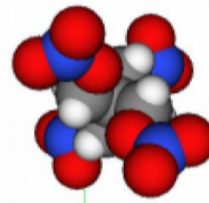


## GSAS-II USER MEETING

(NEWS SINCE  
SEPTEMBER 2017)

# GSAS-2



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## INTEGRATION STEPS IN GSAS-II

### Single Image integration

- Read image ( image, background, dark, container, gain map - if any)
- Make x,y → 2th,azm map – usually most expensive
- Apply masks (includes Make masks) – can be expensive if many masks
- Do binning → powder pattern (done in Fortran)
- Clean up
- An example timing:

```

C:\WINDOWS\system32\cmd.exe
Read Mar345 file: C:\work\GSASII\Examples\texture\steel\nx_tex_pre_001.mar2300
image read time: 0.297
Begin image integration
Step times:
  apply masks    0.750s xy->th,azm    1.765s fill map    0.047s
  binning        0.063s cleanup      0.016s
Elapsed time:   2.641s
Integration complete

```

## INTEGRATION STEPS IN GSAS-II

### Speed up by reuse of x,y → 2th,azm map & mask

- Test if image geometry is unchanged & test if mask unchanged
- Use previous ones (in Integrate All & Auto Integrate – not for table lookup)

```

C:\WINDOWS\system32\cmd.exe
Read Mar345 file: C:\work\GSASII\Examples\texture\steel\nx_tex_pre_001.mar2300
image read time: 0.297
Use new image controls; new xy -> th,azm time 1.773
Use new mask; make mask time: 0.516
Read Mar345 file: C:\work\GSASII\Examples\texture\steel\nx_tex_pre_001.mar2300
image read time: 0.281
Begin image integration
Step times:
  apply masks    0.222s xy->th,azm    0.000s fill map    0.048s
  binning        0.049s cleanup    0.000s
Elapsed time:   0.336s
Integration complete
Read Mar345 file: C:\work\GSASII\Examples\texture\steel\nx_tex_pre_002.mar2300
image read time: 0.281
Begin image integration
Step times:
  apply masks    0.222s xy->th,azm    0.000s fill map    0.003s
  binning        0.111s cleanup    0.016s
Elapsed time:   0.352s
Integration complete
Read Mar345 file: C:\work\GSASII\Examples\texture\steel\nx_tex_pre_003.mar2300
image read time: 0.297
Begin image integration
Step times:
  apply masks    0.235s xy->th,azm    0.000s fill map    0.061s
  binning        0.048s cleanup    0.000s
Elapsed time:   0.344s
Integration complete
  
```

Repeated anytime  
new geometry or  
mask mask

0.336s vs 2.64s  
per image



## PYTHON3.X MIGRATION

### GSAS-II is now compatible with Python 2.7 and 3.6

- All code has been updated to meet Python3.6+ standards, not all code has been exercised
- GUI updated to work with wxPython 4.0 (required by Python3.x)
- Build routines with scones have been updated and tested (on 32 & 64 bit Python, w/both 2.7 & 3.6) using Anaconda supplied gfortran
- Anaconda is not ready for us to distribute with Python 3.6 (missing packages)
- Plan is to automate compilation on Jenkins

## SCRIPTING INTERFACE TO GSAS-II

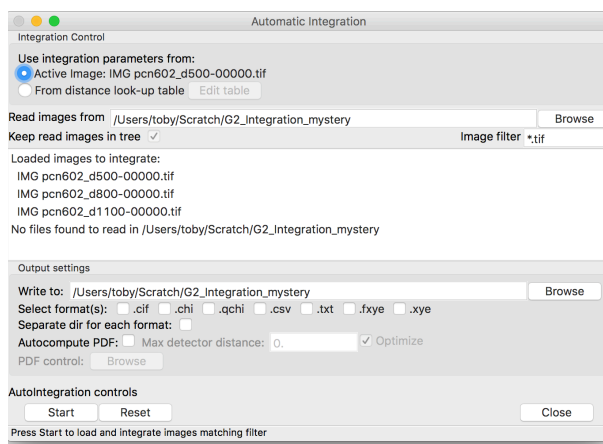
Allows for conducting refinements from Python or bash scripts

- Tutorial written
- Looks good
- Some limitations to be addressed

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## NEW OPTIONS IN AUTOINTEGRATION



Read images:  
directory was  
previously included in  
filter, now has  
separate field &  
Browse button

Keep images in tree:  
Option to be implemented

.qchi: gives access to  
chi file with Q units

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## IMAGE METADATA

- GSAS-II needs at a minimum wavelength, detector-to-sample distance, etc
- For SRS beamlines (.tif files), metadata read from a .metadata file
- For 1-ID: need to pickup data from a column-oriented .par file

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## SUGGESTED IMPROVEMENTS: METADATA

- If the label for a free parameter is changed, that could trigger a search of comments for values matching that keyword (implemented in v. 3193)

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