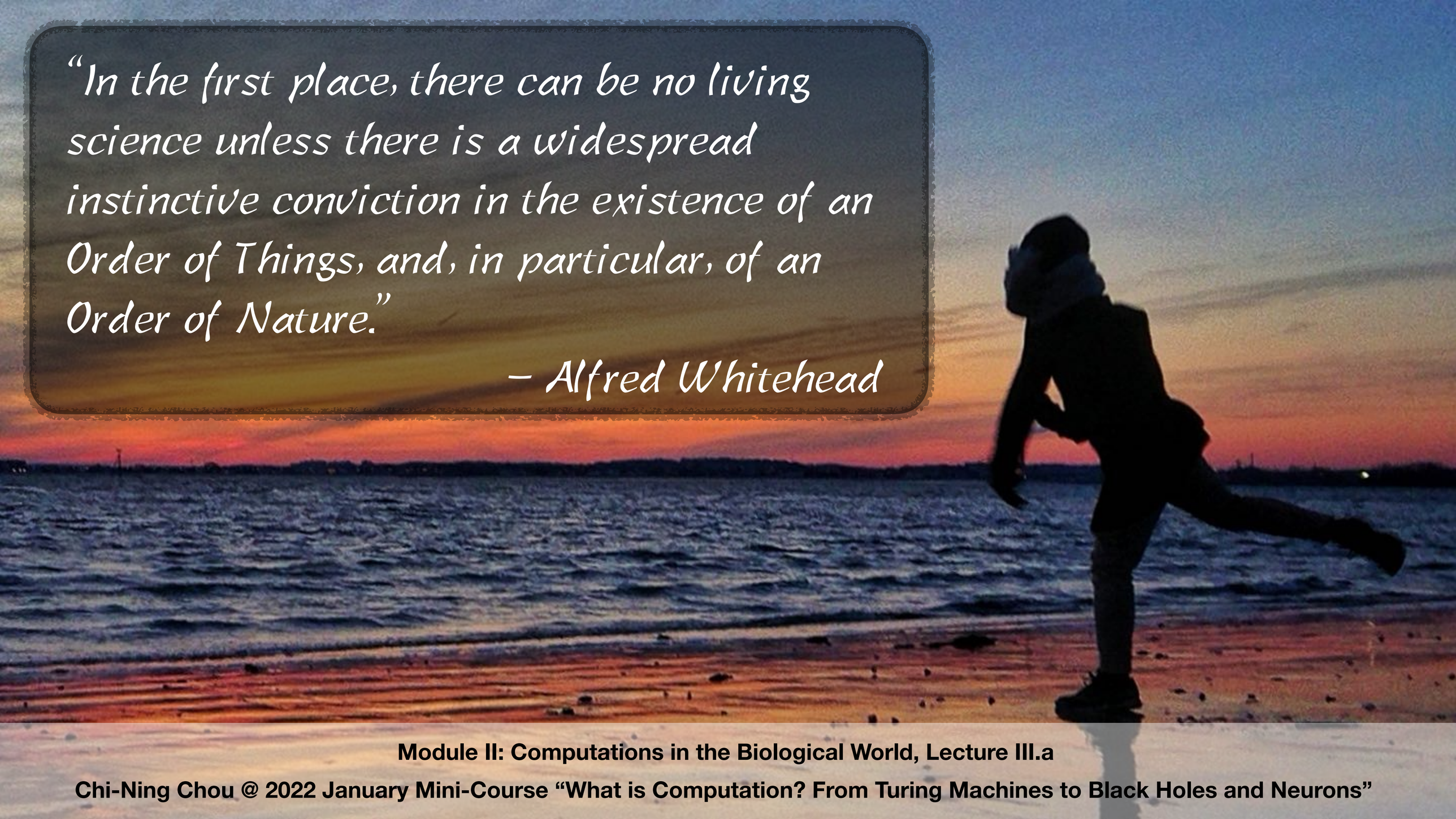


Module II: Computations in the Biological World, Lecture III.a

Chi-Ning Chou @ 2022 January Mini-Course "What is Computation? From Turing Machines to Black Holes and Neurons"

Entering the Living World: Algorithms & Computations in Biology

Module III: Computations in the Biological World

"In the first place, there can be no living science unless there is a widespread instinctive conviction in the existence of an Order of Things, and, in particular, of an Order of Nature."

– Alfred Whitehead

Inspiration

Biology
&
Computation

Tools

What is Biology and Why Care?

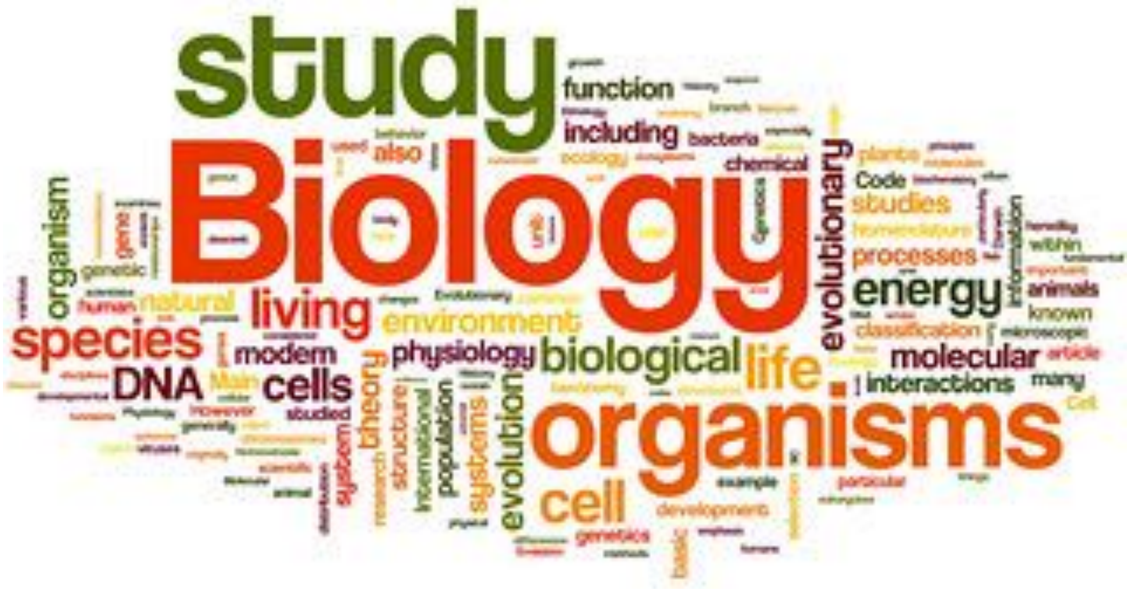
"Biology is the scientific study of life. It is a natural science with a broad scope but has several unifying themes that tie it together as a single, coherent field."

– Wikipedia

- We humans are living beings!
- Computational methods are widely used in the study of biology.

Q: What are the computations in the biological worlds?

Q: Biology as constraints or inspirations?



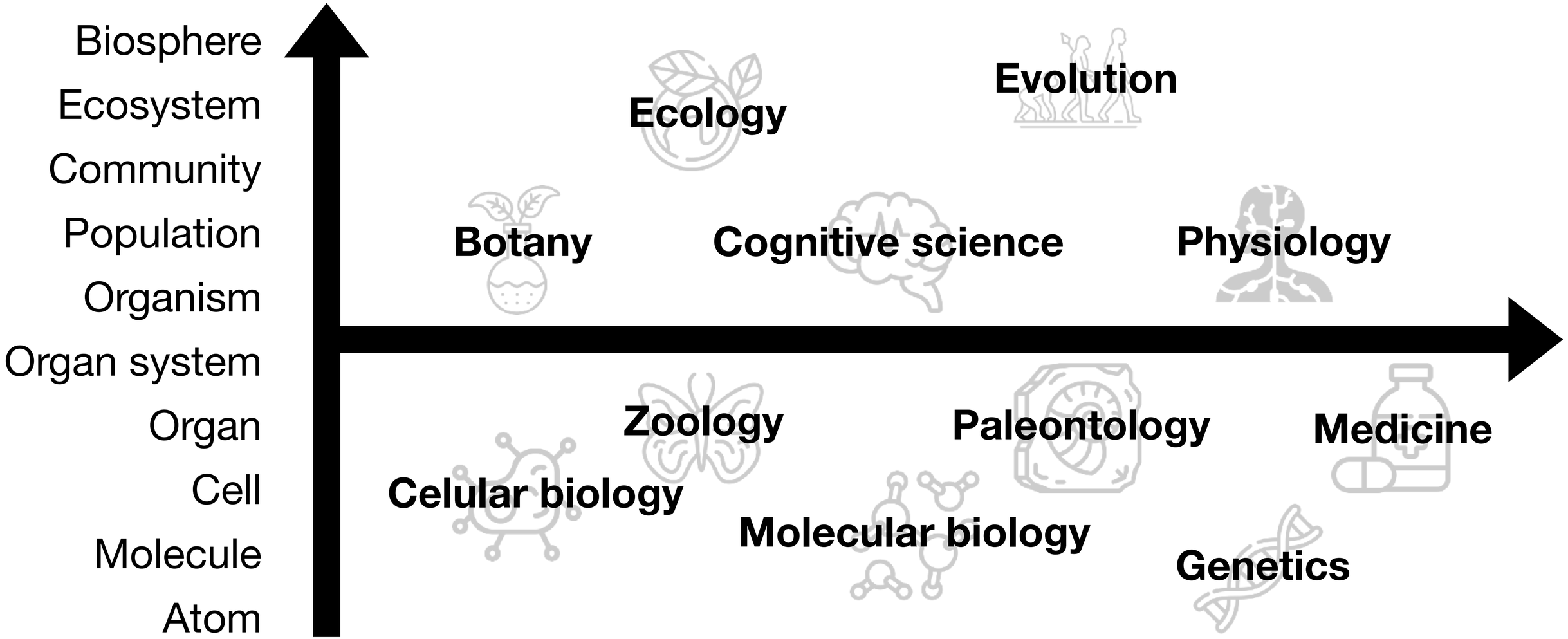
Why Biology?

