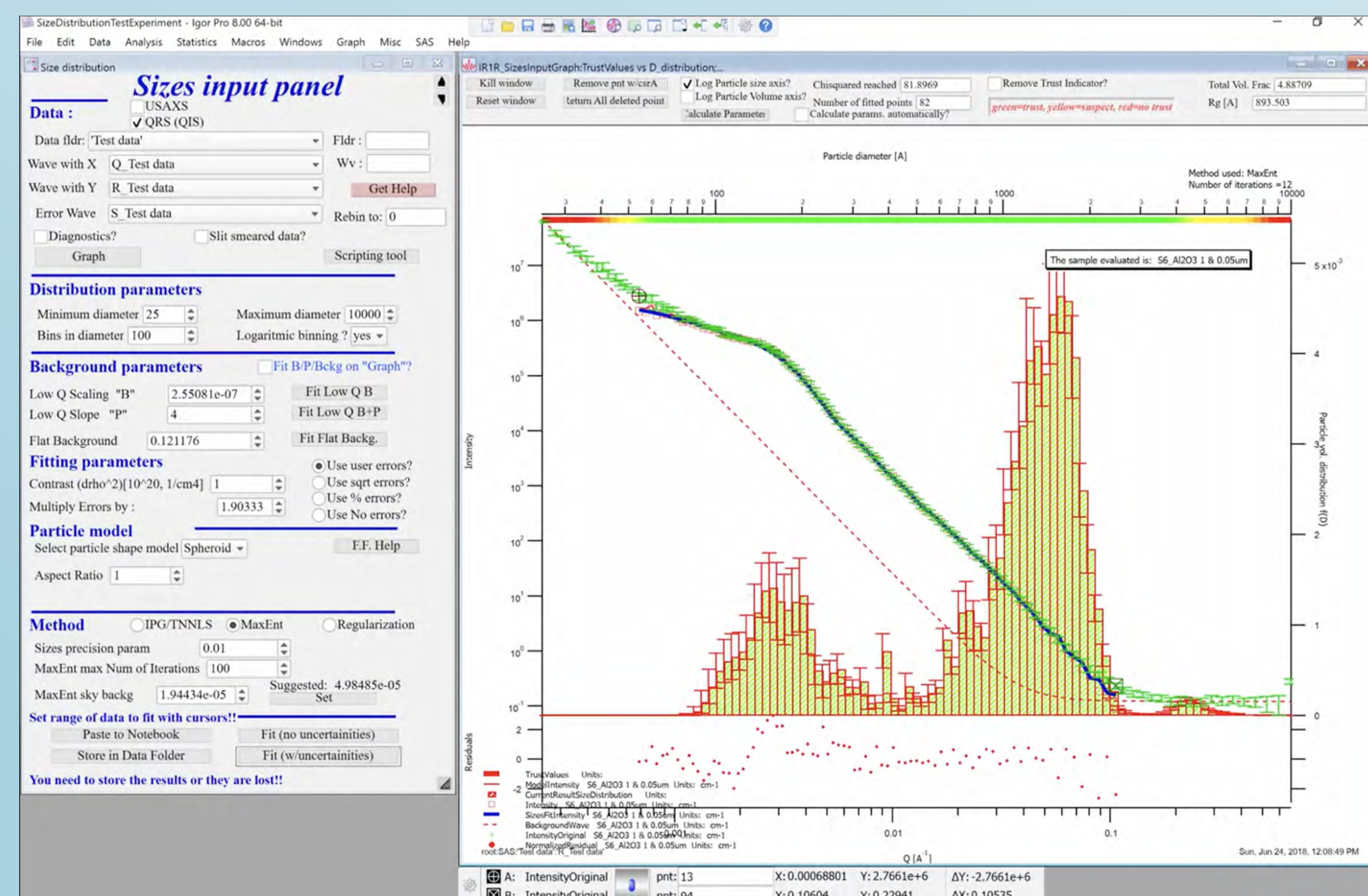


Irena is a data manipulations and analysis toolbox for small-angle scattering (SAXS, SANS, USAXS, USANS) data, written for Igor Pro (from WaveMetrics, Inc) by Dr. Jan Ilavsky, physicist at the X-Ray Science Division of Argonne National Laboratory.

