Universität Bremen

BRUKER

Fabian Schönfeld
Petr Shulpyakov

Center for Industrial Mathematics

Faculty 03

Automatic Tuning of Mass Spectrometers

Mass Spectrometry and Ion Optics

- Mass spectrometers: measure molecular masses in sample
- Measuring time of flight of ionized particles
- Flight path influenced by electric fields
- Voltages of fields need tuning to obtain high quality mass spectra

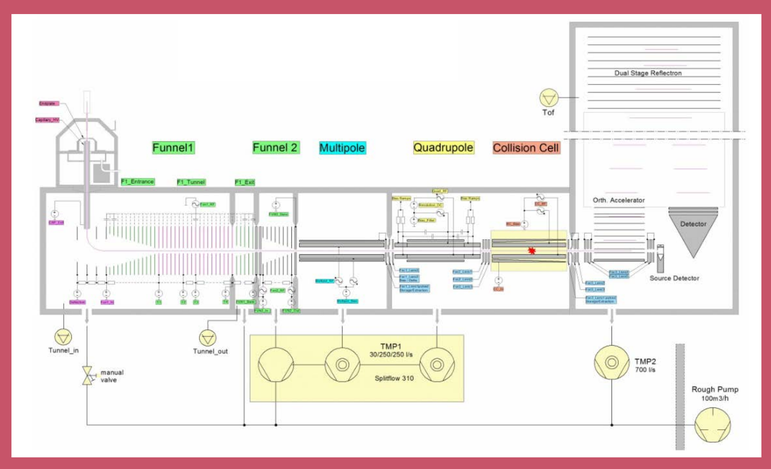


Fig. Schematic of Time-of-Flight mass spectrometer

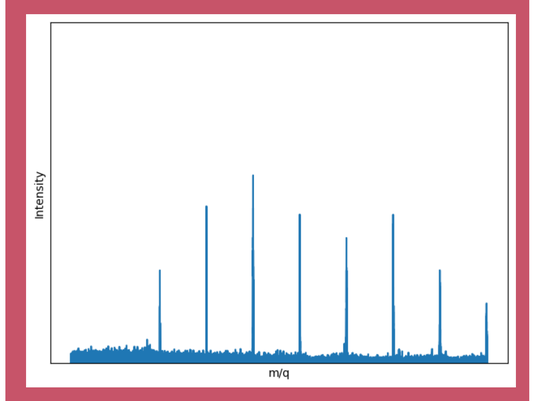


Fig. Mass spectrum

Tuning is performed by trained test field engineers

- labor hours of qualified personnel
- requires expert knowledge
- no guarantees for optimality

Tuning algorithm

- Minimal labor hours required
- Minimal prior experience required
- Finds optimal solution using mathematical algorithms

Optimization Problem

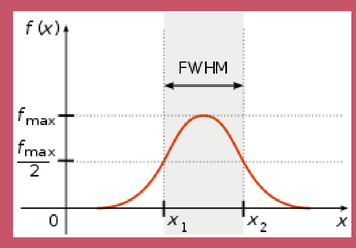
- Tuning of mass spectrometer evaluated based on resulting spectra
- Optimization problem: optimize tuning criterion based on output spectrum (depending on tuning parameters)

$$\max_{p \in \mathbb{R}^n} F(S(p))$$

p: Tuning parameters
S: Spectrum
F: Tuning criterion

Possible tuning criteria:

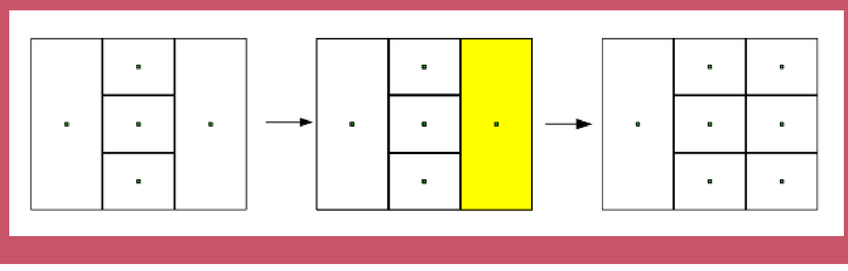
- Intensity of highest peak
- Resolution of highest peak
- Intensity/resolution of specific peak
- Average resolution over multiple peaks



Resolution: peak value / width of peak at half peak height

Optimization Algorithm

- Dividing Rectangles Algorithm used to solve optimization problem
- Algorithm divides search region into subsets, evaluates potentially optimal regions and subdivides further



Procedure:

