Experience at the EMBL with Debian: the viewpoint of a scientist

Sandor Brockhauser

EMBL-Grenoble

Debian for Scientific Facilities Days
ESRF
Grenoble, France
June 24-26, 2012

EMBL - ESRF

Austria 1974
Belgium 1990
Croatia 2006
Denmark 1974
Finland 1984
France 1974
Germany 1974
Greece 1984
Iceland 2004
Ireland 2003
Israel 1974
Italy 1974
Luxembourg 2007
Netherlands 1974
Norway 1985
Portugal 1998
Spain 1986
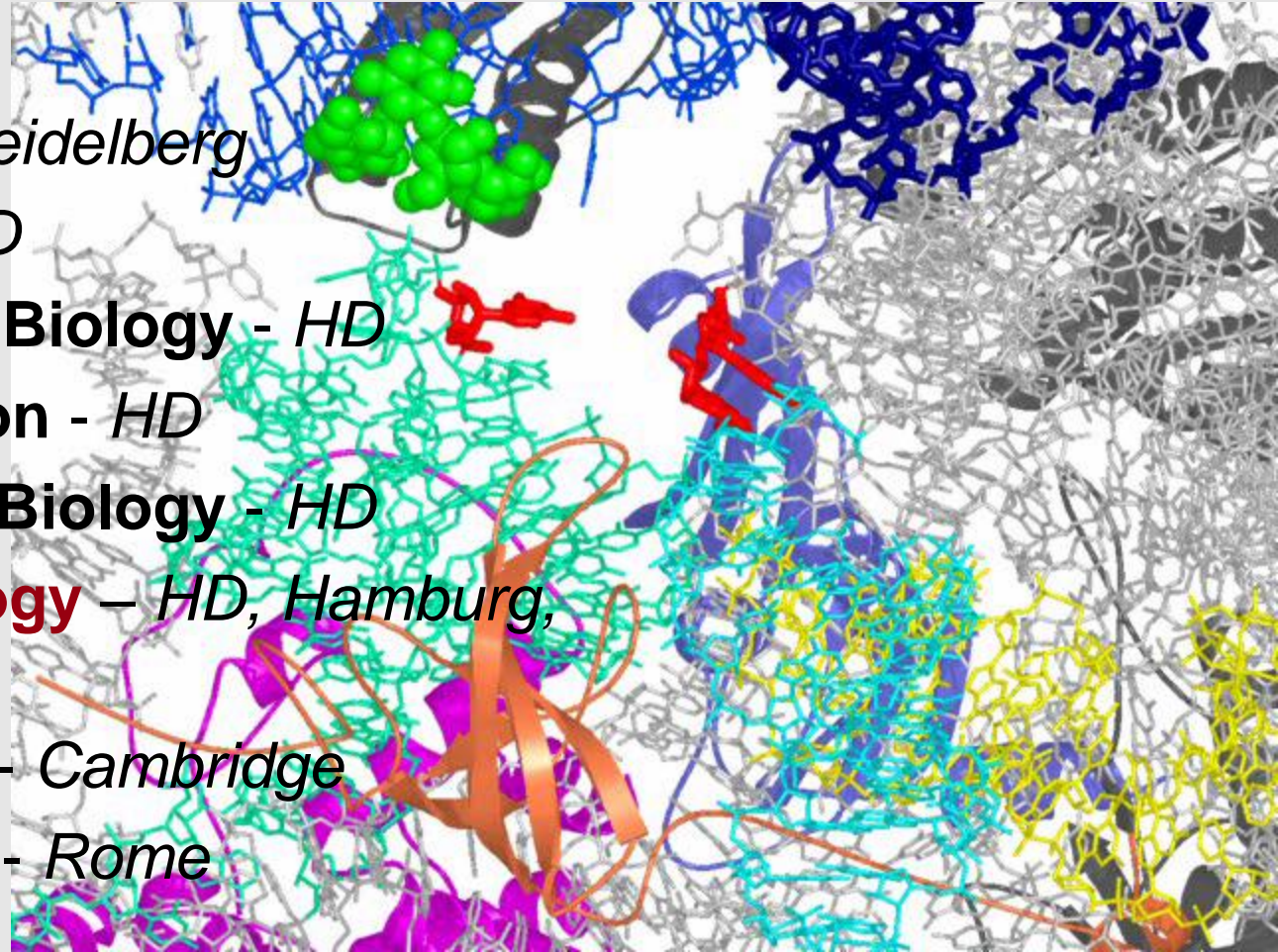Sweden 1974
Switzerland 1974
United Kingdom 1974

EMBL

EMBL Units

- **Cell Biology**- *Heidelberg*
- **Biophysics** - *HD*
- **Developmental Biology** - *HD*
- **Gene Expression** - *HD*
- **Computational Biology** - *HD*
- **Structural Biology** – *HD, Hamburg, Grenoble*
- **Bioinformatics** - *Cambridge*
- **Mouse Biology** - *Rome*

EMBL

EMBL Units

- **Cell Biology**- *Heidelberg*
- **Biophysics** - *HD*
- **Developmental Biology** - *HD*
- **Gene Expression** - *HD*
- **Computational Biology** - *HD*
- **Structural Biology** – *HD, Hamburg, Grenoble*
- **Bioinformatics** - *Cambridge*
- **Mouse Biology** - *Rome*

