Instances of Functional Heterochiral Replication of the J. Byl Structure supported by Two State-Set Permutations

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Abstract

Previous work demonstrates that strict heterochiral replication of self-replicating loops in two-dimensional cellular automaton space is not possible under any single cell-state transition function, but a less-strict functional heterochirality is possible with the introduction of a different broken symmetry: a cell state-set permutation applied exclusively to left- (or right-) handed replication. A new result reported here is that up to two different state-set permutations applied to one replication chirality can support functionally-heterochiral replication of the J. Byl self-replicating structure in one common cellular automata space.

Keywords: Artificial Life, cellular automata, self-replication, origin of life, biological homochirality, broken symmetry

Introduction

Biological homochirality observed today is assumed to have developed from a racemic ancestral proto-metabolism [1, 4]. As a prospective credible model for the emergence of biological homochirality, a hypothetical racemic metabolism would have to become homochiral, so that subsequent development could culminate in a biology incorporating chiral components, *i.e.*, the modern biology of left-handed (L) amino acids and right-handed (D) sugars.

A question to answer about this proposed chemical evolution from the abiotic to the biotic is how the breaking of symmetry from the racemic state to homochirality might have occurred. In 1953, Charles Frank proposed the existence of a mechanism of antagonism between units of opposing chirality within a racemic system, culminating in complete dominance of one chirality within the proto-metabolism and subsequent biology. In his paper, Frank invited researchers to discover systems which develop homochirality by the proposed general process of autocatalysis and mutual antagonism of left- and right-handed replicators.

In 1995, Kenso Soai reported an experimental system (autocatalytic alkylation of pyrimidyl aldehydes) incorporating both the autocatalysis and mutual antagonism features of the Frank model (see [1]), and although the reaction ingredients are unlikely to be consistent with conditions of the early earth, identification of this reaction is recognized as an important step towards understanding biological homochirality [1].

In further work, Jafarpour *et al.* [4] derived a model in which stochasticity of autocatalysis is sufficient to drive racemic metabolism to homochiral biology. The chiral order parameter ω quantifies enantiomeric excess. The rate of change of ω, dω/dt, is modelled by the sum of a decay term and a noise term. The noise in the model is multiplicative, *i.e.*, the noise term is a function of the dependent variable ω so that the noise term coefficient reduces from a maximum at ω= 0 (initially racemic) to zero at |ω| = 1 (complete left- or right-handed homochirality). Under this model, an initial racemic system inevitably drifts to perfect homochirality of one polarity or the other without including the mutual antagonism feature of Frank's proposal.

The research history summarized above describes some of the effort to explain the gradual appearance of homochirality in biology from a likely racemic ancestral origin. A

supplementary approach to studying biochirality may be to look at the inner structure of identified replicators and observe the logic of replication as it occurs. Self-replicating structures in two-dimensional cellular automata (CA) space are potentially useful for investigating ideas about the origin of life and biological homochirality. The first recognized example is John von Neumann's universal constructor, by which an input "tape" is both translated and copied in two-dimensional CA space. If the tape is encoded with the information specifying the constructor itself, the machine plus tape comprises a self-replicator.

Recognizing that complex life we now observe has gradually developed from simple origins, subsequent researchers investigated the question of the minimal-necessary complexity supporting self-replication. Edgar Codd derived a smaller implementation of the von Neumann machine, but inspired by Codd's work and the specificity of biological replication, a huge reduction in size and complexity was achieved by dropping the requirement for universal construction to create a compact specific (not universal) self-replicator [5]. Further successive reductions in size and/or complexity were achieved by J. Byl [2], and H-H. Chou and J. Reggia [3].

My work [6, 7, 8, 9] has repurposed these simple abstractions of self-replication to investigate the biochirality question with specific focus on the J. Byl replicator, a structure of twelve non-quiescent cells which replicates under an appropriate state transition function [2]. In this work, a result which follows the work described in [8] is presented:

Some new results (an addendum to the work described in [8])

Previous work [6, 7, 8, 9] demonstrates that strict heterochiral replication of self-replicating loops in two-dimensional CA space is not possible under any single state-transition function, but a less-strict functional heterochirality is possible with the introduction of a different broken symmetry: a cell state-set permutation applied exclusively to left- (or right-) handed replication [8].

Applying a cell state-set permutation chirally (*i.e.*, to one chirality of self-replication only – in this case, to L-loop replication), and applying the appropriate Moore rules (not von Neumann rules) state-transition function, functional heterochiral replication is achieved [8]. There are six state-set permutations supporting functional heterochiral replication of the J. Byl structure [8]. Since the work described in [8], I have found that the six state-set permutations form four mutually-exclusive categories (shown in Figures 1 to 4 below). Of the six state-set permutations applied to L-Loop replication, there are two pairs each of which correspond to no rule contradictions between the state-transition functions (see Figures 3 and 4 below).