Module III: Computations in the biological world

I encourage you to enjoy the many examples we are going to see throughout the lectures and build up your own story!

The Scope of Biology

An extremely diverse scientific field!



Distinguishing Characteristics of Life

"All these characteristics of living organisms distinguish them categorically from inanimate systems."

– Ernst Mayer

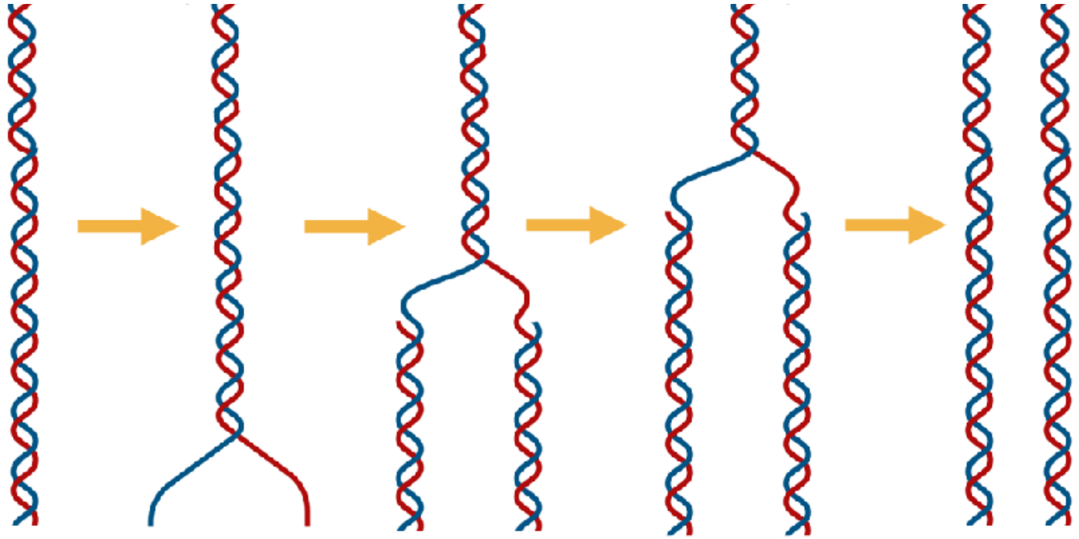
A capacity

- for evolution.
- for self-replication.
- for growth and differentiation via genetic program.
- for metabolism (the binding and releasing of energy).
- for self-regulation, to keep the complex system in steady state.
- for response to stimuli from the environment through perception and sense organs.
- for change at two levels, that of the phenotype and that of the genotype.

Life is Complicated!!

Biological Algorithms vs. Computer Algorithms

Example: copying strings



DNA Replication
(An oversimplified version)

```
char *
STRCPY (char *dest, const char *src)
{
  return memcpy (dest, src, strlen (src) + 1);
}

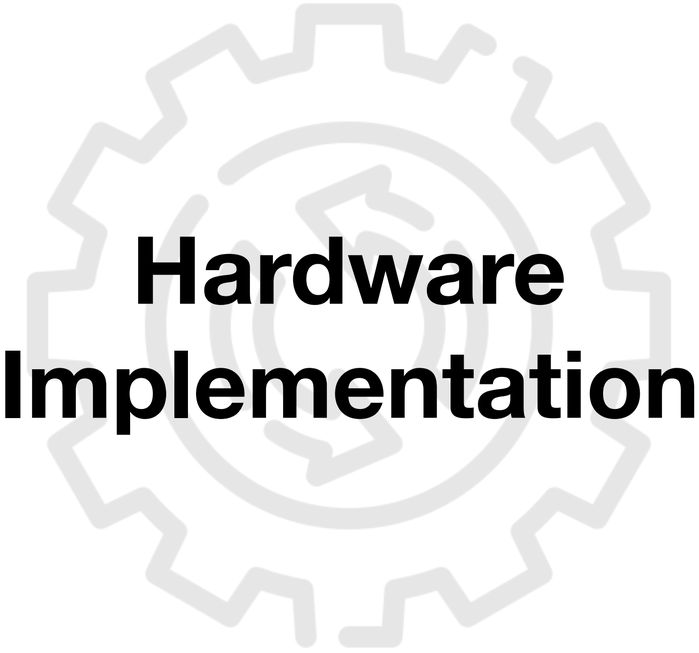
void *
memcpy (void *dest, const void *src, size_t len)
{
  char *d = dest;
  const char *s = src;
  while (len--)
    *d++ = *s++;
  return dest;
}
```

String Copying in C

"Algorithm" in Biology might be Multi-Functional or Goalless!?

