

Squirrel speed and robustness improvement possibilities

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Igor vs Matlab

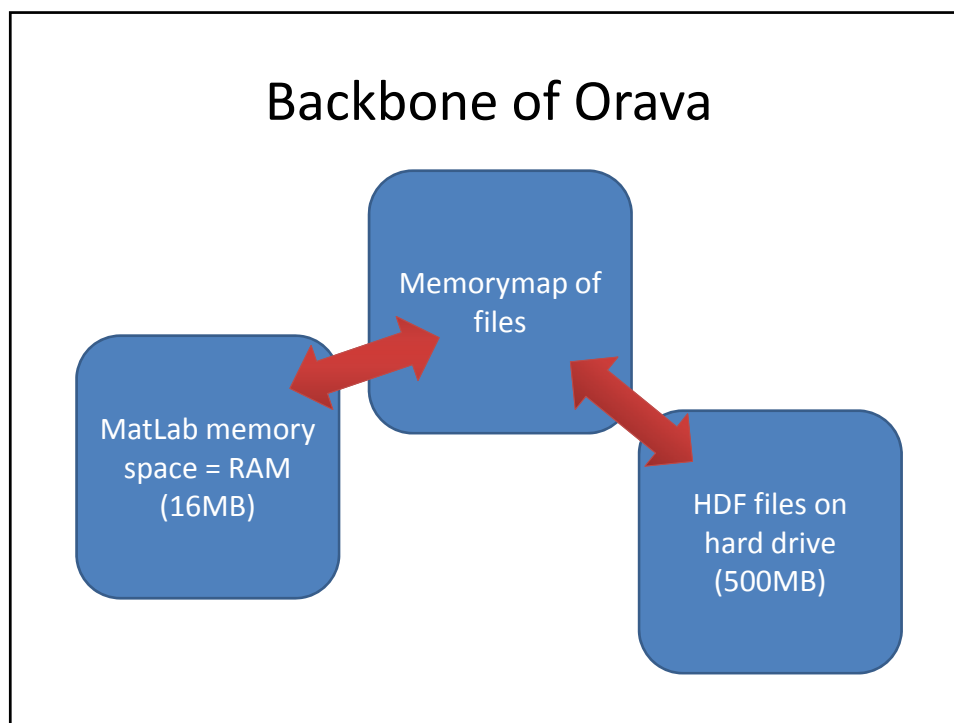
Performance times (s) for 5 days of data

MS mode

	Squirrel	Orava
get index	48	2
load data	-	3
mz - calib	268	54
preprocess	203	106
baseline & sticks		
total (sec)	519	166
total (min)	8.7	2.8

3x faster

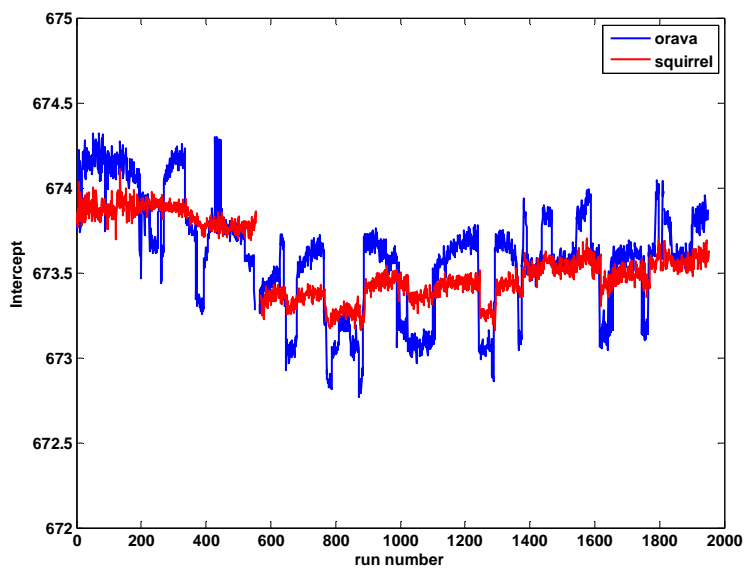
```
amsD=AMS_load_fileInfo_mm([datenum(2007,4
,6),datenum(2007,4,10)])
amsD=AMS_load_ms_mm(amsD,'/MSclosed');
amsD=AMS_load_ms_mm(amsD,'/MSopen');
amsD=AMS_mz_calib_mm(amsD);
amsD=AMS_baseline_mm(amsD,'MSopen');
amsD=AMS_baseline_mm(amsD,'MSclosed');
amsD=ams_calc_diff_mm(amsD);
```



