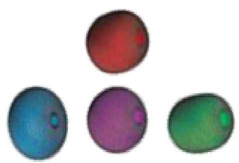
TRIUMF

Space-Charge Effects in Multiple-Reflection Time-of-Flight Devices

Alec Cannon

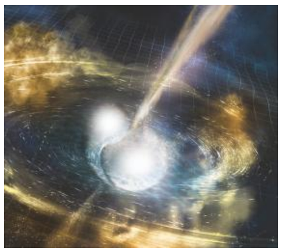
Precision mass measurements far from stability is crucial for our understanding of nuclear structure and astrophysical studies

Nuclear shell structure



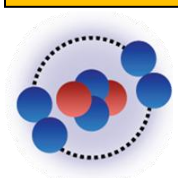
$\delta m/m = 10^{-5} - 10^{-6}$

Nucleosynthesis via the r-process

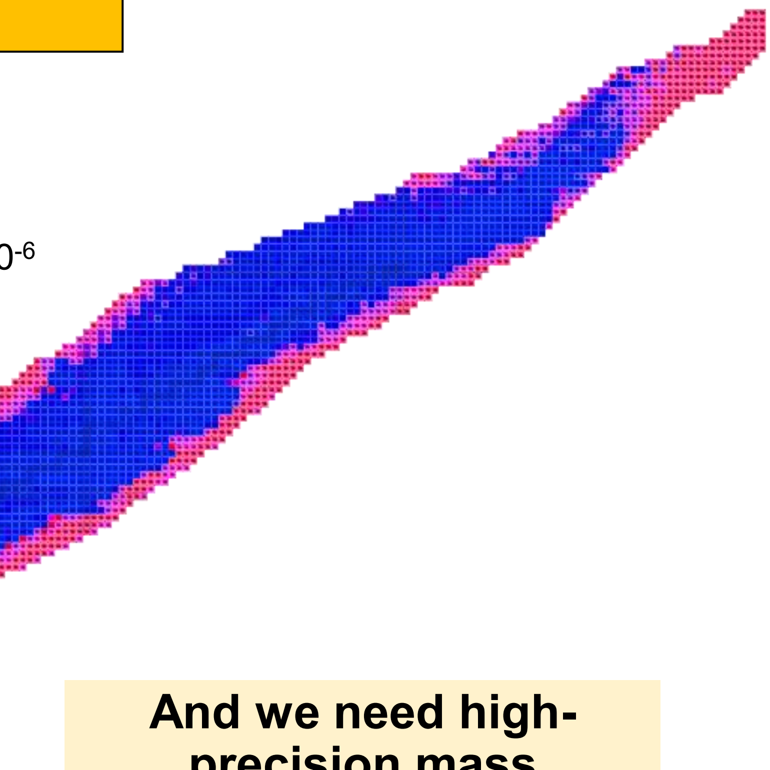


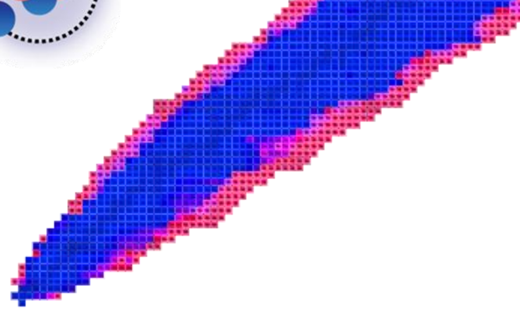
$\delta m/m < 10^{-6} - 10^{-7}$

Halos and skins



$\delta m/m = 10^{-7}$





And we need high-precision mass measurement tools !

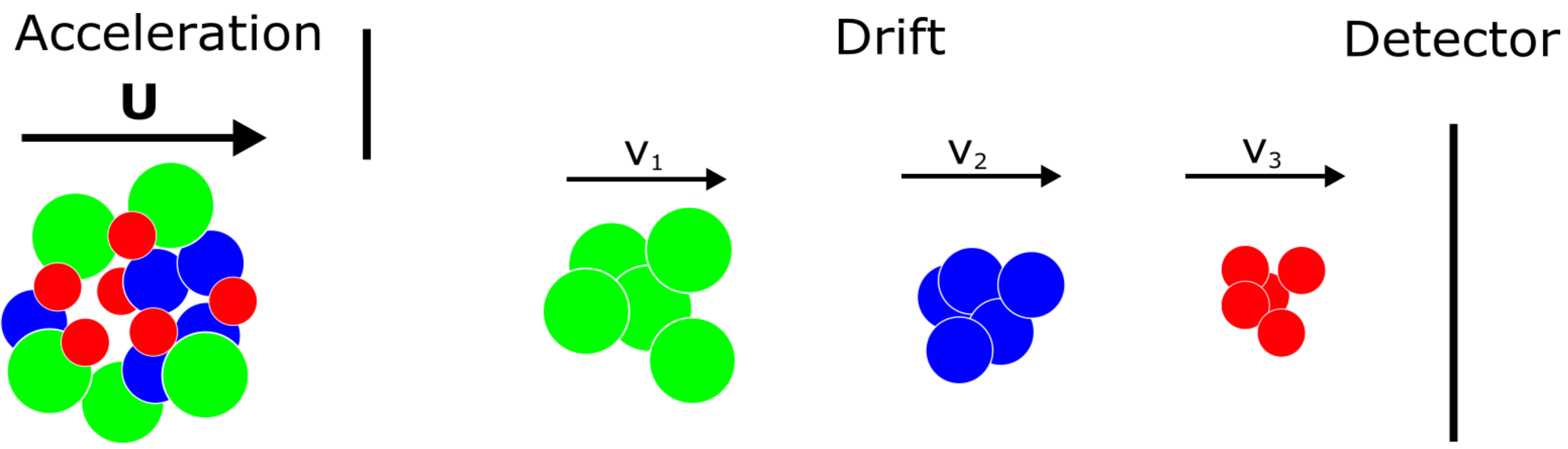
https://people.physics.anu.edu.au/~ecs103/chart/