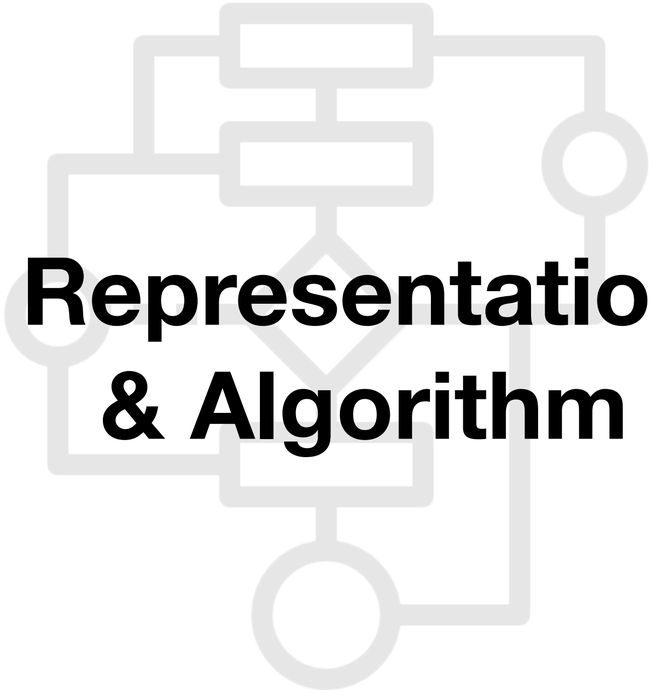
Different Angles to Think

Marr's three levels of analysis



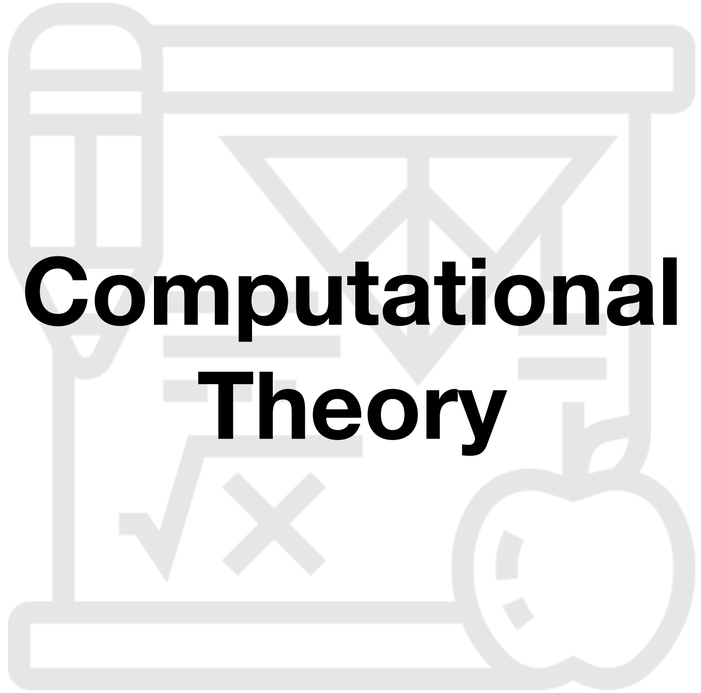
Hardware Implementation

E.g., genotype and phenotype



Representation & Algorithm

E.g., heritable variation, differential reproduction, fitness, competition



Computational Theory

E.g., natural selection

Computation → Biology

Computational Biology & Bioinformatics

Study biology using computational, statistical, and mathematical methods

Structural Biology

System Biology

Theoretical Biology

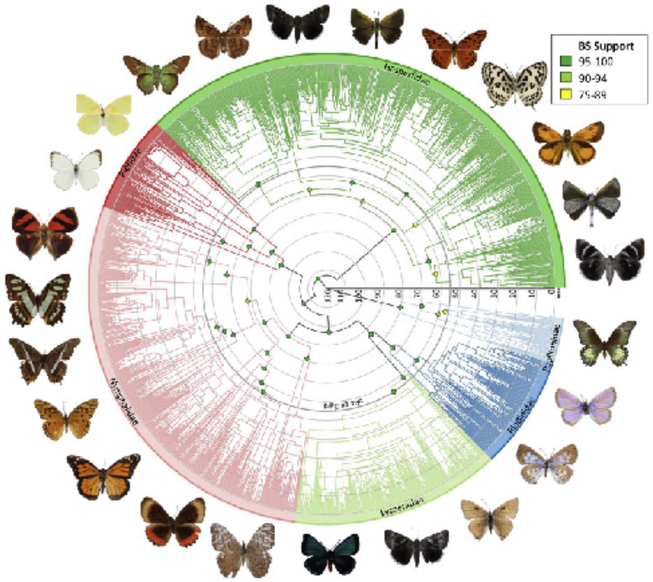
Genomics

Neuroscience

Evolutionary Biology

Example: A Study in Butterflies

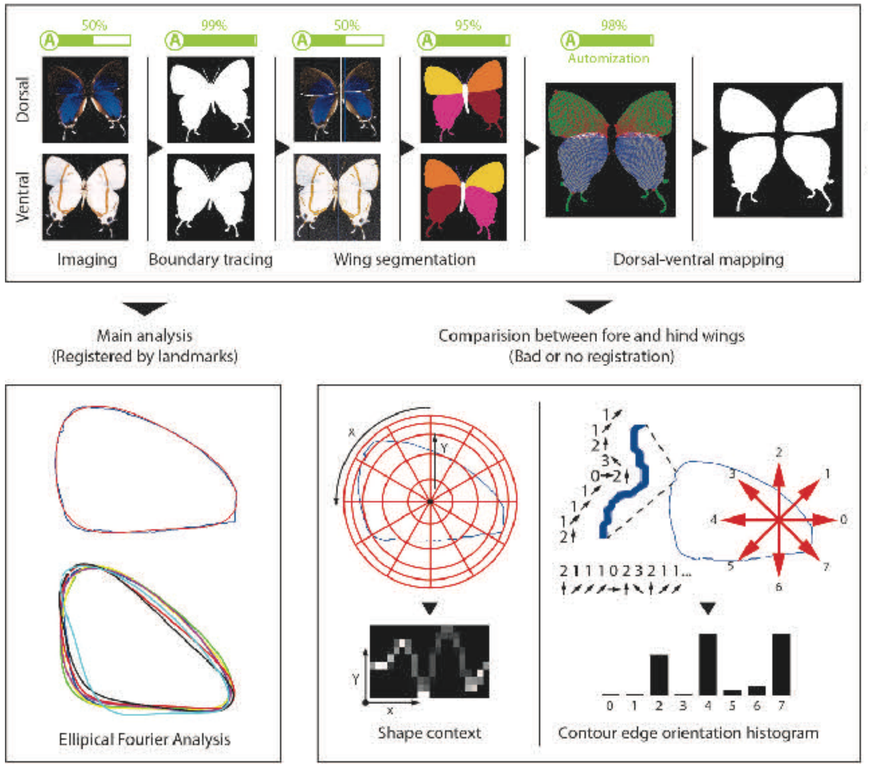
Thank Wei-Ping Chan, my dearest roommate, for sharing his projects!

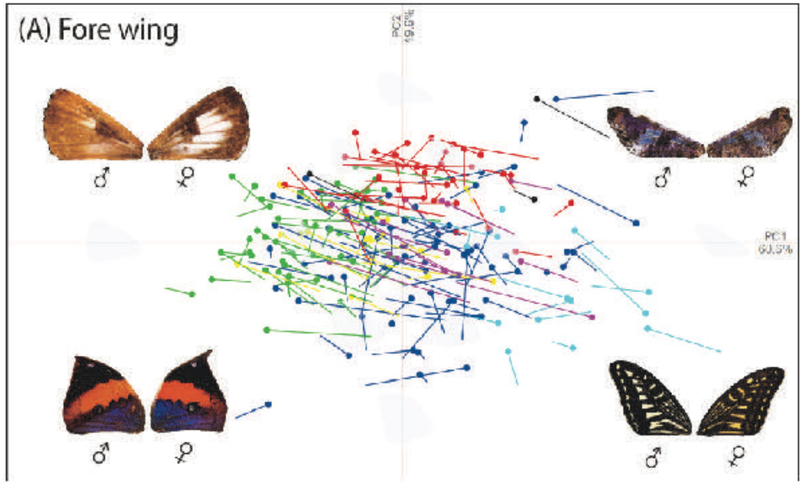


Building phylogenetic tree

[Espeland et al. 2018]

Computer-assisted analysis





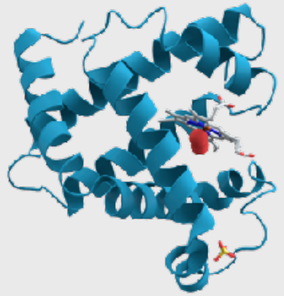
Data analysis

- Principal component analysis (PCA), General linear mixed model (GLMM), Structural equation modeling (SEM), etc.
- Ancestral state reconstruction, morphological disparity through time, etc.

* Chan et al., unpublished, 2022.

AlphaFold

A game changer in the study of protein folding

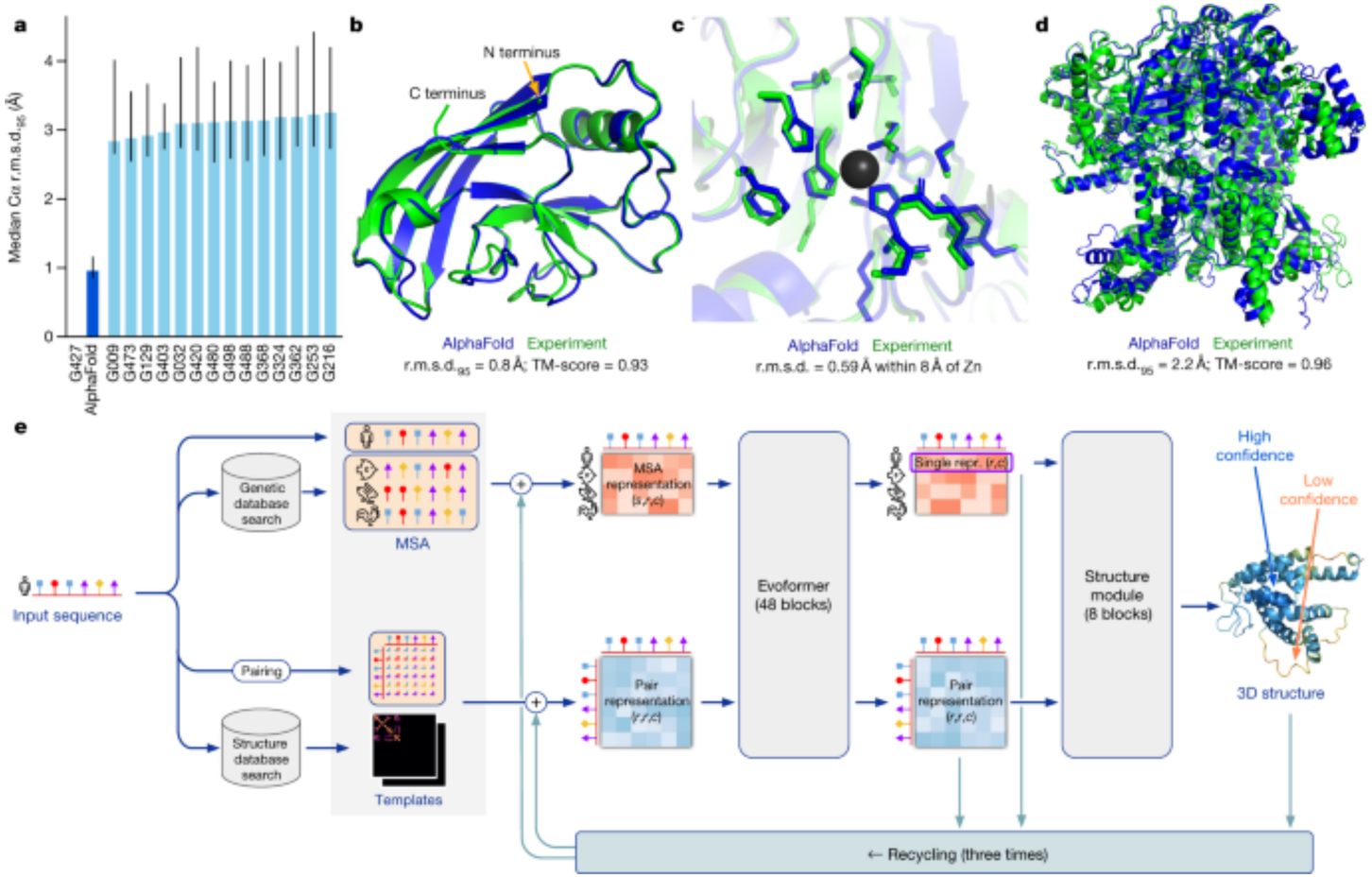


Myoglobin

The 3D shape of a protein determines its function.