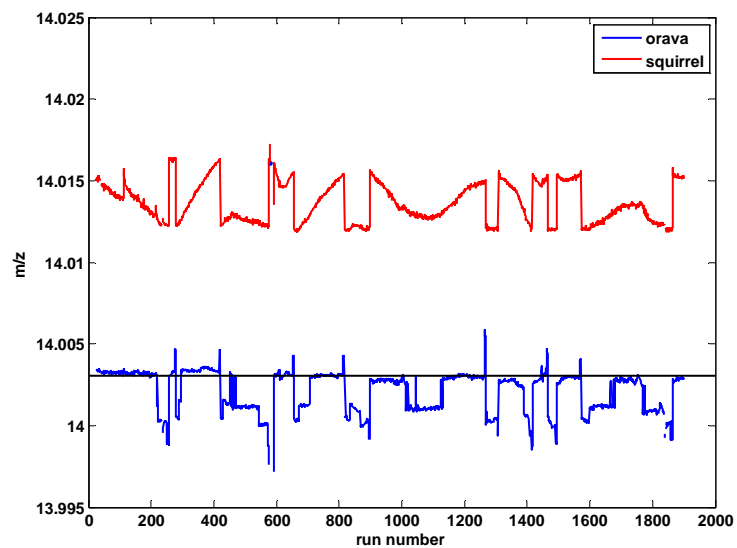
More robust mass calibration

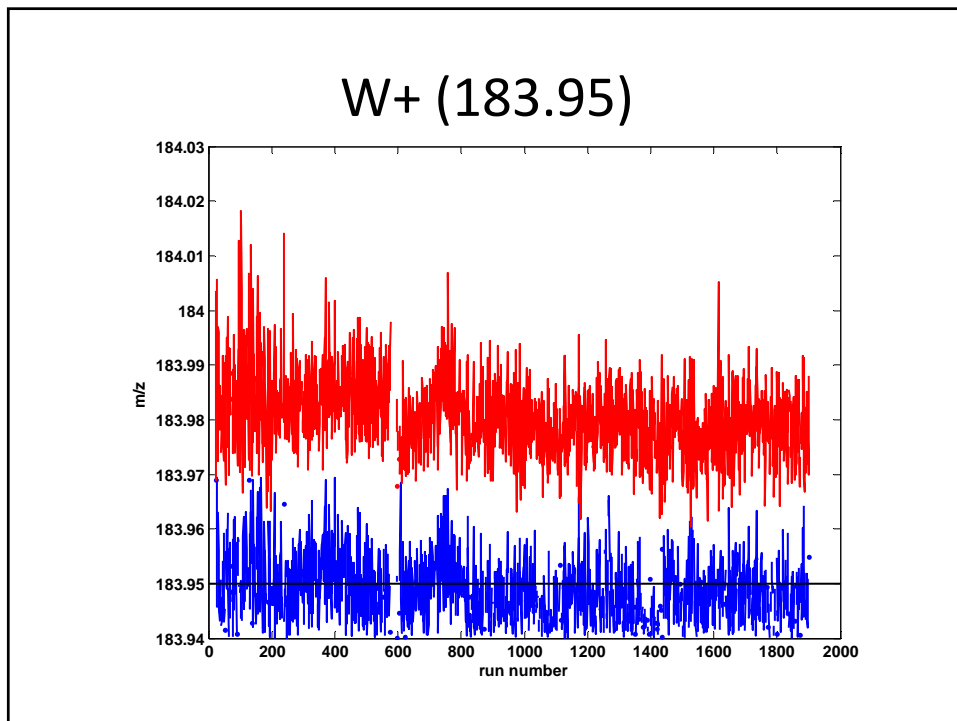
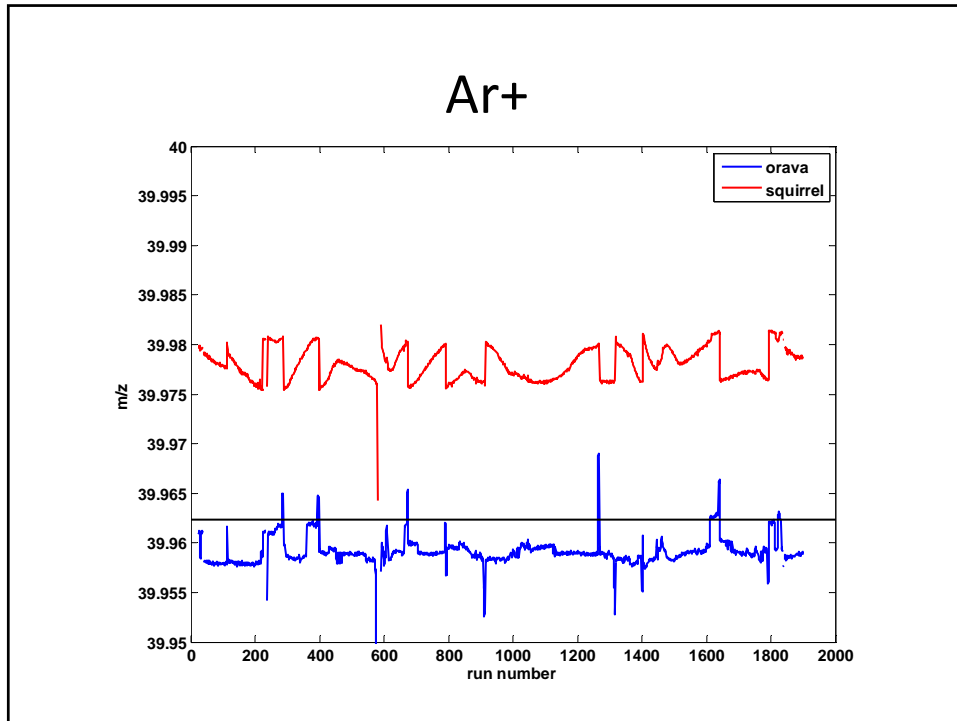
- If DAQs m/z-calibration is completely off
 - Find baseline areas of spectra, calculate average and find intercept and slope that minimize that value
- If DAQs ok (you can find the peaks)
 - List of peaks that should be there, 10-15 known peaks
 - Go through all combination of eg 4-5 peaks and choose the best one
 - "dirty" peaks will be excluded