Irena is used for analysis of data in materials science, chemistry, polymers, metallurgy, physics, and other systems of typically solid or liquid samples.

Main Irena Tools

- Unified fit
- Modeling - Direct modeling of SAS from up to 10 populations on up to 10 data sets at once. Selection of form factors and structure factors, Unified fit, Mass or Surface Fractal, and Diffraction peaks
- **Size distribution** using Maximum Entropy, Total Non-Negative Least Squares and Regularization methods



- Guinier-Porod model
- Fractal model (combination of mass and surface fractals)
- Debye-Bueche, Cicciariello-Benedetti, and Treubner-Streus models
- X-ray and Neutron reflectivity using Parrat's recursive method
- Small-angle diffraction tool (up to 6 diffraction peaks)
- Pair distance distribution function (PDDF, P(r), see GNOM from D. Svergun for more details)
- Powder diffraction peak fitting tool (WAXS)

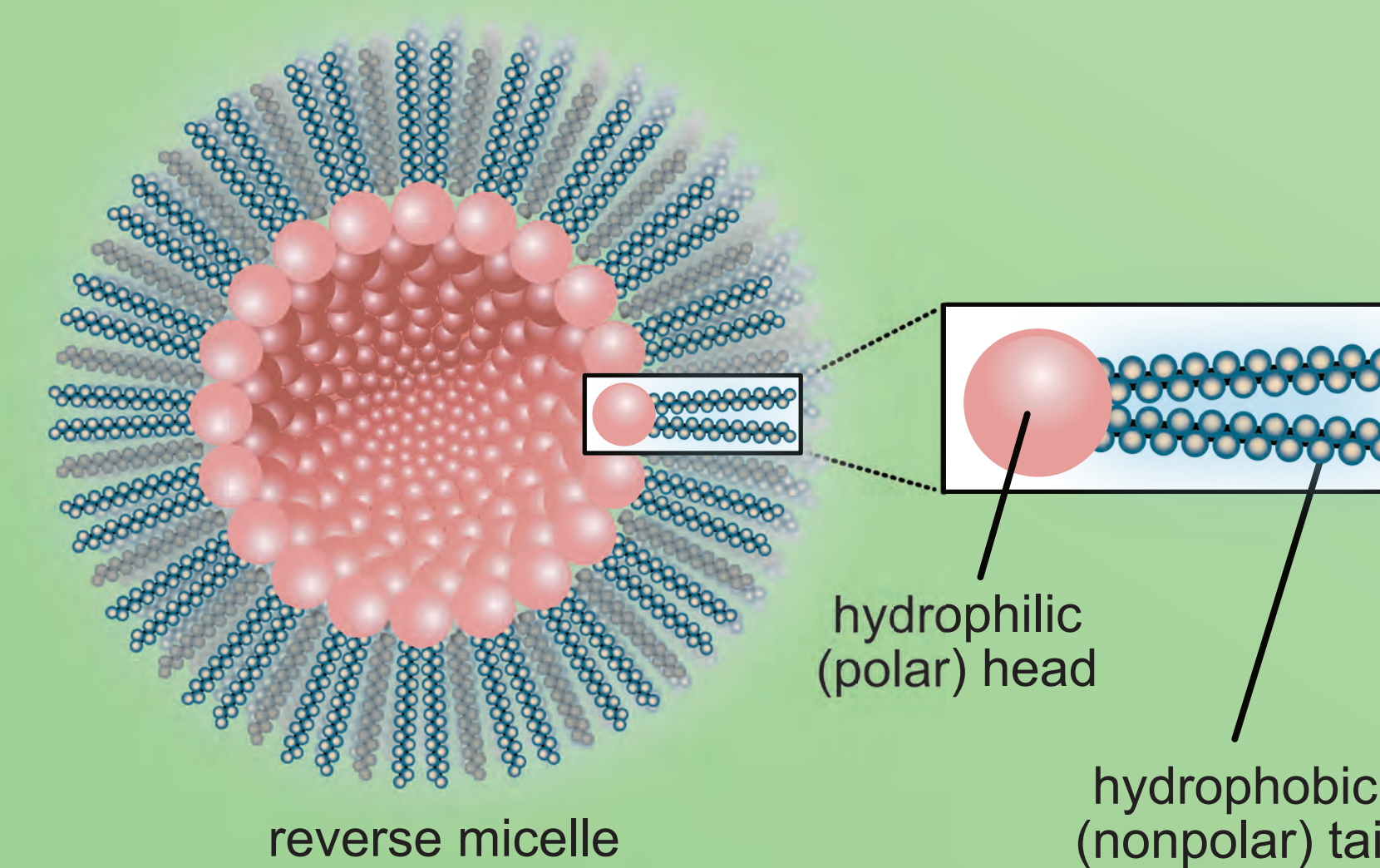
<https://usaxs.xray.aps.anl.gov/software/irena>

