# FPGA-BASED NMR AND DECONVOLUTION OF 1D NMR SPECTRA USING DEEP LEARNING

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# 1
# INTRODUCTION

Nuclear Magnetic Resonance (NMR) spectroscopy is a powerful and theoretically complex analytical tool that is widely utilized in chemistry, biochemistry, and biology for elucidating the molecular structure of compounds and studying molecular dynamics. The technique is pivotal in various scientific and industrial applications, such as determining the content and purity of a sample as well as its molecular integrity. However, the implementation of NMR spectrometry, particularly in portable and low-cost formats, has been a subject of ongoing research and development.

One viable solution to the challenges of miniaturization and efficiency enhancement lies in the development of Application-Specific Integrated Circuits (ASICs). ASICs, with their specially designed chips, are tailored to maximize both miniaturization and efficiency in specific applications, such as NMR spectrometry. For instance, Bürkle *et al.*[1], Dreyer *et al.*[2], and Krüger *et al.*[3] have designed ASICs that facilitate the creation of notably compact NMR spectrometers without compromising performance(figure 1).

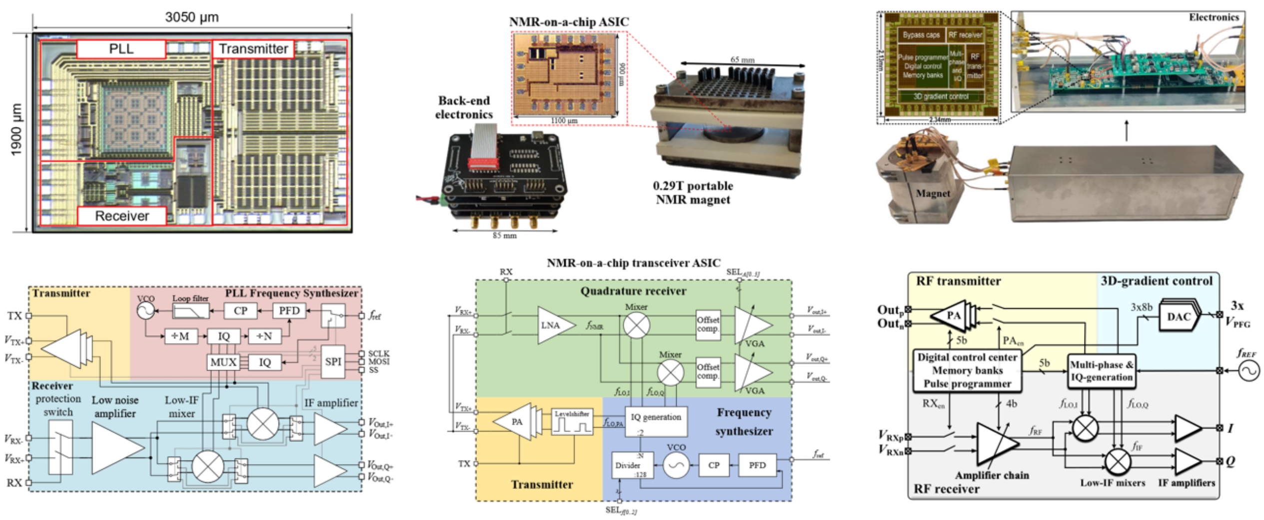


Figure 1: Photographs of ASICs and their architectures. Reprint from [1][3][2].

While the design and manufacturing of ASIC offer a pathway towards miniaturized and efficient NMR spectrometers, the associated costs can be prohibitively high. Consequently, Field-Programmable Gate Arrays (FPGAs) emerge as a compelling alternative, striking a balance between performance and development costs. Pioneering work by Takeda [4][5] around 2007 underscored the viability of FPGAs in constructing a home-built NMR spectrometer. The subsequent, rapid evolution of Integrated Circuit technology, characterized by an exponential growth in transistor count, has precipitated a significant leap in performance capabilities. More recently, researchers such as Louis-Joseph A *et al.*[6], Webber J B W *et al.*[7], and Ariando *et al.*[8] have demonstrated the construction of a compact NMR spectrometer utilizing a contemporary FPGA. Louis-Joseph A *et al.* provided a comprehensive overview of the ongoing development and prevailing challenges in creating low-cost, portable Fourier Transform NMR (FT-NMR) systems[6]. Furthermore, Ariando *et al.*ingeniously integrated a System-on-Chip (SoC) that amalgamates an ARM microprocessor and an FPGA(figure 2), facilitating fully autonomous operation without necessitating an external computer[8].

