A multi-purpose simulator of coupled spin systems for MR localized spectroscopy and spectroscopic imaging

Z. Starcuk jr. 1, J. Starcukova1, and D. Graveron-Demilly2

1Magnetic Resonance and Bioinformatics, Institute of Scientific Instruments, Academy of Sciences of the Czech Republic, Brno, Czech Republic, 2Creatis-LRMN, Université Claude Bernard Lyon 1, France

Introduction. In spite of the fact that numerous MR simulators exist, the choice progressively narrows when more functionality for in vivo MR spectroscopy and spectroscopic imaging is required. A practical spectroscopist or a pulse sequence developer alike reach an impasse if the requirements include coupled homo- as well as heteronuclear spin systems undergoing relaxation, cross-relaxation and/or magnetization transfer, which are to be exposed to spatially and/or frequency-selective excitation, potentially involving phase cycles and/or RF and gradient modulation not excluding simultaneous modulation. The wish list further includes simple pulse sequence programming tightly matching the underlying physics, and its combination with protocol-oriented interface appealing to a practical user. The possibility to determine functional dependences and to inspect quantum mechanical features not available in the bulk M

Method: The substantial components of the simulator are the (a) spin system model and (b) the protocol and pulse sequence editor and interpreter, each of them includes a calculation core and a graphical user interface.

(a) The number of coupled spins is limited only by the available memory and calculation time. Each spin system is defined by the list of nuclei (heteronuclear systems allowed), their chemical shifts and J-couplings, which are treated as weak for heteronuclear and as strong for homonuclear couplings. Additionally, the whole spin system may be characterized by its spatial position. The principal data structures used in calculations are product ket-space operators and the density matrix, but relaxation is nevertheless simulated according to the Redfield relaxation superoperator, including general mixing of populations by T

Acknowledgements: The work was supported by the ASCR grant AV0 Z20650511, GACR grant GA102/09/1861, and EU Marie Curie Research Network ‘FAST’, MRTNCT-2006-035801.

References.

Discussion: Simulation is an indispensable tool in spectroscopic pulse sequence design and in the preparation of basis sets for spectroscopic quantitation. This simulator gives an MR spectroscopist the power to calculate the necessary signals with the real shaped pulses used in the experiment, to obtain proper spectral patterns including line phases, which may be affected by frequency selective excitation, and to study the effects of various parameters with no or very little traditional programming. Thanks to the Redfield-matrix based treatment of relaxation phenomena, this simulator can be used for deepening the knowledge of relaxation as well as magnetization transfer in spectroscopic measurements. The merger of imaging and spectroscopic approaches may be found useful for NMR education. The current restriction to the Windows platform is only temporary. This simulator is intended to be released with jMRUI by May 1, 2011 and will be available together with this software package.

Figure 1. Pulse sequence GUI showing the protocol (left) and the low-level pulse sequence (right).

Figure 2. Part of a pulse sequence for dual-band excitation showing overlaid AM RF pulse superposition is produced automatically.

Figure 3. SE spectrum of myo-inositol simulated with and without water/fat presaturation (B0=3T, T2=1400ms, T1=200ms, 0Hz: 4.7ppm).

Results: The code has been found to run reliably on a range of PCs – netbooks to workstations. The calculation time depends heavily on the computer, the pulse sequence, spin system, and cycling requirements; 7-8 coupled spins seem to be the current practical limit. Typical simple tasks (individual spectra, excitation profiles, B1 dependences etc.) can be determined mostly in 0.5-5 min. Typically 70-80% of the total calculation time is spent at 2 code lines performing matrix exponentiation or matrix multiplication. Fig. 1 illustrates the simulator GUI, the sequence in Fig. 2 leading to the spectrum of Fig. 3 illustrates one practical application.