

# *Analysing tool for residual gas spectra*

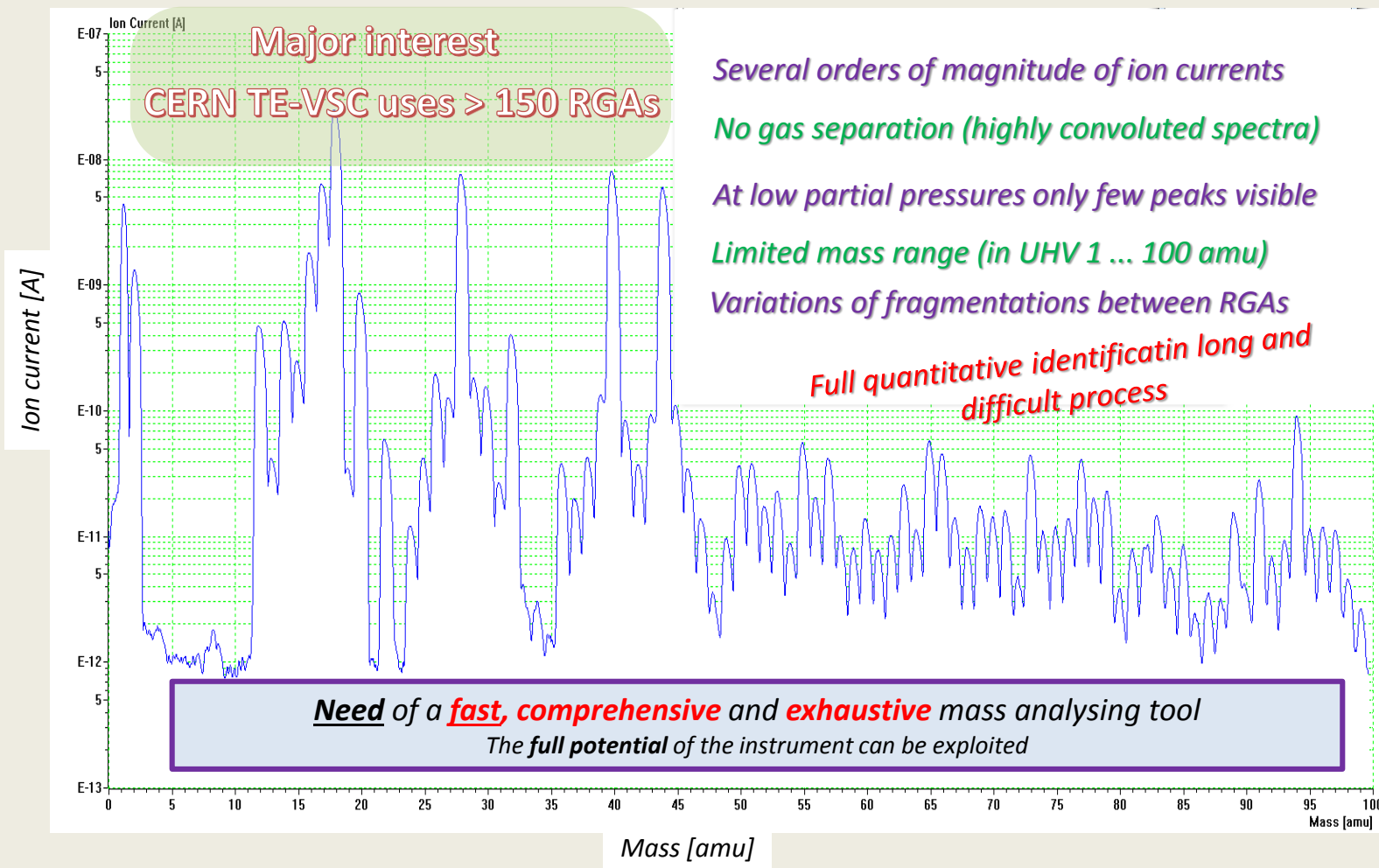
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- 1. Why*
- 2. What / Idea*
- 3. Who / What*
- 4. Next steps*
- 5. Possible use outside HEP*

