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Laboratory(ies) of affiliation: LASIRE CNRS (UMR 8516)
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Thesis director: Ruckebusch, Cyril, Full Professor, cyril.ruckebusch@univ-lille.fr
Co-supervisor (non HDR): Vitale, Raffaele, Associate Professor, raffaele.vitale@univ-lille.fr

Title of the thesis: Towards chemometrics-driven spectral data acquisition

Many modern analytical platforms are capable of generating massive amounts of data based on which one can characterize complex systems and phenomena with a high level of detail. As an example, today's microscopes permit to investigate chemical and biochemical issues not only with an unprecedented spatial resolution but also providing fundamental insights of physico-chemical relevance into them, by allowing, *e.g.*, infrared spectra, Raman spectra, fluorescence intensity decays, *etc.*, to be registered for each individual pixel of the images they yield. Nevertheless, these incredibly quick advances risk to be practically useless for two main reasons:

1. it is well-established nowadays that, for many of the aforementioned systems and phenomena, only reduced subsets of measurements can actually encode the essential and most useful information required for tackling a wide variety of tasks, from multivariate classification (for, *e.g.*, cancer diagnostics) to object recognition (for, *e.g.*, microplastic detection and pharmaceutical counterfeit determination) and linear unmixing (for, *e.g.*, chemical reaction monitoring and endmember extraction);

2. generally, traditional computing systems exploited in such contingencies cannot perform analytics on-the-fly, that is to say as long as the recording operations are still ongoing. This somehow prevents users and operators from, for instance, collecting data in a targeted fashion or processing them on-line, two strategies which may dramatically reduce the time-to-result since, this way, the data acquisition procedure could be ideally interrupted as soon as all the aforementioned useful information has been recovered.

This Ph.D. thesis project aims at overcoming both these issues towards the conception of innovative instrumental tools integrating built-in algorithms for chemometrics-driven data acquisition. More concretely, the Ph.D. candidate will be expected to:

1. design methodologies for essential information selection in three different application scenarios (multivariate classification, spectral unmixing and exploratory analysis);

2. adapt them for on-the-fly calculations in order to enable the real-time identification of those fewer measurements that need to be performed for retrieving in a faster way the maximum possible content of meaningful information. In practice, this implies developing novel approaches for the reduction,

compression, rational handling and processing of time-evolving, virtually ever-lasting flows of streaming instrumental recordings.

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Contact (e-mail address): cyril.ruckebusch@univ-lille.fr