Paromomycin binding to 30S
http://www.mrc-lmb.cam.ac.uk/ribo/homepage/mov_and_overview.html

EMBL

Techniques for Structural Biology
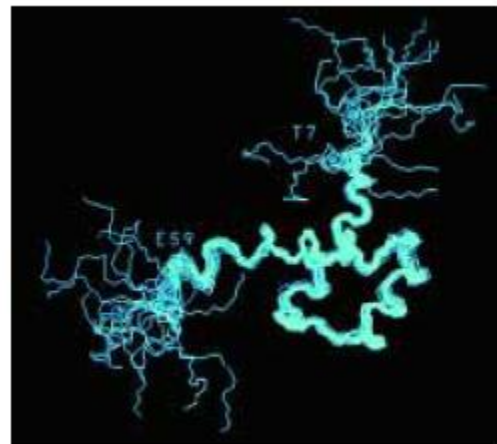
- Nuclear Magnetic Resonance (NMR)

Figure 1. NMR structure of the *Antennapedia* homeodomain (1). A bundle of 20 superimposed conformers represents the polypeptide backbone. For the polypeptide segment 7–59 the tight fit of the bundle indicates that the structure is defined with high precision, whereas the two chain ends are disordered.

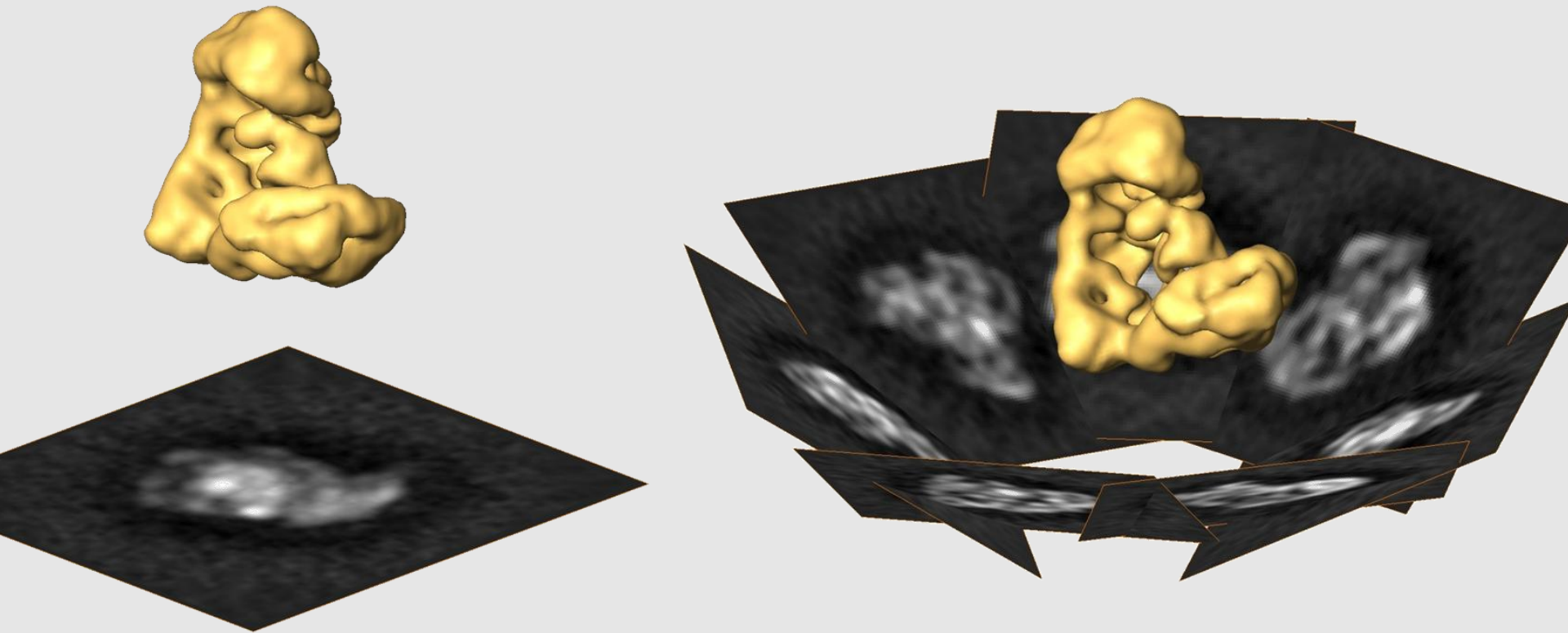NMR STUDIES OF STRUCTURE AND FUNCTION OF BIOLOGICAL MACROMOLECULES
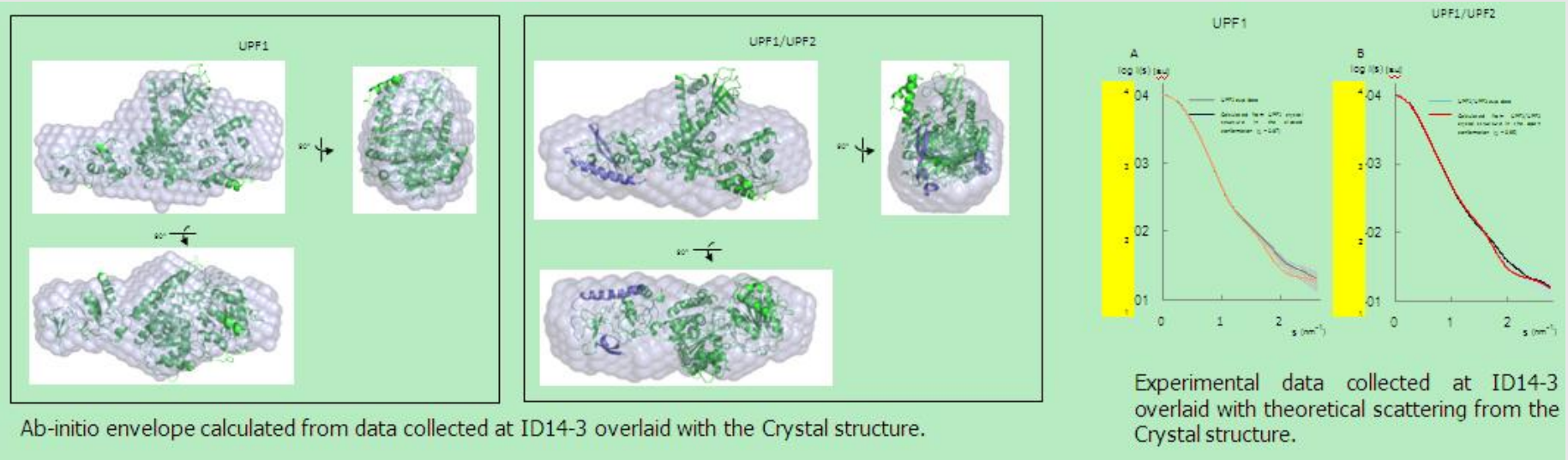
Nobel Lecture, December 8, 2002