# Why / Problem

Residual gas analysers used since decades  
Still today: No analysing tool available that covers our needs

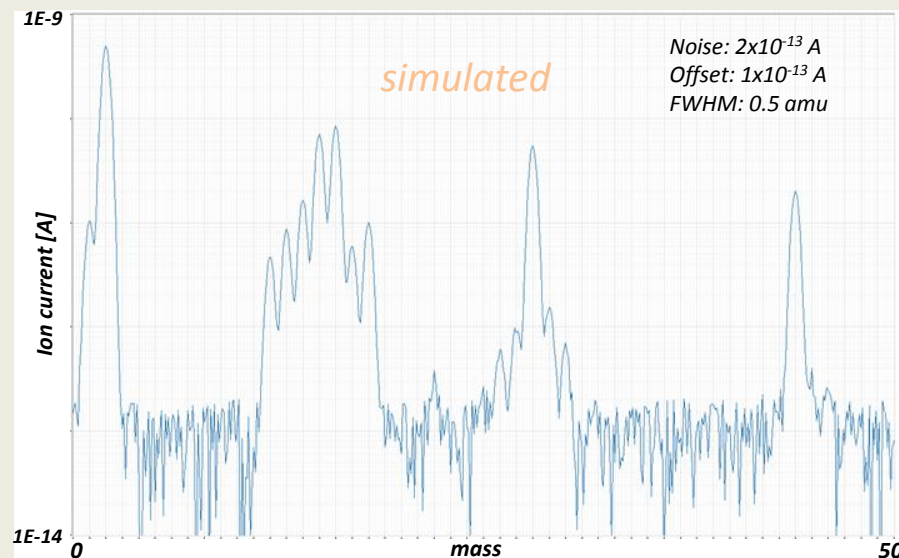


## Software

# Analysing tool for residual gas spectra

Adapted to the needs in Ultra-High Vacuum (UHV)

- UHV-dedicated fragmentation pattern libraries
- Specific features for simulating, analysing and handling spectra



## Simulations

(partial pressures and fragmentation patterns)  
**automatic**

### manually

Include analyser-specific parameters  
(mass **resolution**, **sensitivity**, noise,  
offset ...)

Case studies, training of personal ...

## Iterative deconvolution

(in logarithmic scale)

Deconvolution: Identify composition and determine  
partial pressures

Comparison: **measured** and **simulated** spectra

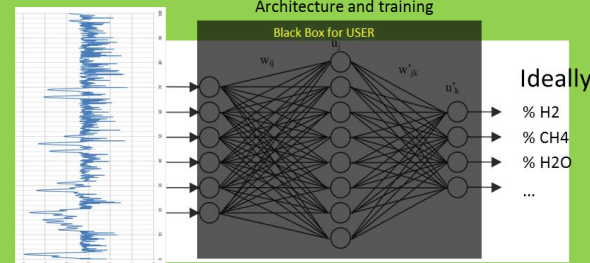
Variation of partial pressures -> simulate spectrum -> determine error

Search: **Global Minimum Integral Error**

## Machine-Learning

Recognition of residual gas composition by **pattern**  
Extensive **training** with random **simulated spectra**