Nika is a package of Igor Pro macros designed to reduce 2D (area) detector (e.g., CCD) data into 1D "lineouts" for SAXS or WAXS - providing correctly calibrated Intensity, q (2θ or d), and errors.

Nika provides multiple methods to extract the data:

- Sector and circular averages ("cake")
- Intensity along linear and elliptical path (vertical/horizontal lines, line under an angle and ellipse of arbitrary aspect ratio)
- Intensity along linear path but for Grazing incidence geometry
- Intensity vs azimuthal angle image intended for manual inspection of geometry

<https://usaxs.xray.aps.anl.gov/software/nika>



Reverse Micelles (RMs) are macromolecular structures consisting of water, a surfactant and a non-polar solvent.

Much work has been spent studying RMs comprised of NaAOT (sodium bis(2-ethylhexyl) sulfosuccinate) as the surfactant and i-octane as the solvent and are liquid at ambient temperature.

In order to understand the internal dynamics of the micelles it has proved necessary to quench or freeze out the overall micellar rotation and translation in solution.

This is accomplished by replacing the i-octane with higher carbon number alkanes which exhibit melting points near room temperature.

This figure displays SARMs made with eicosane ($C_{20}H_{42}$) which has a melting point of 37 deg C. These SARMs are small pools of softly confined water immobilized in a solid paraffin matrix.

X-ray scattering was performed on such samples to confirm that the freezing process has not destroyed the micellar structure.

Several samples are presented (collected on a Rigaku S-max3000 pinhole camera and initially processed using Jan Ilavsky's Nika package on Igor Pro).

The main Bragg Diffraction peaks were fitted to single gaussian line shape using Igor Pro.