by

KURT WÜTHRICH

EMBL

Techniques for Structural Biology

- Nuclear Magnetic Resonance (NMR)
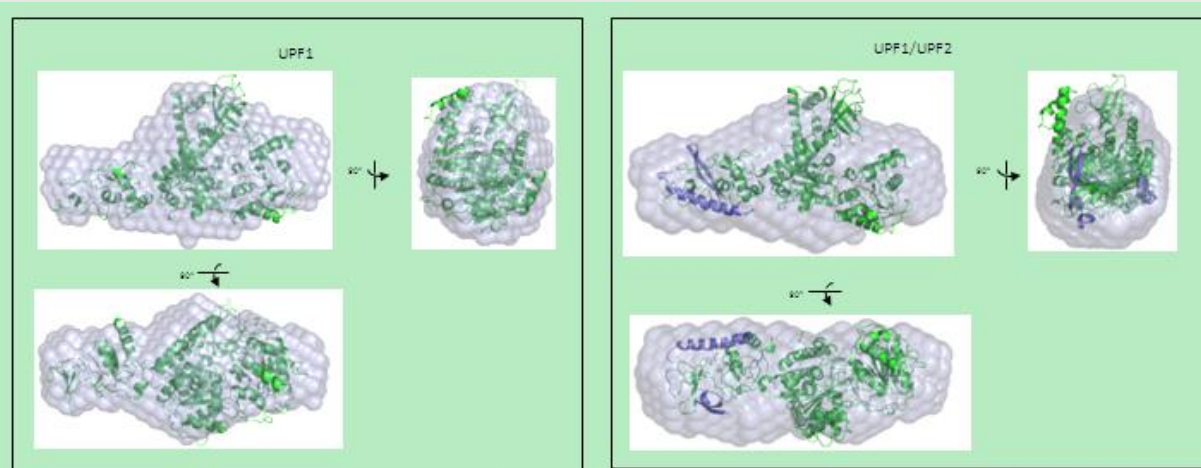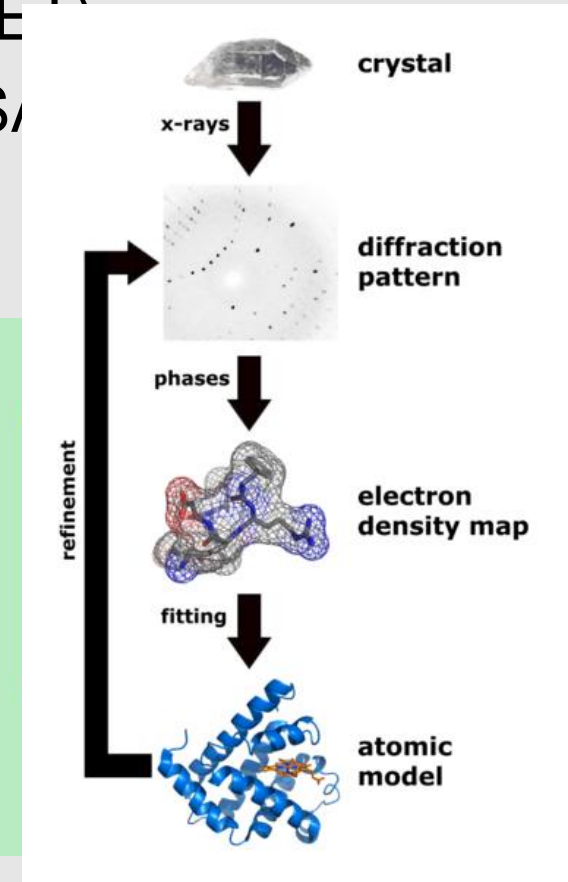- Electron Microscopy/Tomography (EM/ET)

Techniques for Structural Biology

- Nuclear Magnetic Resonance (NMR)
- Electron Microscopy/Tomography (EM/ET)
- Small Angle Xray/Neutron Scattering (SAXS/SANS)

Ab-initio envelope calculated from data collected at ID14-3 overlaid with the Crystal structure.

