

Software tools for magnetic diffraction

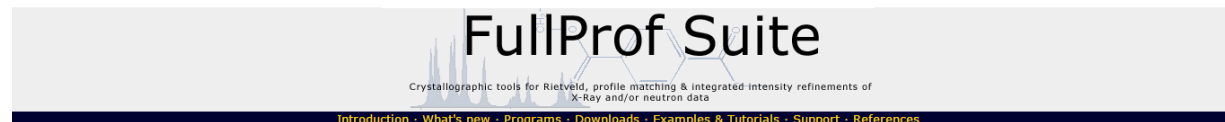
- ❑ Rietveld packages
- ❑ Symmetry analysis tools
- ❑ Visualization tools

Ovi Garlea (Neutron Scattering Division, Oak Ridge National Laboratory)



Rietveld packages for refining magnetic structures

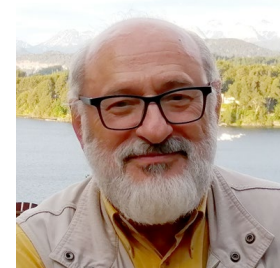
FullProf_Suite: <https://www.ill.eu/sites/fullprof/>



The FullProf Suite (for Windows and Linux) is formed by a set of crystallographic programs (FullProf, WinPLOTR, EdPCR, GFourier, etc...) mainly developed for Rietveld analysis (structure profile refinement) of neutron (constant wavelength, time of flight, nuclear and magnetic scattering) or X-ray powder diffraction data collected at constant or variable step in scattering angle 2theta.

The different programs can be run either in stand alone form (from a console window or clicking directly in a shortcut) or from the interfaces WinPLOTR and/or EdPCR.

The programs within the FullProf Suite are distributed in the hope that they will be useful, but WITHOUT ANY WARRANTY of being free of internal errors. In no event will the authors (or their institutions) be liable to you for damages, including any general, special, incidental or consequential damages arising out of the use or inability to use the programs (including but not limited to loss of data or data being rendered inaccurate or losses sustained by you or third parties or a failure of the program to operate with any other programs). The authors are not responsible for erroneous results obtained with the programs.



Juan Rodríguez Carvajal

GSAS-2 : <https://advancedphotonsource.github.io/GSAS-II-tutorials/#>

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Welcome to the home page for GSAS-II, a unique and comprehensive open source Python project for determination of crystal structures and diffraction-based materials characterization for crystalline solids on all scales, from perovskites through proteins, using both powder and single-crystal diffraction and with both x-ray and neutron



Robert Von Dreele



Brian H. Toby

Rietveld packages for refining magnetic structures

JANA: <http://jana.fzu.cz/>



JANA

Jana2006 is a crystallographic program focused to solution, refinement and interpretation of difficult, especially modulated structures. It calculates structures having up to three modulation vectors from powder as well as single crystal data measured with X-ray or neutron diffraction. The input diffraction data can be unlimitedly combined, the combination of powder neutron data with single crystal X-ray data being a typical example. The structure solution can be done using the built-in charge flipping algorithm or by calling an external direct methods program. Jana can handle multiphase structures (for both powder and single crystal data), merohedric twins as well as twins with partial overlap of diffraction spots, commensurate and incommensurate structures. It contains a powerful transformation table for summation.

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Dept of Structure Analysis | Laboratory of Crystallography
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CRYSTALLOGRAPHIC COMPUTING SYSTEM FOR STANDARD AND MODULATED STRUCTURES
Václav Petříček, Michal Dusek & Lukáš Palatinus

News

June 24 - 28, 2024 Aperiodic 2024 - The 11th International Conference on Aperiodic Crystals: Caen, France
abstract deadline 15 May 2024

COFUND project Physics for Future: Postdoctoral fellowships at the Institute of Physics, Prague, offer training in various disciplines including crystallography.

Jana2020 publication in Zeitschrift für Kristallographie: Please cite this article if you publish structures calculated with Jana2020.

