SAS data reduction and analysis

Jan Ilavsky

Content

- Igor Pro as platform for SAS data analysis
  - Why?
  - Capabilities
  - Installation etc…
- Data reduction tools
  - Nika package (pinhole cameras)
  - Indra package (USAXS)
  - Other
- Data analysis tools
  - NIST tools
  - Old (IPNS) tools
  - Irena package
- Conclusions…

Igor Pro as SAS data reduction & analysis platform

- What is Igor Pro?
- Where to get it?
- Why to use it?
- Advantages - disadvantages

What is Igor Pro?

- Software package (now version 6.32) from Wavemetrics Inc. (www.wavemetrics.com)
  - Available for both Mac (OSX) and PC platforms
  - Same scripting code runs on both platforms
  - Scripting code is simple text file = open source
  - Extendable with C-code (xop, platform specific)
  - High-level programming language with very little programming experience needed to write code
    - Data management, import/export
    - GUI capabilities, same code for both platforms
    - Highly optimized library of mathematical operations (build-in Numerical recipes and more)
    - Publication quality graphs
    - Notebooks,…
  - Excellent support: active user community, responsive company
- Lot of data analysis software already available for this platform

Igor Pro II

- Installation : ~100Mb download of installation (demo) package
- When installed it can be simply moved/copied as folder to another folder or even another computer (does not require installation, behaves like “Mac” software)

- Philosophy:
  - 0D data – variables, strings
  - 1D – 4D data – “waves”
  - Waves are:
    - Vectors (1D), Images (2D), volumetric data (3D), and 4D data if needed…
    - Can have scaling for each dimension or use two or more waves as x, y, and z points.
    - For 1D SAXS data need q, intensity, error = 3 waves. More waves may be needed to describe smearing (SANS).
    - Wave notes – associated text file for notes taking.

Data reduction tools

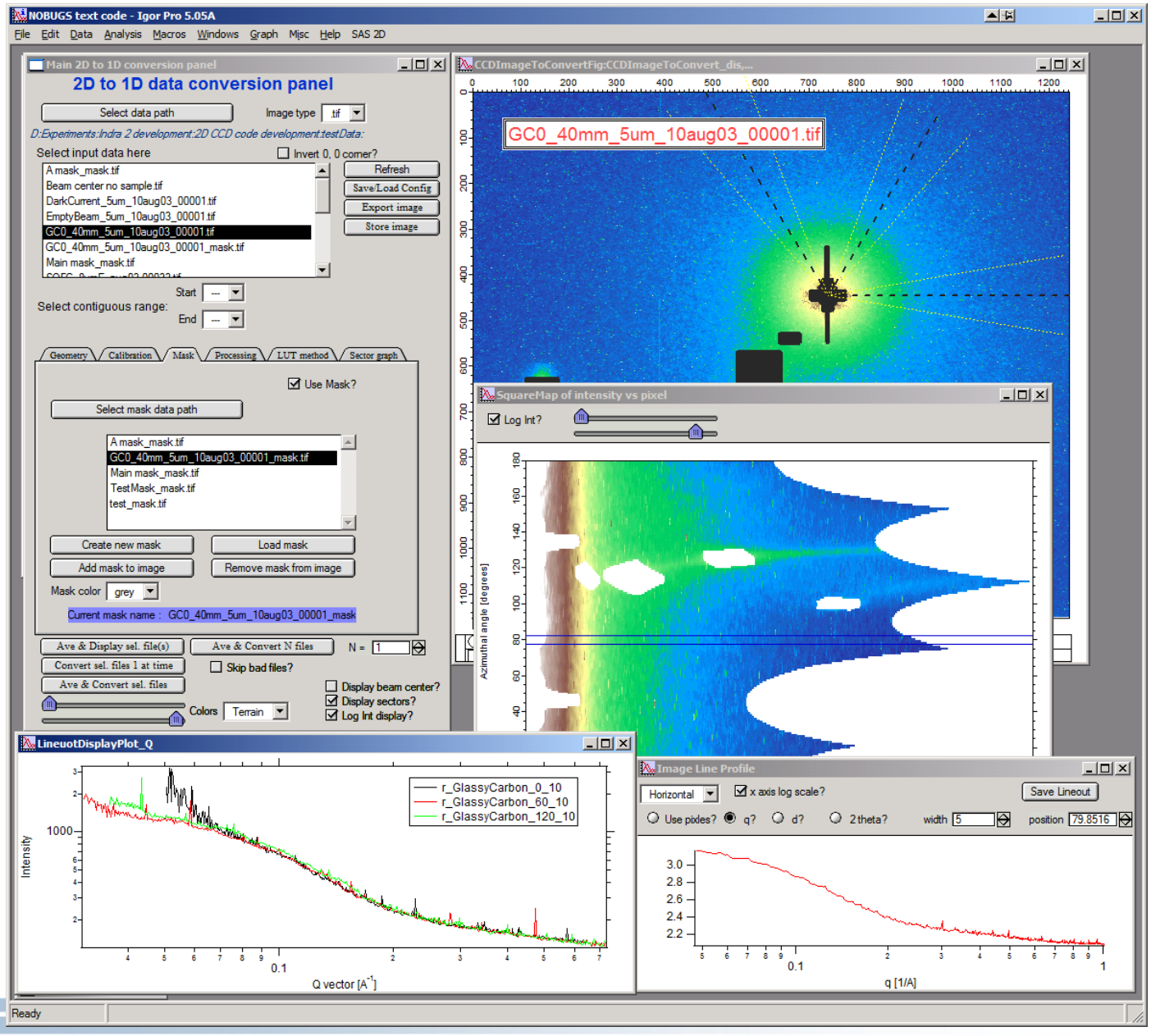
- 2D data using Igor Pro:
  - Nika package (generic package for analysis of any 2D data)
  - Instrument specific:
    - BIOCAT
    - IPNS, ORNL, NIST (SANS & USANS)
- 2D data not using Igor Pro:
  - Fit2D (generic)
  - Datasqueeze (generic)

- USAXS
  - Indra package

Area detectors data reduction package "Nika"

- Provides some of the functionality of Fit2D within Igor
- Seamless collaboration with "Irena", similar GUI, easy to use for Irena users
- Targeted for flexible SAS/WAS data processing, built in batch processing
- Optimized for speed for processing multiple data sets with same parameters
- Capabilities:
  - Import images natively (~10 types) or through Fit2D (Windows, OSX 10.4)
  - Display image (linear intensity or log intensity, different color maps)
  - Create line outs in angular sections
  - Create map of lineout vs azimuthal angle
  - Generate intensity profiles on arbitrary line
  - Tools to create Mask, Pixel sensitivity
  - Subtract empty/dark, sum data sets
  - Tool to calibrate distance/energy & get beam center for measurements of known or user standards (Ag behenate)
  - Look up parameters (thickness/I0/exposure time, etc) using user developed Igor lookup functions from ASCII records loaded into Igor

Nika example



Data analysis packages for Igor Pro

- NIST SANS analysis package
- IPNS/ORNL SANS (Ken Littrell) tools
- Irena package
- Motofit (Reflectivity), FitGISAXS (GISAXS, DWBA), …

- The good … wide variety of tools which can analyze many different datasets
  - NIST
    - Lot of structure factors and form factors for fitting, optimized for speed
    - Fitting tool for linearization plots
    - Various other tools
    - Excellent documentation (including QT movies on web site)
    - Nice installation tool
  - IPNS/ORNL macros
    - Fitting & plotting tools, not much experience with new versions
  - Irena
    - Size distributions, unified fit, fractals, gels model, …
    - Plotting tools, support tools
    - Extensive documentation (tutorial)

Data analysis SAS tool in Igor

- The bad:
  - Different philosophy in data management (history)
  - Different approach to GUI and level of needed user Igor proficiency
  - Different data naming system (note: Irena handles all)

- Data management philosophy:
  - NIST:
    - Data in ASCII files outside Igor experiment, Igor mostly transient (work area) and results are immediately exported
    - Use of Igor data folders to organize data
  - IPNS/ORNL
    - Igor experiment is place for data
    - Naming structure is challenge for larger data sets (IMHO)
  - Irena
    - Igor experiment is place for data
    - Data organized in potentially complex Igor folder structure

Igor tools… cont.