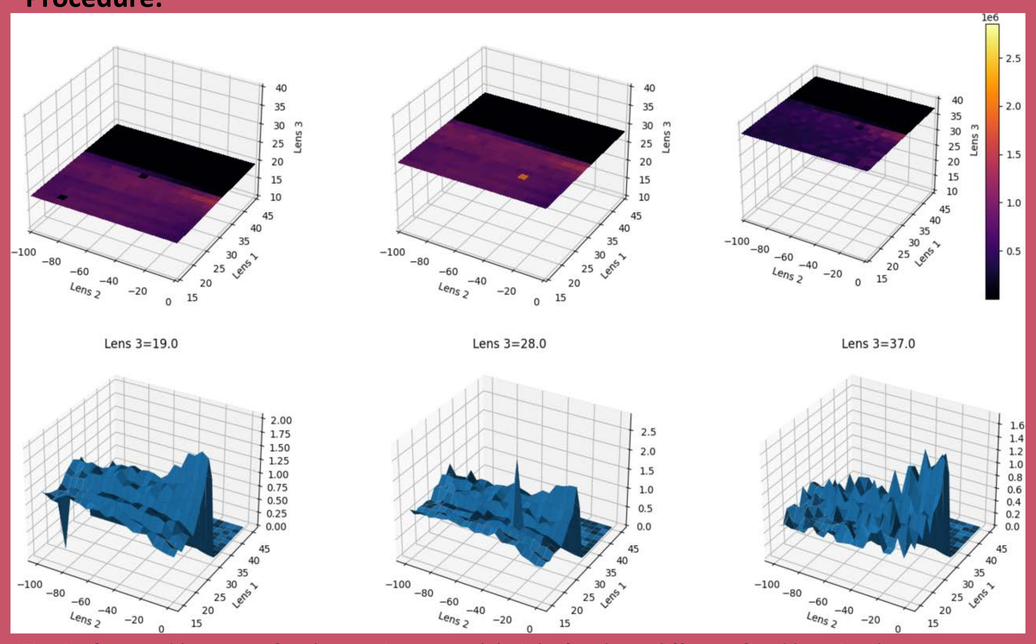


Fig. Surface and heatmap for the maximum peak height for three different fixed lens 3 voltages

First 3 Independent Parameters:

- Start optimizing voltages with respect to maximum-peak height and resolution for a group of 3 ion lenses
- Multiple recordings of spectra on grids with various resolutions.
- Visualization of recorded data
- Analyzing data with respect to maximum peak height and resolution
- Testing non-gradient based global optimization algorithms on recorded data
- Tuning/optimizing with respect to resolution not sensible

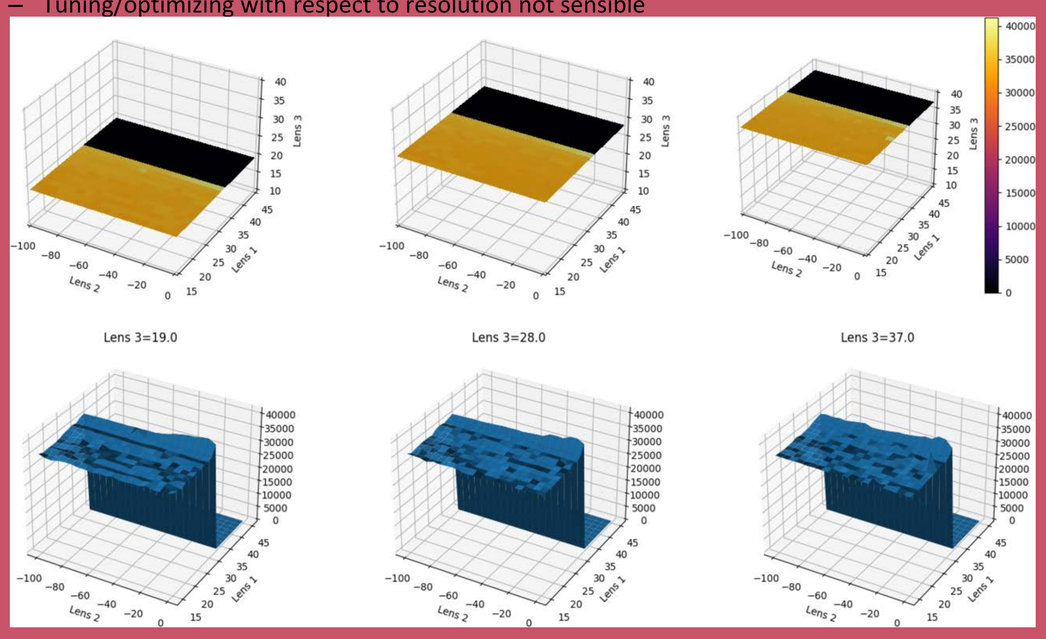


Fig. Surface and heatmap for the maximum peak resolution for three different fixed lens 3 voltages