Architecture and training



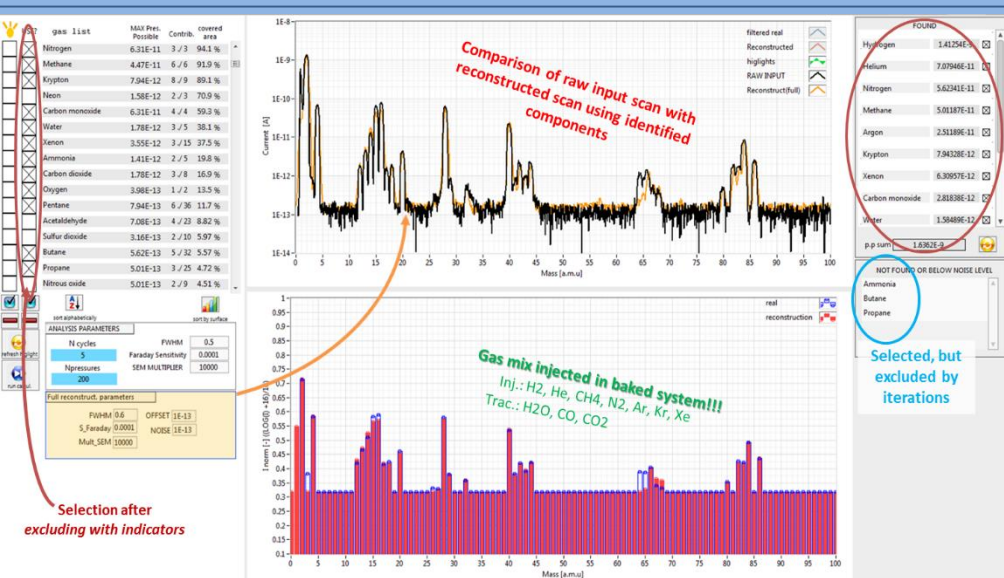
Both need rapid  
simulation of thousands  
of mass spectra

## Iterative deconvolution & reconstruction

## Idea & driving project TE-VSC

## Machine-Learning

Prototype application in LabVIEW



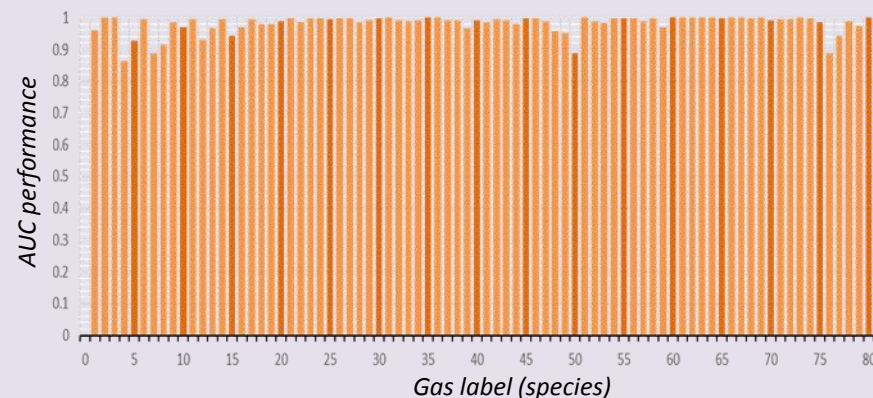
(feasibility study, collaboration KE3129-TE)

**Intelligent Data Analysing Laboratory**

(University of Valencia, Spain)



**IDAL**



**Training sets:** 50000 random spectra

**Learning rate:** 0.1 x presentation of test set: 200

**Test set:** another 50000 random spectra

*Impressive in identification of complex molecules*

*Iterative tool is required to determine partial pressures*

Very fast reconstruction with identified components

Can be applied to a full library for identification  
(in combination with indicators)

**Iterations:** 80000 simulations + error calculation: 6 seconds  
(80 species, 5 iterations, 10 decades, 20 pp-steps per decade)

