# Linking Biological Data with Modeling and Simulation

Bioinformatics Student Symposium

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20230522 v5| https://doi.org/10.5281/zenodo.7955393



Silakan berdiskusi asinkron setelah simposium ini di https://github.com/dudung/bi3209-00-2022-2/issues/1

# Keterangan (disclaimer)

- Apa yang akan disampaikan tidak terkait langsung dengan bidang bioinformatika, akan tetapi lebih merupakan sharing pengalaman penelitian selama ini.
- Rujukan, yang telah dipilih, mengenai suatu hal dituliskan di bagian bawah slide terkait untuk dapat ditelusuri lebih lanjut.
- Hal-hal yang disampaikan tidak dapat terlepas dari pendapat pribadi dan pengalaman penyaji, sehingga belum tentu merupakan informasi yang paling tepat.

# Kerangka

<ul> <li>Model</li> </ul>	6	<ul> <li>Penelitian (penyaji)</li> </ul>	
<ul> <li>Simulasi</li> </ul>	14	saat ini	39
<ul> <li>Akurasi dan keseder-</li> </ul>		<ul> <li>Diskusi</li> </ul>	<b>-</b> 3
hanaan	22		
<ul> <li>Bioinformatika</li> </ul>	32		
<ul><li>Fiksi atau impian?</li></ul>	36		

#### Model

# Model

- A model is a product (physical or digital) that represents a system of interest.
- A model is similar to but simpler than the system it represents, while approximating most of the same salient features of the real system as close as possible.
- A good model is a judicious tradeoff between realism and simplicity.

Vinod Kumar Soni, "Answer to What is the difference between simulation and modeling?", ResearchGate, 21 Feb 2020, url https://www.researchgate.net/post/What\_is\_the\_difference\_between\_simulation\_and\_modeling [20230519].

# Model (lanj.)

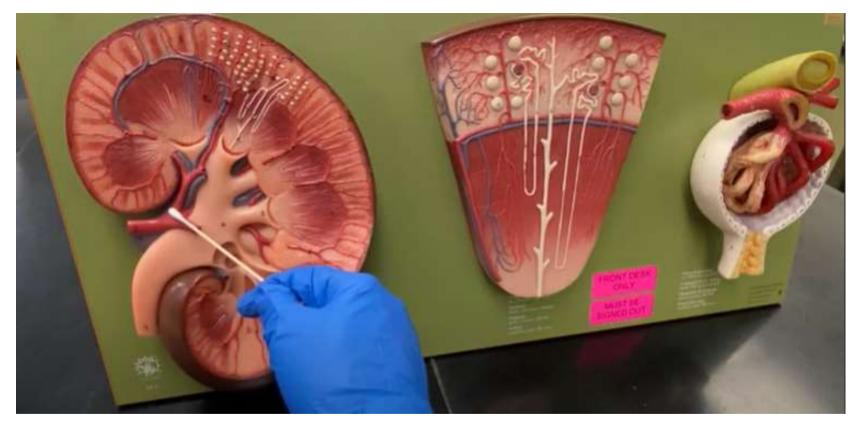
- A key feature of a model is manipulability.
- A model can be:
  - a physical model (for example a physical architectural house scale model, a model aircraft, a fashion mannequin, or a model organism in biology research); or
  - a conceptual model (for example a computer model, a statistical or mathematical model, a business model).







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#### **Simulasi**

# Simulation

- A simulation is the process of using a model to study the behavior and performance of an actual or theoretical system.
- In a simulation, models can be used to study existing or proposed characteristics of a system.
- The purpose of a simulation is to study the characteristics of a real-life or fictional system by manipulating variables that cannot be controlled in a real system.

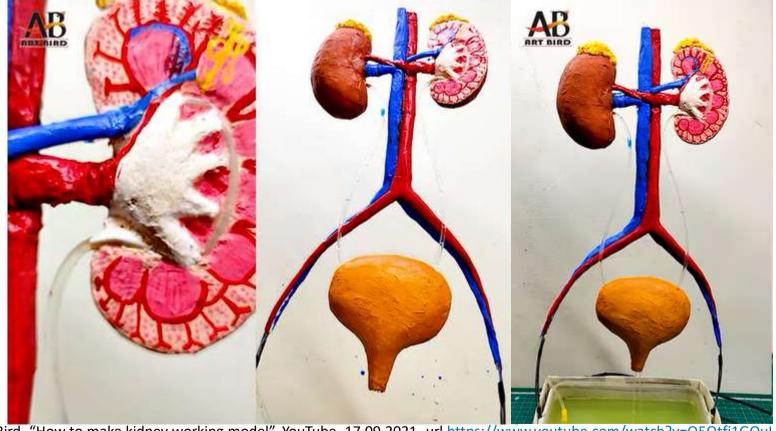
Vinod Kumar Soni, "Answer to What is the difference between simulation and modeling?", ResearchGate, 21 Feb 2020, url https://www.researchgate.net/post/What\_is\_the\_difference\_between\_simulation\_and\_modeling [20230519].

