00: Course Overview

CSCI4181/6802 Bioinformatics Algorithms

Finlay Maguire (finlay.maguire@dal.ca)

Why am I teaching this course?

Maguire Lab Overview

Genomic Epidemiology

Affiliations:

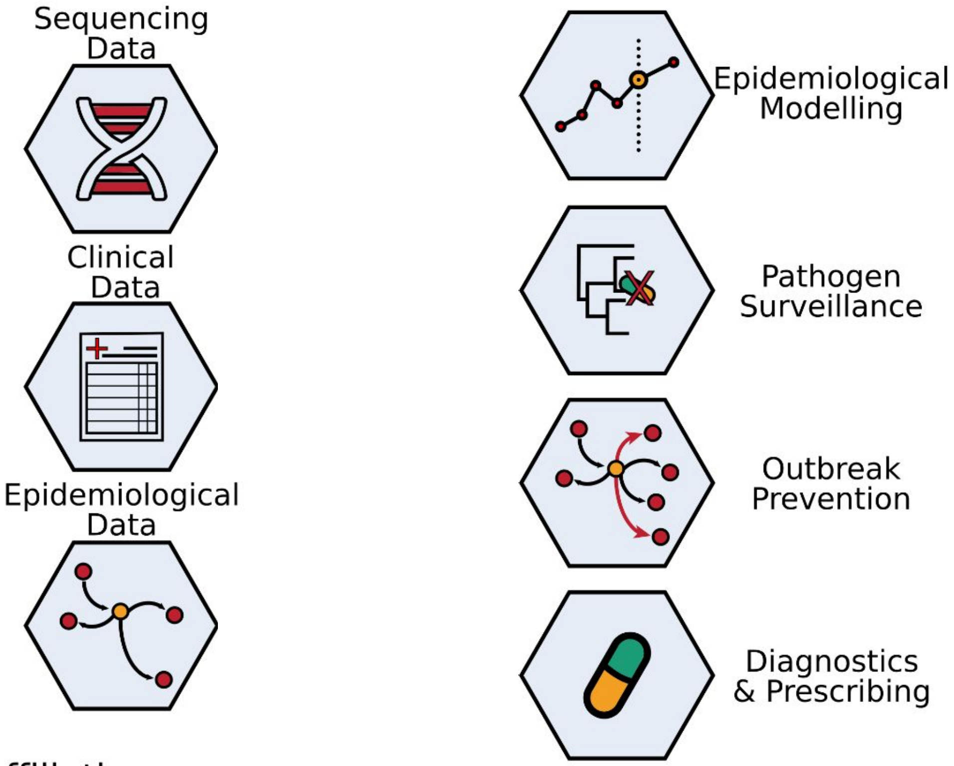
DALHOUSIE UNIVERSITY
Computer Science
Community Health & Epidemiology
Institute of Comparative Genomics

Sunnybrook HEALTH SCIENCES CENTRE
Sunnybrook Research Institute
Shared Hospital Laboratory

Public Health Alliance for Genomic Epidemiology

Maguire Lab Overview

Genomic Epidemiology



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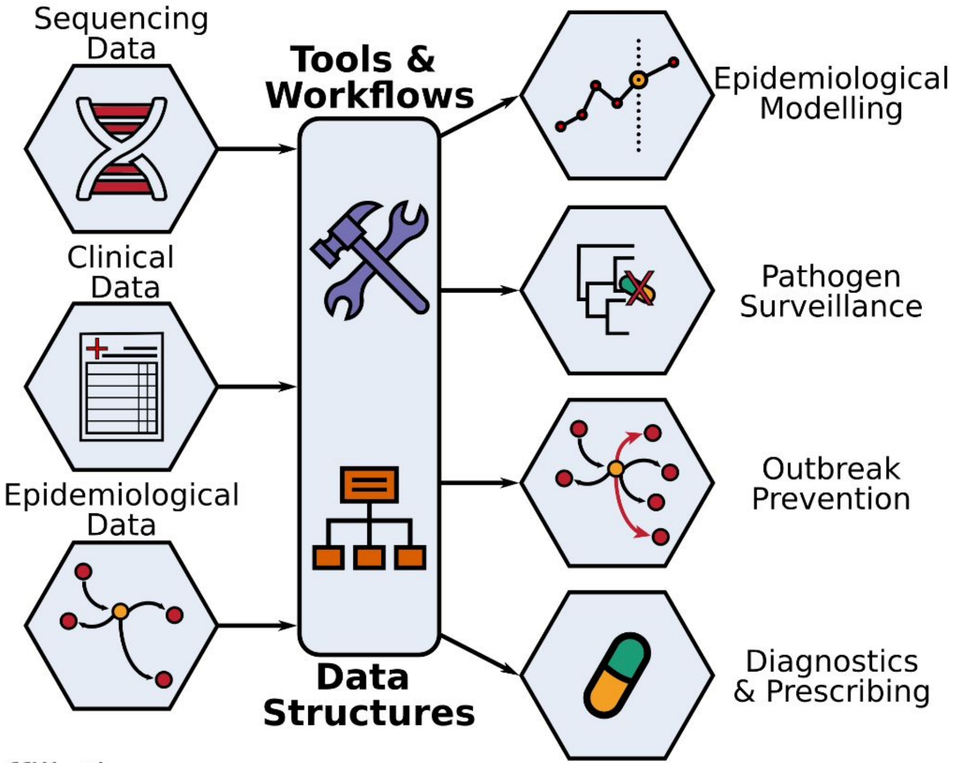

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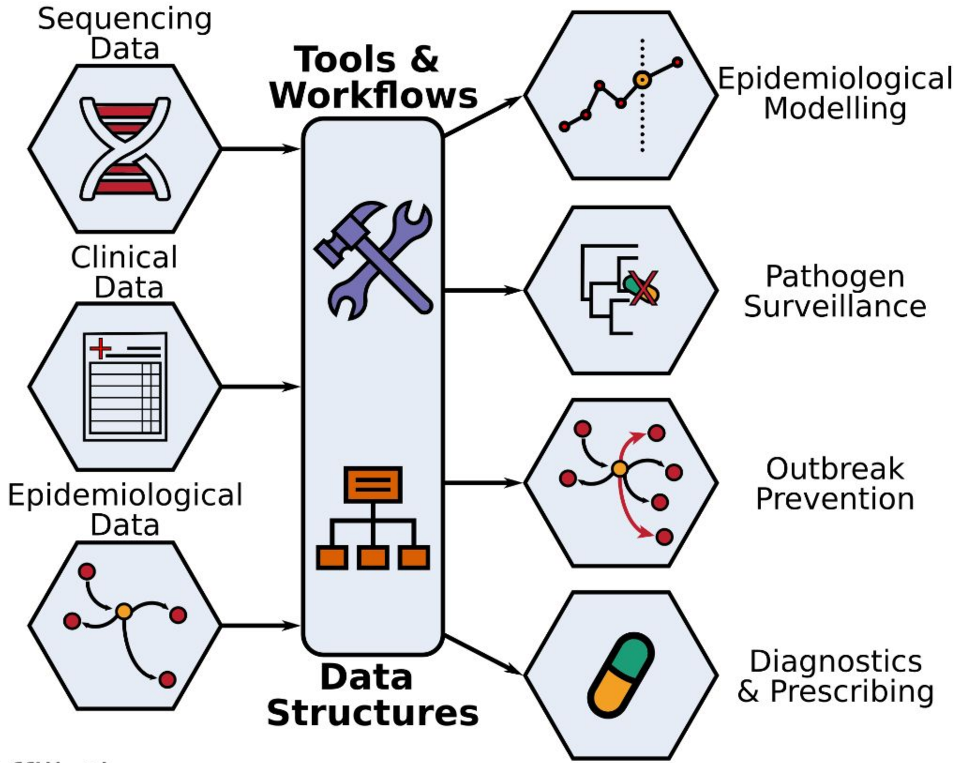
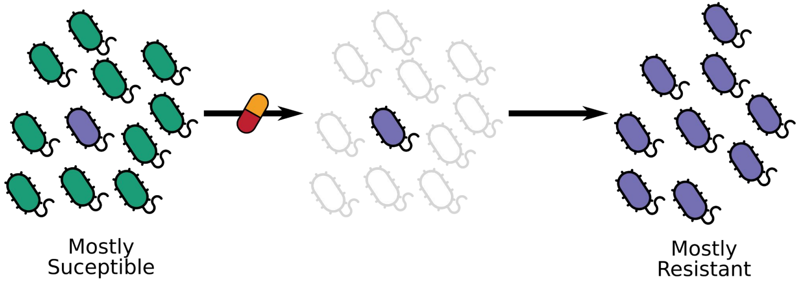


Antimicrobial Resistance



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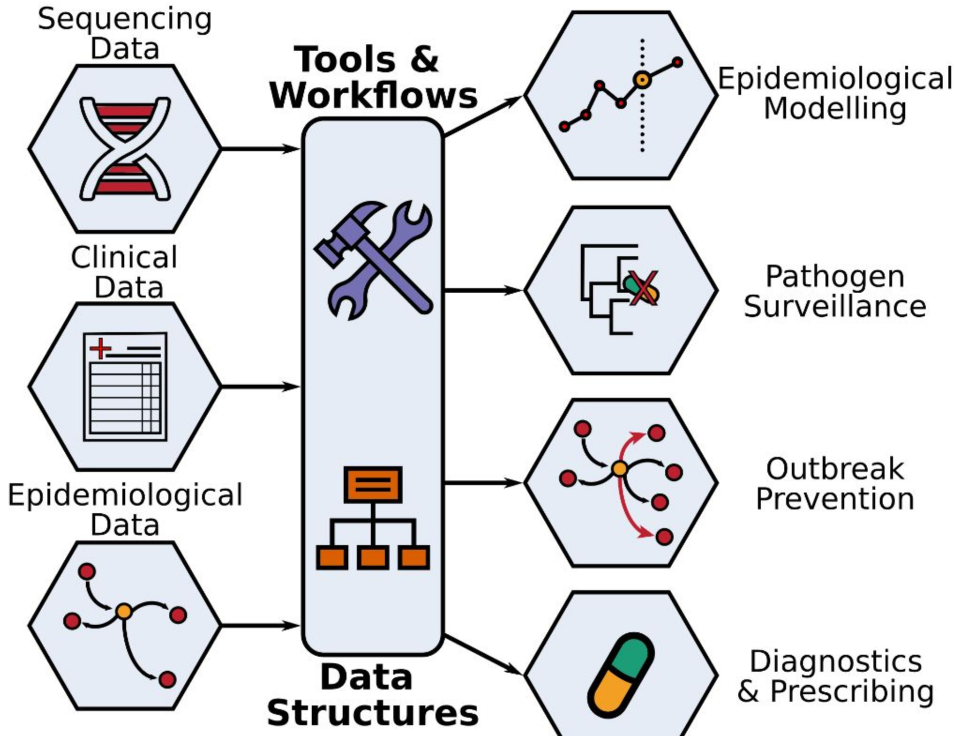

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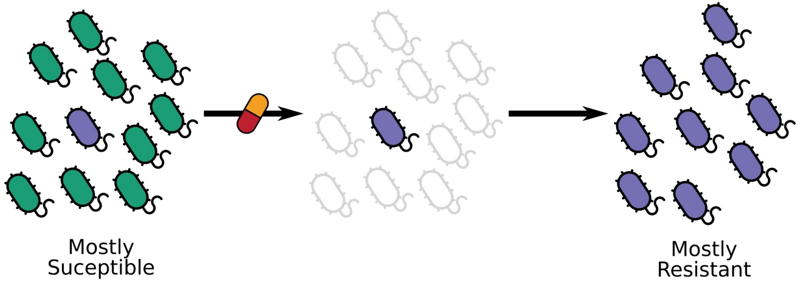
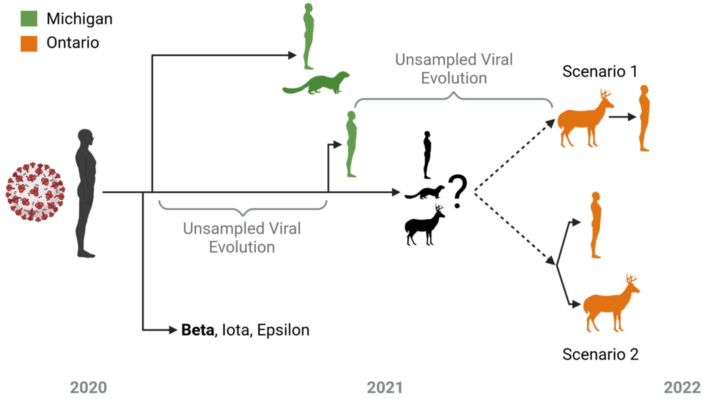


SARS-CoV-2 Evolution



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What is bioinformatics?