The Universal Quest for Purity: Radioactive Ion Beams

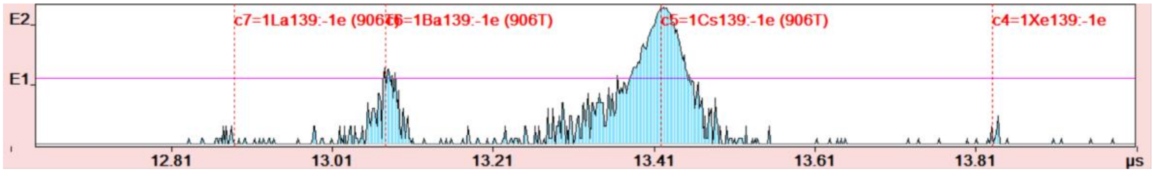
Mass Separator	Resolving Power	Max Rate	Time
Magnetic Dipole	~1E3	~1mA	Continuous
Magnetic Multipole	~1E4	~100pA	Continuous
MR-TOF	~1E5	~100 ions	~10ms
Penning Trap	~1E6	~10 ions	~50ms

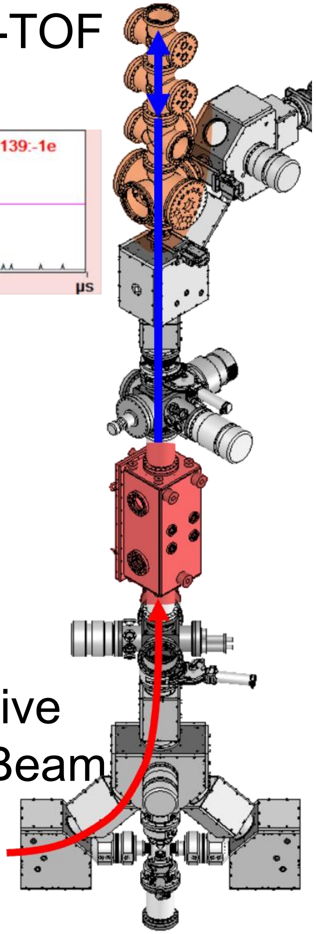
Time-of-Flight Beam Purification

- Time-of-Flight devices are used for beam purification or mass measurement
- Ions are injected with the same energy
- Different mass ions travel different speeds in the trap, $\mathrm{KE} = \frac{1}{2}mv^2 \propto \frac{1}{t^2}$
- Resolving power, $\mathrm{R} = \frac{m}{\Delta m} = \frac{t}{2\Delta t}$, on the order of 1E5

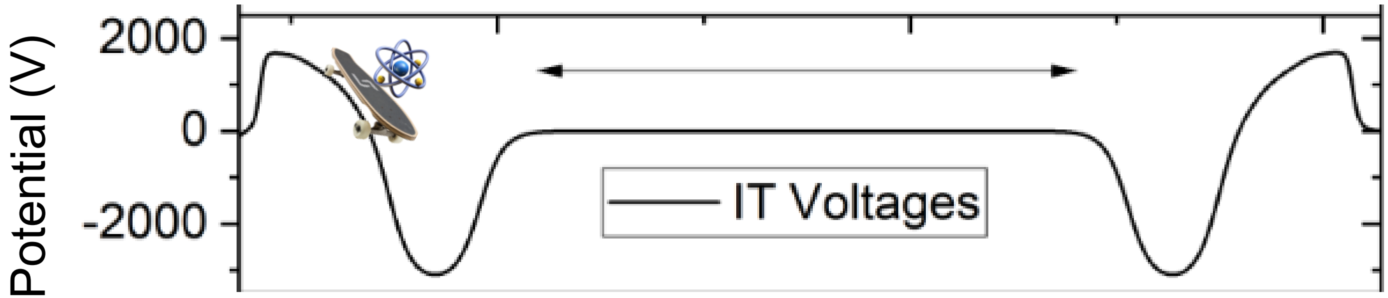


TITAN MR-TOF-MS



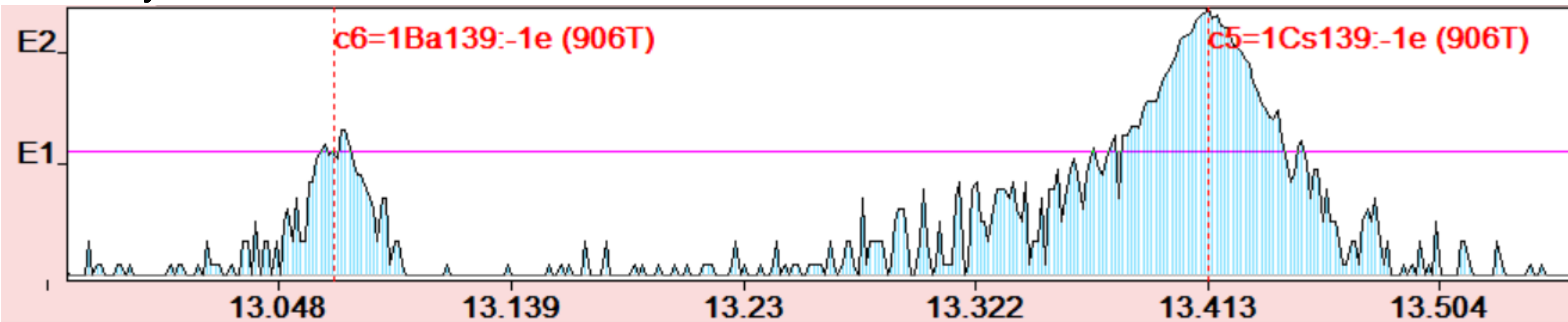


- The TITAN Multiple-Reflection Time-of-Flight Mass Spectrometer (MR-TOF-MS) measures ion time of flight
- Electrostatic Mirrors extend flight path (~1km)
- Atomic mass can then be calculated from this time of flight
- $\mathrm{R} = \frac{m}{\Delta m} = \frac{t}{2\Delta t} = {\sim}5E5$ when operated as a mass spectrometer
- Spectra are $t \propto \sqrt{m}$ vs. counts
- Useful for nuclear astrophysics and structure

