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# On Irreducible Reaction Systems

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## ABSTRACT

Reaction system, introduced by Ehrenfeucht and Rozenberg as a computational model inspired by biochemical reactions in the living cells, has been widely studied from diverse directions. Our work belongs to the research line that concentrates on the mathematical property of the state transition functions specified by reaction systems and, particularly, focuses on irreducibility and reaction system rank. We showed that for any state transition function $f$ and any integer $n$ between the reaction system rank of $f$ and some upper bound depending on $f$, an irreducible reaction system of size $n$ that specifies $f$ can be obtained.

**Keywords:** Natural Computing, Biochemical Reaction, Reaction System Rank, Functionally Equivalent, Focus Function.

# 1. Introduction

Reaction system, introduced in Ehrenfeucht and Rozenberg (2007b), is a formal model of computation motivated by biochemical reactions taking place in the living cells. The central idea is that the interactions between individual reactions are regulated according to the mechanisms of facilitation and inhibition. The simple and crisp definition of reaction system facilitates qualitative analysis of the biological process.

The basic framework of reaction systems allows for various biological motivated extensions, including dynamic causalities [Barbuti et al. (2016)], mass conservation [Azimi et al. (2015)], time [Ehrenfeucht and Rozenberg (2009)], and events [Ehrenfeucht and Rozenberg (2007a)]. Furthermore, a few newfound studies are based on reaction systems, including reaction automata [Okubo et al. (2012)], zoom structures [Ehrenfeucht and Rozenberg (2014)], a proof calculus called reaction algebra [Pardini et al. (2014)], and a new genetic programming framework called evolutionary reaction system [Manzoni et al. (2013)]. Just recently, Ehrenfeucht et al. (2017) proposed a more general framework where the set of reactions of a reaction system can evolve over time, which opens up wide range of further study.

Our work pertains to purely mathematical study of reaction systems, which has largely focused on two sub-directions, namely, state sequences generated by state transition functions [Ehrenfeucht et al. (2011), Salomaa (2015a), Salomaa (2012a), and Salomaa (2012b)] and minimal reaction systems [Ehrenfeucht et al. (2012), Manzoni et al. (2014), Salomaa (2013), and Salomaa (2015b)]. Particularly, we focus on irreducibility and reaction system rank, two rather new notions introduced in Teh and Atanasiu (2017a). A reaction system is said to be irreducible if no proper subset of its set of reactions can specify to the same state transition function. This leads canonically to a classification of an individual state transition function according to the size, called reaction system rank, of a minimal set of reactions that specifies the function. This work is motivated by the following question, attempted by the first author while working on Teh and Atanasiu (2017b).

**Question 1.1.** *What is the largest possible size of an irreducible reaction system over a given background set?*

Throughout the work of Teh and Atanasiu (2017b), a canonical assumption was adopted that requires distinct reactions in a reaction system do not have the same reactant set and inhibitor set. Under that assumption, the reaction system produced in Example 18 in Teh and Atanasiu (2017b) was believed to be an irreducible reaction system having the largest possible size, coincidently also 18, for a background set of size three. However, a theoretical proof remains elusive from us and a computational verification is not feasible due to hardware limitation.

Surprisingly, when that assumption is dropped, there is a clean simple answer to the question. This initial result is generalized in this paper and the largest possible size of an irreducible reaction system specifying a given state transition function is obtained. Finally, we show the existence of an irreducible reaction system specifying a given state transition function such that its size is any given integer between two established bounds.

# 2. Preliminaries

If $S$ is an arbitrary finite set, then $\sharp S$ denotes its cardinality and $2^S$ denotes its power set.

**Definition 2.1.** *Suppose $S$ is a finite nonempty set. A* reaction in $S$ *is a triple $a = (R_a, I_a, P_a)$, where $R_a$ and $I_a$ are disjoint (possibly empty) subsets of $S$ and $P_a$ is a nonempty subset of $S$. The sets $R_a$, $I_a$, and $P_a$ are the* reactant set, inhibitor set, *and* product set *respectively.*

**Definition 2.2.** *A* reaction system *is a pair $\mathcal{A} = (S, A)$ where $S$ is a finite nonempty set and $A$ is a (possibly empty) set of reactions in $S$. The set $S$ is called the* background set of $\mathcal{A}$.