October 18 - 20, 2023 Jana2020 workshop: Garching, Germany

June 18 - 23, 2023 The 15th conference on quasicrystals: Tel Aviv, Israel

The 26th IUCr Congress: abstract deadline 21 February 2023

August 22 - 25, 2023 The 26th IUCr Congress: Melbourne, Australia

June 28 - 23, 2023 The 15th International Conference on Quasicrystals, ICQ15: Tel Aviv, Israel

June 19 - 24, 2022 APERIODIC2022 - 10th International Conference on Aperiodic Crystals: Sapporo, Japan

May 23 - 27, 2022 5th international school on aperiodic crystals: Kutná Hora, Czechia

August 22 - 30, 2020 The 25th IUCr Congress: Prague, Czech Republic



Václav Petříček

MAG2POL <https://www.ill.eu/users/instruments/instruments-list/d3/software>

MAG2POL

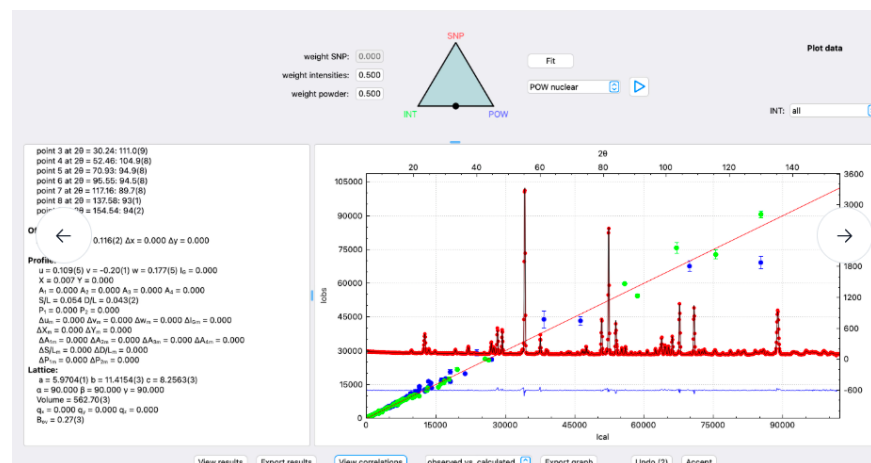
Mag2Pol is a program for the analysis of single-crystal and powder diffraction data. Nuclear and magnetic structures can be refined from spherical polarimetry and flipping ratio data as well as from integrated intensities and powder patterns.



A program for the analysis of neutron and X-ray diffraction data.

Mag2Pol is distributed under the LGPLv3 (Lesser GNU Public License version 3). A copy of the license text can be invoked from the About window within the program. The source code of the dynamically linked Qt libraries can be obtained (<https://code.qt.io/licenses/>) (note that the original code was not modified). The QtCustomPaint library can be downloaded (<https://code.qt.io/licenses/>) or from www.qt.io/licenses/. The Eigen library was obtained here (<https://eigen.tzema.org/>). You can also consult the [Eigen](https://eigen.tzema.org/) website.

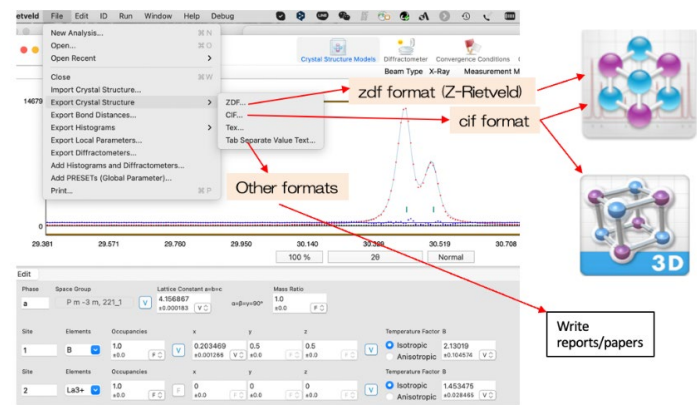
If this program was useful for analyzing and publishing your data, please cite it as [Mag2Pol, Qureshi, 2020](https://doi.org/10.1107/2020.0000000000000000).



