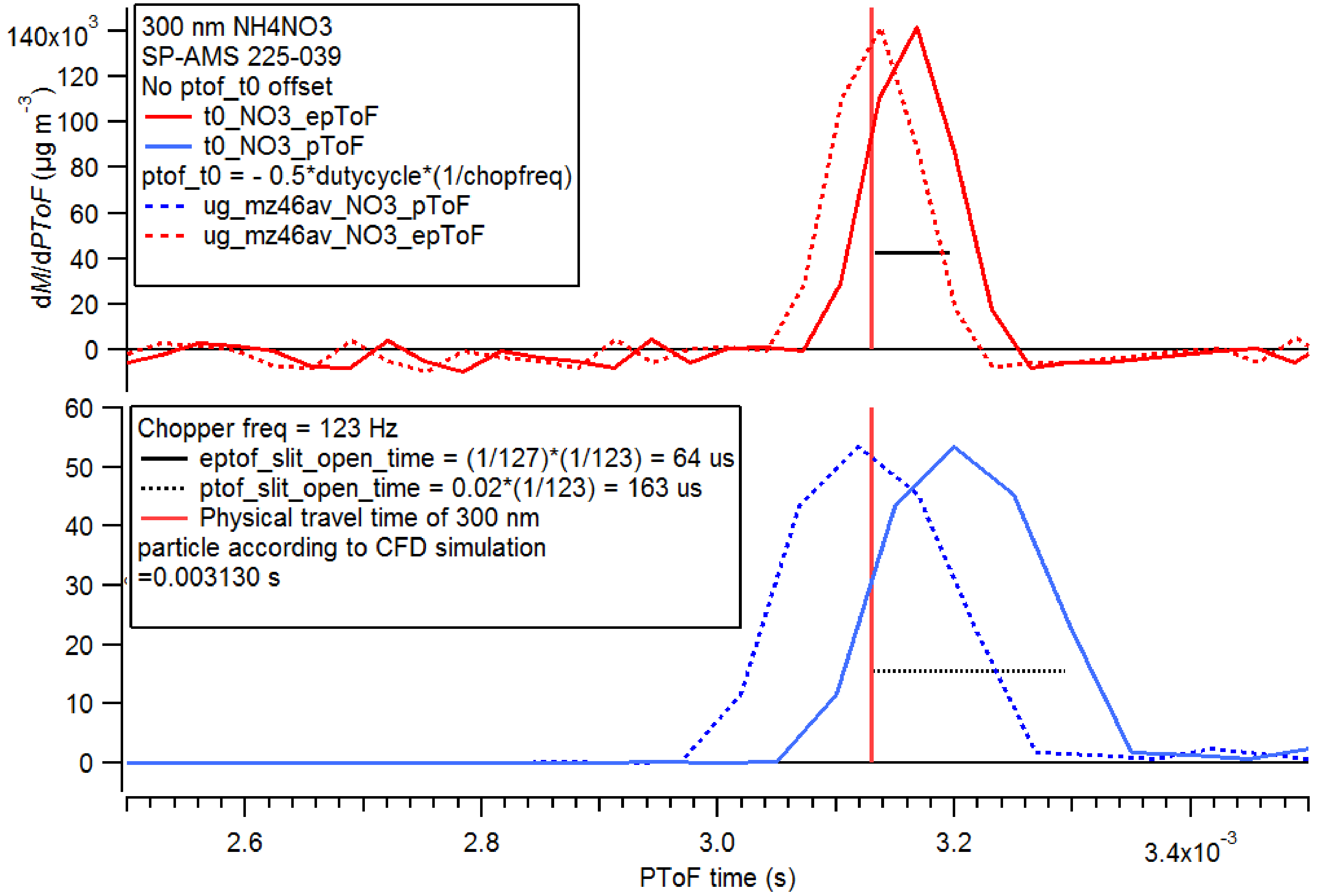
AMS Users Meeting
October 23, 2016
Leah Williams

Can I use the same velocity calibration for pToF and epToF?

