Artificial Neural Networks for high-resolution 3D imaging

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Motivation and Objectives

Rutherford Backscattering Spectrometry (RBS) spectra, when recorded using a nuclear microprobe, allows visualizing the elemental distribution in 2D maps, to identify the elemental matrix of an unknown sample and the depth profiling of those elements.

Metallic nanoparticles (NPs) have emerged as promising tools with broad applications in diagnostics, therapy, and vaccines among other biological and biomedical areas. However, their interactions with cells and their biological effects are largely unknown.

The possibilities offered by nuclear microscopy techniques, specially RBS, enable visualizing NPs distribution in cells with high-resolution, inspect volume distribution and quantify their uptake.

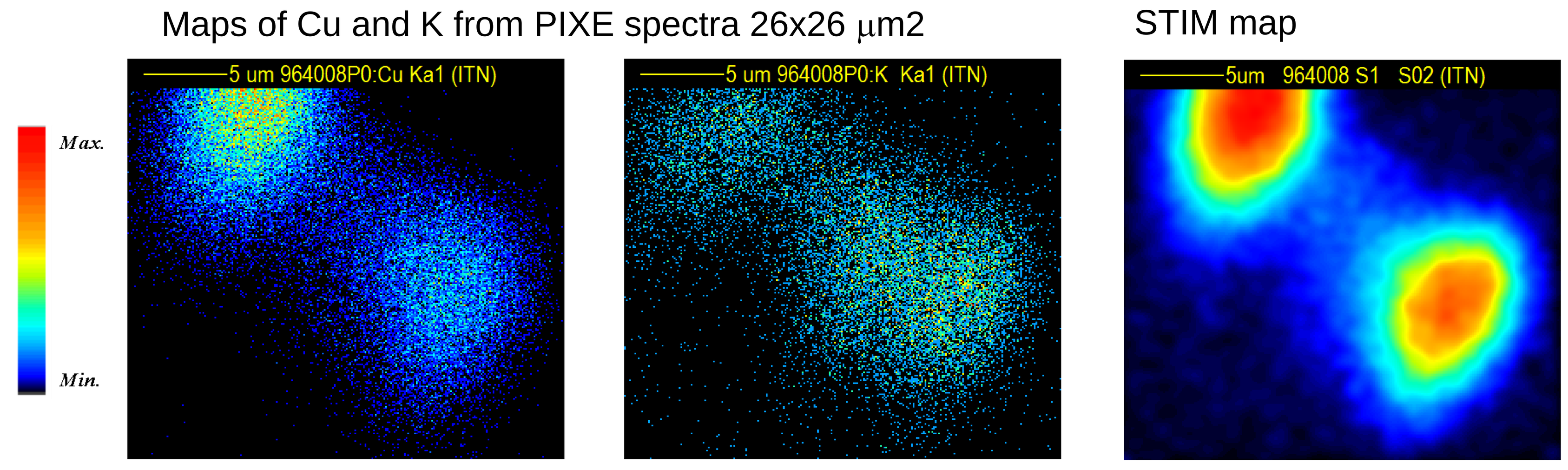
Using RBS spectra as input and calculating the energy loss, MORIA code [1] allows to visualize NPs in a 3D environment.

In this work, we propose the use of Convolutional Neural Networks (CNN) [2], to handle the analysis of large data sets of RBS spectra recorded during nuclear microscopy analysis of cells exposed to Cu NPs.

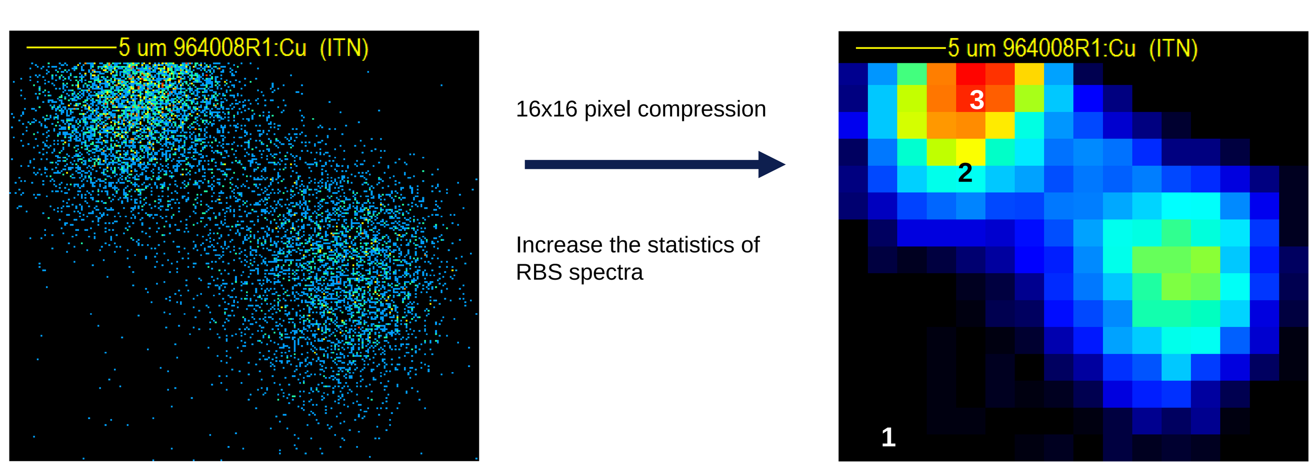
Are results comparable to those obtained using MORIA?

