

Origin of Left- or Right-Handed B1 cellular Automata Replicators: An Analogy for the CISS Theory of Biological Homochirality Origin

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Abstract

Homochiral biology can be recognized as the outcome of an ancestral breaking of chiral symmetry which has subsequently propagated through a broadening range of descendant dynamic networks. Recently published research provisionally accounts for the establishment of biological homochirality by demonstrating that the chiral symmetry of ribo-aminooxazoline (RAO) in racemic solution is broken by exclusive adsorption of D-RAO, a precursor of RNA, on to a naturally-magnetized mineral surface (magnetite). This proposed mechanism in the prebiotic environment would allow for subsequent unidirectional propagation of homochirality through homochiral RNA to homochiral peptides (including enzymes) to homochiral metabolism. Noting these recent chemical and physical results, I show that an origin out of broken chiral symmetry and subsequent homochiral replication of the B1 cellular automata replicator (1989) can be seen as an analogy to the origin and propagation of biological homochirality.

Keywords: artificial life, B1 replicator, cellular automata, CISS effect, D-RAO, homochirality, origin of life, prebiotic environment, replicator, ribo-aminooxazoline, RNA world.

Introduction

The electrons of currents conducted through chiral molecules have been observed to become spin-polarized, *i.e.*, the intrinsic angular momenta of the electrons align with a chirality-dependent specific direction. This phenomenon is referred to as Chiral Induced Spin Selectivity (CISS). CISS promises a deeper understanding of chemistry and its physics, particularly in the biological context. Reference [2] is a recent review of CISS and its implications.

The CISS effect offers a credible mechanism for the breaking of chiral symmetry in the prebiotic environment, setting the conditions for the development of homochiral biology. Combined with a credible prebiotic environmental scenario, and assuming the “RNA world” picture of ancestral biology, S.F. Ozturk and colleagues have proposed a model [4] for the origin of a pool of homochiral (D-) ribonucleotides, the monomer units of RNA.

A precursor of D-ribonucleotides is D-ribo-aminooxazoline (D-RAO). A racemic solution of RAO in a shallow body of water over sediments of naturally-magnetized magnetite (Fe_3O_4) is taken to be a credible prebiotic environment for a proposed mechanism of accumulating D-RAO from racemic solution. Solar UV light incident on magnetite surfaces stimulates photoemission of electrons and with the action of the CISS effect, the natural magnetism of a magnetite surface corresponds to adsorption of one particular enantiomer and exclusion of its mirror complement. Accumulating crystallization of the adsorbed enantiomer enhances the field strength and range of the mineral surface’s magnetism, and by this positive feedback, amplification of chiral selection occurs [3,6].

As demonstrated by experiments, the CISS effect and enhancement of magnetization on a magnetite surface by feedback between accumulating D-RAO and the surface results in homochiral selection to 100% enantiomeric excess [5].

The “central dogma of molecular biology” is the principle that genetic information flows one-way: DNA → mRNA → peptides (proteins, including enzymes) → metabolism. As a corollary, chirality also flows unidirectionally: selection of D-RAO from a racemic RAO pool → homochiral RNA → homochiral peptides → homochiral metabolism [6]. My previous work, *e.g.* [7, 8], describes the homochirality of both origin and subsequent replication of the Byl cellular automata (CA) replicator [1], demonstrating initial breaking of chiral symmetry followed by propagation of homochirality to larger spatial scales. These results represent an algorithmic analogy to the conclusions of Ozturk *et al.*, as detailed further below.