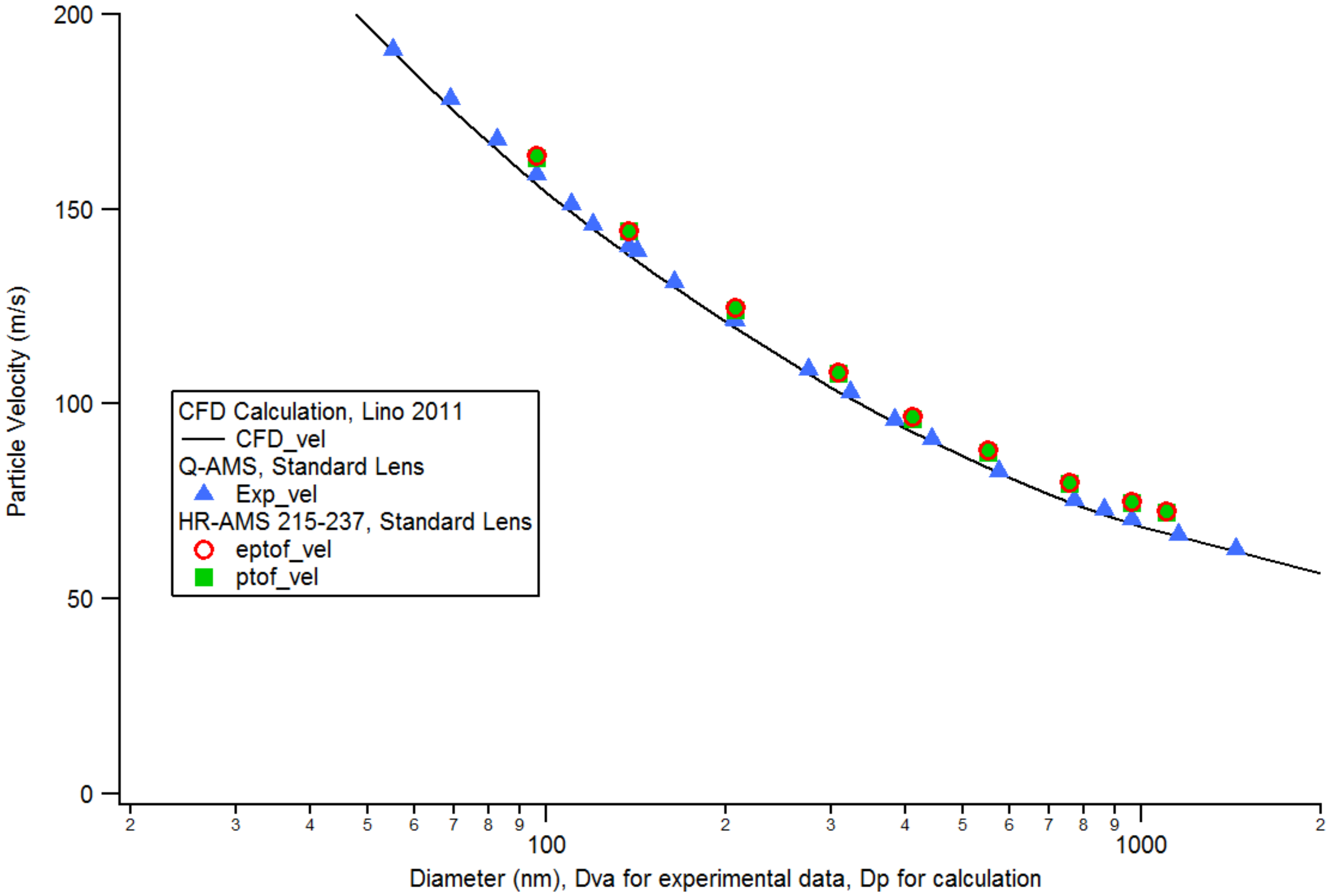
Yes, but…

eptofvsptof ExplanationofArrivalTimev3.pptx



- Solid lines: DAQ recorded pToF
- Dashed lines: pToF corrected for slit width time
  - pToF correction -0.5*chopper_duty/ChopperFreq
  - epToF correction -0.5*(1/127)/ChopperFreq

CalData_07122014.pxp



- Excellent agreement between epToF and pToF velocity calibration
- Reasonable agreement with Q-AMS, no longer setting t0 carefully during instruement build.