Mass calibration parameters

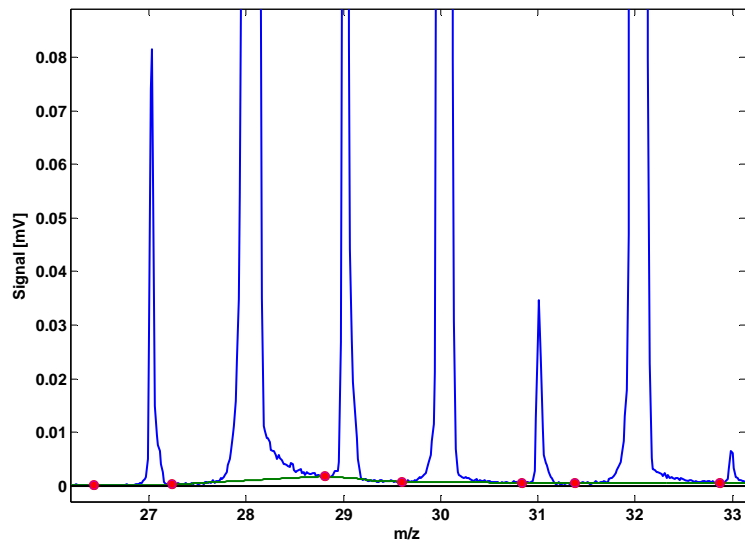


N+

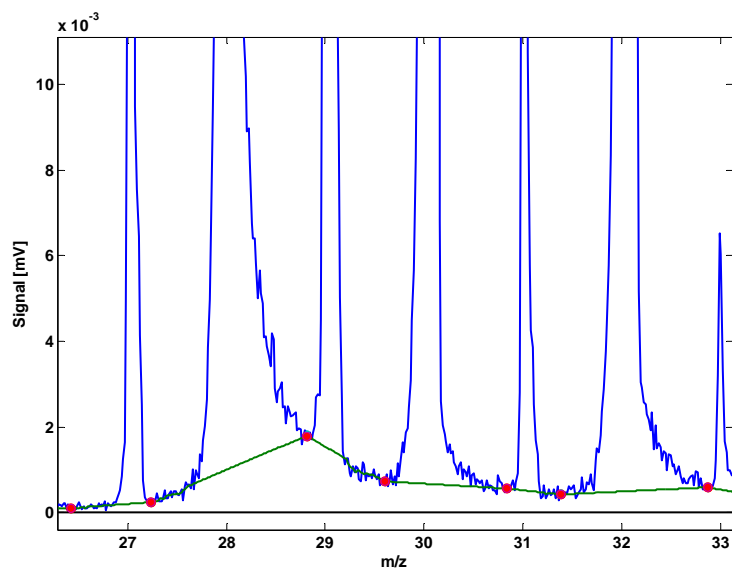




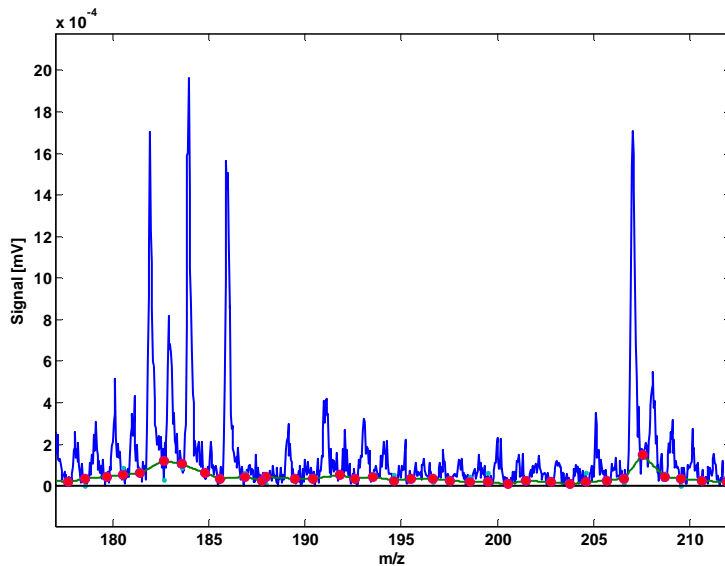
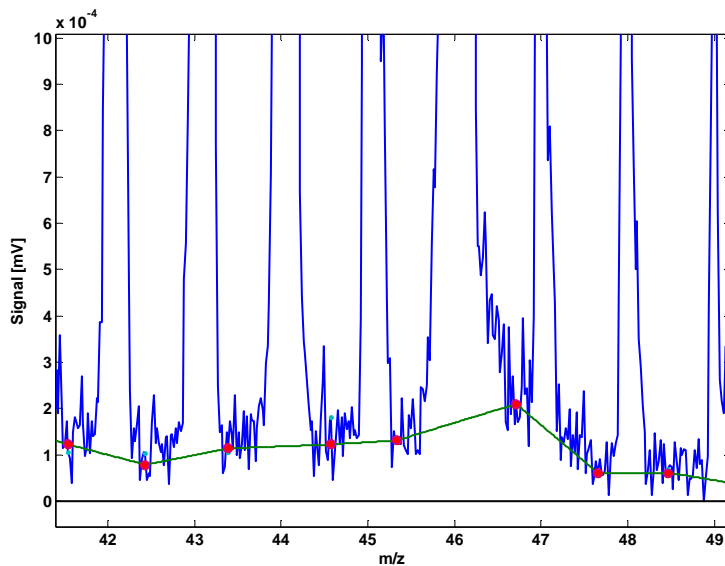
Robust baseline determination