Using **computers** to understand **biology**

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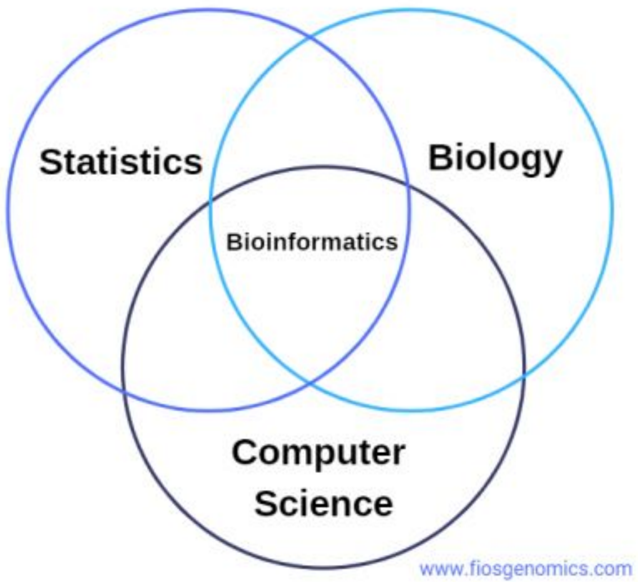
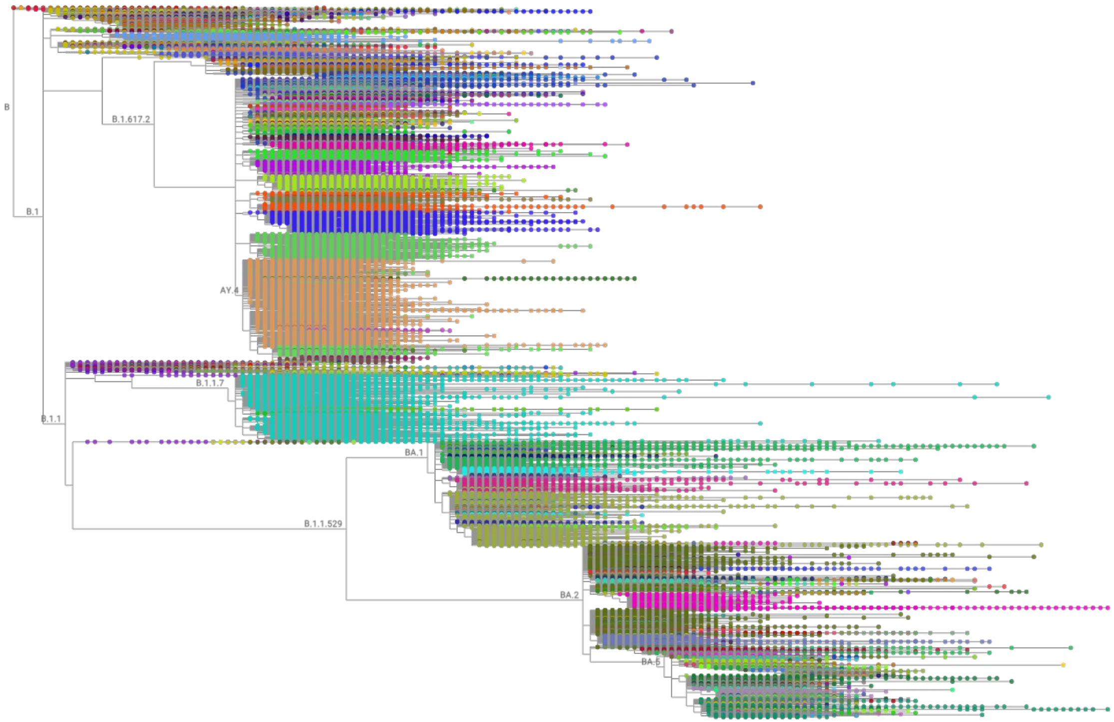


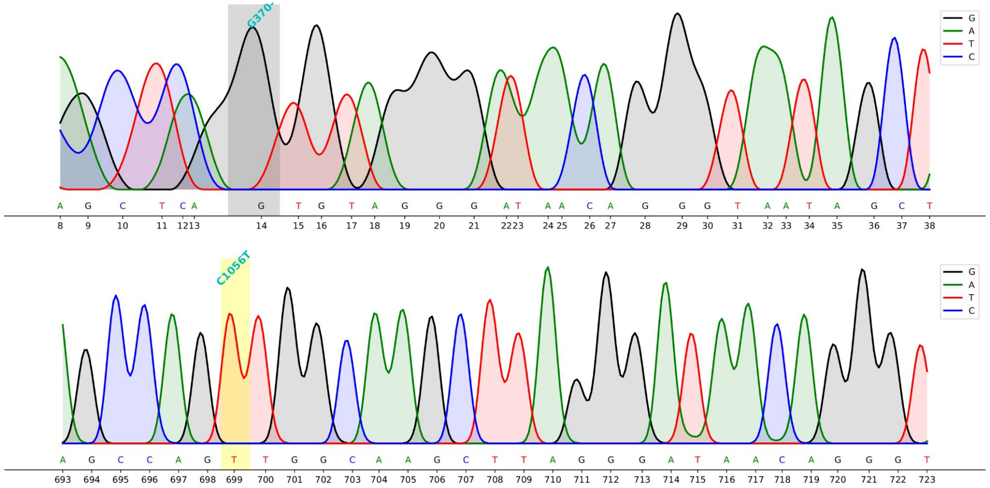
Why do we care about algorithms in bioinformatics?

Lots of data

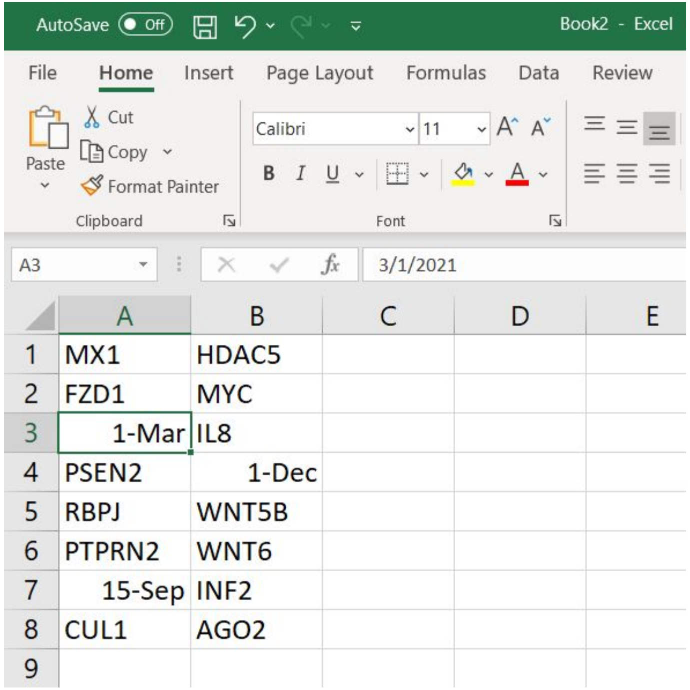


Cov2tree: taxonium 13.4 million SARS-CoV-2 Genomes

Lots of messy data



https://github.com/y9c/cfutils



https://cosmosmagazine.com/science/excel-autocorrect-errors-still-plague-genetic-research/

Lots of messy **biological** data

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  Philosophy of Biology infuses what we do in many interesting ways

What are we actually going to learn?

1.

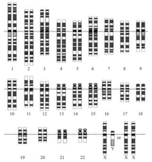
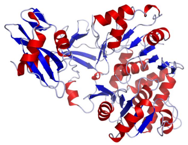
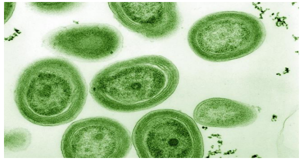
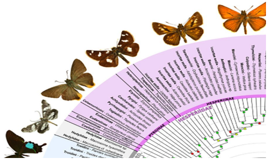
2.

3.

4.

5.

1. **Introduction:** Biological foundations

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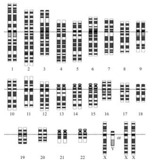
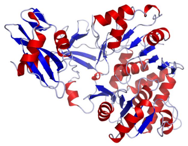
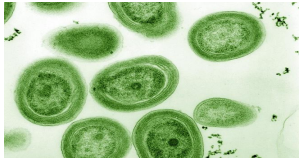
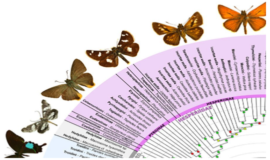

2. **Homology:** Comparing biological sequences

```
K-ELQRAASLTIEV
KDEGQK--SLVIDV
```

AWGHE vs. AWHEA		A	W	G	H	E
	0	-5	-10	-15	-20	-25
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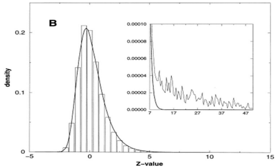

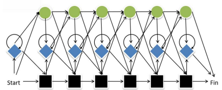


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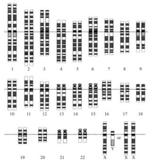
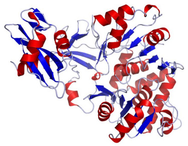
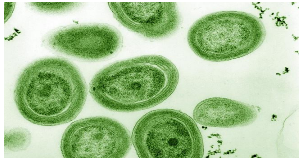
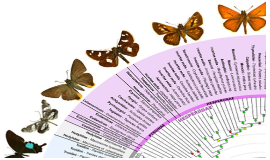

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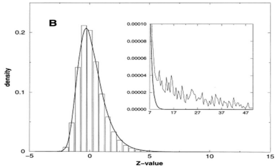

