Numerical modeling of cell membrane electromagnetic behaviour and nanoparticles interaction

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1. Summary

Computational modelling and analysis in biology and medicine have received major attention in recent years.. Multi-scale and Multiphysics computational modeling and analysis, capable to capture biological and physiological interdependencies across multiple observational scales –not only in time and space, but also in physico-chemical modality– could be very useful. In particular models can be employed to address the basic interaction mechanisms between electromagnetic (EM) fields, nanoparticles and biological cells, and to study biophysical phenomena occurring on spatiotemporal scales that cannot be observed with experimental methods. Starting from the circuital model of cell membranes, the possibility to have the EM cell membrane field distribution will be presented and used to perform in silico analysis of eukaryotic and excitable cells subjected to electromagnetic stimuli.

2. Description of the problem and proposed approaches

Computational modelling and analysis in biology and medicine have received major attention in recent years. The interdisciplinary efforts developed so far aimed at elucidating structures and functions of living systems with major challenges in computational modelling to understand, analyze and predict the complex mechanisms of biological systems [1-2]. Researchers are now beginning to address the grand challenge of multi-scale computational modeling and analysis, such as in the case of carbon-based nanoparticles presence [3] used to interact with cells: effectively capturing biological and physiological interdependencies across multiple observational scales –not only in time and space, but also in physico-chemical modality– and doing so in a computationally efficient manner [4]. In this scenario analytical and numerical models can be employed to address the basic interaction mechanisms between EM fields, nanoparticles and biological cells, and to study biophysical phenomena occurring on spatiotemporal scales that cannot be observed with experimental methods. Starting from a circuital model of cell membranes [5-6], the use of equivalent medium theory is exploited in order to derive a field model of cell membrane EM behaviour taking in to account the presence of voltage controlled ionic channels and the field induced membrane non linearity [4,7]. The systems of equations to be solved is obtained by coupling suitable differential equations describing these two phenomena with the Electro-quasistatic formulation of Maxwell equations. A finite element solution of the system in a commercial software (Comsol multyphysics) is here reported and used to perform in silico analysis of excitable cells and of agglomerate of eukaryotic cells subjected to electromagnetic stimuli in presence of nanoparticles [8].

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