Experimental data collected at ID14-3 overlaid with theoretical scattering from the Crystal structure.

Techniques for Structural Biology

- Nuclear Magnetic Resonance (NMR)
- Electron Microscopy/Tomography (EM/E~~)
- Small Angle Xray/Neutron Scattering (S~
- Macromolecular Crystallography (MX)

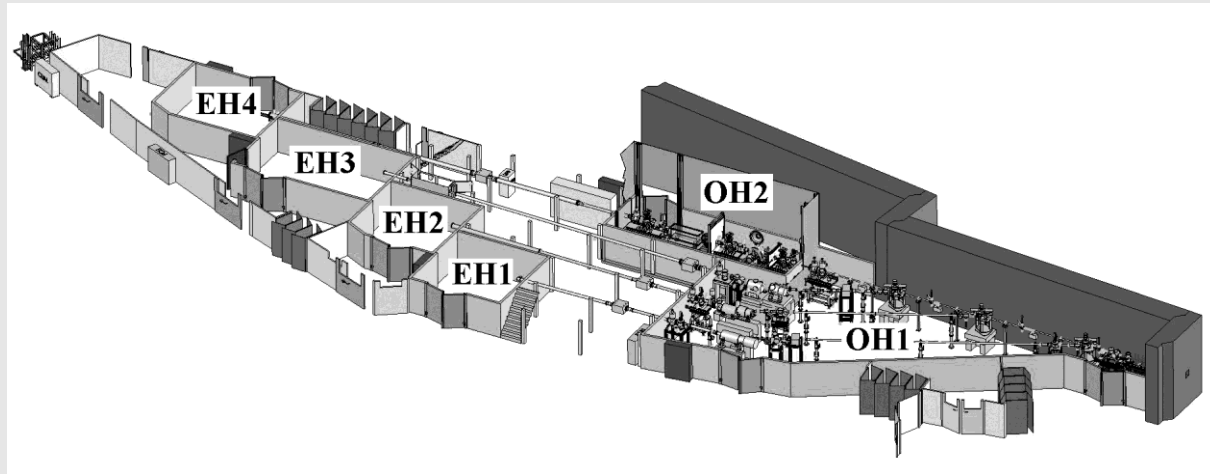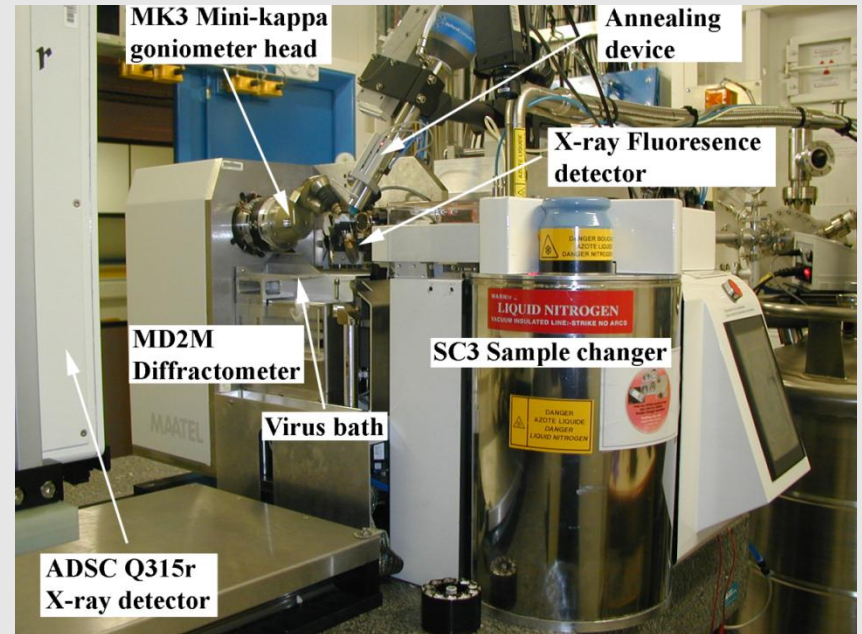Ab-initio envelope calculated from data collected at ID14-3 overlaid with the Crystal structure.