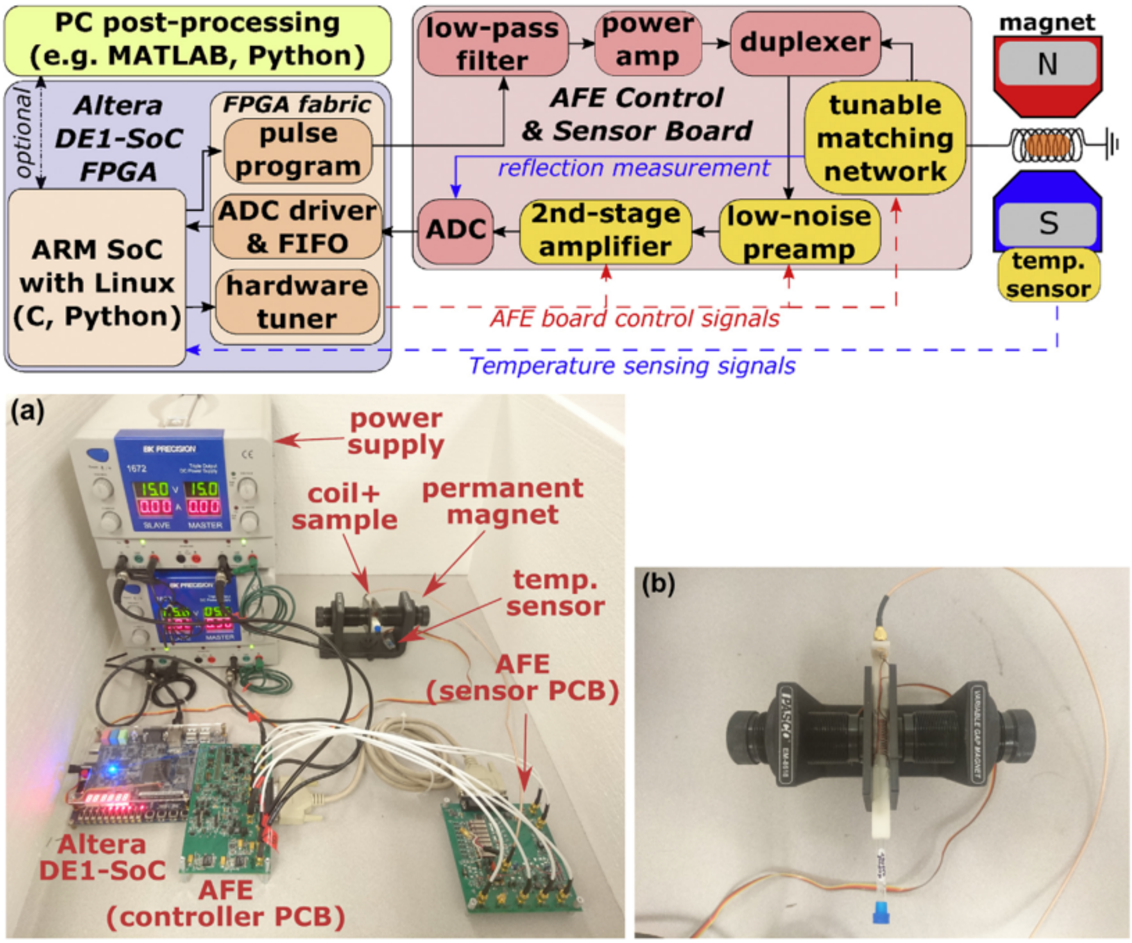


Figure 2: Photograph of SoC and his architecture. Reprint from Ariando *et al.*[8].