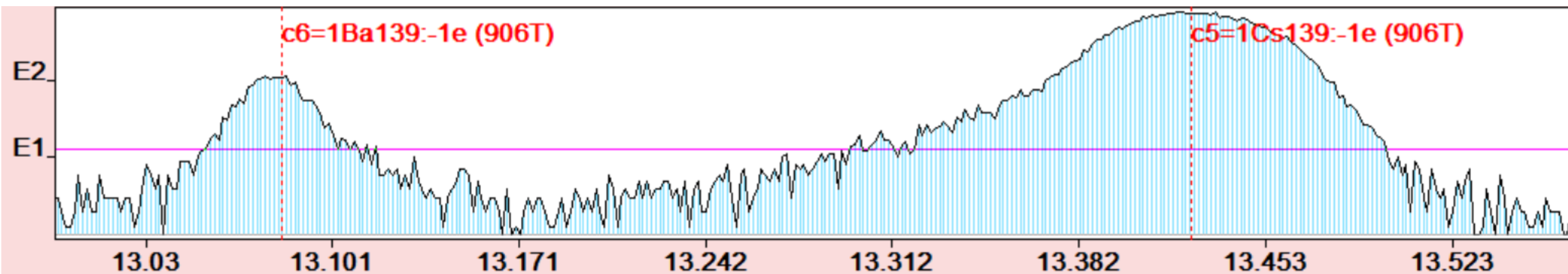


Problems with Increasing Number of Trapped Ions

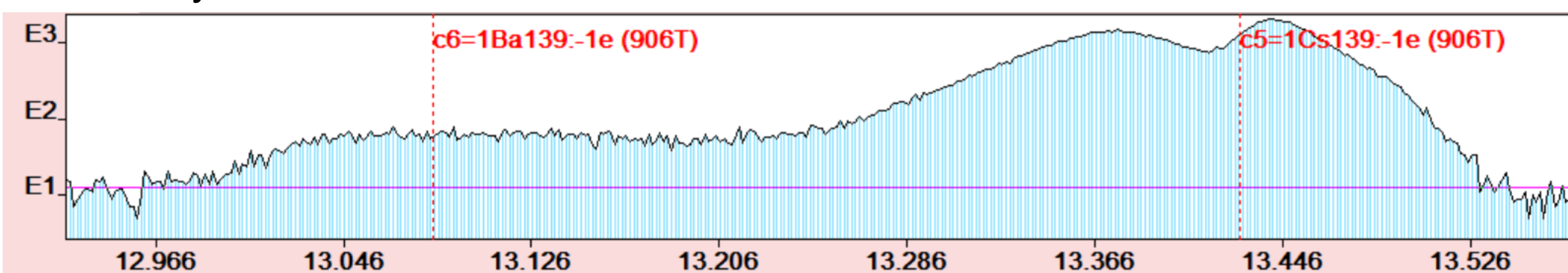
1 ion/cycle



9 ions/cycle

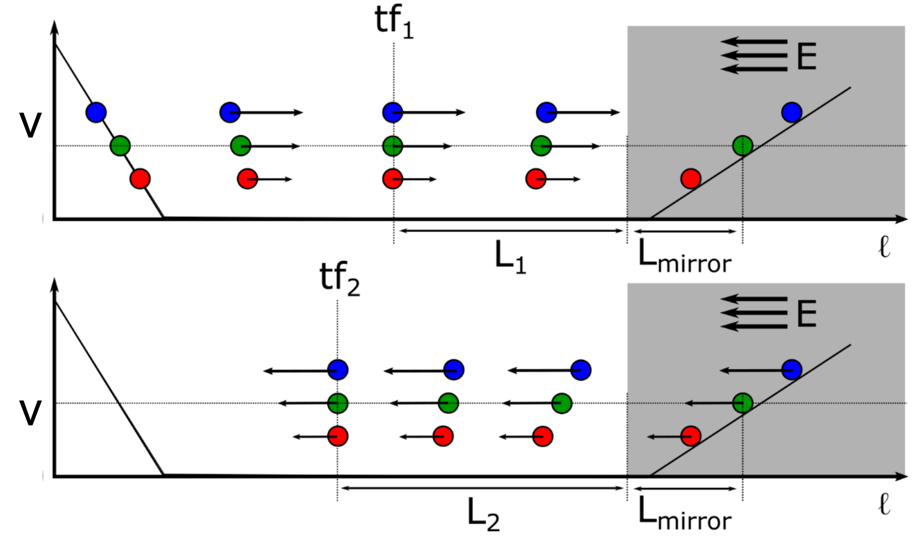


270 ion/cycle

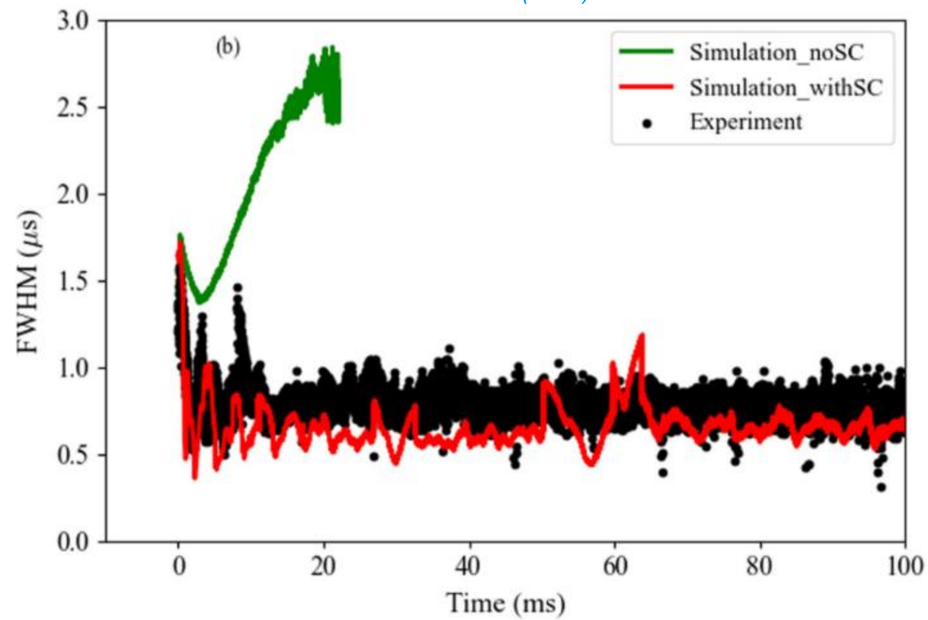


Known Problem 1:
Self Bunching

- We need to know how many ions we can measure at once in our trap
- Storing too many ions at a time causes Coulomb interactions among trapped ions
- Traffic jams in the mirror electrodes forces ions together
- This deviation makes mass measurement unreliable
- **Key variable: interaction time**