crystal

x-rays

diffraction pattern

phases

electron density map

fitting

atomic model

refinement

EMBL

EMBL at the SB Beamlines

Hassan Belrhali, Babu Manjasetty

Sandor Brockhauser, Andrew McCarthy

Max Nanao

- MX:
  BM14, ID14-1, ID14-4, ID23-1, ID23-2, ID29
- BioSAX:
  BM29

Adam Round,
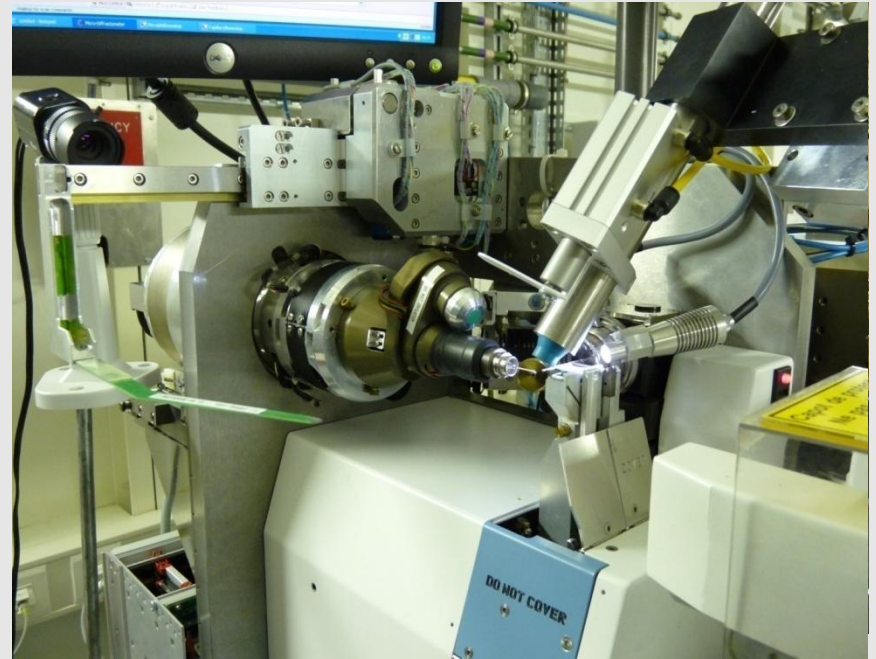*Petra Pernot (ESRF)*

EH4
EH3
EH2
EH1
OH2
OH1

EMBL

EMBL/ESRF developments

- Diffractometer
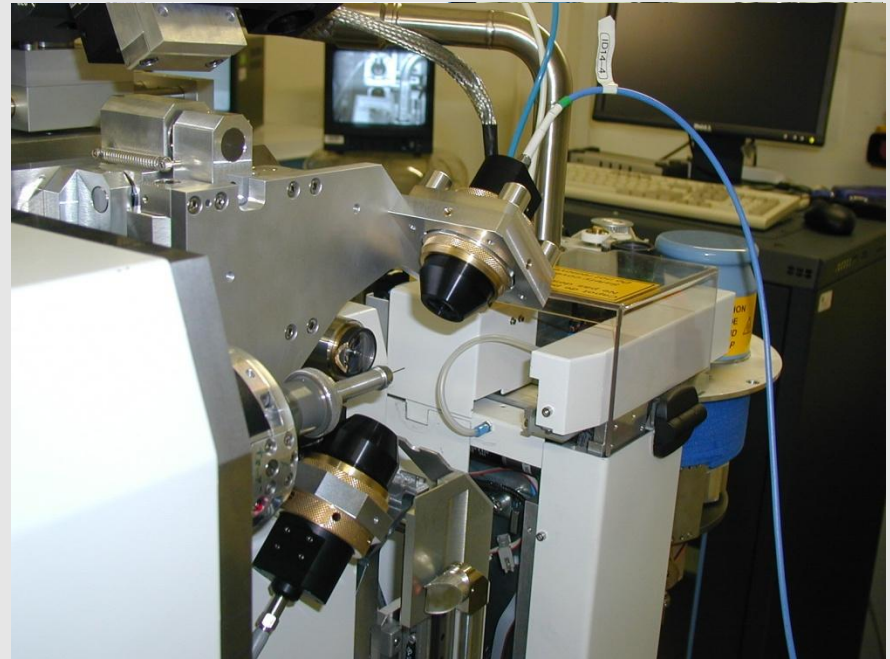- On-axis-view
- Sample Changer

