

Department of Mathematics Drganizes International Faculty Development Programme (FDP) On **APPLIED MATHEMATICS IN ENGINEERING AND TECHNOLOGY** 27.03.2024 0 10.30 AM -12.30 PM

Mode : Online

**Resource Person** 

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Applications of DNA Computation in Industrial Technology

Convenor Dr. S. Radhakrishanan , AssistantProfessor/Mathematics, Coordinator Dr.K. lyappan, Associate Professor/Mathematics. Organizing Secretary Dr.S.Sridevi, AssistantProfessor/ Mathematics,

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AssistantProfessor/ Mathematics, FOR ENQUIRIES 1800 202 2535



## "Applications of DNA Computation in Industrial Technology"

International Faculty Development Program on Applied Mathematics in Engineering and Technology

#### Organized by

Department of Mathematics, SRM TRP Engineering College, Tiruchirappalli, India

#### 27 March 2024

**Innovating Solutions** 

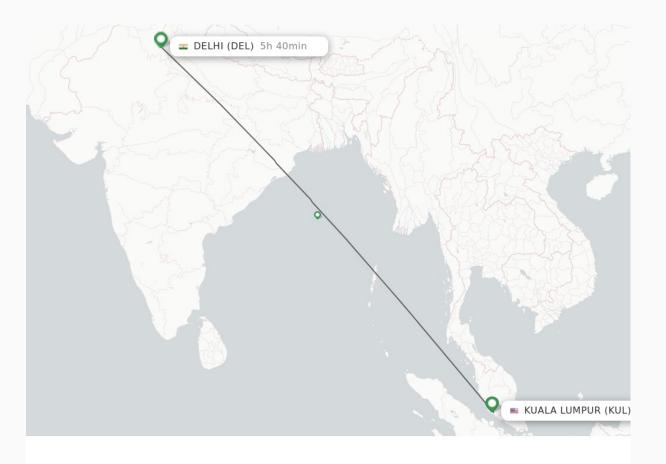
### **PROF DR NOR HANIZA SARMIN**

Department of Mathematical Sciences, Faculty of Science, Universiti Teknologi Malaysia nhs@utm.my

## Malaysia in the World Map



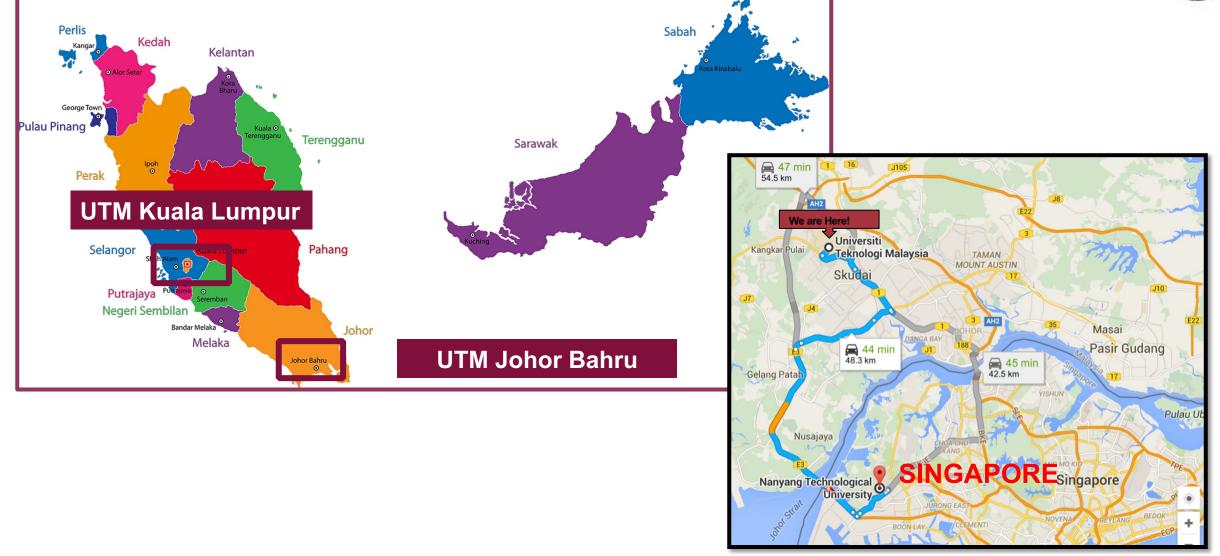
## From India to Malaysia



- The distance between India and Malaysia is estimated at 4,218 km or 2621 miles.
- A typical flight would have a flying time of about 4 5 hours.
- Time difference between India and Malaysia is 2:30 hours.







## **Faculties in UTM**

#### **12** Faculties

Civil Engineering	Mechanical Engineering	Chemical & Energy Engineering	Electrical Engineering	Computing	Built Environment & Surveying
<ul> <li>Structure Materials</li> <li>Geotechnics and Transportation</li> <li>Water and Environmental Engineering</li> </ul>	<ul> <li>Applied Mechanics &amp; Design</li> <li>Thermo Fluids</li> <li>Aeronautics, Automotive &amp; Ocean Engineering</li> <li>Materials, Manufacturing &amp; Industrial Engineering</li> </ul>	<ul> <li>Chemical Engineering</li> <li>Petroleum Engineering</li> <li>Bioprocess &amp; Polymer</li> <li>Energy Engineering</li> <li>Petroleum</li> <li>Engineering</li> <li>#44 &amp; 2 in</li> <li>MAS</li> </ul>	<ul> <li>Communication Engineering</li> <li>Control and Mechatronics Engineering</li> <li>Electronic and Computing Engineering</li> <li>Electrical Power Engineering</li> </ul>	<ul> <li>Computer Science</li> <li>Applied Computing</li> <li>Software Engineering</li> </ul>	<ul> <li>Architecture</li> <li>Quantity Surveying</li> <li>Urban and Regional Planning</li> <li>Landscape Architecture</li> <li>Geoinformation Real Estate</li> </ul>
Management	Science Environmental Sciences TOP 200 & #3 in MAS	Social Sciences & Humanities	Faculty of Artificial Intelligence	Azman Hashim International Business School	Malaysia-Japan International Institute of Technology
<ul> <li>Management</li> <li>Accounting</li> <li>Marketing</li> <li>Technology Management</li> <li>Information Technology</li> <li>Information Systems</li> </ul>	<ul> <li>Biosciences</li> <li>Physics</li> <li>Chemistry</li> <li>Mathematical Sciences</li> </ul>	<ul> <li>School of Education</li> <li>School of Human Resource Development &amp; Psychology</li> <li>Academy of Islamic Civilisation</li> <li>Language Academy</li> <li>Centre for Advanced Studies on Islam, Science, and Civilisation</li> <li>FSSH KL</li> </ul>	<ul> <li>Engineering &amp; Technology</li> <li>Science, Management &amp; Design</li> <li>Advanced Informatics</li> <li>Perdana Centre</li> </ul>	<ul> <li>Business Administration</li> <li>Accounting and Finance</li> <li>Information System</li> <li>Accounting &amp; Finance TOP 250 &amp; #7 in MAS</li> </ul>	<ul> <li>Electronic System Engineering</li> <li>Mechanical Precision Engineering</li> <li>Chemical and Environmental Engineering</li> <li>Management of Technology</li> <li>Software Engineering</li> </ul>



DEPARTMENT OF MATHEMATICAL SCIENCES FACULTY OF SCIENCE UNIVERSITI TEKNOLOGI MALAYSIA https://science.utm.my/mathematics/



## POSTGRADUATE PROGRAMMES

We offer Masters and Doctoral Programmes in Mathematics.