2D Elemental distribution

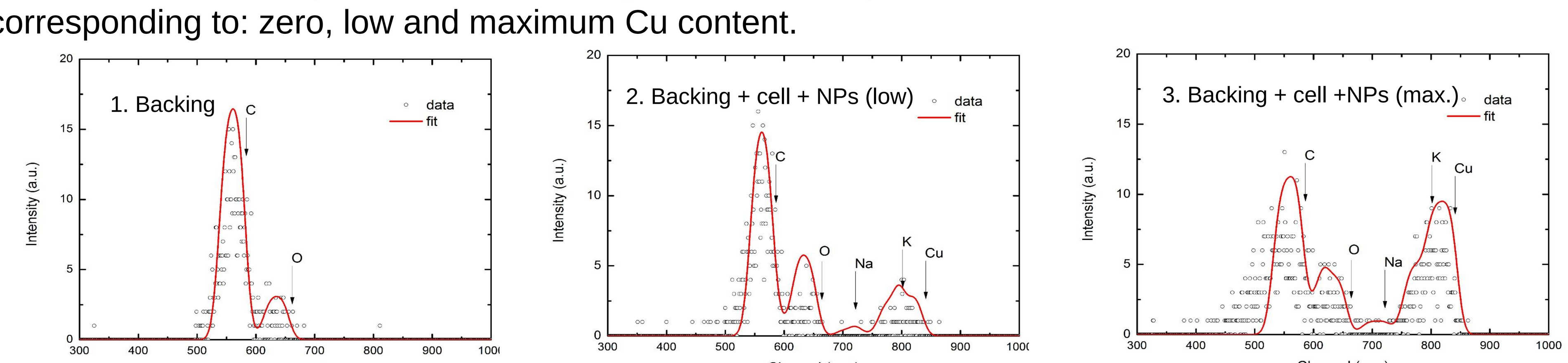
Maps of Cu and K from PIXE spectra 26x26 μm2 — STIM map



Map of Cu from RBS spectra



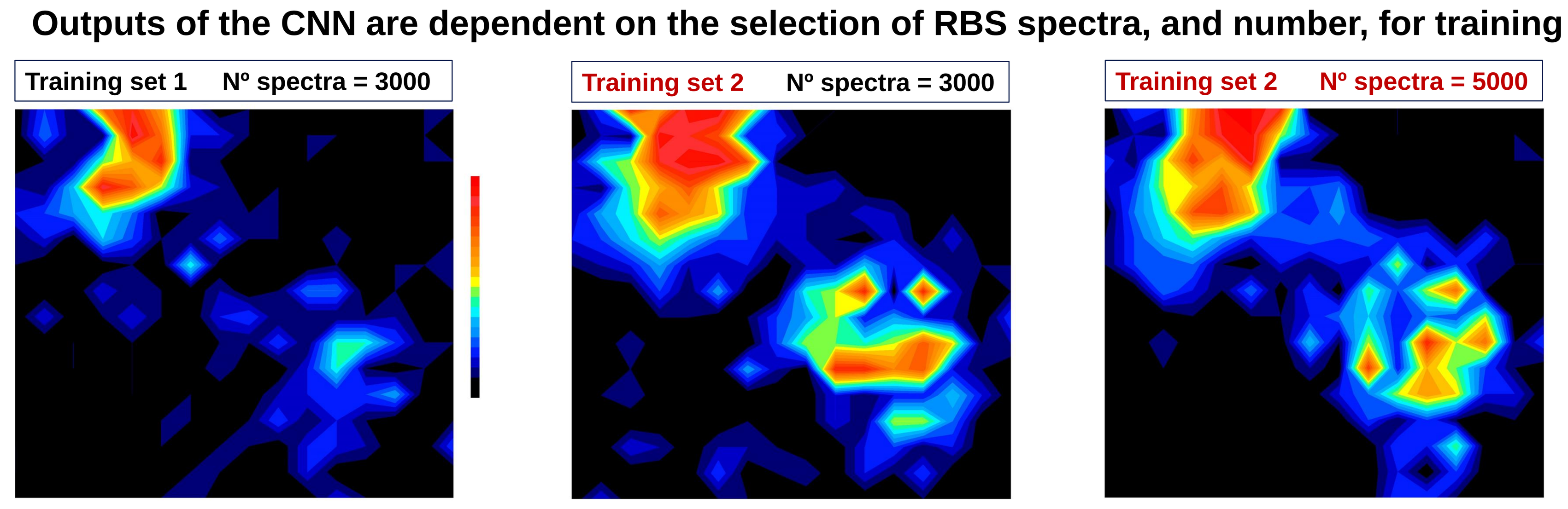
Three different RBS spectra chosen among the 256 RBS spectra extracted from the LMF file, corresponding to: zero, low and maximum Cu content.



