

# Development of a Mathematica-based tool for simulation of Dynamic Nuclear Polarization via Solid Effect on a 3D lattice.

S. Colombo Serra<sup>1</sup>, A. Rosso<sup>2</sup>, F. Tedoldi<sup>1</sup>

<sup>1</sup> CRB - Bracco Imaging Spa, via Ribes 5, Colletterto Giocosa (TO), Italy

<sup>2</sup> University of Paris Sud (LPTMS), 15 rue G. Clemenceau, 91405 Orsay, France

Nuclear Magnetic Resonance (NMR) signal, providing information about molecular structure and chemical environment modifications of an examined compound, may be a useful probe for *in vivo* metabolism. Unfortunately, the intrinsic low sensitivity of NMR technique has always opposed this development opportunity.

In the last years, the possibility of using previously known methods for enhancing the polarization of a nuclear spin system (such as optical pumping, *Para*Hydrogen Induced Polarization and Dynamic Nuclear Polarization (DNP)) for *in vivo* Magnetic Resonance Imaging applications has been demonstrated. This new and promising perspective consists in an *ex-vivo* hyper-polarization (i.e. establishment of a non-thermal polarization as much as possible close to unity) of a metabolic compound and in its intravenously injection into the subject under investigation. Following the metabolic fate of that compound, by NMR spectroscopy or Chemical Shift Imaging techniques, healthy and pathological behaviour can be differentiated and characterized.

A nuclear spin system is hyperpolarized by DNP through three steps: preparation of the sample, with a vitreous solvent and a free organic radical, transfer of that sample to low temperature and high field, microwave (MW) irradiation to transfer polarization from unpaired electrons to nuclei. The interaction between nuclear and electronic spin systems can be described by Solid Effect (SE), Cross Effect or Thermal Mixing theories, depending on the values of the experimental boundary conditions.

Besides strong experimental evidences of DNP method efficiency, a full theoretical comprehension of these physical mechanisms is still not completely achieved.

In the present work, a computational approach has been proposed as method to simulate the SE phenomenon and analyze the system under the effect of different experimental conditions.

Using a home-developed Mathematica tool, a 3D lattice of nuclear spins doped with electrons (randomly distributed or clustered) and their reciprocal interactions have been simulated. The following mechanisms have been considered: nucleus-nucleus interactions (i.e. spin diffusion mechanism), spontaneous nucleus-electron relaxation, MW forced nucleus-electron interactions, intrinsic nuclear relaxation. The probability rates have been computed for each spin (in the case of single spin process) and for each couple of spins (in the case of two spins process). At each computational step a random selection of the subsequent event (normalized according to individual rates) is carried out.

The simulation tool has been entirely developed in Mathematica, from numerical computation to data reporting in graphical form. After a complete optimization and check, it will allow to analyze build-up time and maximum level of the nuclear polarization as function of MW experimental setup parameters (power and frequency) and sample experimental features (electrons distribution, inter-nuclear distances, radical features, etc.). The analysis and the comprehension of these last issues, hardly describable from a pure theoretically point of view, is the very final goal of the present work.