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# Efficient numerical integrator based on Fer expansion: Application to solid-state NMR experiments

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Numerical methods for differential equations are one of the notable glories of contemporary science. Coupled with much algorithmic ingenuity, numerical methods are widely applied across science and engineering fields. One of the most important numerical methods is the numerical integration which has been the focus of intense research since its development in 1915 by David Gibb. In this abstract, we present the study of numerical integrator based on Fer expansion in the integration of the time-dependent Schrodinger equation (TDSE) which is a central problem to nuclear magnetic resonance (NMR) in general and solid-state NMR in particular. Numerical simulations of NMR experiments are often required for the development of new techniques and for the extraction of structural and dynamic information from the spectra. The development and design of various pulse sequences and understanding of different NMR experiments are based on the form of effective Hamiltonian or effective propagator that satisfies the TDSE which is difficult to solve unless the Hamiltonian is time independent or commutes with itself at two different times. The evolution operator allows obtaining the density matrix of the spin system that has evolved from the equilibrium density matrix due to the application of RF irradiation. The signal intensity depends on the final density matrix of the spin system. For example, if the numerical model is implemented with the approximate solutions of Fer or Magnus, the results of the simulation will show incorrect or undesirable effects of finite pulses and ring-down mainly when dealing with quadrupolar nuclei (I>1/2). In this study we proposed an efficient numerical integrator based on Fer expansion for solving the TDSE to obtain an effective propagator that continually improves the detected NMR signal. We will also compare the performance of the numerical integrator based on Fer expansion with respect to other Lie-group solvers, namely Magnus and Cayley methods.

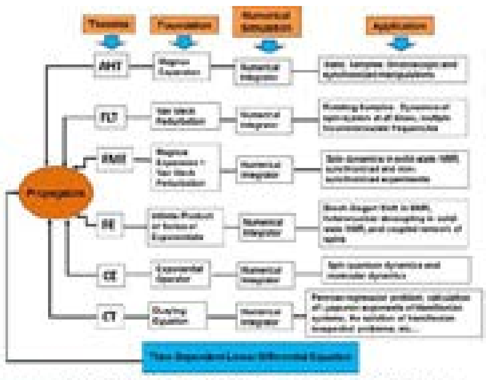


Figure 1: Flow chart of the theories, numerical simulations and applications in NMR.

## Biography

Eugene Stephane Mananga is a Faculty Member in the Physics Doctorate Program and in the PhD Program in Chemistry at the Graduate Center of the City University of New York. He is an Assistant Professor of Physics and Nuclear Medicine at BCC of CUNY, and an Adjunct Professor of Applied Physics at New York University. He completed his PhD in Physics from the Graduate Center of the City University of New York, and holds six additional graduate degrees and training from various institutions including Harvard University (HMS), Massachusetts General Hospital (MGH), and City College of New York. He did his Postdoctoral studies in the National High Magnetic Field Laboratory of USA, Harvard Medical School, and Massachusetts General Hospital. Prior to joining Harvard - MGH, he was a Research Engineer in the French Atomic Energy Commission and Alternative Energies. He has published more than 40 peer-review scientific articles including prestigious scientific journals and he has been serving as Editorial Board Member for more than 20 remarkable journals. He currently serves as Editor-in-Chief of the *Journal of Imaging Science*. His scientific contribution was honored during the 70th anniversary (1946-2016) of the Russian Academic of Sciences.

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