Navid Qureshi

Rietveld packages for refining magnetic structures

Z-Rietveld: <https://z-code-software.com/>



Takashi Kamiyama (CSNS),
Toru Ishigaki (CROSS),
Yoshihisa Ishikawa (CROSS)
Masato Hagihara (JAEA),
Ryoko Oishi-Tomiyasu (Kyushu Univ.)
Satoshi Tamura (VIC)

RIETAN : <https://jp-minerals.org/rietan/> Fujio Izumi

RIETAN-FP・VENUS system distribution file

We analyze powder X-ray and neutron diffraction data, develop programs to visualize the results and electronic state calculation results in three dimensions, and make these works available free of charge on the Internet to promote structural analysis and visualization technology, and to give back our research results to society. It will also contribute to correcting disparities in research environments. This web page provides archive files for Windows and macOS that include manuals, programs, execution examples, RIETAN-FP and VENUS integrated support environments, etc. All archive files have been checked for viruses by [Avast Security](#). Note that VESTA, which is updated relatively frequently among the members of the VENUS system, is not included.

1. Overview of the RIETAN-FP/VENUS System

This system includes the following programs, macros (Windows: Hideamaru Macro *.mac, mac OS: AppleScript *.scpt), and bash scripts (*.command) as its main components. All Fortran programs are 64-bit applications. Windows shell scripts use [BusyBox](#), a lightweight Linux tool set, as a backend.

1. RIETAN-FP 3.12 is a multipurpose pattern fitting system that can be used for the Rietveld method, pattern decomposition, and MPF (MEM-based Pattern Fitting).
2. cif2ins Imports crystal data in *.cif into input file *.ins for RIETAN-FP
3. Combins creates an input file for multiphase Rietveld analysis, multi_phase.ins, from multiphase *.ins
4. *ins → *.dat → *.cif conversion utility ins2cif
5. cif2pdf converts the *.cif file obtained by ins2cif into a LaTeX document file *.tex, and then typesets it into a report on the crystal structure *.report.pdf
6. [Dynamica](#) is a maximum entropy method (MEM) program that implements the L-BFGS algorithm.
7. MPE_multi is a shell script that uses RIETAN-FP and Dynamica as the MPF analysis engine to calculate density distributions by varying the standard uncertainty of the observed structure factor as specified.
8. ALBA: A maximum entropy Patterson (MEP) program that can improve the structure factor of overlapping reflections obtained by pattern decomposition
9. MADEL: A program for calculating Madelung energy and site potentials using the Fourier method
10. Utility xdc to graph the wavelength dependence of the real part f' and imaginary part f'' of the anomalous dispersion correction term: and the mass attenuation coefficient μ_m of a specified element
11. Shell script sda for sequentially executing Rietveld analysis with some strings replaced in the input file hoge.ins for RIETAN-FP
12. VESTA is a 3D visualization system that was developed with close integration with RIETAN-FP and related software in mind, and has achieved widespread use on a global level.

1. RIETAN-FP・VENUS システムの概要

本システムは以下に列挙するプログラム、マクロ (Windows: 秀丸マクロ *.mac, mac OS: AppleScript *.scpt), bash スクリプト (*.command) を主要コンポーネントとします。Windows 用シェルスクリプトは軽量 Linux ツール群 [BusyBox](#) をバックエンドとして使います。

1. リートベルド法、パターン分解、MPF (MEM-based Pattern Fitting) に使える多目的パターンフィッティング・システム RIETAN-FP 3.12
2. *.cif 中の結晶データを RIETAN-FP 用入力ファイル *.ins に導入する cif2ins
3. 複数相の *.ins から多相リートベルド解析用入力ファイル multi_phase.ins を作成する combins
4. *ins → *.dat → *.cif 変換ユーティリティ ins2cif
5. ins2cif で得られた *.cif を LaTeX 文書ファイル *.tex に変換してから結晶構造に関する報告書 *.report.pdf として組版する cif2pdf
6. [Dynamica](#) は最大エントロピー法 (MEM) プログラム [Dynamica](#)
7. RIETAN-FP と [Dynamica](#) を MPF 解析エンジンとし、観測構造因子の標準不確かさを指定通りに変換させて密度分布を求めるためのシェルスクリプト MPE。
8. パターン分解で求めた重量百分の構造因子を改善しうる最大エントロピー・パターン (MEP) 法プログラム ALBA
9. フーリエ法によるマデルング・エネルギーとサイト・ポテンシャルの計算プログラム MADEL
10. 指定元素の質量分極補正項の実際の f' と虚部 f'' 、質量減断係数 μ_m の波長依存性をグラフ化するユーティリティ xdc
11. RIETAN-FP 用入力ファイル hoge.ins 中の文字列を一部置換したリートベルド解析を連続実行する外圍り計算用シェルスクリプト sda
12. RIETAN-FP や周辺ソフトとの密接な連携を念頭に開発され、世界レベルの普及を果たした三次元可視化システム VESTA

