Task 10.4: interoperable data treatment software

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Pietro Bonfà, University of Parma, Italy

- Automated user-friendly workflows
- Atomistic modeling software
- μSR specific software release

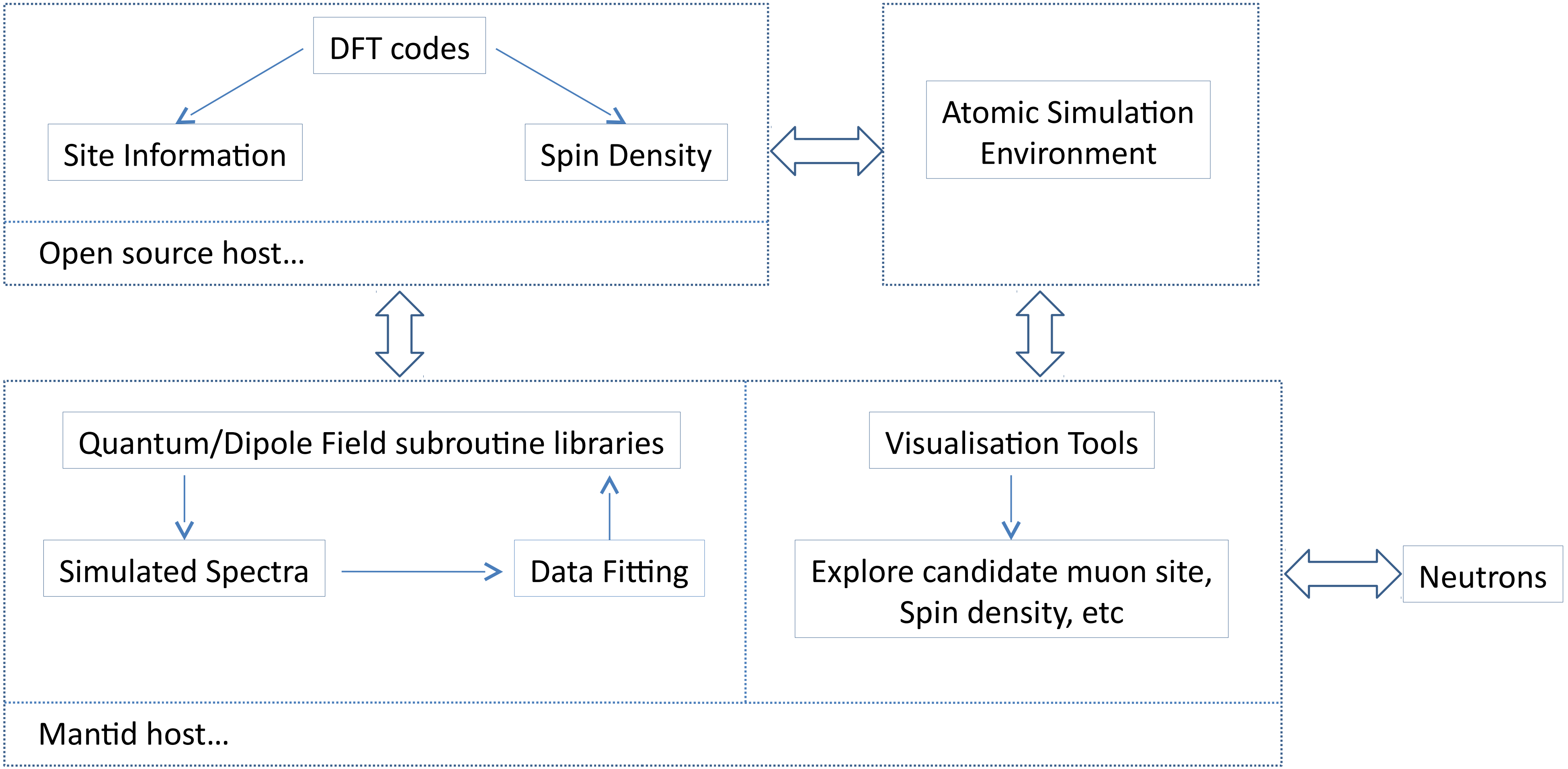
Context of the Task…

- Muon spectroscopy is a complementary technique
- User groups increasingly make use of both neutrons and muons in their research – there are examples of studies where results would not have been possible without a muon experiment
- *Interoperability* under an established platform is therefore beneficial
  - to the users … e.g. familiar environment, well supported, many features
  - to the developers … e.g. established environment, well supported, code reuse
- Experiments are becoming more diverse and systems more complex
  The user community is becoming more diverse and less specialised
- A detailed knowledge of muon sites is a huge asset to effective analysis
- However, reaching this goal is complex, methods for reliable modelling/simulation not yet properly understood
- Therefore, *bringing together groups working in this area* and *exploiting wider expertise* will be hugely beneficial to the project

Developing Interoperability

Mantid appears to be an ideal platform for hosting …

- Python subroutine library for site refinement
- visualisation tools



Bringing interested groups together

Several μSR groups (incl. Parma, Oxford and Durham) are …

- working to develop DFT methods for predicting the muon site
- exploring methods for simulating μSR data, such as dipole field calculations

There have been a very successful series of site calculation meetings (NMI3 I/II)
We suggest following this up with a Workshop (end 2016?) …

The Workshop will allow (at least) …

- sharing of ideas and strategies for both DFT and dipole field calculations
- Understanding requirements for the visualisation of results