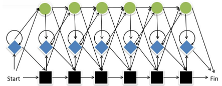


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3. **Assembly:** Recovering genomes from sequencing data

```
Reference  TCCTAGAGATCCGCCTCTTAGCGGATATAATACAGCCGAATCTTAGCGGAATTGCCAGCACAG
Reads       CCTAGAGATCCG
                GAGATCCGCCTC
                   ATCCGCCTCTTA
                       GCCTCTTAGCGG
                           CTTAGCGGATAT
                             TAGCGGATATAA
                                    TATAATACAGCC
                                          ACAGCCGAATCT
                                              CCGAATCTTAGC
                                                GAATCTTAGCGG
                                                   TCTTAGCGGAAT
                                                       AGCGGAATTGCC
                                                          GGAATTGCCAGC
                                                            AATTGCCAGCAC
                                                              TTGCCAGCACAG
Contigs     CCTAGAGATCCGCCTCTTAGCGG
                           CTTAGCGGATATAATACAGCCGAATCTTAGCGG
                                                   TCTTAGCGGAATTGCCAGCACAG
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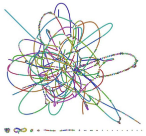
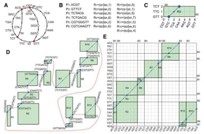

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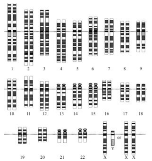
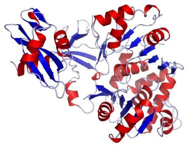
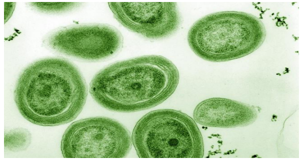
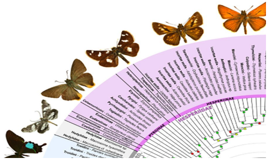

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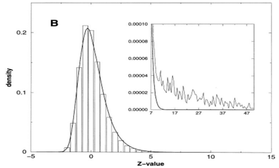

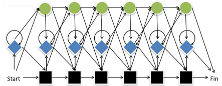


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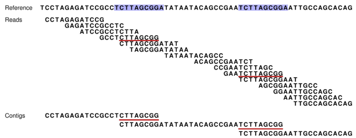

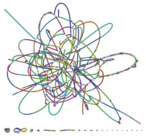
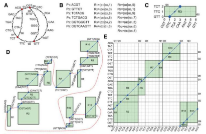

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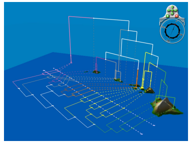
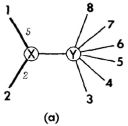

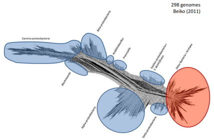

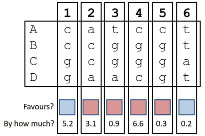

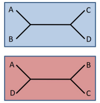

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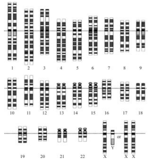
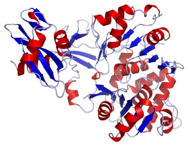
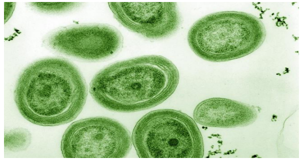
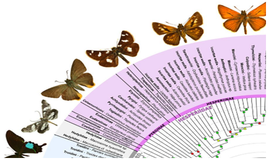

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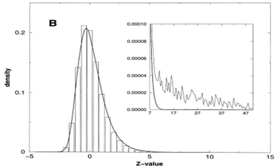

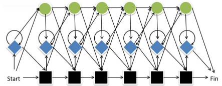

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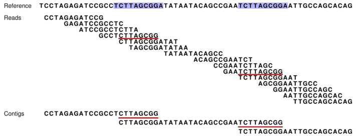

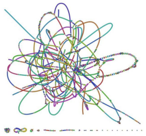
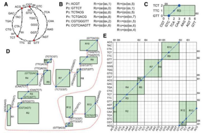

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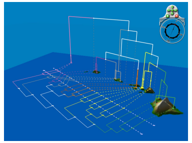
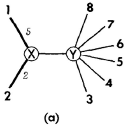
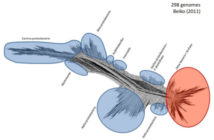
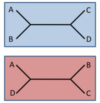
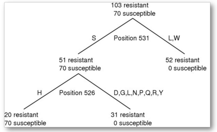



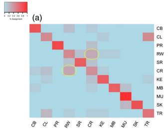
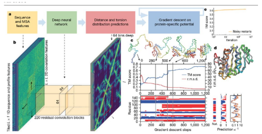
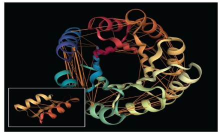


	1	2	3	4	5	6
A	c	a	t	c	c	t
B	c	c	g	g	g	t
C	g	c	g	g	g	a