RIETAN-FP は比較的軽いソフトなので、CPU に対する負荷が高い並列処理を控えました。ノート PC 上でも他のプログラムを使いながら余裕をもって動かせます。

TOPAS : <http://www.topas-academic.net/>

TOPAS-Academic V7

by Coelho Software

Brisbane, Australia

August, 2020

Australian Business Number

70 827 688 789

AlanCoelho@bigpond.com

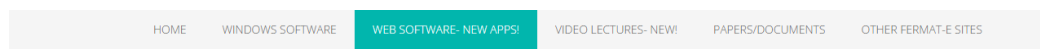
Introduction

Version 7 of TOPAS-Academic [Technical Reference.pdf](#) is now available to:

Symmetry analysis tools for creating magnetic models:

SARAh Representational Analysis:

<http://fermat.chem.ucl.ac.uk/spaces/willsgroup/web-software.html>



SARAh webRefine - FullProf

Two pieces of advice for using SARAh webRefine : 1. change your browser settings to allow you to select where you save downloads (and overwrite files). 2. when you click <evaluate>, it will look like nothing is happening for a few seconds. Look in the tab '4. Help and Strategies' for more information.

-Andrew (February 2022)



Space group : $[2, P-1, C1]$
Propagation vector :
0 0 0
Crystallographic coordinates with each atom on a separate line :
e.g. Cu2 1/2 1/2 -1/2
Cu1 1/2 1/2 -1/2

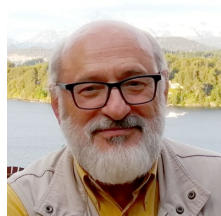
Submit



Andrew Wills

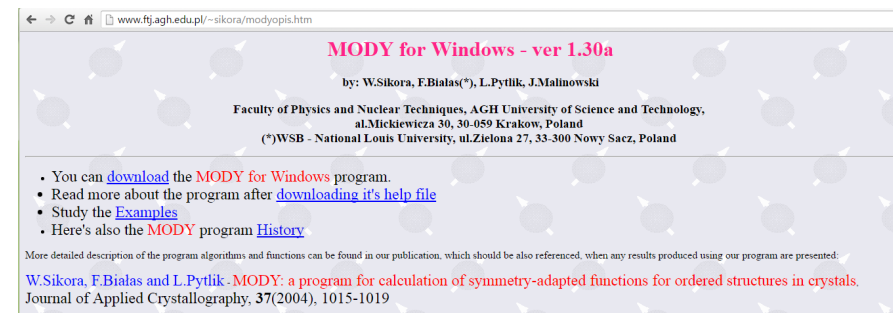
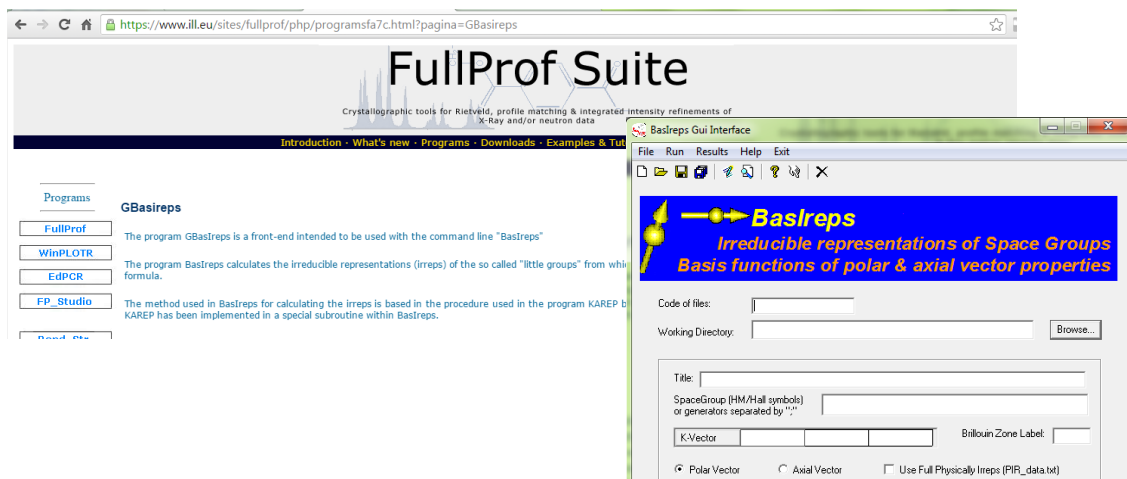
Basireps (FullProf_Suite)