- Naming systems for Q, Intensity and errors
  - NIST : name_q, name_i, name_s
  - “IPNS” = “QRS” : qname, rname, sname
  - USAXS : DSM_Q, DSM_Int, DSM_Error (or SMR_Q, SMR_Int, SMR_Error)
  - “Irena” :
    - USAXS
    - NIST and QRS (= “QRS” choice)
    - Arbitrary (user can choose any wave names)

- All packages attempt to limit need for user Igor proficiency

SAS data evaluation package – "Irena"

- General use SAS tools (http://usaxs.xray.aps.anl.gov/staff/ilavsky/irena.html)
  - ASCII Data import/export tool (for general SAS)
  - Data manipulation tool (subtract, combine, divide, sum, smooth, etc.)
  - Data plotting tool with basic fitting functions
  - Desmearing [Lake, Pete Jemian]
  - Size distribution (Maximum entropy, TNNLS, …) [Pete Jemian, Jan Ilavsky]
  - Unified model [Greg Beaucage] with LSQF
  - Modeling of size distributions (two versions) with LSQF & Genetic Opt.
  - Gels model [Debye-Bueche] with LSQF
  - Fractals model [Andrew Allen] with LSQF
  - Reflectivity tool [L. G. Parratt, Andy Nelson] with LSQF & Genetic Opt.
  - Scattering contrast (X-ray & neutron) calculator (inc. Cromer-Liberman code) – available also separately: http://usaxs.xor.aps.anl.gov/staff/ilavsky/AtomicFormFactors.html
  - Some other useful tools
  - Can use both slit smeared data or pinhole collimated data

Data import tool, Data manipulation

- Import ASCII data (columns)
  - Preview data
  - Select appropriate columns (Intensity, q, error)
  - Convert units (nm -> Å)
  - Scale imported data (intensity), rebin, trim, …
  - Generate estimated errors (2 methods) if experimental are not available
- Data manipulation
  - Change one or manipulate two data sets
  - Remove points
  - Smooth result of the manipulation
  - Propagate errors as best as possible
  - One data set:
    - Scale
    - Re-bin in **q** (change number of points)
  - Two data sets
    - Mathematical operations (+, -, /, and various combinations)
    - Combine
    - Re-bin in **q** one with the **q** values from the other

SAS Data analysis tools

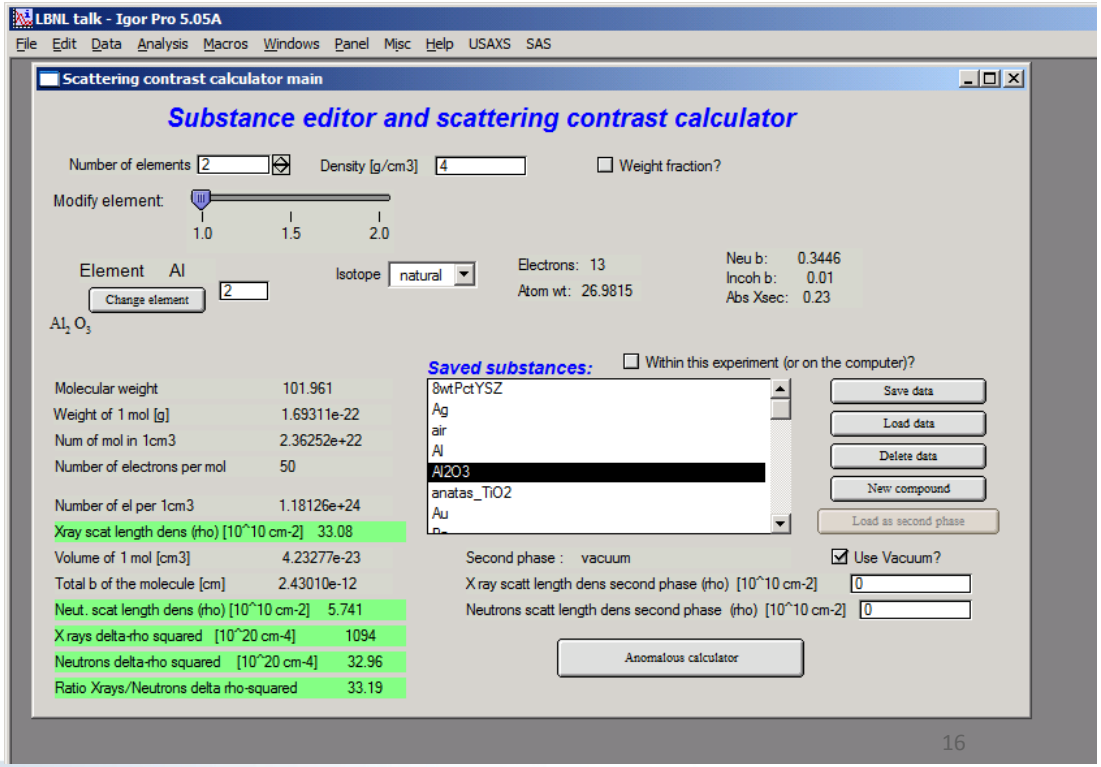
- Unified fit with Least square fitting build in
  - Method author: Greg Beaucage (U. Cinn.)
  - Relatively generic method for SAS data analysis
- Direct modeling with least square fitting
  - Two tools available.
  - Multiple populations of scatterers, diffraction peaks & Unified levels
  - Dilute limit with simple approximate method for accounting for interparticle interferences for more concentrated systems
  - Library of form factors included
  - Applicable for analysis of SAS from discrete scatterers
- Maximum entropy/ TNNLS
  - MaxEnt implementation author: Pete Jemian (APS)
  - TNNLS implementation author: Jan Ilavsky (APS)
  - Dilute limit, discrete scatterers
- Fractals:
  - Method author: Andrew Allen (NIST)
  - Modeling of fractal systems (two mass & two surface fractals available)
- Gels
  - Uses Debye-Bueche model & low-q power law slope to model SAS from gels

Reflectivity

- Method for calculation of X-ray & neutron reflectivity from layered structures (using Parratt's code L. G. Parratt, *Phys Rev*, **95**(2), 359-369, 1954)
- Analysis package using code (xop/Igor code) provided by Andrew Nelson "Mottofit" (ANSTO, http://www.ansto.gov.au)
- Simple tool with limitations:
  - Number of layers available (5)
  - Fitting to one data set at time
- Used by reflectivity users at 1BM and general community
- Great tool for support of first time reflectivity users or for solution of relatively simple structures
  - Easy to test influence of various parameters on result
- For more complex problems available Andy's program "Mottofit" (more challenging to use, need to be more Igor proficient) http://motofit.sourceforge.net/