D	g	a	a	c	g	t
Favours?						
By how much?	5.2	3.1	0.9	6.6	0.3	0.2



5. **Machine Learning:** Encoding and using biological data in machine learning



General Overarching Theme

Biology → Biological Data → Questions → Models → ?

Biology

Underlying messy world of the (mostly microbial) biology

Biological Data

Biological sequence data we measure or extract from the biology.

Questions

1. What does this sequence do?
2. Has this pathogen acquired a new resistance gene?
3. Where did this pathogen come from?
4. Will this bacteria be resistant to this antibiotic?

Models

1. Similar sequences do similar things
2. Genomes contain mobile elements
3. Similar sequences may be related to one another via evolution
4. Parts of genome are associated with observed phenotype

?

Bioinformatics Algorithms!

How are we going to learn?

Lectures, practical assignments, and a paper review

- 22 lectures (every Tuesday and Thursday)
    - Guest lectures by Dr. Ryan Fink, Prof. Robert Beiko, and Alex Manuele

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  2. Genome Assembly (20%)
  3. SARS-CoV-2 Genome Analysis (20%)
  4. Prediction of AMR Phenotypes (20%)

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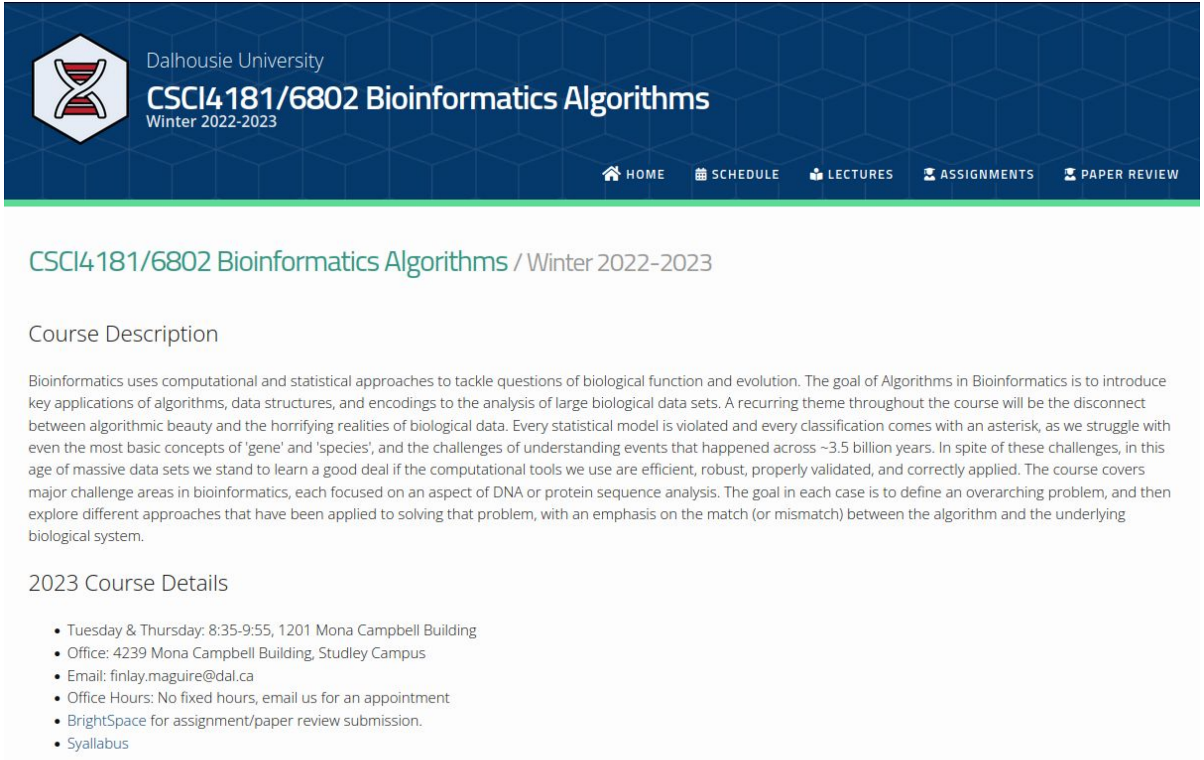
  2. Genome Assembly (20%)
  3. SARS-CoV-2 Genome Analysis (20%)
  4. Prediction of AMR Phenotypes (20%)
- Paper Review
  - Review of recent bioinformatics paper (selection due 2023/03/21)
  - Written Summary due 2023/04/04 (10%)
  - Oral Presentation 2023/04/04 to 2023/04/11 (10%)

Other Class Logistics

- Details on course website
- Contact for office hours
- **TA: Jee-in Kim (remote)**
- Assignment must be submitted via Brightspace as .docx or .pdf and named:

  "BannerID_LastName_AssignmentX.{pdf,docx}"



Dalhousie University

CSCI4181/6802 Bioinformatics Algorithms

Winter 2022-2023

HOME SCHEDULE LECTURES ASSIGNMENTS PAPER REVIEW

CSCI4181/6802 Bioinformatics Algorithms / Winter 2022-2023

Course Description

Bioinformatics uses computational and statistical approaches to tackle questions of biological function and evolution. The goal of Algorithms in Bioinformatics is to introduce key applications of algorithms, data structures, and encodings to the analysis of large biological data sets. A recurring theme throughout the course will be the disconnect between algorithmic beauty and the horrifying realities of biological data. Every statistical model is violated and every classification comes with an asterisk, as we struggle with even the most basic concepts of 'gene' and 'species', and the challenges of understanding events that happened across ~3.5 billion years. In spite of these challenges, in this age of massive data sets we stand to learn a good deal if the computational tools we use are efficient, robust, properly validated, and correctly applied. The course covers major challenge areas in bioinformatics, each focused on an aspect of DNA or protein sequence analysis. The goal in each case is to define an overarching problem, and then explore different approaches that have been applied to solving that problem, with an emphasis on the match (or mismatch) between the algorithm and the underlying biological system.