Moreover, advancements in artificial intelligence, particularly in machine learning, are beginning to permeate various facets of NMR spectroscopy, enhancing its capabilities and applications. For instance, Manu V S *et al.*[9] has explored the utilization of AI-designed NMR spectroscopy RF pulses to expedite acquisition at both high and ultra-high magnetic fields, showcasing the potential of artificial intelligence in optimizing data acquisition processes. Similarly, Schmid N *et al.*[10] has employed deep learning algorithms to resolve one-dimensional NMR spectra, demonstrating the efficacy of deep learning in enhancing the resolution and interpretability of spectral data(figure 3). Furthermore, Kuhn S *et al.*[11] has leveraged deep learning to identify substructures in two-dimensional NMR spectra of mixtures, illustrating the potential of artificial intelligence in deciphering complex spectral data and revealing underlying structural information.

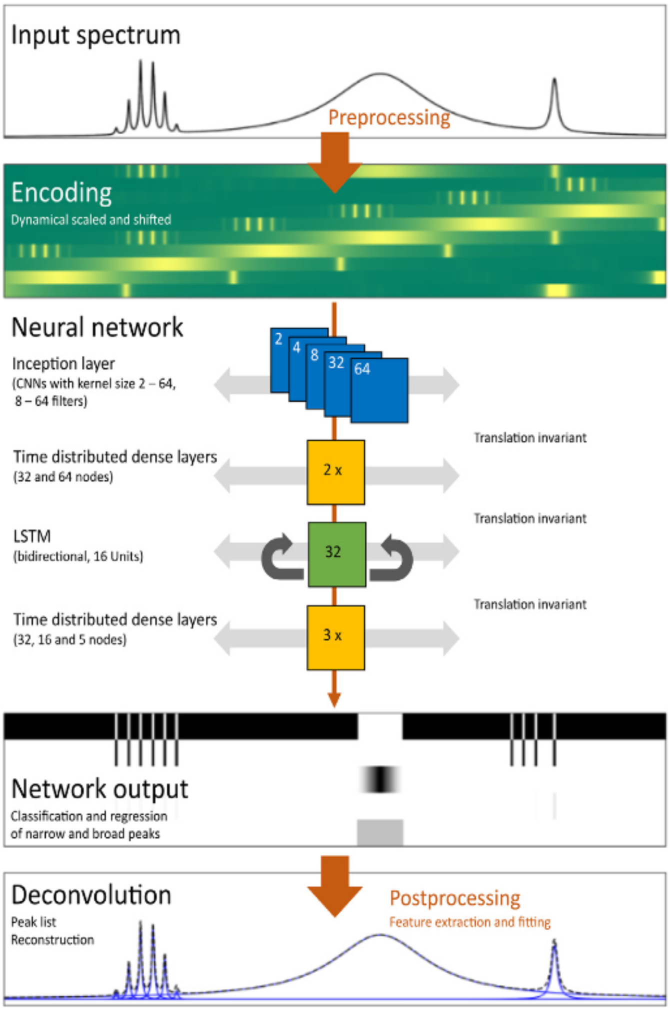


Figure 3: Data flow diagram for the neural network. Reprint from Schmid N *et al.*[10].

# 2
# OBJECTIVES

## 2.1 Primary Objective

Leveraging my prior experience with machine learning projects, the initial focus will be on reproducing the findings from "Deconvolution of 1D NMR Spectra: A Deep Learning-Based Approach.[10]" The first step involves requesting the training data from the authors of the paper by Schmid N, which will be utilized to construct a neural network architecture, adhering to the methodologies delineated within the paper. Subsequent to building the architecture, the model will be trained and tested to validate the results against the original findings. In a bid to foster collaborative development and knowledge sharing, the code will be open-sourced to the GitHub community. Furthermore, alternative neural network architectures, such as Variational Autoencoders (VAE), will be explored to ascertain if they yield enhanced results, thereby contributing to the ongoing evolution of deep learning applications in NMR spectra deconvolution.