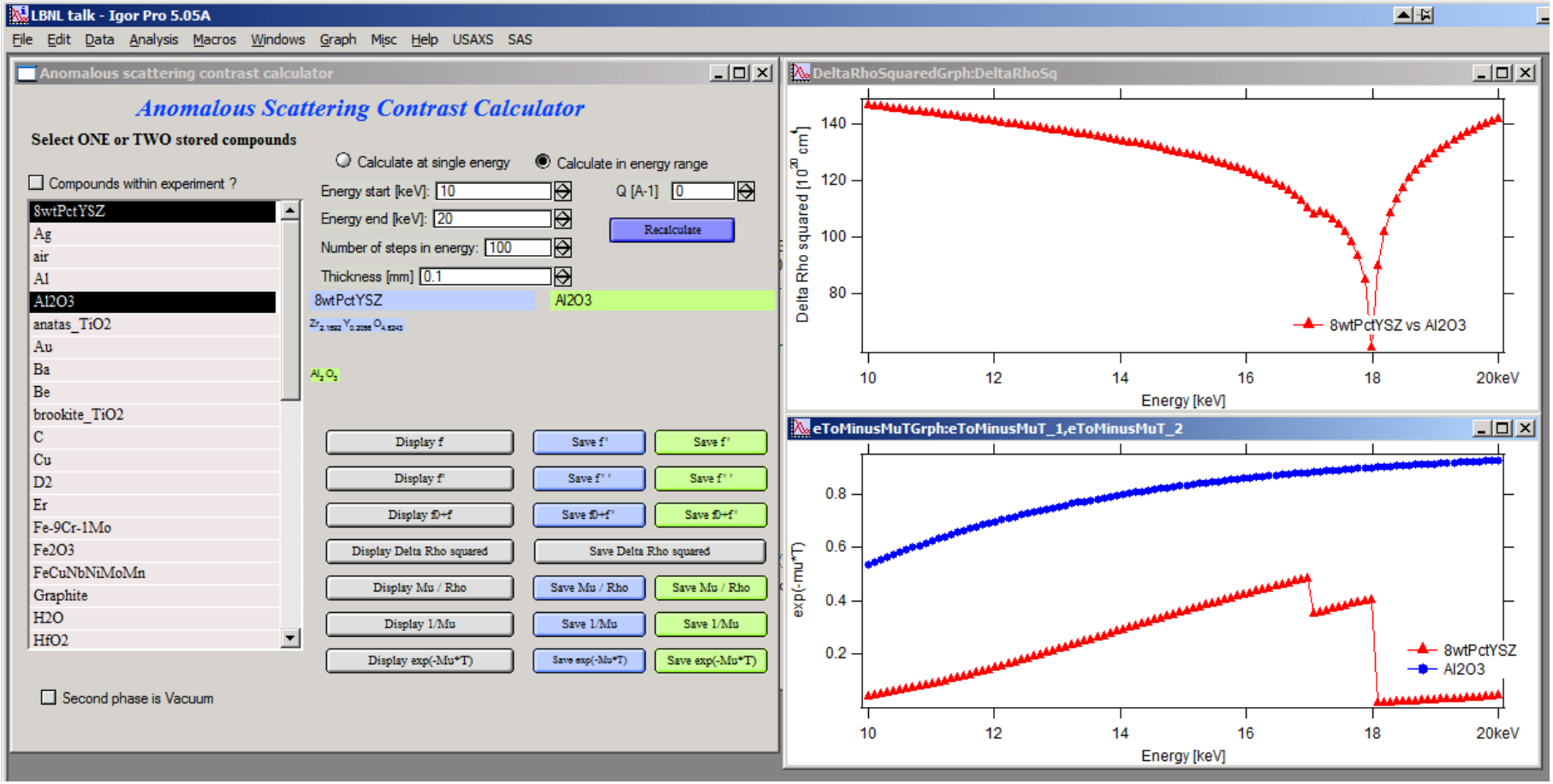
X-ray & neutron contrast calculator

- Calculates X-ray and Neutron contrast for compounds
  - Chemistry in atomic fraction (H_2O) or weight % (50wt% Ni and 50wt%Al).
  - Compounds can be stored on computer (outside Igor) or within Igor experiment.
- Two calculators actually:
  - Neutron and non-energy dependent X-ray contrast (approximation) – f0 only.
  - Anomalous X-ray contrast using Cromer-Liberman code (available also separately for download)
- Anomalous data available for saving