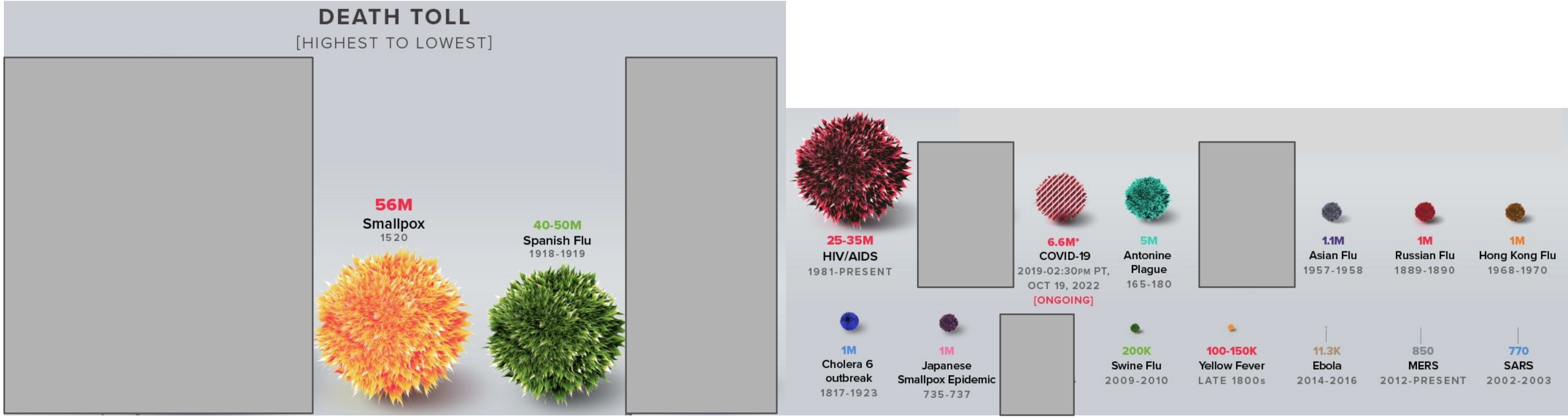
2023 Course Details

- Tuesday & Thursday: 8:35-9:55, 1201 Mona Campbell Building
- Office: 4239 Mona Campbell Building, Studley Campus
- Email: finlay.maguire@dal.ca
- Office Hours: No fixed hours, email us for an appointment
- BrightSpace for assignment/paper review submission.
- Syallabus

https://maguire-lab.github.io/bioinformatics_algorithms

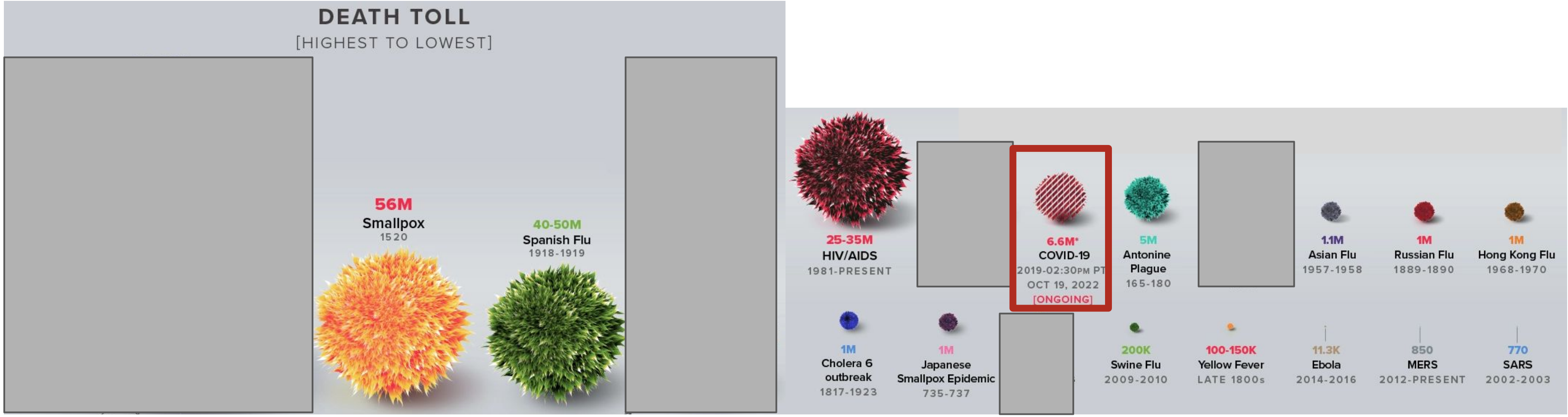
Why does any of this matter?

Pandemics matter to humans



https://www.visualcapitalist.com/history-of-pandemics-deadliest/

Pandemics matter to humans



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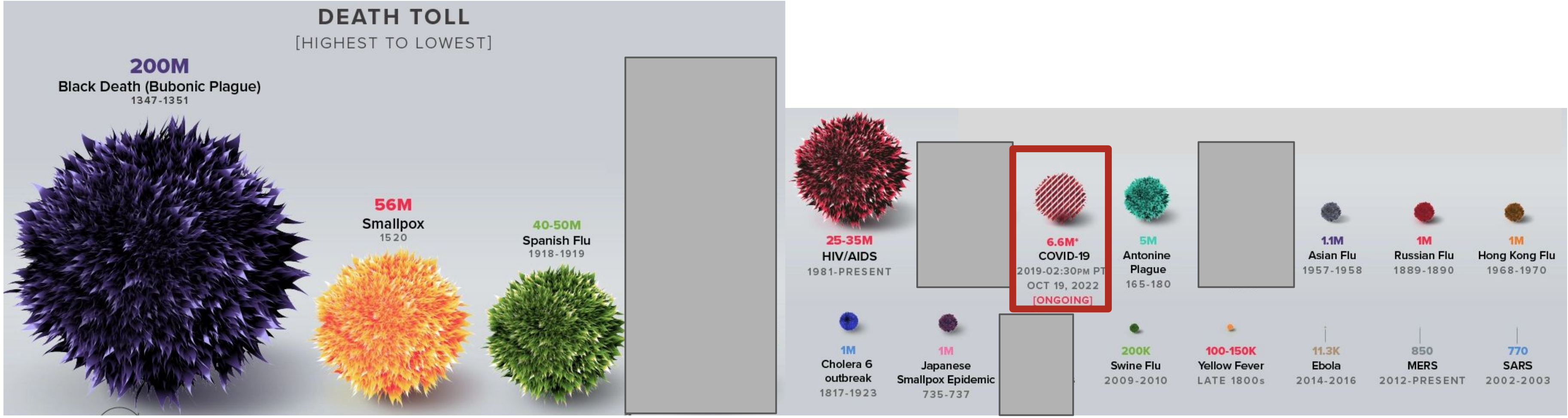

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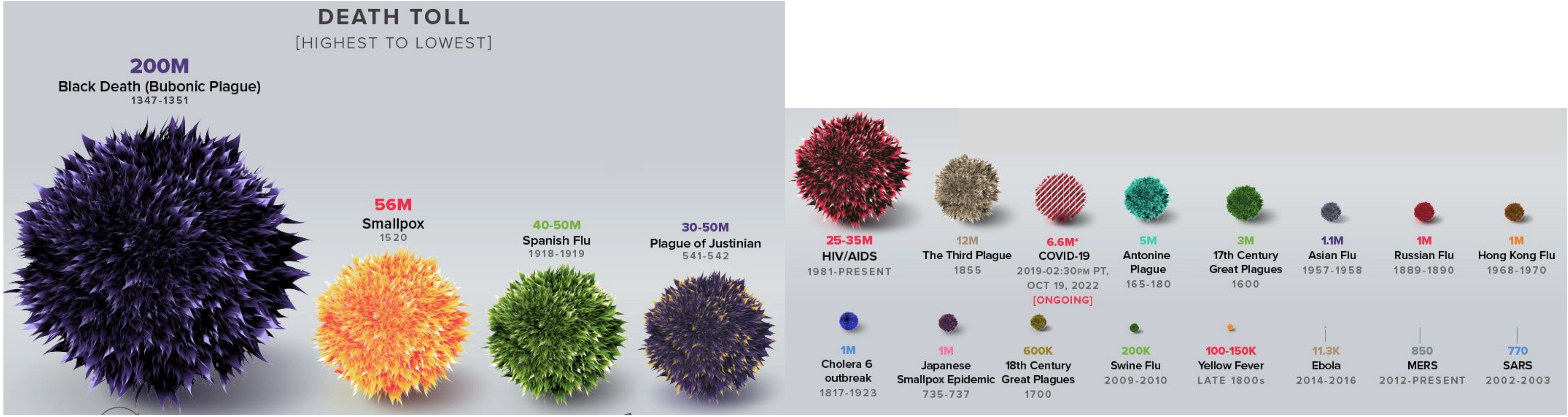

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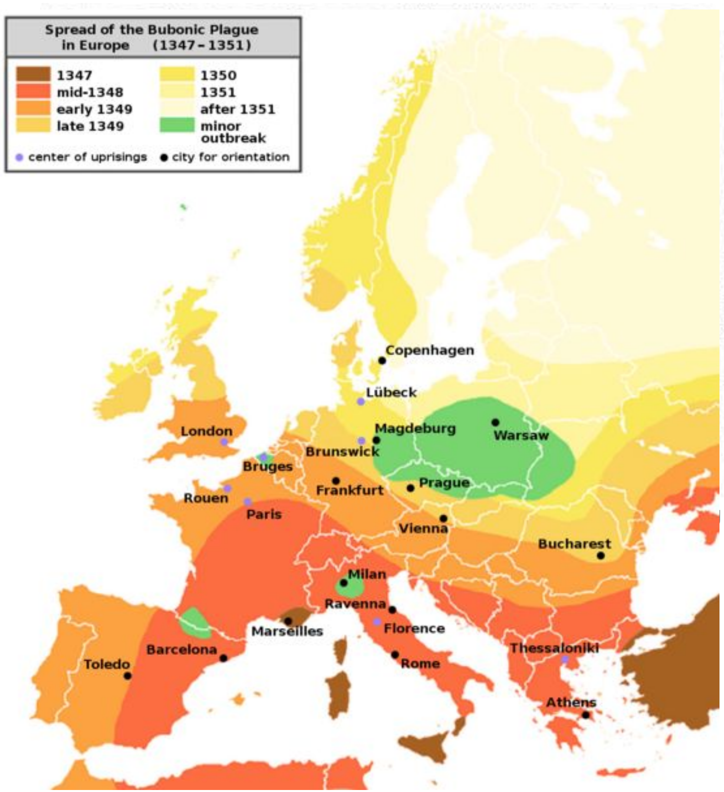
Plague Huge Impact on Human History

- Justinian Plague (541–549)

https://origins.osu.edu/connecting-history/covid-justinianic-plague-lessons?language_content_entity=en

Plague Huge Impact on Human History

- Justinian Plague (541–549)
- Black Death (1347-1351 / 1330s to 1830s)



https://commons.wikimedia.org/wiki/File:Bubonic_plague_map.PNG

Plague Huge Impact on Human History

- Justinian Plague (541–549)
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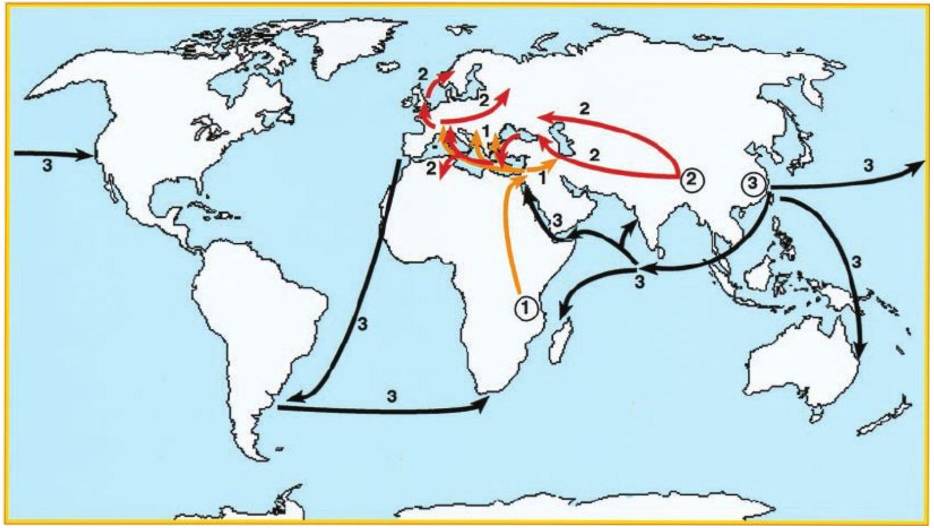
https://commons.wikimedia.org/wiki/File:Lord_haue_mercy_on_London.jpg

Plague Huge Impact on Human History

- Justinian Plague (541–549)
- Black Death (1347-1351 / 1330s to 1830s)
- 3rd Plague (1855-1960 / Today)



https://doi.org/10.1073/pnas.96.24.14043

Plague Huge Impact on Human History

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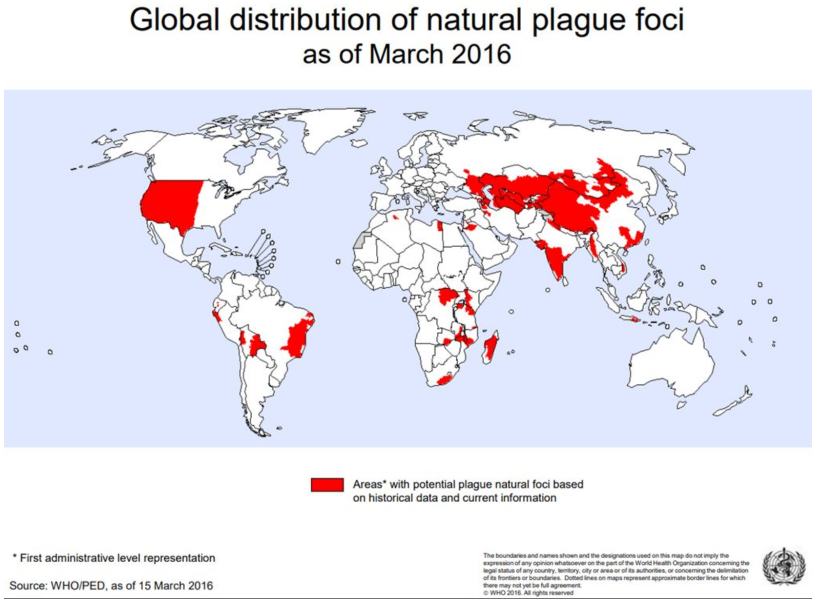
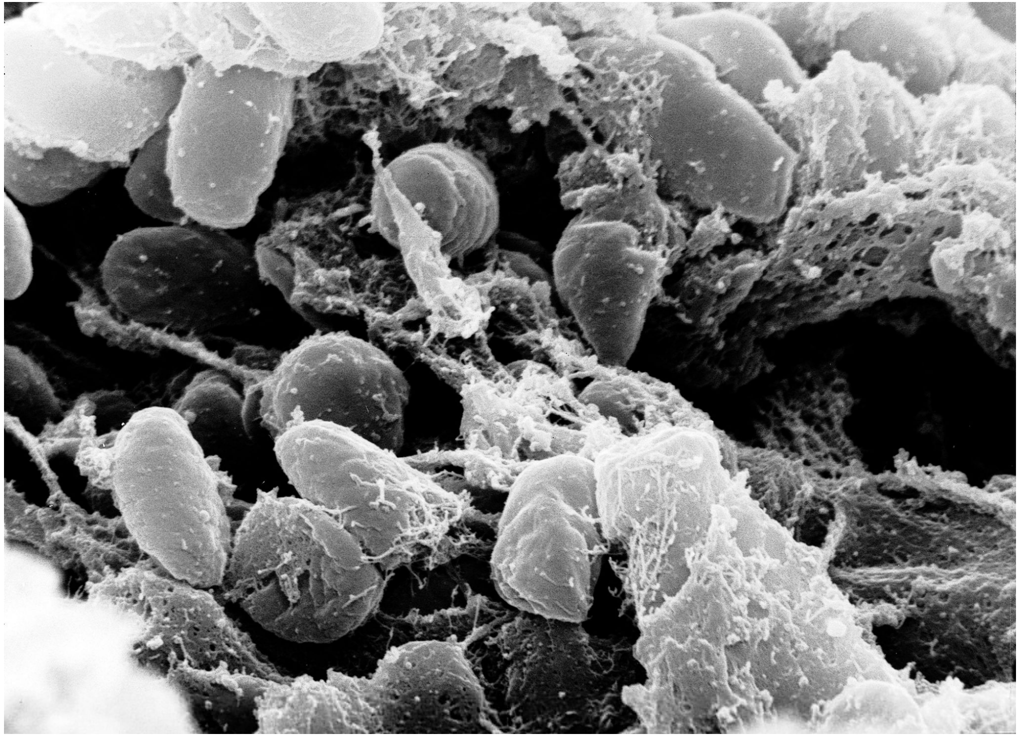


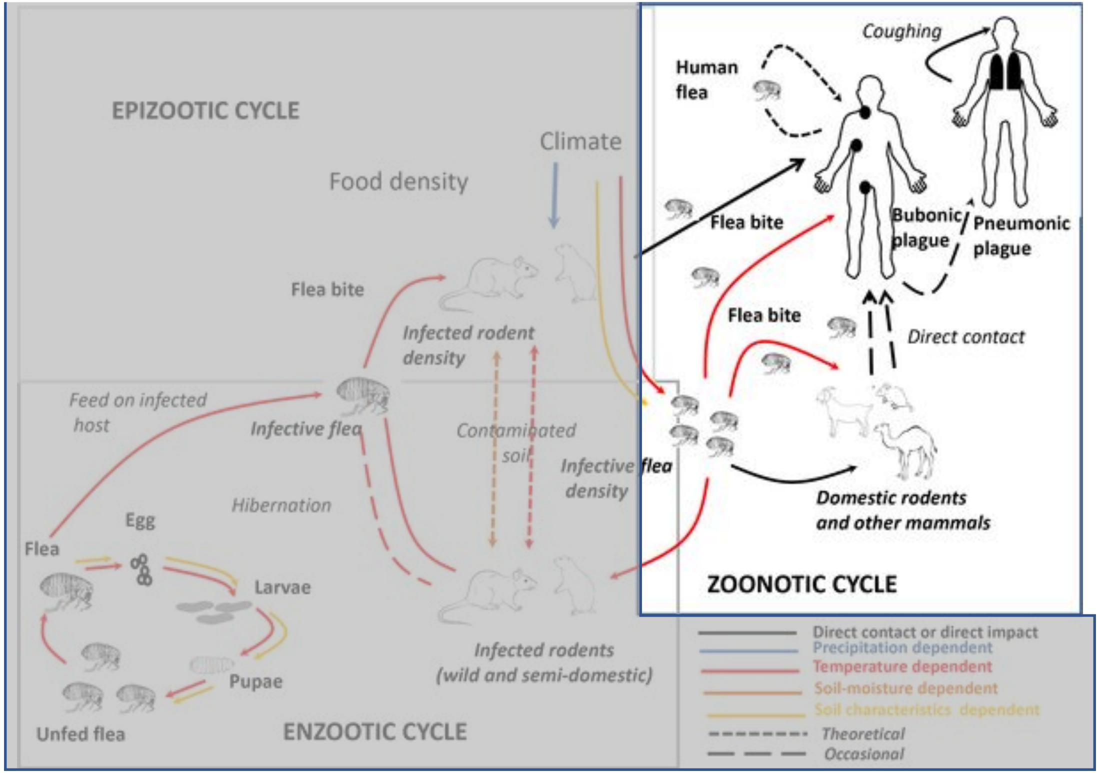
Working out the cause of the plague

- **1546 Fracastro:** disease from invisible “seeds”
- **1683 Van Leeuwenhoek:** microscopic creatures
- **1857 Pasteur:** microbes are living creatures that don’t spontaneously appear
- **1876 Koch:** microbes cause disease (Koch’s Postulates)
- **1894 Shiabasaburō & Yersin:** Isolation of microbe in 3rd Plague
- **1896 Simon:** Isolation of microbe in fleas

Bubonic plague is caused by *Yersinia pestis*

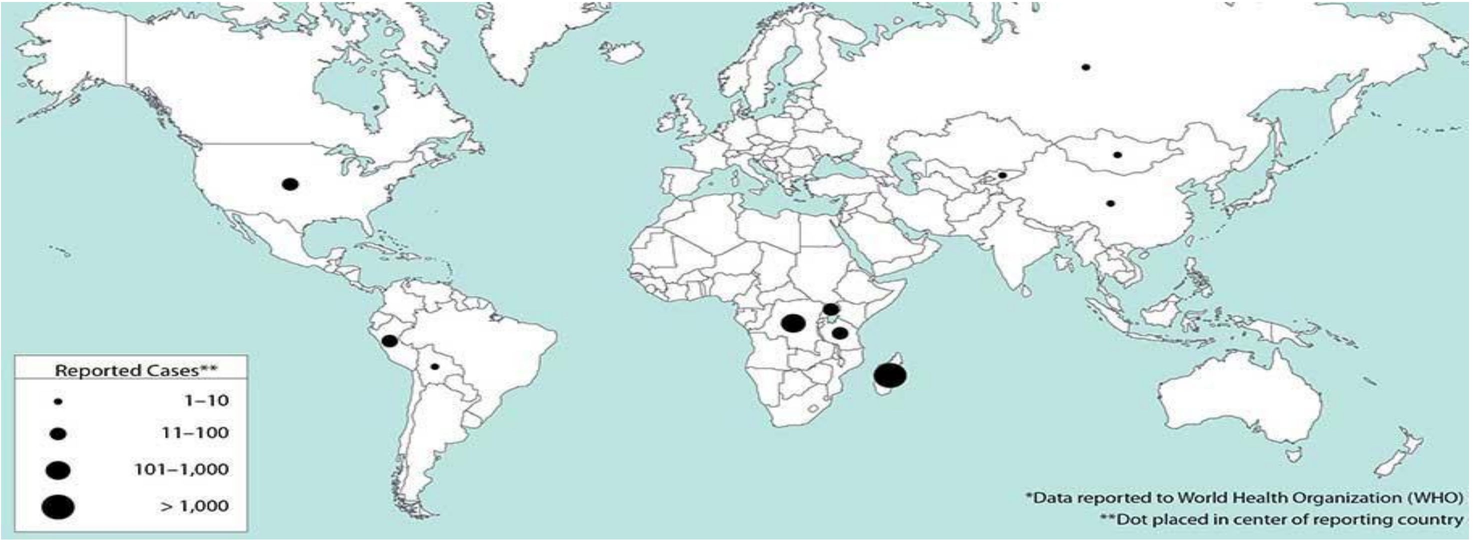


Complex life cycle including fleas and rodents



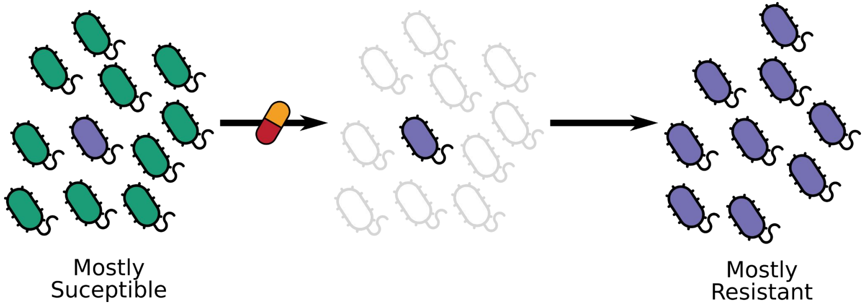
Vallès X, Stenseth NC, Demeure C, Horby P, Mead PS, et al. (2020) Human plague: An old scourge that needs new answers. PLOS Neglected Tropical Diseases 14(8): e0008251.

Still causes disease but is treatable



Fatality rate (untreated) = **40%-70%**
Fatality rate (treated) = **5%-15%**

Becoming less treatable



Becoming less treatable

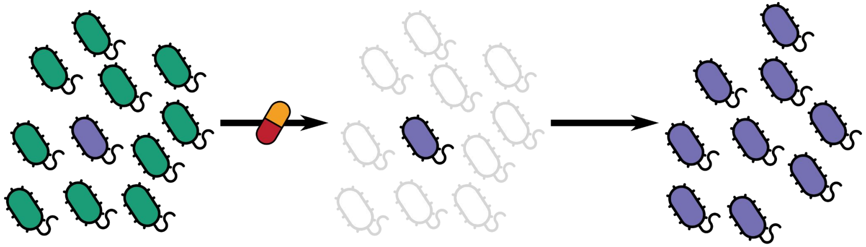
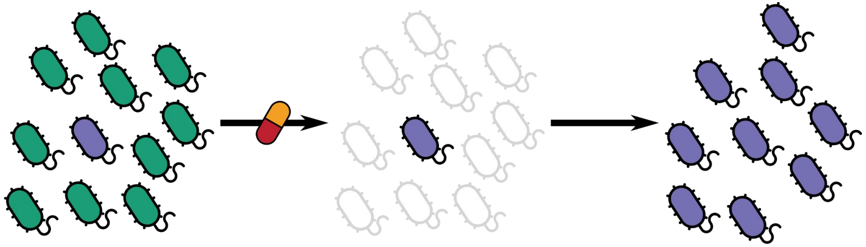


TABLE 2 Antimicrobial MIC distributions for *Y. pestis* isolates in this study ($n = 392$)

