Splicing System: from Biology to Computer Science & Mathematics

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DNA Computing

• DNA computing has emerged in the last twenty years as an exciting new research field at the intersection of Biology, Computer Science, Mathematics and Engineering.







- The field has blossomed rapidly, with development of significant **theoretical** and **experimental** results by researchers from **interdisciplinary** areas.
- **Different models** of molecular computation have been proposed in scientific society including Splicing Models and Sticker Models.











• DNA, or deoxyribonucleic acid, is the hereditary material in humans and almost all other organisms (animals, plants etc).













• Two single strands of DNAs can be linked together with the hydrogen bonds between their bases and hence form a helical shape called double stranded DNA (dsDNA).







• In 1953, it was shown that the bases can join only complimentarily, A with T and G with C respectively.















• DNA molecules can be cut by restriction enzymes at specific places based on the cutting sites of the restriction enzymes.

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Sticky end (e.g. Acil)
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5′...C▼CGC...3′
3′...GGC▲G...5′
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Blunt end (e.g. Afel)

5'....AGC▼GCT....3' 3'....TCG▲CGA....5'





- Every restriction enzyme has a triple known as the cleavage pattern of the enzyme.
- The triple is denoted as a rule for the restriction enzyme which consists of left context, crossing and right context (Head, 1998).
- The restriction enzyme *EcoRI* is isolated from the bacterium Escherichia coli with strain serotype *R*; I indicates the first enzyme discovered from the bacterium.
- The cleavage pattern of restriction enzyme *EcoRI* is



left context crossing right context

Head, T. (1998). Splicing Representations of Strictly Locally Testable Languages. *Discrete Applied Mathematics*, 87(1), 139-147.





• A restriction enzyme is an enzyme that cuts double-stranded or single stranded DNA at specific recognized nucleotide sequences, known as restriction sites.







*EcoR*I: ([G/C],[A/T],[A/T],[T/A],[T/A],[C/G])



MfeI: ([C/G], [A/T], [A/T], [T/A], [T/A], [G/C])







• DNA ligase is an enzyme that can catalyze the linking of DNA strands together by forming a phosphodiester bond.









S = (A, I, B, C)



Previous Molecular Works on Splicing Systems

Author	Description
Laun and Reddy 1999	The first experiment on the splicing system using restriction enzymes Bgll and Drall
Fong 2008	The adult and limit languages from Head's splicing model using restriction enzymes <i>Hpa</i> ll and Acil
Karimi 2013	Verification of the persistency properties of splicing systems involving restriction enzymes CvaQI and Acc65I
Yusof et al. 2015	Yusof-Goode splicing system with restriction enzymes Acll and Acil using limit graph approach
Ahmad et al. 2018	Experiment on second order limit language from Yusof-Goode splicing system using restriction enzyme <i>Dpn</i> II
Ismail 2020	Experiment using the restriction enzymes <i>CviQl</i> and <i>Acil</i> to verify the generalisation of splicing system involving palindromic and non-palindromic rules

Laun, E., & Reddy, K. J. (1999). Wet Splicing Systems. Paper presented at the 3rd DIMACS Workshop on DNA Based Computers, University of Pennsylvania, Philadelphia. Fong, W. H. (2008). Modelling of Splicing Systems using Formal Language Theory. (Ph.D. Thesis), Universiti Teknologi Malaysia, Skudai, Malaysia.

Karimi, F. (2013). Mathematical Modelling of Persistent Splicing Systems in DNA Computing. (Ph.D. Thesis), Universiti Teknologi Malaysia, Johor, Malaysia.

Yusof, Y., Lim, W. L., Goode, T. E., Sarmin, N. H., Heng, F. W., & Wahab, M. F. A. (2015). *Molecular Aspects of DNA Splicing System*. Paper presented at the International Conference on Mathematics, Engineering and Industrial Applications 2014 (ICoMEIA 2014), Penang, Malaysia.

Ahmad, M. A., Sarmin, N. H., Abdul-Wahab, M. F., Heng, F. W., & Yusof, Y. (2018). Biomolecular Aspects of Second Order Limit Language. *Malaysian Journal of Fundamental and Applied Sciences*, 14(1), 15-19.

Ismail, N. I. (2020). Generalisations of Splicing Languages From DNA Splicing Systems. (Ph.D. Thesis), Universiti Teknologi Malaysia, Skudai, Malaysia.

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Visit to wet lab, State University of New York, Binghamton, New York, USA 2007





























Definition 1 (Head, 1987) Splicing System and Splicing Language

A splicing system, S = (A, I, B, C) consists of

- A: finite alphabet
- *I*: a finite set of initial strings in *A**
- B and C: finite sets of triples (c, x, d) with c, x and d in A*
- Triples in *B* are called left patterns
- Triples in *C* are called right patterns

For each such triple the string *cxd* is called a site and the string *x* is called a crossing.

