Post-doctoral position

Development of an advanced data fusion method in physical chemistry to push back the analysis limits of conventional instruments for complex samples.

1. Context

The subject of the post-doctorate is part of the ICEEL Carnot Transverse project entitled **TRANSFUSION**. There is currently a great deal of interest in nanoscience in many fields, including physics, chemistry and biology. In order to meet this demand, instrumentation needs to be ever more efficient. Vibrational spectroscopy, atomic force microscopy (AFM) and electron microscopy are formidable analytical techniques for characterising complex samples. They provide access to a wealth of molecular and elemental information. Coupling microscopes with spectrometers has made it possible to generate chemical maps representing the spatial distributions of the components or chemical elements characterising a complex sample. Numerous instrumental advances now make it possible to acquire more and more spectra in an increasingly short space of time.

Interpreting this data requires the use of high-performance mathematical tools to extract the most relevant information quickly and without preconceptions. At first sight, it might seem that managing this growing mass of data is a disadvantage, but in reality, it is a real asset when it comes to solving an analytical problem, provided you have the right chemometrics tools. What's more, there today many different kinds of data, whether it's organised or not. Chemometrics is a science that emerged in the 1970s under the impetus of two physical chemists, Svante Wold and Bruce R. Kowalski. This science applies and develops mathematical and statistical methods to design or select optimal measurement procedures and experiments, and to improve the characterisation, modelling and understanding of complex reaction systems and/or samples. To achieve these objectives, chemometrics integrates several fundamental approaches derived from mathematics: data dimension reduction, classifications, unmixing, modelling, prediction, data fusion and topology.

Spectroscopic and microscopic imaging have also benefited from this recently, with data fusion methods for multivariate curve resolution capable of simultaneously extracting the spectra of pure products or elements and their associated chemical or elemental mappings. However, despite the wealth of molecular and/or elemental information available, coupled with the development of high-performance chemometrics tools, some techniques are still poorly suited to imaging micrometric and submicrometric samples. Over and above the experimental conditions, their spatial resolution is inherent in the instrumentation used. Increasing spatial resolution is therefore still a major challenge if the samples analysed are to be better characterised. Two approaches have therefore emerged to push back the spatial limits. The first focuses on instrumental development, where the economic costs can quickly become exorbitant, while the second attempts to reduce spatial resolution using an algorithmic approach.

The aim of the **TRANSFUSION** project is to develop innovative, high-performance numerical tools to push back the current instrumental limits when generating spatial data coupled with elementary, molecular and mechanical chemistry information. The improvement will focus on the size of the smallest observable object, the identification of its composition and the computing time. The other interest lies in the cross-disciplinary nature of the expected tools, through their ability to take into account variable environments and data of multiple natures and scales, applicable, in the current pilot phase, largely to the scientific fields of ICEEL's partner components, namely : Process Engineering and Energy (**LERMAB**), Resources and Environment (**LIEC, GeoRessources**, and **LCPME**), Materials (**LMOPS**) and Industrial Technologies (**TJFU**), where the current instrumental platforms **must offer finer and faster characterisation of the samples analysed for their users in the public and private sectors**.

2. Description of the postdotoral position

The consortium has chosen to work on four analysis methods: hyperspectral Raman imaging (**LMOPS, LCMPE**), the Castaing probe (**GeoRessources**), atomic force microscopy (**LCPME, LIEC**) coupled with Raman (**LCPME**), on which data fusion methods (**LIEC**) will be developed to characterise biomass samples (**LERMAB**), innovative materials (**TJFU, LCPME**) and biological samples (**LIEC, LCPME**). These techniques have been chosen for two main reasons:

- They are sensitive and selective and, in some cases, allow precise and accurate quantification of the elements or molecules characterising the sample.
- They allow molecular, elemental or mechanical characterisation of surface and/or volume samples with a lateral and azimuthal spatial resolution of 1µm.

Consequently, a first part of the work will involve overcoming this spatial limitation of the various techniques by using super-resolution methods. This concept is based on the fusion of several so-called low-resolution (LR) images of the same object observed from different viewpoints in order to obtain a so-called high-resolution (HR) image. Understanding the principle of super-resolution means formulating the link between BR images and a HR image for each instrument. The very first work on super-resolution in Raman hyperspectral imaging enabled us to go from a resolution of 600 to 200 nanometres. The candidate will have to consider the construction or purchase of specific test patterns to determine the intrinsic spatial resolution of these devices and use the super-resolution algorithms already tested at the **LIEC**. The second part of the work will concern the extraction of the most relevant information from these devices for the characterisation of complex samples. To do this, several chemometric strategies can be envisaged. The use of multivariate curve methods to extract particular signals or learning methods. The final objective is to propose a data fusion method to best characterise a complex sample, both spatially and chemically.

3. Areas of expertise

The candidate should have solid skills in physical chemistry (particularly spectroscopy) and mathematics (chemometrics). He/she should also have a particular taste and a certain autonomy for experimental work, as well as for programming (MATLAB, PYTHON, R or any other language).

The contract is for 1 year (with the possibility of being renewed once) in LIEC at Nancy (France) and starts at €2 130 (gross salary), depending on experience.

Contact: marc.offroy@univ-lorraine.fr