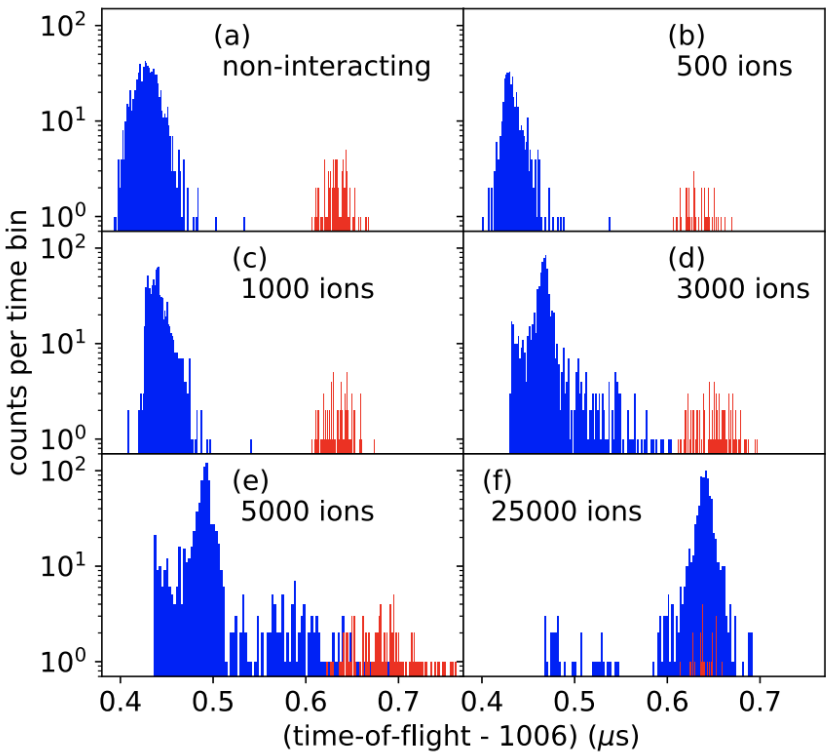
A. Jacobs, PhD. Thesis, University of British Columbia (2023)



D. Gupta et al., Phys. Rev. E **104**, 065202 (2021)

Known Problem 2: Peak Coalescence

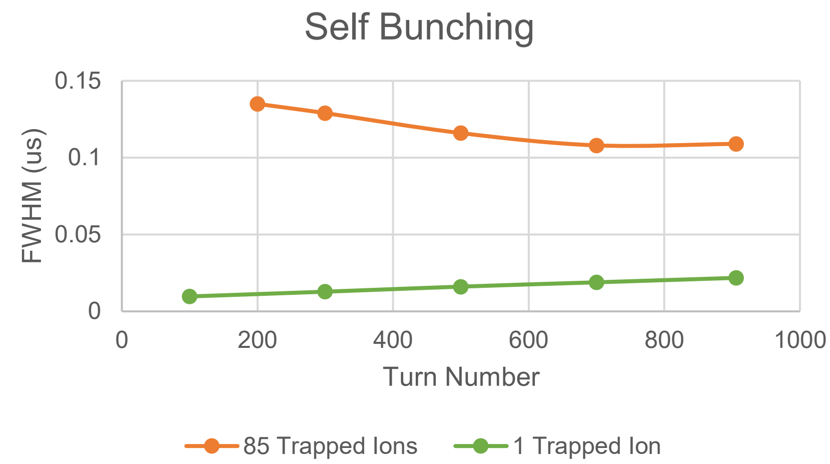
- Similar to self-bunching, too many ions creates space-charge effects for multiple species
- Peak coalescence happens when the self bunching of 2 different ion peaks causes them to merge
- Effect is stronger the closer in mass
- This makes mass separation unreliable
- **Key variable: trapped ions**