eptofvsptof.pxp

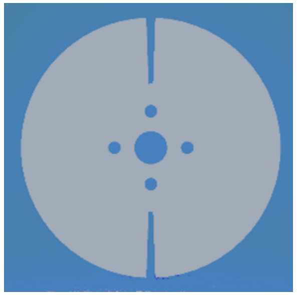
Velocity Calibration Best Practices:

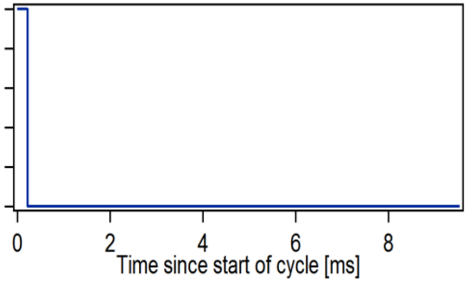
- Always do calibration under same conditions as data acquisition
  - Do velocity calibration in epToF for epToF data
- There was a mistake in the timing correction for epToF in SQ 1.57
  - Error will be corrected in next SQ release –1.58
- VERY IMPORTANT:
  - If you have an epToF velocity calibration that you analyzed in 1.57, you MUST reanalyze it in 1.58 before you apply it to data in 1.58.

Signal and PToF for both PToF and ePToF (from Pedro)