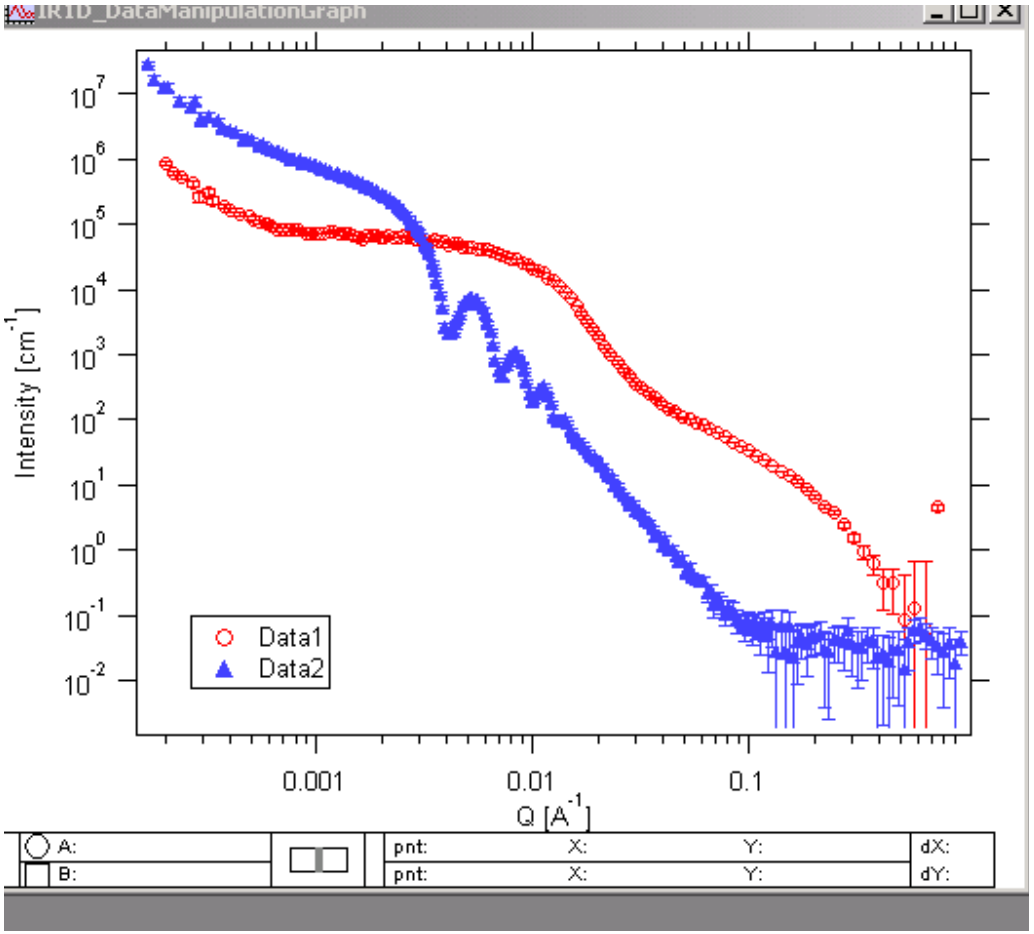


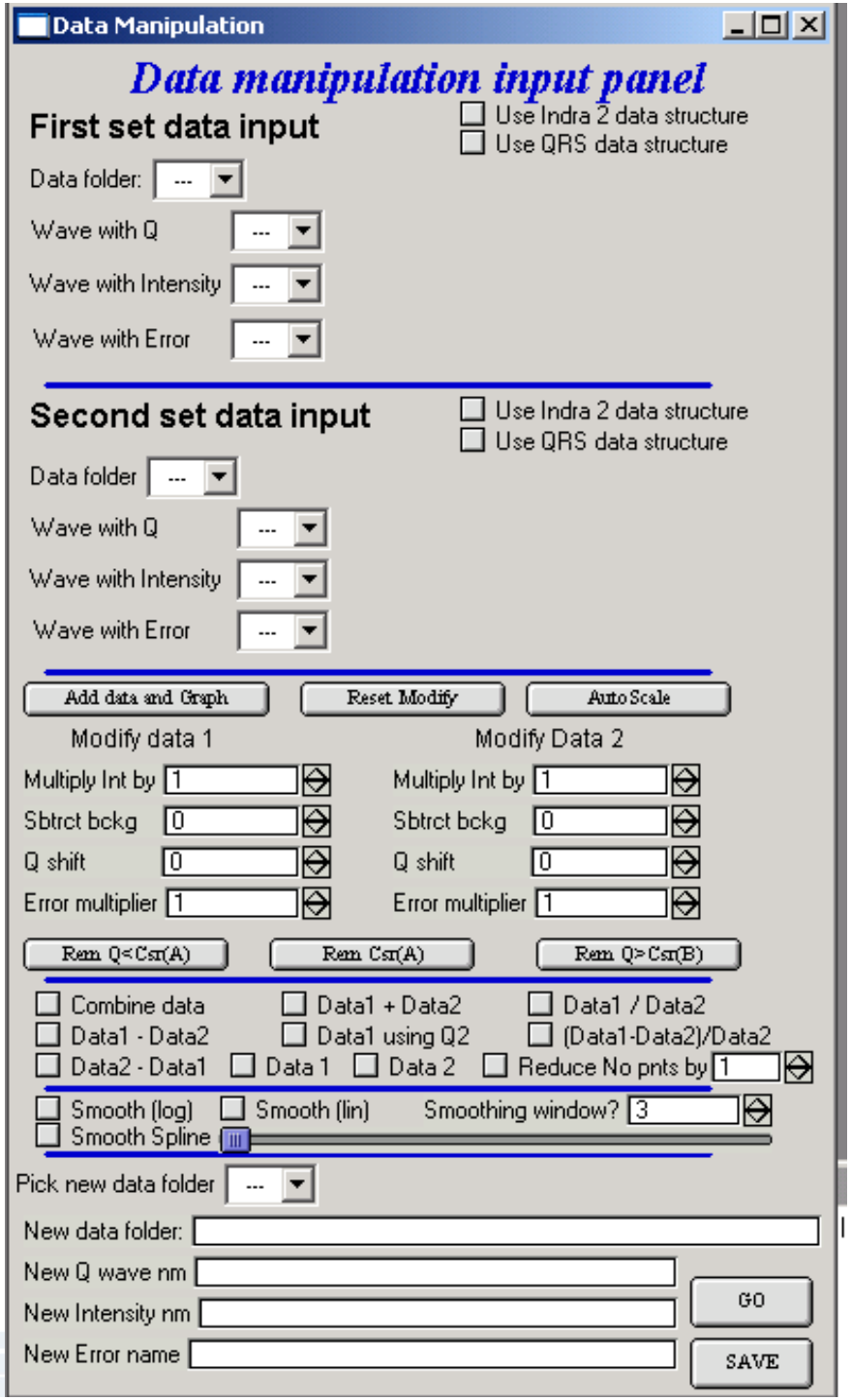
X-ray Calculator II - anomalous effects

- Calculates f_0, f', f'', $\Delta\rho^2$, μ, also transmission for known thickness