## 2.2 Secondary Objective

Trying to implement the FPGA part of the paper "Autonomous, Highly Portable NMR Spectrometer Based on a Low-Cost System-on-Chip (SoC)[8]" on an Altera DE2 in the lab. Since the lab does not have an FPGA with an integrated microprocessor (Altera DE1 SoC), I thought I could build the system using the Altera DE2 in cooperation with a computer.

# 3
# EXPECTED OUTCOMES

## 3.1 Deep Learning-Based Deconvolution

Python code open-sourced on github.

## 3.2 Implementation of FPGA-Based NMR

VHDL code used to build the system.

# REFERENCES


[1] Heiko Bürkle, Tobias Klotz, Reiner Krapf, and Jens Anders. A 0.1 MHz to 200 MHz high-voltage CMOS transceiver for portable NMR systems with a maximum output current of 2.0 App. In *ESSCIRC 2021 - IEEE 47th European Solid State Circuits Conference (ESSCIRC)*, pages 327–330, September 2021.

[2] Frederik Dreyer, Qing Yang, Belal Alnajjar, Daniel Krüger, Bernhard Blümich, and Jens Anders. A portable chip-based NMR relaxometry system with arbitrary phase control for point-of-care blood analysis. *IEEE Transactions on Biomedical Circuits and Systems*, pages 1–12, 2023. Conference Name: IEEE Transactions on Biomedical Circuits and Systems.

[3] Daniel Krüger, Aoyang Zhang, Behdad Aghelnejad, Henry Hinton, Victor Marrugat Arnal, Yi-Qiao Song, Yiqiao Tang, Ka-Meng Lei, Jens Anders, and Donhee Ham. A Portable CMOS-Based Spin Resonance System for High-Resolution Spectroscopy and Imaging. *IEEE Journal of Solid-State Circuits*, 58(7):1838–1849, July 2023.

[4] Kazuyuki Takeda. A highly integrated FPGA-based nuclear magnetic resonance spectrometer. *Review of Scientific Instruments*, 78(3):033103, March 2007.

[5] Kazuyuki Takeda. OPENCORE NMR: Open-source core modules for implementing an integrated FPGA-based NMR spectrometer. *Journal of Magnetic Resonance*, 192(2):218–229, June 2008.

[6] Alain Louis-Joseph and Philippe Lesot. Designing and building a low-cost portable FT-NMR spectrometer in 2019: A modern challenge. *Comptes Rendus Chimie*, 22(9):695–711, September 2019.

[7] J. Beau W. Webber and Pavel Demin. Credit-card sized field and benchtop NMR relaxometers using field programmable gate arrays. *Magnetic Resonance Imaging*, 56:45–51, February 2019.

[8] David Ariando, Cheng Chen, Mason Greer, and Soumyajit Mandal. An autonomous, highly portable NMR spectrometer based on a low-cost System-on-Chip (SoC). *Journal of Magnetic Resonance*, 299:74–92, February 2019.

[9] V. S. Manu, Cristina Olivieri, and Gianluigi Veglia. AI-designed NMR spectroscopy RF pulses for fast acquisition at high and ultra-high magnetic fields. *Nature Communications*, 14(1):4144, July 2023. Number: 1 Publisher: Nature Publishing Group.

[10] N. Schmid, S. Bruderer, F. Paruzzo, G. Fischetti, G. Toscano, D. Graf, M. Fey, A. Henrici, V. Ziebart, B. Heitmann, H. Grabner, J. D. Wegner, R. K. O. Sigel, and D. Wilhelm. Deconvolution of 1D NMR spectra: A deep learning-based approach. *Journal of Magnetic Resonance*, 347:107357, February 2023.

[11] Stefan Kuhn, Eda Tumer, Simon Colreavy-Donnelly, and Ricardo Moreira Borges. A pilot study for fragment identification using 2D NMR and deep learning. *Magnetic Resonance in Chemistry*, 60(11):1052–1060, 2022. _eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1002/mrc.5212.