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A language, L is a splicing language if there exists a splicing system S for which L = L(S).
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DNA Splicing System (Cont.)



Example 1

Suppose that S = (A, I, B, C) is a splicing system in which $A = \begin{cases} A, C, G, T \\ T & G & C & A \end{cases}$ is the set of dsDNA symbols, $I = \begin{cases} GAATTCTCTGTAAT \\ CTTAAGAGACATTA \end{cases}$ is the set consisting of an initial string of molecules, set $B = \{ \begin{pmatrix} G & AATT & C \\ C' & T & TAA' & G \end{pmatrix} \}$ is the set of cleavage pattern for the enzyme **EcoRI** and set *C* is the empty set.

The initial string is shown in the following:

5'-GAATTCTCTGTAAT-3' 3'-CTTAAGAGACATTA-5''

or written 180 degree wise,

5'-ATTACAGAGAATTC-3' 3'-TAATGTCTCTTAAG-5'



DNA Splicing System (Cont.)





Wet Splicing System involving CviQI and Acil

	Lane 1	Lane 2	Lane 3	Lane 4	Lane 5
	(LMW ladder)	(0 minute)	(30 minutes)	(60 minutes)	(2 hours)
766				· ·	
500					\equiv
350					
300	, <u> </u>				
250					
200					
150	<				
100				/	
75					
50			/	/	/
25	·				

	Lane 1 (LMW ladder)	Lane 2 (0 minute)	Lane 3 (30 minutes)	Lane 4 (60 minutes)	Lane 5 (2 hours)	
766 -						
500						🕳 336 bp
250 -				Summer and summer and	-	🛶 248 bp
150-					l	 160 bp 125 bp
100- 75 -			-			← 79 bp, 81 bp ← 72 bp
50 —	_					
						🗲 44 bp
						🍨 35 bp
25 -						

• Lane 1: LMW ladder

• Lane 2 (0 minute): 79 bp (or 81 bp), 125 bp and 160 bp

- Lane 3 (30 minutes): 35 bp, 44 bp, 79 bp, 81 bp, 125 bp, 160 bp, 248 bp
- Lane 4 (60 minutes): 35 bp, 44 bp, 79 bp, 81 bp, 125 bp, 160 bp, 248 bp
- Lane 5 (2 hours): 35 bp, 44 bp, 72 bp, 79 bp, 81 bp, 125 bp, 160 bp,

248 bp, 336 bp

Theoretical vs Lab Results



Wet Splicing System involving CviQI

	Lane 1	Lane 2	Lane 3	Lane 4	Lane 5
	(LMW ladder)	(0 minute)	(30 minutes)	(60 minutes)	(2 hours)
766					
500					
350					
300					
250					
200					
150					
100			/	/	/
75	· ·				
50			/	/	/
25					

	Lane 1 (LMW ladder)	Lane 2 (0 minute)	Lane 3 (30 minutes)	Lane 4 (60 minutes)	Lane 5 (2 hours)	
	· ·			·*···		
766 -						
350 - 300 -						240 h -
250 -						🔶 248 бр
150 -	_					+ 160 bp
100 —			and the second second			🔶 125 bp
75 —						🔶 72 bp
50 —						
						🛨 35 bp
25 -						

- Lane 1: LMW ladder
- Lane 2 (0 minute): 160 bp
- Lane 3 (30 minutes): 35 bp, 72 bp, 125 bp, 160 bp and 248 bp
- Lane 4 (60 minutes): 35 bp, 72 bp, 125 bp, 160 bp and 248 bp
- Lane 5 (2 hours): 35 bp, 72 bp, 125 bp, 160 bp and 248 bp

Theoretical vs Lab Results



Wet Splicing System involving Acil





- Lane 1: LMW ladder
- Lane 2 (0 minute): 79 bp (or 81 bp) and 160 bp
- Lane 3 (30 minutes): 79 bp, 81 bp and 160 bp
- Lane 4 (60 minutes): 79 bp, 81 bp and 160 bp
- Lane 5 (2 hours): 79 bp, 81 bp and 160 bp

Programming Code



• A C++ program is created in **Microsoft Visual Studio** to **develop the GUI** for DNA splicing systems involving palindromic and non-palindromic rules.