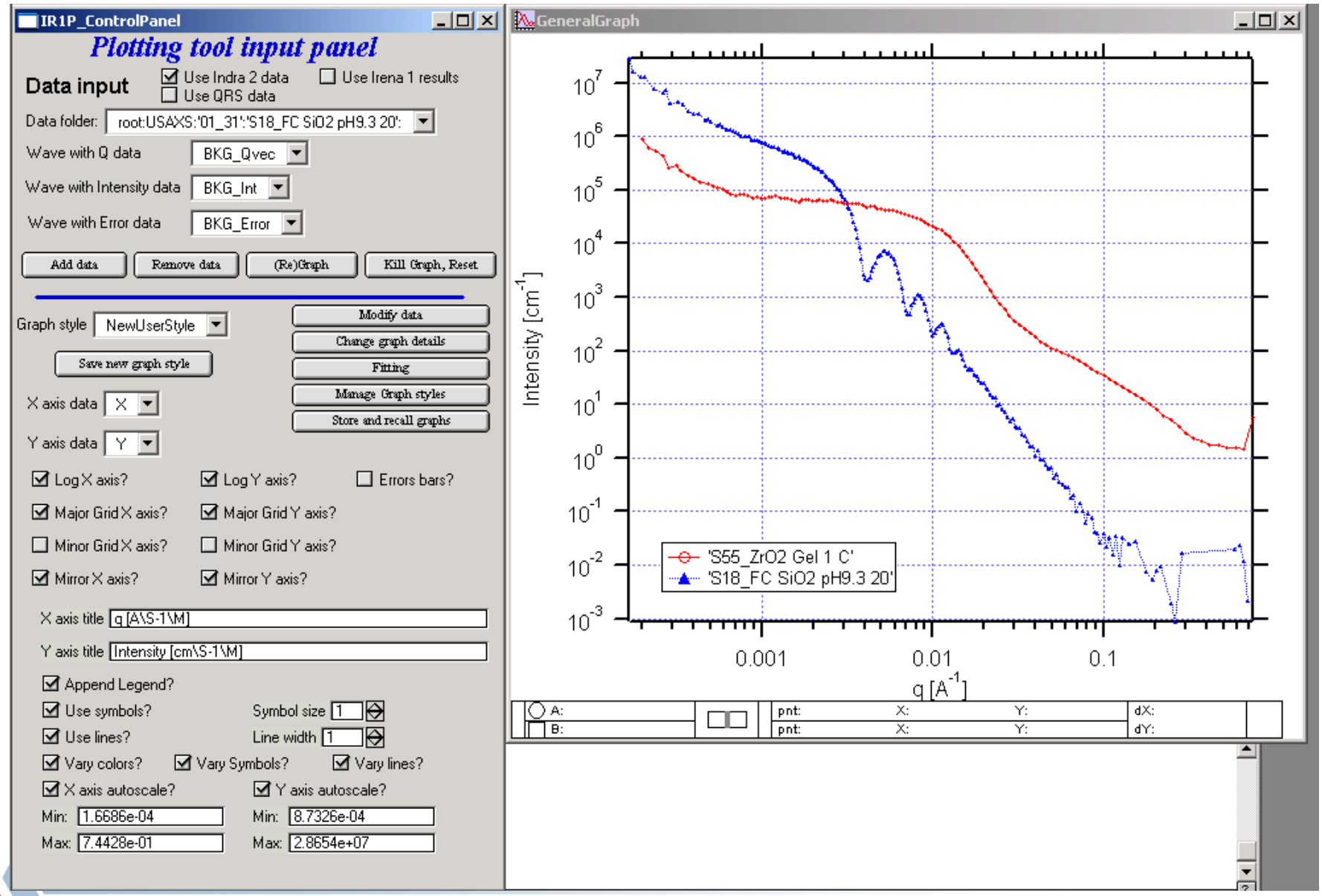


Manipulate data



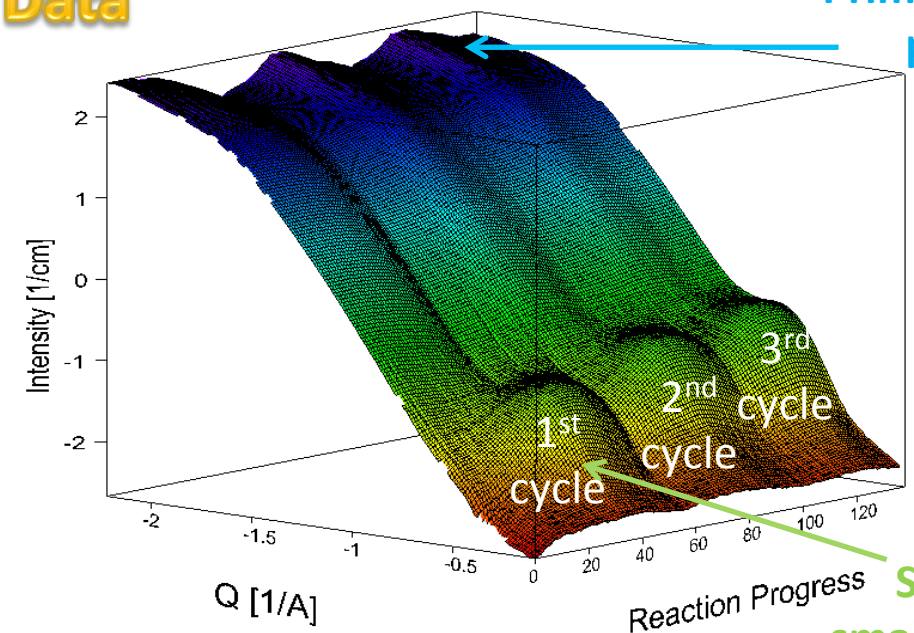


Example plotting tool

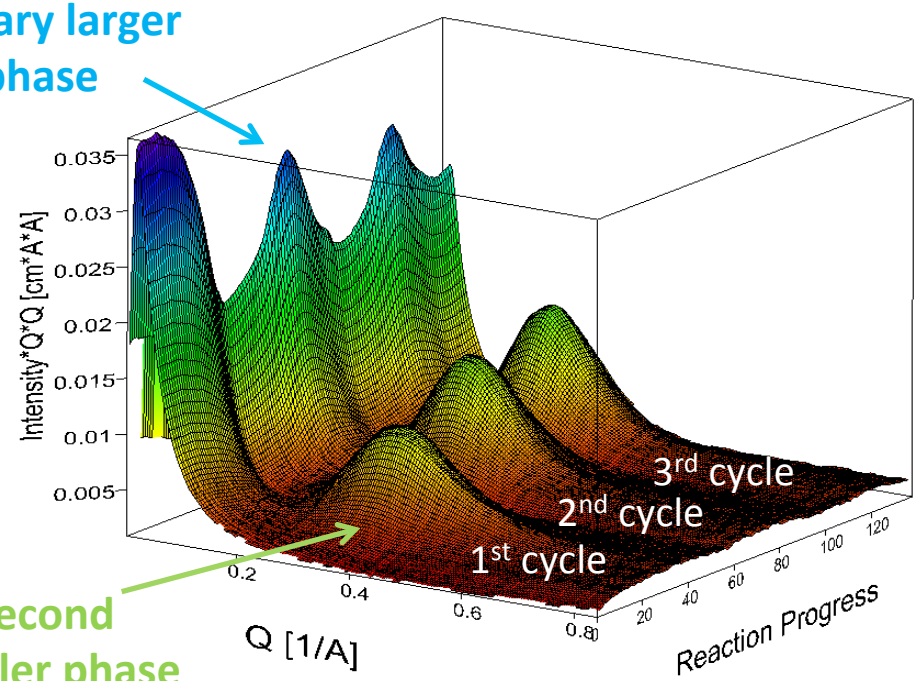


3D EXAMPLE : SAXS DATA COLLECTED USING AMPIX CELL DURING FIRST THREE DISCHARGE-CHARGE BATTERY CYCLES

Data

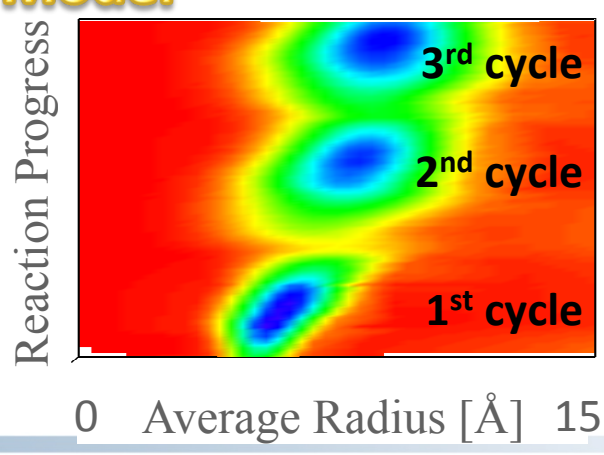


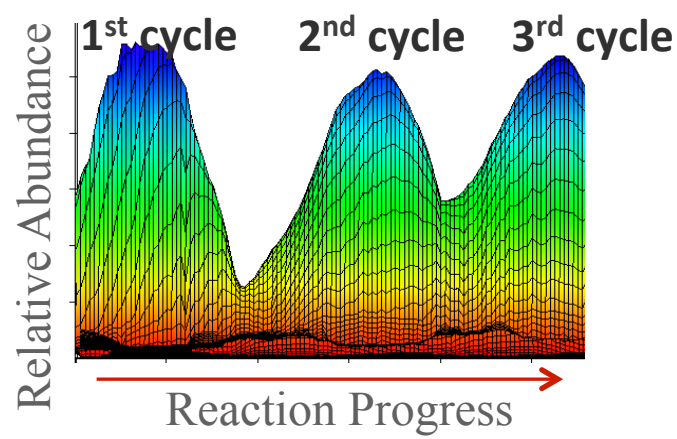
Primary larger phase



Second smaller phase

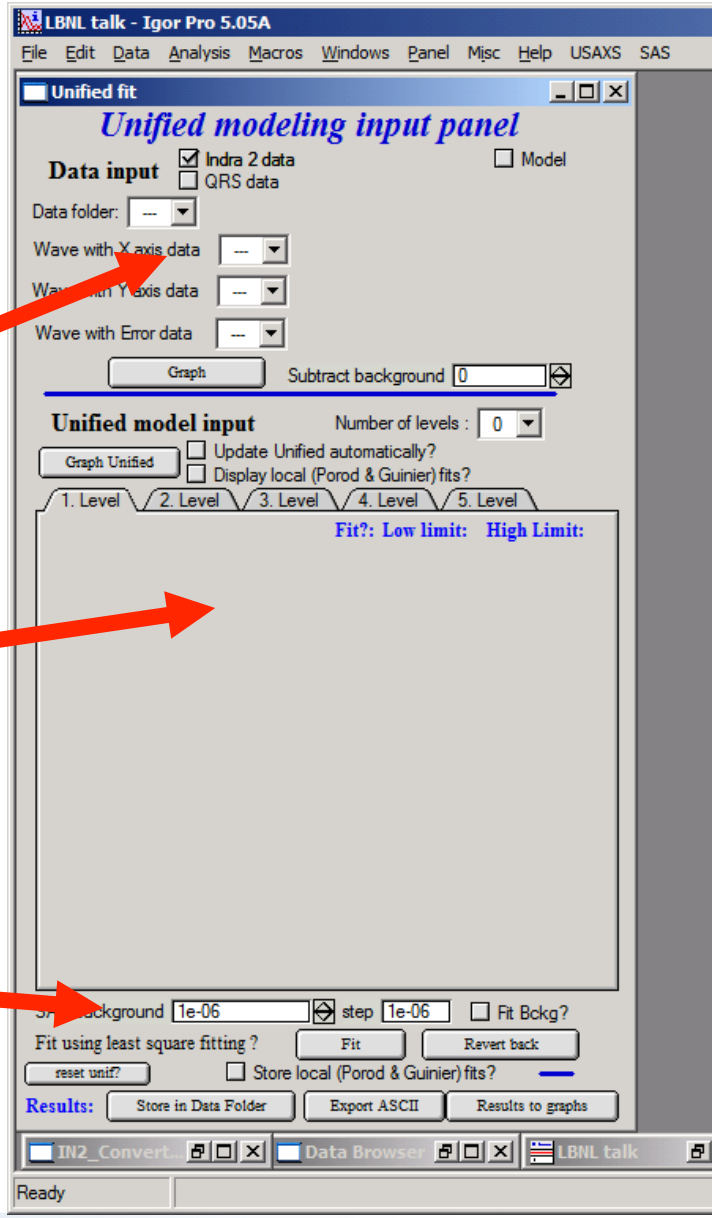
Small Phase Model





Example of data processing - Unified fit…

- Unified fit is method developed By Greg Beaucage (U Cinn). Unified fit models SAS data by sequence of Guinier knees and Power law areas. Uses Least-square fitting to optimize multiparameter function. Complex data may need large number of parameters (>40 possible).