EMBL/ESRF developments

- Diffractometer

- On-axis-view

- Sample Changer

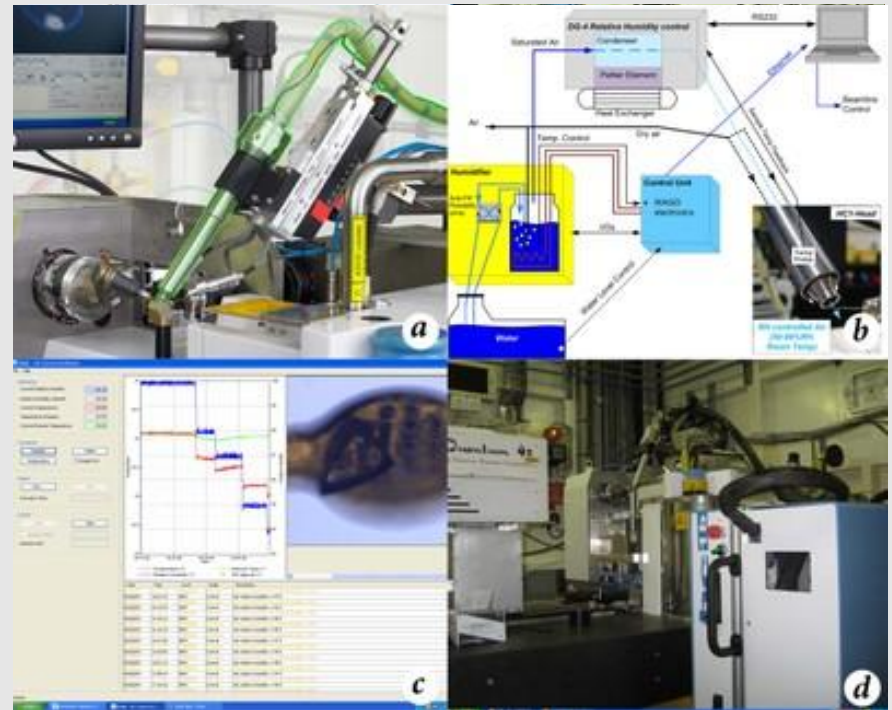- MiniKappa

- Low-resolution beamstop

EMBL/ESRF developments

- Diffractometer
- On-axis-view
- Sample Changer
- MiniKappa
- Low-resolution beamstop
- On-line Microspec

EMBL

EMBL/ESRF developments

- Diffractometer

- On-axis-view

- Sample Changer

- MiniKappa

- Low-resolution beamstop

- On-line Microspec

- Humidity Control Device
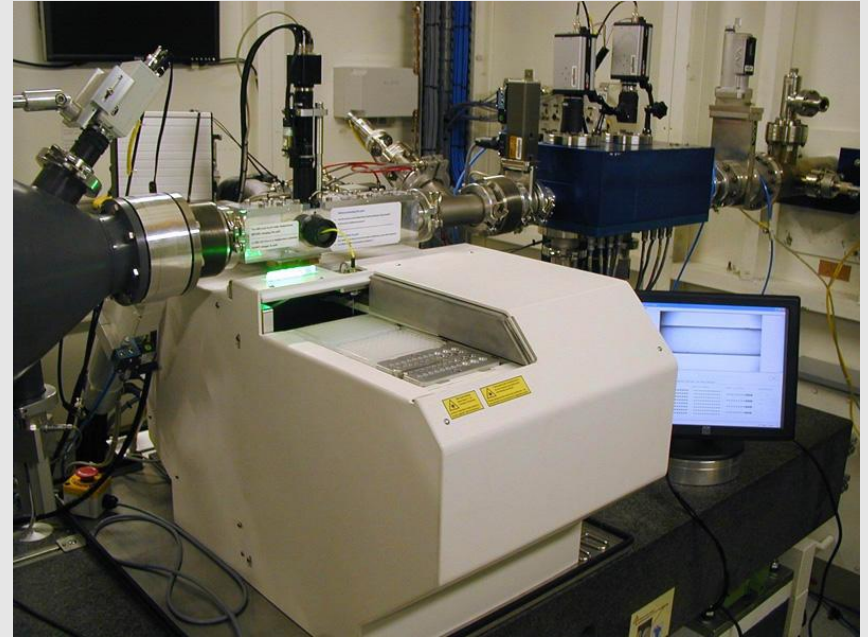
EMBL

EMBL/ESRF developments

- Diffractometer

- On-axis-view

- Sample Changer

- MiniKappa

- Low-resolution beamstop

- On-line Microspec

- Humidity Control Device

- SAX Sample Changer

EMBL

EMBL/ESRF developments

- Diffractometer
- On-axis-view
- Sample Changer
- MiniKappa
- Low-resolution beamstop
- On-line Microspec
- Humidity Control Device
- SAX Sample Changer
- Tomography