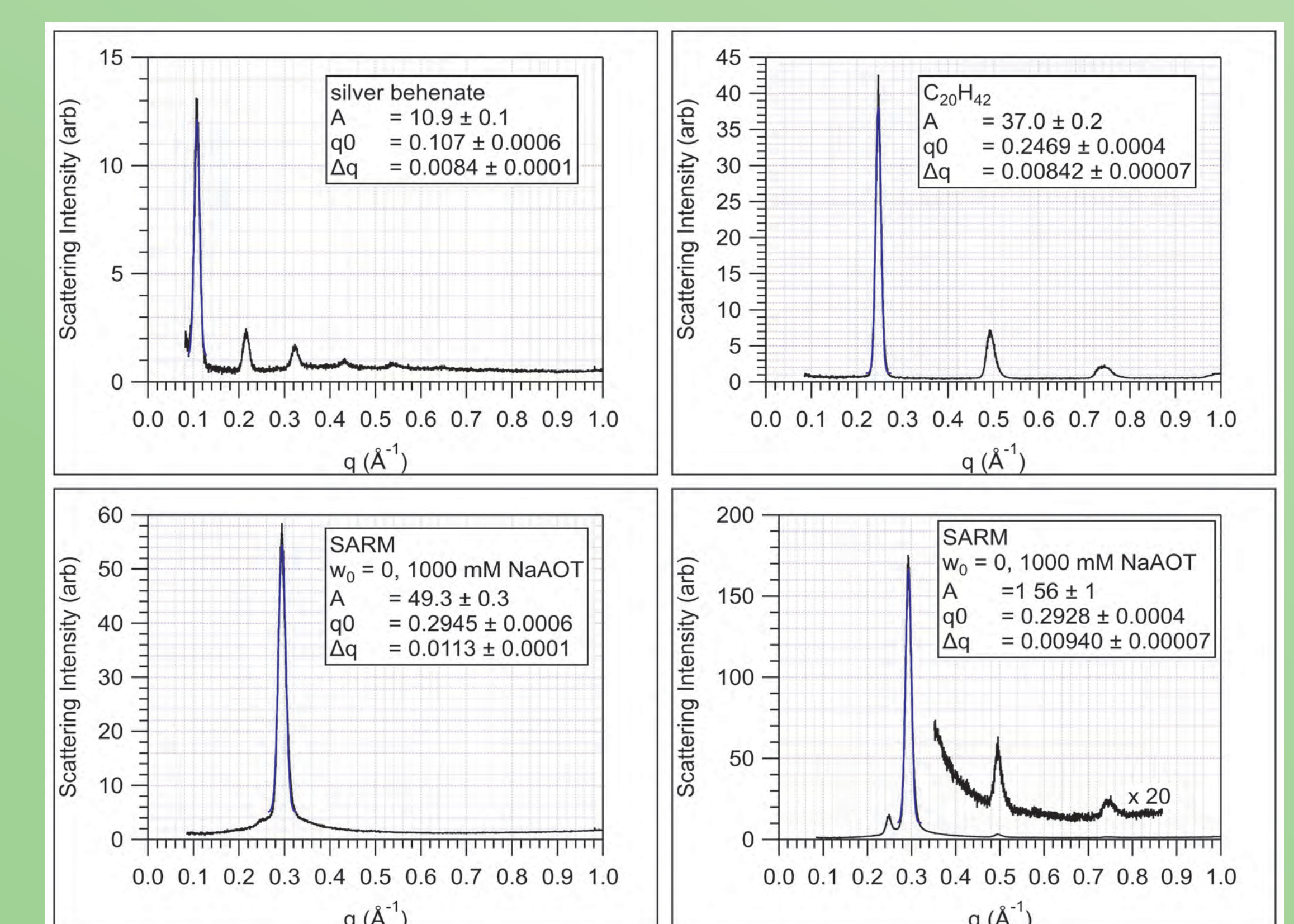


Figure and description by Joseph A. DiVerdi, Ph.D., M.B.A., Special Associate Professor of Chemistry, Colorado State University.

Igor Pro is a fully interactive software environment where you can import and analyze your scientific and engineering data and produce publication-quality graphs and graphics:

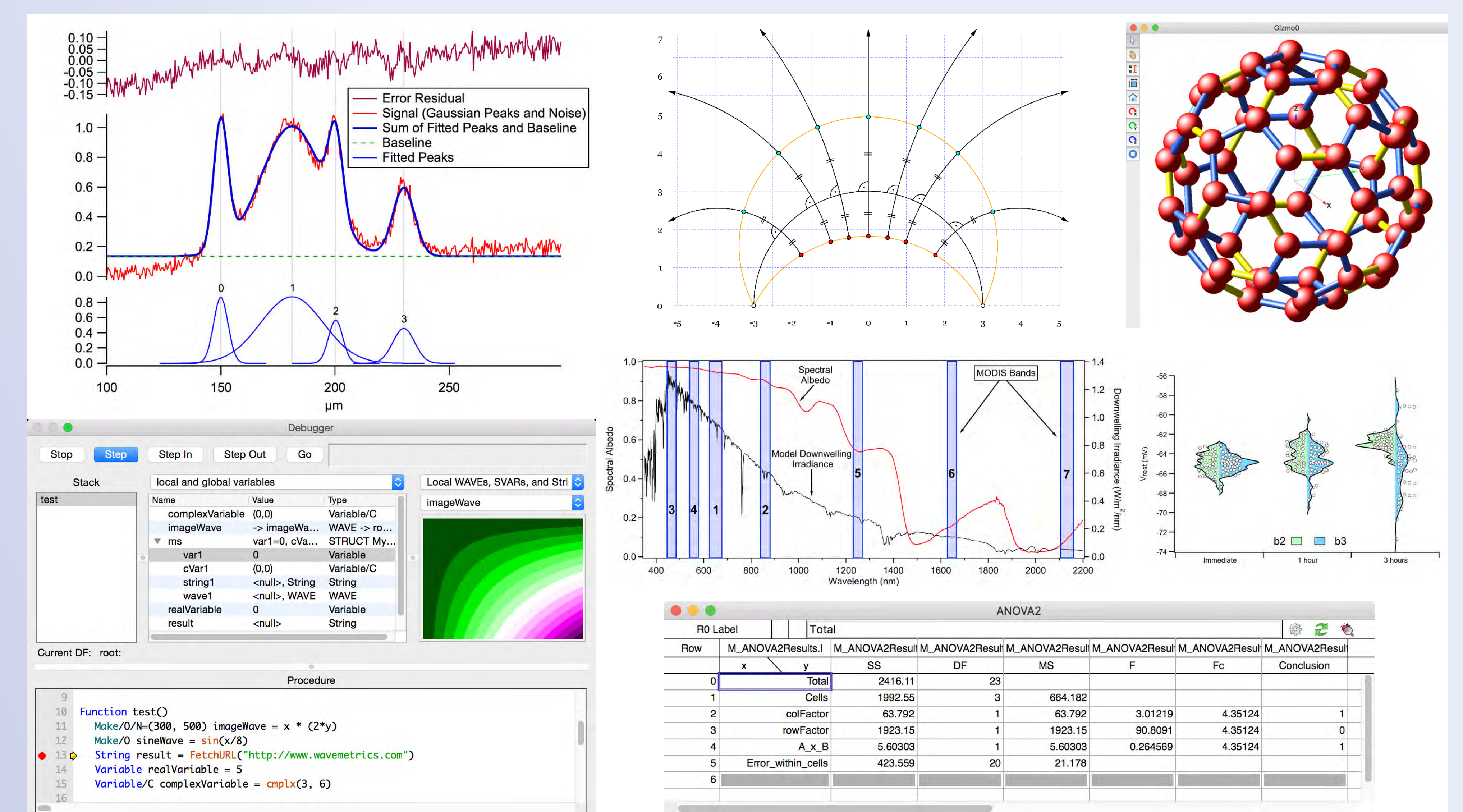
- Quickly analyze and graph large data sets
- Visualize your data with scientific journal-quality graphs
- Comprehensive statistics and curve fitting for data analysis
- Import data in many formats or acquire data from hardware devices
- Cross-platform compatible: macOS and Windows

Point-and-click is just the beginning. Add your custom programming using Igor's powerful built-in language to automate your data analysis:

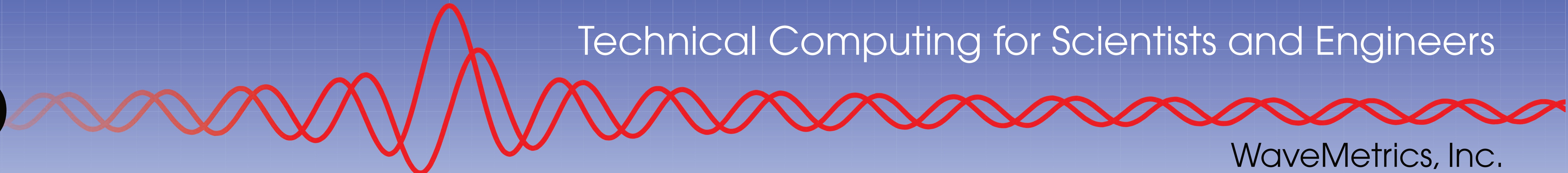
- Automate data import, file i/o, analysis, graphs, images, and 3D plots
- Troubleshoot Igor Pro code with the symbolic debugger tool
- Igor Pro includes hundreds of pre-programmed analysis and control commands for rapid algorithm development
- Create custom GUIs with controls that perform analyses and display results

Standard, Academic, and Student licensing options for Igor Pro are available for purchase online at:

<https://wavemetrics.com>



IGOR Pro



Technical Computing for Scientists and Engineers

WaveMetrics, Inc.