

Software

Table 1 : Software evaluated

Name	Description	Site
DAVE	Data Analysis and Visualization Environment	http://www.ncnr.nist.gov/dave
Frida	Flexible rapid interactive data analysis	http://apps.jcns.fz-juelich.de/doku/frida/start
LAMP	Large Array Manipulation Program	http://www.ill.eu/instruments-support/computing-for-science/cs-software/a
ISAW	Integrated Spectral Analysis Workbench software project	ftp://ftp.sns.gov/ISAW
iFit	A simple library to analyse data	http://ifit.mccode.org/
Mantid	High-performance computing and visualisation of scientific data.	http://www.mantidproject.org/
GenX	The differential evolution algorithm for fitting X-ray and neutron reflect	http://genx.sourceforge.net/
Mfit	fit any type of (x,y) data with any fit function (even combinaisons)	http://www.ill.eu/instruments-support/computing-for-science/cs-software/a
Mview	manipulate and display up to 20 data files	http://www.ill.eu/instruments-support/computing-for-science/cs-software/a
Rescal/Matlab	compute 4D resolution ellipsoid for inelastic scattering instrument	http://www.ill.eu/instruments-support/computing-for-science/cs-software/a
Sansview	data analysis and modelling	http://danse.chem.utk.edu/sansview.html
Grasp	Reduction and Analysis	http://www.ill.eu/instruments-support/instruments-groups/groups/lss/grasp
Sasfit	Analysing and plotting small angle scattering data (no reduction?)	http://kur.web.psi.ch/sans1/SANSSoft/sasfit.html
GSAS	General Structure Analysis System	http://www.ncnr.nist.gov/xtal/software/gsas.html
Gsas-ii	Crystallography Data Analysis Software	https://subversion.xor.aps.anl.gov/trac/pyGSAS
EXPGUI	Graphical user interface to GSAS	https://subversion.xor.aps.anl.gov/trac/EXPGUI/wiki
FullProf Suite	Rietveld analysis of neutron/ X-ray powder diffraction data.	http://www.ill.eu/sites/fullprof/
PDFgui	Pair distribution function fit (Gui for PDFFit2)	http://www.diffpy.org
PDFfit2	Python version of PDFfit	http://www.diffpy.org
McStas	Monte Carlo Simulation of TAS	http://www.mcstas.org
Restrax	Monte Carlo simulations and data analysis	http://neutron.ujf.cas.cz/restrax/
Vitess	Virtual Instrumentation Tool for the ESS	http://www.helmholtz-berlin.de/forschung/grossgeraete/neutronenstreuung
Vtas	virtual Three Axis Spectrometer	http://www.ill.eu/?id=2048

Software

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Fields

Table 2: Scientific categorizes software has been applies to. Category Structure covers the sub-categorizes powder and single crystal diffraction beamlines and

	Structure			Spectroscopy		Reflectometry	Backscattering	Spin-echo
	Powder	SANS	Single-crystal	Time-of-flight	Muon	Triple-axis		
DAVE				x	?	x		x
Frida				x	?			x
LAMP	x	x		x	?		x	x
ISAW			x	x	?			
iFit					?			
Mantid	x	x	x	x	x		x	x
GenX					?		x	
Mfit					?	x		
Mview					?	x		
Rescal/Matlab				x	?	x		
Sansview		x			?			
Grasp		x			?			
Sasfit		x			?			
GSAS	x		x		?			
GSAS-II	x		x		?			
EXPGUI	x		x		?			
FullProf Suite	x		x		?			
PDFgui	x		x		?			
PDFfit2	x		x		?			
McStas	x	x	x	x	?	x	x	x
Restrax	x		x		?	x		
Vitess	x	x		x	?			x
Vtas					?	x		

Fields

I large scale structure beamlines (SANS). Category Spectroscopy covers beamlines on time-of-flight, reactor source (triple-axis) and Muon spectroscopy

Fields

beamlines.

Versions

Table 3A : Software versions, which were tested July 2012.

Name	Stable version	Development version	Language	Libraries
DAVE	v2.0 (2010)	Yes (IDL 8, http)	IDL 7.0	
Frida	v2.1.4c (2012)	Yes (svn)	C++	Yacc, Flex, Bison, GSL, gnuplot
LAMP	2012	Yes (ftp)	IDL 8.1	
ISAW	v. 1.9.1_12a (2012)	Yes (ftp)	Java	Jython
iFit	1.2 (2012)	Yes (svn)	Matlab	
Mantid	V2.2 (2012)	Yes (git)	C++, Python	Several
GenX	2.0.0 (2011)	Yes (svn)	Python	wxPython
Mfit/MView/Rescal	2005	No	Matlab	
Sansview	2.1.1 (2012)	Yes (svn)	C++, Python	NumPy, SciPy, Matplotlib
Grasp	6.60 (2012)	Yes (http)	Matlab	
Sasfit	0.93.3 (2011-05-4)	Yes (svn)	C	BLT for plotting
GSAS	2009	No	Fortran	
GSAS-II	0.2 (2012)	Yes (svn)	Python, Fortran	WxPython, NumPy, SciPy, Matplotlib
EXPGUI	2011	Yes (svn)	TCL	
FullProf Suite	2012	Yes	Fortran	CrysFML, Winteractor
PDFgui	2.0-r3067` (2009)	Just bug fixes (http)	Python	
PDFfit2	3.0-r3067` (2009)	No	C++, Python	
McStas	1.12 (2012)	Yes (svn)	C, Perl	PGPLOT (Matlab)
Restrax	2011	Yes (http)	F77/90	RESCAL, VTAS
Vitess	2.11(2011)	Yes (http)	C	BLTwish, IDL, PV-Wave
VTAS	4.1 (2010?)	No	Java	

Facilities

Table 3 : Here is a list of some of the facilities which uses the reviewed software. Should there not be a Muon column, after all the software evaluated is for NM

Supported / Used in													
Name	X-ray	Neutrons	ILL	NIST	PSI	LLB, Fr	Isis	HMI	Julich	ORNL SNS	ANSTO	FRM2	JAEA
DAVE	No	yes	yes	yes	yes								
Frida	No	yes											
LAMP	yes	yes	yes	?	yes	?	?	yes	?	?	yes	yes	?
ISAW	No	yes	No	?	?	?	?	?	?	?	?	?	?
iFit	yes	yes	yes				yes					yes	
Mantid	(muons)	yes					yes			yes			
GenX	yes	yes	?										
Mfit/Mview	?	yes	yes	?	?	?	?	?	?	?	?	?	?
Rescal													
Sansview	no?	yes	yes							yes			
Grasp	No	yes	yes	yes	yes	?	?	yes	yes	yes	yes	yes	yes
Sasfit	yes	yes	?	?	yes								
GSAS	yes	yes											
GSAS-II	yes	yes											
EXPGUI													
FullProf Suite	yes	yes	yes	?	?	yes	yes						
PDFgui		yes								yes			
PDFfit2		yes								yes			
McStas	(McXtrace)	yes	yes	yes	yes	yes	yes	?	yes	yes	yes	yes	yes
Restrax		yes	yes										
Vitess		yes						yes	yes			yes	
Vtas		yes	yes										

Facilities

I3 (Neutron scattering and Muon Spectroscopy). Also specify what “Supported” means? Should this table not be Table 4?