Second 3 Interdependent Paramters:

- Multiple recordings of spectra on grids with various resolutions
- Visualization & Analyziation of recorded data
- Coordinate transformation with Principle Component Analysis (PCA)
- Testing non-gradient based optimization algorithms on recorded data

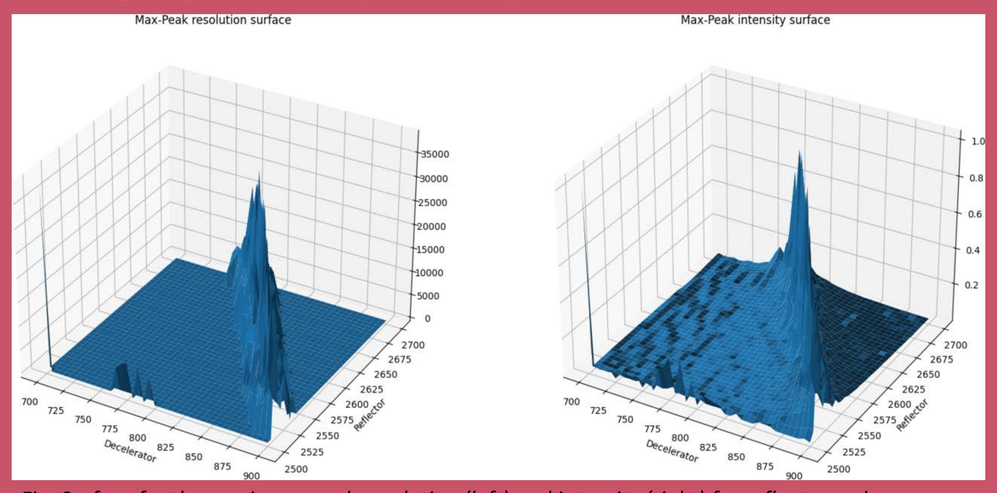


Fig. Surface for the maximum peak resolution (left) and intensity (right) for reflector and decelerator voltages

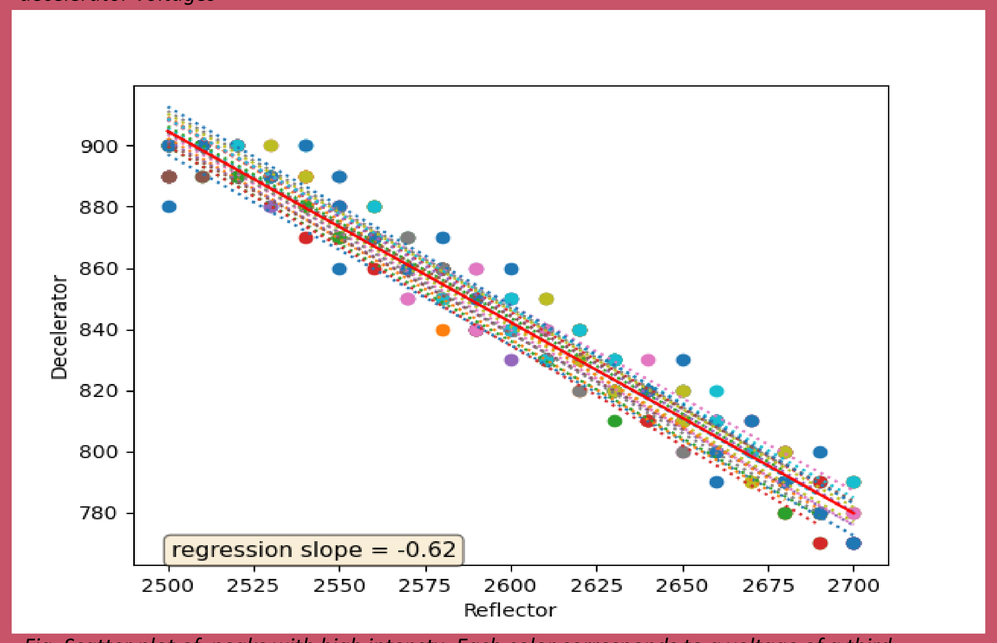


Fig. Scatter plot of peaks with high intensty. Each color corresponds to a voltage of a third parameter

Results on real timsTOF devices:

- At first unsufficient results with respect to resolution and max-peak height
- With increased settling time and decreased spectra rate the algorithm is able to find high resolution and high intensity spectra even if the device was mistuned.