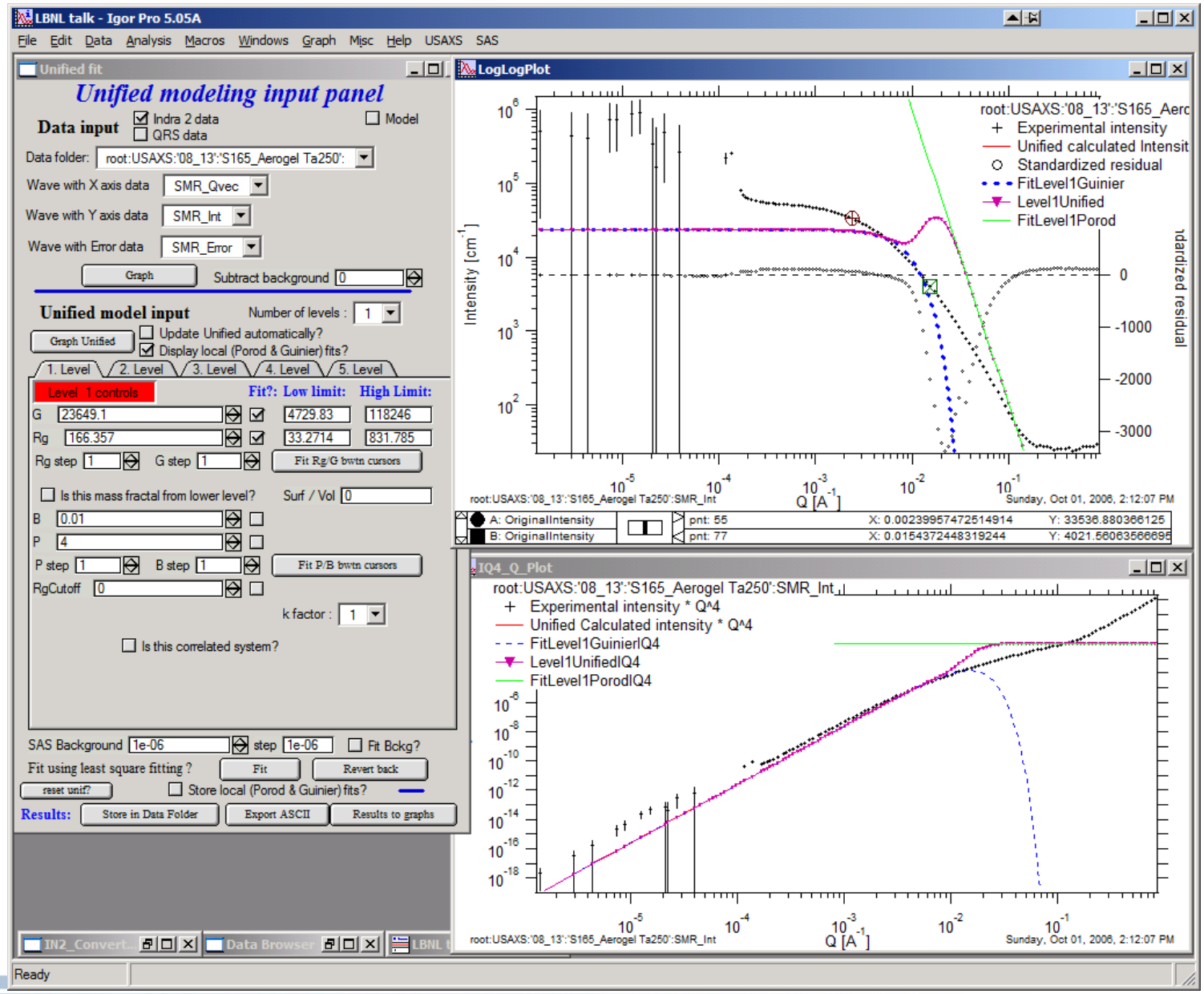


Data selection area

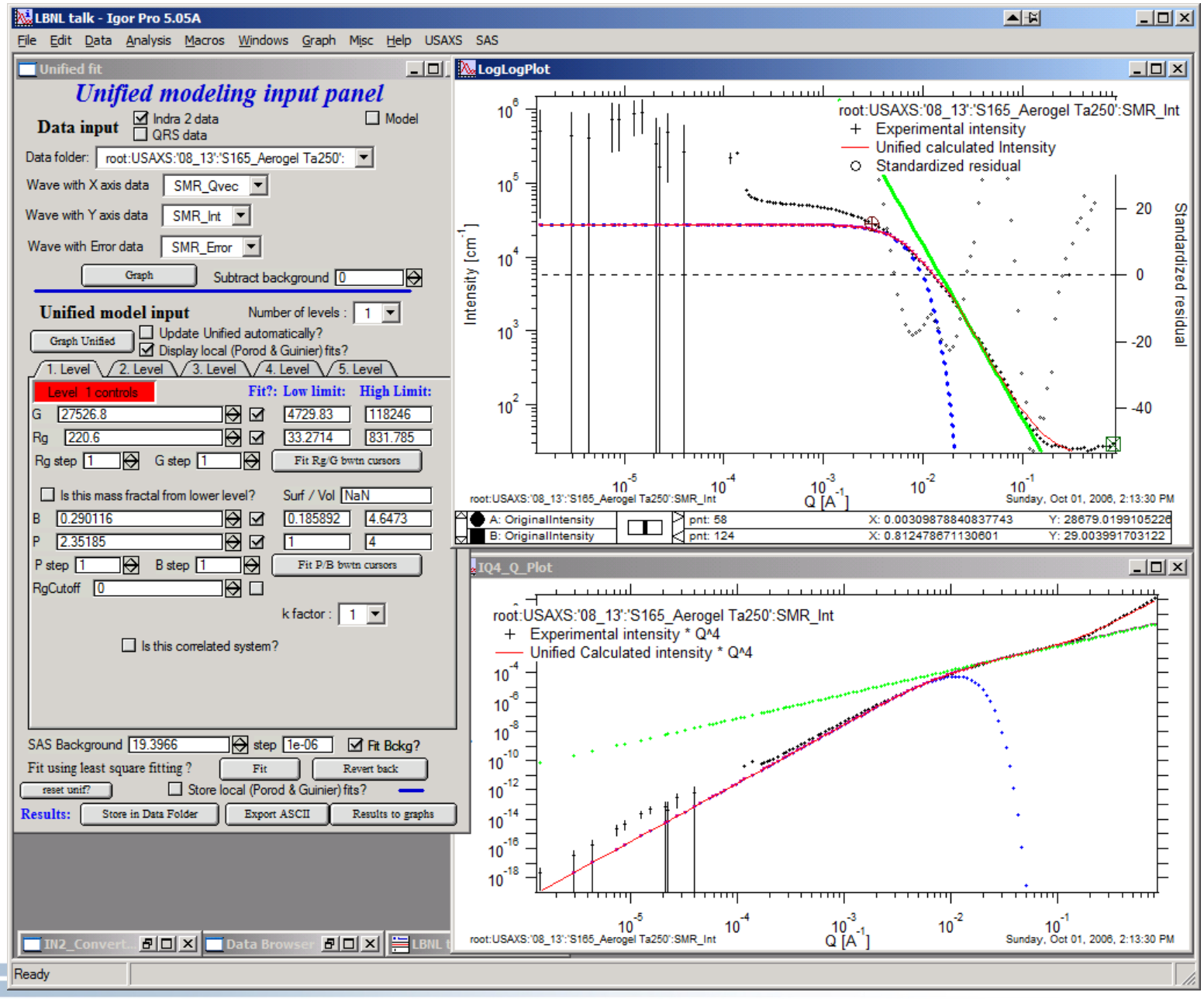
Model control area

Other controls

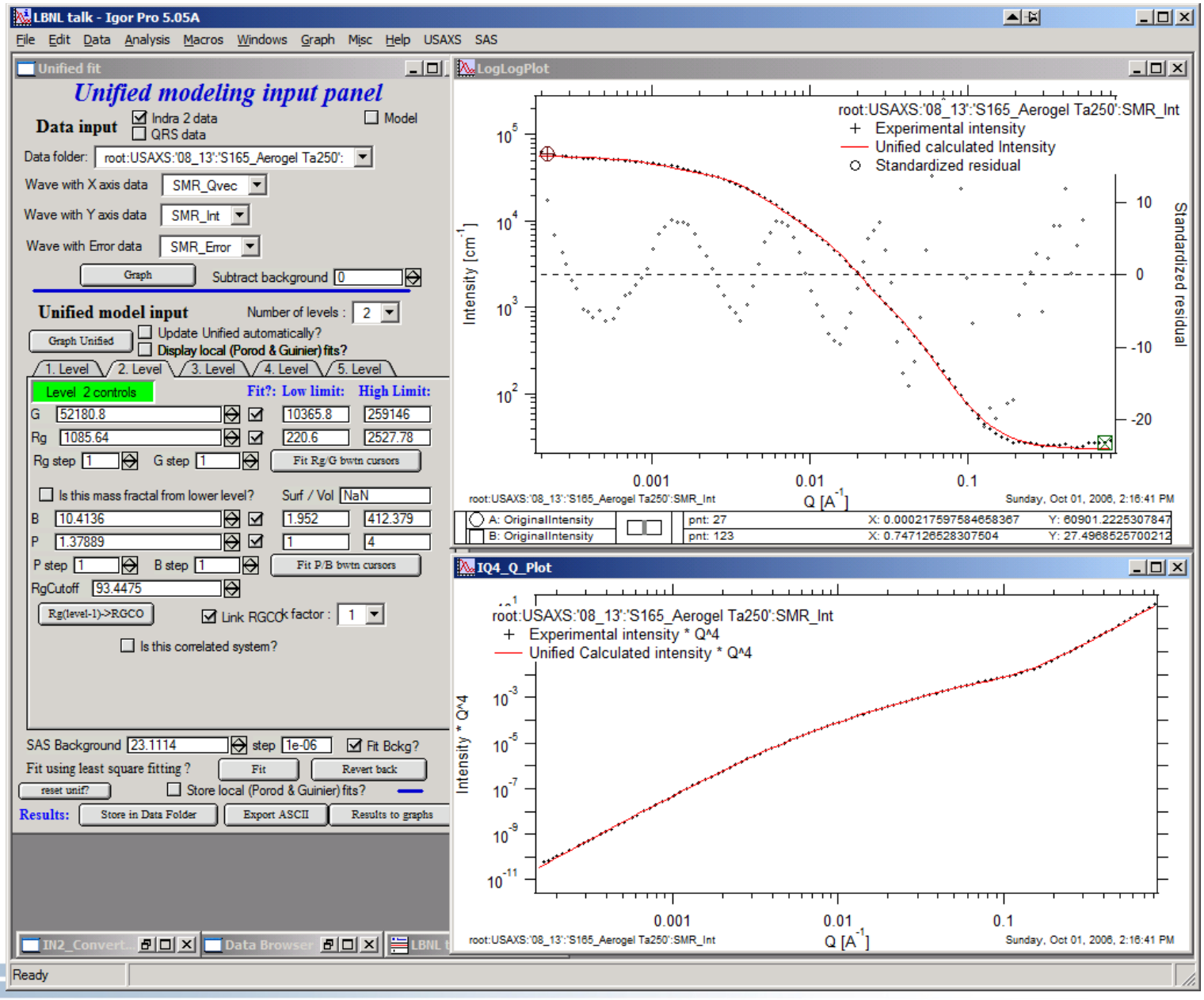
Unified cont…