# Simulation (lanj.)

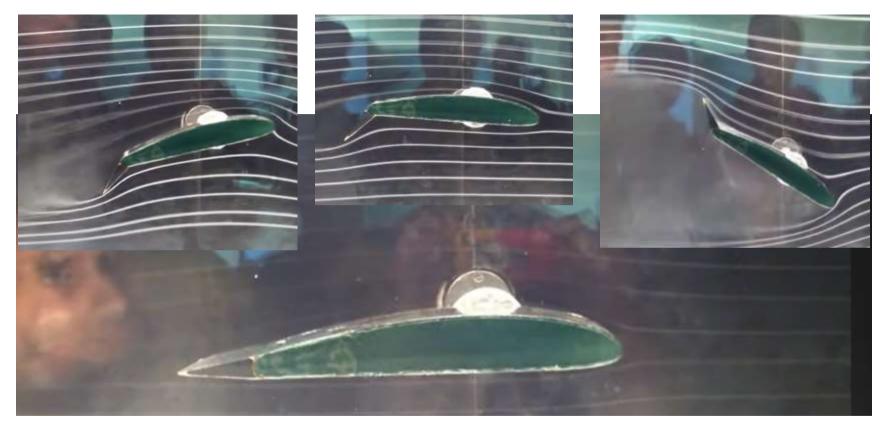
- Simulations allow evaluating a model to optimize system performance or to make predictions about a real system.
- Simulations are useful to study properties of a model of a real-life system that would otherwise be too complex, too large/small, too fast/slow, not accessible, too dangerous or unacceptable to engage.
- While a model aims to be true to the system it represents, a simulation can use a model to explore states that would not be possible in the original system.



Dimetrius Darwin, "Anleitung zur Herstellung eines Miniaturhauses mit LED-Licht | Maßstab 1/64", YouTube, 04.03.2022, url https://www.youtube.com/watch?v=US5tpFVJqvY [20230519].

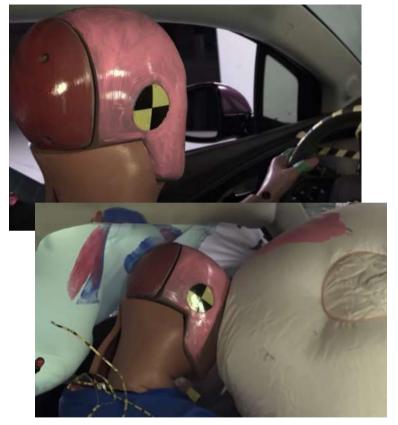


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Ruhou Gao, "Cambered Airfoil in Smoke Tunnel", YouTube, 15.09.2012, url https://www.youtube.com/watch?v=Png0fnG0b\_U [20230519].





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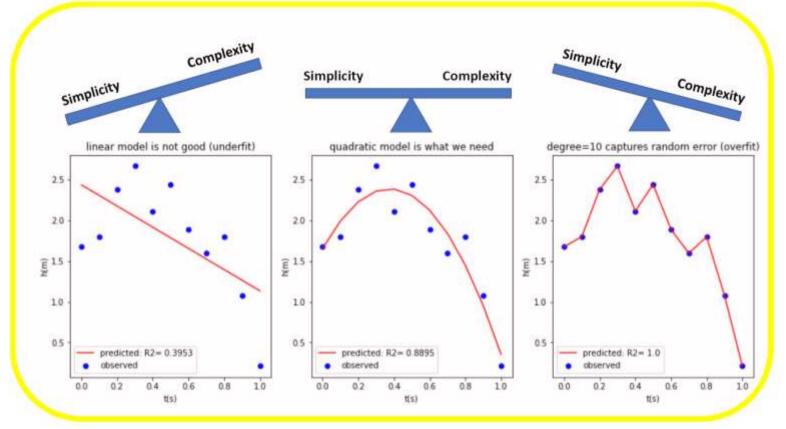


Vaccine Makers Project, "A Virus Attacks a Cell" YouTube, 28.07.2017, url https://www.youtube.com/watch?v=jkNxmTrrZSk [20230519].