The following defines the state transition function specified by a reaction system.

**Definition 2.3.** *Suppose $\mathcal{A} = (S, A)$ is a reaction system. The* function specified by $\mathcal{A}$, *denoted* $\mathrm{res}_{\mathcal{A}}$, *is given by*

$$\mathrm{res}_{\mathcal{A}}(X) = \bigcup_{\substack{a \in A \\ R_a \subseteq X, I_a \cap X = \emptyset}} P_a \quad , \quad \textit{for all } X \subseteq S.$$

From now on, we fix a finite nonempty background set $S$. For a reaction $a$ in $S$ and $X \subseteq S$, if $R_a \subseteq X$ and $I_a \cap X = \emptyset$, then we say that $a$ is *enabled by* $X$. The collection of subsets $X$ of $S$ such that $a$ is enabled by $X$ is denoted by $\mathrm{encoll}(a)$, that is,

$$\mathrm{encoll}(a) = \{\, X \subseteq S \mid R_a \subseteq X \text{ and } I_a \cap X = \emptyset \,\}.$$

Every function $f\colon 2^S \to 2^S$ is called an *rs function over* $S$. It is said to be *null* if $f(X) = \emptyset$ for all $X \in 2^S$ and *nonnull* otherwise. Hence, every function specified by a reaction system is an rs function over the corresponding background set. Conversely, every rs function over $S$ can be canonically specified by a *maximally inhibited* reaction system $(S, A)$ in the sense that $I_a = S \backslash R_a$ for every reaction $a \in A$.

**Definition 2.4.** *Suppose* $\mathcal{A} = (S, A)$ *is a reaction system. If* $a \in A$*, we say that* $(R_a, I_a)$ *is the* core of $a$*, denoted by* $\mathrm{core}(a)$*. The* core of $\mathcal{A}$ *is*

$$\mathrm{core}(\mathcal{A}) = \{\, \mathrm{core}(a) \mid a \in A \,\}.$$

We emphasize that in this work, distinct reactions in a reaction system can have the same core.

**Definition 2.5.** *Suppose* $\mathcal{A}$ *and* $\mathcal{B}$ *are reaction systems with the same background set* $S$*. Then* $\mathcal{A}$ *and* $\mathcal{B}$ *are functionally equivalent iff* $\mathrm{res}_{\mathcal{A}} = \mathrm{res}_{\mathcal{B}}$*, that is,* $\mathrm{res}_{\mathcal{A}}(X) = \mathrm{res}_{\mathcal{B}}(X)$ *for all* $X \subseteq S$*.*

When the background is understood, a reaction system $\mathcal{A} = (S, A)$ can be identified with $A$. Hence, we may write $\mathrm{res}_A$ for $\mathrm{res}_{\mathcal{A}}$.

The next two definitions were recently introduced in Teh and Atanasiu (2017a).

**Definition 2.6.** *Suppose* $\mathcal{A} = (S, A)$ *is a reaction system. We say that* $\mathcal{A}$ *is irreducible if and only if* $\mathrm{res}_A \neq \mathrm{res}_B$ *for every proper subset* $B$ *of* $A$*.*

**Remark 2.1.** *A reaction system* $\mathcal{A} = (S, A)$ *is reducible if and only if* $\mathrm{res}_A = \mathrm{res}_{A\backslash\{a\}}$ *for some* $a \in A$*.*

**Definition 2.7.** *Suppose* $f$ *is an rs function over* $S$*. The* reaction system rank of $f$*, denoted* $\mathrm{rsrank}(f)$*, is defined by*

$$\mathrm{rsrank}(f) = \min\{\, \sharp A \mid \mathcal{A} = (S, A) \textit{ is a reaction system such that } \mathrm{res}_{\mathcal{A}} = f \,\}.$$

If $f = \mathrm{res}_{\mathcal{A}}$ and $\sharp A = \mathrm{rsrank}(f)$, then we say that $\mathcal{A} = (S, A)$ witnesses the reaction system rank of $f$. Note that if $\mathcal{A}$ is a witness of $\mathrm{rsrank}(f)$, then $\mathcal{A}$ must be irreducible.

The following notion plays a key role in the classfication of functions specified by minimal reaction systems [Ehrenfeucht et al. (2012) and Teh and Atanasiu (2017b)].