- establishing standards for a subroutine library for sharing codes

Meeting to discuss techniques for calculation of the Muon Site

12:00pm, 19th March, 2014

CR16 and 17, R80, Rutherford Appleton Laboratory

12:00	Buffet Lunch (conference room)	
12:55	Welcome	(Adrian Hillier)
13:00	Presentations (maximum 15 minutes + 5 minutes questions) (session chair: Adrian Hillier)	
	Re-examination of muon sites in La_2CuO_4	(Isao Watanabe, RIKEN)
	Muon Sites in $V_4S_9Br_4$	(Mohamed Ismail Mohamed-Ibrahim, USM)
	DFT investigation of muon sites in T' La_2CuO_4	(Pietro Bonfa, Parma)
	Muon site estimation in $Ce(Ru_{1-x}Rh_x)_2Al_{10}$	(Aina Adam, RIKEN)
	Playing quantum Hyde-and-seek with the muon	(Johannes Moeller)
15:00	Coffee	
15:30	Presentations (continued)	(session chair: Paul McClarty)
	Muon stopping states from first principles calculations using CASTEP	(Dominik Jochym, STFC)
	DFT calculations on Cu-based metal-organic hybrid magnets	(Edi Suprayog, RIKEN)
	Muonium Sites in ZnO	(Shukri Slaiman, USM)
	Theoretical isotropic hyperfine coupling constants of muoniated benzene: Exploring the effects of anharmonicity, methods and basis sets	(Ke Wang, QMUL)
	ALC spectra of molecular solids: effects of multiple sites, crystalline environment and quantum delocalisation	(Francis Pratt, STFC)
17:30	Coffee and Discussion	
18:00	Meeting close	
19:30	Dinner	

Sharing expertise beyond μSR

Potential for sharing DFT knowledge/skills/resources through (for example) …

- links with Theoretical and Computational Physics group within STFC Scientific Computing department
- possible use of resources such as CASTEP and HPC
- building links (as appropriate) with DFT work ongoing in the neutron community
- …

For example …

- Two year PDRA recently appointed by the Theoretical and Computational Physics group to work on research projects in collaboration with the muon community
- Francis Pratt (ISIS) is guiding this collaboration
- PDRA gave a presentation at the recent Muon School

