

Simulations in aid of experiments

The problem: to identify the muon site(s). The project of a simulation program implies defining

Functionalities and algorithms: calculation of electrostatic and magnetic fields, validation with experiments;

Interface: input (crystallographic and magnetic structure), output, visualization;

Implementation: choice of available data meta-formats (CIF) and possible extensions (MCIF), usage of calculation and visualization engines (Matlab/Octave, Jmol);

Development plan

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Tasks for JRA

Level I: computation methods

- Solve the electrostatic problem in a point charge approximation; let's call potential minima E-sites
- Calculate local dipolar fields at E-sites from electron/nuclear moments
- Choose suitable algorithms and strategies
- Validate model with experiments

The muon site(s)

Criteria

- Pure guess of a suitable site

Voids

- Electrostatic potential minima constrained e.g. to spheres centred on O^{2-} at $\sim 1.1 \text{ \AA}$

Model validation

Many strategies:

- Internal fields in magnetic materials

- Internal rms fields from nuclear dipoles (+ quadrupoles)

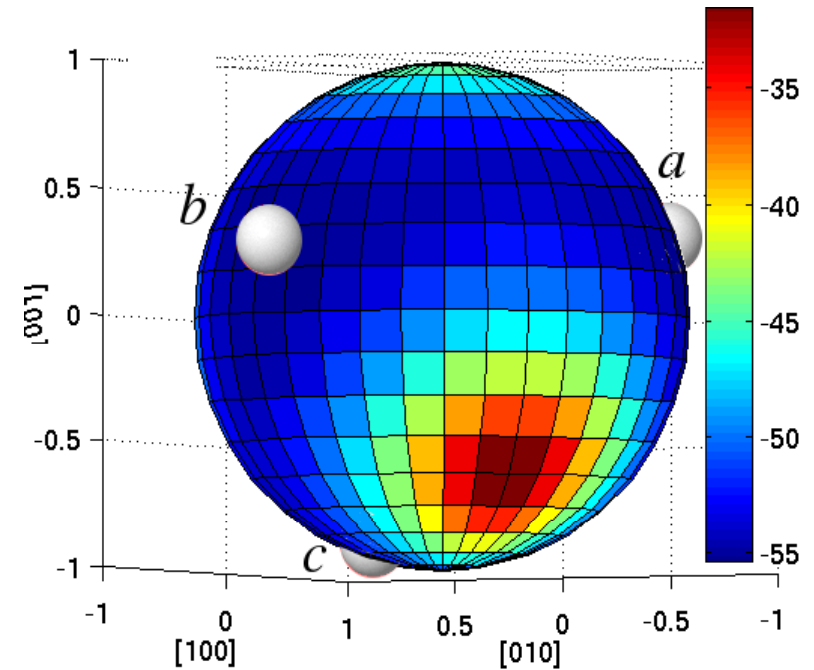
- Single crystal experiments in field

Several strategies require lattice sums

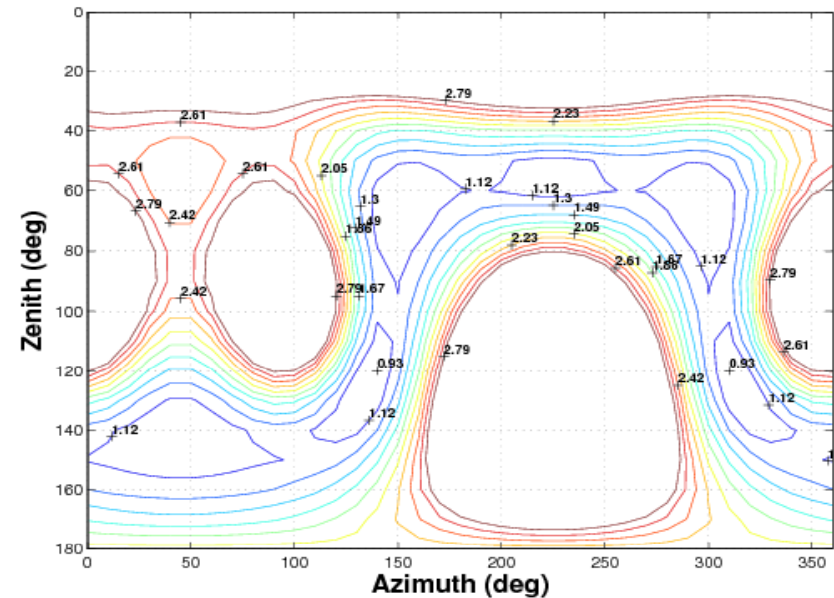
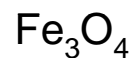
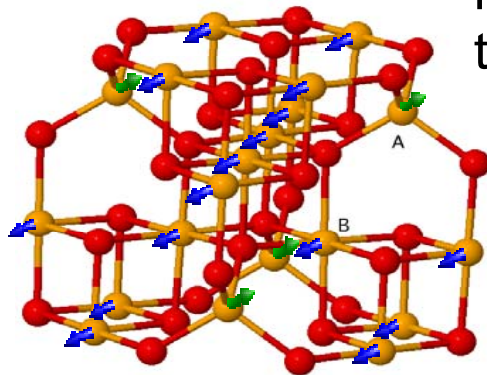
Minimal muon suite capabilities

Lattice sums for

Electrostatic potential
(e.g. around O^{2-})



Dipolar sums: Magnetic field modulus around the sphere



Level II: Interface

Essential features

Data input: define a convenient user-friendly format to enter crystallographic cell and magnetic structure (it needn't be CIF);

Import/export CIF files for data interchange with existing databases and programs;

3-D visualization for atomic positions within the cell, magnetic sublattices, candidate muon stopping sites;

Gui interface?

