

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.jcms.fz-juelich.de/doku/frida/start
LAMP	Large Array Manipulation Program	http://www.ill.eu/instruments-support/computing-for-science/cs-software/all-software/lamp/
ISAW	Integrated Spectral Analysis Workbench software project (ToF)	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 reflections	http://genx.sourceforge.net/
Mfit	fit any type of (x,y) data with any fit function (even combinations)	http://www.ill.eu/instruments-support/computing-for-science/cs-software/all-software/matlab-ill/mfit/home
Mview	manipulate and display up to 20 data files	http://www.ill.eu/instruments-support/computing-for-science/cs-software/all-software/matlab-ill/mfit/home
Rescal/Matlab	compute 4D resolution ellipsoid for TAS	http://www.ill.eu/instruments-support/computing-for-science/cs-software/all-software/matlab-ill/mfit/home
Sasview	SAS data analysis and modelling	http://sasview.org/
Grasp	SANS Reduction and Analysis	http://www.ill.eu/instruments-support/instruments-groups/groups/iss/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 (diffraction)	http://www.ncnr.nist.gov/xtal/software/gsas.html
Gsas-ii	Crystallography Data Analysis Software (diffraction)	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, diffraction)	http://www.diffpy.org
PDFfit2	Python version of PDFfit (diffraction)	http://www.diffpy.org
McStas	Monte Carlo Simulation of TAS and other neutron instruments	http://www.mcstas.org
Restrax	Monte Carlo simulations and data analysis (TAS, diffraction)	http://neutron.ujf.cas.cz/restrax/
Vitess	Virtual Instrumentation Tool for the ESS	http://www.helmholtz-berlin.de/forschung/grossgeraete/neutronenstreuung/vitess_en.html
Vtas	virtual Three Axis Spectrometer	http://www.ill.eu/?id=2048
qtiKWS	SANS data reduction and analysis	http://www.ill.eu/~pipich/dokuwiki/doku.php/qtikws

Fields

Table 2: Scientific categories where software has been applied to.

	Structure			Spectroscopy			Reflectometry	Backscattering	Spin-echo
	Powder	SANS	Single-crystal	Time-of-flight	Muon	Triple-axis			
DAVE				X		X		X	X
Frida				X				X	
LAMP	X	X		X			X	X	
ISAW			X	X					
iFit	X	X		X		X			
Mantid	X	X	X	X	X		X	X	
GenX							X		
Mfit						X			
Mview						X			
Rescal/Matlab				X		X			
Sasview		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	X
Restrax	X		X			X			
Vitess	X	X		X					X
Vtas						X			
qtiKWS		X							

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	
Sasview	2.2 (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	2.0 (2012)	Yes (svn)	C, Perl, Python	PGPLOT, Matlab, Matplotlib/Chaco, x3d
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 4 : Here is a list of some of the facilities which uses the reviewed software.

Name	Used at										
	ILL	NIST PSI	LLB, Isis	HMI	ORNL	SANSTO	FRM2/Jü	JAEA	X-ray	Muons	
DAVE	yes	yes	yes								
Frida									yes		
LAMP	yes	?	yes	?	?	yes	?	yes	yes	?	yes
ISAW		?	?	?	?	?	?	?	?	?	
iFit	yes				yes				yes		yes
Mantid	yes				yes		yes				yes
GenX	yes										yes
Mfit/Mview	yes	yes	?	?	?	?	yes	?	?	?	?
Rescal	yes	yes					yes				
Sasview	yes						yes				yes
Grasp	yes	yes	yes	?	?	yes	yes	yes	yes	yes	
Sasfit	?	?	yes								yes
GSAS											yes
GSAS-II											yes
EXPGUI											yes
FullProf Suite	yes	?	?	yes	yes						yes
PDFgui							yes				yes
PDFfit2							yes				yes
McStas	yes	yes	yes	yes	yes	?	yes	yes	yes	yes	(McXtrace)
Restrax	yes										
Vitess						yes			yes		
Vtas	yes										
qtiKWS									yes		