



Simple mechanisms of early life – simulation model on the origin of semi-cells



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ABSTRACT

The development of first cellular structures played an important role in the early evolution of life. Early evolution of life probably took place on a molecular level in a reactive environment. The iron-sulfur theory postulates the formation of cell-like structures on catalytic surfaces. Experiments show that H₂S together with FeS and other metallic centers drive auto-catalytic surface reactions, in which organic molecules such as pyruvic and amino acids occur. It is questionable which mechanisms are needed to form cell-like structures under these conditions. To address this question, we implemented a model system featuring the fundamentals of molecular dynamics: heat, attraction, repulsion and formation of covalent bonds. Our basic model exhibits a series of essential processes: self-organization of lipid micelles and bilayers, formation of fluid filled cavities, flux of molecules along membranes, transport of energized groups towards sinks and whole colonies of cell-like structures on a larger scale. The results demonstrate that only a few features are sufficient for discovering hitherto non described phenomena of self-assembly and dynamics of cell-like structures as candidates for early evolving proto-cells.

Significance statement

The quest for a possible origin of life continues to be one of the most fascinating problems in biology. In one theoretical scenario, early life originated from a solution of reactive chemicals in the ancient deep sea, similar to conditions as to be found in thermal vents. Experiments have shown that a variety of organic molecules, the building blocks of life, form under these conditions. Based on such experiments, the iron-sulfur theory postulates the growth of cell-like structures at certain catalytic surfaces. For an explanation and proof of such a process we have developed a computer model simulating molecular assembly of lipid bilayers and formation of semi-cell cavities. The results demonstrate the possibility of cell-like self-organization under appropriate physico-chemical conditions.

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1. Introduction

The quest for a possible origin of life continues to be one of the most fascinating problem in biology. Most theories consider the origin of life as an evolutionary process during which a pre-biotic physico-chemical environment developed (Eigen and Winkler, 1992; Luisi, 2006; Huber et al., 2012). Among the earliest approaches were experimental investigations, which have been conducted under reasonable conditions for different molecular mixtures in aqueous solution, leading to the formation of essential organic molecules (Miller, 1953; Wächtershäuser, 1990; Alpermann et al., 2011) and stable lipid vesicles of various size

(Stano et al., 2005; Budin and Szostak, 2011; Carrara et al., 2012). The formation of vesicles was supported by corresponding physical models and mathematical simulations (Bernardes, 1996; Tobias et al., 1997; Marrink and Mark, 2003; Müller et al., 2006; Reynwar et al., 2007). However, these biosynthetic or theoretical reconstructions of vesicles as cell precursors are based on broth scenarios, supposing the formation of readily closed cell units in free solution. Alternative scenarios postulate a chemical and cellular evolution on catalytic surfaces as found in deep-ocean hydrothermal volcanic vents including white and black smokers.

White smokers are characterized by temperatures of up to 200 °C. Successive hydroxylation, growth and fracture of carbonate surfaces can form inorganic cavities called micro-pores, in which steady geothermal flows create temperature-, redox- and pH-gradients towards the outside ocean water (Martin and Russell, 2007; Lane et al., 2010). These gradients and the presence of metal-

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based catalysts may have produced hydrophobic lipids that coated the micro-pores from inside, thus forming a surface-supported bilayer membrane. Eventually, the membrane would close itself and detach as a substrate-independent envelope, including an already developed biochemistry within a thus emerging free-living prokaryotic cell (Martin and Russell, 2003). Though these authors refer to possible ways of synthesizing lipids under different conditions within such a scenario (cf. (Budín et al., 2009)), only few physical models feature the postulated dynamics of surface coating and membrane formation in detail.

At black smokers there are strongly acidic hydrothermal volcanic flows, with even higher pressures and temperatures of about 350°C. These high pressures and temperatures provide enough energy and supply of substances such that the inorganic rocky iron-nickel/sulfur (e.g., pyrite) surface on the crust of the vents could have served as an auto-catalytic carrier for carbon fixation, successive production and enrichment of surface bound organic molecules as well as an establishment of first metabolic cycles (Wächtershäuser, 1988; Wächtershäuser, 2006). Among those surface-captured organic compounds could easily have been simple amino acids and several types of polyphosphates, e.g., produced from P₄O₁₀ in volcanic vents (Wächtershäuser, 2006). The phosphates may serve as energizing (phosphorylating) agents and initiate the formation of isoprenoid lipid chains. For a retrospective explanation of the process called cellular revolution, Wächtershäuser (Wächtershäuser, 1988; Wächtershäuser, 1997) postulated a successive condensation and growth of adhesive lipids forming surface-bound mono-layer patches, a partial flip-over of lipids by hydrolysis of their hydrophilic heads and, thus, the formation of lipid bilayer membranes. These are generally supported by the reactive surface, but they might span over eventual caverns in the non-smooth crust surface (Wächtershäuser, 2006). Such a semi-cellular structure would be able to grow by accumulating water due to osmosis, stabilize its membrane bilayer by inserting several lipophilic compounds and develop an own sheltered metabolism in its interior.

