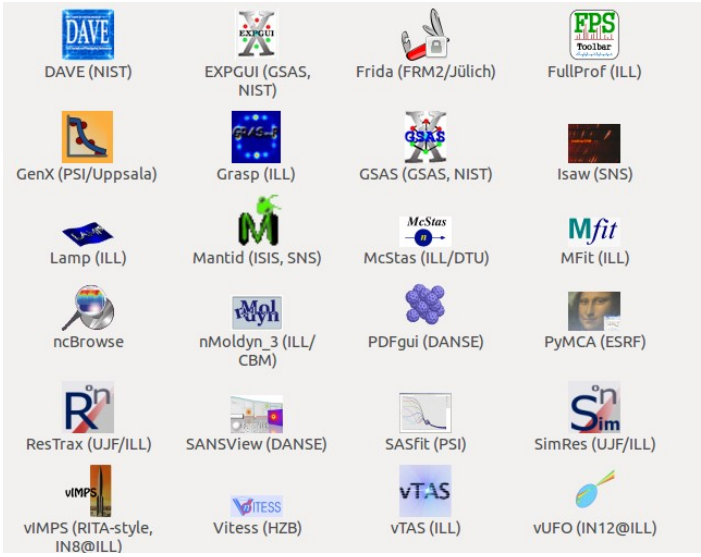
Welcome to the NMI3/ILL Ubuntu Live DVD distribution

E. Farhi, May 2012
[ILL Computing for Science] [NMI3 Data Analysis]



It comes with some neutron community related software (pre-installed):

***Generic*: LAMP, DAVE, Mantid, nMoldyn, Frida**
***Monte-Carlo simulation*: McStas, Vitess, SimRes,**
***TAS*: Mfit/MView, vTAS, ResTrax,**
***Diff*: PDFgui, FullProf, F.O.X,**
***SANS*: SASfit, GSAS, SANSView, GRASP, GenX**

as well as many other scientific/computing software:

- *C, C++ and Fortran compilers, Java, Python, Perl, Tcl/Tk, OpenMPI, Python libs (Matplotlib, numpy, scientific, tk, numeric),* ***AbInit****, Chemtool, Gelemental, Ghemical, Gperiodic, Gromacs, mopac, MPQC, PyMol, Rasmol, Viewmol, BallView, Avogadro, DrawXtl, CBFlib, DX, Fityk, Gabedit, Garlic, Gcrystal, Octave, PerlDL, PGPLOT, netcdf, ncview, hdf4, hdf5,* ***nexus****, hdfview, GeomView, OpenBabel, ParaView, Maxima, Java3d, gimp, freewrl,PyMCA,* ***FOX****, OpenMX, JMol,*

This DVD is bootable. It contains a Ubuntu 12.04 system with pre-installed applications. You may just run it without touching the current computer disk. You may also install it (with all software) on a 30 Gb+ disk. The Ubuntu system runs on all machines, including Apple ones. The CPU needs to support 64bit architecture (will not run on some *netbooks* and older machines). Perfect for testing software, tutorials and schools, and machine deployment. Find Applications from either the Desktop directory, or type '**neutron**' in the *Dash Home*.
MacOSX*: Press '**C**' at boot to start from the DVD.*

NOTE. Remember to check *System Settings* / Network and Keyboard

INSTALL the DVD: requires a 30GB+ partition. **Be cautious** not to erase existing systems/data ! See ***notes below*** for Mac OSX systems. You may also run the ISO in a **virtual machine** using e.g.. VirtualBox: define a new machine, attach a 30Gb disk and this ISO, then boot and install the system on the virtual disk. You can of course change the layout/settings after installation.

INSTALL applications for Windows, Linux, Mac OSX: use source codes in the **Desktop/Packages** directory. All binaries are installed in /usr/local and /opt.

Credits and References

This DVD is a product of the EU FP7 NMI3-II [INFRA-2011-1.1.17.] grant 233883
Work package 6 "Standards for Data Analysis Software"
members: ILL, STFC/ISIS, TUM, Jülich, PSI, HZB, CEA, HZG, ESS

LAMP © ILL (Apr 12th, 2012)
Large Array Manipulation Program
D. Richard, M. Ferrand and G.J. Kearley, J. Neutron Research **4**, 33-39, 1996.
<http://www.ill.eu/instruments-support/computing-for-science/cs-software/all-software/lamp/>

McStas © ILL and DTU NMI3/ESS (1.12c, June 3rd, 2011)
Monte Carlo simulation of neutron instruments
K. Lefmann and K. Nielsen, Neutron News 10, 20, (1999).
P. Willendrup, E. Farhi and K. Lefmann, Physica B, 350 (2004) 735.
<www.mcstas.org>

Mfit/MView © ILL (Aug 23rd 2005)
Data Analysis Suite based on Matlab v7.13 (2010a), for neutrons
<http://www.ill.eu/instruments-support/computing-for-science/cs-software/all-software/matlab-ill/>