Antimicrobial	No. of isolates with MIC (μg/ml)[a]											
Gentamicin			3	260	110	18	1					
Streptomycin					2	6	119	263	2			
Tetracycline				11	154	224	3					
Doxycycline			4	66	245	77						
Ciprofloxicin	371	20	1									
Levofloxacin	385	7										
Chloramphenicol					34	86	201	71				
Trimethoprim-sulfamethoxazole	9	333	49	1								

Urich et al. (2012) Antimicrob Agents Chemoterapy

Becoming less treatable



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Urich et al. (2012) Antimicrob Agents Chemoterapy

Multidrug Resistance in *Yersinia pestis* Mediated by a Transferable Plasmid

Marc Galimand, Ph.D., Annie Guiyoule, Guy Gerbaud, Bruno Rasoamanana, M.D., Suzanne Chanteau, Ph.D., Elisabeth Carniel, M.D., Ph.D., and Patrice Courvalin, M.D.

Plasmid-mediated doxycycline resistance in a *Yersinia pestis* strain isolated from a rat

Nicolas Cabanel [a], Christiane Bouchier [b], Minoarisoa Rajerison [c], Elisabeth Carniel [a,*]

Transferable Plasmid-Mediated Resistance to Streptomycin in a Clinical Isolate of *Yersinia pestis*

Annie Guiyoule,* Guy Gerbaud,* Carmen Buchrieser,* Marc Galimand,* Lila Rahalison,† Suzanne Chanteau,† Patrice Courvalin,* and Elisabeth Carniel*
*Institut Pasteur, Paris, France; and †Institut Pasteur, Antananarivo, Madagascar

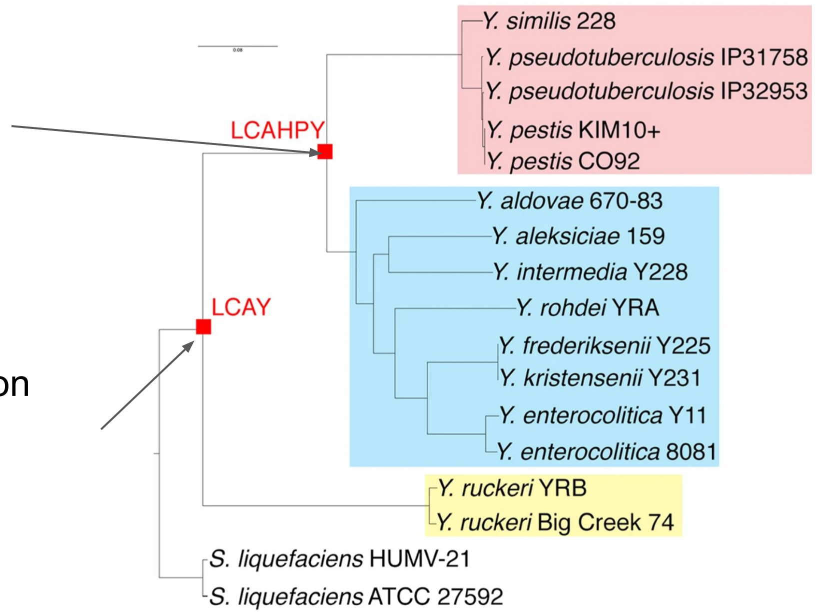
How can we control *Yersinia pestis*?

Need to learn about pathogen to control it

How did *Y. pestis* evolve?

Last common ancestor of human pathogenic *Yersinia*

Last common ancestor of *Yersinia*



Tan et al. (2016) Sci Rep https://www.nature.com/articles/srep36116

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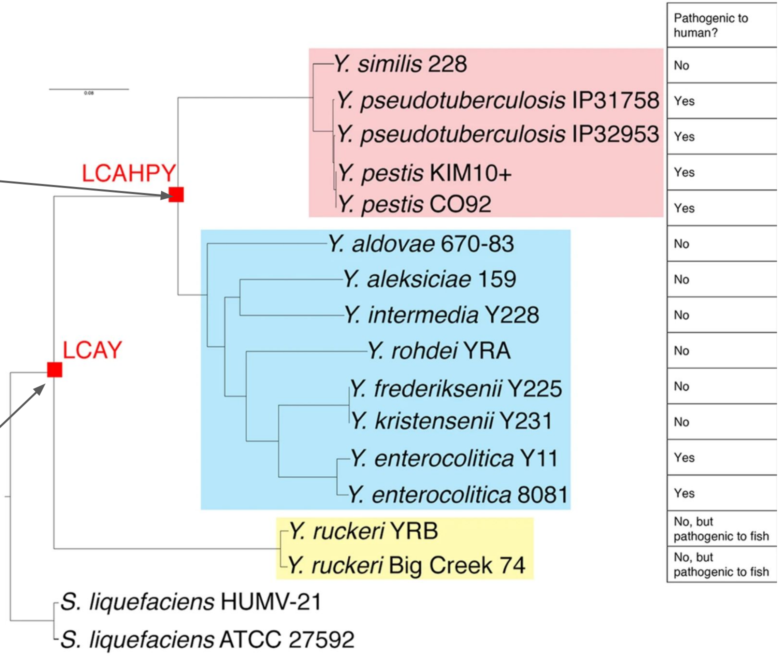
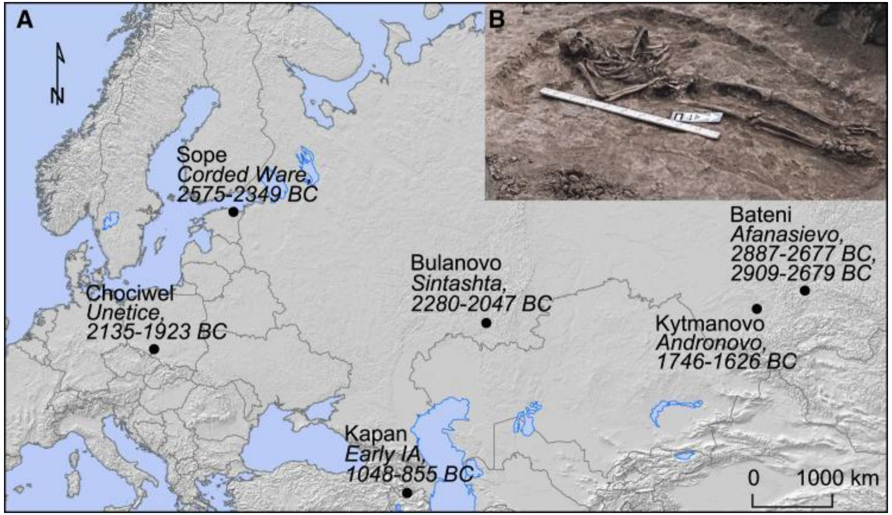
Last common ancestor of human pathogenic *Yersinia*

Last common ancestor of *Yersinia*



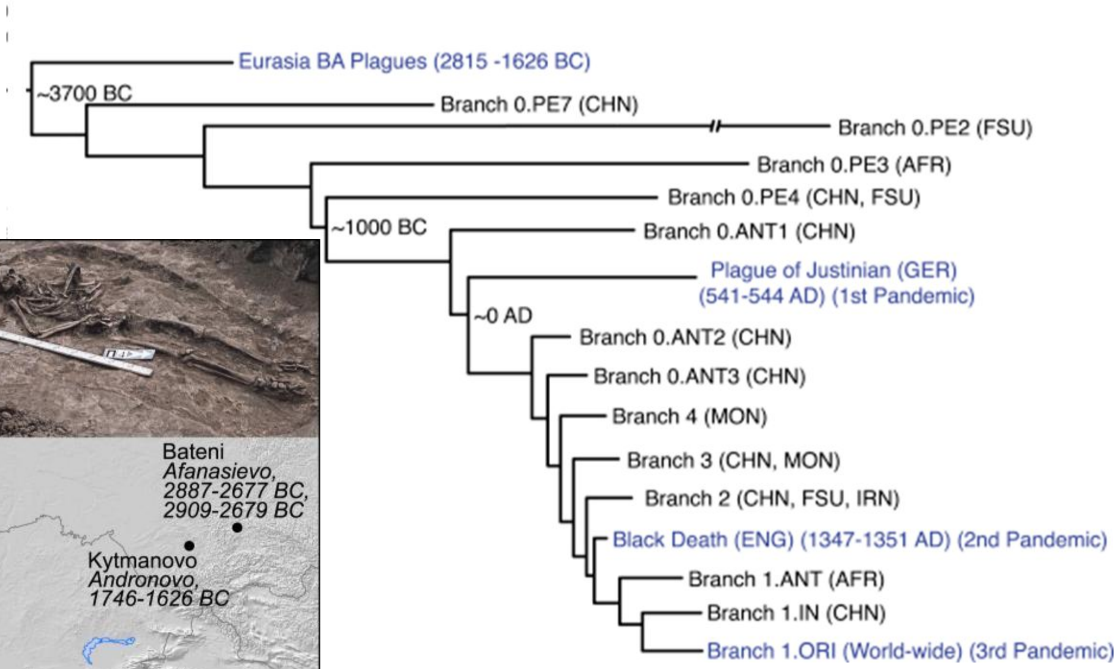
Tan et al. (2016) Sci Rep https://www.nature.com/articles/srep36116

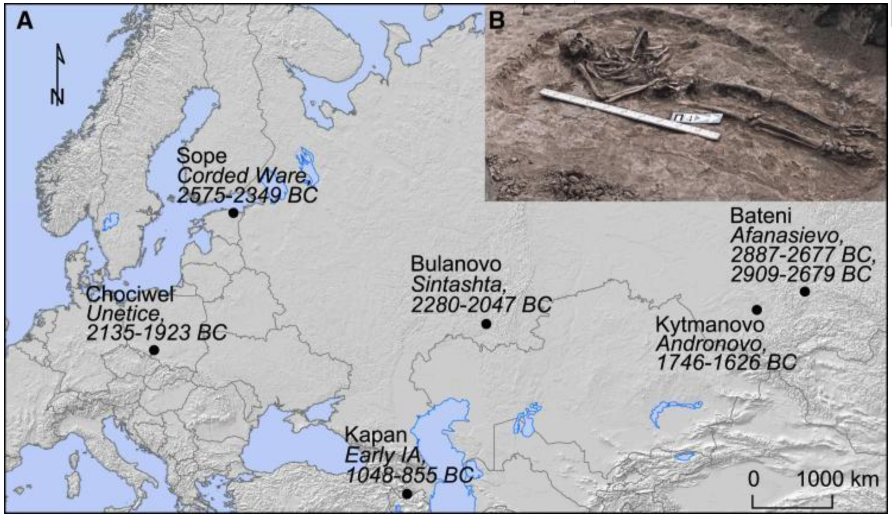
How old is *Y. pestis?*



Rasmussen et al. (2015) *Cell*
https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4644222/

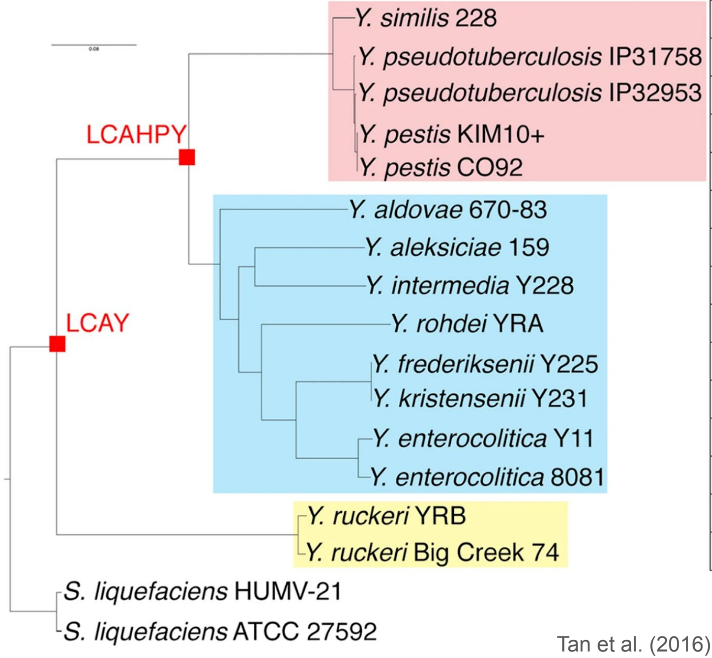
How old is *Y. pestis?*





Rasmussen et al. (2015) *Cell*
https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4644222/

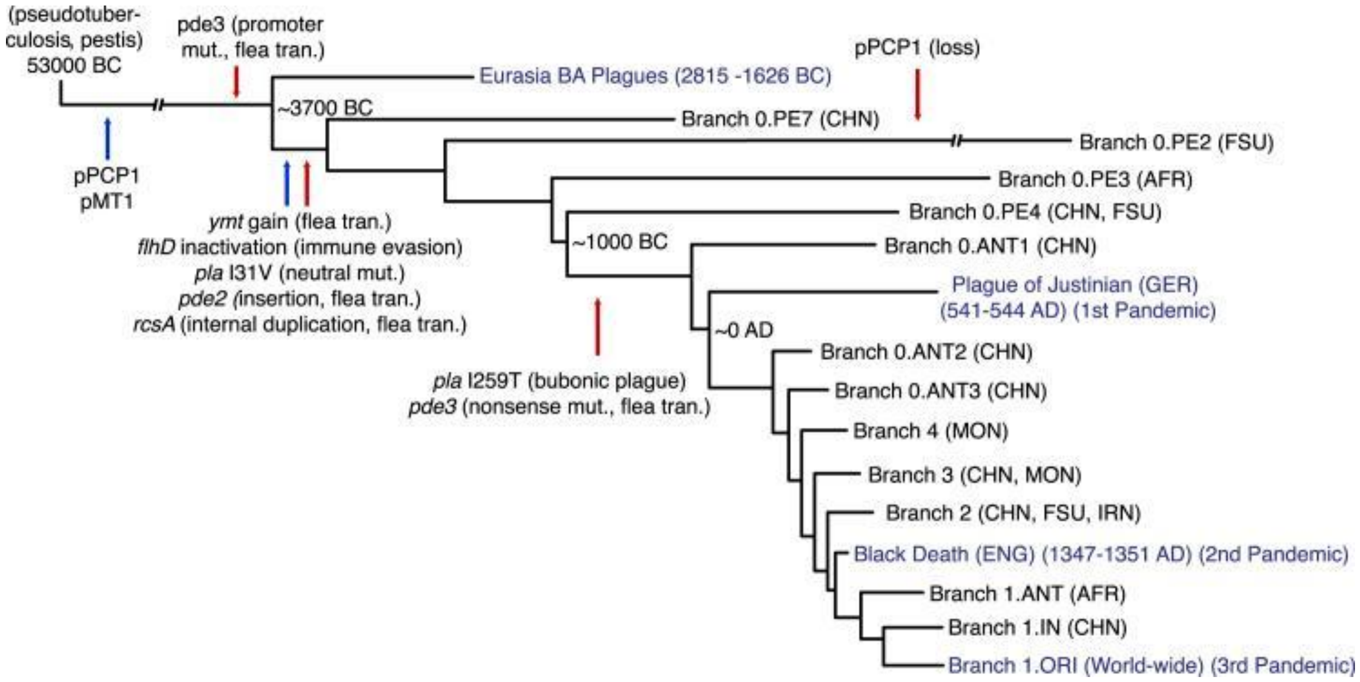
What makes it so virulent?



Pathogenic to human?	Presence of pYV plasmid?	Presence of CRISPR spacer to become immune to pYV or pYE854 plasmid?	Presence of *inv* homolog and N-terminal?	Number of copy of *ail* homolog?
No	No	Yes	Yes	4
Yes	Yes	No	Yes	4
Yes	Yes	Immune to pYV of *Y. enterocolitica*	Yes	4
Yes	Yes	Immune to pYV of *Y. enterocolitica*	No	4
Yes	Yes	Immune to pYV of *Y. enterocolitica*	No	4
No	No	No	No	1
No	No	No	No	1
No	No	No	No	1
No	No	No	No	1
No	No	Yes	No	1
No	No	Yes	No	1
Yes	Yes	No	Yes	2
Yes	Yes	No	Yes	2
No, but pathogenic to fish	No	No	No	1
No, but pathogenic to fish	No	No	No	1

Tan et al. (2016) Sci Rep https://www.nature.com/articles/srep36116

How did it become so deadly?



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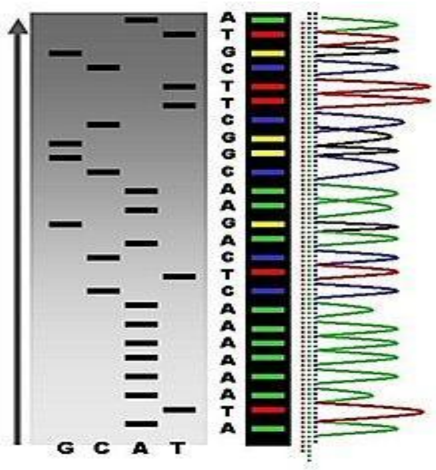