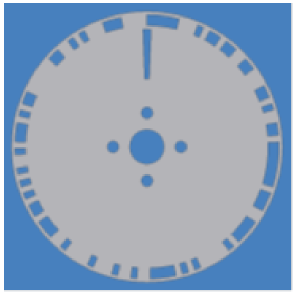
Beam Open/Closed at 104 Hz

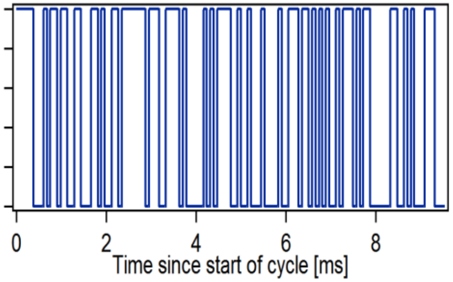
PToF



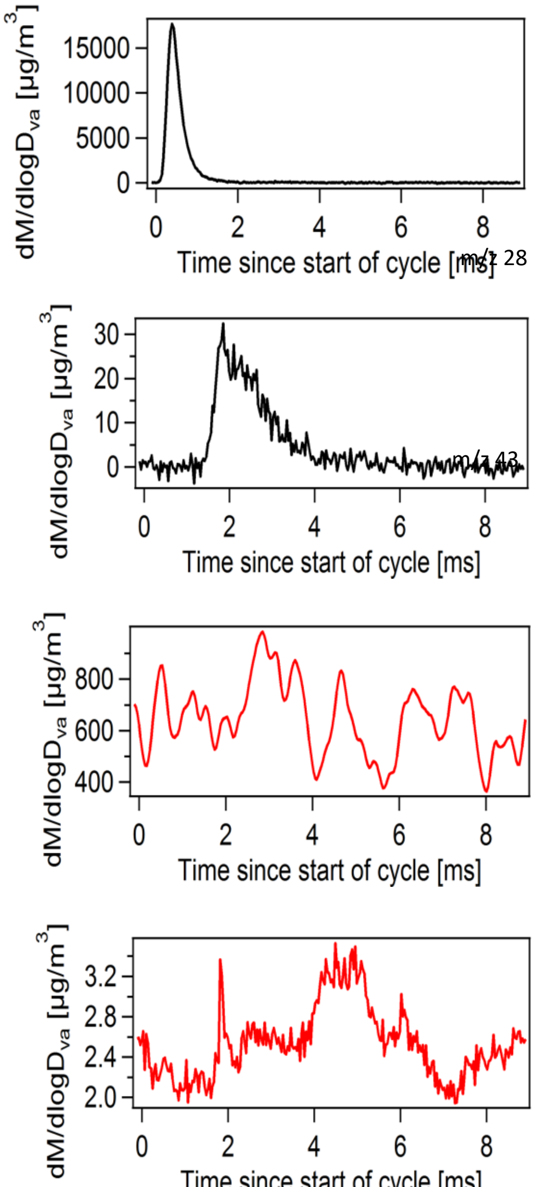


ePToF

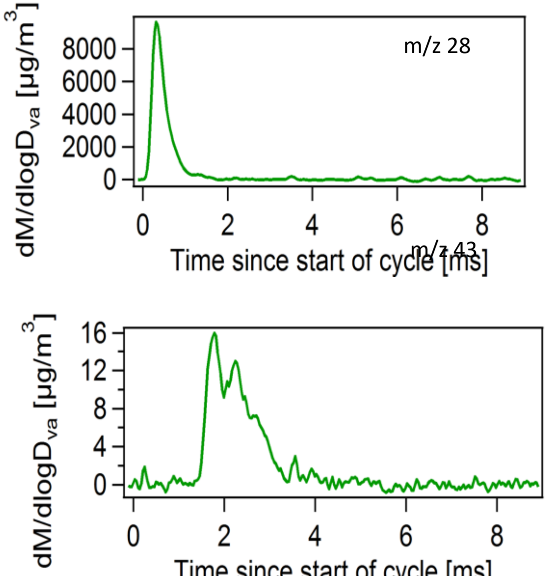




Signal as recorded



ToF after Transform (ePToF only, matrix)