Enrollment

- 1st Nov.: Ph.D. student Ifeanyi John Onuorah
  - Experience:
    - Master degree @ International Centre for Theoretical Physics
    - Thesis: Ab-initio Simulations of Sodium Superoxide
  - Work:
    - DFT & code development and deployment under the supervision of Prof. Roberto De Renzi (RDR).
    - De Renzi will charge 300 h over 3 year to the project.
  - De Renzi charged hours + Onuorah Ph.D project will fulfill the Parma task.
- 16th Jen.: Postdoc Research Fellow Pietro Bonfà
  - Fund provided from University of Parma
  - Working full time on DFT+μ

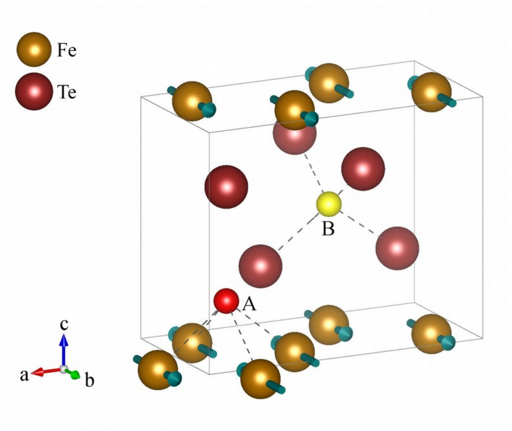
DFT & μSR

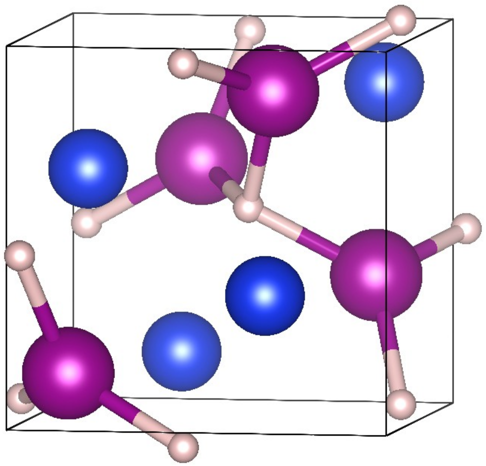
Quoting from PSI website:

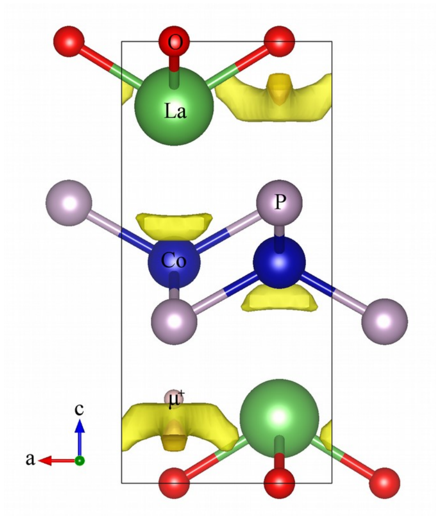
“The majority of the proposals is devoted to magnetism and superconductivity.”

DFT & μSR

- Muon site identified in
  - MnSi PRB **89**, 184425 (2015) - J.Phys.Chem.C 119, 4278 (2015)
  - MnGe arXiv:1602.01756
  - MnP arXiv:1603.03367
  - T'-La_2CuO_4 P.B. Doc. Thsis
  - Fluorides PRB **87**, 121108 (2013)
  - Iron Pnictides SC
  - …







Convinced?

Requirements

- Medium size computer cluster (~64 cores)

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Titan X550 - Dual CPUs Intel Xeon E5-2600 Haswell V3 Series Quad Tesla GPU Computing Server up to 36 Cores

Starting Price: $3,725.00

★★★★★ (2)

Paying taxes and the Titan X550 are the only things you can be certain of in life. This is what happens when you ask us to "make you one with everything": we do and this is it, well as far as dual CPU workstations go. Scientific, creative or any computing task is no problem for even the base model X550. Need more power? Capable of using up to four Tesla cards for GPU Computing and up to 36 CPU Cores with these expansion options the sky is practically the limit.