#### **UNDERGRADUATE PROGRAMS**

Bachelor of Science (Mathematics) with Honours

Bachelor of Science (Industrial Mathematics) with Honours



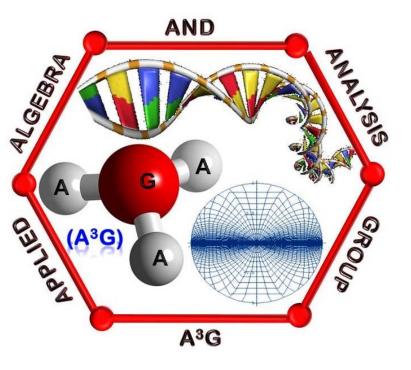
### DEPARTMENT OF MATHEMATICAL SCIENCES FACULTY OF SCIENCE UNIVERSITI TEKNOLOGI MALAYSIA https://science.utm.my/mathematics/

The department is divided into 5 broad research areas/academic panels:

- 1. Algebra & Analysis
- 2. Applied Mathematics
- 3. Numerical & Computational
- 4. Operations Research
- 5. Statistics

Members belong to specific research groups focused on diverse studies.

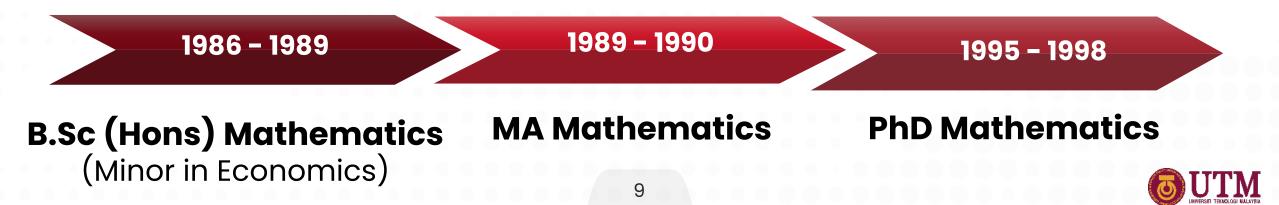
Joined Department of Mathematics, Faculty of Science, UTM on 2 May 1991



## **MY BACKGROUND**



State University of New York at Binghamton (now known as Binghamton University), New York, USA



### "Applications of DNA Computation in Industrial Technology"

### Abstract

The diversity of mathematical applications in various scientific concepts has led to significant advancements in understanding complex biological processes. One area where this interdisciplinary collaboration thrives is DNA Computing, specifically DNA Splicing, a basic biological process in manipulating genetic information and simulated by the technique of recombinant DNA molecules that relies on restriction enzymes. This presentation explores the idea of DNA splicing in various concepts. Firstly, the fundamental mathematical framework behind DNA splicing is presented. Also, the interplay between mathematical models and wet lab experiments is shared to validate the theoretical findings. The emergence of DNA splicing in industrial technology, particularly in computer science where some computational models such as graphical user interface (GUI) are discussed. Finally, the graphical approach in mathematics to studying DNA splicing is presented to emphasize the role of visual representation in comprehending complex biological processes.

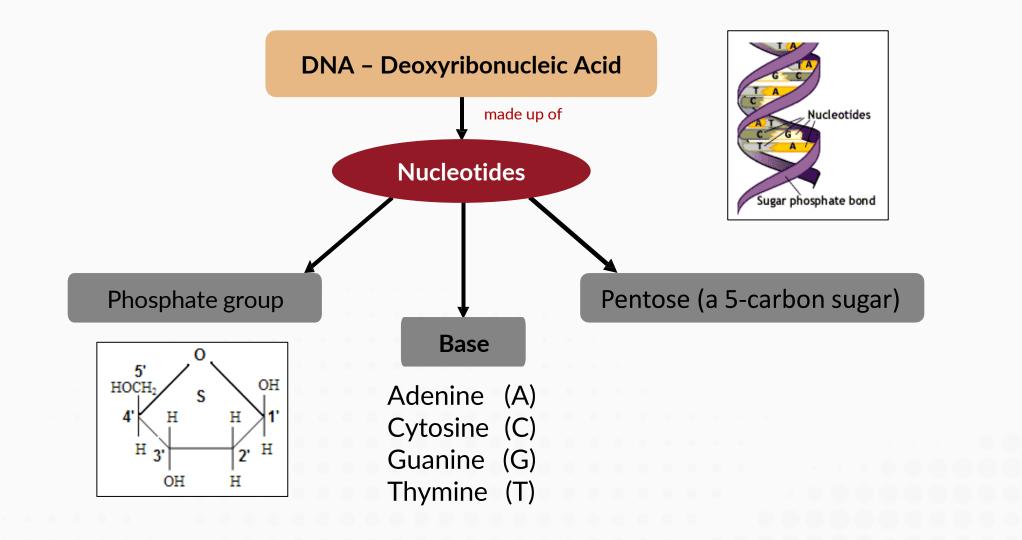


# **DNA Structure**

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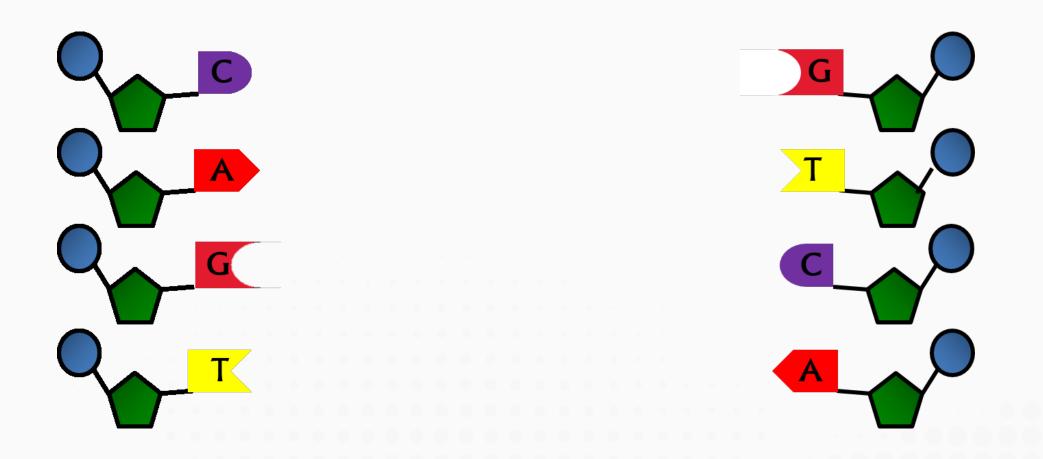