DNA Splicing System with Palindromic and N	Ion-Palindromic Rules			- <u></u> -		х
Instruction: Insert the initial string a	and the cleavage pattern of the enzyme	(s).				
Initial string]		Insert the initial	DNA stri	ing	
Enzyme 1 ,		Ins	ert the cleavage pat	tern of	the e	enzyr
Compute	Clear					
Click 'Compute'	Click 'Clear' button					
button to generate the results	to reset the interface					

Graphical User Interface (GUI)



Output of GUI for DNA Splicing System involving One Rule

E DNA Splicing System	with Palindromic and Non-Palindromic Rules	– 🗆 X
Instruction: Inse	rt the initial string and the cleavage pattern of the enzyme(s).	l.
Initial string	aggactagtct	
Enzyme 1	c , ta , g ,	One restriction enzyme is inserted by user
The ini		
5'	A G G A C T A G T C T -3' T C C T G A T C A G A -5'	oxes indicate the cutting site of the restriction enzyme found in the initial string
Restric	tion site of the enzyme :	
Tł	5'-CTAG-3' e enzyme 3'-GATC-5'	dromic crossing. The algorithm determines if the restriction enzyme is palindrome or not a palindrome including crossing
The nu The re	mber of cutting sites found: 1 The a sulting molecules: Case 1	algorithm states the number of cutting sites
5' 3'	(A G G A + A G A) C T A G [T C T + T C C (T C C T + T C T) G A T C [A G A + A G G	C T J -3' G A J -5'
	4 2	
The algorit	nm generates all the splicing languag	iges in the second s

Additional features:

- Certain messages are displayed on the interface if the number of cutting sites found exceeds two
- The interface prompts the users if the cutting sites of restriction enzyme overlap
- The users will be notified if the inputs are incorrect.

DNA Splicing System with Palindromic and Non-Palindromic Rules

Compute

The initial molecule:

Restriction site of the enzyme :

Initial string

Enzyme 1

Enzyme 2

Instruction: Insert the initial string and the cleavage pattern of the enzyme(s).

cg

cg

5'-ATTCGACTGCGCAGA-3'

3'-TAAGCTGACGCGTCT-5'

attcgactgcgcaga

С

Clear

Two restriction enzymes are inserted by user

Output of GUI for DNA Splicing System involving Two Rules





Splicing System in Graph Theory





Splicing System in Graph Theory (Cont.)

5'-GAATTCTCTGTAAT-3' 3'-CTTAAGAGACATTA-5'



Graph representation of the DNA string

Splicing System in Graph Theory (Cont.)

 Graph splicing system is originally introduced by Freund in 1995 to describe the DNA splicing system in the form of graphs instead of one-dimensional strings.



Freund, R., Splicing systems on graphs, in 1st Int. Symp. On Intelligence in Neural and Biological Systems, INBS'95 (IEEE, Washington, DC, 1995), 189-194.

Graph Splicing Scheme

Definition (Freund, 1995) Graph Splicing Scheme

A graph splicing scheme is a pair $\sigma = (A, P)$ where A is a set of finite alphabets and P is a set of finite splicing rules. A finite set P with k number of graph splicing rules, can be written in the form

((h[1],E'[1]);(h[2],E'[2]),...,(h[k];E'[k]);R)

such that $k \ge 1$ where $k \in \mathbb{N}$ and for all *i* with $1 \le i \le k$, where

- h[i] = (N[i], E[i], L[i]) weakly connected graph, where E[i] is the edges of the *i*th graph splicing rule,
- $E'[i] \subseteq E[i]$, where E'[i] is the cutting pattern for the *i*th graph splicing rule,
- the nodes N[i] are mutually disjoint,
- *R* obeys the following rules:
- i. Each edge $(n,m) \in E'[i]$ is supposed to be divided into two parts; i.e the start part (n,m] and the end part [n,m),
- ii. The elements of *E* are of the form ((n,m], [n',m')), where (n,m) and (n',m') are edges from $\bigcup_{1 \le i \le k} E'[i]$,
- iii. Every element from $\{(n,m], [n,m) \mid (n,m) \in \bigcup_{1 \le i \le k} E'[i] \text{ must appear exactly once in a pair of } E.$

- Graph splicing scheme described the whole process of the graph splicing system where the graph splicing rule(s) is defined.
- Similar as enzymes in DNA splicing, splicing rules are used to control and restrict the edges to be cut on the initial graphs.

Graph Splicing Scheme (Cont.)