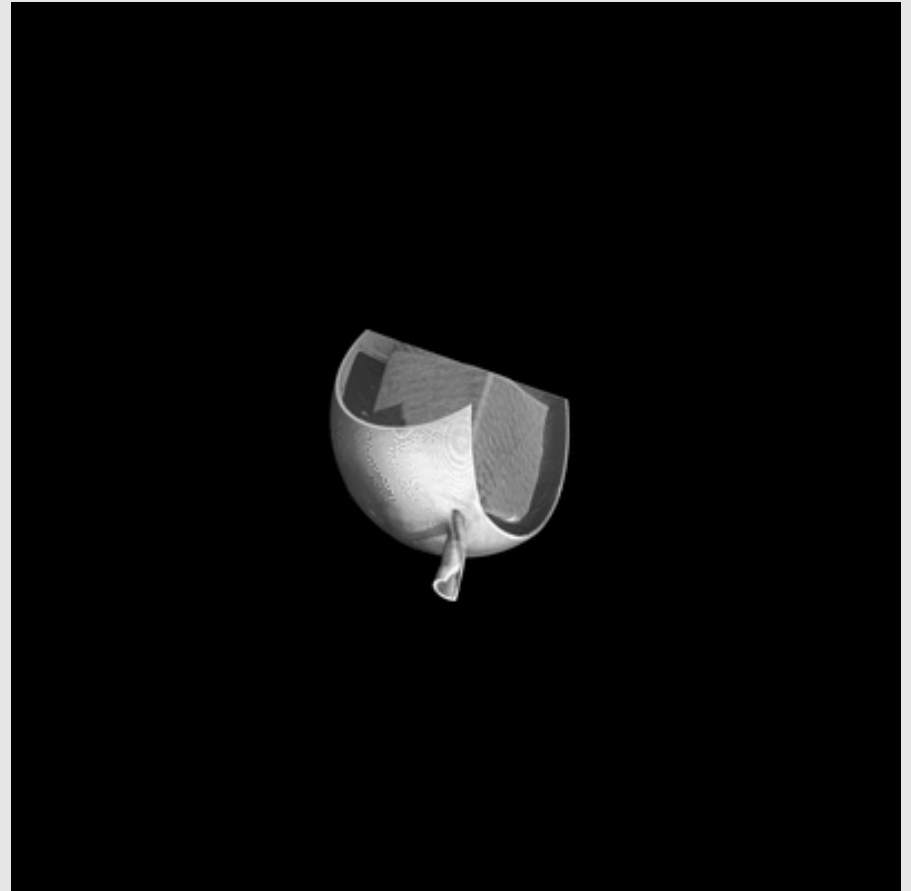# EMBL/ESRF developments

- Diffractometer
- On-axis-view
- Sample Changer
- MiniKappa
- Low-resolution beam
- On-line Microspec
- Humidity Control De
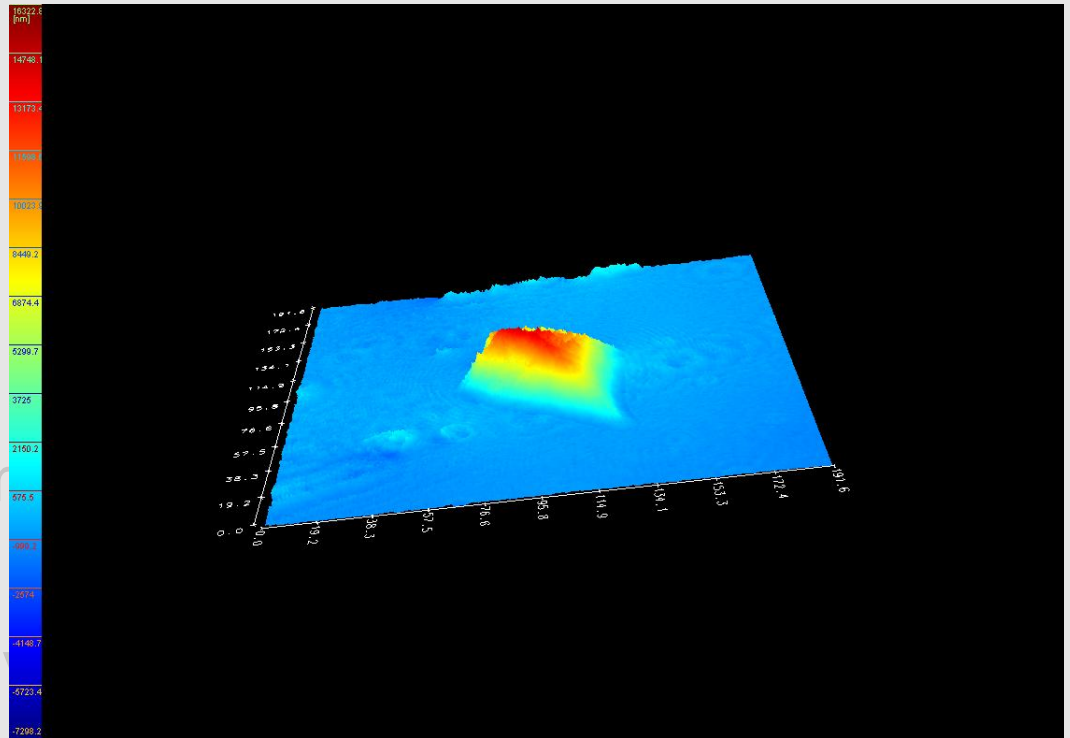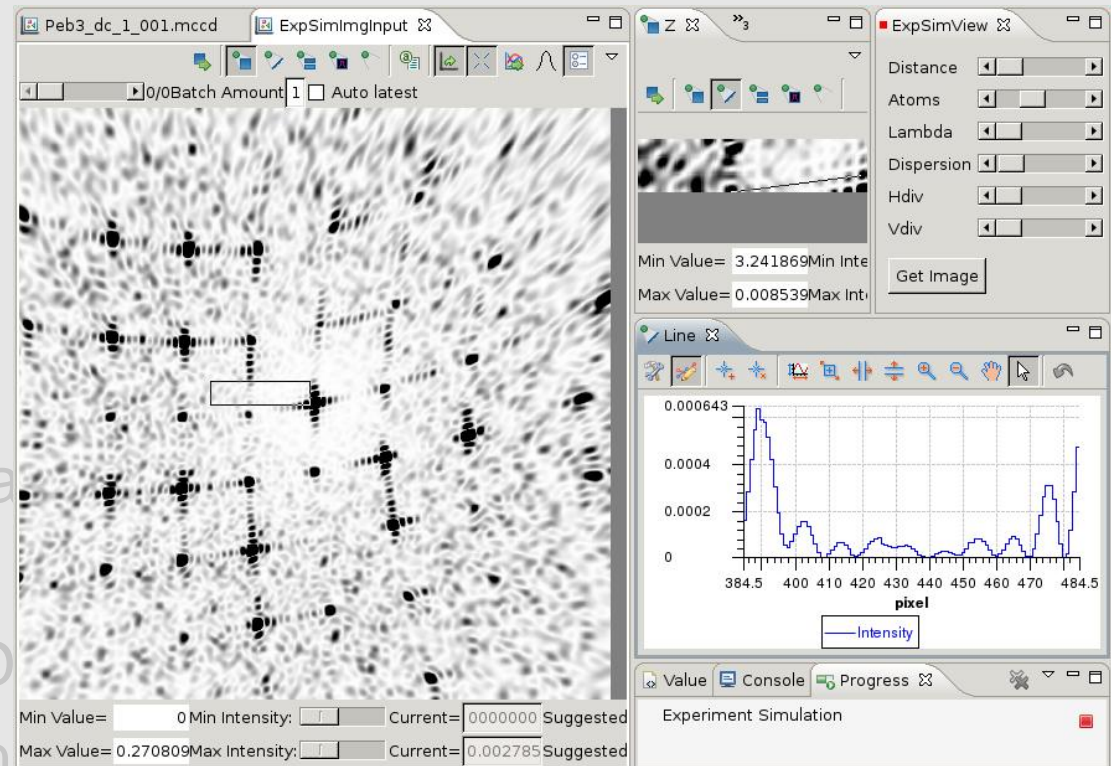- SAX Sample Changer
- Tomography
- Holography