## **Structure of DNA**





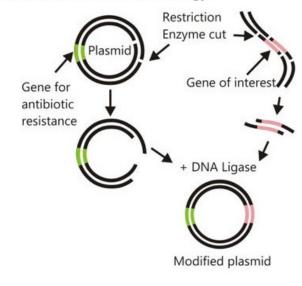
## Structure of DNA (Cont.) Watson-Crick Complementary





# Recombinant DNA

**Recombinant DNA Technology** 



 $\bullet \bullet \bullet \bullet$ 

## VARIOUS APPLICATIONS OF RECOMBINANT DNA TECHNOLOGY

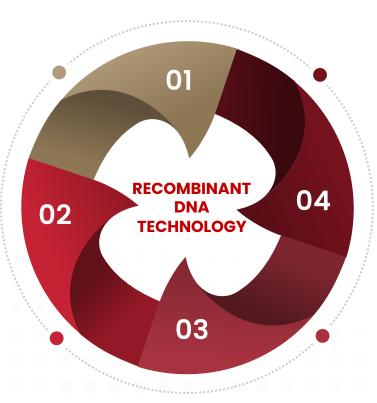
#### **2. THERAPEUTIC PRODUCTS**

Vaccines Growth hormones Antibodies Anticancer drugs Recombinant protein

#### Gene therapy Monitoring device Therapeutic strategies

CRISPR

**3. DIAGNOSIS** 



#### **1. GENETICALLY MODIFIED PRODUCTS**

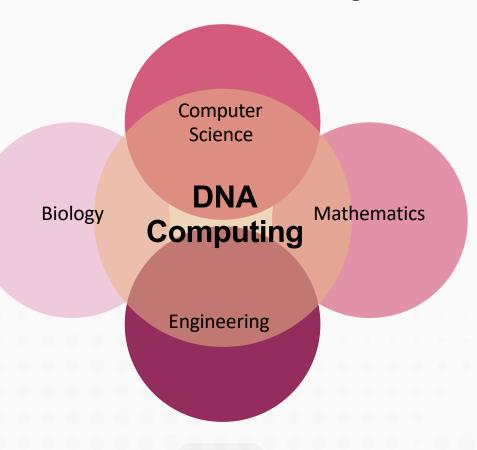
Fruits Vegetables Crops Microbs Animals

#### 4. ENERGY APPLICATIONS Biohydrogen Bioethanol Biomethanol Biobutanol



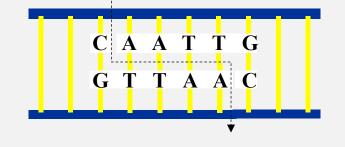
## **DNA Computing**

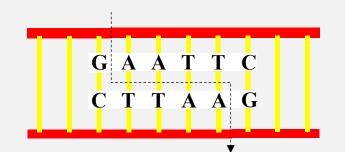
• DNA computing has emerged in the last twenty years as an exciting new research field at the intersection of Biology, Computer Science, Mathematics and Engineering.





# DNA Splicing System





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## Mathematics and DNA Splicing System

- The mathematical modelling of splicing system was first defined by Tom Head in 1987.
- It was introduced as a mathematical model of the generative capacity of a biological system containing DNA molecules in the presence of appropriate enzymes.

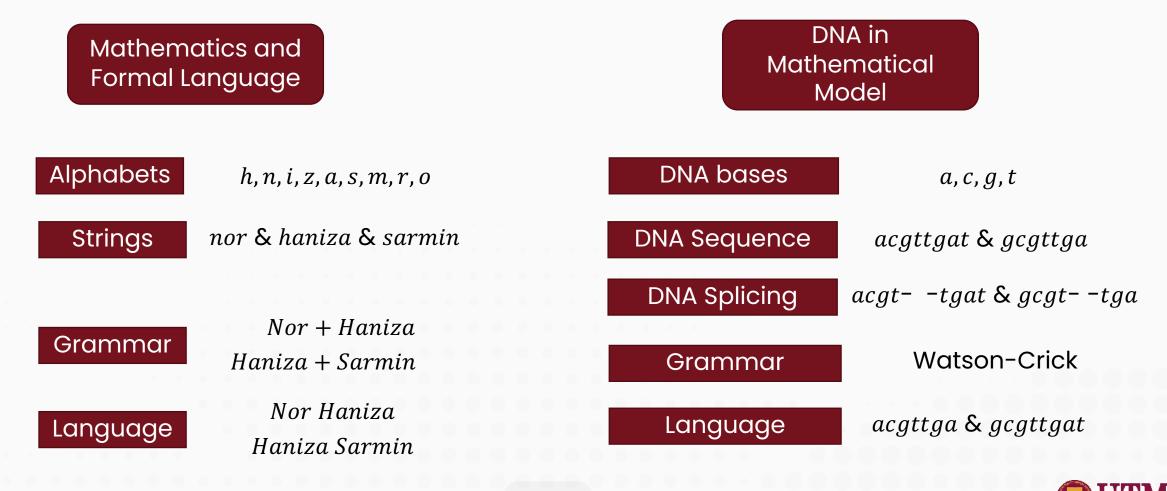




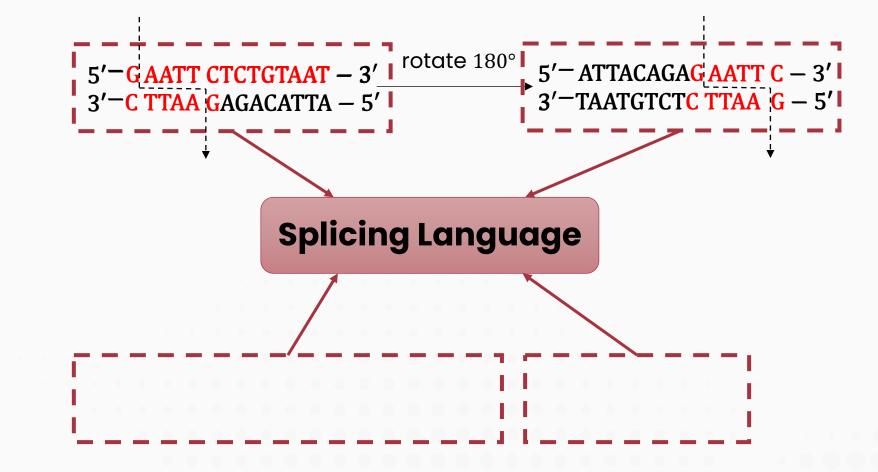
## **Prof Head's visit to UTM,**

## Mathematical Modelling of DNA Splicing System

How do we model it?



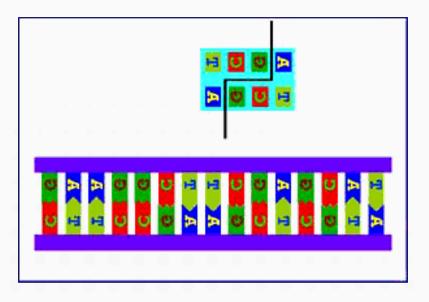
## Mathematical Modelling of DNA Splicing System (Cont.)





