Stochastic simulations of minimal cell model systems

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The top-down synthesis of artificial cells and bottom-up self-assembly of protocells are becoming scientifically feasible targets [1-4]. In that context, the properties of closed lipid bilayers or vesicles (e.g., their stability, permeability, growth dynamics, potential to host reactions or undergo division processes…) are being experimentally explored by an increasing number of labs and are raising more and more interest as plausible models for minimal or proto-cellular systems, in combination with different chemical or biochemical reaction networks. Thus, from a theoretical standpoint, it would be a highly attractive goal to determine, under a set of assumptions as broad as possible, the conditions that allow the robust implementation of this type of complex (chemically reacting) compartmentalized systems, as well as their controlled reproduction[5].

On the other hand, in compartmentalized reacting systems where the molecular population of the reactants is very low, random fluctuations due to the stochastic nature of reacting events (intrinsic stochasticity) can bring an open system towards unexpected time evolutions [6]. Additionally, this effect can be enlarged by the spreading of different initial concentrations of biological molecules encapsulated in lipid compartments, depending on the experimental preparation procedure (extrinsic stochasticity). In recent years we developed a computational platform [7, 8] suitable for studying the stochastic time evolution of reacting lipid compartments in order to elucidate the role of randomness [9] in the time behaviour of chemically reacting and self-reproducing lipid compartments, such as vesicles or micro emulsions.

As it stands, the general project we have started is divided in two main lines of research. The first consists in modelling and simulating the structural properties and dynamic behaviour of lipid vesicle populations [8, 9], comparing them directly with real experimental data. This gives us the opportunity to test our approach and our simplifying assumptions and to estimate dynamic and structural parameters, by fitting experimental data. The second line of research explores hypothetical protocell models that keep a relatively low degree of molecular complexity like for instance the ‘minimal lipid-peptide cell’[10] and the ‘Ribocell’ [11, 12]. In all these cases, random fluctuations can play an important role in determining the time behaviour of the studied systems.