The Structure Problem

Given a string of different amino acids, what's the shape of protein?



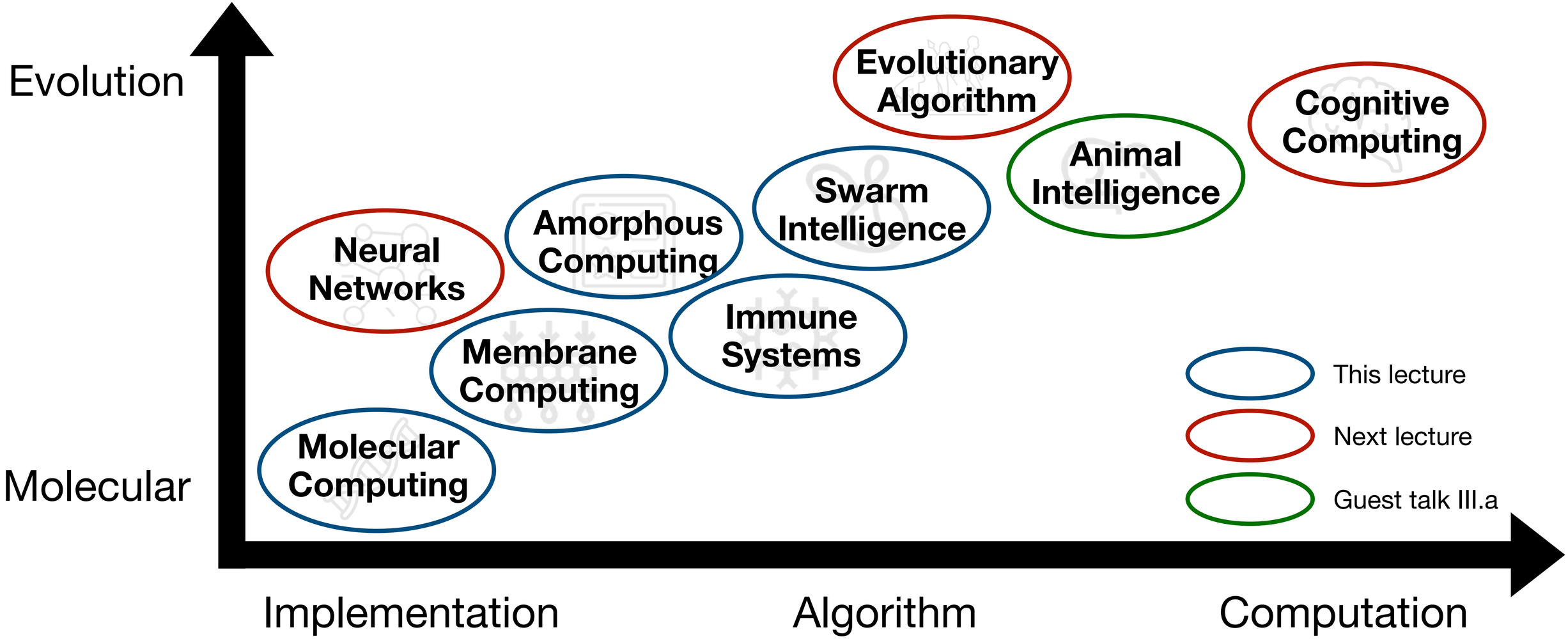
* Jumper, John, et al. "Highly accurate protein structure prediction with AlphaFold." *Nature* 596.7873 (2021): 583-589.

Biology → Computation

Disclaimer: I’m not an expert in any of the example, so please feel comfortable to correct me!

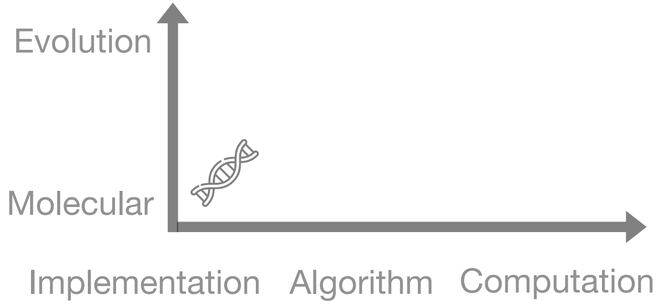
Biological Computation

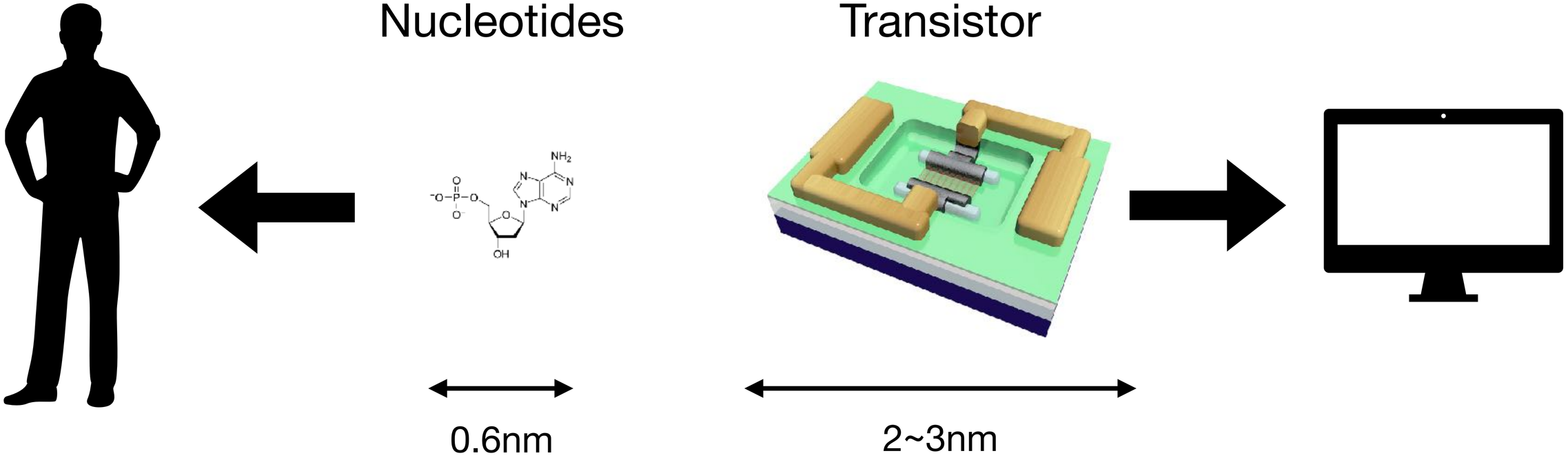
Also known as natural computing, bio-inspired computing, etc.



Molecular Computing

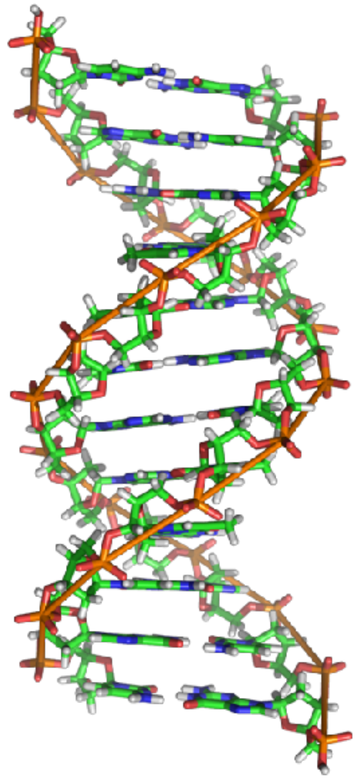
With a focus on DNA computing



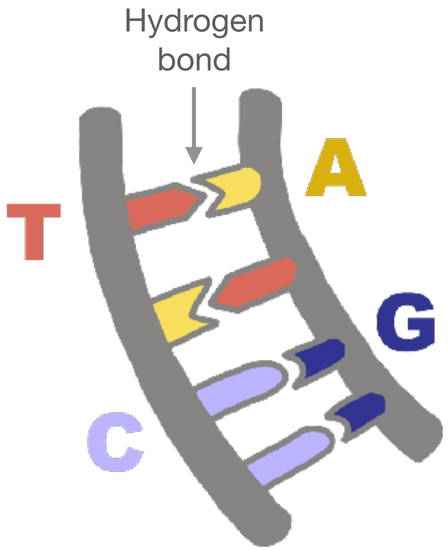


Use molecules to perform basic computational operations!?