#### Akurasi dan kesederhanaan

# Accuracy vs simplicity

- Accuracy vs. Simplicity: A Complex Trade-Off (E. Aragones, I. Gilboa, A. Postlewatite, D. Schmeidler, 2002).
- Simplicity and Accuracy Trade-Off in Science: Simple metric for model selection (P. Niinen, 2013). pdf
- An Analysis of Accuracy and Simplicity in Relation to Knowledge (Kibin, 2023). html
- Simplicity vs Complexity in Machine Learning Finding the Right Balance (Tayo, 2019). html



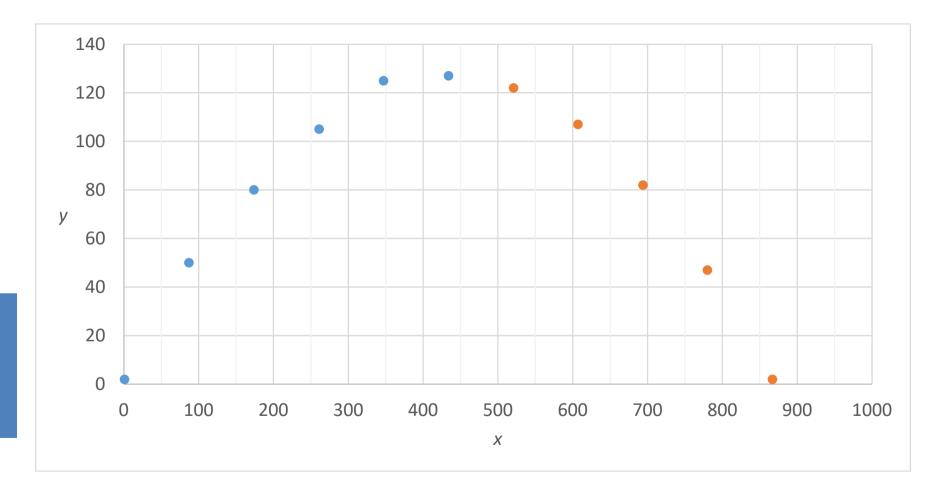
Benjamin Obi Tayo, "Simplicity vs Complexity in Machine Learning — Finding the Right Balance", Towards Data Science, 11 Nov 2019, url https://towardsdatascience.com/p-c9000d1726fb [20230519].

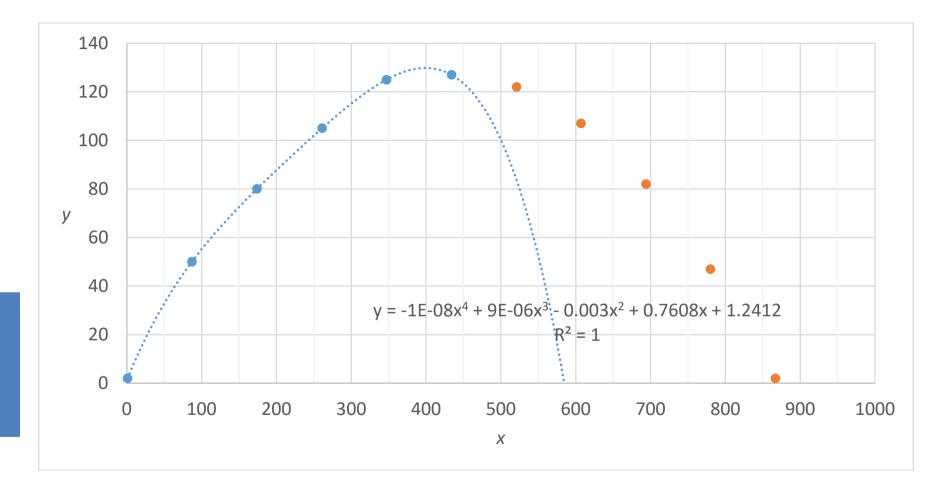
# Simple model is preferred over a complex one