Processors:	Memory:	Video Card:	Hard Drive:	Warranty:
Dual Intel Xeon E5-2600 v3 Series Haswell Up to 36 Physical cores and 72 cores w/ Hyper Threading.	16GB (4 x 4GB) 288-Pin DDR4 SDRAM DDR4 2133 (PC4-17000) ECC Server Memory Expandable to 1TB (RDIMM)	NVIDIA Quadro K620 2GB 128-bit DDR3 PCI Express 2.0 x16 Workstation Video Card and Up to four Nvidia Quadro or Tesla Cards.	10x SATA3 (6Gbps) ports. RAID 0/1/5/10 Capable.	Lifetime labor & Technical Support + 2 Years Replacement Parts. Also covers International customers.

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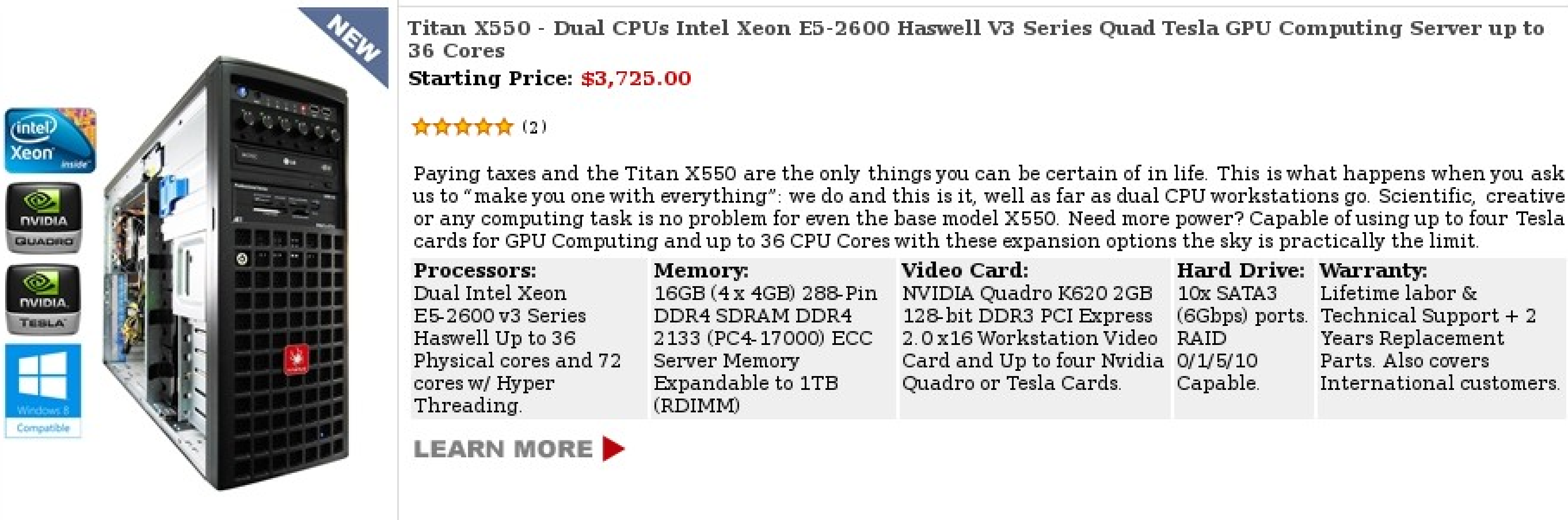


- Some experience with DFT
  (difficulties with pseudopotentials, accuracy of mean-field approaches for magnetic materials)

Gotcha/Fiasco

✔ Candidate muon sites

● Stable muon sites

✗ Population of muon sites

✗ Fermi contact interaction (?)

