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System dynamics through individual behaviour simulation

Abstract: The study of physical systems by computational means has two major approaches: At a macroscopic level, the system is described by a set of differential equations, and solved by numerical methods while at a microscopic level, the system is described by particles, groups and interaction rules. Both ways require, for accuracy, intensive computational resources, spanning two or more scales. We are trying a somewhat different approach. The idea is that, to replicate a given system, some of the micro dynamics, resulting from sub-scale interactions, can be forged by macro behaviours.
We describe our work done so far: the implementation of a software framework where we can simulate 3D multi-agent systems and the (on-going) development of a case study, rooted on pharmaceutic research about the set-up of a reasonably accurate computational simulation of the action of Heparin in the Coagulation Cascade of the blood.