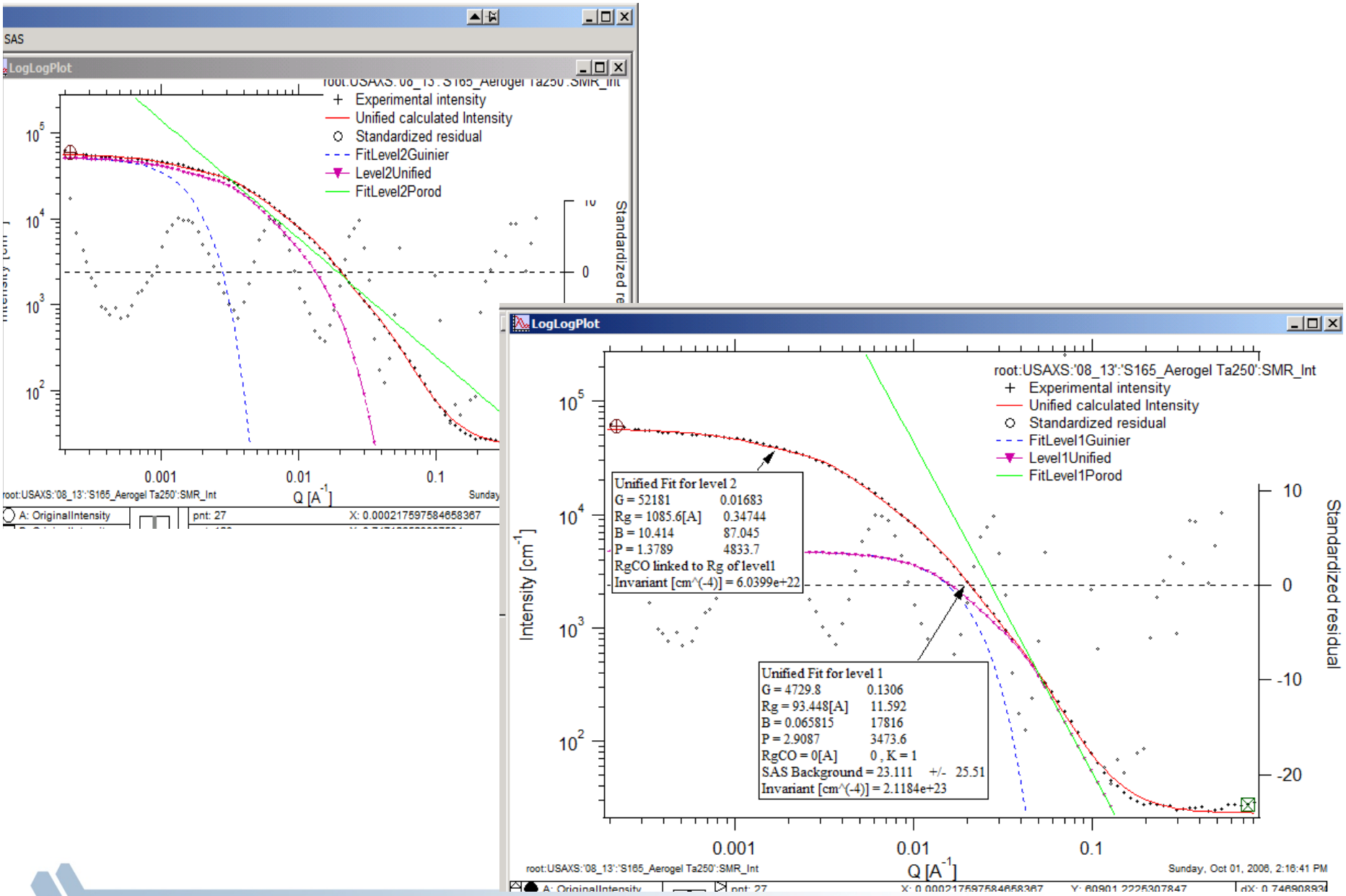
Unified cont…



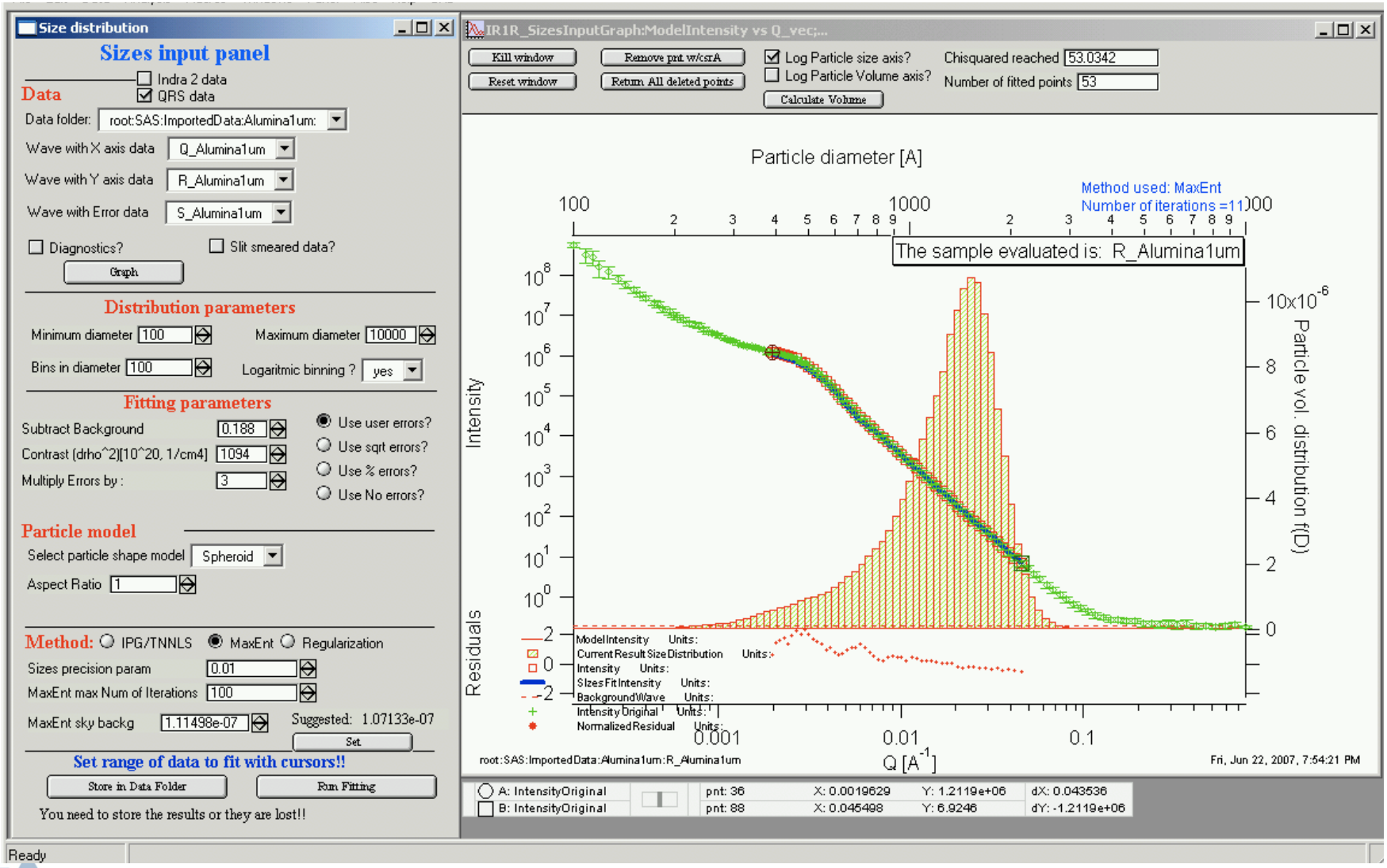
Unified cont…



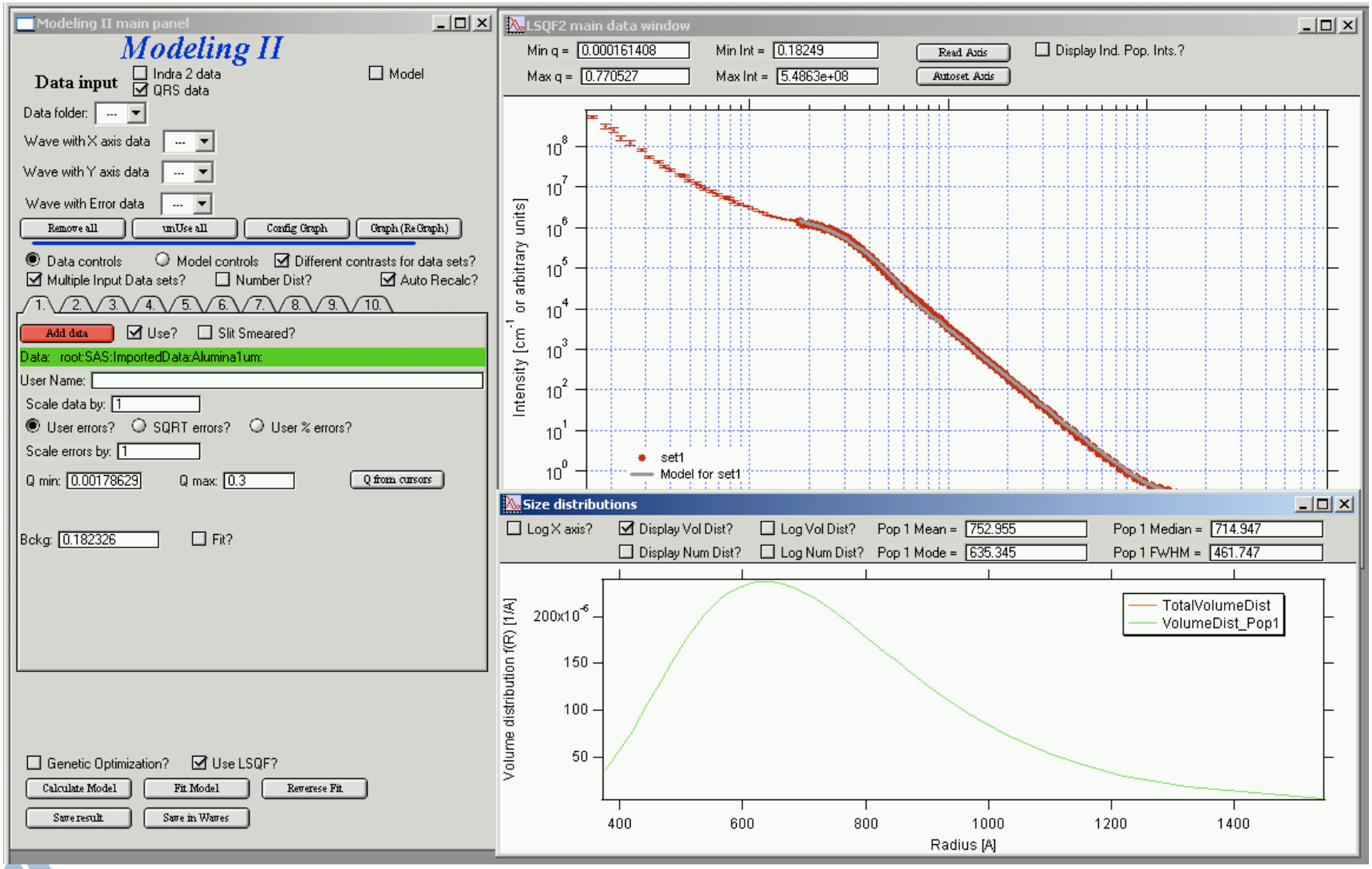
Unified cont…



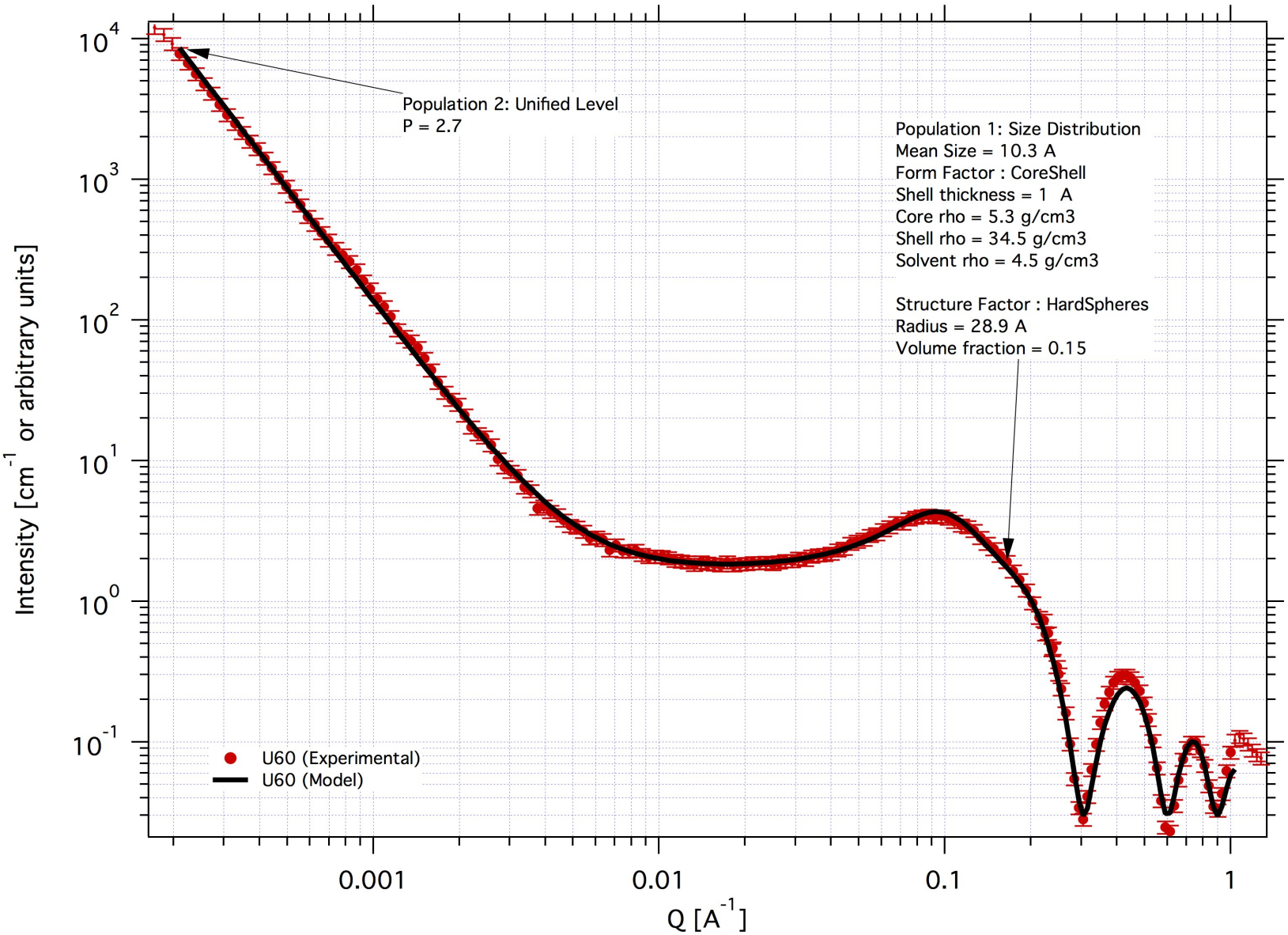
Size distribution - dilute system of SAME particles



Modeling II – Size distribution + Unified Fit + Diff. peaks



Modeling II results example:



Now to installation on your computer…