**Definition 2.8.** *An rs function $f$ over $S$ is a* focus function *iff $f$ is null or there exists $q \in S$ such that*

$$\textit{for every } X \subseteq S, \textit{ if } f(X) \neq \emptyset, \textit{ then } f(X) = \{q\}.$$

Suppose $f$ is an rs function over $S$ and $q \in S$. Let $f^q$ be defined by

$$f^q(X) = f(X) \cap \{q\} \text{ for all } X \subseteq S.$$

Then $f^q$ is a focus function. Also, $f = \bigcup_{q \in S} f^q$, that is, $f(X) = \bigcup_{q \in S} f^q(X)$ for all $X \subseteq S$.

Suppose $\mathcal{A} = (S, A)$ is a reaction system and $q \in S$. Define a reaction system $\mathcal{A}^q = (S, A^q)$ by

$$A^q = \{ (R_a, I_a, \{q\}) \mid a \in A \text{ and } q \in P_a \}.$$

If $f = \text{res}_{\mathcal{A}}$, then $f^q = \text{res}_{\mathcal{A}^q}$. Additionally, $\text{res}_{\mathcal{A}} = \bigcup_{q \in S} \text{res}_{\mathcal{A}^q}$. Furthermore, if $\mathcal{A}$ and $\mathcal{B}$ are functionally equivalent, then $\mathcal{A}^q$ and $\mathcal{B}^q$ are functionally equivalent for every $q \in S$.

The following is an equivalent reformulation of Theorem 35 in Teh and Atanasiu (2017b). Both the theorem and the ensuing lemma are needed for our main result.

**Theorem 2.1** (Teh and Atanasiu (2017b))**.** *Suppose $f$ is an rs function over $S$. Then* $\text{rsrank}(f)$ *is equal to*

$$\min\{ \sharp \bigcup_{q \in S} \text{core}(\mathcal{A}_q) \mid \mathcal{A}_q \textit{ is irreducible and } f^q = \text{res}_{\mathcal{A}_q} \textit{ for each } q \in S \}.$$

**Lemma 2.1.** *Suppose $\mathcal{A} = (S, A)$ is a reaction system. If $\mathcal{A}^q$ is irreducible for every $q \in S$ and $P_a \cap P_{a'} = \emptyset$ whenever $a$ and $a'$ are distinct elements of $A$ such that* $\text{core}(a) = \text{core}(a')$*, then $\mathcal{A}$ is irreducible.*

*Proof.* We argue by contradiction. Assume $\mathcal{A}$ is reducible. Then $\text{res}_A = \text{res}_{A \setminus \{a\}}$ for some $a \in A$. Choose $q \in P_a$. By the hypothesis, $q \notin P_{a'}$ for every $a' \in A$ distinct from $a$ such that $\text{core}(a') = \text{core}(a)$. Hence, $(R_a, I_a, \{q\}) \in A^q \setminus (A \setminus \{a\})^q$. Therefore, $(A \setminus \{a\})^q$ is a proper subset of $A^q$. However, $\text{res}_A = \text{res}_{A \setminus \{a\}}$ implies that $\text{res}_{A^q} = \text{res}_{(A \setminus \{a\})^q}$, contradicting the irreducibility of $\mathcal{A}^q$. □

Conversely, irreducibility of $\mathcal{A}$ does not imply irreducibility of $\mathcal{A}^q$ for every $q \in S$. For example, let $\mathcal{A} = (\{1,2,3\}, A)$ where

$$A = \{(\{1\},\{3\},\{1,2\}),(\{1,2\},\{3\},\{1,3\})\}.$$

Then $\mathcal{A}$ is irreducible but $\mathcal{A}^1$ is reducible.

