Squirrel Overview

7th AMS Users Meeting
U of Minnesota, Minneapolis, Sun., Sept. 17, 2006 17:00

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Aerodyne, University of Colorado, Boulder

Outline

✓ Squirrel Motivation
   What, Why, How

✓ Squirrel Analysis Flow Chart
   Outline major steps, Quick & Thorough Analysis

✓ Squirrel Features
   AMS Igor Panel Screen Shots, Resulting Graphs

✓ Squirrel Future
   Bug list & Feature request

✓ Closing Remarks
**What is Squirrel?**

- SQUIRREL (SeQUential Igor data RetRiEvaL) is an AMS data management and analysis tool for Igor
- Ongoing, collaborative effort
  - Silke Hings, Frank Drewnick
  - James Allan, Jonny Croiser
  - Ed Dunlea, Donna Sueper
  - Tim Onasch
  - And many other AMS Users!

**Why Squirrel?**

- Aerodyne AMS generates large data sets
  - Not feasible to load all data into memory
  - The squirrel approach is to load sufficient data for task at hand (diagnostics, quick look…)

- Recreation of James’ quad program
  - Generates mass spectra averages, size distributions, time trends; uses same frag list and batch files
  - WHAT IS NEW: size binned mass spectra

- Familiarity with Igor
  - Publication-quality graphs
  - Users can write custom code
How does Squirrel work?

✓ Access Raw HDF files generated from DAQ
  * HDF is a general purpose file format for storing scientific data
  * Raw data remains on the disk in randomly accessible HDF format

✓ Create intermediate hdf files (pre-processing)
  * Files name example: AMS_intermediate_000001.hdf
  * Some operations which create intermediate files: conversion to Hz, stick recalculation, application of DC markers for Ptof size distributions

✓ Select runs to analyze via Todo waves
  * Todo waves are made up of run numbers, have a special format
  * For quad users, Todo waves are generalized and versatile mask waves

How does Squirrel access data?

✓ RAW DATA REMAINS UNMODIFIED in original HDF files

✓ MSSDiff_p matrix (run vs m/z sticks) stays in memory

✓ Intermediate HDF files, written to disk, hold processed MS and PToF data
  (open and closed MS sticks, raw MS spectra, PToF sticks and PToF raw spectra)

✓ This has implications for how to organize, store Igor experiments!!!
Screen Shots
AMS Panel

Squirrel Credits, Web link

Select Analysis Action
* Always read top to bottom, left to right
* Buttons make things go
* Checkboxes indicate options
* Gold buttons are popular
* Most default settings are appropriate
* Italicized items aren’t functional

Select Data to Act Upon
Create, view todo waves

Manipulate Output, Other Info

Is it done yet?

Squirrel Data Analysis Flow Chart

Quick Look

Get Index

Pre-Process

_p data (DAQ sticks)

HDF Index Tab

MS Tab

PTOF Tab

time series, avg spectrum
image, avg size dist, size binned spectrum
Screen Shots
HDF tab Output

Screen Shots
MS Tab

<table>
<thead>
<tr>
<th>Image, avg size dist, size binned spectrum</th>
<th>time series, avg spectrum</th>
<th>m/z</th>
<th>Nitrate equivalent mass (µg m^-3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>MSSD all 112.709</td>
<td>MSSD Air 110.953</td>
<td>MSSD Water -0.762827</td>
<td>MSSD NO3 0.133794</td>
</tr>
<tr>
<td>MSSD SO4 0.257086</td>
<td>MSSD Org 0.703696</td>
<td>MSSD NH4 0.166322</td>
<td>MSSD Chl 0.00246195</td>
</tr>
</tbody>
</table>
**Screen Shots**

**Check m/z calibration**
- View fit info for many runs
- Choose which peaks to fit
- View peak fits for individual runs
- Filter out bad runs

**Check baseline**
- Choose fitting parameters
- View many runs
- Choose stick compliment parameters
- View details of one run
Screen Shots
Modify SI

![Screen Shot Image]

Change these values IF daq values wrong

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Squirrel Data Analysis Flow Chart

**Quick Look**

1. Get Index
2. Pre-Process
3. PToF Tab

**Thorough Look**

1. Get Index
2. Pre-Process
3. HDF Index Tab
4. PToF Tab
5. Corr Tab
6. Frag Checks Tab

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**Flow Chart Diagram**

- Quick Look
  - Get Index
  - Pre-Process
  - PToF Tab

- Thorough Look
  - Get Index
  - Pre-Process
  - HDF Index Tab
  - PToF Tab
  - Corr Tab
  - Frag Checks Tab

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- Diagnostics
  - Plot
  - MS Tab
  - FF Tab
  - Calc Loadings
  - Tweak Frag table

- Mass spec, image, etc.
  - Loading waves
  - plot
  - size dist, mass spec, image, etc.
  - DC marker
What do I need to do to use Squirrel?

✓ Latest version of Igor
✓ HDF5 xop to be placed in your Igor Extensions folder
✓ Latest Squirrel software, a packed Igor template

http://cires.colorado.edu/jimenez-group/ToFAMSRessources/ToFSoftware/SquirrelInfo/

What is next for Squirrel?

✓ Continued bug fixing
✓ Implement existing feature requests
  * Error Analysis
  * Normalize PToF to MS
  * Finish Jose’s Mission Diagnostics Panel
  * Think about using 4 separate correction factors
  * Journal interface
  * Misc panel & graph tweaking
Where can I go for more Squirrel info?

✓ http://cires.colorado.edu/jimenez-group/ToFAMSRessources/ToFSoftware/SquirrelInfo

Thanks to fellow coders

✓ Special Thanks to James Allan

✓ Thanks in advance for the ongoing collaboration

We are squirrel!