Figure 1 follows on the next page.

(The content of Figure 1 is reproduced from [8]).

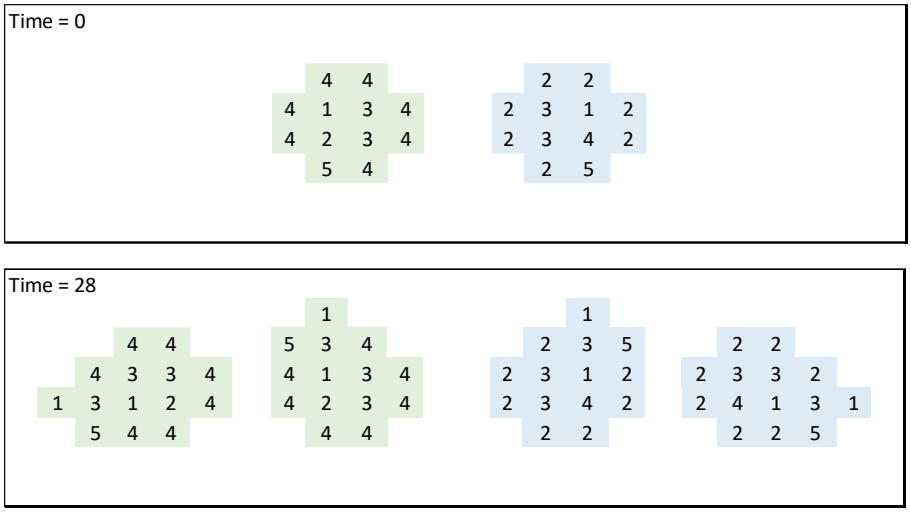

Figure 1. Applying the 12345 → 14325 cell state set permutation to L-loop replication, and the corresponding comprehensive and consistent (*i.e.*, no internal contradictions) Moore rules state transition function to both L-loop (green structure) and R-loop (blue structure) replication, functional heterochirality of self-replication is achieved. From the Time = 0 configuration shown in the upper frame, both left- and right-handed structures have replicated by Time = 28 (lower frame), and replication cycles continue subject to available surrounding quiescent (state 0) white space. Note that the R-loop structures (blue) and the L-loop structures are not strictly mutual mirrors of each other due to the state-set permutation applied only to L-loop replication, *i.e.*, the heterochiral replication depends on the introduction of a broken symmetry of cell-state assignment. All of the steps from Time = 0 to 28 are explicitly shown in [8].

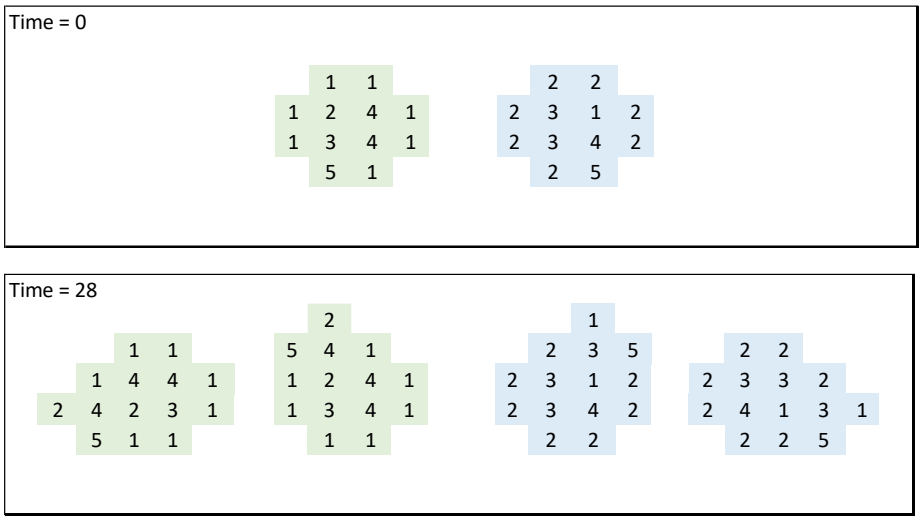

Figure 2. As for the functional heterochiral replication shown in Figure 1, an alternative functional heterochiral replication is achieved with the state set permutation 12345 → 21435 applied to L-loop replication. State-set permutations 12345 → 21435 (this Figure) and 12345 → 14325 (Figure 1) applied to L-loop (or R-loop) replication cannot coexist in a common CA universe.