## **Restriction Enzymes**

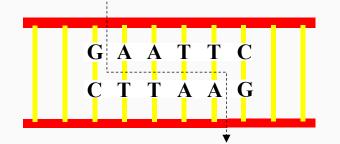
• A restriction enzyme is an enzyme that cuts double-stranded or single stranded DNA at specific recognized nucleotide sequences, known as restriction sites.



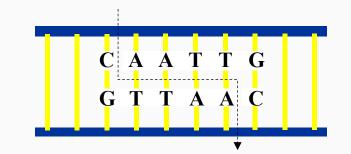


## Restriction Enzymes (Cont.)

*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])





## **Types of DNA Splicing Systems**



- Head, T. (1987). Formal Language Theory and DNA: An Analysis of the Generative Capacity of Specific Recombinant Behaviors. Bulletin of Mathematical Biology, 49(6), 737-759. doi:https://doi.org/10.1007/BF0248177
- Păun, G. (1996). On the Splicing Operation. Discrete Applied Mathematics, 70(1), 57-79. doi:https://doi.org/10.1016/0166-218X(96)00101-1
- Pixton, D. (1996). Regularity of Splicing Languages. Discrete Applied Mathematics, 69(1-2), 101-124. doi:https://doi.org/10.1016/0166-218X(95)00079-7
- Goode, E., & Pixton, D. (2004). Splicing to the Limit. In N. Jonoska, G. Păun, & G. Rozenberg (Eds.), Aspects of Molecular Computing, Lecture Notes in Computer Science (pp. 189-201). Germany: Springer-Verlag.
- Yusof, Y., Sarmin, N. H., Fong, W. H., Goode, T. E., & Ahmad, M. A. (2013). *An Analysis of Four Variants of Splicing System*. Paper presented at the 20th National Symposium on Mathematical Sciences Research in Mathematical Sciences: A Catalyst for Creativity and Innovation (SKSM 2012).
- Karimi, F., Turaev, S., Sarmin, N. H., & Fong, W. H. (2014). Fuzzy Splicing Systems. In D. Hwang, J. J. Jung, & N. T. Nguyen (Eds.), Computational Collective Intelligence. Technologies and Applications, ICCCI 2014, Lecture Notes in Computer Science (pp. 20-29). Cham, Switzerland: Springer International Publishing.



## Types of DNA Splicing Systems (Cont.)

Splicing System	<b>Head</b> S = (A, I, B, C)	$Paun \\ \sigma = (A, R)$	<b>Pixton</b> $\zeta = (R, I)$	Goode-Pixton ( <i>w</i> , <i>w</i> ′)⊢ <sub>r</sub> z	<b>Yusof-Goode</b> S = (A, I, R)	<b>Fuzzy</b> S = (A, T, I, R, ⊙)
Initial String	u <mark>cxd</mark> v pexfq	u <mark>u<sub>l</sub>u</mark> 2v u'u3u4v'	ξ <mark>α</mark> η ξ'α'η'	w = x u v y $w' = x' u' v' y'$	α <mark>υχν</mark> β γyzδ	$(ua, x)$ $(bv, y)$ $x, y \in [0, 1]$
Rule	( <mark>c</mark> , x, d) (e, x, f)	<mark>u₁#u₂</mark> \$u₃#u ₄	<b>(α</b> , α': β)	r = ( <b>u</b> , <b>v</b> ; <b>u</b> '; <b>v</b> ')	( <b>u</b> , x, <b>v</b> : y, x, z)	u#a\$b#v
Splicing Language	u <mark>c</mark> xfq pexdv	น <mark>น</mark> าน <sub>4</sub> v′	ξ <mark>β</mark> η′	z = x u v' y'	αuxzδ γyxvβ	( <i>uv</i> , x ⊙ y) ⊙ is fuzzy operation

- S: splicing system
- $\sigma$  and  $\zeta$ : splicing schemes
- A: finite alphabet
- $T \subseteq A$ : terminal alphabet

- *I*: set of initial strings
- B: set of rules with left pattern
- C: set of rules with right pattern
- $R = B \cup C$  : set of rules

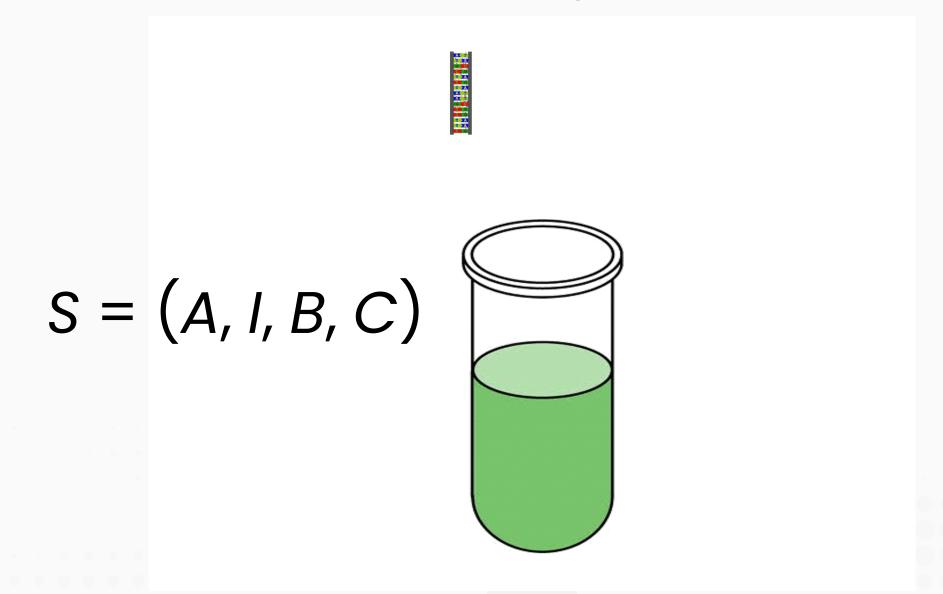


# Theoretical vs Wet Lab



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## Wet Experiment on Splicing System





## Theoretical vs Lab Results Wet Splicing System involving *Cvi*Ql and *Aci*l

- An initial DNA molecule *I* used in this splicing model is a small segment taken from bacteriophage lambda between 42958 and 43117 with the length of 160 base pairs (bp).
- The initial molecule contains one cutting site each of the restriction enzymes CviQI and Acil where the genome locations for the cutting sites are found at 42992–42995 and 43036– 43039 respectively.
- Five sticky ends of molecules  $\alpha$ ,  $\beta$ ,  $\gamma$ ,  $\alpha \beta$  and  $\beta \gamma$  are produced by the restriction enzymes when cutting the initial molecule. The lengths of fragments for the sticky ends are given in the following.