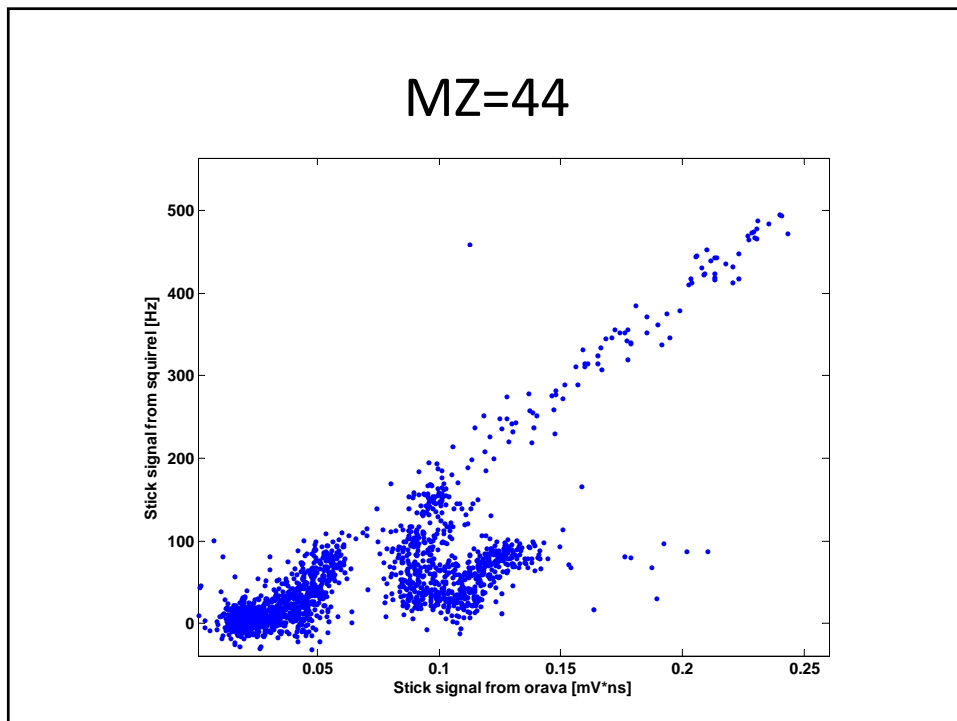
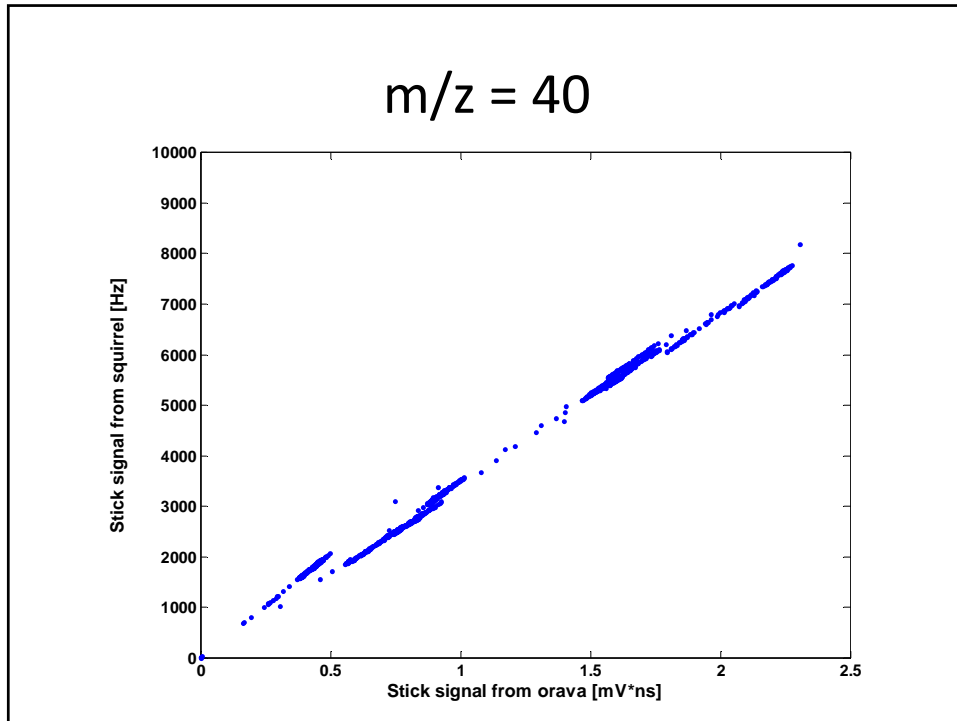