GRASP © ILL (6.47, Apr 30th, 2012)
Small-Angle Neutron Scattering (SANS) data analysis based on Matlab v7.6 2007a
Charles Dewhurst, ILL
<http://www.ill.eu/instruments-support/instruments-groups/groups/lss/grasp/>

nMOLDYN © ILL (3.0.9, January 2011)
Molecular Dynamics Trajectory Analyzer
Eric Pellegrini, ILL, Konrad Hinsen and Gerald Kneller, CNRS
<http://forge.ill.fr/projects/show/nmoldyn>

vTAS © ILL (0.6d1, January 2011)
TAS-type machine simulator with direct and reciprocal space handling
With TAS, Flat Cone, IMPS (IN8 multiplexed) and UFO (IN12)
Press R key to compute resolution function with McStas in the background
Martin Boëhm, Alain Filhol, Yannick Raoul, ILL 2009-2011
<http://www.ill.eu/instruments-support/computing-for-science/cs-software/all-software/vtas/>

DAVE © NIST (2.1 beta, Oct 2nd, 2012)
R.T. Azuah, L.R. Kneller, Y. Qiu, P.L.W. Tregenna-Piggott, C.M. Brown, J.R.D. Copley, and R.M. Dimeo, **J. Res. Natl. Inst. Stan. Technol. 114, 341** (2009).
<http://www.ncnr.nist.gov/dave/>

SASfit © PSI (0.93.2 - 2010-07-08)
Software package SASfit for fitting small-angle scattering curves
Joachim Kohlbrecher, PSI
<http://kur.web.psi.ch/sans1/SANSSoft/sasfit.html>

Mantid © ISIS and SNS (2.1, May 4th, 2012)
Framework for computing on neutron and muon data
<http://www.mantidproject.org>

PyMCA © ESRF (4.5.0, May 2012)
EDF and HDF data analysis, for X rays.
<http://pymca.sourceforge.net/>

ncBrowse © NOAA/PMEL/EPIC (1.6.3, August, 28, 2006)
NetCDF browser
<http://www.epic.noaa.gov/java/ncBrowse/>

Isaw @ SNS (1.9.1, Feb 17th 2012)
Time-of-flight data analysis
Dennis Mikkelson (mikkelsond@uwstout.edu) University of Wisconsin-Stout Menomonie, USA
<ftp://ftp.sns.gov/ISAW/>

DiffPy/PDFgui @SNS/DANSE (1.0-r3067 2009-04-10)

a program for full-profile fitting of the atomic pair distribution function (PDF) derived from x-ray or neutron diffraction data

C. L. Farrow, et al. *J. Phys.: Condens. Matter* **19**, 335219 (2007)

<http://www.diffpy.org/>

ResTrax @UJF/ILL (5.2.3 Apr 2011) and SimRes (6.1.2)

Monte Carlo simulations and data analysis for three-axis neutron spectrometers

J. Šaroun, J. Kulda, "RESTRAX - a program for TAS resolution calculation and for scan profile simulation", *Physica B* **234-236** (1997) 1102-1104.

<http://neutron.ujf.cas.cz/restrax/>

SANSView @NIST/DANSE (2.1 Feb 2012)

SANS dana analysis and modeling with an emphasis on the 2D analysis of oriented systems.

Dr. P. Butler DANSE/SANS Project Leader NIST

<http://danse.chem.utk.edu/sansview.html>

Vitess @HZB/NMI3/ESS (2.11)

Virtual Instrumentation Tool for Neutron Scattering at Pulsed and Continuous Sources

G. Zsigmond, K. Lieutenant & F. Mezei, Neutron News 13, 2002

<http://www.helmholtz-berlin.de/vitess>

GSAS @NIST (2012)

Generalized Analysis Structure System

A.C. Larson and R.B. Von Dreele, "General Structure Analysis System (GSAS)", Los Alamos National Laboratory Report LAUR 86-748 (2000).

B. H. Toby, *EXPGUI*, a graphical user interface for *GSAS*, *J. Appl. Cryst.* **34**, 210-213 (2001)

<http://www.ncnr.nist.gov/xtal/software/gsas.html>

FullProf ©ILL and LLB (May 2010)

Rietveld analysis (structure profile refinement) of neutron or X-ray powder diffraction data

Rodriguez-Carvajal, J., Physica B.(1993), 192, 55

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

GenX @ PSI/Uppsala (2.0.0 March 2011)

X-ray and neutron reflectivity data

M. Björck and G. Andersson, J. Appl. Cryst. 40, 1174 (2007).

<http://genx.sourceforge.net/index.html>

DISCLAIMER: This custom Ubuntu system comes with no guaranty.
Use it carefully, especially when installing the system (back-up).

INSTALL notes

The installation is straight forward, and lasts about 30 minutes. It is highly recommended to back-up your personal data before you start. A new partition and swap space will be created during the first installation.

Mac OSX users will need to install rEFIt before. Refer to:
<https://help.ubuntu.com/community/MactelSupportTeam/AppleIntelInstallation#Dual-Boot:%20Mac%20OSX%20and%20Ubuntu>.