<https://www.ill.eu/sites/fullprof>



Juan Rodríguez Carvajal

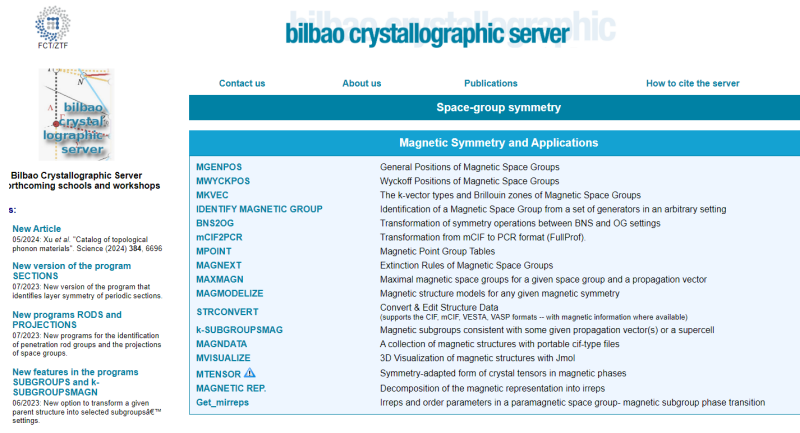
MODY: <http://www.ftj.agh.edu.pl/~sikora/modyopis.htm>



Symmetry analysis tools for creating magnetic models:

Bilbao Crystallographic Server

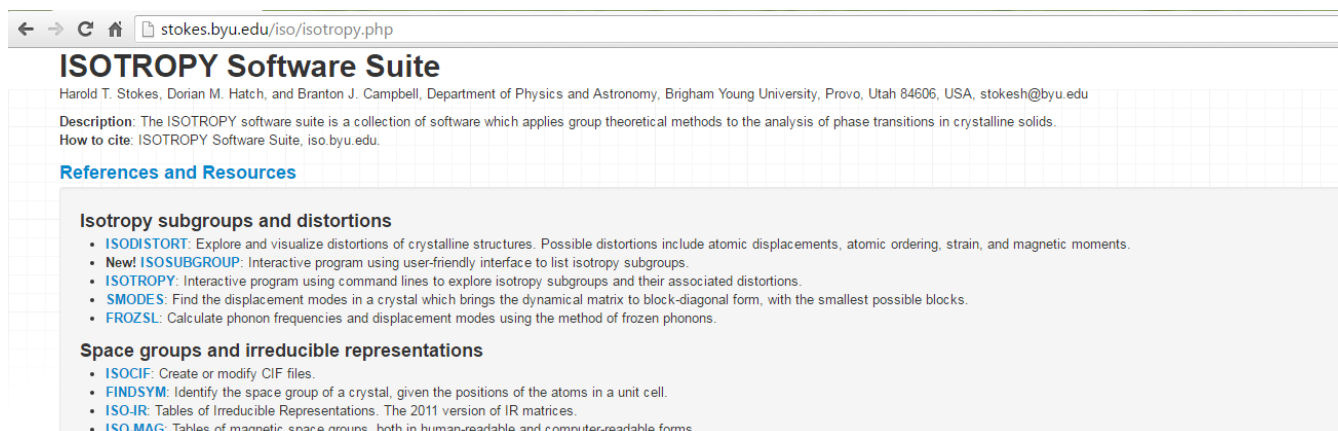
<https://www.cryst.ehu.es/#msgtop>



Manuel
Perez-Mato

Luis Elcoro,
Mois I. Aroyo

ISOTROPY Software Suite: <http://stokes.byu.edu/iso/isotropy.php>



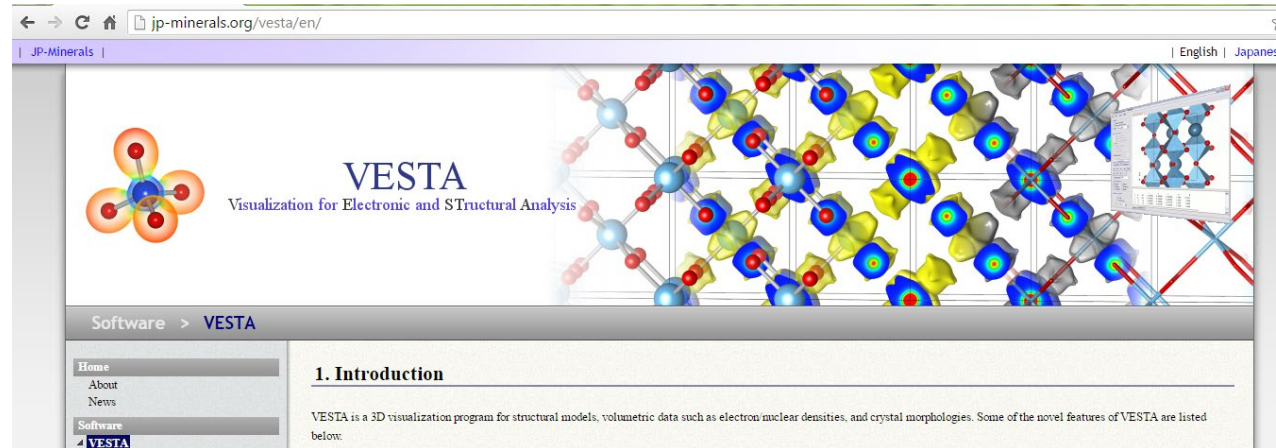
Branton J.
Campbell



Harold
T. Stokes

Visualization tools:

VESTA: <http://jp-minerals.org/vesta/en/>

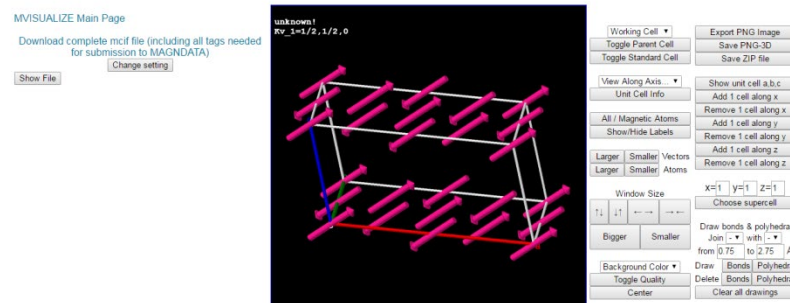


MVISUALIZE: Bilbao Crystallographic Server

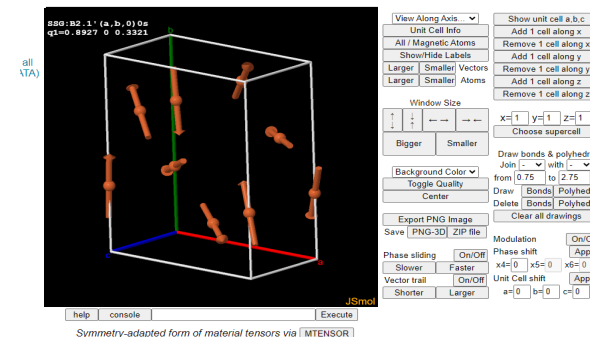
https://www.cryst.ehu.es/cgi-bin/cryst/programs/msglist_mod.pl