# 3. Main Results

**Definition 3.1.** *Suppose $f$ is an rs function over $S$. Define*

$$\mathscr{G}_f = \{\, (X,q) \in 2^S \times S \mid q \in f(X) \,\}.$$

**Theorem 3.1.** *Suppose $f$ is an rs function over $S$ and suppose $\mathcal{A} = (S, A)$ is an irreducible reaction system such that $\mathrm{res}_{\mathcal{A}} = f$. Then $\sharp A \le \sharp \mathscr{G}_f$ and equality holds if and only if $A = \{\, (X, S\backslash X, \{q\}) \mid q \in S, X \subseteq S, \text{and } q \in f(X) \,\}$.*

*Proof.* For each $(X,q) \in \mathscr{G}_f$, since $q \in \mathrm{res}_{\mathcal{A}}(X)$, we can choose a reaction $a \in A$ such that $a$ is enabled by $X$ and $q \in P_a$; each such choice will be denoted by $a_{(X,q)}$. Let $A' = \{\, a_{(X,q)} \mid (X,q) \in \mathscr{G}_f \,\}$. Note that $A' \subseteq A$ and $\sharp A' \le \sharp \mathscr{G}_f$. (The choices made may coincide for distinct elements of $\mathscr{G}_f$.)

**Claim 3.1.** $\mathrm{res}_{A'} = \mathrm{res}_A$.

*Proof of claim.* Suppose $X \subseteq S$. Obviously, $\mathrm{res}_{A'}(X) \subseteq \mathrm{res}_A(X)$ because $A' \subseteq A$. Conversely, suppose $q \in \mathrm{res}_A(X)$. Then $(X,q) \in \mathscr{G}_f$ by the definition of $\mathscr{G}_f$. By our choice, $a_{(X,q)}$ is enabled by $X$ and $q \in P_{a_{(X,q)}}$. Since $a_{(X,q)} \in A'$, it follows that $q \in \mathrm{res}_{A'}(X)$ by definition. Thus $\mathrm{res}_A(X) \subseteq \mathrm{res}'_A(X)$. □

Since $A' \subseteq A$ and $A$ is irreducible, by the claim, $A' = A$ and thus $\sharp A \le \sharp \mathscr{G}_f$.

Now, let $B = \{\, (X, S\backslash X, \{q\}) \mid q \in S, X \subseteq S, \text{and } q \in f(X) \,\}$. Note that $B$ is irreducible, $\mathrm{res}_B = f$, and $\sharp B = \sharp \mathscr{G}_f$. If $A = B$, then $\sharp A = \sharp \mathscr{G}_f$. Conversely, suppose $\sharp A = \sharp \mathscr{G}_f$. To see that $A = B$, it suffices to show that $A \subseteq B$. Suppose $a \in A$, $X \in \mathrm{encoll}(a)$, and $q \in P_a$. Then $(X,q) \in \mathscr{G}_f$ and we can choose $a_{(X,q)}$ to be $a$. Assume there exists $(X', q')$ distinct from $(X,q)$ such that $X' \in \mathrm{encoll}(a)$, and $q' \in P_a$ as well. Then we can also choose $a_{(X',q')}$ to be $a$. Hence, we may obtain $A'$ based on our choices where $\sharp A' < \sharp \mathscr{G}_f = \sharp A$. However, by the claim, this contradicts the irreducibility of $\mathcal{A}$. Therefore, it must be the case that $\mathrm{encoll}(a) = \{X\}$ and $P_a = \{q\}$, which means $a = (X, S\backslash X, \{q\})$. It follows that $a \in B$ as required. □

**Corollary 3.1.** *Suppose $\mathcal{A} = (S, A)$ is an irreducible reaction system. Then $\sharp A \le 2^{\sharp S} \times \sharp S$ and the upper bound is attainable exactly when*

$$A = \{\, (X, S\backslash X, \{q\}) \mid X \subseteq S \text{ and } q \in S \,\}.$$

*Proof.* Let $f = \mathrm{res}_{\mathcal{A}}$. The inequality follows by Theorem 3.1 because $\mathscr{G}_f \subseteq 2^S \times S$. The upper bound is attainable when $\mathscr{G}_f = 2^S \times S$, that is, when $f(X) = S$ for all $X \subseteq S$ and thus, by Theorem 3.1 again, when $A = \{\, (X, S\backslash X, \{q\}) \mid X \subseteq S$ and $q \in S \,\}$. □

**Lemma 3.1.** *Suppose $f$ is a focus function over $S$. For every integer $n$ such that $\mathrm{rsrank}(f) \le n \le \sharp\{\, X \subseteq S \mid f(X) \neq \emptyset \,\}$, there exists an irreducible reaction system $\mathcal{A} = (S, A)$ such that $\mathrm{res}_{\mathcal{A}} = f$ and $\sharp A = n$.*