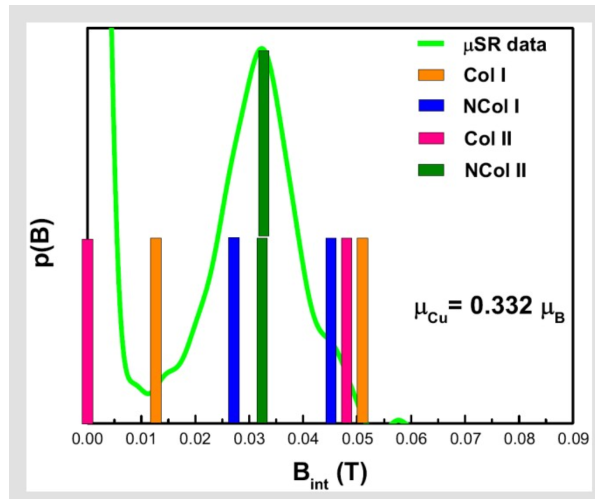
✗ Interaction with light nuclei

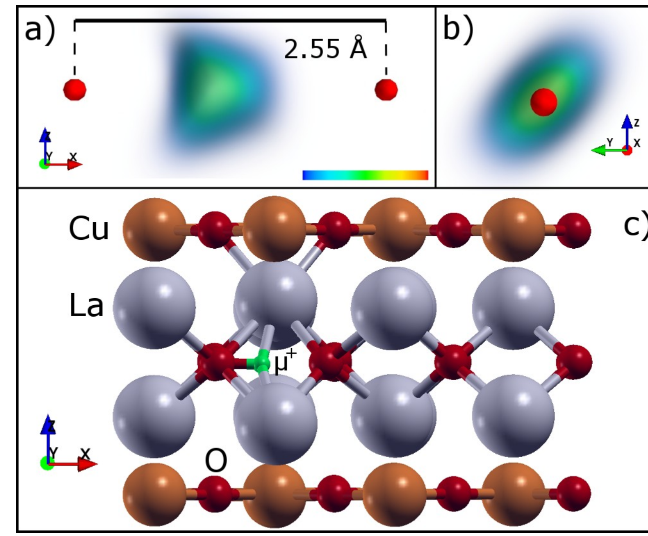
In sight...

Stability of candidate muon sites

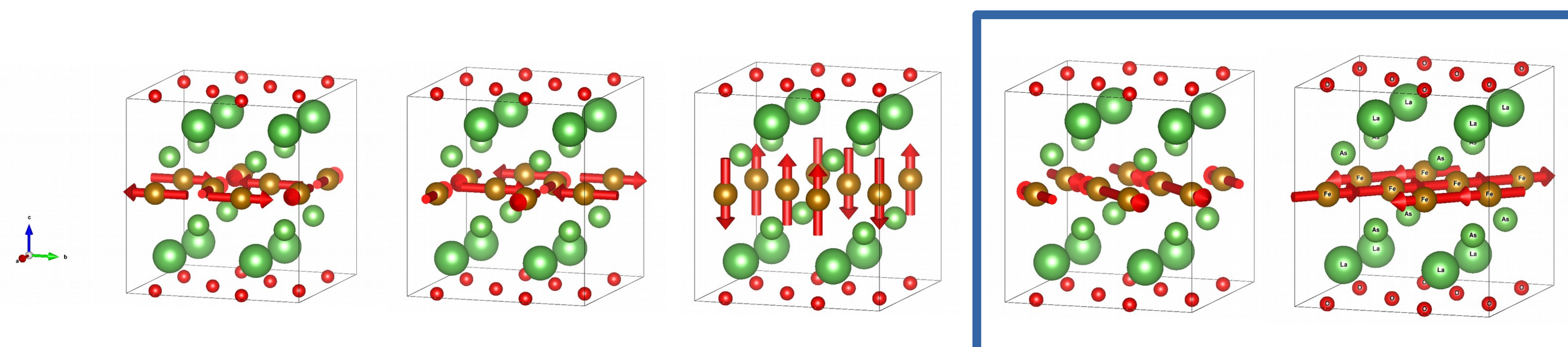
Quantitative results

- T’ La_2CuO_4





- LaFeAsO



Dealing with uncertainty

- Bayesian analysis

Available online at www.sciencedirect.com

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Physics Procedia 30 (2012) 113 – 116

