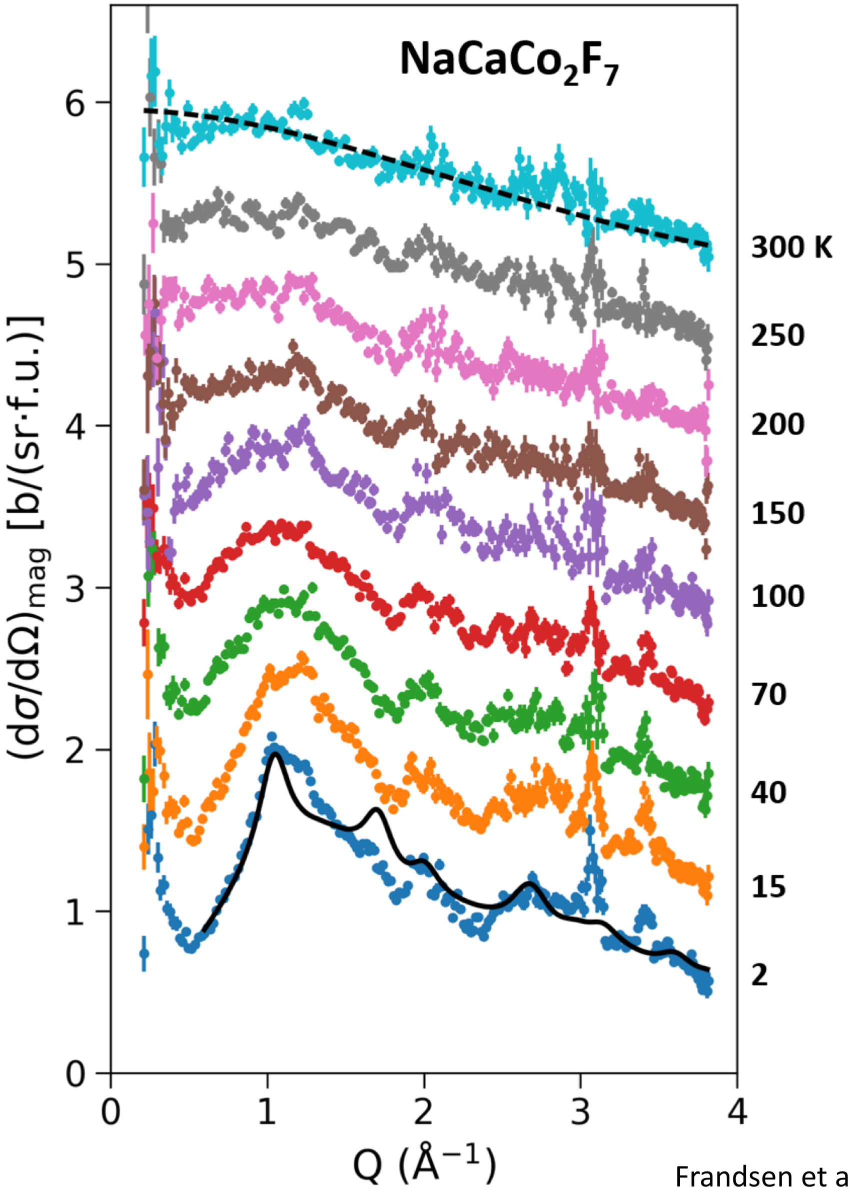
Frandsen et al, *Phys. Rev. Mater.* **1**, 074412 (2017)

Comparison to polarized neutron scattering



Frandsen et al, *Phys. Rev. Mater.* **1**, 074412 (2017)