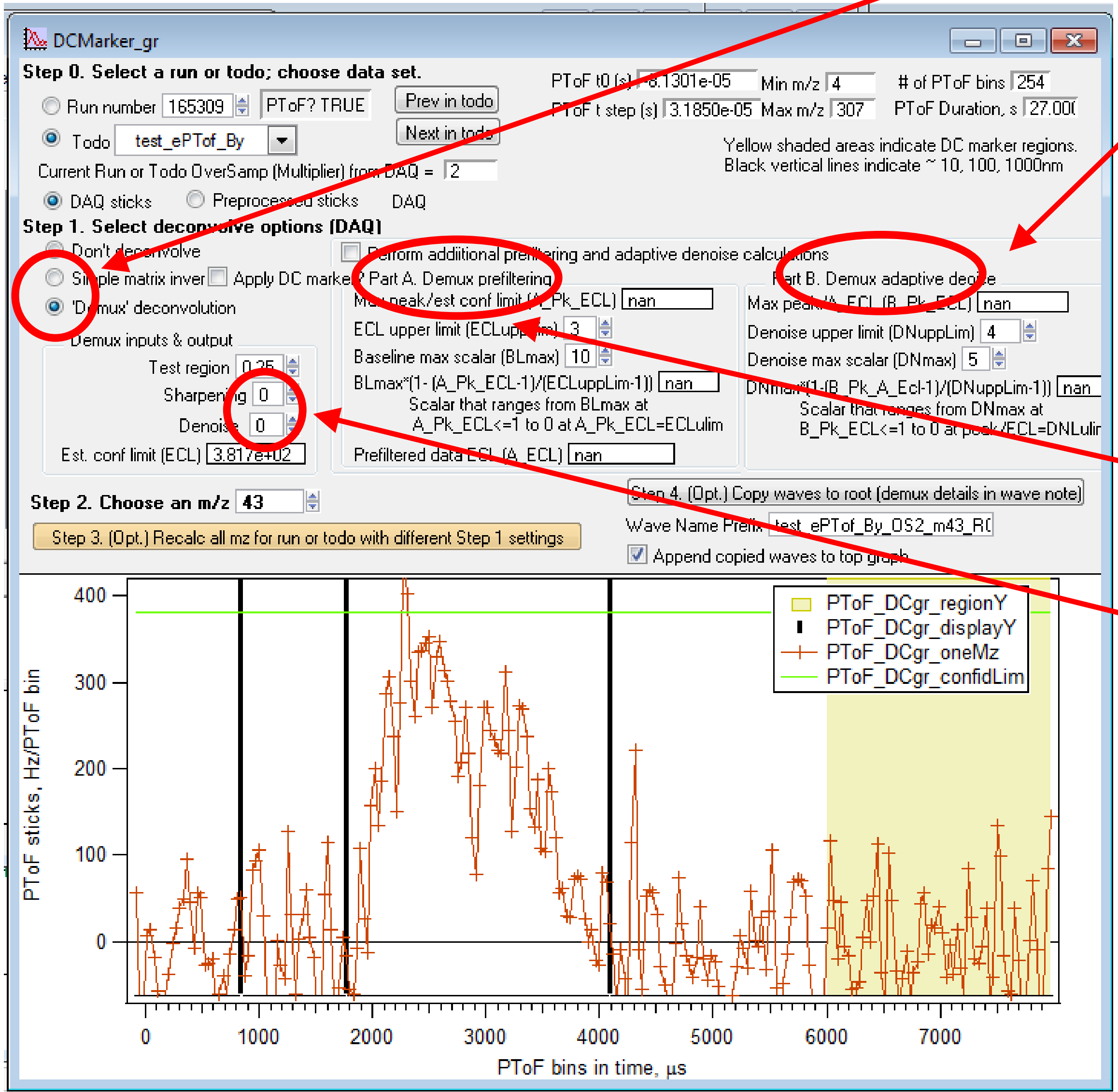


Advantages:

- Higher throughput (48% vs 1-2%)
- Better size resolution
- Run epToF/Closed mode

Originally developed for CIMS data

- Want to pull a narrow blip out of a lot of noise, and don’t care what the shape is.
- But, for AMS pToF data, signal is broad and we do care about the shape.
- Squirrel evolution: simple eptof panel → very complicated eptof panel → simple eptof panel (coming soon).



DCMarker_gr

Step 0. Select a run or todo; choose data set.

○ Run number 165309 PToF? TRUE

● Todo test_ePTof_By

Current Run or Todo OverSamp (Multiplier) from DAQ = 2

● DAQ sticks ○ Preprocessed sticks DAQ

PToF t0 (s) -8.1301e-05 Min m/z 4 # of PToF bins 254

PToF t step (s) 3.1850e-05 Max m/z 307 PToF Duration, s 27.00(

Yellow shaded areas indicate DC marker regions.
Black vertical lines indicate ~ 10, 100, 1000nm

Step 1. Select deconvolve options (DAQ)

○ Don't deconvolve

○ Simple matrix inver □ Apply DC marker?

● 'Demux' deconvolution

Demux inputs & output

Test region 0.25

Sharpening 0

Denoise 0

Est. conf limit (ECL) 3.817e+02

□ Perform additional prefiltering and adaptive denoise calculations

Part A. Demux prefiltering

Max peak/est conf limit (A_Pk_ECL) nan

ECL upper limit (ECLuppLim) 3

Baseline max scalar (BLmax) 10

BLmax*(1- (A_Pk_ECL-1)/(ECLuppLim-1)) nan

Scalar that ranges from BLmax at
A_Pk_ECL<=1 to 0 at A_Pk_ECL=ECLulim

Prefiltered data ECL (A_ECL) nan

Part B. Demux adaptive denoise

Max peak/A_ECL (B_Pk_ECL) nan

Denoise upper limit (DNuppLim) 4

Denoise max scalar (DNmax) 5

DNmax*(1-(B_Pk_A_Ecl-1)/(DNuppLim-1)) nan

Scalar that ranges from DNmax at
B_Pk_ECL<=1 to 0 at peak/ECL=DNLulir

Step 2. Choose an m/z 43

Step 3. (Opt.) Recalc all mz for run or todo with different Step 1 settings

Step 4. (Opt.) Copy waves to root (demux details in wave note)