*Proof.* The result follows trivially when $f$ is null because then $\mathrm{rsrank}(f) = 0$ and $\mathrm{res}_{\emptyset} = f$. Suppose $f$ is nonnull. Let $\mathscr{F} = \{\, X \subseteq S \mid f(X) \neq \emptyset \,\}$. We argue by contradiction. Let $n$ be the least integer such that $\mathrm{rsrank}(f) \le n \le \sharp\mathscr{F}$ and no irreducible reaction system $\mathcal{A} = (S, A)$ such that $\mathrm{res}_{\mathcal{A}} = f$ and $\sharp A = n$ exists. By definition of $\mathrm{rsrank}(f)$, we know that $n > \mathrm{rsrank}(f)$.

Now, let $\mathcal{B} = (S, B)$ be an irreducible reaction system such that $f = \mathrm{res}_{\mathcal{B}}$, $\sharp B = n-1$, and $\sum_{b \in B} \sharp\, \mathrm{encoll}(b)$ is minimal among such reaction systems. Since $\sharp B < \sharp\mathscr{F}$ and $\bigcup_{b \in B} \mathrm{encoll}(b) = \mathscr{F}$, we can choose $b_0 \in B$ such that $\mathrm{encoll}(b_0)$ is not a singleton and thus $I_{b_0} \neq S\backslash R_{b_0}$. Choose any $x \in S\backslash(R_{b_0} \cup I_{b_0})$. Let $b_1 = (R_{b_0} \cup \{x\}, I_{b_0}, P_{b_0})$ and $b_2 = (R_{b_0}, I_{b_0} \cup \{x\}, P_{b_0})$. Then $\mathrm{res}_{\{b_1, b_2\}} = \mathrm{res}_{\{b_0\}}$ because $\mathrm{encoll}(b_0) = \mathrm{encoll}(b_1) \cup \mathrm{encoll}(b_2)$.

Let $B' = \{b_1, b_2\} \cup (B\backslash\{b_0\})$. Then

$$\mathrm{res}_{B'} = \mathrm{res}_{\{b_1,b_2\}} \cup \mathrm{res}_{B\backslash\{b_0\}} = \mathrm{res}_{\{b_0\}} \cup \mathrm{res}_{B\backslash\{b_0\}} = \mathrm{res}_B = f.$$

Since $B'$ has size $n$, $\mathcal{B}' = (S, B')$ must be reducible. Note that if $C$ is any subset of $B'$ such that $\mathrm{res}_C = f$, then $B\backslash\{b_0\} \subseteq C$; otherwise,

$$f = \mathrm{res}_{C \cup \{b_1,b_2\}} = \mathrm{res}_{\{b_1,b_2\}} \cup \mathrm{res}_{C \cap B\backslash\{b_0\}} = \mathrm{res}_{\{b_0\}} \cup \mathrm{res}_{C \cap B\backslash\{b_0\}} = \mathrm{res}_{\{b_0\} \cup (C \cap B\backslash\{b_0\})},$$

contradicting the irreducibility of $\mathcal{B}$. Hence, $f = \mathrm{res}_{\{b_i\} \cup (B\backslash\{b_0\})}$ for some $i \in \{1, 2\}$.

Let $B'' = \{b_i\} \cup (B\backslash\{b_0\})$. Since $f \neq \mathrm{res}_{B\backslash\{b_0\}}$, it follows that $\mathcal{B}'' = (S, B'')$ is an irreducible reaction system such that $f = \mathrm{res}_{\mathcal{B}''}$ and $\sharp B'' = n - 1$. However, $\sum_{b \in B''} \sharp\, \mathrm{encoll}(b) < \sum_{b \in B} \sharp\, \mathrm{encoll}(b)$ because $\sharp\, \mathrm{encoll}(b_i) < \sharp\, \mathrm{encoll}(b_0)$, contradicting the minimality of $B$. □

**Theorem 3.2.** *Suppose $f$ is an rs function over $S$. For every integer $n$ such that* $\operatorname{rsrank}(f) \leq n \leq \sharp\mathscr{G}_f$*, there exists an irreducible reaction system* $\mathcal{A} = (S, A)$ *such that* $\operatorname{res}_{\mathcal{A}} = f$ *and* $\sharp A = n$.

