PhD DISSERTATION PROJECTS

Novel Algorithms and Software Tools for LR-NMR Applications
in Food Science and Technology

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This PhD research project is aimed at the development of software tools for the evaluation of Low Resolution (LR) Nuclear Magnetic Resonance (NMR) data pertinent to applications in food science and technology. This software would be a necessary tool to develop new applications and for the optimisation of the analysis in terms of precision and reproducibility of the results. The software, written in C++, will include basics operations along with innovative algorithms, which will be tested on both simulated and experimental data.

Nuovi Algoritmi e Strumenti Software per Applicazioni NMR a Bassa Risoluzione
in Scienze e Tecnologie Alimentari

Questo progetto di ricerca di dottorato prevede lo sviluppo di strumenti software per l’elaborazione di dati di Risonanza Magnetica Nucleare a Bassa Risoluzione pertinenti ad applicazioni in scienze e tecnologie alimentari. Il software sarebbe uno strumento necessario per lo sviluppo di nuove applicazioni e per l’ottimizzazione del processo di analisi in termini di precisione dei risultati e della loro riproducibilità. Il software, scritto in C++, comprenderà operazioni di base a fianco di algoritmi innovativi, i quali verranno testati con dati sia simulati che sperimentali.

# **1. State-of-the-Art**

Food technology impacts on all steps of food processing, starting from the production of foodstuffs, to their storage, various transformations, and even cooking. Each step must include proper concurrent quality assessment and safety controls.

Nuclear Magnetic Resonance (NMR) is a very useful method to study and characterize several chemical and physical properties of the soft matter, including all kinds of materials and therefore also foodstuffs. The salient features of NMR include a large penetration depth, a totally non-invasive nature, the capability to discriminate even small variations in chemical composition as well as in molecular aggregation and mobility, an intrinsic quantitative response and good reproducibility. The drawbacks of NMR, in some contexts, are its relatively low sensitivity and the need to apply a relatively strong and very homogeneous magnetic field.

NMR comprises three distinct branches: relaxometry, spectroscopy, and imaging. Relaxometry studies the temporal evolution of nuclear magnetization and the ways it is affected by the molecular dynamics of the sample, spectroscopy is concerned mostly with highly resolved radio spectrum of a sample which reflects its chemical properties (molecular structure and composition), and imaging specializes in obtaining various kinds of visual images of the internal parts of a sample.

NMR have been widely used to solve many problems in the general area of food technology. While in NMR spectroscopy many useful high-resolution applications were developed by focusing on the chemical assignments and quantification of various spectral peaks, in NMR relaxometry the situation is different. There exist hundreds of publications proposing various Low Resolution (LR)-NMR applications related to food quality and processing, but relatively few of these potential applications were so far actually refined to the stage of practical assessment procedures.

LR-NMR applications cover many recognizable categories, such as the distinction of sample components or phases (muscle/fat, solid/liquid) or inner states (ripe or damaged), rheological and textural properties (Glicerina *et al.*, 2017) monitoring melting/freezing processes or diffusion processes (Bertram *et al.*, 2005), determination of particle/droplet sizes in emulsions (milk, cream), ageing of materials (stocked food, cheese ripening), or even the assessment of products authenticity, as Mengucci *et al*. (2021) carried out on PDO buffalo mozzarella cheese.

Despite the great number of applications, there are not many complete software tools dedicated to data analysis for specific use in industries. LR-NMR instruments are usually equipped with different hardware features from each other and with low software support to any particular application. In general, data format and the evaluation procedures do not follow any universal standard. In this situation application developers struggle and find difficult to guarantee reproducibility of the results. So, there is a great need for a uniform, vendor-agnostic software tool, one sufficiently sophisticated to allow an expert user, once he selects a potential application, to optimize it, to assess its precision and its reproducibility, to automate it, and to make it suitable for practical use in industrial environments.

In this PhD I plan to develop a complete package for the optimization of some specific LR-NMR applications in food science and technology. I will select some specific food or products; I will do sampling and acquisition of data. Then I will develop software dedicated to the data analysis, in order to obtain results which ought to be reliable and reproducible. The entire process, from data acquisition to results, will be proposed as a complete method for a practical use in an industrial environment.

# **2. PhD Thesis Objectives and Milestones**

An application developer employs one or more LR-NMR instruments to acquire data and a software tool for the data analysis, in order to optimize and automate the whole process. The goal of this project is the development of high-level software tools for the evaluation of LR-NMR data pertinent to possible applications in food technology and testing. This would provide support for the development and optimisation of specific applications. The software will be mostly written in C++ and will be based on either innovative algorithms and on improvements of the existing ones, and it will be focused on obtaining quantitative information about the sample physical and chemical properties, structure, quality. Simulated data will be generated to test the algorithms correct operation; then, real data will be acquired to test the effective robustness and stability of the software routines. The quality of the results achieved during the PhD course will be verified through the feedback received from potential users, who will employ the alpha version of the application software to analyse food products selected for verification.

The doctoral project may be organised in the following activities, resumed in the Gantt chart shown in table 1:

**A1) Preparation:** bibliographic research about LR-NMR applications in food science and technology.

**A2) Software development:** research of the currently available software tools for NMR data evaluation, research of innovative algorithms and their implementation and testing.

**A3) Experiments:** data acquisition and sequence optimization.

**A4) Application development**: choice of one or two potential applications to optimise in terms of analysis workflow from the data acquisition to the final extrapolation of results.

**A5) Writing and publishing:** scientific papers, posters, final thesis and oral presentation.

***Table 1*** *Gantt diagram for this PhD thesis project*.

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| Activities Month | **2** | **4** | **6** | **8** | **10** | **12** | **14** | **16** | **18** | **20** | **22** | **24** | **26** | **28** | **30** | **32** | **34** | **36** |
| A1) | ***Preparation*** |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
|  | 1) Bibliographic research  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| A2) | ***Software development*** |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
|  | 1) Research of currently available software tools and algorithms |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
|  | 2) Software project and implementation |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
|  | 3) Testing algorithms |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| A3) | ***Experiments*** |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
|  | 1) Data acquisition |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| A4) | ***Applications development*** |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| A5) | ***Preparation of papers and thesis*** |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |

# **3. Selected References**

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