Wave Name Prefix test_ePTof_By_OS2_m43_R(

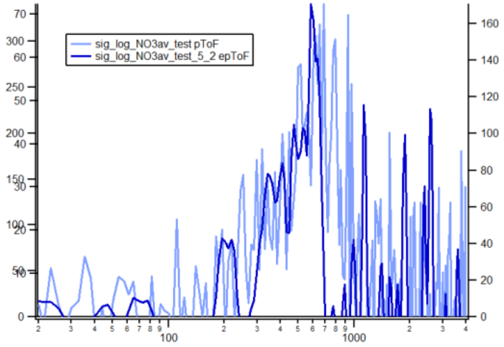
☑ Append copied waves to top graph

Simple matrix vs demux: demux makes deconvolution less noisy. ☺

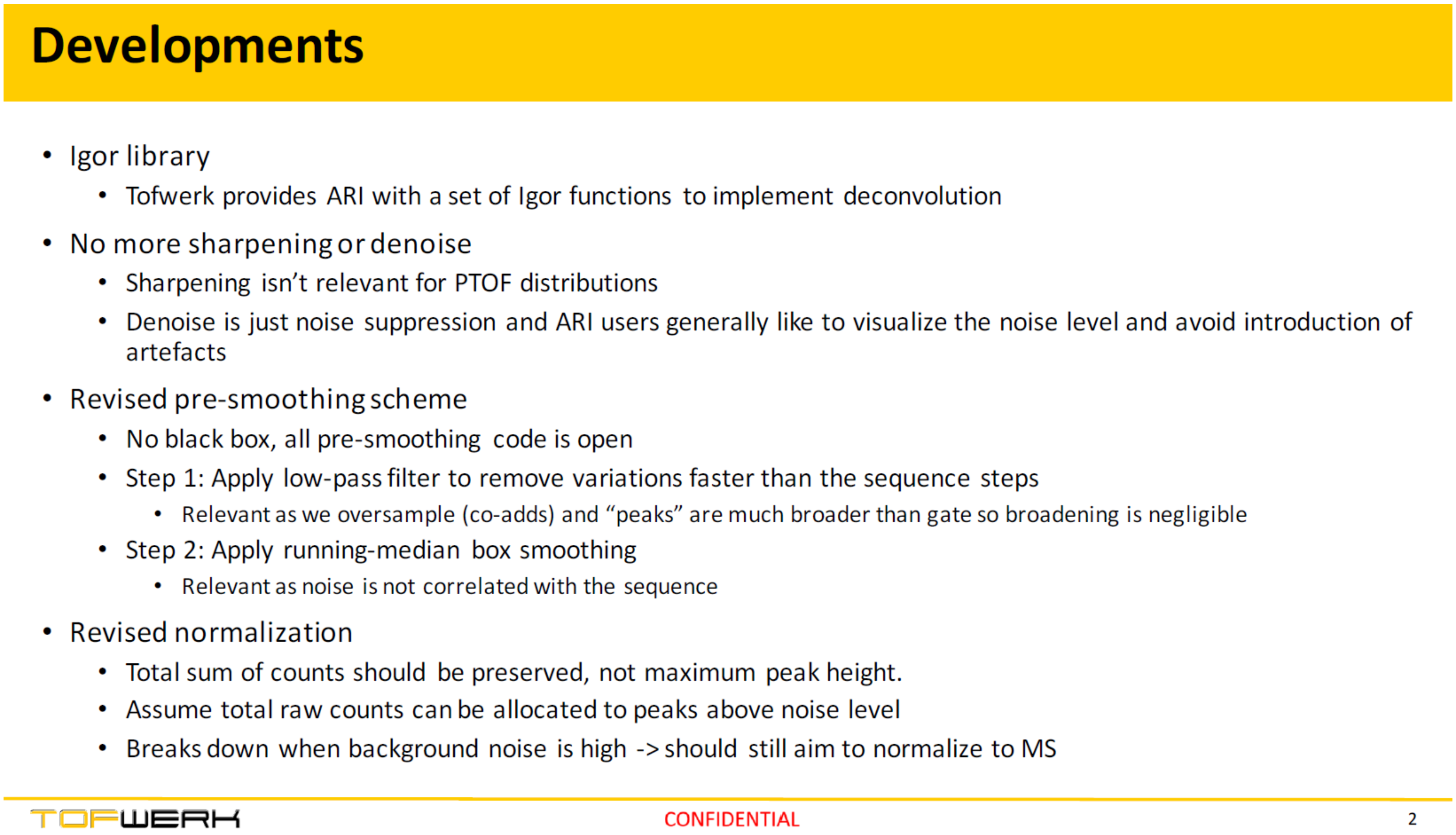
Adaptive denoise: apply different denoise to each m/z. ☹

Prefiltering: smooth before demux, reduces noise, but different degree of smoothing applied to each m/z. And air peaks included in signal-to-noise estimate. ☺ ☹

Sharpening and denoise: reduce noise, but change shape and area. ☹



New deconvolution code from Mike Cubison.