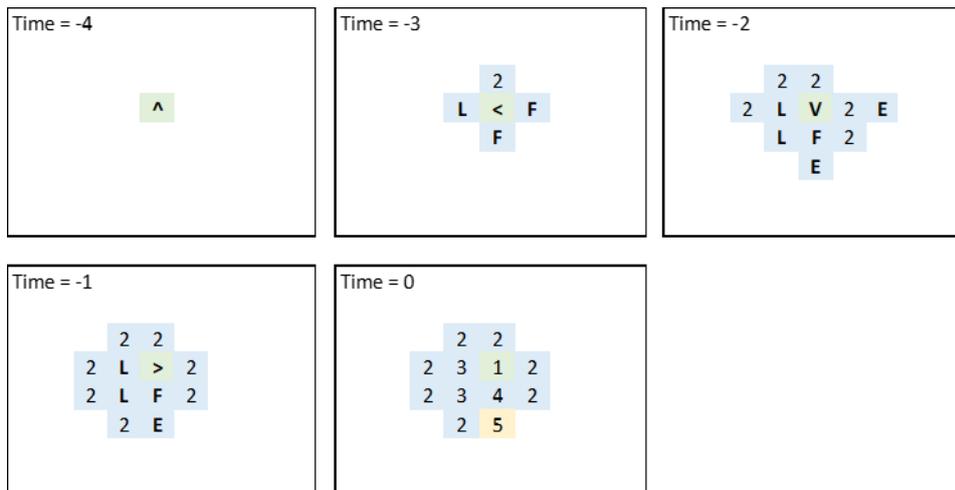
A homochiral origin pathway to a Byl replicator and subsequent homochiral replication

Reference [8] describes an origin pathway to the J. Byl CA replicator [1] from an initially isolated non-quiescent cell in an oriented state (\wedge). This origin pathway requires addition of states \wedge , E, F and L to the state set $\{0, 1, 2, 3, 4, 5\}$. These added states permanently disappear from a developing structure by the time the replicating structure is established. Figure 1 below shows: **A** - origin of the originally-published (right-handed) Byl replicator, and **B** - origin of its complementary mirror (L-) form. The origin of the R-form shown in Figure 1, **A** is reproduced from [8].

The initial oriented state \wedge can either rotate counterclockwise ($\wedge \rightarrow < \rightarrow v \rightarrow >$) or clockwise ($\wedge \rightarrow > \rightarrow v \rightarrow <$). The symmetry of its potential to rotate either way is broken by application of the specific right- or left-handed state transition function [8]. From here, homochirality propagates through an increasing spatial range.

(Article continues with Figure 1, next page)

A: Origin of the right-handed (R-) replicator, established at Time = 0.



B: Origin of the left-handed (L-) replicator, established at Time = 0.

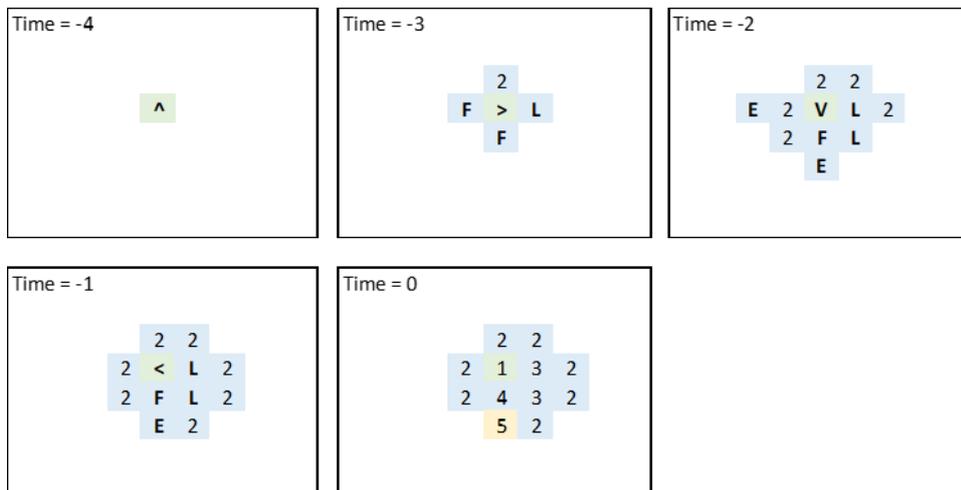


Figure 1. Comparison of **A**: an origin of the right-handed Byl replicator (as originally published [1]) with **B**: its mirror-complement representing origin of the left-handed form of the replicator. The origin state transition function is given in [8] and the replication state transition function originally given in [1] is later redescribed and analysed in the context of chirality in [7]. The white space corresponds to quiescent state 0.

Figure 1 shows that as the initial state \wedge rotates right or left in accordance with the corresponding chiral state transition function applied [8], the accumulation of non-quiescent states of surrounding cells culminates in the appearance of a right- or left-handed Byl replicator at Time = 0.