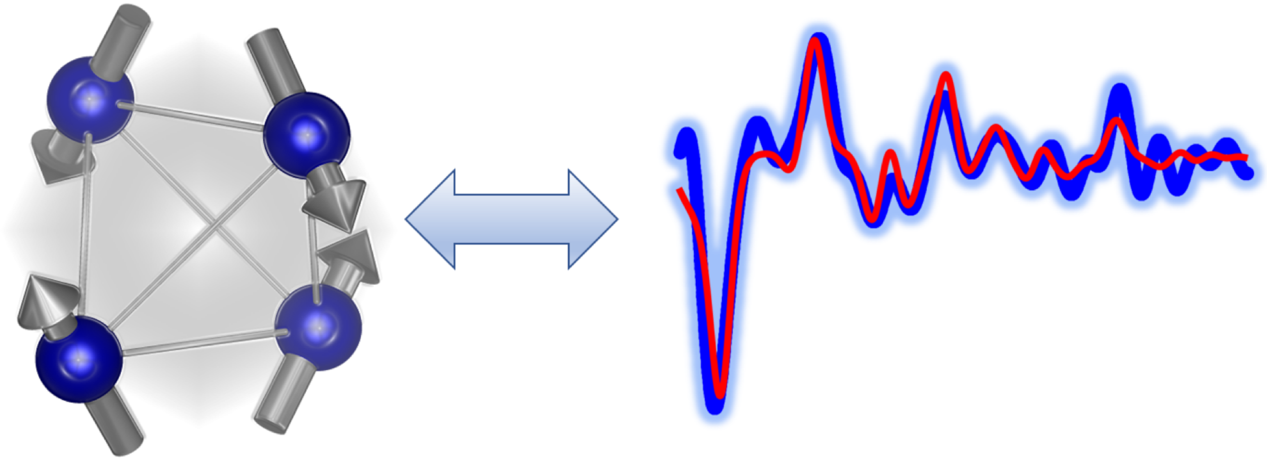
Comparison to polarized neutron scattering



Frandsen et al, *Phys. Rev. Mater.* **1**, 074412 (2017)

$NaCaCo_2F_7$ Summary

- Refinement of local magnetic structure against mPDF data confirms single-crystal results: ψ_2/ψ_3 + collinear AF
- New fluoride pyrochlores are promising platform for frustrated magnetism at relatively high temperatures
- mPDF enables real-space inspection and analysis of short-range magnetic correlations in frustrated materials



Reference: Frandsen et al, *Phys. Rev. Mater.* **1**, 074412 (2017)

I WANT YOU

TO START DOING mPDF

Software Overview

- diffpy.mpdf (http://www.diffpy.org/products/mPDF.html)
  - Open-source python package
  - Runs on Linux and MacOS
  - Requires other packages in the DiffPy-CMI suite as dependencies
- Features
  - Calculate the normalized and unnormalized mPDF from an arbitrary magnetic structure
  - Build magnetic structures of arbitrary complexity using propagation vectors or a magnetic unit cell
  - Include multiple magnetic species in one structure
  - Easily refine magnetic models against mPDF data
  - Atomic/magnetic PDF co-refinements within DiffPy-CMI, or sequential refinements with convenient interface to PDFgui
  - Easily customizable for your own tailored calculators/refinements
  - Do simple 3D visualizations of your magnetic structure
  - Calculate magnetic scattering pattern from magnetic structure
  - And many more features!

Installation

Conda installation

```
conda config --add channels diffpy
conda config --add channels benfrandsen
```

```
conda create --name diffpy python=2.7
source activate diffpy
```

```
conda install diffpy.mpdf
```

