UPDATE NOTES

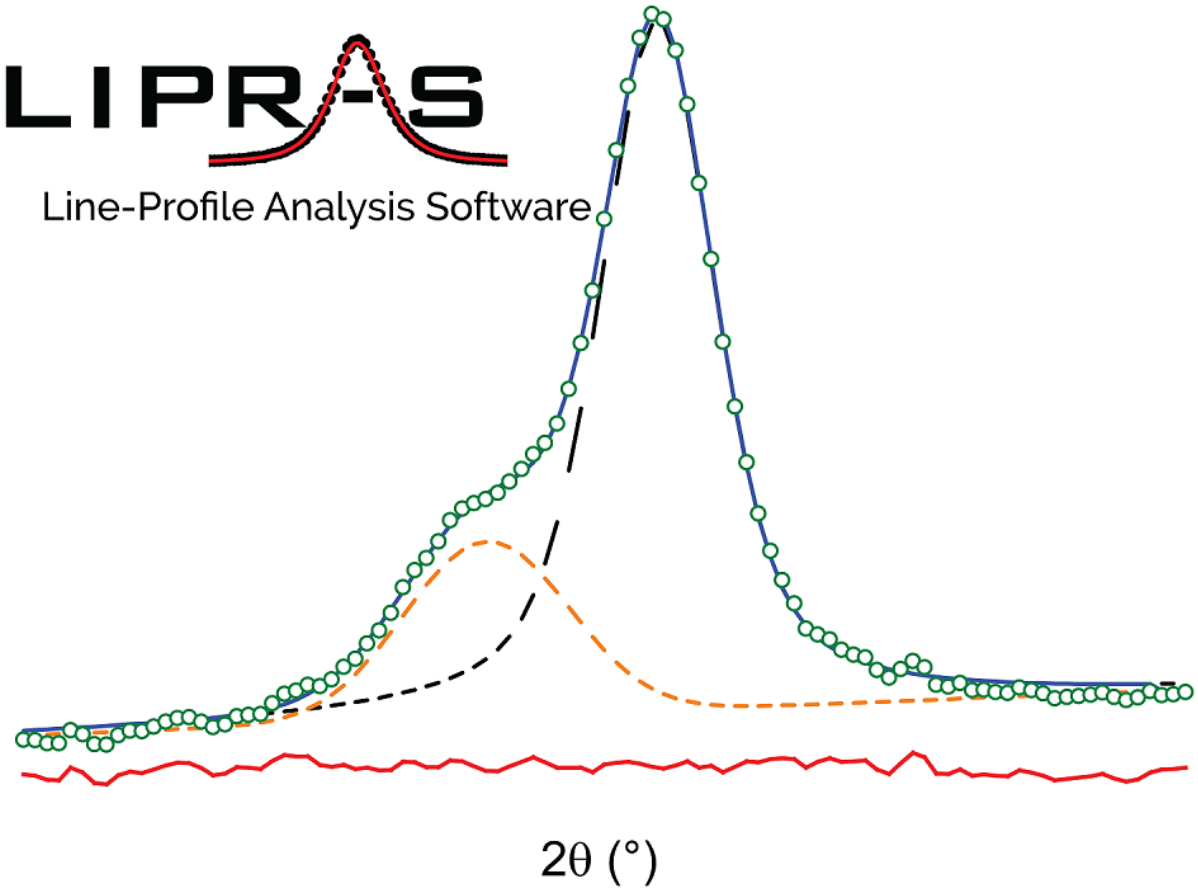

TABLE OF CONTENTS

April 24, 2017

1. Exported images are now printed at 100 dpi by default and can be uniquely saved based on preference selection
2. Export image now creates a separate figure that conducts all plotting and saves it, this prevents unnecessary cycling of the GUI, Export saves the current axes 1 as is, meaning if its zoomed in, it will save the zoomed in region
3. No error message when canceling exporting plot
4. Code clean up from GitHub merge conflicts
5. Reduced font size on title of plots and statistics plot from 14 to 12
6. Added the following to Preference tab: Image resolution selection, image format, save all images instead of one
7. Preference file is now read on start up after all classes have been formed; previously this would happen when a file was read
8. Preference can now be launched with Ctrl+P
9. Image export can now be launched with Ctrl+F
10. When viewing coefficients, export plot will export only that plot and not the fits. Will add Coeffs to the filename as well
11. Removed 'truesize' command so that Image Processing Toolbox would not be needed to view the about section
12. (MATLAB Only) On startup save the current directory in case user navigates away and would try to reset LIPRAS
13. Individual Fmodels are no longer written, never had a use for opening one since the master Fmodel contained all the data. The lines were just commented out so MATLAB users can reactivate this whenever
14. Added individual Kalpha2 peaks to Fdata file. FData now writes peak 1, peak 2, peak… then the Kalpha2 for all peaks

May 19, 2017

IMPORTANT: ***Users who use weights need to ensure they use LIPRAS version 398 or higher.***

LIPRAS version labeling now reflects the commit number on GitHub.

1. Fixed an issue where weights of the first pattern were applied to all the patterns instead of being file dependent
2. Changed 'Weights' in preference tab to have only [Default, None, 1/obs ($1/\sigma^2$), and 1/sqrt(obs) ($1/\sigma$)]. The 'Default' is for files that have errors associated with measured intensity. To force 1/obs or to have no weights, this must be changed in Weights and can be reverted by going back to 'Default'
3. Weights for least squares are now written in Fdata
4. Rp, Rwp, and GOF (Reduced-χ^2) are now written in the Fmodel file
5. Rp, Rwp, and Reduced-χ^2 are now displayed for each diffraction pattern after a fit below the graphics window
6. Fdata now prints to 8 decimal places

7. FXYE and CSV/Excel now reads in the errors columns and sets the weights to the errors in accordance to $1/\sigma^2$. To override, set weights to 'None'
8. LIPRAS now reads .xye which is twotheta, intensity, error, no header can be present. Errors for these files are set as weights
9. Import parameter file does enable 'Fit Data' when importing
10. Added feature that can check for updates based on the commits to the master file on GitHub. This is done by reading the html page source and finding the current commit displayed on the GitHub webpage pertaining to LIPRAS
11. Interactive help is no longer visible, this requires more work to be useful.
12. (MATLAB) Jacobian matrix from resulting least squares is stored and can be accessed by those using LIPRAS in MATLAB. To do this, type the following into the command Window, after a fit: handles.profiles.FitResults{1}{filenumber}.FitInfo.Jacobian

May 25, 2017

* *Commits 415, 416*

1. Fixes to Reduced chi-square, 'Default' weight options for CHI files were incorrect. This was a typo, although could be forced by specifying '1/obs'. Found out GOF or (reduced chi-square) is sse/dfe which are values found in the Fmodel files. In the case of Weights being set to 'None' GOF is calculated the same way as when weights are set to '1/obs'.
2. LIPRAS assumes sqrt(intensity) for error when reading XRDML files.

June 8, 2017

* *Commit 417*

1. **Significant improvement to background refinement**. Realized that the background needs to be evaluated and modeled with the proper scaling and centering. Therefore, refined model now refines with x=(x-mean(x))/std(x) for the bkg coefficients and is properly evaluated. This change improves the initial guess for bkg coefficients and results drastically. To evaluate the resulting coefficients manually, the x=(x-mean(x))/std(x) must be used.
2. Round Rp, Rwp, and GOF to 4 decimal places. For reporting purposes, users should use 2 decimal places.