Consider the set of natural numbers denoted by $\mathbb{N} = \{0, 1, 2, ...\}$ and $\mathbb{N}_{\infty} = \mathbb{N} \cup \infty$. Let M be any set, and r be a function representing \mathbb{N}_{∞} -subset of set $M, r : M \to \mathbb{N}_{\infty}$, where r can be written as formal power series $r = \sum_{m \in M} (r(m) \circ m)$. The idea of r(m) is to count the number of occurence of the object m. Since there is an infinite number of copies of m, then $r(m) = \infty$. The set $\{m \in M \mid r(m) \neq 0\}$ is called as the support of r, denoted as supp(r). Assume every \mathbb{N}_{∞} -subset to have finite support and denote the set of all \mathbb{N}_{∞} -subset of M by $\langle \langle M \rangle \rangle$. Then $r \in \langle \langle M \rangle \rangle$ can be written as

 $r = \{ (m, r(m)) \mid m \in \text{supp}(r) \}.$

Definition (Freund, 1995) Graph Splicing Rule

Let p = ((h[1], E'[1]), ..., (h[k], E'[k]); R) be a graph splicing rule and $r \in \langle \langle \gamma_c(A) \rangle \rangle$ where $\gamma_c(A)$ is a set of connected graphs over alphabet A. If there are k different graphs g[1], ..., g[k] from r, in the sense that n copies of the graph $g \in \gamma_c(A)$ are n objects selected, provides that $r(g) \ge n$, then p can be applied to r, which yields some $s \in \langle \langle \gamma_c(A) \rangle \rangle$ in the following way:

- i. for all *i* with $1 \le i \le k$, h[i] is a subgraph of g[i], where f[i] establishes the injective node embedding h[i] into g[i],
- ii. the union of g[i], ..., g[k] can be looked at as a single graph $g \in \gamma_c(A)$ and the union of the functions f[i] as single function f embedding h[i] into g. Eliminate all edges from $\bigcup_{1 \le i \le k} f(E'[i])$ from g and add all edges (f(n), f(m')) such that $((n,m], [n',m')) \in E$, which yields the uniquely determined union of k' connected graphs g'[i], ..., g'[k],
- iii. the new \mathbb{N}_{∞} -subset *s* is obtained from *r* by successively decrementing r(g[1]), ..., r(g[k]) by one and incrementing r(g'[1]), ..., r(g'[k]) by one.

• A graph splicing rule consisting the enzyme Acl can be written as follows.

Definition (Freund, 1995) Graph Splicing System

Let $\sigma = (A, P)$ be any graph splicing scheme and consider $I \in \langle \langle \gamma_c(A) \rangle \rangle$ where $I = \{(g, k)\}$, for any $g \in \langle \langle \gamma_c(A) \rangle \rangle$ and $k \ge 0$ is the number of copies of g. Then there exists the set of all $I' \in \langle \langle \gamma_c(A) \rangle \rangle$ denoted by $\sigma(\{I\})$, obtained by applying one graph splicing rule of P to I. By applying the graph splicing rule repeatedly, for every $n \ge 2$, $\sigma^n(\{I\})$ is defined by $\sigma^n(\{I\}) = \sigma(\sigma^{n-1}(\{I\}))$ and note that $\sigma^0(\{I\}) = \{I\}$. Also, note that $\sigma^n(\{I\})$ is simply denoted as $\sigma^*(\{I\}) = \bigcup_{n \in \mathbb{N}} \sigma^n(\{I\})$, by extending $\sigma^n(\{I\})$, where \mathbb{N} is the set of natural numbers. Hence, there is a set of triple S = (A, P, I) is called as a graph splicing system.

• In 2011, Jeyabharathi *et. al.* introduced one type of splicing called as *n*-cut splicing.

S. Jeyabharathi, J. Padmashree, S. S. Selvi, and K. Thiagarajan, Semigraph structure on DNA splicing system, in 6th Int. Conf. on Bio-Inspired Computing: Theories and Applications, BIC-TA (IEEE Computer Society, Washington, DC, 2011), 182–187.

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Semigraph representation of DNA molecule

An *n*-cut splicing is applied

Two components of *n*-cut spliced semigraphs are generated

Example of *n*-cut splicing & *n*-cut spliced semigraph

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n-Cut Splicing (Cont.)

• An *n*-cut splicing will cut *n*+2 number of edges and the two vertices from the left most of the graphs as well as the two vertices from the right most of the graphs will never be cut.

Folding Technique *n*-Cut Semigraphs (Cont.)

Examples of *n*-cut spliced semigraphs folding

List of Publications

Link: https://people.utm.my/nizasarmin/

2010

Nor Haniza Sarmin, Yuhani Yusof and Fong Wan Heng, Some Characterizations in Splicing Systems, International Conference on Mathematical Sciences (ICMS 2010), Abant Yzzet Baysal Üniversitesi, Bolu, Turkey, 23 – 27 Nov 2010, American Institute of Physics (AIP) Conference Proceedings, Melville, New York, Vol 1309, pg. 411-418, (ISBN 978-0-7354-0863-0).