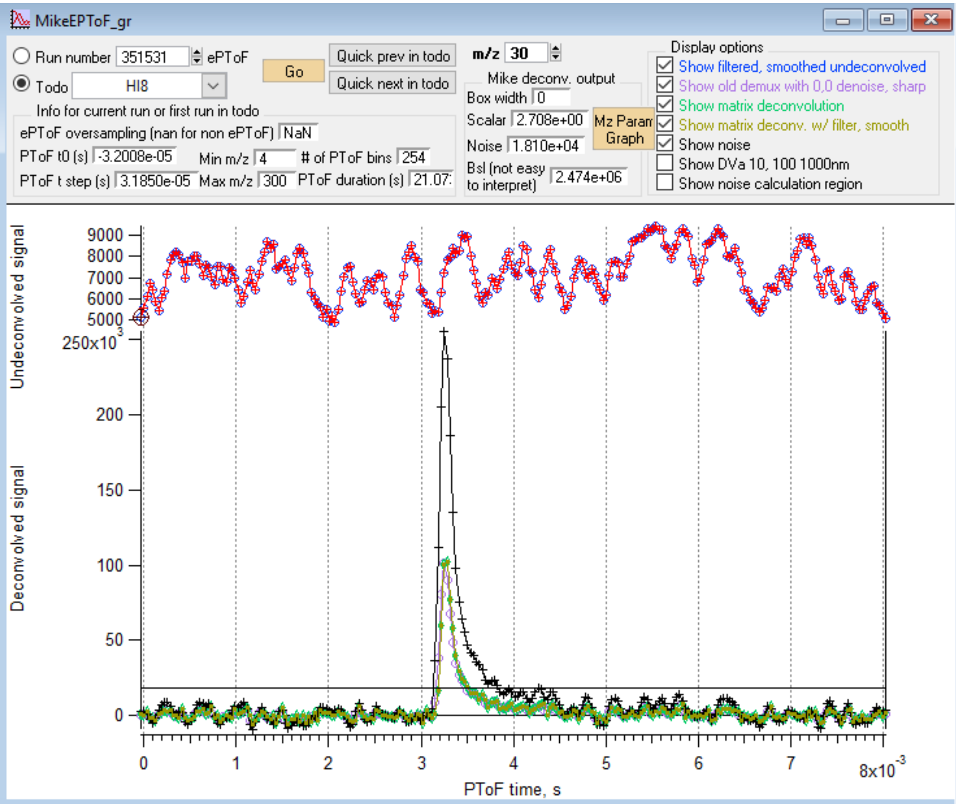


Developments

- Igor library
  - Tofwerk provides ARI with a set of Igor functions to implement deconvolution
- No more sharpening or denoise
  - Sharpening isn’t relevant for PTOF distributions
  - Denoise is just noise suppression and ARI users generally like to visualize the noise level and avoid introduction of artefacts
- Revised pre-smoothing scheme
  - No black box, all pre-smoothing code is open
  - Step 1: Apply low-pass filter to remove variations faster than the sequence steps
    - Relevant as we oversample (co-adds) and “peaks” are much broader than gate so broadening is negligible
  - Step 2: Apply running-median box smoothing
    - Relevant as noise is not correlated with the sequence
- Revised normalization
  - Total sum of counts should be preserved, not maximum peak height.
  - Assume total raw counts can be allocated to peaks above noise level
  - Breaks down when background noise is high -> should still aim to normalize to MS

New panel from Donna

- Ready soon
- Remaining issues:
  - Average runs, then deconvolve vs Deconvolve each run, then average.
  - Ion counts in background vs particle signal – difficult to allocate when background is high.
  - ALWAYS need to normalize to MS.