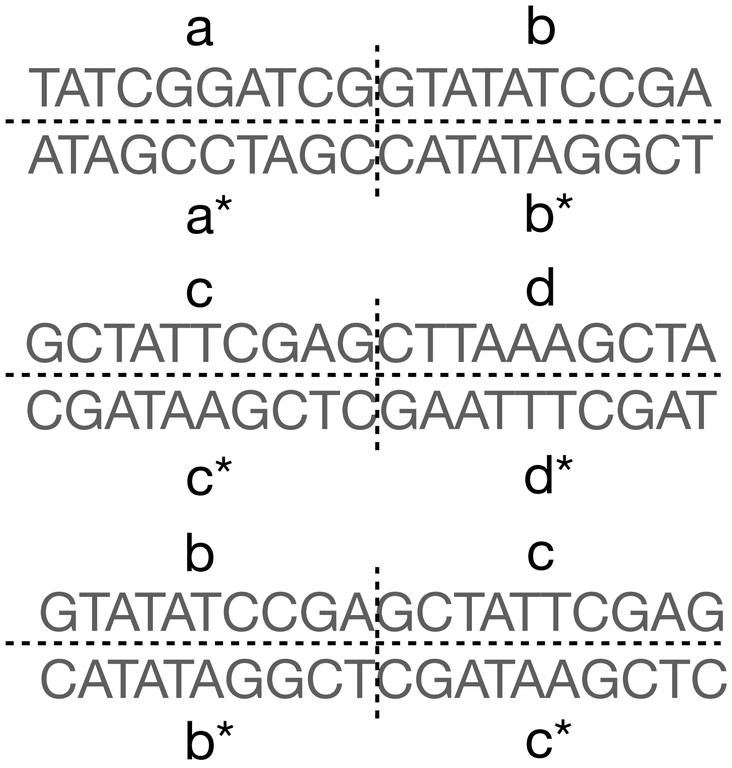
Basic Facts about DNA



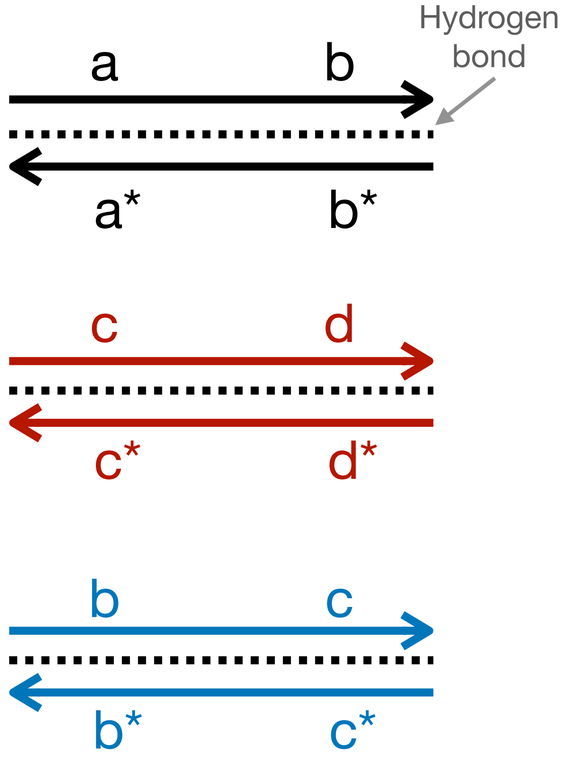
DNA



Nucleotides



Oligonucleotide

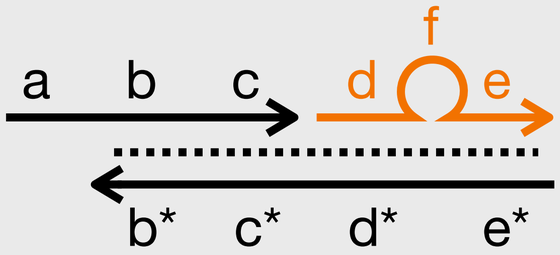


An abstraction

Nucleotides provide basic elements to encode information!

A Simple Logical AND Gate via DNA

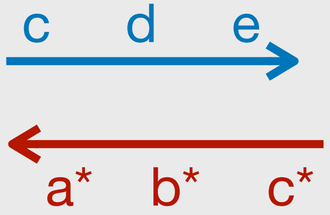
AND gate



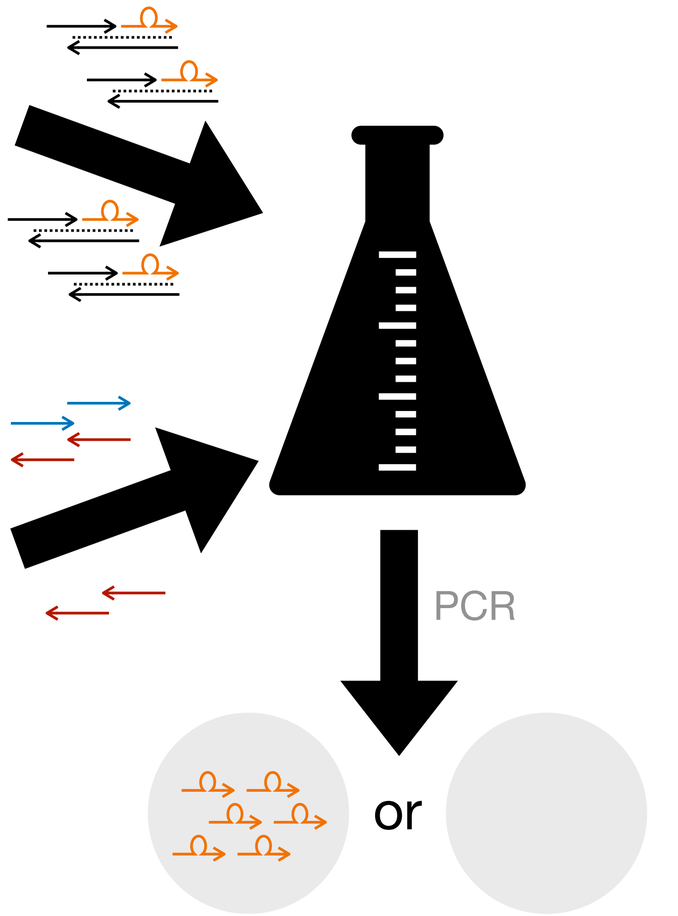
Inputs

(The presence of the Oligonucleotide encodes 0/1)

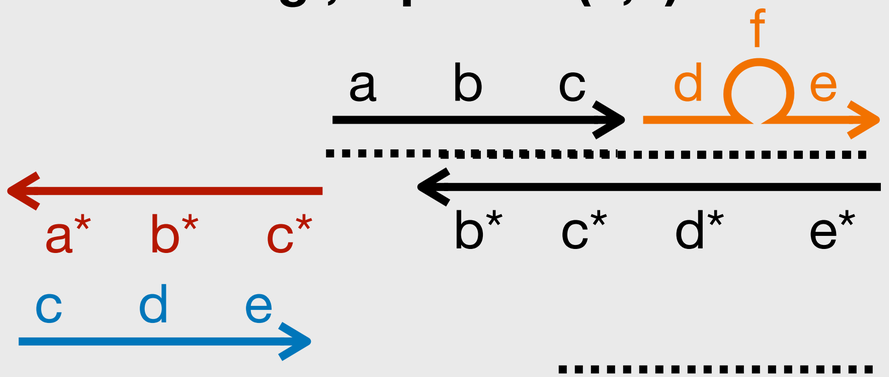
- Inputs = (1,1)



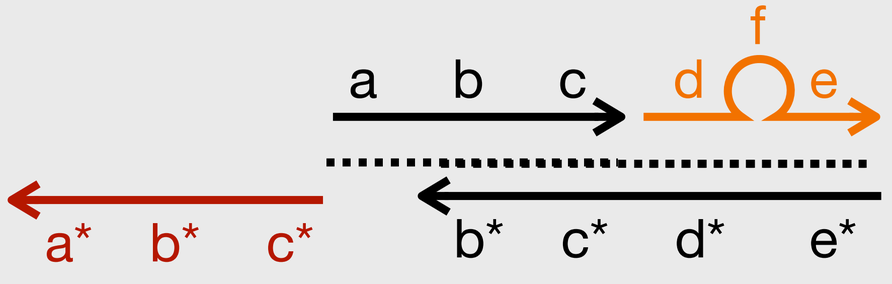
- Inputs = (0,1)



E.g., inputs = (1,1)



E.g., inputs = (0,1)



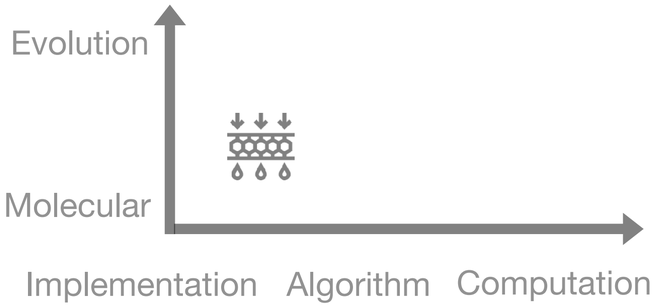
* There's animation for the complete version of this slide.