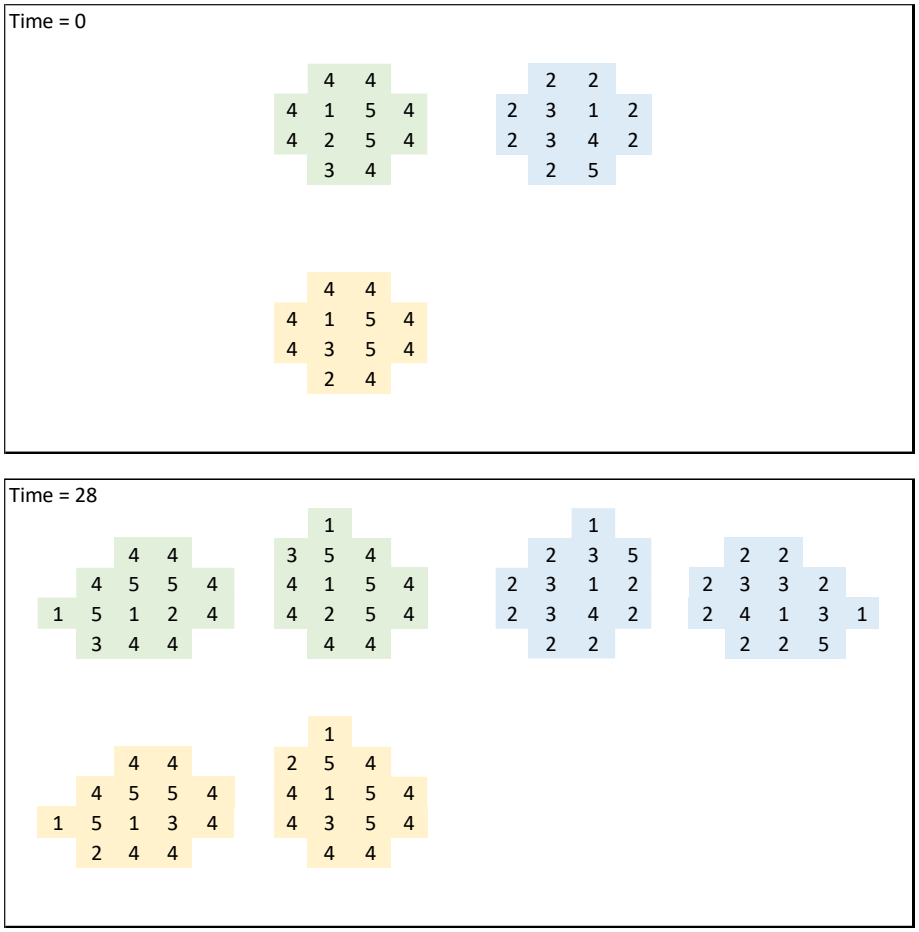

Figure 3. The Moore rules state-transition functions supporting L-loop replication under state-set permutations 12345 → 14523 (green), and 12345 → 14532 (gold) incorporate no contradictory rules, so a pooling of the 12345 → 12345 R-loop (blue) replication state transition function with these two L loop state-transition functions delivers a comprehensive, consistent transition function which supports replication of the blue, green and gold structures in a common CA universe.

Figure 4 follows on the next page:

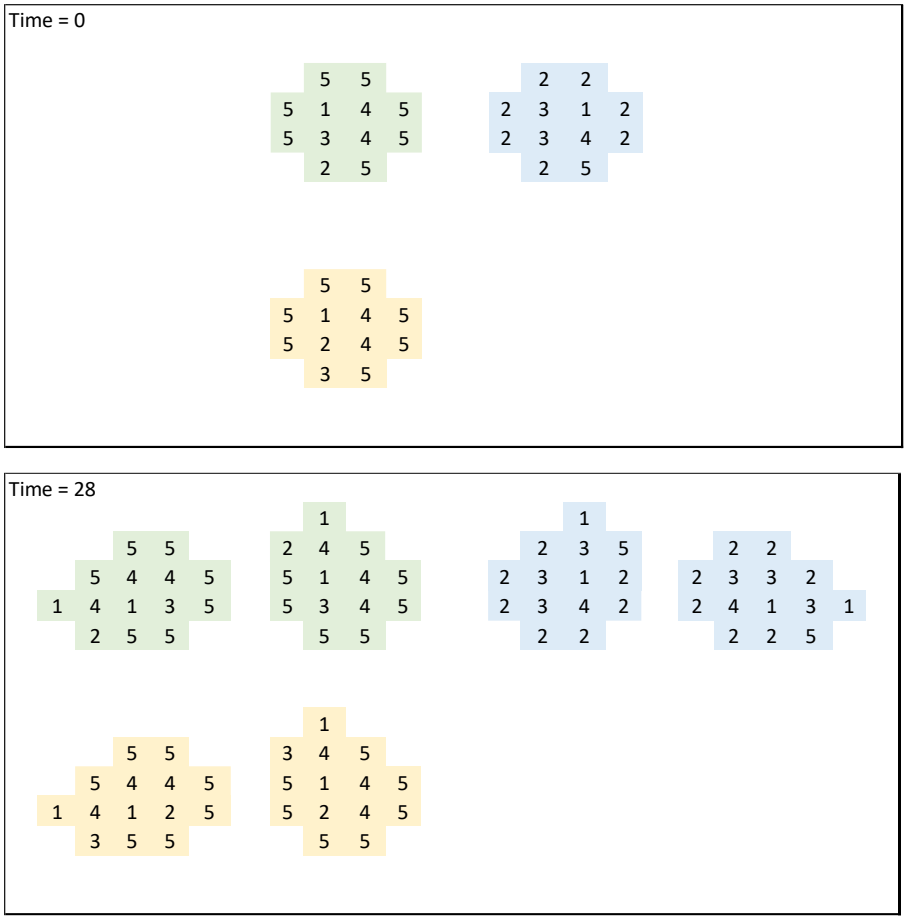

Figure 4. The Moore rules state-transition functions supporting L-loop replication under state-set permutations 12345 → 15432 (green), and 12345 → 15423 (gold) incorporate no contradictory rules, so a pooling of the 12345 → 12345 R-loop (blue) replication state transition function with these two L loop state-transition functions delivers a comprehensive, consistent transition function which supports replication of the blue, green and gold structures in a common CA universe.

The coexistence of self-replication under state-set permutations 12345 → 14523 and 12345 → 14532 (Figure 3), and 12345 → 15432 and 12345 → 15423 (Figure 4) depends in each case on corresponding Moore rules state-transition functions, but the pairs of coexisting L-loop replications in each case cannot coexist under their corresponding von Neumann rules state-transition functions. Within the L-Loop von Neumann rules state-transition functions, there are 19 rule contradictions in each case (analysis not shown).

Discussion

In the H-H Chou and JA Reggia model [3], the cell state-transition function incorporates both achiral and chiral rules which respectively support the appearance of replicators, and the replication of these structures [7]. Spontaneous replicator formation (analogous to non-autocatalytic formation) occurs by implementation of an achiral subset of rules within the cell state-transition function, then “autocatalytic” replication occurs by implementation of “bound” rules which include chiral rules. Chirality in the system appears immediately on the appearance of 2x2 cell chiral replicating structures {O, O; L, >} which replicate by application

of the bound rules subset (which includes the chiral rules) within the cell state-transition function.

The dynamics of the model described in [3] differs from the models described in [1, 4] where a hypothetical ancestral system includes a racemic mixture of left- and right-handed replicators, and one chirality only gradually becomes permanently dominant. In [3], chirality is always inherent in the system by the presence of a subset of “bound” rules which includes the chiral rules of the system’s cell state-transition function, therefore there cannot be any racemic mixture of replicating structures in the system. Reviewing all models of replicating loops in CA space, the historical emergence of replicators is generally not considered (*e.g.*, [2, 5]), as the intent in these studies was restricted to the question of the minimal degree of complexity required for the phenomenon of replication. Considering all studied systems of self-replicating loops in CA space ([2, 3, 5] and others) the logical impossibility of racemic mixtures of replicators may indicate a fundamental difference between the logic of replication of earth’s biological replicators and the essentially-chiral logic of replication of two-dimensional loop structures in CA spaces.

While strict heterochiral replication of loop structures in CA spaces is not supported, a less-strict functional heterochiral replication can be implemented in which right-handed replication can coexist with left-handed replication of a structure consisting of a different arrangement of cell states, but which replicates by the same mechanism.

Instances of functional heterochiral replication can be achieved by expanding the number of active cell states in the cell state set. This simple solution can work by creating two disjunct cell state-transition functions (one for each chirality) within one comprehensive, consistent transition function. However, it was shown in [8] that functional heterochiral replication of the J. Byl structure is more-economically achieved by applying a cell state-set permutation from a set of six suitable permutations to just one chirality (left- **or** right-handed replication), without adding any more states to the set of possible cell states. It is an interesting observation that removing one broken symmetry (achievement of functional heterochiral replication) is only possible with the introduction of a different broken symmetry.

References

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