So far, experimental studies on self-assembly of lipid vesicles (Budín et al., 2009) could not reconstruct the formation of semi-cellular structures. Therefore our attempt was to seek for principal mechanisms and conditions, under which semi-cells might occur. To do so, we implemented a particle model featuring the fundamentals of molecular dynamics: heat, attraction, repulsion and formation of covalent bonds. For a wide range of conditions we explored the appropriate parameters for a successful semi-cell development.

2. Materials and methods

The employed multi-particle simulation aims to follow the Wächtershäuser scenario of a catalytic surface with associated particle attachment, reactions and isoprenoid chain elongation (Wächtershäuser, 2006; Wächtershäuser, 1997). In our surface catalysis model, solute molecules (white particles in Fig. 1) are assumed to be particles of a fluid containing the precursors of amphiphilic chains as well as energized and non-energized molecules. The reactions of our solutes are catalyzed by surface particles (gray and yellow particles Q and Q_E in Fig. 1) and lead to amphiphilic chains, similar to Wächtershäuser's (Wächtershäuser, 1988) idea of catalytic surface induced lipid chain formation. Surface particles are energized by solute particles E as energized variants of solute particles H (Fig. 1), thereby catalyzing the formation of chains from two other solutes (particles A and B in Fig. 1). Short chains (constituted by 2 particles) are able to elongate to long chains (constituted by 3 particles), again by means of a catalytic surface reaction. Both short and long chains consist of hydrophilic

heads (pink A_Q and red A₀ particles) and hydrophobic tails (light B_E, B_Q and dark B₀ blue particles). Hydrophilic heads of short and long chains may either be strongly (pink particles A_Q) or less surface-affine (red particles A₀), see Fig. 1 and the parameter choices for attractive interaction between particles in Table 1.

In our interactive multi-particle system all these reagents (Q, Q_E, H, E, A, B, A_E, A_Q, A₀, B_E, B_Q and B₀) are assumed to be molecular structures of similar size and, for ease of numerical computation, are represented by ball-like particles R_i of same radius $r = 1$ and mass $m = 1$, concentrated as a point mass at position P_i. Notice that, in our simulation model, time, space and other units are dimensionless.

Each simulated particle, indexed by i , moves with velocity V_i and is able to interact and react with other particles. At long distance range, interactions become zero. Once two particles approach, they attract each other according to their physical properties. At close range, particle interaction is strongly repulsive. The Newtonian equations of motion for each particle i are:

$$\frac{dP_i}{dt} = V_i \quad (1)$$

$$\frac{dV_i}{dt} = \frac{F_i}{m} + G_i + \frac{k_n \sigma}{\sqrt{dt}} \quad (2)$$

with interaction force F_i , drag G_i , normally distributed noise σ and noise strength $k_n = 0.32$. Mutual drag depends on the velocity difference vector $V_j - V_i$ for each neighbor particle j :

$$G_i = \sum_{j=1}^{N_i} \mu \left((V_j - V_i) \frac{(P_j - P_i)}{|P_j - P_i|} \right) (P_j - P_i) \quad (3)$$

where $\mu = 0.001$ is a kind of viscosity constant and summation is performed over all j with number N_i of neighbor particles. Interaction forces F_i are the sum of repulsive forces F_{ri} , attractive forces F_{ai} and forces due to bonds between connected particles F_{bi} . In order to reduce computational effort, force terms are implemented as kernels depending piecewise linearly on particle distances $P_j - P_i$:

$$F_{ri} = - \sum_{j=1}^{N_i} k_r (1 - |P_j - P_i|) \frac{(P_j - P_i)}{|P_j - P_i|} \quad \text{for } |P_j - P_i| < 1 \quad (4)$$

$$F_{ai} = \sum_{j=1}^{N_i} k_{ij} \left(1 - \frac{1}{3} |P_j - P_i| \right) \frac{(P_j - P_i)}{|P_j - P_i|} \quad \text{for } |P_j - P_i| < 3 \quad (5)$$

$$F_{bi} = - \sum_{h=1}^{M_i} k_b (L_b - |P_h - P_i|) \frac{(P_h - P_i)}{|P_h - P_i|} \quad (6)$$

with constants for uniform repulsion ($k_r = 0.1$), particle type dependent attraction (k_{ij} , see Table 1) and again uniform Hook spring interaction in bonds (stiffness $k_b = 1$, spring length $L_b = 1$). Bond forces were computed for all bonded particles. h , with number M_i of particles in covalent bonds. In addition, an angular spring was implemented in case of three particles inside a molecular compound. This spring connects the outermost particles with rest length $L_b = 1.633$ and strength $k_b = 0.01$. Note that if $k_r \gg k_{ij}$ a linear interpolation of the Lennard-Jones potential is achieved. The intensity of attractive forces between neighboring particles depends on their reagent type, see reference values of attraction parameters k_{ij} in Table 1. Attractive forces have been adjusted such that hydrophilic solutes and chain heads (A_Q and A₀) strongly attract each other. In contrast, hydrophobic chain tails (B₀, B_E, B_Q) are merely attractive, whereas attractive forces between surface particles (Q, Q_E) are extraordinarily strong, so that they tend to aggregate firmly.

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