Fragment: 
$$\alpha \frac{CviQI \text{ site }}{|\alpha|} \beta \frac{Acil \text{ site }}{|\gamma|} \gamma$$
  
 $|\alpha| = 35 \text{ bp}$   
 $|\beta| = 44 \text{ bp}$   
 $|\gamma| = 81 \text{ bp}$   
 $|\alpha - \beta| = 79 \text{ bp}$   
 $|\beta - \gamma| = 125 \text{ bp}$ 



### Theoretical vs Lab Results (Cont.) Wet Splicing System involving *Cvi*QI and *Aci*I

• Initial Molecule (42958 and 43117 from bacteriophage lambda)

• Enzyme CviQI (palindromic)

5′...G▼TAC...3′ 3′...CAT<sub>▲</sub>G...5′

• Enzyme Acil (non-palindromic)

5′...C▼CGC...3′ 3′...CGC\_C...5′



### Theoretical vs Lab Results (Cont.) Wet Splicing System involving *Cvi*QI and *Aci*I

The splicing language from this splicing system *S* invoving one cutting site each of palindromic restriction enzyme CviQI (*g*, *ta*, *c*) and non-palindromic restriction enzyme AciI (*c*, *cg*, *c*) with different palindromic crossings is shown in the following:

 $L(S) = \{ \alpha gtac(\beta ccgg\beta' gtac)^{n-1}(\alpha' + \beta ccgc\gamma) \}$ 

+{ $\gamma'$ gcg(g $\beta'$ gtac $\beta$ ccg)<sup>n-1</sup>( $c\gamma$  +  $g\beta'$ gtac $\alpha'$ )}.

where  $n \in \mathbb{Z}^+$ . The fragments of DNA strings in the splicing language L(S) are stated as follows:

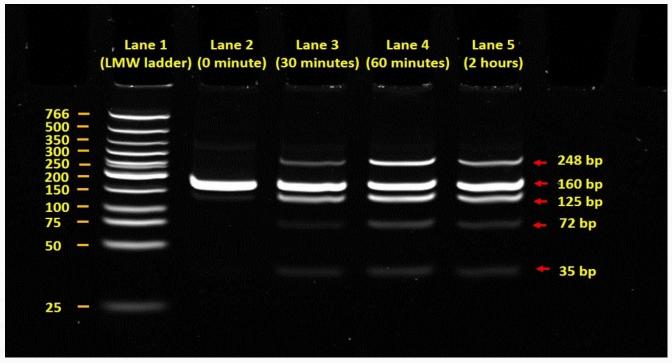
$$\alpha \frac{\text{gtac}}{\alpha} \left( \beta \frac{\text{ccgg}}{\beta} \beta' \frac{\text{gtac}}{\beta} \right)^{n-1} \alpha',$$
  
$$\alpha \frac{\text{gtac}}{\alpha} \left( \beta \frac{\text{ccgg}}{\beta} \beta' \frac{\text{gtac}}{\beta} \right)^{n-1} \beta \frac{\text{ccgc}}{\gamma},$$
  
$$\gamma' \frac{\text{gcg}}{\gamma} \left( \frac{g}{\beta} \beta' \frac{\text{gtac}}{\beta} \beta \frac{\text{ccg}}{\gamma} \right)^{n-1} \frac{g}{\gamma} \gamma \text{ and}$$
  
$$\gamma' \frac{\text{gcg}}{\gamma} \left( \frac{g}{\beta} \beta' \frac{\text{gtac}}{\gamma} \beta \frac{\text{ccg}}{\gamma} \right)^{n-1} \frac{g}{\gamma} \beta' \frac{\text{gtac}}{\gamma} \alpha'$$

where  $n \in \mathbb{Z}^+$  represents multiple copies of the specific strings.



### Theoretical vs Lab Results (Cont.) Wet Splicing System involving *Cvi*QI

	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			1	/	/
25	()				

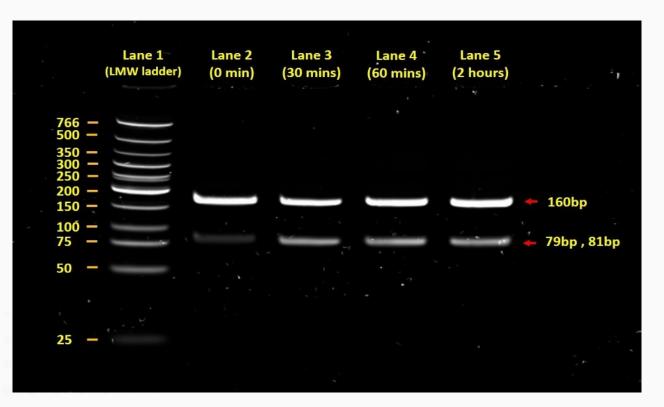


- Lane 1: LMW ladder
- Lane 2 (0 minute): 160 bp
- Lane 3 (30 minutes): 35 bp, 72 bp, 125 bp, 160 bp and 248 bp
- Lane 4 (60 minutes): 35 bp, 72 bp, 125 bp, 160 bp and 248 bp
- Lane 5 (2 hours): 35 bp, 72 bp, 125 bp, 160 bp and 248 bp



### Theoretical vs Lab Results (Cont.) Wet Splicing System involving Acil

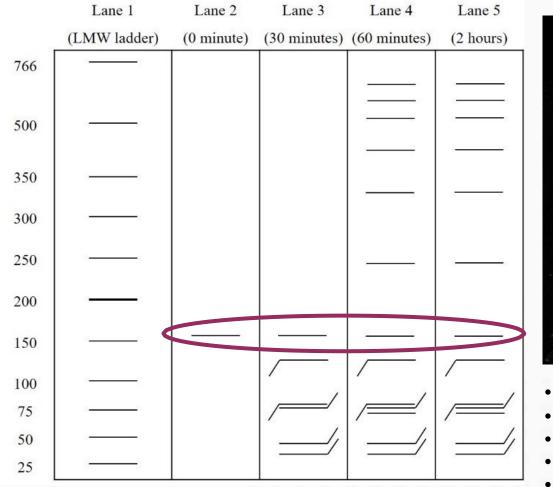
	Lane 1	Lane 2	Lane 3	Lane 4	Lane 5
	(LMW ladder)	(0 minute)	(30 minutes)	(60 minutes)	(2 hours)
766					
500					
350					
300					
250					
200	· · · · · · · ·				
150	·				
100				,	
75					
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25	()				

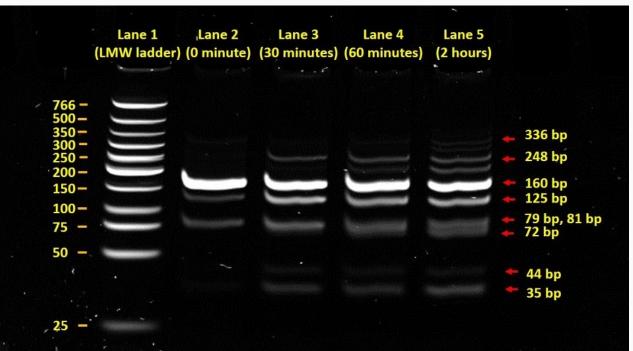


- Lane 1: LMW ladder
- Lane 2 (0 minute): 79 bp (or 81 bp) and 160 bp
- Lane 3 (30 minutes): 79 bp, 81 bp and 160 bp
- Lane 4 (60 minutes): 79 bp, 81 bp and 160 bp
- Lane 5 (2 hours): 79 bp, 81 bp and 160 bp