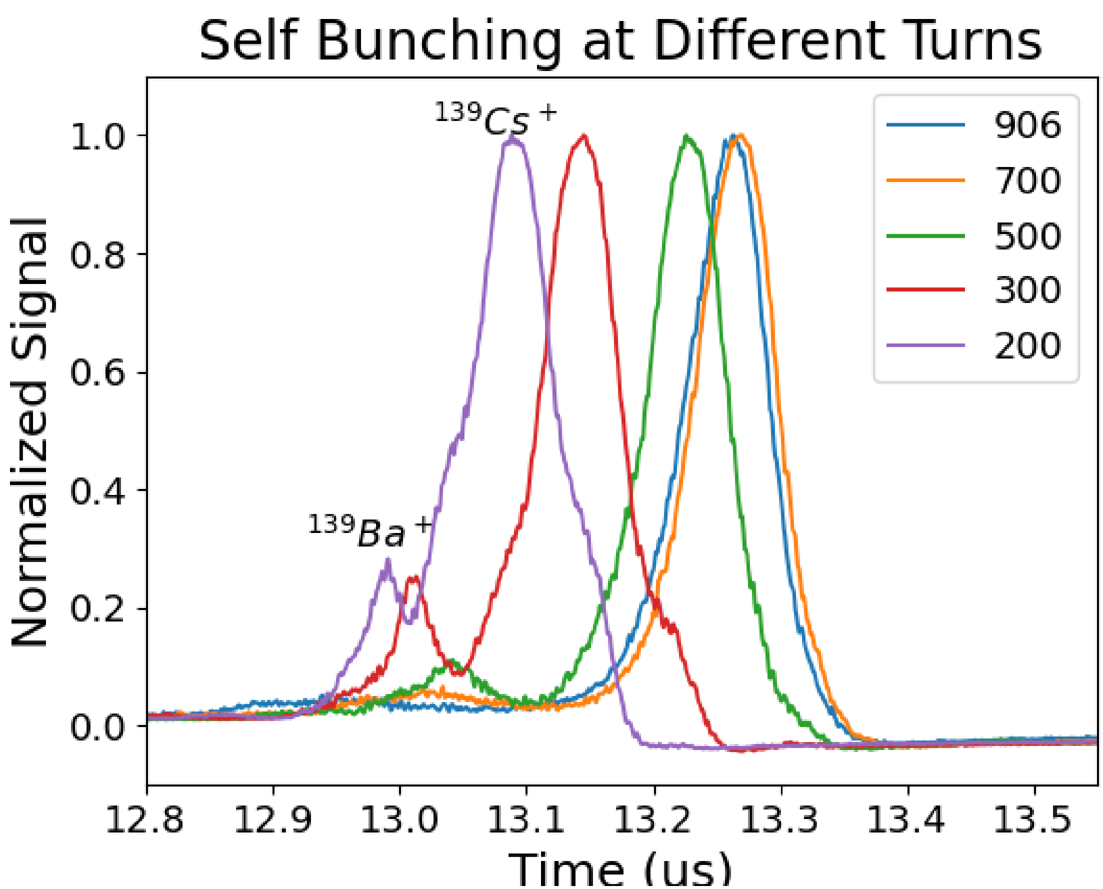


F. M. Maier et al., Nucl. Instrum. Methods. Phys. Res. A 1056, 168545 (2023)

Measurements of Self Bunching vs Time

- Each turn takes ~23.2μs
- 85 simultaneously trapped ions
- Should trap less than 20 ions simultaneously
- **20x more than current operation**



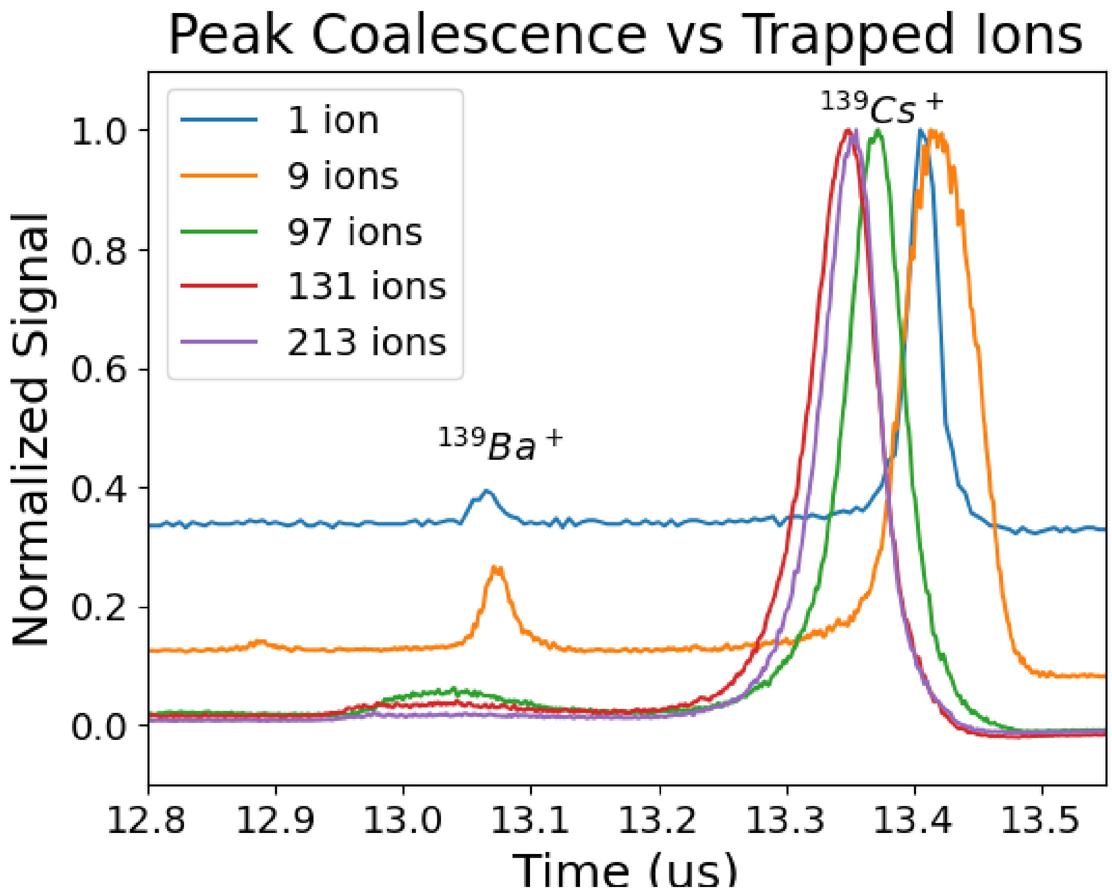


- Bunch width of $^{139}Cs^+$ with increasing interaction time
- Self-bunching hinders accuracy during analysis
- Can still function as mass separator for high rates with low interaction time