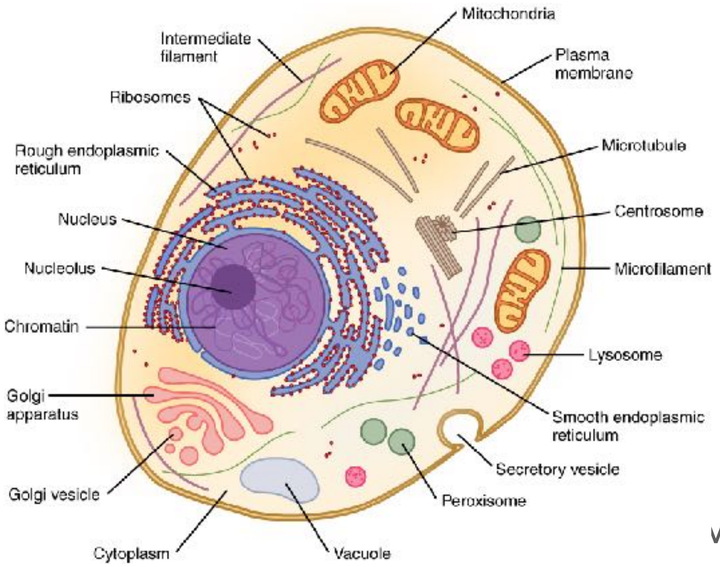
Salvador
(Jan. 19
2pm-3pm ET)

"DNA Computing, Cellular Automata, and Beyond"

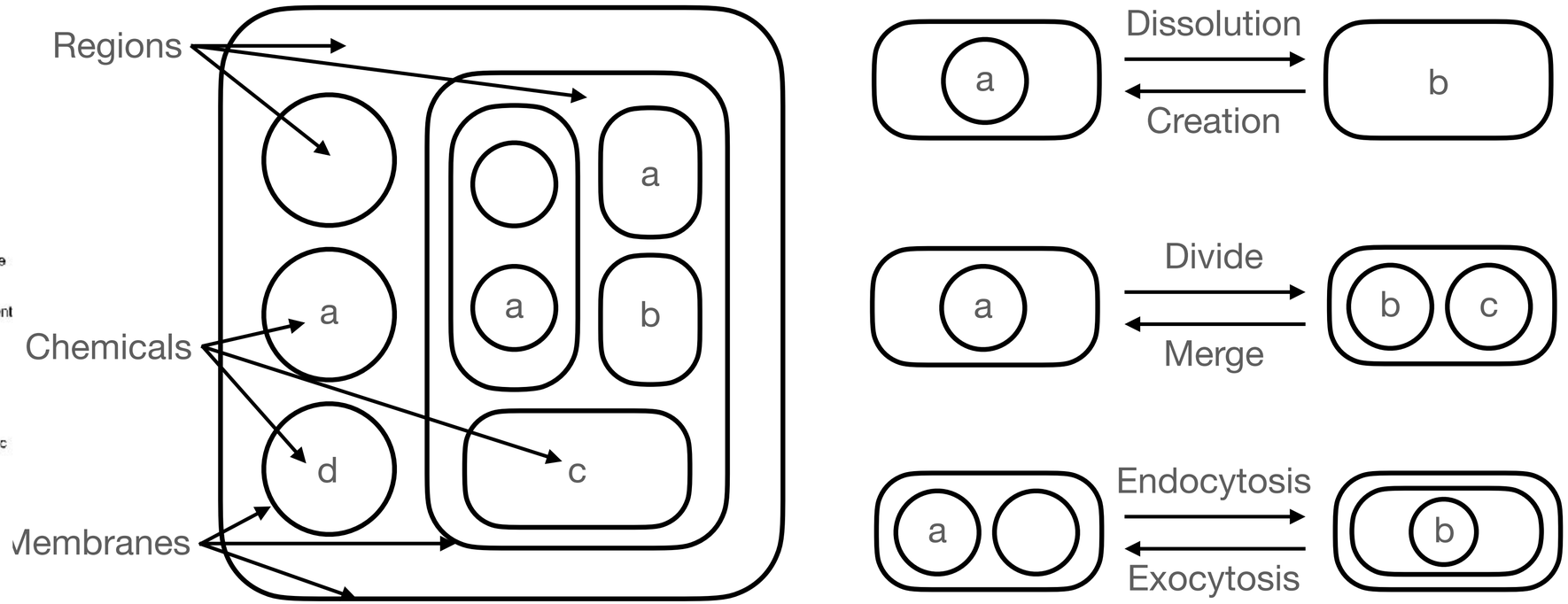
Membrane Computing

Sometimes called cellular computing





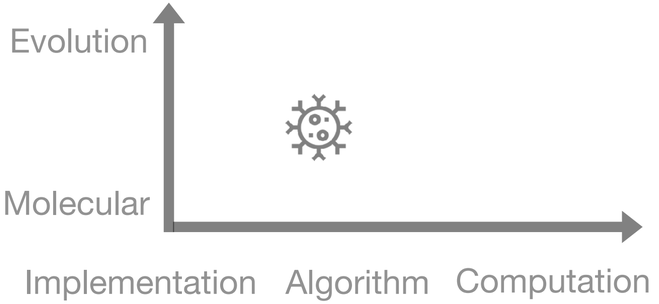
A cell

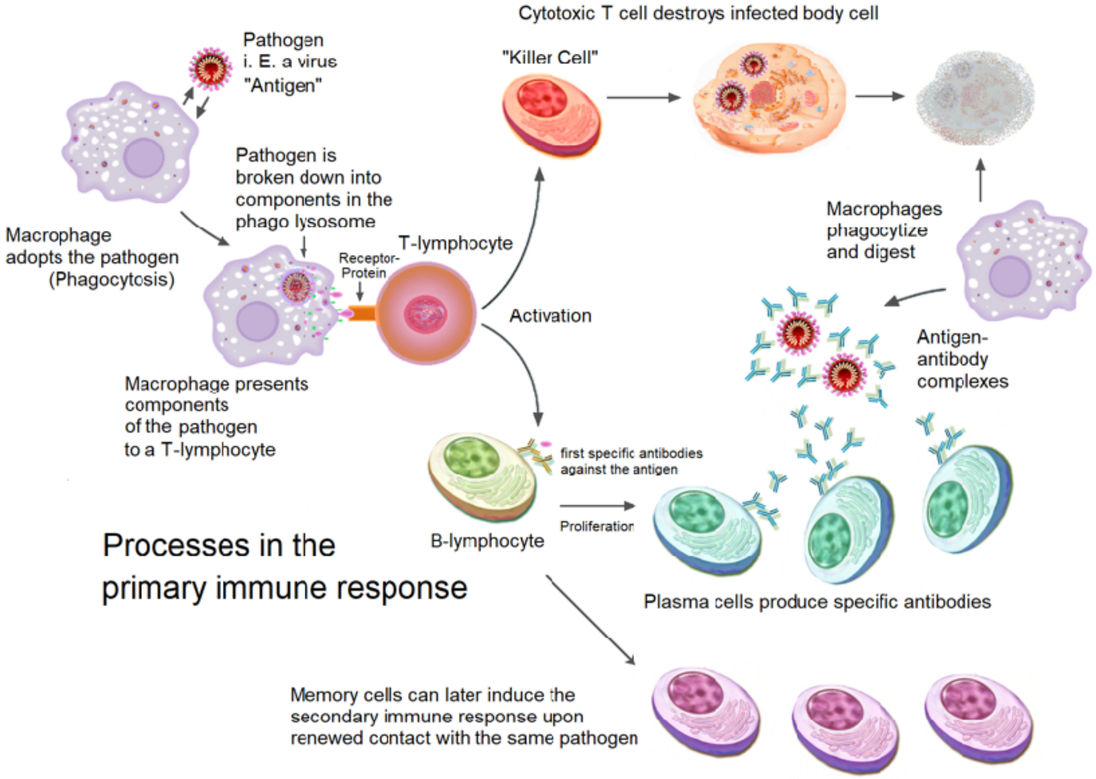


An abstraction (e.g., P system)

Many models here (e.g., P system & Cellular automata) are Turing-complete*!