Level III: Implementation

Suggested programming **environment and language:**

Matlab (commercial) or Octave (free):

Interpreted high level languages, quick development and debugging cycle;

Platform independent;

Efficient (moderate performance penalty vs. C++ compilers);

Programming interfaces (API) to external DLL are available;

Advanced graphic capabilities, GUI programming (Matlab only).

File meta-formats: CIF & MCIF (todo)

CIF: suggested metaformat for encoding of structural data.

CIF is already a standard <http://ww1.iucr.org/cif/>
(a standard way to specify different atoms in the unit cell).
Employing an accepted standard ensures data interchange and interoperability with different data sources and programs.

Extended CIF with magnetic structure (MCIF) can be based

- on existing work

<http://www.ftj.agh.edu.pl/~pytlik/msdb/msdb.htm>

- or on the electron density extension of CIF

http://www.iucr.org/_data/iucr/cifdic_html/1/cif_rho.dic/index.html

(just need a way to store local spin direction and magnitude at each atom)

Structure visualization: external engines

Ready-available free-software tools; they use CIF as input language

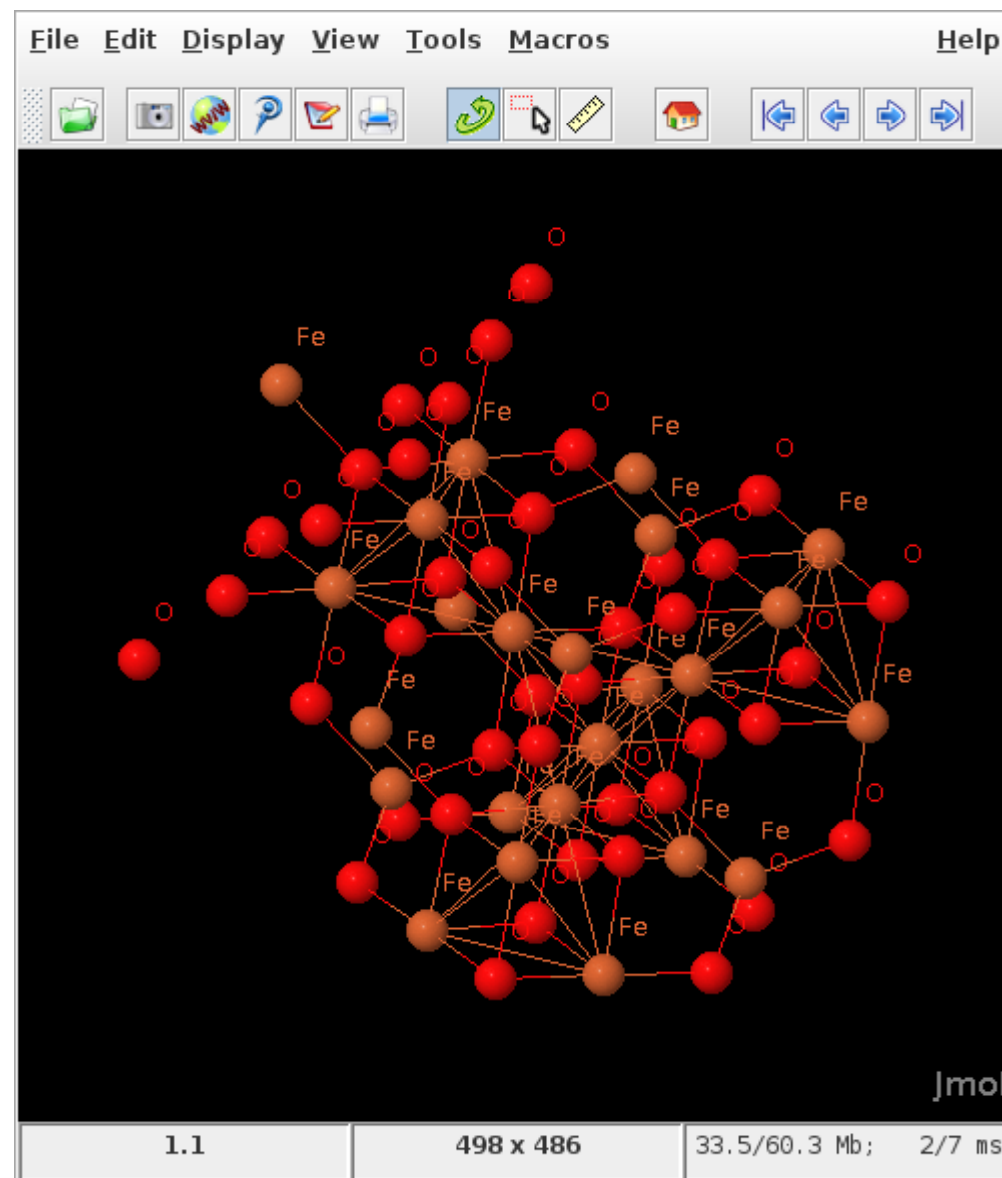
Jmol (platform-independent)

Rasmol

Mercury

(also commercial tools may be considered)

May use colours to distinguish sublattices.



Plans for the muon JRA

Acceptance of CIF as a meta-file standard (**done**)

Identification of MCIF standard (essential sub-standard) (**preliminary**).

Structure visualization (also magnetic) (**done**)

Minimal muon suite: in matlab or octave (**todo**)

Availability via a web page at ISIS and PSI (**todo**) with

Muon localization: an introduction

Definition of CIF ([link](#)), MCIF

Download of minimal set of tools and basic software in an open language (e.g. octave or matlab)