MikeEPToF_gr

○ Run number 351531 ePToF

● Todo HI8

Info for current run or first run in todo

ePToF oversampling (nan for non ePToF) NaN

PToF t0 (s) -3.2008e-05 Min m/z 4 # of PToF bins 254

PToF t step (s) 3.1850e-05 Max m/z 300 PToF duration (s) 21.07:

m/z 30

Mike deconv. output

Box width 0

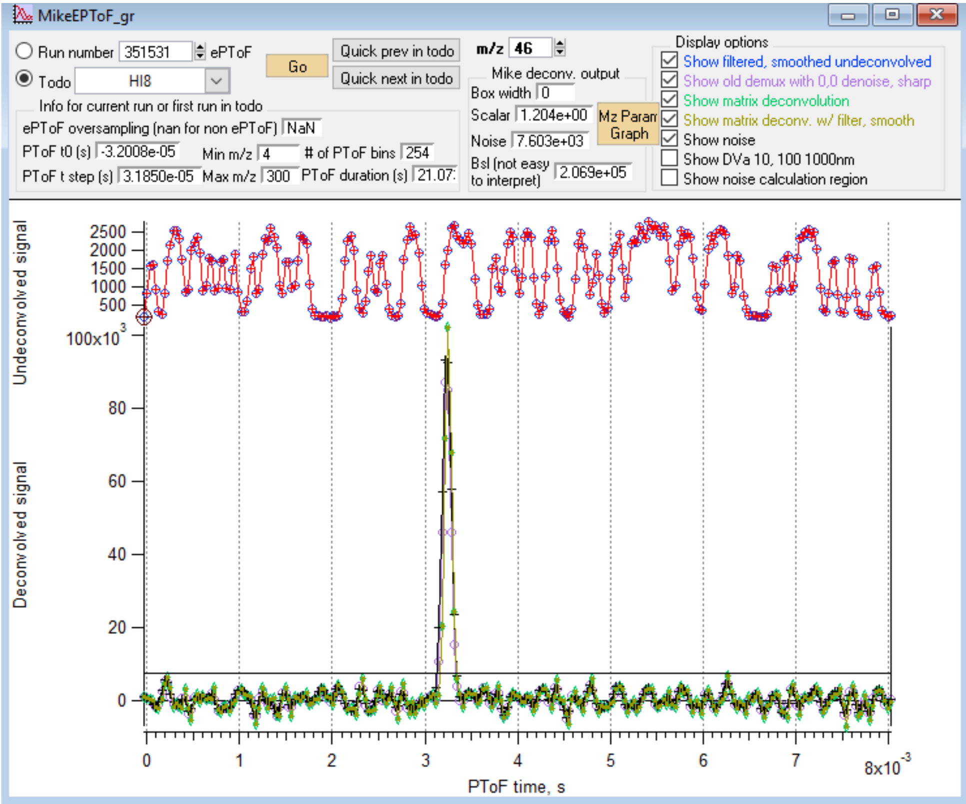
Scalar 2.708e+00

Noise 1.810e+04

Bsl (not easy to interpret) 2.474e+06

Display options

☑ Show filtered, smoothed undeconvolved
☑ Show old demux with 0,0 denoise, sharp
☑ Show matrix deconvolution
☑ Show matrix deconv. w/ filter, smooth
☑ Show noise
☐ Show DVa 10, 100 1000nm
☐ Show noise calculation region



MikeEPToF_gr

○ Run number 351531 ePToF

● Todo HI8

Info for current run or first run in todo

ePToF oversampling (nan for non ePToF) NaN

PToF t0 (s) -3.2008e-05 Min m/z 4 # of PToF bins 254

PToF t step (s) 3.1850e-05 Max m/z 300 PToF duration (s) 21.07:

m/z 46

Mike deconv. output

Box width 0

Scalar 1.204e+00

Noise 7.603e+03

Bsl (not easy to interpret) 2.069e+05

Display options

☑ Show filtered, smoothed undeconvolved
☑ Show old demux with 0,0 denoise, sharp
☑ Show matrix deconvolution
☑ Show matrix deconv. w/ filter, smooth
☑ Show noise
☐ Show DVa 10, 100 1000nm
☐ Show noise calculation region