Physics Procedia

A Bayesian approach to magnetic moment determination using μSR

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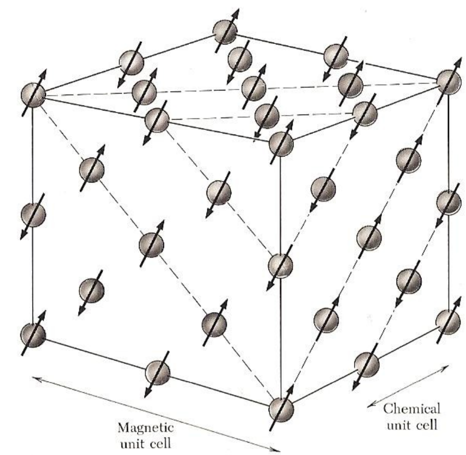
Dealing with uncertainty

Example: MnO

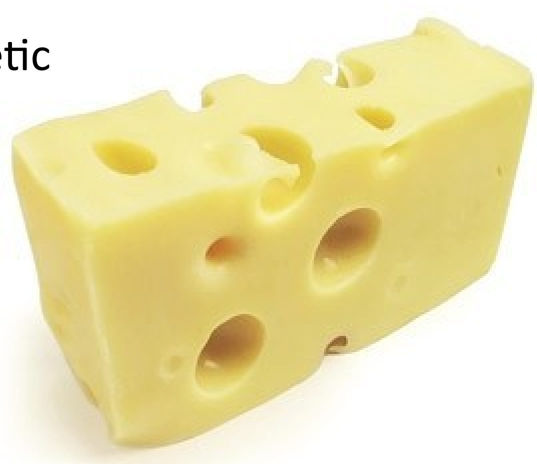


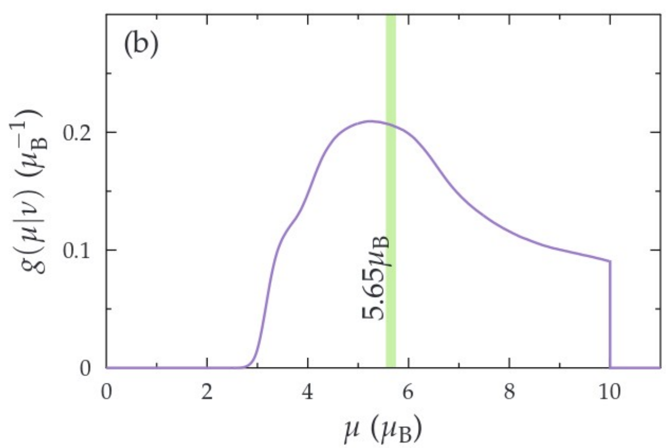
pdf of manganese moment Mn moment μ given the observed ν

the pdf of dipole fields for $r_{\mu\text{-any}} > 0.17$ nm

$$g(\mu|\nu) = \frac{\frac{1}{\mu} f(\nu/\mu)}{\int_0^{\mu_{\max}} \frac{1}{\mu'} f(\nu/\mu')\, d\mu'},$$

Uniform probability for magnetic moment





Kindly asking for NS tools

- The analysis of μSR data in magnetic systems is getting progressively similar to the refinement of neutron scattering data!

MAGNETIC STRUCTURE DETERMINATION FROM POWDER DIFFRACTION USING THE PROGRAM *FullProf*

JUAN RODRIGUEZ-CARVAJAL

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E-mail: juan@llb.saclay.cea.fr

Kindly asking for NS tools

- The analysis of muSR data in magnetic systems is getting progressively similar to the refinement of neutron scattering data!