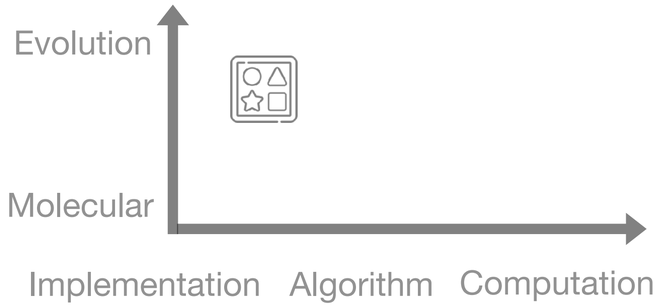
Immune Systems

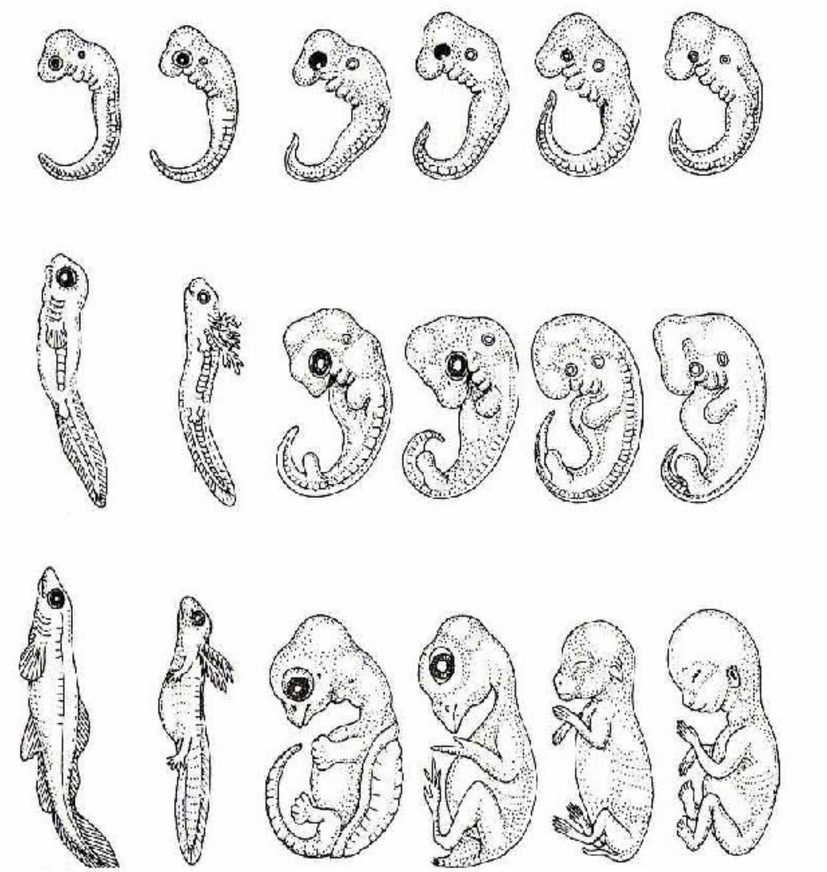




What is foreign and what is a part of its own system?

Amorphous Computing





How do organisms form reliably and consistently while the cells

- are asynchronous,
- are interconnected in an unknown and time-varying ways,
- communicate locally,
- and identically programmed!?

Emergent phenomena!

What's the underlying computational aspect of emergent properties?

Example: Turing's Leopards' Spots Problem

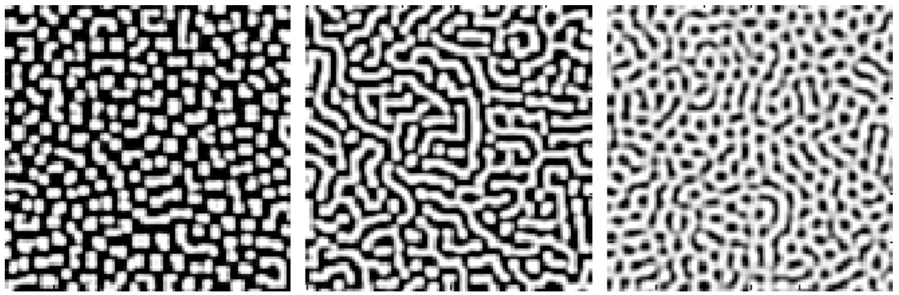
Q: How do the diverse patterns appear ubiquitous in nature?

Q: Why these patterns are hexagons, spirals, stripes, etc.?

THE CHEMICAL BASIS OF MORPHOGENESIS

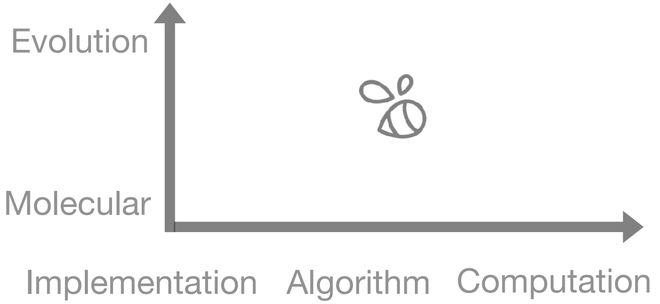
By A. M. TURING, F.R.S. *University of Manchester*

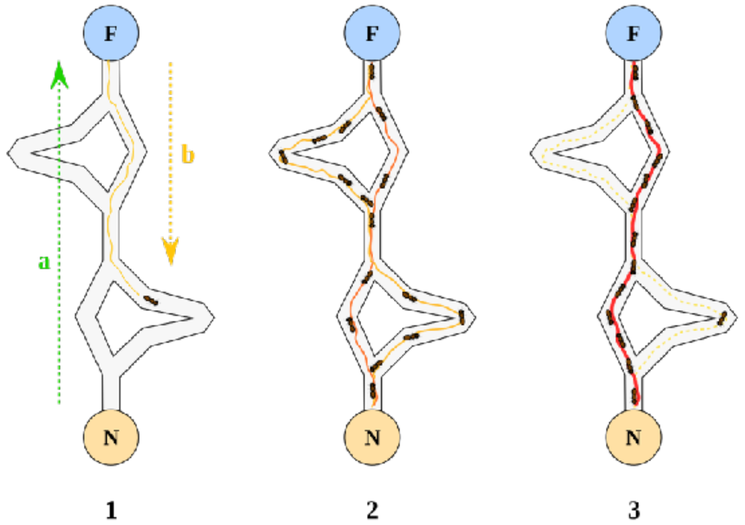
(*Received* 9 *November* 1951—*Revised* 15 *March* 1952)

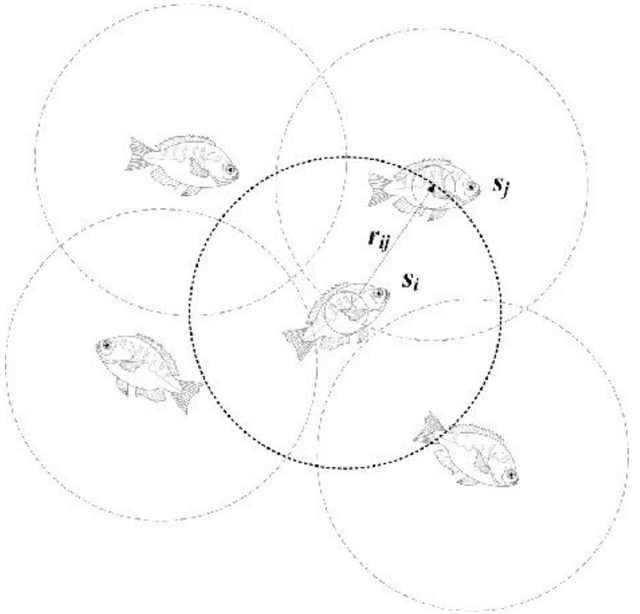


The diffusion and reaction between two "morphogens" would introduce complex pattern that looks like coming from random chaos!