## Theoretical vs Lab Results (Cont.) Wet Splicing System involving *Cvi*QI and *Aci*I





- 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



### Wet-lab Experiment on Splicing System



Universiti Teknologi Malaysia, 2007



### Wet-lab Experiment on Splicing System





State University of New York, Binghamton, New York, and Towson University, USA, 2010



### Wet-lab Experiment on Splicing System



Universiti Teknologi Malaysia, 2012



### Wet-lab Experiment on Splicing System



Universiti Teknologi Malaysia, 2015



### Wet-lab Experiment on Splicing System



Universiti Teknologi Malaysia, 2020



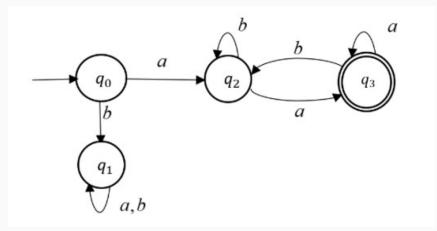
# DNA Splicing in Computer Science



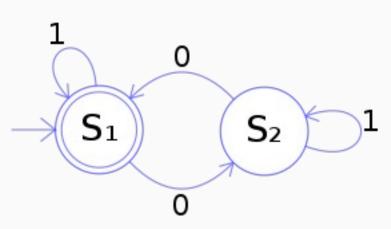
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# Automata of Splicing System

**Automata theory** is the study of <u>abstract</u> <u>machines</u>, as well as the <u>computational</u> <u>problems</u> that can be solved using them. It is a theory in <u>theoretical computer science</u>.



The automaton diagram for regular language



The automaton described by this <u>state</u> <u>diagram</u> starts in state  $S_1$ , and changes states following the arrows marked 0 or 1 according to the input symbols as they arrive. The double circle marks  $S_1$  as an accepting state. Since all paths from  $S_1$  to itself contain an even number of arrows marked 0, this automaton accepts strings containing even numbers of 0s.

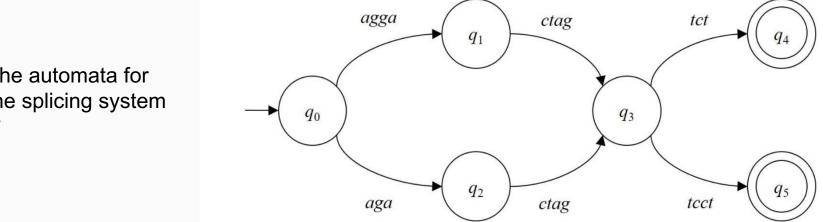


Given a splicing system S = (A, I, B, C) where  $I = { AGGACTAGTCT$  $TCCTGATCAGA } is the set of$ 

initial string, set  $B = \left\{ \begin{pmatrix} C & TA \\ C & AT \end{pmatrix} \right\}$  is the set of cleavage pattern for the enzyme *BfaI*, and set C is the empty set.

The enzyme *BfaI*, 5' - CTAG - 3' is a palindromic rule since the base 3' - GATC - 5'

sequence of enzyme *BfaI* reads the same forwards and backwards.



The automata for the splicing system S

### Graphical User Interface (GUI) for DNA Splicing System

#### DNA Splicing Language Generator (DNASpliceGen)

A C++ program that is created in **Microsoft Visual Studio** to **develop the Graphical User Interface (GUI)** for DNA splicing systems involving palindromic and non-palindromic rules.

DNA Splicing System with Palindromic and Non-	Palindromic Rules		- 🗆 X	
Instruction: Insert the initial string and	the cleavage pattern of the enzyme(s).			
Initial string		Insert the initial DNA	string	
Enzyme 1 , Enzyme 2 , Enzyme 2		Insert the cleavage patter	n of the enzyr	ne(s)
Compute	Clear			
		_		
Click 'Compute' button to generate the results	Click 'Clear' button to reset the interface			
				· •



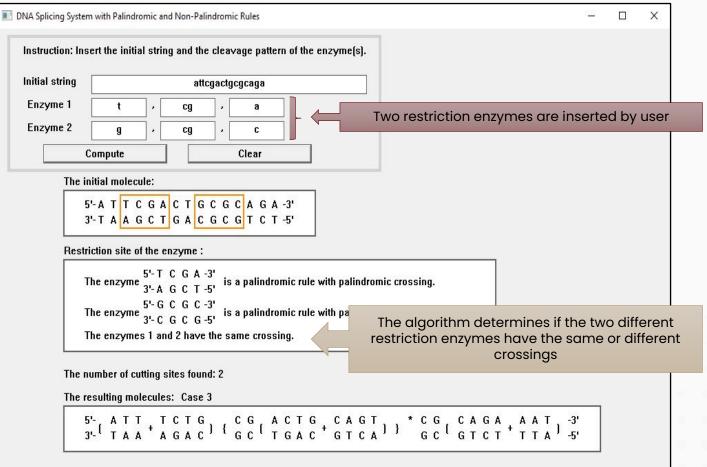
### DNA Splicing Language Generator (DNASpliceGen)

DNA Splicing System	m with Palindromic and Non-Palindromic Rules	- 🗆 ×
Instruction: Ins Initial string Enzyme 1	sert the initial string and the cleavage pattern of the enzyme(s).       aggactagtct       c     ,       ta     ,	One restriction enzyme is inserted by user
	Compute Clear	
	initial molecule: 5'-A G G A C T A G T C T -3' 3'-T C C T G A T C A G A -5'	es indicate the cutting site of the restriction enzyme found in the initial string
	riction site of the enzyme : 5'- C T A G -3' The enzyme 3'- G A T C -5' is a palindromic rule with palindro	romic crossing. The algorithm determines if the restriction enzyme is a palindrome or not a palindrome including crossing
	number of cutting sites found: 1 The	e algorithm states the number of cutting sites
	5'- A G G A + A G A   C T A G   T C T + T C C ] 3'- ( T C C T + T C T ) G A T C ( A G A + A G G A	T 1 -3' A 1 -5'
The algoi	rithm generates all the splicing languages	



### DNA Splicing Language Generator (DNASpliceGen)

Output of GUI for DNA Splicing System involving Two Rules

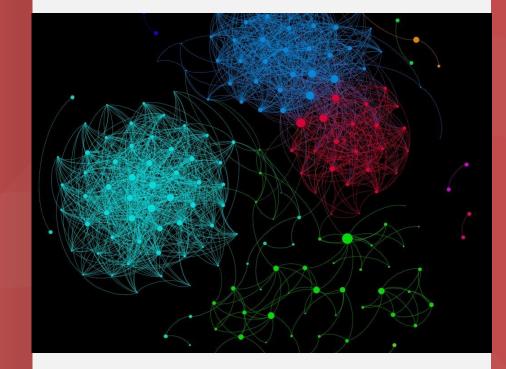


### Additional features:

- 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.