How do we know this?

Molecular biology

How do we know this?

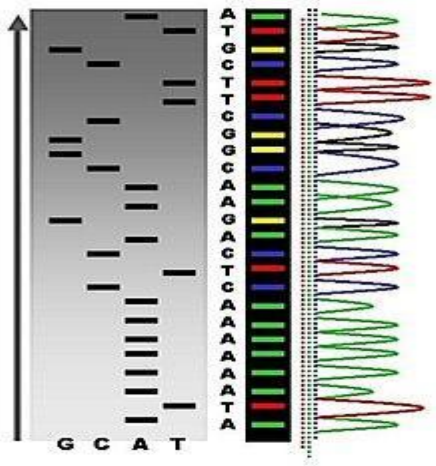
Molecular biology



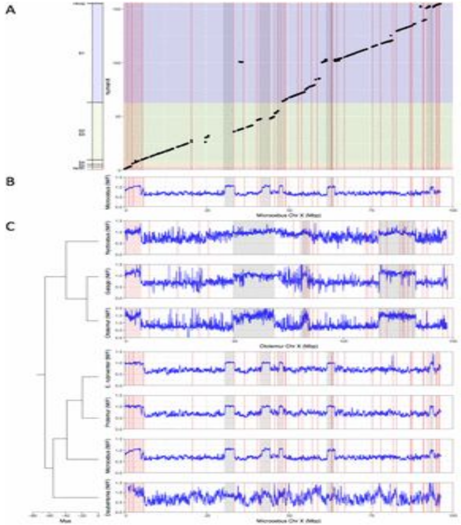
DNA sequencing

How do we know this?

Molecular biology



DNA sequencing



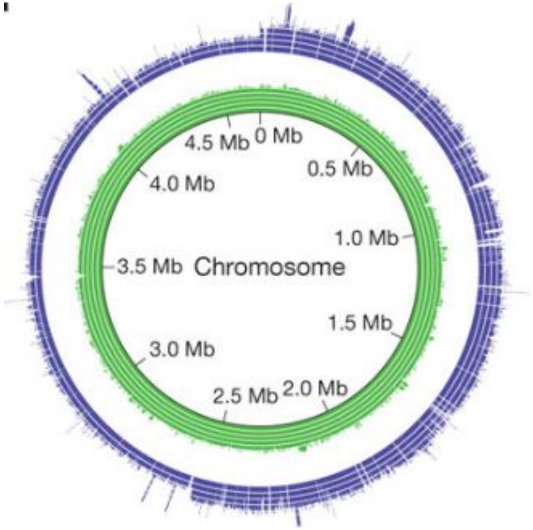
Bioinformatics!

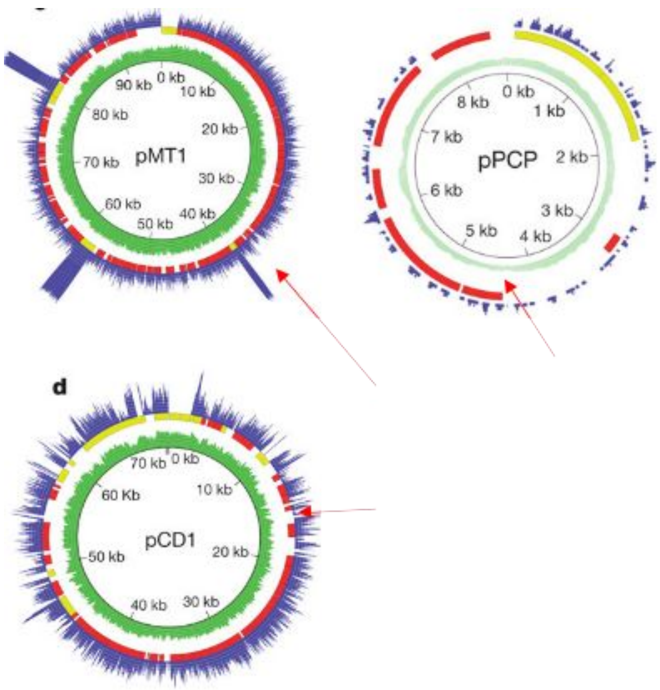
We can sequence the Black Death Genome

LONDON, 1593. By JOHN NORDEN.

Bos et al. (2011) Nature doi:10.1038/nature10549

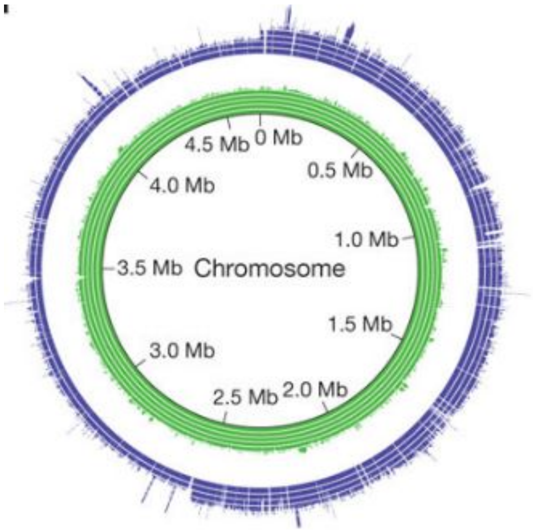
Need assembly algorithms to get genome



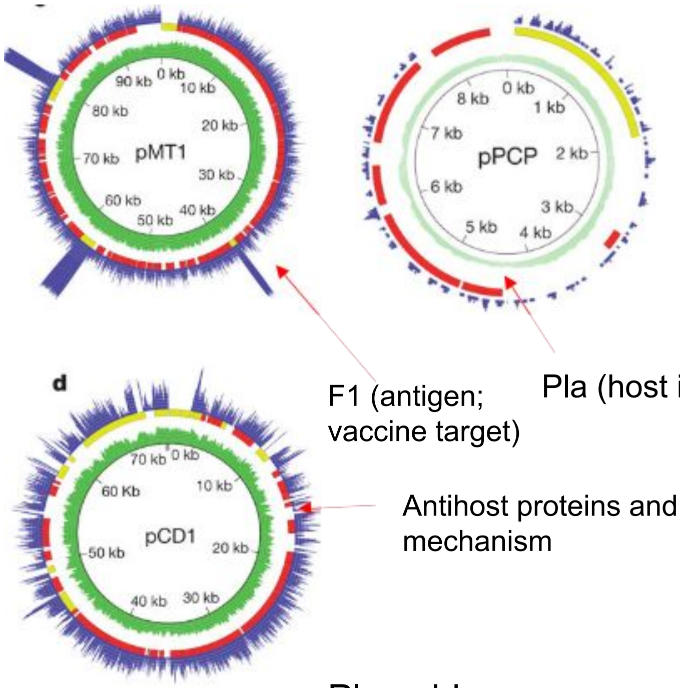


Bos et al. (2011) Nature doi:10.1038/nature10549

Need homology algorithms to decipher genome



Main Chromosome



F1 (antigen; vaccine target)

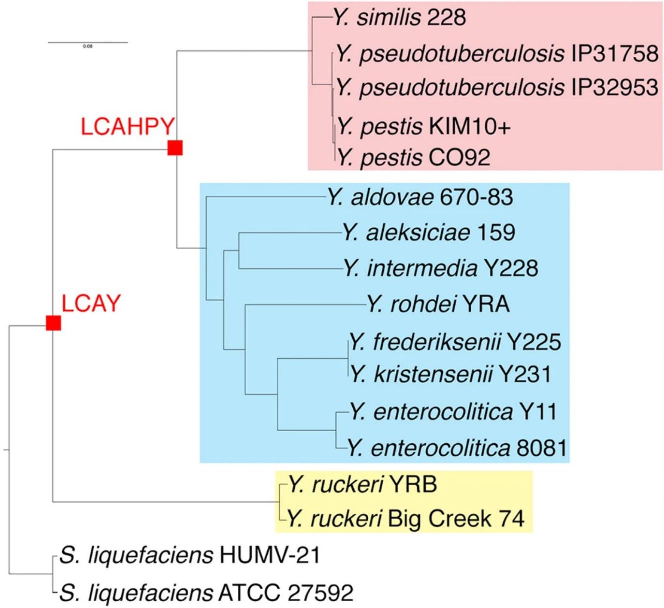
Pla (host invasion)

Antihost proteins and cellular delivery mechanism

Plasmids

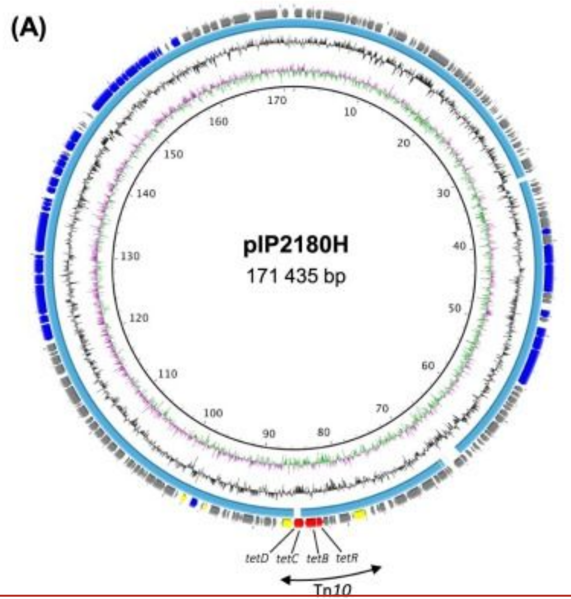
Bos et al. (2011) Nature doi:10.1038/nature10549

Need phylogenetic algorithms to trace



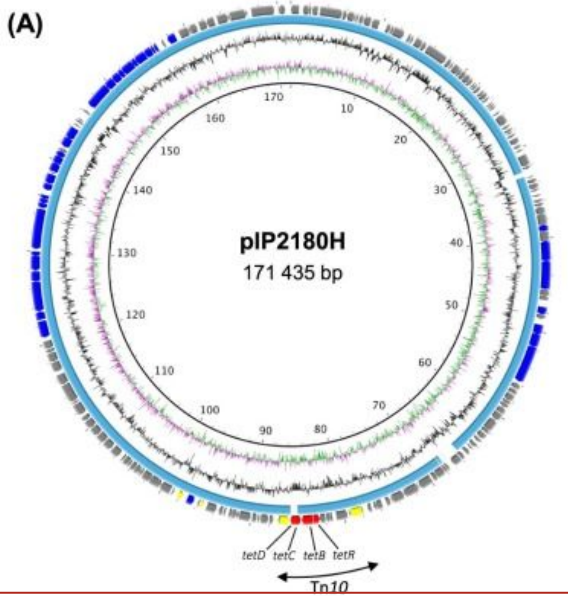
Pathogenic to human?
No
Yes
Yes
Yes
Yes
No
No
No
No
No
No
Yes
Yes
No, but pathogenic to fish
No, but pathogenic to fish

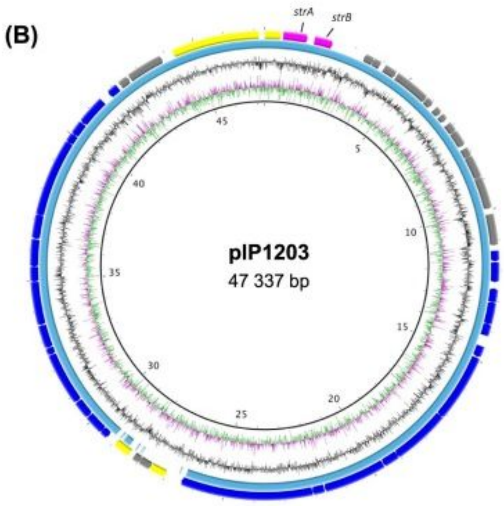
Need ML algorithms to predict resistance



Doxycycline resistance genes (from *Salmonella*)

Need ML algorithms to predict resistance





Doxycycline resistance genes (from *Salmonella*)

Streptomycin resistance genes (from *Acidovorax*)

Summary!

- Bioinformatics is using **computers** to understand **biology**

- **Algorithms** are vital to doing this effectively

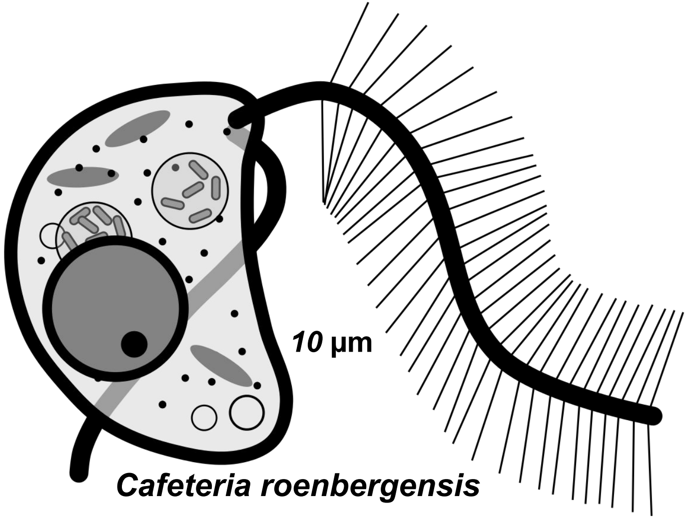
- We need **bioinformatic algorithms** to solve important problems including in human health

01: Life at Resolution: Organisms, Genomes, Sequences, and so on

CSCI4181/6802 Bioinformatics Algorithms

Finlay Maguire (finlay.maguire@dal.ca)

Even single microbial life covers a large range

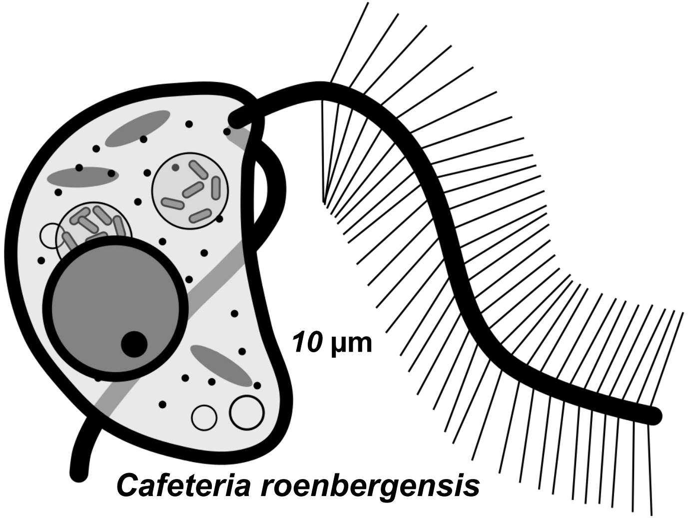


https://commons.wikimedia.org/wiki/File:CafeteriaRoenbergensis.jpg

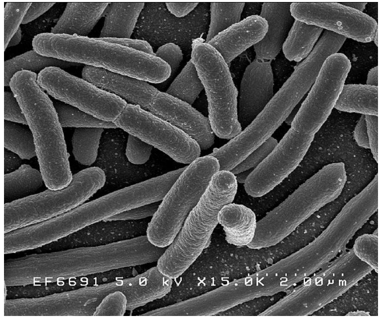
https://www.cam.ac.uk/sites/www.cam.ac.uk/files/styles/content-885x432/public/news/research/news/mitochondria.jpg?itok=CIFE3yjc

https://upload.wikimedia.org/wikipedia/commons/f/f7/Giant_virus_CroV_with_its_virophage_Mavirus.png

Even single microbial life covers a large range



Cafeteria roenbergensis



2 µm

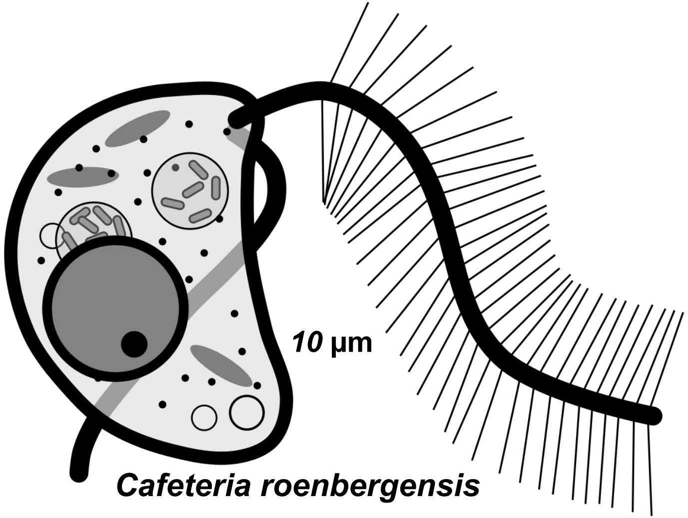
Escherichia coli

https://commons.wikimedia.org/wiki/File:CafeteriaRoenbergensis.jpg

https://www.cam.ac.uk/sites/www.cam.ac.uk/files/styles/content-885x432/public/news/research/news/mitochondria.jpg?itok=CIFE3yjc

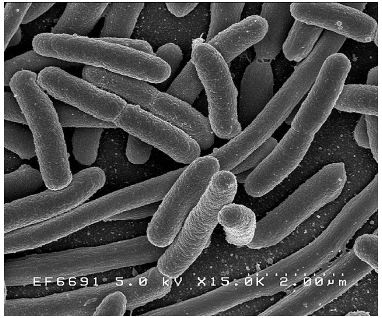
https://upload.wikimedia.org/wikipedia/commons/f/f7/Giant_virus_CroV_with_its_virophage_Mavirus.png

Even single microbial life covers a large range



10 µm

Cafeteria roenbergensis



2 µm

Escherichia coli

0.5 µm

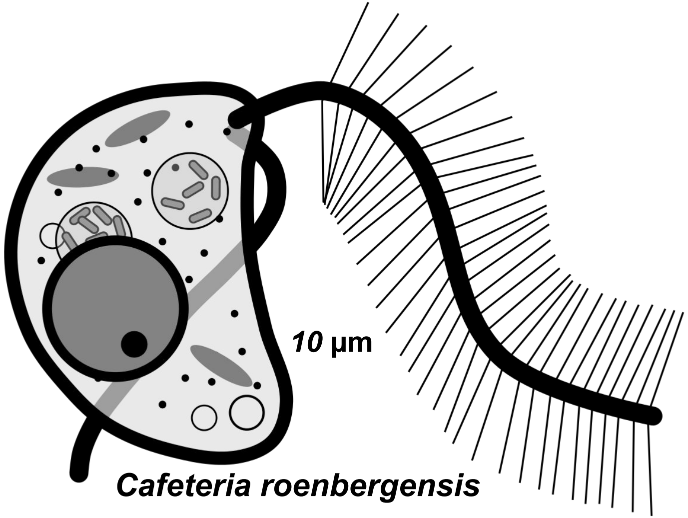
Mitochondria

https://commons.wikimedia.org/wiki/File:CafeteriaRoenbergensis.jpg