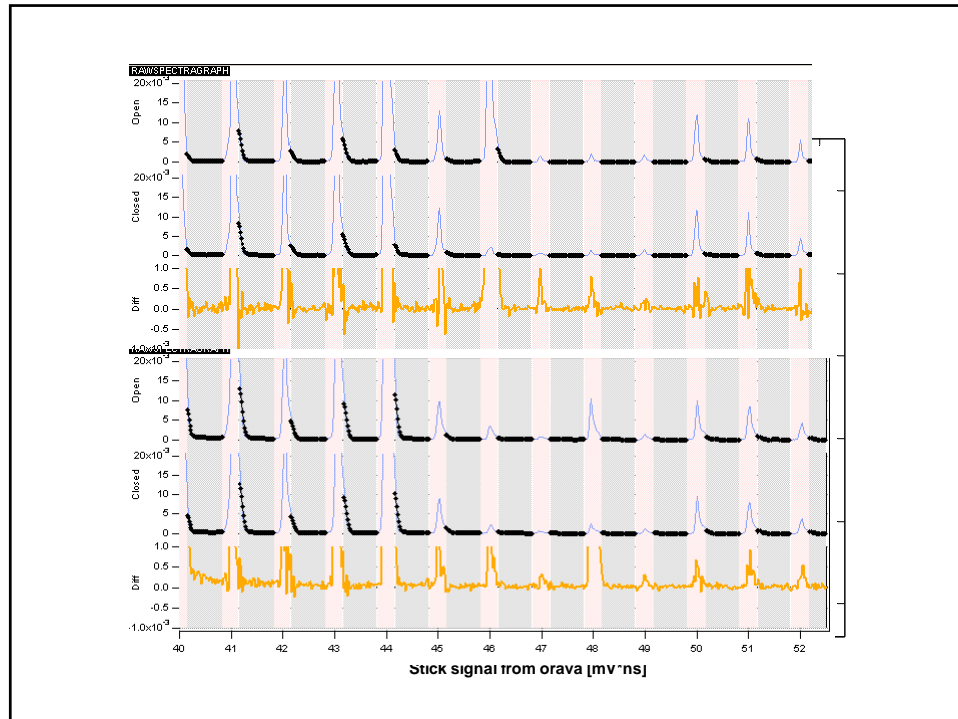
Robust baseline determination



Robust baseline determination







Faster squirrel is possible

If you don't care about software development have a look at soccer prediction at www.betpredict.com