Pip installation

```
pip install diffpy.mpdf
```

Installation from source

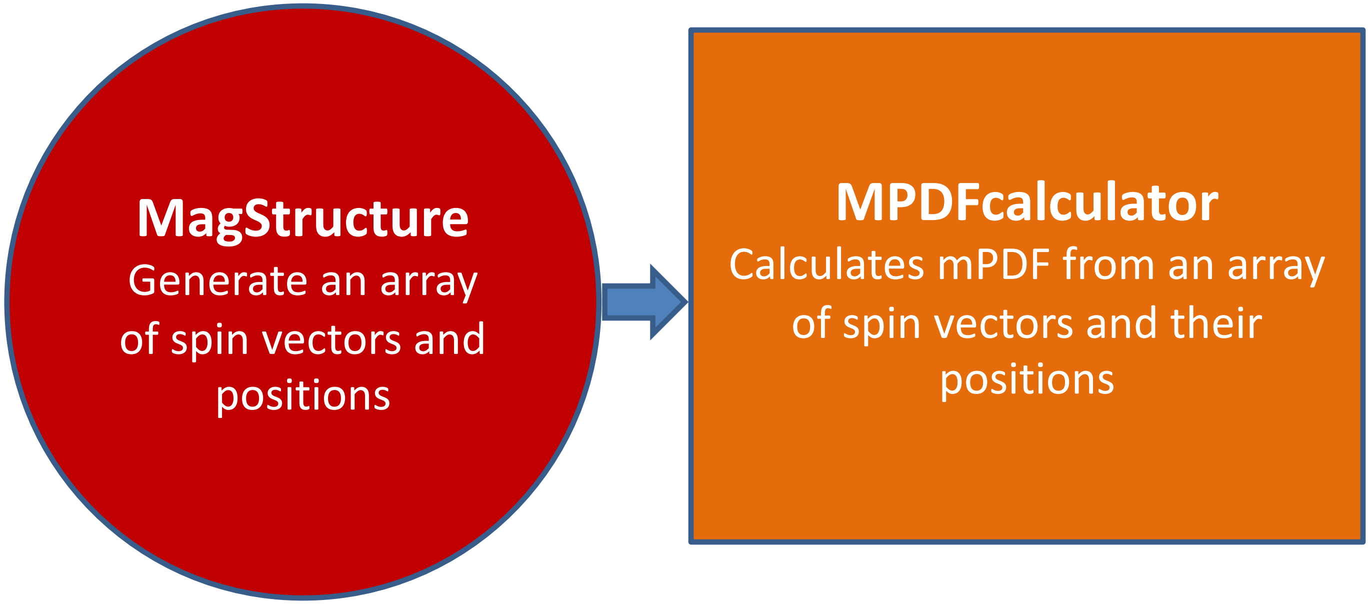
Download source files from
https://github.com/benfrandsen/diffpy.magpdf

```
python setup.py install
```