Alec Cannon

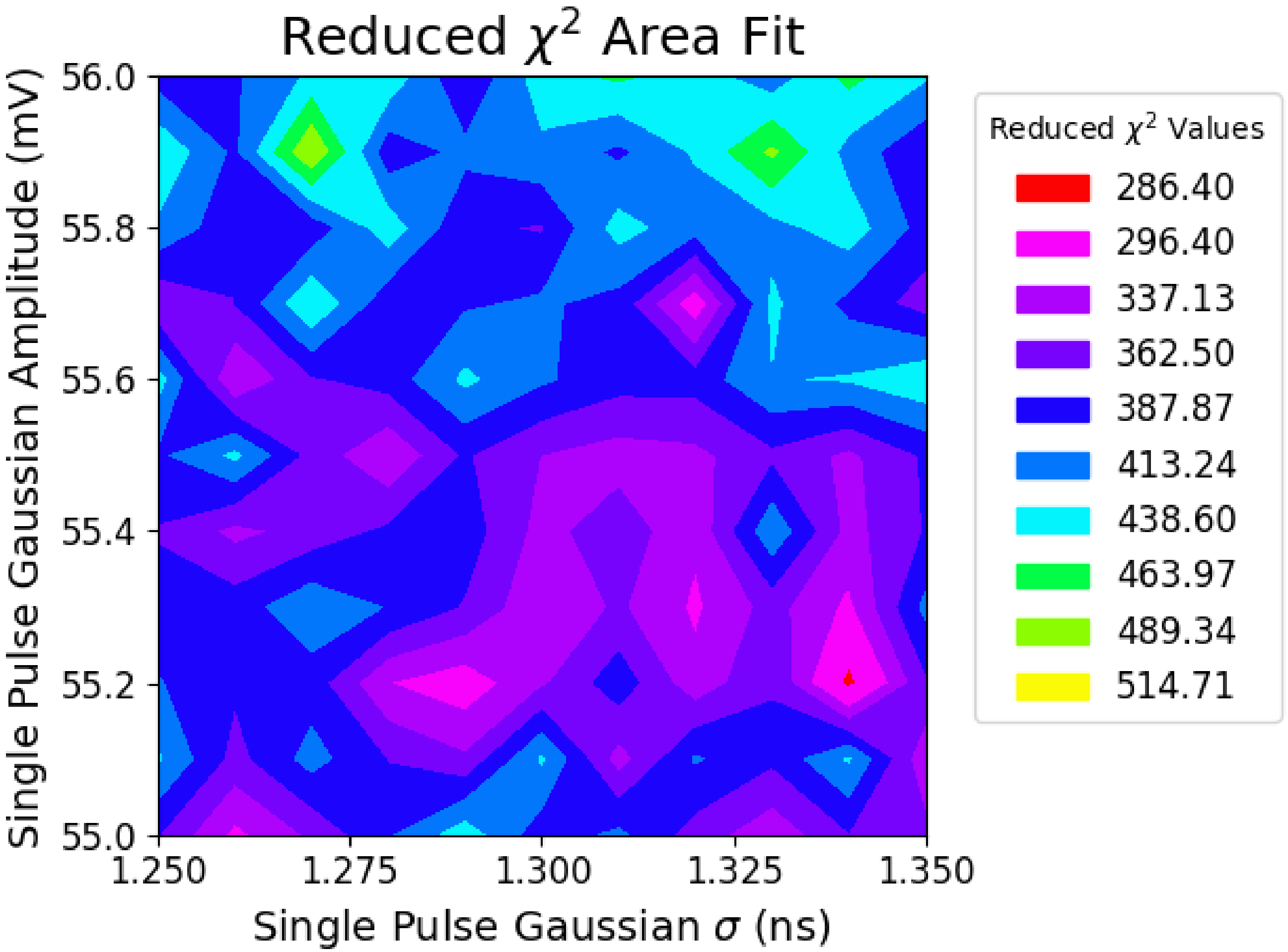
Measurements of Peak Coalescence vs Ion Rate

- Data taken for maximum interaction time
- **$^{139}Ba^{+}$ peak could be missed entirely or an inaccurate measurement made with this data**



Simulations Probing Detector Response for Space-Charge Studies

- Detector Deadtime means we need to calibrate to signal area
- Simulation reproduces spectra
- Scans individual ion amplitudes and widths