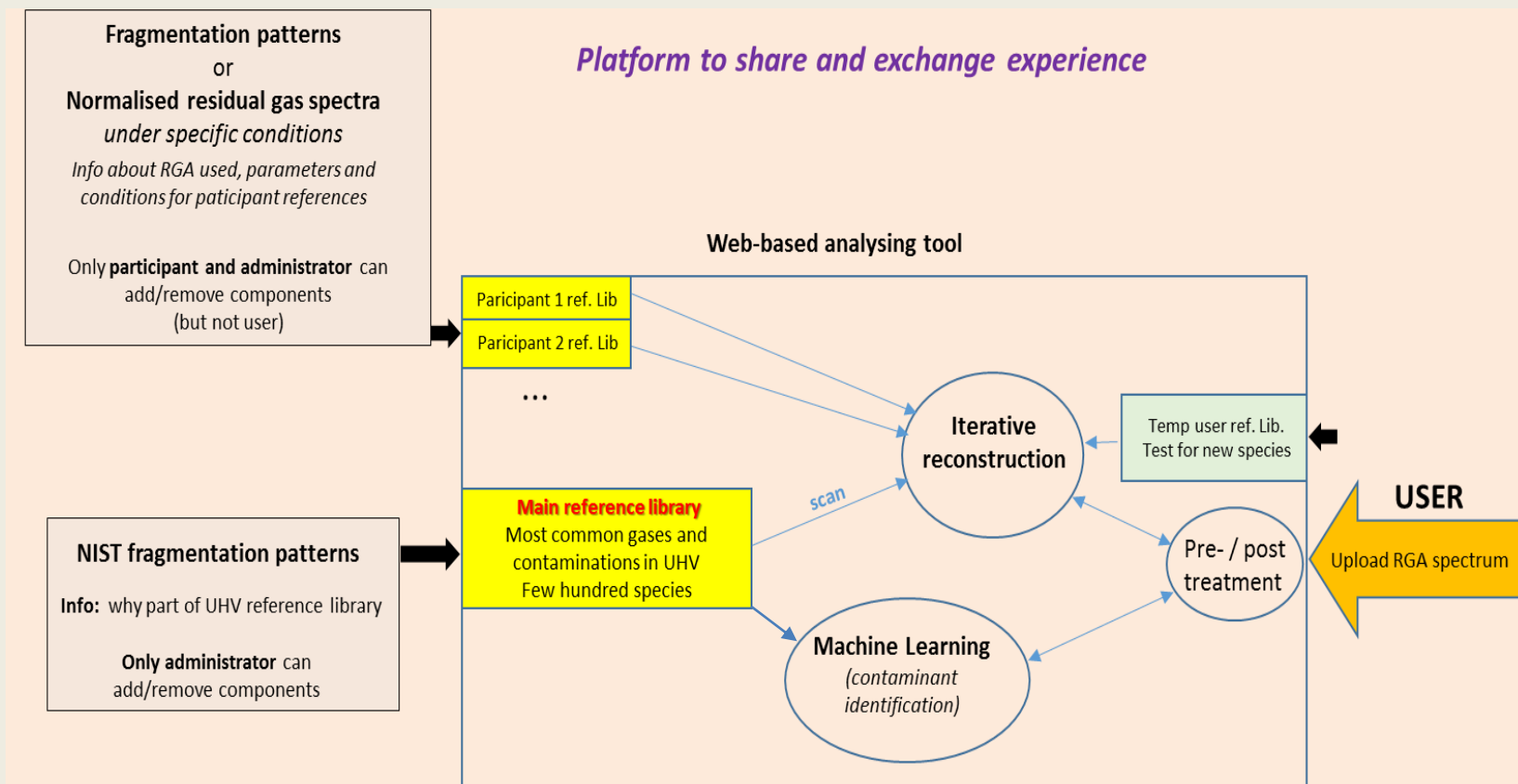
## *Towards a real-world application*

- Iterative deconvolution:**
- ➔ Enhanced pre- post-analysis treatments
  - ➔ Large & multiple fragmentation pattern libraries (few hundred species)
  - ➔ Include calibration features
  - ➔ Subtraction of species from pre-treated measured spectra
  - ...

- Machine-Learning:**
- ➔ Implement basic pre- post-analysis treatments
  - ➔ Adapt architecture for large libraries
  - ➔ Include variable noise cut-off limits in training
  - ➔ Explore possibility to identify components that are not in library
  - ...

**Combination in a web-based application:**

## Web-based platform



➡ Universities and institutes with research facilities using **high quality vacuum**

➡ Semi-conductor industries (process control ...)

...

Basically everywhere where residual gas analysers are used



Web-tool must be user friendly and intuitive  
(and stable)

➡ *People will use it*

THANK YOU