Subsequently, replication of the emergent Time = 0 right- or left-handed replicator structure is driven by the corresponding right- or left-handed state transition function [7]. The von Neumann neighbourhood state transition functions facilitating origin of and subsequent replication of R-replicators contain rules which contradict state transition rules within the complement L-state transition functions, so broken chiral symmetry is perpetuated: no common state transition function

supports coexistence of origin and replication of *both* right- and left-handed replicators in a common CA environment.

After Time = 0, subsequent replication cycles correspond to rotation of the 2x2 cell information loop (3,1;3,4) which is both interpreted as instructions for construction of descendant replicators, and copied into descendant replicator instances [1]. The rotation of the information loop in the course of a replication cycle is either counterclockwise or clockwise as determined by the chirality of the structure and of the corresponding state transition function applied [7], so we note here that the homochirality of the replicator's origin extends to the larger spatial scale of a replication cycle.

Subsequent replication of the Time = 0 replicators is not shown in Figure 1 above, but subsequent replication of an isolated replicator occurs into adjoining state 0 quiescent space [1]. Given the orientation of the ancestral Time = 0 right-handed replicator shown in Figure 1, **A**, the first descendant develops to the right ("east") of the parent. With the east direction subsequently blocked by the completion of a descendant, a second replication cycle of the initial replicator is diverted up ("north"). By sequential blockage of quiescent space into which replications can be directed, the orientation of the initial R-replicator instance rotates counterclockwise. When descendants have been generated sequentially in east, north, west and south directions, no further replication is possible, but replication of descendants continues into available quiescent space indefinitely. The replication process of the left-handed Time = 0 structure (Figure 1, **B**) is driven by the mirror complement state transition function: given the orientation shown, the first left-handed replication occurs to the left ("west") and as directions available for replications are sequentially blocked, the orientation of the parent rotates clockwise.

Discussion

One hope of my work has been to relate the abstract CA investigation of homochirality origin and homochiral replication to real chemical and physical phenomena. The analogous relationship of the CA work to the Ozturk *et al.* results is perhaps a meaningful beginning. The following discussion matches aspects of the CISS theory of homochiral abiogenesis to analogous aspects of my work on the homochirality of origin and replication of the Byl CA replicator.

The initial breaking of chiral symmetry

The CISS theory describes the initial breaking of chiral symmetry by association of natural magnetization of a magnetite surface to adsorption of D-RAO from racemic solution and exclusion of the levorotatory RAO complement. The analogous mechanism for the initial symmetry-breaking in the origin of the Byl CA replicator is that a chiral state-transition function applied to state \wedge determines its direction of rotation, *e.g.*, The right-handed state transition function causes the \wedge state to rotate counterclockwise (the initially-applicable rule of form $CNESW \rightarrow C'$ is $\wedge 0000 \rightarrow <$) which excludes clockwise rotation.

Propagation of homochirality to a larger scale of organization

D-RAO is a candidate precursor of D-nucleotides, the monomer units of RNA. The homochiral RNA of biology can only be a product of polymerization of homochiral monomers. Analogously, the rules of the Byl replicator right-handed state transition function facilitating its origin [8] collectively

determine the accumulation of non-quiescent states around the oriented state \wedge simultaneously with its rotation $\wedge \rightarrow < \rightarrow v \rightarrow >$, culminating in a homochiral replicating structure comprising more cells (12) in non-quiescent states.

Propagation of homochirality continues to ever increasing scales up to a biosphere of homochiral life

The breaking of chiral symmetry inherent in selection of D-RAO from a racemic RAO pool propagates to homochiral RNA which on translation delivers homochiral peptides which participate in homochiral metabolism [6]. The determination of homochiral replication is implied. Following establishment of a Byl replicator structure, propagation of homochirality continues as the descendants of the ancestral parent inherit the same chirality. As an isolated parent generates descendants, its orientation rotates in a direction determined by the direction set by the initial broken chiral symmetry, so homochirality is observed to propagate to increasing spatial scales.

My work on the Byl CA replicator demonstrates emergence of non-trivial homochiral replication from small, simple origins, and additionally, demonstrates a modest, capped degree of coexistent variability by means of specific state set permutations [9]. However, the challenge of finding a simple abstraction that fully captures the indefinitely open-ended development characteristic of real biology remains.

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