Swarm Intelligence







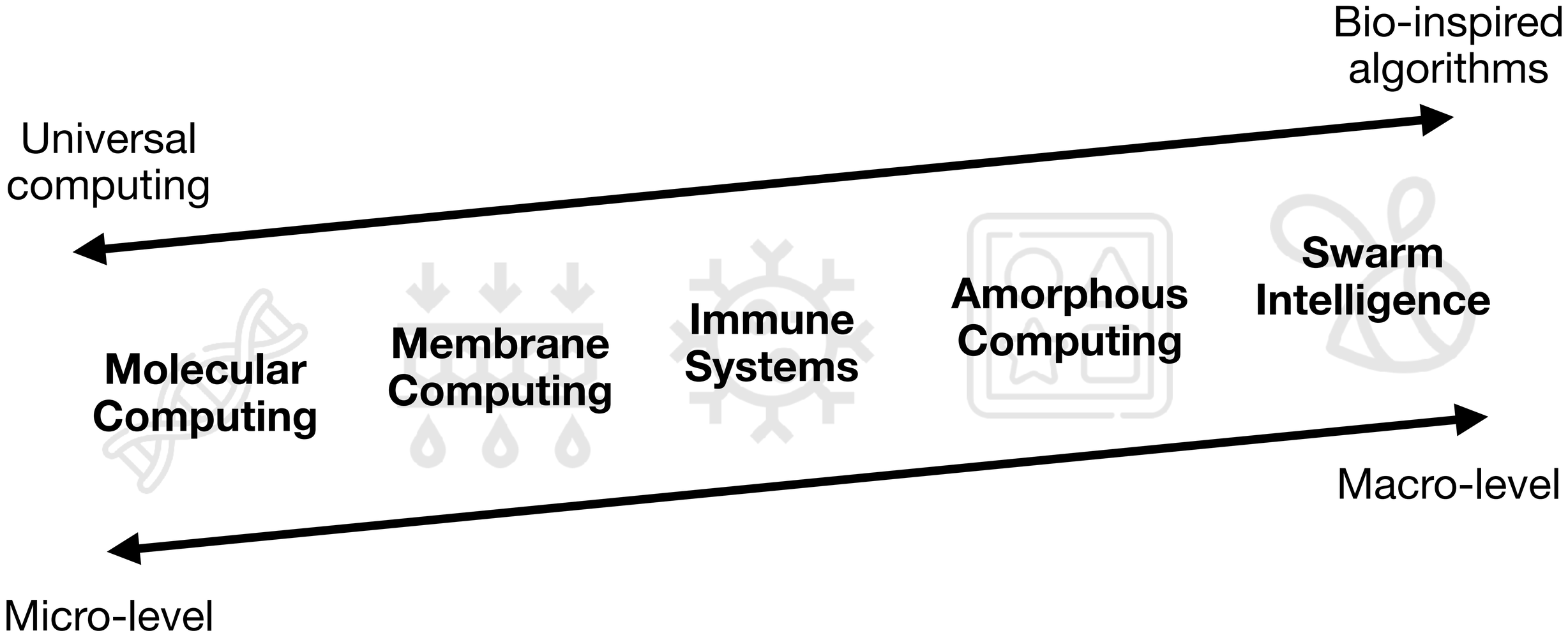
Slime mold solving maze

Ant colony optimization

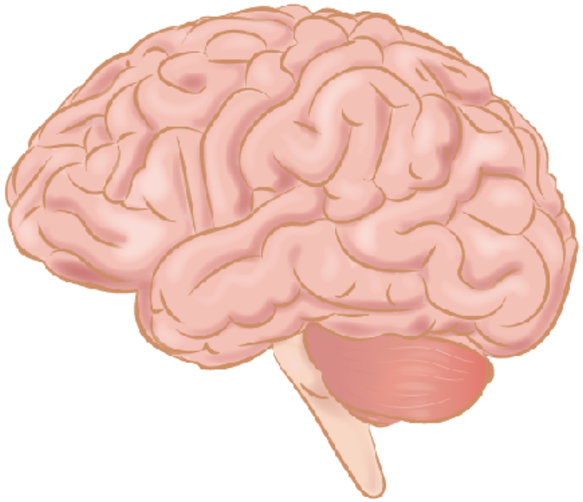
Fish Swarm algorithm

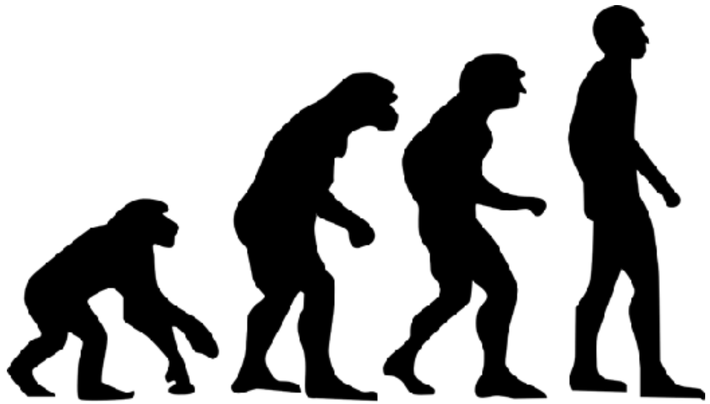
Inspired lots of algorithms and metaheuristics!

A Bird-Eye View



More to Come…





Neuroscience & Cognitive Science

Evolution

Animal Intelligence

Lecture III.b

Guest Talk III.c

Summary

Key Concepts

What is Biology and Why Care?

"Biology is the scientific study of life. It is a natural science with a broad scope but has several unifying themes that tie it together as a single, coherent field."
– Wikipedia

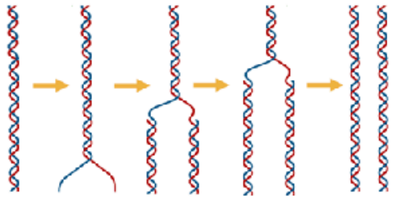
- We humans are living beings!
- Computational methods are widely used in the study of biology.

Q: What are the computations in the biological worlds?

Q: Biology as constraints or inspirations?

Biological Algorithms vs. Computer Algorithms

Example: copying strings



DNA Replication
(An oversimplified version)

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    *d++ = *s++;
  return dest;
}
```

String Copying in C

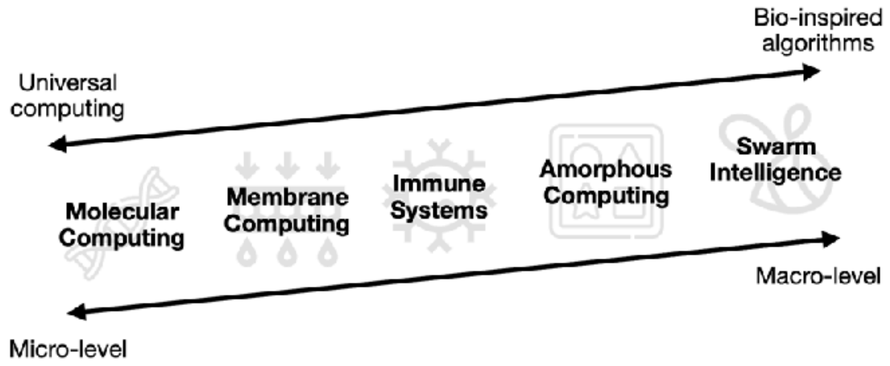
"Algorithm" in Biology might be Multi-Functional or Goalless!?

Different Angles to Think

Marr's three levels of analysis

Hardware Implementation	Representation & Algorithm	Computational Theory
E.g., genotype and phenotype	E.g., heritable variation, differential reproduction, fitness, competition	E.g., natural selection

A Bird-Eye View



Guest Speakers for Module III

Angel Hsing-Chi Hwang
(Jan. 17 11am-12pm ET)

"Into the Unknown: (De)constructing Creativity in the Age of Human-Machine Partnership"

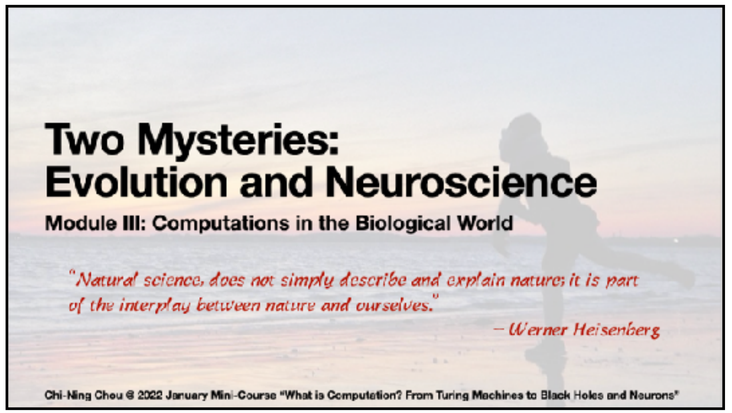
"A Road to Totality: Between Art and Computation"

Zhiqian Wang
(Jan. 19 11am-12pm ET)

Brabeeba Wang
(Jan. 20 11am-12pm ET)

"Animal Intelligence: Flexible Computation Under Uncertainty"

Next



Lecture III.b

(Jan. 14 10am-10:50am ET)

Salvador

(Jan. 19
2pm-3pm ET)

"DNA Computing, Cellular Automata, and Beyond"

Check them out on the calendar!

Food for Thought

Q: How do you think the “computations” done in the biological world differ from that in the physical world as well as the mathematical formulation?

Q: Can you come up with some examples of biological computation from your own life experience?

Q: Do you think the current studies (at lease those being discussed in this lecture) of biological computation have captured most of the computational insights?

Exercise

- If you have come up with some example of biological computation, try to formalize it and abstract out the computational insight.
- Find one example you like the most from this lecture and look into it!

References

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- Chelly Dagdia, Z., Avdeyev, P. & Bayzid, M.S. Biological computation and computational biology: survey, challenges, and discussion. Artif Intell Rev 54, 4169–4235 (2021), link.

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- Nowak, Martin A. Evolutionary dynamics: exploring the equations of life. Harvard university press, 2006, link.
- Jones, Neil C., Pavel A. Pevzner, and Pavel Pevzner. An introduction to bioinformatics algorithms. MIT press, 2004, link.
- Gillespie, John H. Population genetics: a concise guide. JHU Press, 2004, link.

Fun reads:

- Stanley, Kenneth O., and Joel Lehman. Why greatness cannot be planned: The myth of the objective. Springer, 2015, link.
- Schrödinger, Erwin. What is life?: With mind and matter and autobiographical sketches. Cambridge university press, 1992, link.
- Mayr, Ernst. This is biology : the science of the living world. Harvard University Press, 2001, link.
- Banatre, Jean-Pierre, et al., eds. Unconventional Programming Paradigms: International Workshop UPP 2004, Le Mont Saint Michel, France, September 15-17, 2004, Revised Selected and Invited Papers. Vol. 3566. Springer Science & Business Media, 2005, link.

* Many icons in the slides were made by Freepik from www.flaticon.com