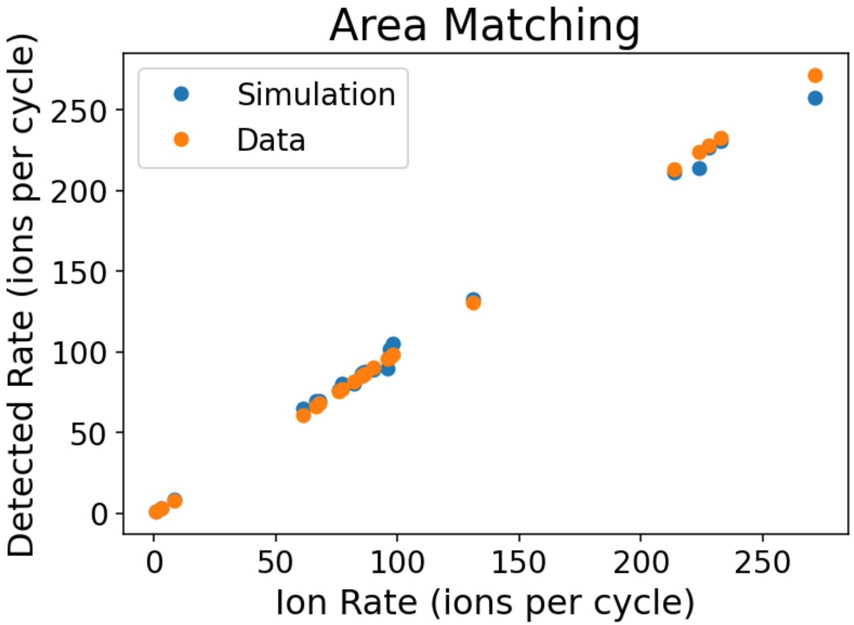


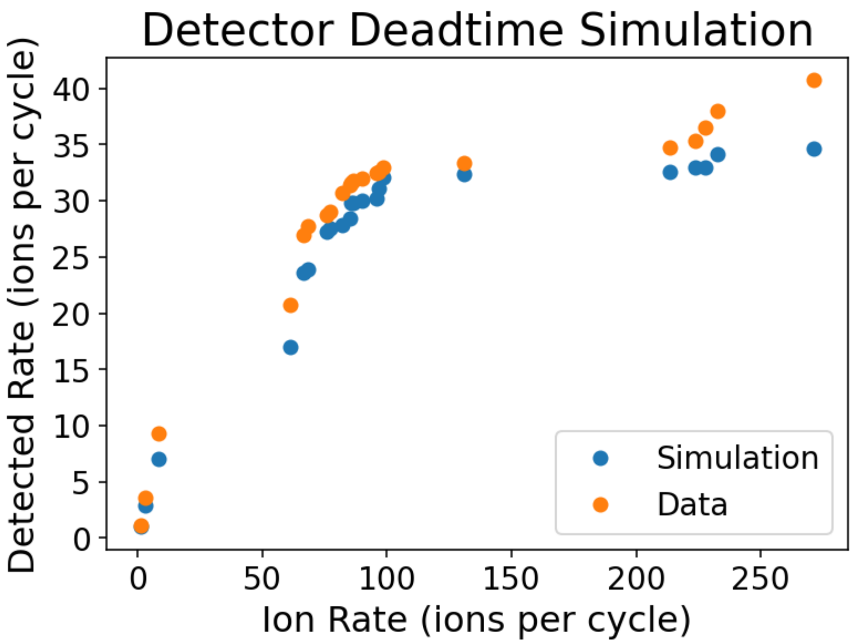
Simulation Results

- Amplitude of 55.2mV and width of 1.34ns reproduces both datasets (single counts and signal area)

- Detector begins to undercount at around 20 ions per cycle

- **Adjusting the detector threshold could help avoid deadtime at higher rates**





Summary

- MR-TOF devices are powerful mass separators and spectrometers
- Too many trapped ions causes self bunching and peak coalescence
- These space charge effects make mass separation unreliable, limiting the rate MR-TOF devices can effectively process
- The TITAN MR-TOF can handle ~20 trapped ions

Outlook

- Accept higher rates to measure faster
- Adjust threshold to keep detector from deadtime

TRIUMF is located on the traditional, ancestral, and unceded territory of the xʷməθkʷəy̓əm (Musqueam) people, who for millennia have passed on their culture, history, and traditions from one generation to the next on this site.

TRIUMF's home has always been a seat of learning.

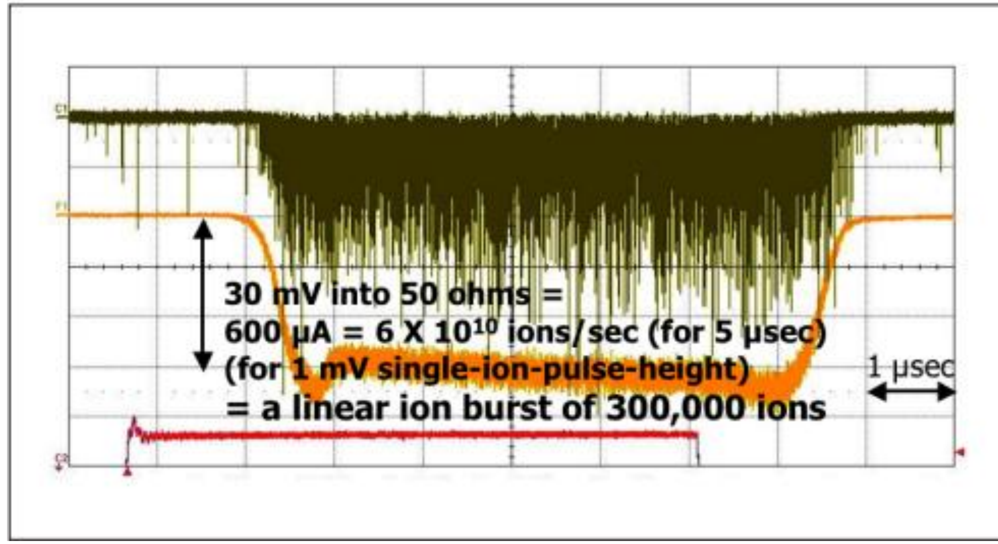
TRIUMF
University of Manitoba
University of Calgary
McGill
University of Notre Dame
Oak Ridge National Laboratory
Justus-Liebig-Universität Giessen
Central Michigan University
Max-Planck-Institut für Kernphysik Heidelberg
university of groningen
kvi - center for advanced radiation technology

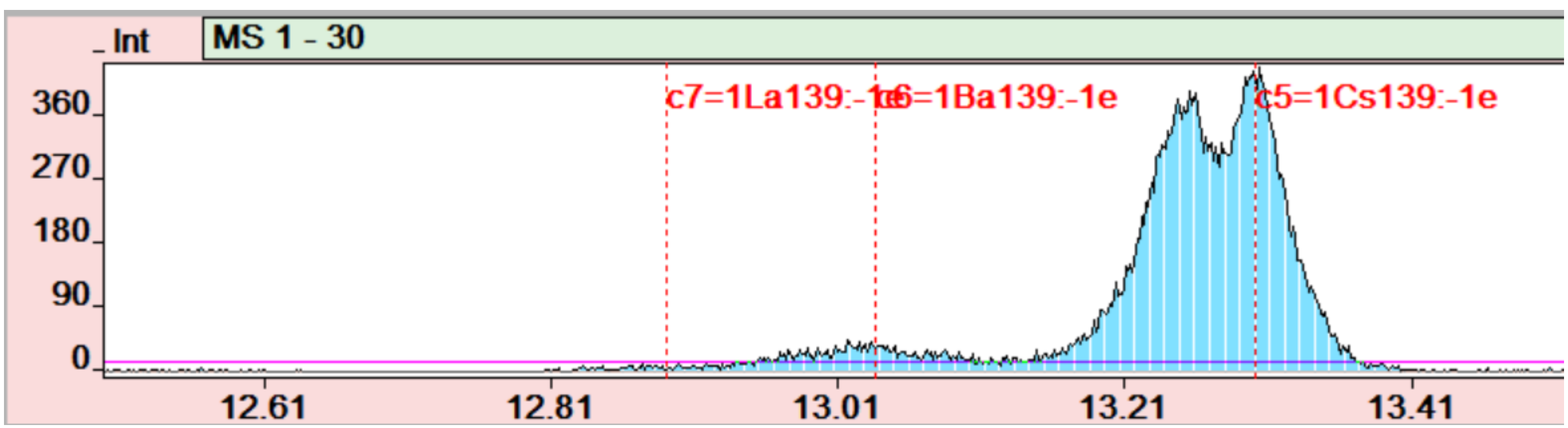
SFU
University of Victoria
The University of Edinburgh
cnrs
Colorado School of Mines