Process

- 21 RBS spectra, with different Cu contents and depth profiles, were used as starting point to train the CNN.
- For each RBS spectrum, 5000 spectra were generated to train the CNN (Training Set).
- The weights between nodes are adjusted during the training, and the outputs of the last layer (results) are compared with the known results. The difference between the outputs and the known results are minimized along the process.
- After training the CNN with these 105 000 generated spectra, the 256 RBS spectra extracted from the LMF file using the RLModeP code, are introduced as input to the CNN.
- In less than a minute the CNN classifies the 256 RBS spectra into the 21 classes, according to the Cu contents and thicknesses.

Outputs of the CNN are dependent on the selection of RBS spectra, and number, for training



References

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Experimental

Nuclear Microprobe

Data acquired at the nuclear microprobe (OM 150 triplet system, Oxford Microbeams Ltd., UK) installed at one of the beam lines of the 2.5 MV Van de Graaff accelerator at IST-CTN, Portugal [1].
2 MeV proton beam; Current: 100 pA; Vacuum conditions; Resolution: 3x4 μm^2. Acquisition time: 1 hour. Data acquisition: OMDAQ software, each scanned area is acquired as a 256x256 pixel map.
RBS spectra were analysed using WiNDF code.

Cell model

Saccharomyces cerevisiae cells incubated with CuO-NPs (40 mg Cu/L), deposited on 1.5 mm thick polycarbonate foil (backing). More details in [1].

Data Manipulation

Data recorded during a single run are stored in a Listmode (LMF) file, a collection of event-by-event data blocks with information of energy of the detected event and the position on the sample at the moment of detection.

RLModeP code, developed by one of the authors, is able to extract the individual IBA spectra for each position. To increase the event counting statistics in RBS analysis, RLModeP enables different pixel compression levels.

