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Facility for Optimization of Mass Spectrometers

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Abstract

A semi automatic facility for the optimization of mass spectrometers (or more generally space instruments) is presented. Complexity and requirements on performance of space instruments is increasing. Utilizing optimization algorithms decreases the amount of work and time dedicated to the fine-tuning of these instruments on ground and, even more important, in space. Computer based optimization typically outperforms manual tuning of the instrument in both time consumption and final instrument performance. The optimization method presented can be used from designing the hardware to finding the optimal voltage parameters, be it in the first test phases or even during flight in case of degradation of the sensor performance due to anomalies or simple aging. Increase in performance is shown on three different time of flight mass spectrometers e.g. the RTOF instrument on board the ESA mission Rosetta.

1. Introduction

Adaptive Particle Swarm Optimization (APSO) was introduced by Zhan [1]. It belongs to the direct search methods used to find a global maximum in a multidimensional search space. The swarm consists of several solution candidates, referred to as particles. The quality (fitness) of each solution candidate is calculated from a user defined fitness function and is represented as a single number. Minimization of this number is the goal of the optimization. According to APSO algorithm a new generation of solution candidates is created for the next iteration step until a stopping criterion is reached. In terms of time of flight mass spectrometry the fitness (f) of a solution is usually expressed as function of the measured peak curve, e.g. peak height and full width at half maximum which are obtained from fitting of analytical (Gauss, Lorentz etc.) functions to the recorded dataset (Fig. 1), say

$$f = \frac{A}{\Delta T} \quad (1)$$

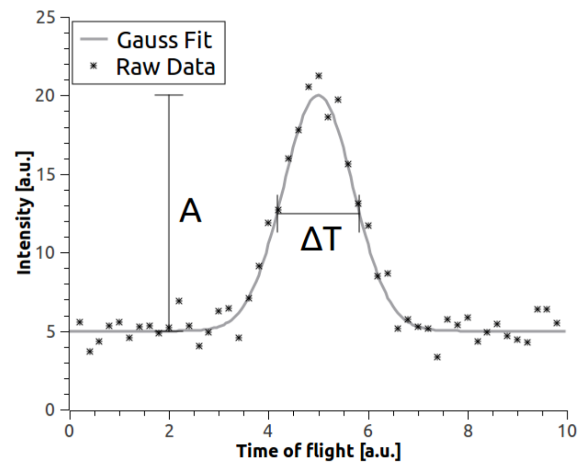

Figure 1: Example of a fitted dataset from a time of flight instrument used during optimization.

Introduction of penalty functions, where undesired solutions are artificially punished, is necessary to keep the optimization process stable. The cause of undesired solutions can e.g. be errors from the data acquisition system or from the peak fitting routine.

From experience with the Rosetta mission it became obvious that also fully automatic optimization of instruments in space is needed. A malfunction of a power supply causes the RTOF instrument to operate at a drift voltage well below nominal conditions, therefore the whole ion optical system has to be re-tuned before rendezvous with comet 67P/Churyumov-Gerasimenko. With signal travel times of more than 45 minutes there is no efficient way of ground based optimization, hence the algorithm has to be directly implemented into the data processing unit enabling in situ tuning of the instrument.

2. Measurements and Results

Three different time of flight instruments have been optimized with the adaptive particle swarm algorithm. A linear time of flight instrument (LTOF) consisting of an orthogonal ion source and a drift tube. The flight spare instrument of the Reflectron Time Of Flight (RTOF) mass spectrometer and a prototype of a novel type of Laser Mass Spectrometers (LMS) used to measure surface compositions on future space missions. Increase in performance is shown for all three instruments with a typical optimization duration of several hours. A typical result can be seen in Fig. 2.

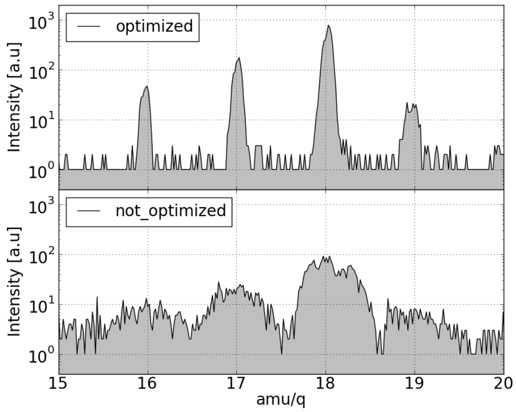

Figure 2: Pre and post optimization spectra of the LTOF instrument.

References

[1] Z-H Zhan, J. Zhang, Y. Li, H.S-H. Chung. Adaptive particle swarm optimization. 2009 IEEE Transactions on Systems Man, and Cybernetics - Part B: Cybernetics, 39 (6), pp. 1362-1381.