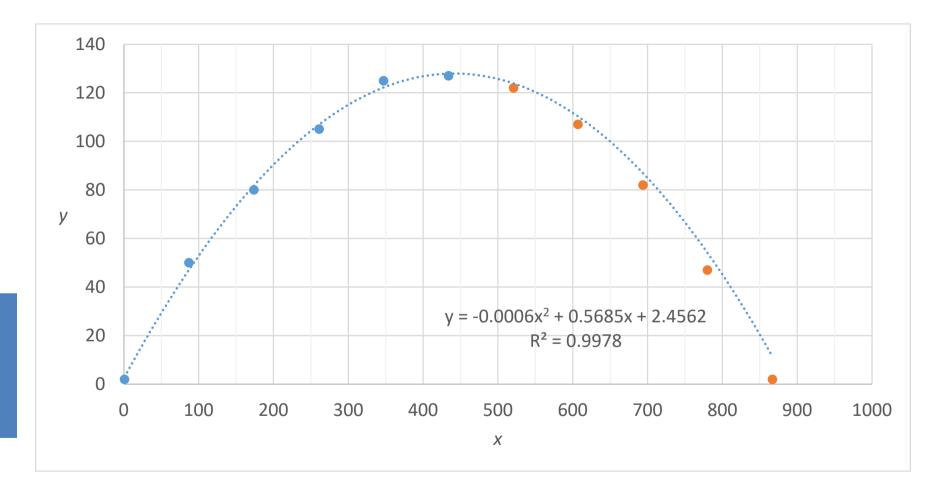
- Prevents Overfitting: A high-dimensional dataset having too many features can sometimes lead to overfitting (model captures both real and random effects).
- Interpretability: An over-complex model having too many features can be hard to interpret especially when features are correlated with each other.
- Computational Efficiency: A model trained on a lowerdimensional dataset is computationally efficient (execution of algorithm requires less computational time).

# Gerak parabola

- Materi fisika dasar yang banyak dimanfaatkan, terutama dalam perang (sains tidak berpihak, tergantung yang memanfaatkanya ③).
- Dapat ditingkatkan kompleksitasnya dengan menambahkan gesekan udara dan adanya angin yang berubah-ubah arah dan besarnya.
- Ilustrasi yang digunakan masih tanpa angin dan tanpa gesekan udara.







# **Formula**

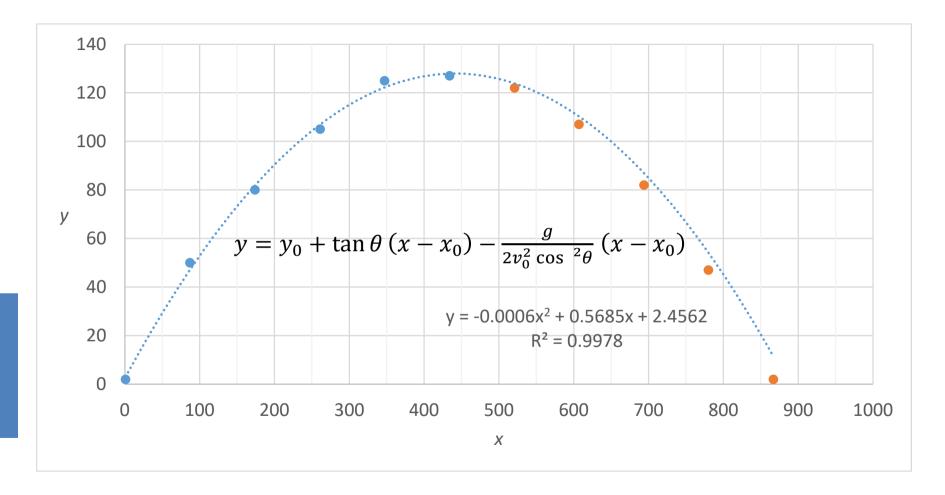
Fungsi parametrik (dari kinematika)

$$x = x_0 + v_0 \cos \theta t$$

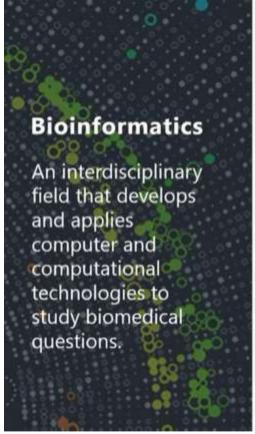
$$y = y_0 + v_0 \sin\theta \, t - \frac{1}{2}gt^2$$

