A Highly Integrated HVNMR Spectrometer with AI-Driven Second-Order Shimming

Zhibin Zhao[1], Yitian Chen[1], Zhenghe Sun[1], Bernhard Blümich[2], Michal Kern[1], Jens Anders[1,3]

[1]Institute of Smart Sensors, University of Stuttgart, Germany

[2]RWTH Aachen

[3]Institute for Microelectronics Stuttgart (IMS CHIPS)

Magnetic field homogeneity is a fundamental requirement for high-resolution nuclear magnetic resonance (NMR) spectroscopy, particularly in compact systems where space constraints limit passive field correction methods. In this work, we present a highly integrated high-voltage NMR (HVNMR) spectrometer equipped with an AI-driven, second-order active shimming system. The system is designed to dynamically compensate for magnetic field inhomogeneities using bi-planar shim coils embedded directly into the core of a permanent magnet.

The shim coils are designed using a target field approach, with eight channels corresponding to the most relevant terms in the spherical harmonic field expansion of the used magnet. The coil structure is fabricated using laser-cut printed circuit boards (PCBs), and controlled via an FPGA-driven octal digital-to-analog converter (DAC) that powers five current drivers with a total power consumption of 6.5 W.

To speed the shimming process and make it more automated, we deploy a hybrid optimization algorithm on the FPGA. This algorithm combines a pre-trained neural network emulator – accelerated by a Xilinx Deep Processing Unit (DPU) – with actual measurement data to refine shimming performance using Gaussian process fitting. This edge-AI approach reduces optimization time by approximately 50% compared to conventional iterative search methods.

Experimental validation using acetic acid and distilled water samples demonstrates a significant improvement in spectral resolution. The full width at half maximum (FWHM) of the water sample is reduced from 32 ppm to 2.3 ppm, indicating a nearly tenfold enhancement in magnetic field homogeneity.

This work highlights the potential of integrating AI-based optimization into compact NMR systems, enabling faster and more efficient field shimming without compromising hardware footprint or energy efficiency.