Physically Grounded Simulations of a Self-Replicating Chemical Aggregate

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Extended Abstract

Self-replicating structures have been studied as models of living organisms since the very onset of Artificial Life research, particularly in the abstract mathematical framework of cellular automata (von Neumann (1966); Langton (1984)). Here, we study self-replicating structures in the 3D space-time continuous and physically grounded framework of dissipative particle dynamics (DPD). DPD is essentially a numerical solver of the Navier-Stokes equations with incorporated thermal fluctuations. The framework is particularly suited for coarse grained simulations of complex liquids and soft condensed matter systems on microscopic length scales. (Groot (1997))

Such a DPD based physical embedding allows us to study self-replicating structures not only as abstract mathematical entities, but to regard them as models of real-world physical objects. In particular, we model super-molecular lipid aggregates (surfactant-coated oil droplets) equipped with an internal metabolism that drives their replication due to a natural aggregate instability. In addition, the aggregate is equipped with inheritable carriers of regulatory chemical information that enables the container-metabolism-information system (commonly referred to as protocell) to undergo Darwinian evolution (Fellermann (2007,b)). Our model is directly related to the minimal protocell design of Rasmussen and coworkers that is currently being pursued both experimentally and through theory (Rasmussen (2008)).

The simulation generates spontaneous self-assembly and self-replication of the entire container-metabolism-information aggregates as well as a fitness function for the inheritable information carriers. These findings are emergent, generic, and robust properties of the systems dynamics.

We analyze the performance of the system for all steps of the replication cycle consisting of (i) nutrient feeding, (ii) information-regulated metabolic turnover, (iii) template-directed replication of the information component, and (iv) aggregate replication by growth and division (see Figure). Interestingly, the model predicts that the most difficult obstacle to be overcome in the life-cycle of this protocell model is product inhibition of the replicating information molecules - a well-known issue from experimental studies (Sievers (1994)).

In conclusion, we argue that physical embedding allows for self-replicating structures of seemingly unanticipated simplicity. Furthermore, the physical foundations of the model opens up for applications of established knowledge and methods, e.g. from statistical physics and, therefore, allows to relate model findings to laboratory results in a qualitative manner. As such, the model provides a systemic consistency check for laboratory implementation issues (which enabled us to discover an earlier ”design bug” with consequences for the experimental implementation).

References

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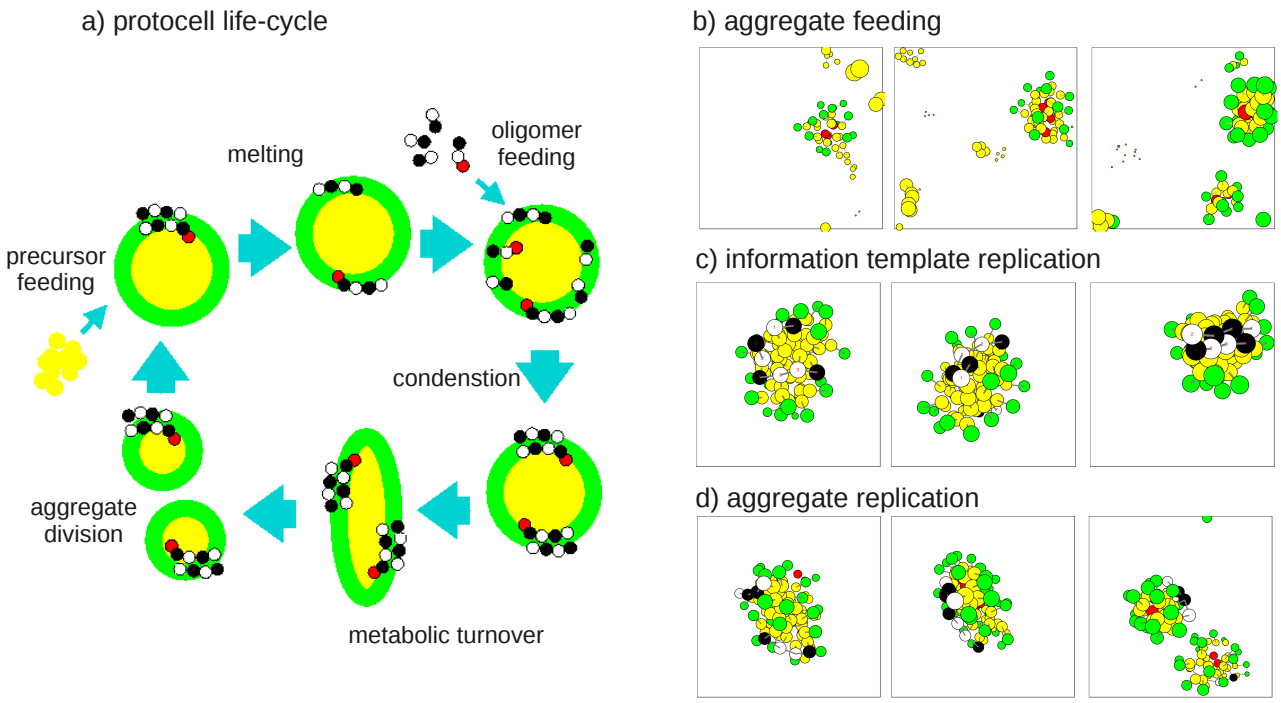

Figure 1: *(a)* The life-cycle of the protocell: Precursos molecules (yellow), surfactants (green), information polymers (black and white), and a photo-sensitizer (red) spontaneously self-assemble in water to form protocells (lower left). Feeding additional precursors increases their volume and stabilizes them when melting the information double strands. Feeding complementary oligomers allows for template-directed replication through condensation. Metabolic turnover of precursors into surfactants induces an aggregate instability that leads to division. Panels *(b)* through *(d)* show simulation snapshots of these processes.

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