The WinGX Program system
Automatic structure determination: Challenges for the future

Louis J. Farrugia,
Department of Chemistry
University of Glasgow
GLASGOW G12 8QQ
Scotland
Automatic structure determination requires:

- automatic data collection & data reduction
- automatic structure solution
- automatic structure refinement, publication & archiving

Automation must save time and effort - remove bottlenecks
Automatic data collection is already a reality for macromolecules MX beamlines at ESRF

(a) automatic sample changer  (b) microdiffractometer
Commercial BruNo robotics

Auto sample changer for cryo-cooled samples

Uses automated goniometer head

Table top liquid N\textsubscript{2} dewar
The WinGX Program system
Automatic structure determination: Challenges for the future
ECM21-2003

WinGX is a general single-crystal structure determination package for MS-Windows™. It is based on refinement with SHELXL and is intended for small-molecule crystallography.


First put on Web in 1997 - more than 2700 users in > 60 countries
New registered downloads ~ 15 per day
http://www.chem.gla.ac.uk/~louis/software/wingx

Philosophy of WinGX program system

• to provide a seamless linking of the best “publicly available” software
• to provide a user friendly environment - Windows operating system
• designed as a “hands-on” system - user decision driven
• easy integration of external programs into main menu system
WinGX provides for most needs in small molecule crystallography

• Data reduction (CAD4 /Siemens P4/ KappaCCD/ SMART)
• Data examination - reciprocal lattice plots, peak profiles
• Absorption corrections (analytical, semi-empirical, ref-deIF)
• Structure solutions - SHELXS, DIRDIF, SIR programs
• Structure refinement - SHELXL-97 (CRYSTALS/Jana2000)
• Analysis of results - THMA, PLATON, PARSIT, GEOM
• Graphics - ORTEP, CAMERON (Schakal, RasMol, POV-Ray ...)
• Publication - CIF creation, validation (CIFtbx tools)

WinGX also provides link mechanisms to external programs
Data processing

WinGX provides for a flexible treatment of area-detector data from Bruker-Nonius diffractometers. No integration software though.

Import data from various sources

Filter data by $\sin(\theta)\lambda$ or batch no.

All facilities in Sortav accessible from GUI - scaling, empirical abs correction and merging
The WinGX Program system
Automatic structure determination: Challenges for the future

Flowchart for data reduction of Bruker Nonius KappaCCD images

KappaCCD images *.kcd

Denzo
.x files
Scalepack-merge
call_all.sca
Cifin
ImportKappaCCD
name.hkl

Scalepack-dcos
scale_all.sca
ImportKappaCCD
import_hkl.sortav
Sorav
sortav.hkl

EvalCCD
gaussian

Sadabs
gaussian_hkl.sortav
Sortav
denzo_hkl.sortav

Denzox
denzo_sad
Sadabs
sad.hkl
Sadabs

Any

final.y

shelx.sad

Export Refln

sad.hkl

Export Refln

export_hkl.sortav
Sortav

nanny.hkl

sortav.hkl

Intermediate files
file.hkl merged reflection file for SHELX
file.hkl unmerged SHELX reflection file

Bruker-Nonius program
WinGX program
WinGX provides KCD Image tool for visualisation of KappaCCD images on a Windows PC.

- Number of tools
- Examine images for twinning
- See which reflections have been integrated
- Examine reflection profiles
Data processing

*WinGX* provides KCD Image tool for visualisation of KappaCCD images on a Windows PC.

**Number of tools**
- Examine images for twinning
- See which reflections have been integrated
- Examine reflection profiles
Automatic phase determination

*WinGX* include most of the popular structure solution packages - GUI for SIR and SHELXD programs.

Input files generated automatically.

AUTO-START option for “first stab” approach

Resultant solution can be examined rapidly with the utility SXGRAPH.

DIRDIF and particularly SIR programs provide an efficient (almost completely) automatic structure solution.

System-S (PLATON) not available in Windows
The WinGX Program system
Automatic structure determination: Challenges for the future

Automatic phase determination

To enhance usability, all structure solution packages in WinGX have GUI’s
Automation of structure solution in WinGX

AUTO-START is a (limited) automatic entry into WinGX

Recommended for any structure since important files are built

• converts CAD4 or KappaCCD (import.cif) files to SHELX HKL format
• examines $E$-statistics to determine whether a center of symmetry is present.
• examines the lattice type
• checks the metrical symmetry using LEPAGE algorithm
• checks Laue symmetry and attempts an automatic determination of space group
• launches SHELXS (ab initio direct methods /Patterson)
• open SXGRAPH
Problems in automated structure solution


• Peak heights in Fourier maps unreliable
• Integrated density an improvement?
• Automatic assignment must be reliable if auto-solutions are to be trusted

Novel approaches include

MOGUL - CSD based geometrical comparison implemented in CRYSTALS.

Bader analysis of density topology recently implemented in DIRDIF
Refinement

Refinement in *WinGX* strongly based on SHELXL

*WinGX* provides an easy migration to other refinement programs
- CRYS*TALS* (David Watkin *et al*)
- JANA2000 (Vladimir Petricek & Michal Dusek)
- XTAL (Syd Hall *et al*)

*WinGX* provides tools for refinement of twinned data

- ROTAX (Simon Parsons)
- TwinRotMat (PLATON - Ton Spek)
- MakeHKLF5
The WinGX Program system
Automatic structure determination: Challenges for the future

Refinement

SXGRAPH

Graphical model editor for SHELX files

Most SHELX parameters can be edited from SXGRAPH
Structure interpretation

Visualisation of Fourier maps
MAPVIEW displays maps as contour plots, interpolated plots, height fields, isosurfaces
Structure interpretation

WinGX has direct links to the CCDC programs Mercury & enCIFer

Mercury has excellent facilities for analysis of H-bonding networks

enCIFer is a useful GUI tool for editing and manipulation of CIF’s
WinGX has direct links to the CCDC programs Mercury & enCIFer

Mercury has excellent facilities for analysis of H-bonding networks

enCIFer is a useful GUI tool for editing and manipulation of CIF’s
Important information in *WinGX* stored in CIF’s

- **STRUCT.CIF** - colour, space group, crystal size
- **DREDDUC.CIF** - data reduction
- **SORTAV.CIF** - data reduction
- `<name>.CIF` - SHELX refinement details

*WinGX* has a general and automatic CIF merging program

- concatenates all requested CIF’s
- reads *request list* - contents of this are user definable
- searches CIF’s in order to extract required data items

CIF’s should not contain redundant information

Validation using IUCRVAL (IUCr criteria), enCIFer & PLATON
**Conclusions & observations**

- atom type determination from structure solution is still far from automatic
- human intervention is often the quickest solution
- GUI based interfaces speed up many processes
- GUI design is important - aesthetics and usability

**Acknowledgements**

- University of Glasgow
- all users who have provided bug-reports and suggestions
- Lachlan Cranswick
The future of data display?

Actuality Systems 100 million Voxel 3D-display

http://www.actuality-systems.com