2012

Sherzod Turaev, Gan Yee Siang, Mohamed Othman, **Nor Haniza Sarmin** and Fong Wan Heng, **Weighted Splicing Systems**, Computational Intelligence and Intelligent Systems, Communications in Computer and Information Science (CCIS), ISBN 978-3-642-34288-2, Volume 316, 2012, pg 416-424, Proceedings in *The 6th International Symposium on Intelligence Computation and Applications (ISICA 2012)*, Wuhan, China, 27-28 October 2012.

2013

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Yuhani Yusof, Nor Haniza Sarmin, Fong Wan Heng, T. Elizabeth Goode and Muhammad Azrin Ahmad, An Analysis of Four Variants of Splicing System, Proceedings of the 20th National Symposium on Mathematical Sciences (SKSM 20), AIP Conf. Proc., Vol 1522, 2013, pg. 888-895 (ISSN: 1551-7616).

Mathuri Selvarajoo, Fong Wan Heng, Nor Haniza Sarmin and Sherzod Turaev, Some Characteristics of Probabilistic One-Sided Splicing Systems, Proceedings of the 20th National Symposium on Mathematical Sciences (SKSM 20), AIP Conf. Proc., Vol 1522, 2013, pg. 967-975(ISSN: 1551-7616).

Sherzod Turaev, Mathuri Selvarajoo, Mohd Hasan Selamat, **Nor Haniza Sarmin** and Fong Wan Heng, **Probabilistic Splicing Systems**, Advanced Methods for Computational Collective Intelligence, Studies in Computational Intelligence, ISBN 978-3-642-34300-1,Volume 457, 2013, pg 259-268, proceedings in 4th International Conference on Computational Collective Intelligence Technologies and Applications (ICCCI 2012), Ho Chi Minh city, Vietnam, 28-30 November 2012.

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List of Publications (Cont.)

Link: https://people.utm.my/nizasarmin/

2014

Muhammad Azrin Ahmad, Nor Haniza Sarmin, Fong Wan Heng, Yuhani Yusof, An Extension of First Order Limit Language, Proceedings of the 3rd International Conference on Mathematical Sciences (ICMS3), AIP Conf. Proc., Vol 1602, 2014, pg. 627-631. (ISBN: 978-0-7354-1236-1)

Mathuri Selvarajoo, Fong Wan Heng, **Nor Haniza Sarmin** and Sherzod Turaev, **Probabilistic Simple Splicing Systems**, *Proceedings of the 3rd International Conference on Mathematical Sciences (ICMS3)*, AIP Conf. Proc., Vol 1602, 2014, pg. 760-766. (ISBN: 978-0-7354-1236-1)

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Fariba Karimi, Sherzod Turaev, **Nor Haniza Sarmin** and Wan Heng Fong, **Fuzzy Splicing Systems**, Lecture Notes in Artificial Intelligence, Computational Collective Intelligence: Technologies and Applications, Volume 8733, ISBN 978-3-319-11288-6, pg 20-29, proceedings in 6th *International Conference on Computational Collective Intelligence Technologies and Applications* (ICCCI 2014), Seoul, Korea, September 24-26, 2014.

2015

Yuhani Yusof, Wen Li Lim, T.Elizabeth Goode, Nor Haniza Sarmin, Fong Wan Heng, Mohd Firdaus Abd Wahab, Molecular Aspects of DNA Splicing Systems, International Conference on Mathematics, Engineering & Industrial Applications 2014 (ICoMEIA 2014), 28-30 May, 2014, The Gurney Resort Hotel & Residences Penang, AIP Conf. Proc., Vol. 1660, 2015, pg. 050045 (ISSN: 1551-7616).

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2016

Wan Heng Fong, Yee Siang Gan, Nor Haniza Sarmin, and Sherzod Turaev, The Generative Capacity of Weighted Simple and Semi-Simple Splicing Systems, Proceedings of the 23rd National Symposium on Mathematical Sciences (SKSM 23), AIP Conf. Proc., Vol 1750, 2016, pg. 050013 1-6 (ISBN: 978-0-7354-1407-5).

List of Publications (Cont.)

Link: <u>https://people.utm.my/nizasarmin/</u>

2017

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2018

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2020 & 2021

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M N S Abdul Razak, W H Fong, **N H Sarmin**. Graph splicing rules with cycle graph and its complement on complete graphs. In: Journal of Physics: Conference Series 1988: 012067 (2021); 1-11. (doi: 10.1088/1742-6596/1988/1/012067)

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