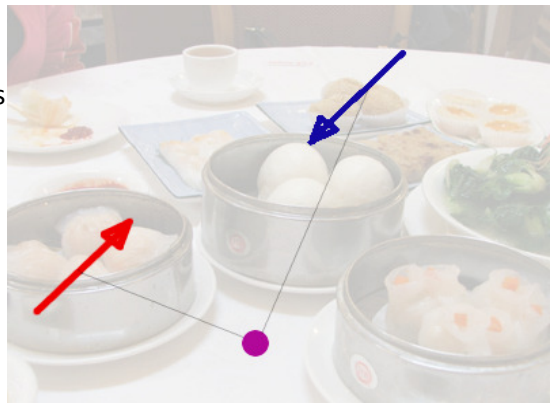
Scope of Simulation Codes to Support µSR Analysis

Abstract

We discuss the plans for a guided procedure through which any MuSR user can calculate dipolar fields at muon sites in a given compound of interest.

Main text

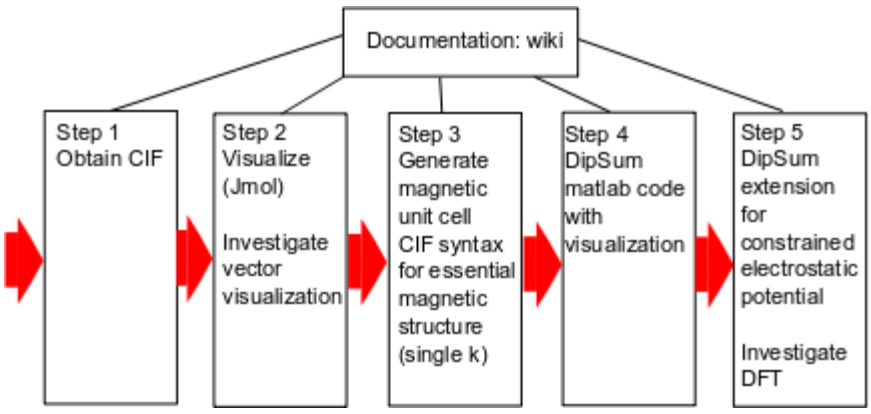
Muon field simulations



The purpose of this procedure, call it DipSum, is to obtain indications of the possible muon localization site(s) in a given magnetic material, starting from the knowledge of its structure and (at lest tentatively) of its magnetic structure. It must be limited initially to simple cases, e.g. ferromagnets, simple antiferromagnets and ferrimagnets, but open to improvements, such as more complex magnetic structures and additional localization strategies.

It will consist of a core DipSum computational part to produce maps of magnetic dipolar fields at plausible locations (e.g. around spheres centred at Oxygen ions in oxides, searching for typical O-Mu bond lengths). The estimated value of the local field and of its orientation in the crystal lattice can be compared to experiments to assign the sites. The full procedure may be already performed by several DFT codes, both commercial and free/open-software versions, but the competence required for their installation and use is an overhead which would probably put off most muon users.

The DipSum core will be sewn in a path, made primarily of existing tools, shown in the flow-chart of Fig. 1.



Its aims are to

1. obtain the structural information in CIF format,
2. check it visually,
3. add the magnetic structure in CIF-compatible syntax,
4. input the CIF file to the computational software,
5. generalize an existing version of the software to face more general cases.

Step 1, to obtain a CIF file (http://www.iucr.org/resources/cif), may be totally straightforward for users with a solid background in crystallography, which is not necessarily the case of a MuSR user. The proposed solution is with the use of standard bibliographic tools and/or Java based tools available on the Bilbao Crystallographic Server at http://www.cryst.ehu.es/ .

This step, with its simple alternative solutions, also highlights the necessity for a suitable documentation, available on the internet. To this purpose we shall start maintaining a local wiki, read-only for the outside world, which may be migrated to the NMI3 portal upon completion of the 1.0 version. In its initial version the wiki will contain examples of how to generate the answer, step by step.

Step 2, lattice visualization, offers several alternatives, commercial and free/open software and it requires only limited documentation.

Old, unmaintained versions of step 3, CIF magnetic structures, are available for guidance (http://www.ftj.agh.edu.pl/~pytlik/msdb/msdb.htm). Our first purpose is to convey the extra information compatibly[1] with the operation of the step-2 software. Solutions for magnetic moment visualization will be considered.

Step 4 and 5 will be developed in matlab for a version 1.0, because of its more powerful visualization tools. Porting to an open software version (e.g. octave) will be considered later. This part will require a more substantial documentation, within the wiki.

Step 5 could include calculations of constrained electrostatic potentials and, eventually, interfaces with DFT software that can simulate energy minimization for a positive point-like charge like the muon. This aspect will be explored by discussing with experts outside the group of the NMI3 WP20 partners.

1 The contents of a CIF are not restricted to data items defined in the standard Dictionary. The presence of non-standard data does not affect the logical integrity of a CIF nor the access to the standard data.