

GSAS v5.1 Release Notes

GSAS Team

November 03, 2005

Introduction

GSAS Release 5.1 fixes errors in the waveform fitting process.

Product Format/Definition Change Summary

GSAS 5.1 introduces no product format changes. However, the GSAS 5.0 product database had a few errors which we have corrected. Thus, the GSAS 5.1 product database update is only a correction of GSAS 5.0.

Known Problems

Same as noted in Release 5.0.

Release Information

The ClearCase label for this release is RELEASE_5.1.

Products generated by this software will be labelled as Release 25 by SDMS.

The release date is November 03, 2005.

Version numbers have been updated to "V5.1 Nov 2005".

This should be verified during operation by checking the version information in the appropriate ANC06 files.

SMDS Impact

The distribution tarfile is on glasdev.wff.nasa.gov at the following location:

```
/glasdev1/v5/dist/gsas_v5.1.tar.Z.
```

ANC Files

New versions of the ANC45 data files are required.

No ANC07 files were changed.

Bundle Changes

None

Compilation

All libraries and binaries should be recompiled using the top-level Makefile.

The process for making the libraries and binaries is as follows (**NOTE: SDMS ONLY!!**)

```
cd /install_dir/gsas_v5.1
make runtime
make install
```

Note : developers should not use the above procedure. This procedure is for SDMS only!

Detailed Change Notes

0002147: Error In Waveform Fit

When W_LsqFit rejects a fit without iterating, the standard deviation of fit is set to invalid. The V5.0 set standard deviation to zero which caused initial estimates to be return as fits for cases when the estimated signal width was less then minimum allowed width.

0002142: Error in W_NormWF & W_UnNormWF

Corrected W_NormWF & W_UnNormWF. Noise when doing fit to normalized return was not being properly used in the un-normalization of the amplitude of the least squares fit. On occasion this caused small peaks to be omitted in the final returned estimated parameters

0002129: The Setting Of The Compression Array d_comp in W_PerformFit Should Be Moved

Fixed error that caused the compression array in W_PerformFit to be calculated incorrectly.

0002131: Update Development Database with late GSAS 5.0 changes

Added description to the following variables:

GLA06, 12-15: Surface_temp, Surface_pres, & Surface_relh
GLA07, 15: Surface_wind, & Surface_wdir

Added descriptions to the following variables:

GLA01: recNrgAll_EU
GLA05,06,12-15 : recNrgAll
GLA06,12-15 : satRngCorr, satNrgCorr, satPwdCorr, & satCorrFlg

Made correction to the description of the variable LRir_QAflag in GLA09. The flag PDF has been corrected.

0002161: Record length changes need to be added to V5.0 release notes

The following record length changes were omitted from the GSAS 5.0 release notes:

GLA05: 17400
GLA07: 70456
GLA08: 792
GLA09: 6944
GLA10: 14976

Changed ANC07 Parameters:

None

Changed Files:

```
/glas/vob/data/anc45_001_01_0001.dat  
/glas/vob/data/anc45_001_01_0002.dat  
/glas/vob/data/anc45_001_01_0003.dat  
/glas/vob/data/anc45_001_01_0004.dat  
/glas/vob/data/anc45_001_01_0005.dat  
/glas/vob/data/anc45_001_01_0006.dat  
/glas/vob/data/anc45_001_01_0007.dat  
/glas/vob/data/anc45_001_01_0008.dat  
/glas/vob/data/anc45_001_01_0009.dat  
/glas/vob/data/anc45_001_01_0010.dat  
/glas/vob/data/anc45_001_01_0011.dat  
/glas/vob/data/anc45_001_01_0012.dat  
/glas/vob/data/anc45_001_01_0013.dat  
/glas/vob/data/anc45_001_01_0014.dat  
/glas/vob/data/anc45_001_01_0015.dat  
./Makefile  
./src/wf_lib/W_FunctionalFt_mod.f90  
./src/wf_lib/W_LsqFit_mod.f90  
./src/common_libs/platform_lib/const_glob_mod.f90
```