VeSPA: Integrated applications for RF pulse design, spectral simulation and MRS data analysis

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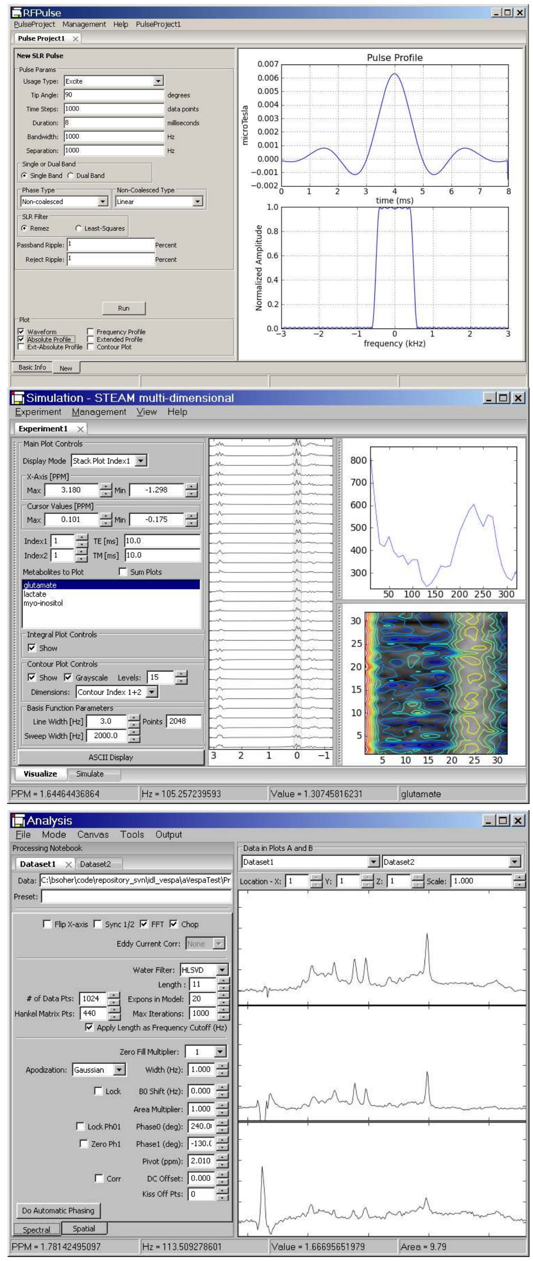
Introduction: Spectral simulation is an effective and efficient means for optimizing data acquisition sequences and for facilitating spectral analysis. The VeSPA-Versatile Simulation, Pulses and Analysis package is an integrated set of open source applications written in that enables users to 1) synthesize RF pulses, 2) explore MRS data acquisition scenarios using multi-parametric spectral simulation and 3) improve MRS data processing/analysis from GE and Siemens scanners.



Software and Methods: The VeSPA project is written in Python which, when combined with Numpy, Scipy and Matplotlib modules, form the basis for an open source, free, replacement for IDL or Matlab. The applications in VeSPA are called RFPulse, Simulation and Analysis and are integrated through the use of a SQLite database (standard in the Python distribution) that allows them to share MR data objects and results. The applications are based on the adaptation and extension of three previous programs, MatPulse [1], GAVA [2] and SITools [3], respectively. Scientific functionality has been ported and extended into the new project while creating a common infrastructure to contain it that is easier to access and maintain (no licensing), simpler to extend (open source, BSD license) and has a consistent style across applications and platforms to ease learning curves.

At the heart of Simulation is the GAMMA [4] spectral simulation library. GAMMA is a powerful C++ library, which can be used to describe and simulate NMR experiments. To facilitate usability, VeSPA has wrapped this resource using SWIG [5] so that its objects can be accessed directly from Python, without the need to compile spectral simulations externally.

Results and Discussion: The three figures show (from top to bottom) 1) development of an SLR pulse in RFPulse application, 2) stack plots, peak integral plots and peak area contour plots for a STEAM simulation with a matrix of 32x32 TExTM values and three metabolites (shown is the glutamate peak integral around 2.4ppm) in the Simulation application, and 3) a short TE and a long TE single voxel PRESS data set and their difference (top, middle, bottom) in the Analysis application. In all cases, more than one pulse/simulation/dataset can be opened and displayed side-by-side. Other significant functionality not shown are: RFPulse - pulse concatenation, rescaling, pole inversion, and export into graphical and manufacturer specific formats; Simulation - a 'pulse sequence' design GUI, full database management dialogs, output to graphical and manufacturer data formats (LC Model, Siemens MetaboliteReport); Analysis - HLSVD signal analysis (for water/lipid removal, etc.), reference deconvolution, metabolite leasts squares basis model fitting iterated with wavelet baseline estimation. In all applications, results can be shared between VeSPA users via an XML import and export. The applications synergize one another. Pulses from RFPulse can be used as building blocks for Simulation pulse sequences, and spectral simulation results could be used in Analysis as part of the data processing or metabolite fitting (fit results not shown in figure). VeSPA application results are accessed by other applications via MR results object browsers from the SQLite database.

There are a variety of predefined algorithms for RF pulse design and pulse sequence definitions that come with VeSPA. Software download and PDF and online documentation available at http://scion.duhs.duke.edu/vespa/

References and Acknowledgements: 1) Matson,GB., MRI, 12, 1205-25, 1994. 2) Soher BJ, et.al. JMR, 185, 291-299, 2007. 3) B.J. Soher et.al. Magn Reson Med 40, 822-831, 1998. 4) S.A. Smith et.al., J. Magn. Reson, Ser. A 106, 75-105, 1994. 5) http://www.swig.org. The authors acknowledge NIH funding - 1R01EB008387-01A1