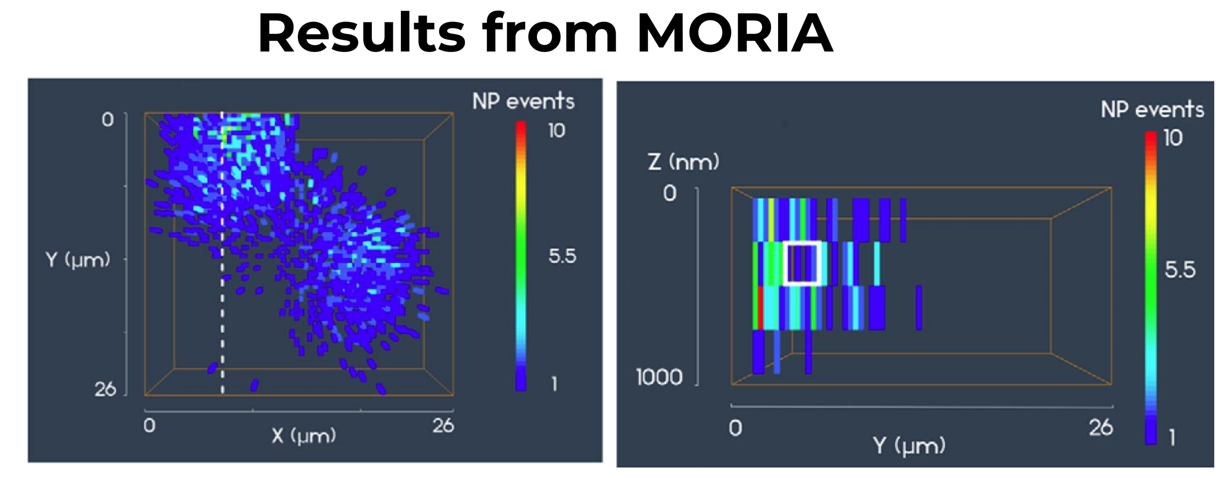
Convolutional Neural Network

Convolutional neural network (CNN) consists of an array of input nodes linked to an array of output nodes through successive intermediate layers and weight parameters.

The architecture, used to study the distribution of Cu atoms in a gold matrix [4], uses 2 Convolutional (C) and 1 Dense (D) layers with 512, 256 and 64 nodes: (I, C512, C256, D64,O).

Computational resources were available through the INCD-Lisbon HPC/HTC clusters [5].

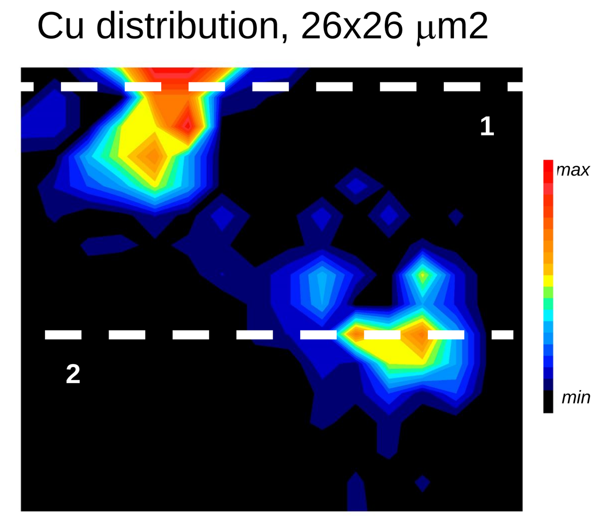
Results from MORIA



MORIA 3D model of the distribution of Cu and the depth distribution of Cu along the white line, from [1].

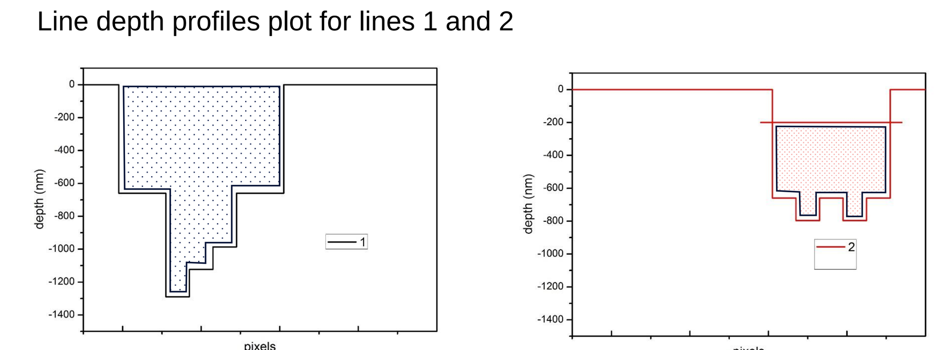
Results from the CNN

Cu distribution, 26x26 μm2



loss: 0.3740 - accuracy: 0.8196

Line depth profiles plot for lines 1 and 2



Depth distribution lines of Cu in lines 1 and 2, showing that some of the Cu atoms are not at the surface.

From both methods, it is possible to visualize the distribution of Cu-NPs in S. cerevisiae cells, which is non uniform in the cellular environment.

Final Remarks and Future work

- Results obtained using CNN are comparable to those obtained using MORIA, validating the CNN model used,
- The CNN used gives fair results, being indifferent of the sample elemental composition. While MORIA deals with heavy elements on a light matrix, the CNN is able to deal with more general cases,
- It is needed to improve the CNN outputs when using input data with very low statistics, to avoid compress the data. An alternative could be to increase the efficiency of the detection system,
- The outputs of the CNN are dependent on the Training Set quality.
- It is needed to implement and an user-friendly interface for output data visualization.

The potential of CNNs to automatically render depth profiles of several types of samples in a 3D environment will definitely extend the imaging capabilities of nuclear microprobes.

Acknowledgments

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