Posisi vertikal sebagai fungsi posisi horizontal

$$y = y_0 + \tan \theta (x - x_0) - \frac{g}{2v_0^2 \cos^2 \theta} (x - x_0)$$



#### **Bioinformatika**

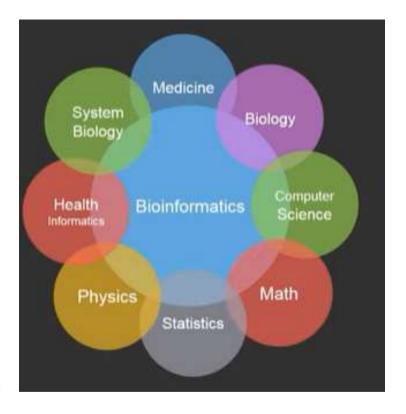


#### TECHNOLOGY

As a technology, bioinformatics is a powerful technology to manage, query, and analyse big data in life sciences.

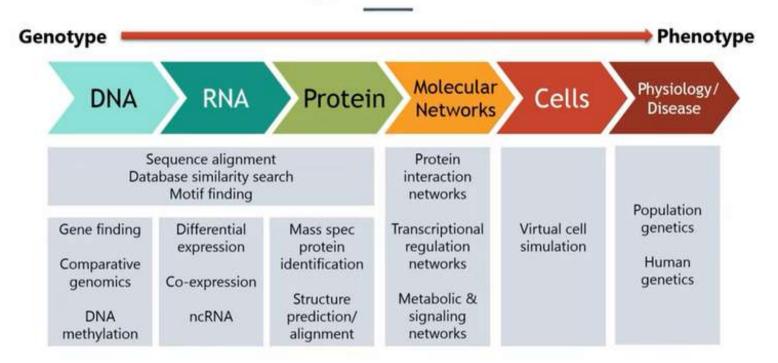
METHODOLOGY

As a methodology, bioinformatics is a topdown, holistic, datadriven, genome-wide, and systems approach that generates new hypotheses, finds new patterns, and discovers new functional elements.

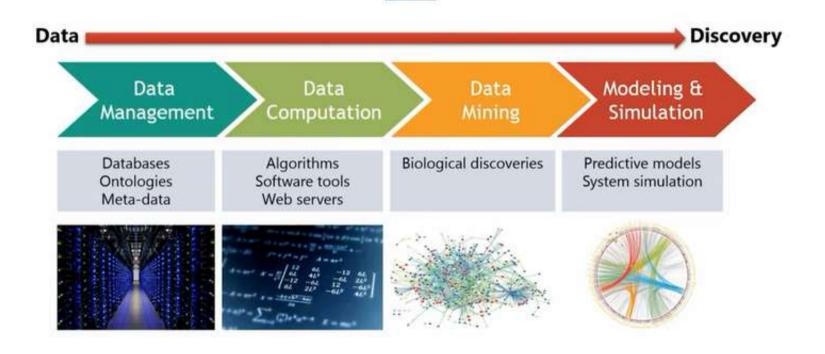


Precision Health, "What is Bioinformatics?" YouTube, 14.05.2021, url https://www.youtube.com/watch?v=7j3atzpjh2c [20230522].