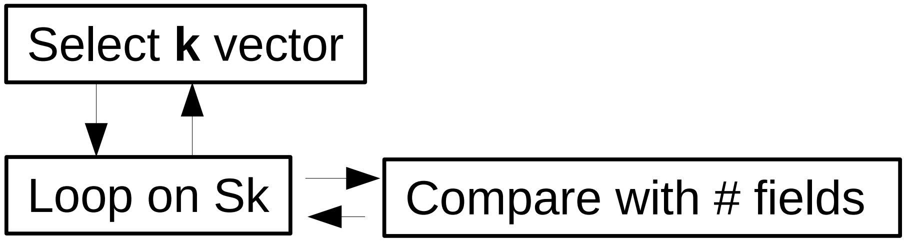
3 The search for the propagation vector and symmetry analysis.

The first problem to be solved before attempting the resolution of the magnetic structure is the determination of the propagation vector(s), i.e. its "periodicity". To find **k** is necessary to index the magnetic reflections appearing below the ordering temperature. With a single crystal the task is somewhat easy, but is tedious for a powder because only the module of reciprocal vectors is available. We have developed a method for searching the propagation vector of a commensurate or incommensurate structure implemented in the program *SuperCell* [5]. Once an approximate propagation vector is obtained the symmetry analysis according to references [4] can be started. The program *BasIreps* may be used for obtaining the vectors $\mathbf{S}_{n\lambda}^{\mathbf{k}\,\nu}(js)$ in Eq.7 for each crystallographic site occupied by magnetic atoms.

μSR magnetic data analysis flow

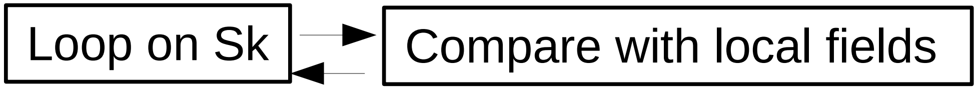
Identify **k** vector

requirements: low symmetry site



Identify long range order

requirements: knowledge of the local moment on magnetic atoms



Complication

- Contact hyperfine field

Additional parameter

Ab initio estimation

Muesr (MUon Embedding Site Refinement)

Tool written in Python+C (simple integration with Mantid).

- Present features
  - Dipolar sums with 1-k commensurate and incommensurate structures.
  - Visualization of magnetic structures
  - Automatic symmetry detection (via spglib)
- Needs adjustments/developments
  - Cumbersome magnetic structure description
  - Magnetic CIF parsing
  - Multiple propagation vectors
  - Contact hyperfine field
  - Documentation (!)
- Open problems
  - Visualization strategies
  - Integration with neutron scattering tools

```
for mcif in mcifs:
# Load all maximally symmetric structures (obtained from bilbao)
#  for propagation vector (1/2,1/2,0)
#  Crystal structure is included and is parsed too.
    m.load_mcif(mcif)
# finds cell symmetries
#  these are inspected from the structure rather than parsed from the cif.
#  The reason for doing this is that structure may be read from files
#  without symmetry informations.
    m.sym_search()
# Sets muon position in fractional coordinates
    m.muon_set_frac('0.375  0.375 0.635')
# Find crystalographically equivalent muon sites. Uses 3 decimal rounding
#  to check if two positions are equivalent.
    m.muon_find_equiv(3)
    res=m.locfield([100,100,50],200)
    print('Structure in file: '+mcif)
    for e in res:
        print(e.T*0.66, "Norm {: 0.4f}".format(np.linalg.norm(e.T*0.66)))

print('\n --> According to PhysRevB 80 094524, the local field at the muon site is about 1700 G')
print('\n --> So long range order is either bcs_file_22902c.mcif or ./bcs_file_22902d.mcif \n')
```

Acknowledgements

S. Blundell, F. Lang, J. Moeller, F. Foronda, ...

University of Oxford

T. Lancaster, F. Xiao, ...

University of Duram

A. Amato, R. Khasanov, H. Luetkens, ...

PSI Bulk μSR Group

You for the attention!