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 reflec	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/gras|
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/neutronenstreuun
Vtas	virtual Three Axis Spectrometer	http://www.ill.eu/?id=2048

Fields

Table 2: fields of application

	Diffraction			Spectroscopy					General	Simulation	Reduction	Analysis
	Powder	Sans	SX	Time-of-flight	3-axis	Reflecto.	Backscatt.	Spin-echo				
DAVE				x	x		x	x				
Frida				x			x				x	
LAMP	x	x		x		x	x		x		x	x
ISAW			x	x								
iFit				x					x	x	x	x
Mantid		x		x							x	
GenX						x						
Mfit					x						x	
Mview					x						x	
Rescal/Matlab				x	x							x
Sansview		x										x
Grasp		x									x	
Sasfit		x										x
GSAS	x		x								x	x
GSAS-II	x		x								x	x
EXPGUI	x		x									
FullProf Suite	x		x								x	x
PDFgui	x		x									x
PDFfit2	x		x									x
McStas	x	x	x	x	x	x	x	x	x	x		
Restrax	x		x		x					x		
Vitess		x		x				x	x	x		
Vtas	x	x			x					x		

Table 3 : Version tested July 2012

Name	Version		Language	Libraries	Extendable	Source code	GUI
	stable	Development					
DAVE	v2.0 (2010)	Yes (IDL 8,	IDL 7.0		No	Yes (need IDL lice	++
Frida	v2.1.4c (2012)	Yes (svn)	C++	Yacc, Flex, Bison, GSL, gnuplot		Yes	No GUI
LAMP	2012	Yes (ftp)	IDL 8.1		yes (IDL scripts)	Yes (need IDL lice-/+	
ISAW	v. 1.9.1_12a	Yes (ftp)	Java	Jython	yes (through operators)	Yes	+ (Swing)
iFit	1.2 (2012)	Yes (svn)	Matlab		Yes (scripts, functions)	Yes	No GUI
Mantid	V2.2 (2012)	Yes (git)	C++, Python	Several	Yes (Python or C++ algo	Yes	++ (Qt)
GenX	2.0.0 (2011)	Yes (svn)	Python	wxPython	yes (scripts, plugins)	Yes	+++ (wxPython)
Mfit/MView/Res	2005	No	Matlab		Yes (routines + fit functio	Yes (need Matlab	+/-
Sansview	2.1.1 (2012)	Yes (svn)	C++, Python	NumPy, SciPy, Matplotlib		Yes	+ wxPython
Grasp	6.60 (2012)	Yes (http)	Matlab		?	Yes (need Matlab	+/-
Sasfit	0.93.3 (2011-	Yes (svn)	C	BLT for plotting	yes (plugins in C)	Yes	TCL/TK
GSAS	2009	No	Fortran		?	No	No GUI
GSAS-II	0.2 (2012)	Yes (svn)	Python, Fortra	wxPython, NumPy, SciPy, Matplc	?	Yes	+ wxPython
EXPGUI	2011	Yes (svn)	TCL		TCL	Yes	+
FullProf Suite	2012	Yes	Fortran	CrysFML, Winteracter	Difficult	Partly (just CrysFM	+/- (winteracter)
PDFgui	2.0-r3067`(20	Just bug fix	Python			Yes	+ wxPython
PDFfit2	3.0-r3067`(20	No	C++, Python			Yes	No Gui
McStas	1.12 (2012)	Yes (svn)	C, Perl	PGPLOT (Matlab)	Yes (modules)	Yes	Perl-TK
Restrax	2011	Yes (http)	F77/90	RESCAL, VTAS	Difficult	Yes	through SIMRES
Vitess	2.11(2011)	Yes (http)	C	BLTwish, IDL, PV-Wave	Difficult	Yes	+ (TCL/TK, IDL, PV
VTAS	4.1 (2010?)	No	Java		No	No	++ / Swing

Table 3 : Supported Facilities

Name	Supported / Used in												
	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	(McXtra)yes	yes	yes	yes	yes	yes	yes	?	yes	yes	yes	yes	yes
Restrax		yes	yes						yes				
Vitess		yes						yes	yes			yes	
Vtas		yes	yes										