*Proof.* For each $q \in S$, let $\mathscr{F}_q = \{ X \subseteq S \mid f^q(X) \neq \emptyset \}$. Note that $\mathscr{G}_f = \bigcup_{q \in S} \{ (X, q) \mid X \in \mathscr{F}_q \}$ and thus $\sharp\mathscr{G}_f = \sum_{q \in S} \sharp\mathscr{F}_q$. By Theorem 2.1, we choose an irreducible reaction system $\mathcal{A}_q = (S, A_q)$ with $f^q = \operatorname{res}_{\mathcal{A}_q}$ for each $q \in S$ such that $\sharp \bigcup_{q \in S} \operatorname{core}(\mathcal{A}_q) = \operatorname{rsrank}(f)$.

First, we show that the required reaction system exists for every integer $n$ such that $\sum_{q \in S} \sharp A_q \leq n \leq \sharp\mathscr{G}_f$. Fix an arbitrary such integer $n$. Since $\sharp\mathscr{G}_f = \sum_{q \in S} \sharp\mathscr{F}_q$, we can choose an integer $n_q$ with $\sharp A_q \leq n_q \leq \sharp\mathscr{F}_q$ for each $q \in S$ such that $\sum_{q \in S} n_q = n$. For each $q \in S$, by Lemma 3.1, we can choose an irreducible reaction system $\mathcal{B}_q = (S, B_q)$ such that $\operatorname{res}_{\mathcal{B}_q} = f^q$ and $\sharp B_q = n_q$. Take $\mathcal{B} = (S, B)$ where $B = \bigcup_{q \in S} B_q$. Note that $\sharp B = \sum_{q \in S} n_p = n$ and $\operatorname{res}_{\mathcal{B}} = \bigcup_{q \in S} \operatorname{res}_{\mathcal{B}_q} = \bigcup_{q \in S} f^q = f$. Furthermore, by Lemma 2.1, $\mathcal{B}$ is irreducible because $\mathcal{B}^q = \mathcal{B}_q$ is irreducible for every $q \in S$.

Now, we show that the required reaction system exists for every integer $m$ such that $\operatorname{rsrank}(f) \leq m < \sum_{q \in S} \sharp A_q$. Fix an arbitrary such integer $m$. Let $U = \bigcup_{q \in S} \operatorname{core}(\mathcal{A}_q)$. Thus $\operatorname{rsrank}(f) = \sharp U$. Note that

$$\sum_{q \in S} \sharp A_q = \sum_{(R,I) \in U} \sharp\{ q \in S \mid (R, I, \{q\}) \in A_q \}.$$

Therefore, we can choose $m_{(R,I)}$ with $1 \leq m_{(R,I)} \leq \sharp\{ q \in S \mid (R, I, \{q\}) \in A_q \}$ for every $(R, I) \in U$ such that $\sum_{(R,I) \in U} m_{(R,I)} = m$. For each $(R, I) \in U$, choose mutually disjoint subsets $P_{(R,I),1}, P_{(R,I),2}, \ldots, P_{(R,I),m_{(R,I)}}$ of $S$ such that

$$P_{(R,I),1} \cup P_{(R,I),2} \cup \cdots \cup P_{(R,I),m_{(R,I)}} = \{ q \in S \mid (R, I, \{q\}) \in A_q \}.$$

Consider the reaction system $\mathcal{C} = (S, C)$ where

$$C = \bigcup_{(R,I) \in U} \{(R, I, P_{(R,I),1}), (R, I, P_{(R,I),2}), \ldots, (R, I, P_{(R,I),m_{(R,I)}})\}.$$

Note that $\sharp C = \sum_{(R,I) \in U} m_{(R,I)} = m$. Furthermore, $C^q = A_q$ and thus $\mathcal{C}^q$ is irreducible for each $q \in S$. Therefore, by Lemma 2.1 again, $\mathcal{C}$ is irreducible. Finally, $\operatorname{res}_{\mathcal{C}} = \bigcup_{q \in S} \operatorname{res}_{\mathcal{C}^q} = \bigcup_{q \in S} \operatorname{res}_{\mathcal{A}_q} = \bigcup_{q \in S} f^q = f$. □

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