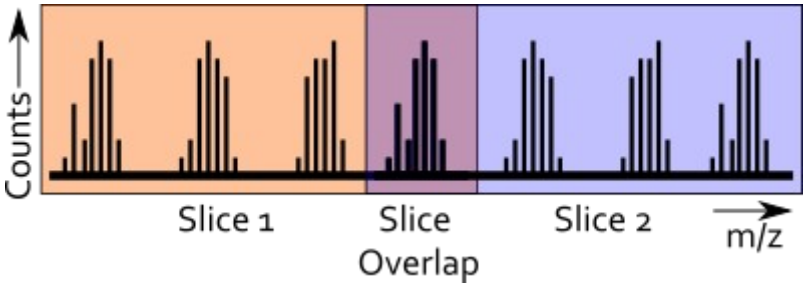
Spectrum Patching



Problem

High Resolving power requires High turn number.
The resulting spectrum has overlapping Turn numbers or a narrow mass range (~3 u).
Just changing the mass center setting and slapping spectra (*slices*) together can bear problems:

1. Manually changing settings hundreds of times (200 u – 700 u in 3 u steps)
2. suppression via RFQ/TTL setting
3. Missmatching calibration
4. change in ion rates changes abundances in between slices
5. suppression in slice border regions
6. double-counting in slice overlap

Data Acquisition per Scan

The MAc voltage optimizer can control TTL and Voltage-Controller values.
For mass scan, one simply has to set up a variable *vara* to control

1. analyzer-center mass (TTL)
2. MRS center mass (TTL)
3. IonGuide (RF Amplitde to pseudopot),
4. Mass filter (RF Amplitude to q value),
5. Cooler (RF Amplitude to Pseudopot)
6. Trap (RF Amplitude to pseudopot).

Voltagecontrol inputs can be calibrated to actually applied RF amplitudes.
Then in Mac optimizer, *vara* is the new center-mass for each iteration.

This setup fixed problem 1 (manually adapting) and 2 (suppression via RFQ/TTL).

The Analysis output is not important. The resulting tof-file has a different setting for each MS, with only the latest spectrum having a correct mass-axis. A simple summed spectrum does not make sense.

Restoring time information

Instead, the Spectra are exported to textfile as matrix (rows = time-bin, column=spectrum, cell=counts).

In an external script each column is separated, a start-time depending on *vara* is added (calculated from TTL or noted in optimizer file) and the resulting total-tof axis calibrated with (a, t_0, b) from MAc.

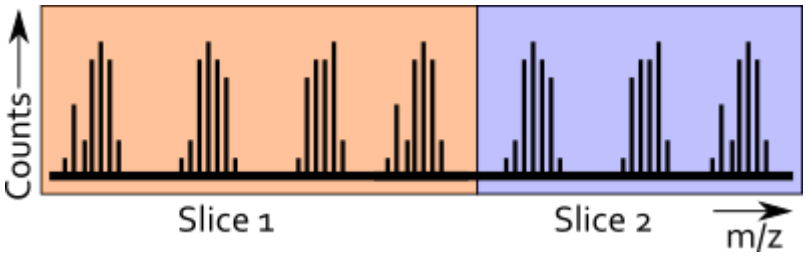
In case calibration is not sufficient, in this stage calibration can be re-done for slices close to calibrant masses (for example tuning Solution 118, 322, 622, 922).

Patching and rescaling

There are different approaches how to scan and patch

1. Simple Patch

The simplest solution. Slices don’t overlap and fit next to each other
After each slice is calibrated, just sum up all events of all slices into a single histogram.

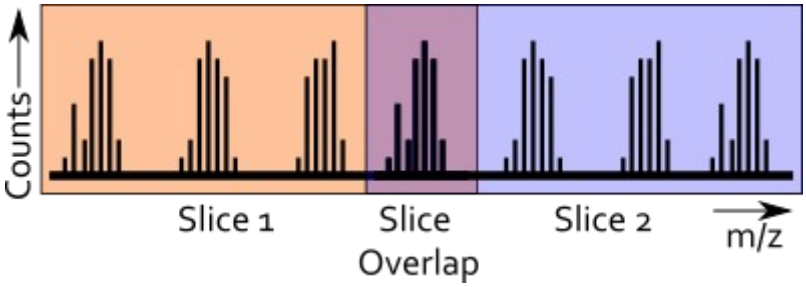


Problems:

- Intensity variations make abundances between slice 1 and 2 incomparable.
- MRS/Analyzer Mirror/Good region might suppress ions close to slice border

2. Border Overlap Patch

The scan is done so there is an overlapping region.
This region serves as reference. Counts in the right spectrum are normalize to fit the left ones.
Normalization can be done with total ion count in the overlapping region.



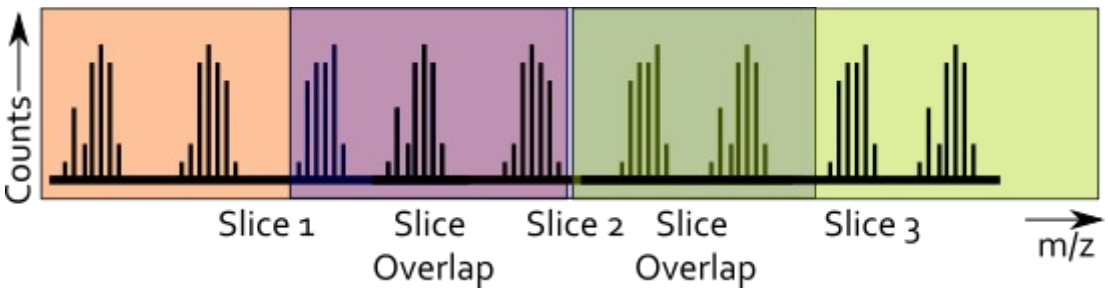
This counters most intensity variations (except signal loss and signal drowning).

Bad-regions can be moved into or even behind the analyzed overlap.
Effects of analyzer-opening or bad regions might still be visible outside overlap.

Simply adding up double-counts ions in overlap-region.
To solve this, One can cut off light masses on right-hand slices.

3. Full Overlap Patch

Two neighboring slices completely cover the center one



This offers full information to eliminate intensity fluctuation and bad-region effects.
Biggest downside is doubling the scan-count.