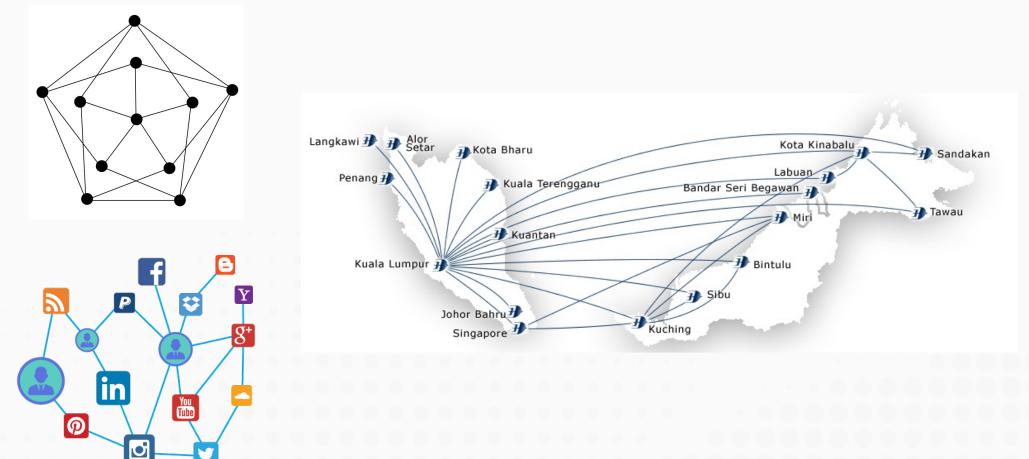
# DNA Splicing on Graph Theory



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### **Graph Theory**

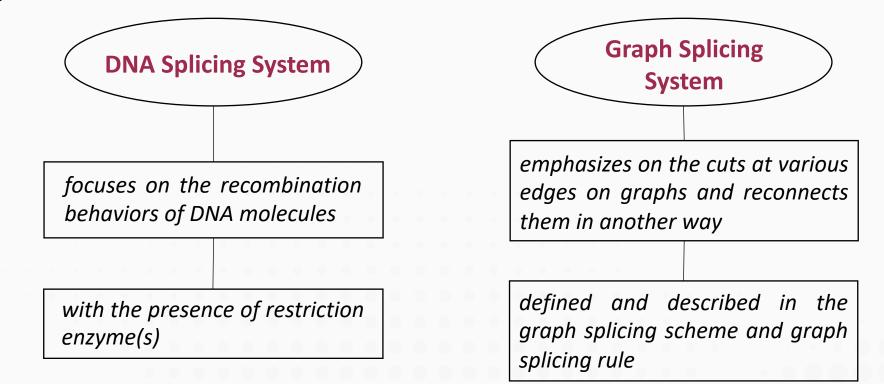
A graph is a mathematical structure consists of two finite sets called the set of vertices, V and edges, E.





# Splicing System in Graph Theory

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 Rule**

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

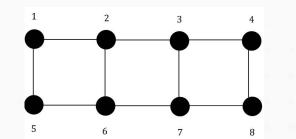


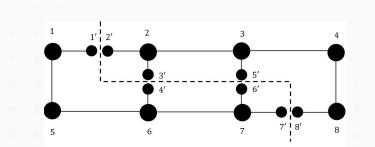
# *n*-Cut Splicing (Cont.)

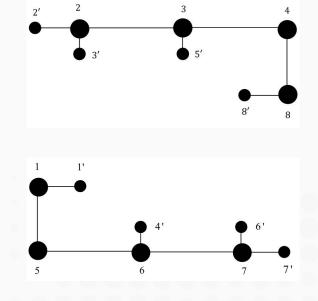
Semigraph representation of DNA molecule

An *n*-cut splicing is applied

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



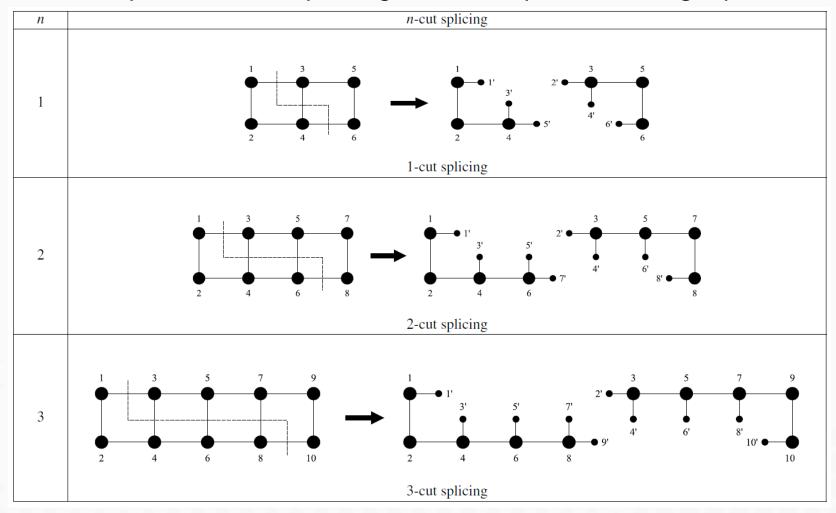






# *n*-Cut Splicing (Cont.)

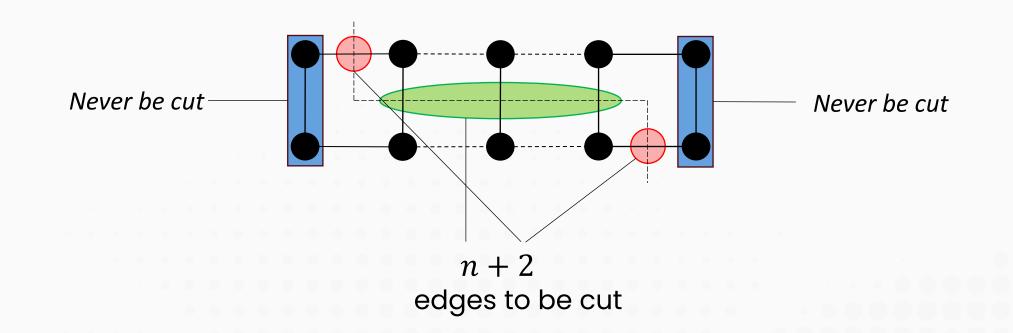
#### Example of *n*-cut splicing & *n*-cut spliced semigraph





# *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.





## **Ongoing Research**

#### A Theoretical DNA Based Computer Model for Food Authentification Process

The authentication of food is an urgent concern owing to the increasing population and direct consequences of food on public health. Food authentication using DNA and omicsbased methods is gaining ground due to critical advantages notably in the areas of food adulteration in plant and animal-based food and feed products and in determining the quality of food and food spoilage. Besides, there is greater demand for the detection of genetically modified foods (GMOs) and the detection of allergens, toxins, and carcinogens like tobacco in the food. Advanced DNA and omics-based methods (genomics, metabolomics, and proteomics) have been used in the food industry including DNA-based methods that rely on specific markers known as reference genes for food authentication. Novel methods like CRISPR-Cas have been recently introduced for the management of beneficial microorganisms relevant to food like probiotics.

