

On Some Sources of Inaccuracy in the Cellular Potts Model Simulations

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ABSTRACT

The cellular Potts model (CPM) is a relatively new (1990s) computational instrument for simulation of 2D and 3D manifolds with application domains in cellular biology and physics of foams, but its bright future in molecular biophysics is also guaranteed. CPM is a development of the Potts model (1951), whose origin is in the Ising model (1924). In simulations each one of these operates as a Monte Carlo algorithm to iteratively re-estimate the mapping of a lattice into subsets of lattice sites, governed by a specific Hamiltonian and engaging certain neighborhood rules. The research presented here is motivated by the understanding that in the monstrous-power-supercomputing era even the tiniest details are able to trigger a butterfly-effect-like deviances in the simulation results, even if the underlying math is not strongly non-linear (which is a rather rare case in the complex natural phenomena). Three distinct kinds of problems in the CPM are investigated: how to avoid the spatial distortion caused by the rectangular-to-hexagonal lattice transition; how to introduce and exploit extremely fine neighborhood relationships; how to handle the assigned non-equilibrium system state transitions.