Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally Mandal, Ranga Reddy Dist., Hyderabad – 500 046

Seminar

Optimal control methods for improving biomolecular NMR experiments

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In my presentation, I will show three examples of how optimal control (GRAPE)-based pulse shapes rescue biomolecular NMR experiments from different problems. In the first example, I will demonstrate how low-power optimal control pulses are essential at 1.2 GHz instruments to achieve the best performance (*Sci. Adv.* 9, eadj1133, 2023). The larger excitation bandwidth required at 1.2 GHz demands higher B_1 power for hard pulses, limiting the coil diameter to 3 mm for a TCI CryoProbe. Using low-power optimal control pulse sequences, we show that a 5 mm TCI probe can be enabled at 1.2 GHz instruments. Such a larger volume cryoprobe is necessary to obtain higher sensitivity for studying concentration limited samples. These sequences are user-friendly and provide boosted sensitivity starting from 800 MHz for bio-NMR experiments. Our pulses are now being used by other facilities with 1.2 GHz instruments to improve their experiments (*JMR*, 2025, 381:107972). In the second example, I will show how a filtered-NOESY experiment-used for studying interactions in protein-protein, protein-RNA, and protein-DNA complexes can be improved using optimal control pulses. The third example will cover improving real-time decoupling in carbon-detected experiments using band-selective optimal control pulses that compensate for the Bloch-Siegert shift (Preprint: 10.2139/ssrn.5415310).

Monday, Feb 16th 2026

11:30 Hrs (Tea / Coffee 11:15 Hrs)

Seminar Hall, TIFRH