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https://people.utm.my/nizasarmin/journal-papers/



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# **Graph Splicing Systems**

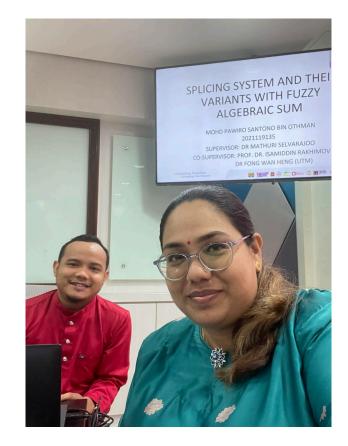
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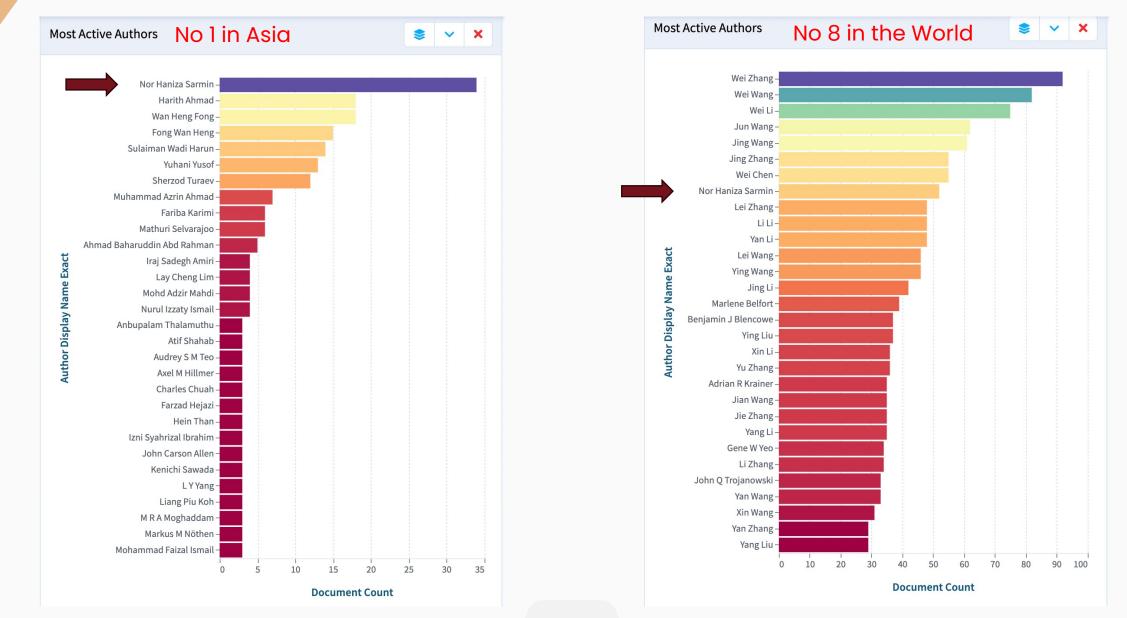
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### Ranking in Splicing Systems (Lens.org)



# **Active Collaborator on DNA Splicing System**



#### **Specialization:**

- 1. Formal Languages and Automata
- 2 DNA Computir
- 2. DNA Computing
- 3. Artificial Intelligence
- 4. Cryptography

#### **Ass. Prof. Dr. Sherzod Turaev** College of Information Technology, United Arab Emirates University

**Co-supervisor for some PhD students** 

# **Active Collaborator on DNA Splicing System**



### **Specialization:**

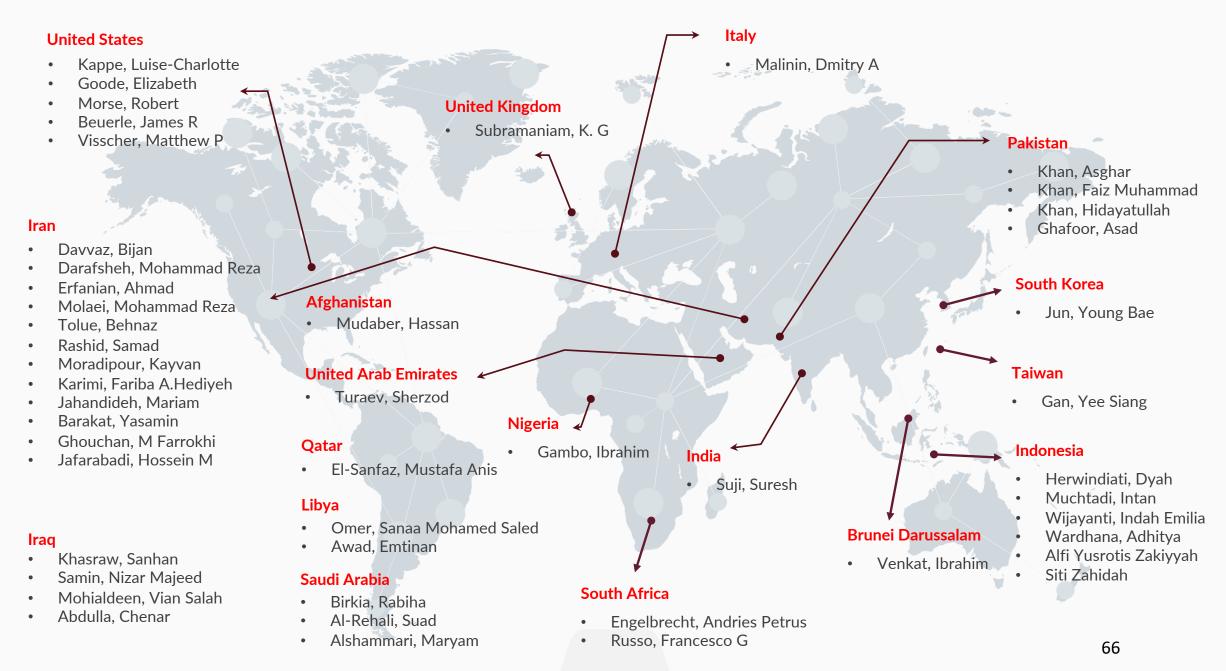
- 1. Spectral of Laplacian Hypergraph and Graph
- 2. Distance Matrices and Quadratic Embedding of Graphs
- 3. Machine Learning
- 4. DNA Sequencing

### Dr. Alfi Yusrotis Zakiyyah

Lecturer in Mathematics and Statistics, School of Computer Science, Bina Nusantara University (BINUS), Jakarta, Indonesia

IndoMS Research Visit Program 2022 to UTM (18 – 30 November 2022)

### My Collaborators Around the World



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In the Name of God for Mankind