EMBL/ESRF developments

- Diffractometer

- On-axis-view

- Sample Changer

- MiniKappa

- Low-resolution bea

- On-line Microspec

- Humidity Control D

- SAX Sample Chan

- Tomography

- Holography

- **Experiment Simulation**

Computing diversity

- Hardware:
  motion control: PMAC/Galil/V-DPAP
  generic computing: i686, x86_64, tesla/fermi

- OS: Windows/MacOS/Linux (suse, redhat, centos, ubuntu, debian, gentoo)

- Local developments
  mostly for specific target platform
  cross platform: java (3D stereo beamline modeling)

- PXSOFT (for *linux* with full support for *multiple versions*):
  applications compiled from source, or
  binary distributions maintained with required libs

EMBL

Using Debian
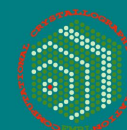
- Open development platform
  Academic spirit
  Democratic management

  HAD problem with redhat
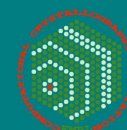
Using Debian

- Open development platform
  Academic spirit
  Democratic management

- Wide package coverage

Centos fails even on libfftw

EMBL

Using Debian

- Open development platform
  Academic spirit
  Democratic management

- Wide package coverage
  Stable releases (also test/unstable releases as well as
        backports for security fixes, and 'non-free' packages)

EMBL

Using Debian

- Open development platform
  Academic spirit
  Democratic management

- Wide package coverage
  Stable releases (also test/unstable releases as well as
      backports for security fixes, and 'non-free' packages)
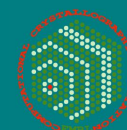 convergence in configuration settings (eg: conf.d)

Using Debian

- Open development platform
  Academic spirit
  Democratic management

- Wide package coverage
  Stable releases (also test/unstable releases as well as
        backports for security fixes, and 'non-free' packages)
  convergence in configuration settings (eg: conf.d)
  powerful packaging system (localisation support:
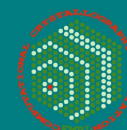   EMBLrepos / EMBLws / EMBLserver packages)

Using Debian

- Open development platform
  Academic spirit
  Democratic management

- Wide package coverage
  Stable releases (also test/unstable releases as well as
          backports for security fixes, and 'non-free' packages)
  convergence in configuration settings (eg: conf.d)
  powerful packaging system (localisation support:
          EMBLrepos / EMBLws / EMBLserver packages)
  easy and robust distribution upgrades

Using Debian

- Open development platform
  Academic spirit
  Democratic management

- Wide package coverage
  Stable releases (also test/unstable releases as well as
        backports for security fixes, and 'non-free' packages)
  convergence in configuration settings (eg: conf.d)
  powerful packaging system (localisation support:
        EMBLrepos / EMBLws / EMBLserver packages)
  easy and robust distribution upgrades
  not too slow updates
        The release of Redhat6 was already slow and
        Centos followed it with an extra 9 months of delay

EMBL

Using Debian

- Open development platform
  Academic spirit
  Democratic management

- Wide package coverage
  Stable releases (also test/unstable releases as well as
        backports for security fixes, and 'non-free' packages)
  convergence in configuration settings (eg: conf.d)
  powerful packaging system (localisation support:
        EMBLrepos / EMBLws / EMBLserver packages)
  easy and robust distribution upgrades
  not too slow updates

- Binary compatibility with other distributions
  can be an issue, but DC

EMBL

Future directions at EMBL

- Up-to-date upgrades for both binary/source packages
- Maintain all configuration and customisation settings as .deb packages

Single Linux OS
DEBIAN 7

EMBL

Thank you for your attention!

S. Brockhauser, *EMBL-Grenoble*

EMBL