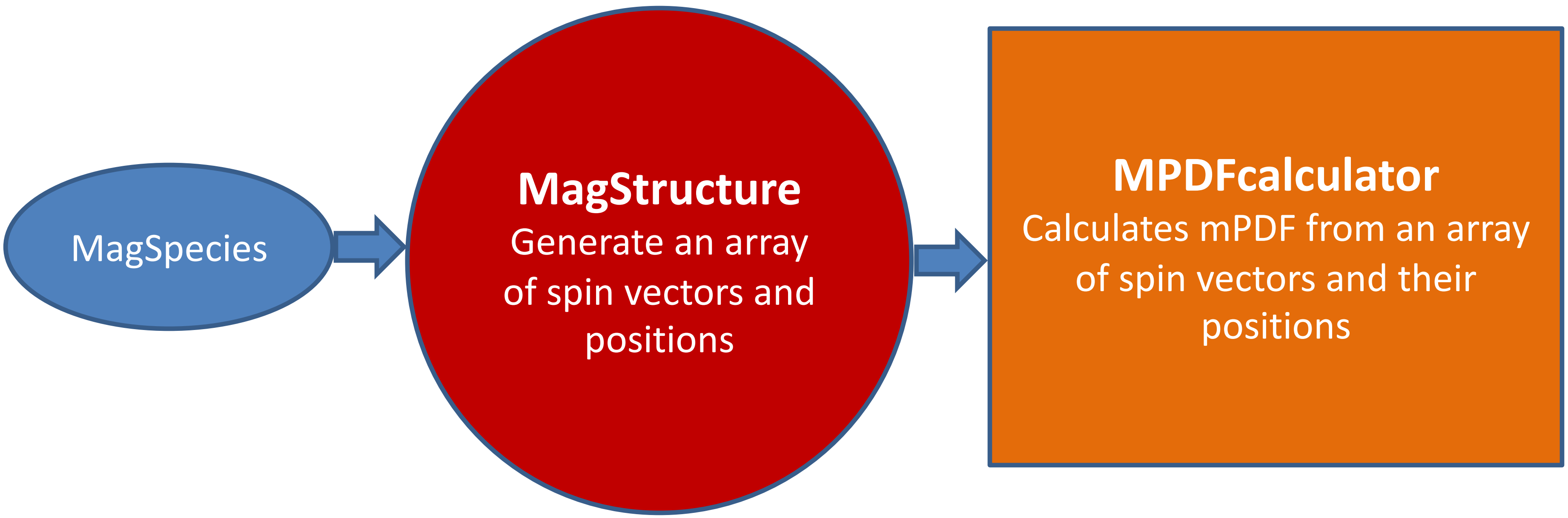
Software Overview

MPDFcalculator
Calculates mPDF from an array of spin vectors and their positions

Software Overview

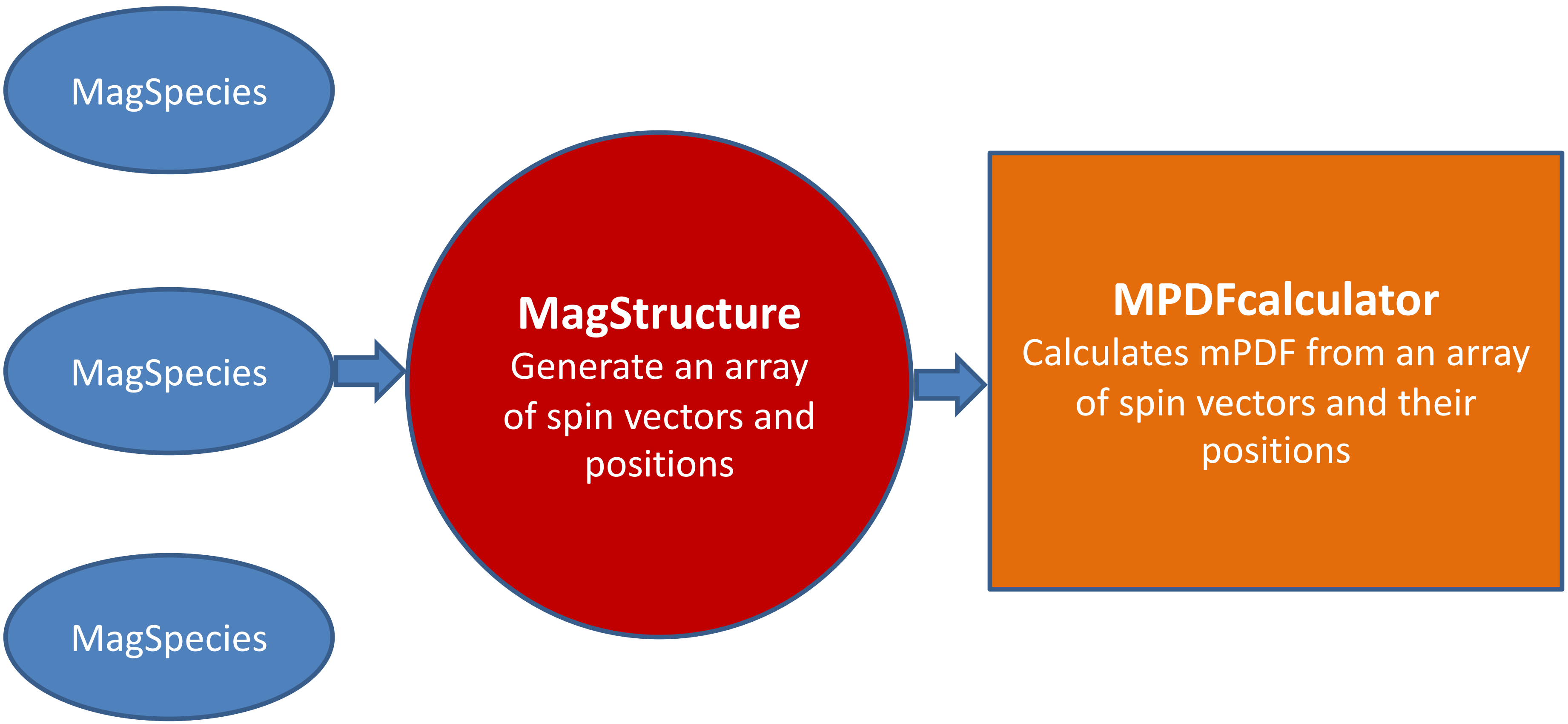


Software Overview



Specify basis vectors,
propagation vectors,
magnetic form factor, etc

Software Overview



Specify basis vectors, propagation vectors, magnetic form factor, etc

Getting started with diffpy.mpdf

Tutorials and example scripts on the CMI Exchange github page:

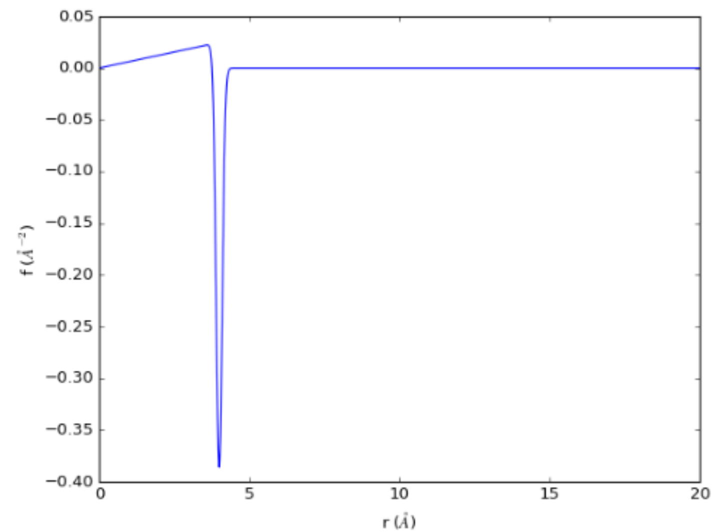
https://github.com/diffpy/cmi_exchange/tree/master/cmi_scripts/mpdf

Simple example: Calculating the mPDF from a spin dimer

We will now create a very simple magnetic structure consisting of just two spins and then calculate the corresponding mPDF.

In [1]:
```
### Import the necessary libraries
import numpy as np
import matplotlib.pyplot as plt
from diffpy.mpdf import *

### Set all plots to be inline
%matplotlib notebook

### Create a MagStructure object
mstr = MagStructure()

### Create two atoms in the structure
mstr.atoms = np.array([[0,0,0],[4,0,0]])

### Create two spin vectors corresponding to the atoms. Let's make them antiferromagnetic.
S=np.array([0,0,1])
mstr.spins = np.array([S,-S])

### Create the MPDFcalculator object and load the magnetic structure into it
mc = MPDFcalculator(mstr)

### Calculate and plot the mPDF!
r,fr = mc.calc() # Use calc() if you want to extract the numerical results of the calculation
mc.plot() # Use plot() if you just want to plot the mPDF without extracting the numerical arrays.
```

<IPython.core.display.Javascript object>



Email me and I will help you get started!

benfrandsen@byu.edu

Summary

- mPDF method provides a way to inspect and model magnetic correlations in real space
- Data can be obtained from conventional neutron beamlines: both standard diffractometers and PDF-optimized instruments (get the mPDF for free along with your atomic PDF!)
- Protocols for successful treatment of weak and/or noisy mPDF signal
- diffpy.mpdf: free and open-source software for mPDF analysis
- Successful application to a variety of magnetic materials with widely varying correlation lengths

References

- *Acta A* **70** 3 (2014)
- *Acta A* **71** 325 (2015)
- *PRL* **116** 197204 (2016)
- *PRB* **94** 094102 (2016)
- *Phys. Rev. Mater.* **1**, 074412 (2017)
- More to come…

Thank you!