[webdcrystal1.ehu.es/magndata/mvisualize.htm?newcif=CuMnO2_45644.png&produced=tmp/mvisualize_45644.mcif&mcif=ly&DcmVhdGVhZGVhZS8BcWwW9W8gQ](https://www.cryst.ehu.es/cgi-bin/cryst/programs/msglist_mod.pl)

MVISUALIZE: 3D Visualization of magnetic structures with Jmol



MVISUALIZE: 3D Visualization of magnetic structures with Jmol



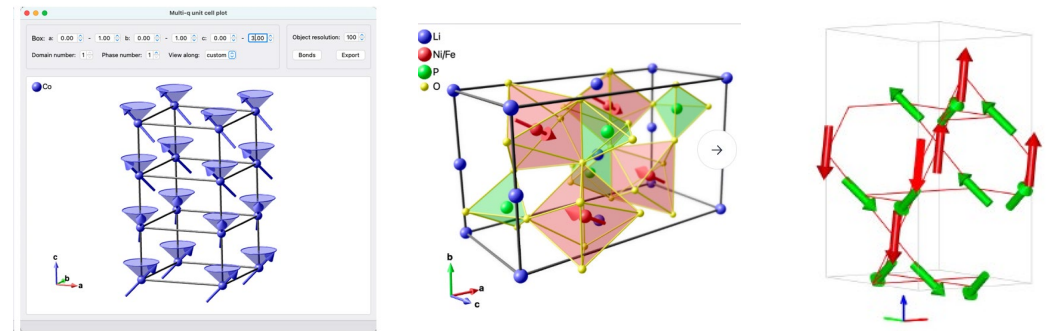
Visualization tools:

FullProf Suite: FPStudio

The screenshot shows the FullProf Suite website at https://www.ill.eu/sites/fullprof/php/programs71b4.html?pagina=FP_Studio. The website header features the 'FullProf Suite' logo and a navigation bar with links: Introduction, What's new, Programs, Downloads, Examples & Tutorials, Support, and References. A sidebar on the left lists programs: FullProf, WinPLOTR, EdPCR, FP_Studio, and Bond_Str. The main content area is titled 'FP_Studio' and describes the version 1.0 of the software, developed by Laurent Chapon and Juan Rodriguez-Carmona, which uses the WINTERACTOR interface. It also mentions that the program is being strongly recommended by the YSGFL community. The software interface itself is shown, displaying a 3D model of a crystal structure with atoms represented by colored spheres and bonds as sticks. The interface includes a 'File' menu, a 'Programs' list, and a 'Tables' section with data for 'Atom' and 'Site'.

MAG2POL, GSAS-2, JANA, Z-3D (Z-Rietveld)

Magnetic structures drawing tools



Diamond: <http://www.crystalimpact.com/diamond/>

The screenshot shows the Crystal Impact website at <http://www.crystalimpact.com/diamond/>. The website header features the 'CRYSTAL IMPACT' logo and a navigation bar with links: About us, Diamond, Endeavour, Match!, and Pearson's CD. A sidebar on the left lists features: Function List, Features, Brochure (PDF), References, Gallery, User Group, Developer blog, Get Diamond, Order Now, Demo Version, Version 4 Support, New Functions, and Feature Tour. The main content area is titled 'Diamond' and describes the software as a 'Crystal and Molecular Structure Visualization' tool. It includes a 'Diamond News' section with updates from March 21, 2016, February 22, 2016, January 4, 2016, and December 17, 2015. The software interface is shown, displaying a 3D model of a crystal structure with atoms represented by colored spheres and bonds as sticks.

CrystalMaker: <http://www.crystallmaker.com/>

The screenshot shows the CrystalMaker website at <http://www.crystallmaker.com/>. The website header features the 'CrystalMaker SOFTWARE' logo and a navigation bar with links: HOME, SOFTWARE, CRYSTALS, STORE, SUPPORT, CONTACT, and ABOUT. The main content area is titled 'Crystal and Molecular Structures Modelling & Diffraction' and includes a 'Visualize Crystal & Molecular Structures' section. It also features a 'Crystal Engineering & Molecular Modelling' section and a 'X-Ray & TEM Single-Crystal Diffraction' section. The software interface is shown, displaying a 3D model of a crystal structure with atoms represented by colored spheres and bonds as sticks.