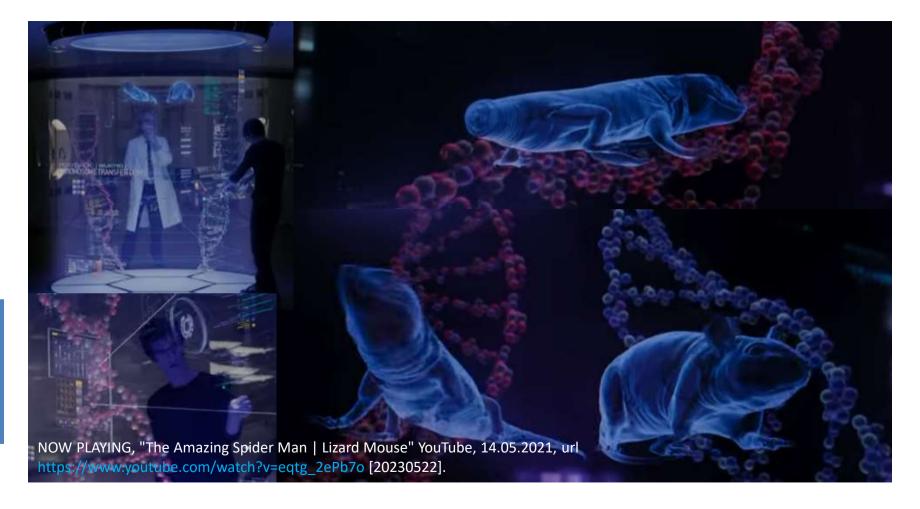
# The Biology in Bioinformatics

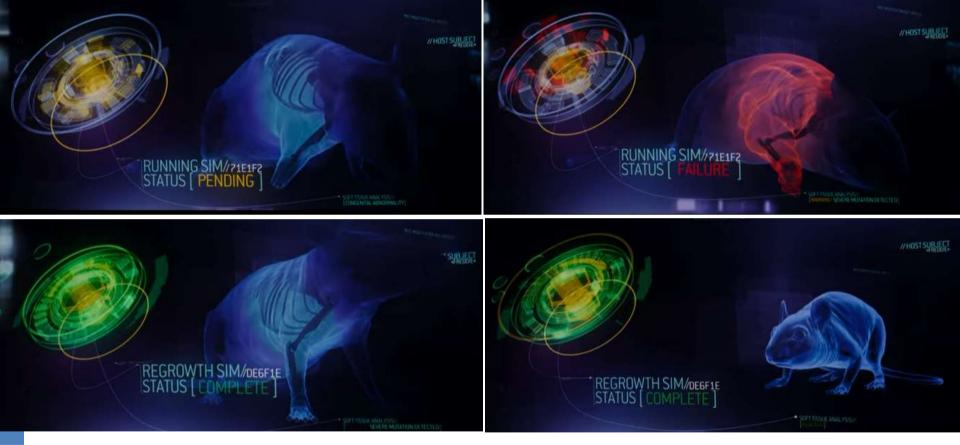


# The Informatics in Bioinformatics

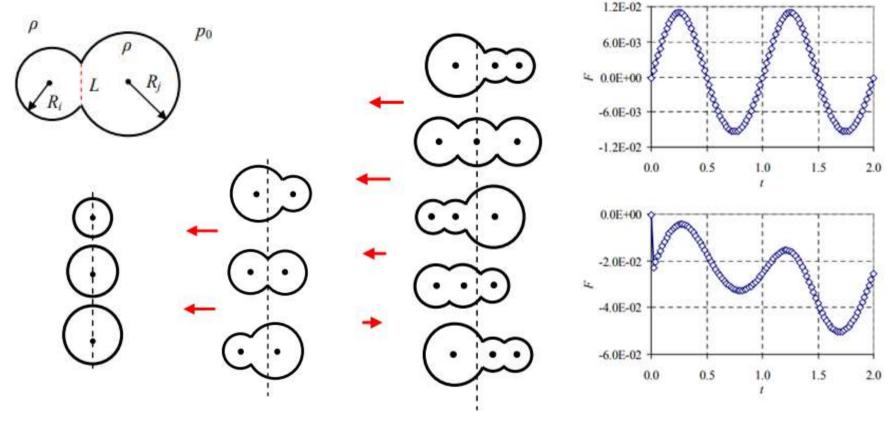


# Fiksi atau impian?

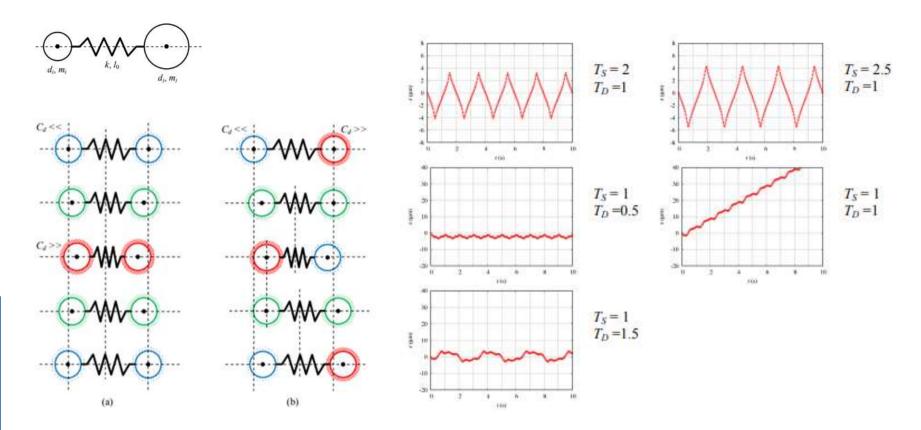




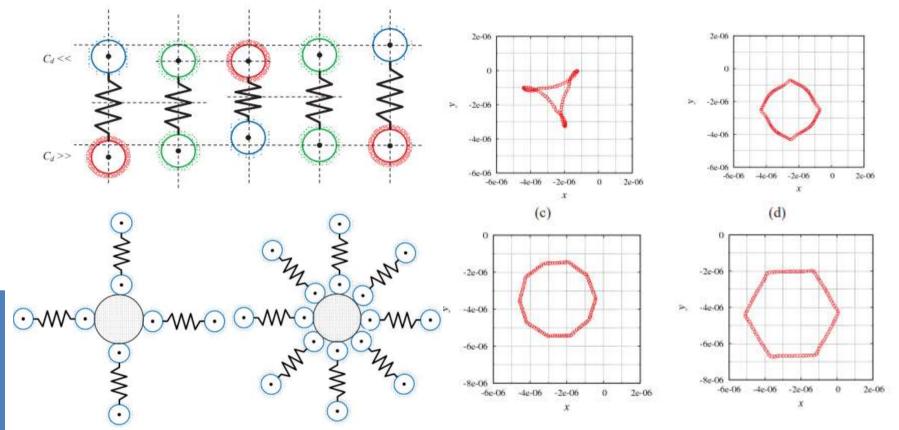
# Penelitian (penyaji) saat ini



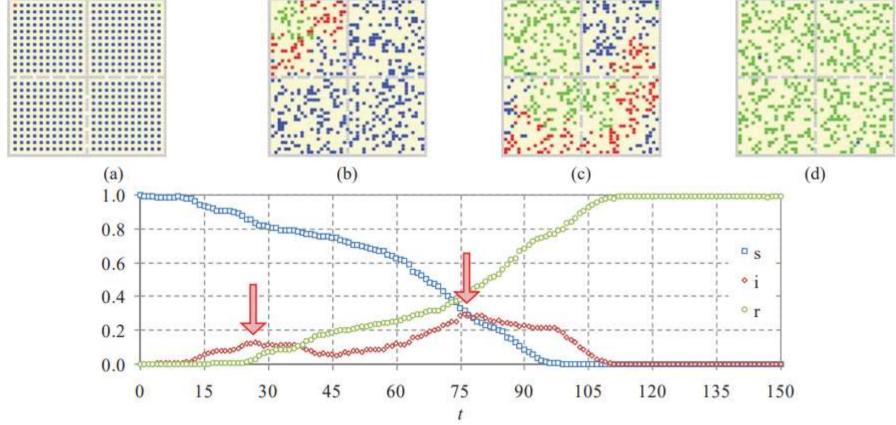
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N. Nuraini, S. Viridi, F. Haryanto, S. N. Khotimah, "Molecular Dynamics Simulation of Microorganism Motion in Fluid Based on Granular Model in the Case of Multiple Simple Push-Pull filaments", in Symposium on Biomathematics-2016, edited by B. Benyamin and Kasbawati, AIP Conference Proceedings 1825, American Institute of Physics, Melville, NY, 2017, pp. 020016.



Armi Susandi, Intan Taufik, Pingkan Aditiawati, Sparisoma Viridi, "The relation between agent-based model and susceptible-infected-recovered model for spread of disease", in The 9th National Physics Seminar, (SNF)-2020, edited by Hadi Nasbey, Riser Fahdiran, Widyaningrum Indrasari, Esmar Budi, Fauzi Bakri, Teguh Budi Prayitno, Dewi Muliyati, AIP Conference Proceedings 2320, American Institute of Physics, Melville, NY, 2021, pp. 050032.

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#### Catatan

 Simulasi sistem biologi yang telah dilakukan terkait kedinamisan biopartikel, baik berupa mikroorganisme ataupun orang.



- Ranah ini merupakan ujung akhir dari Bioinformatika.
- Perlu kolaborasi dan model yang lebih mendalam agar dapat mengaitkan gerak biopartikel dengan informasi genomik.

# Diskusi

# Saran dan pertanyaan

- Silakan menyampaikan saran dan mengajukan pertanyaan.
- Mari kita berdiskusi.

# Terima kasih