NRC CNRC
NSERC CRSNG
DFG Deutsche Forschungsgemeinschaft

Detector Problem

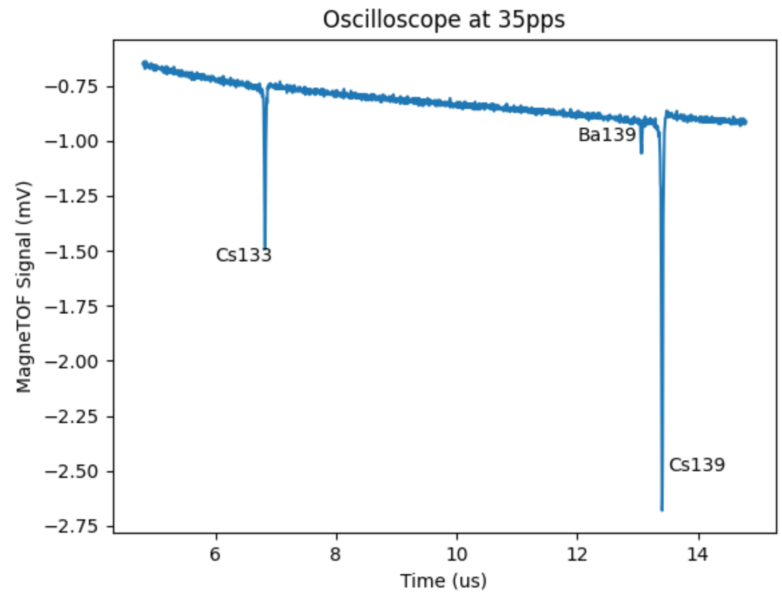
- Measuring high rates makes it impossible to singly count all the ions
- The detector begins to see continuous beam, leading to deformed peak shapes
- Instead, signal area is calibrated to singly counted ions

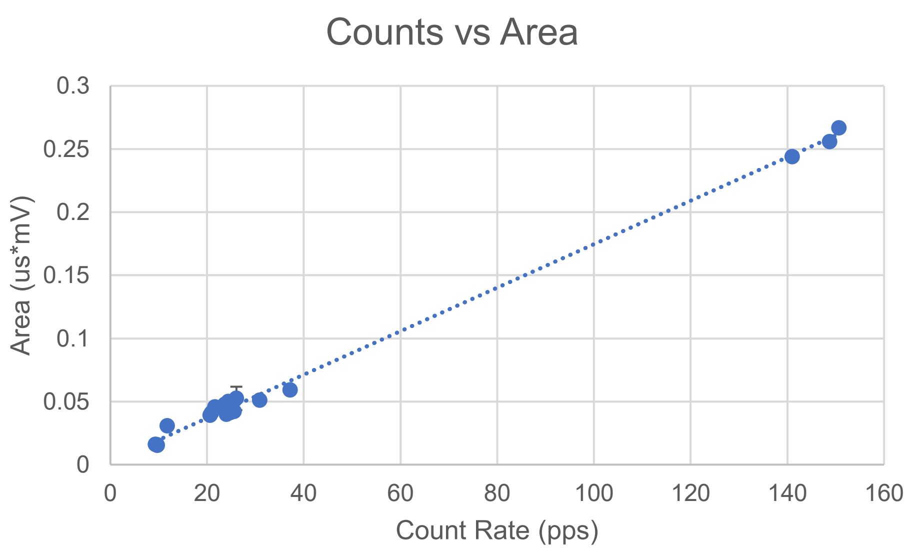




Oscilloscope Calibration

- Using summed Gaussians with a linear or constant background
- Area of the peak is calculated by integrating the fitted function with the trapezoid method and subtracting the manually integrated linear background
- Uncertainty is calculated via error propagation with the uncertainties of each parameter given by the lmfit model





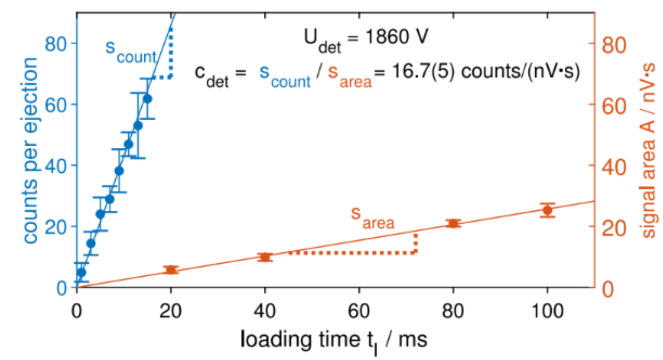


Fig. 7. Ion signal as a function of the loading time, for $U_{det} = 1860\,V$ evaluated with single-ion counting (blue) and signal integration method (orange). For the single-ion counting, a discriminator of 20 mV is used. The calibration factor c_{det} can be calculated as the quotient of the slopes of the fitted lines, where s_{count} is the slope of single-ion counting and s_{area} that of signal-integration evaluation.

F. Simke et al., Int. J. Mass Spectrom. 506 (2024) 117337

Simulation Procedure

Metropolis algorithm MCMC sampling for given probability distribution function

1) Generate random point (x)
2) Generate random jump from point (w)
3) If PDF(w)>PDF(x), accept w as a point
4) If PDF(w)<PDF(x), accept w with probability PDF(w)/PDF(x)
5) If accepted, set x=w and repeat

With this, we can estimate the individual ion pulse heights and widths.