https://www.cam.ac.uk/sites/www.cam.ac.uk/files/styles/content-885x432/public/news/research/news/mitochondria.jpg?itok=CIFE3yjc

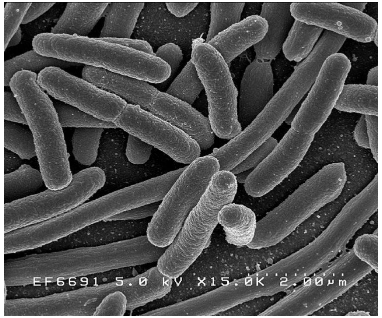
https://upload.wikimedia.org/wikipedia/commons/f/f7/Giant_virus_CroV_with_its_virophage_Mavirus.png

Even single microbial life covers a large range



10 µm

Cafeteria roenbergensis

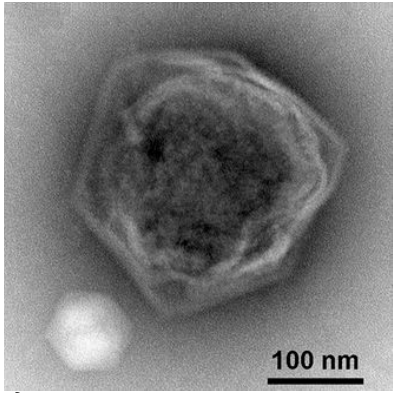


2 µm

Escherichia coli

0.5 µm

Mitochondria



Cafeteria roenbergensis virus

Mavirus virophage

https://commons.wikimedia.org/wiki/File:CafeteriaRoenbergensis.jpg

https://www.cam.ac.uk/sites/www.cam.ac.uk/files/styles/content-885x432/public/news/research/news/mitochondria.jpg?itok=CIFE3yjc

https://upload.wikimedia.org/wikipedia/commons/f/f7/Giant_virus_CroV_with_its_virophage_Mavirus.png

Overview

1. All living organisms have several key essential **properties**

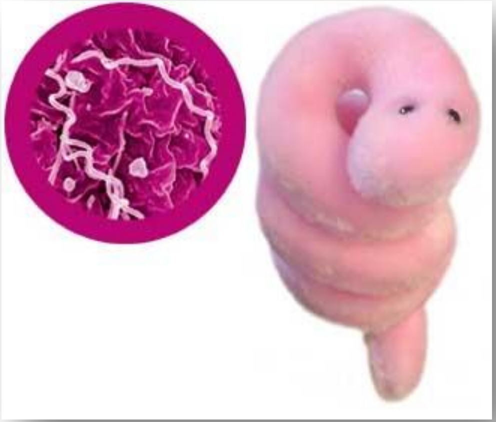
2. Life can be viewed as a **hierarchical structure** with many levels of organization from **genome** (including genomic elements) to the **biosphere**

3. The levels we cannot observe with the naked eye are as (or more) **diverse** as the levels we can observe

Essential properties of an organism

Cellularity

Unicellular



Treponema pallidum
(www.teachersource.com)

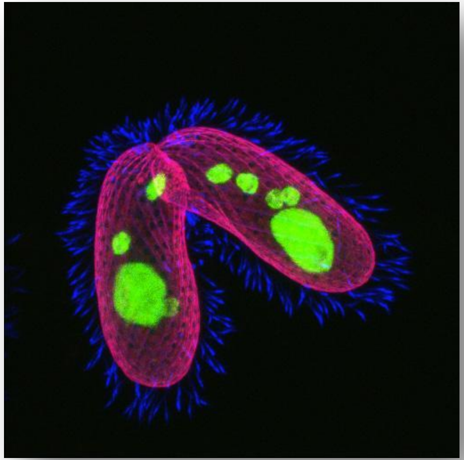
Multicellular

Caenorhabditis elegans (959 cells)
(www.ucl.ac.uk)

Essential properties of an organism

Reproduction

Sexual



Tetrahymena thermophila
(www.isleepinadrawer.com)

Asexual

Amoeba proteus
(www.teachnet.ie)

Essential properties of an organism

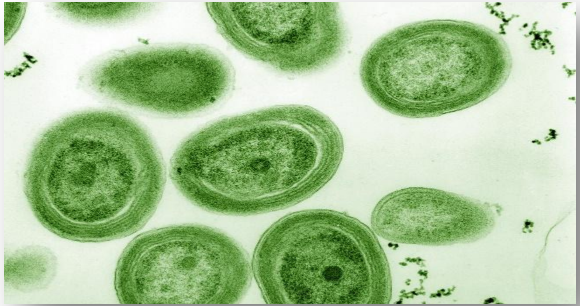
Biochemical Processes and Pathways, such as…

Fermentation

Antibiotic synthesis

Toxin degradation

Photosynthesis

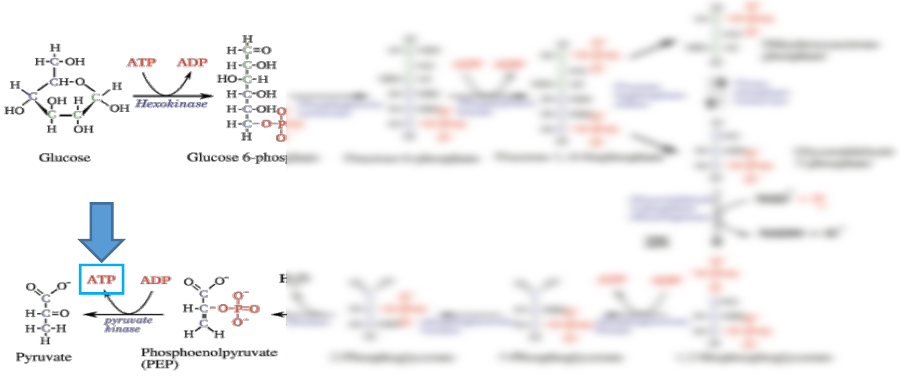


http://en.wikipedia.org/wiki/File:Gimchi.jpg
http://en.wikipedia.org/wiki/File:NOVAMOXIN_antibiotic.jpg
https://www.thestar.com/news/2007/01/28/sydney_tar_ponds_to_be_buried.html
https://commons.wikimedia.org/wiki/File:Prochlorococcus_marinus.jpg

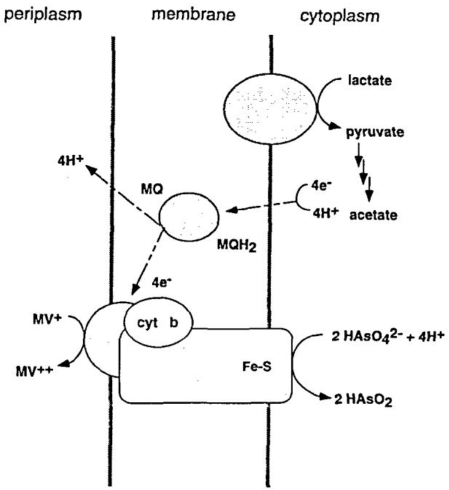
Essential properties of an organism

Respiration

Glucose - boring!



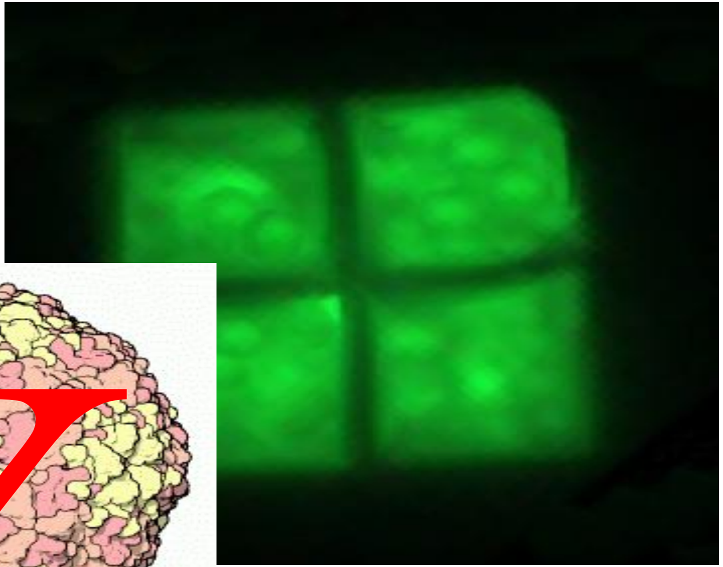
Arsenic - interesting!

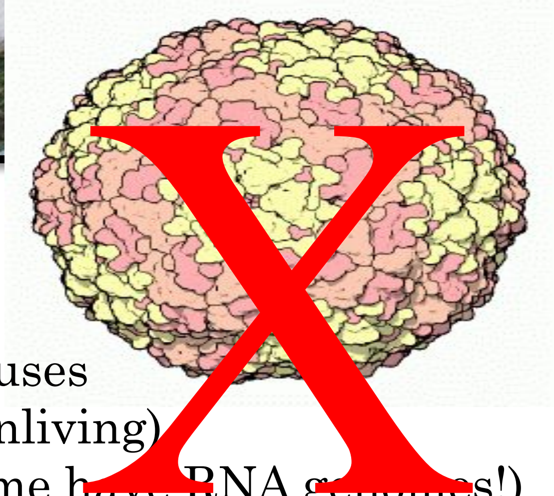


Newmann et al. (1988) *Geomicrobiology Journal*
http://www.opencurriculum.org/5363/powering-the-cell-cellular-respiration-and-glycolysis/

Eukaryotes

Prokaryotes
(Bacteria and Archaea)





Viruses
(nonliving)
(some have RNA genomes!)

Photo: R.Beiko
http://en.wikipedia.org/wiki/File:Haloquadratum_walsbyi00.jpg
http://www.rcsb.org/pdb/101/motm.do?momID=20

Biosphere

Communities and Ecosystems

Populations

Organisms

Cells

Pathways and Systems

Proteins

Genes

Genomes

Groupings

Building blocks

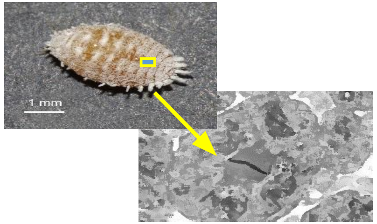
Genome:

The complete set of heritable genetic material

(DNA for all known cellular organisms)

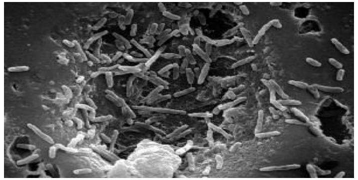
Your Genome and You

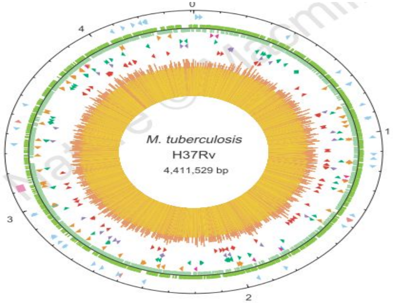
Tremblaya princeps



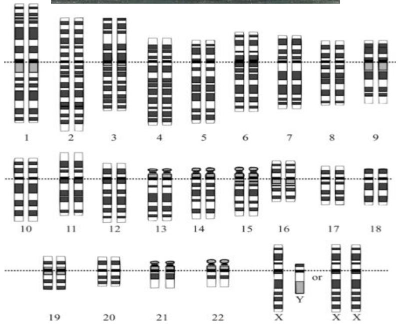
1 chromosome
110 genes
138,931 nucleotides

Mycobacterium tuberculosis H37Rv



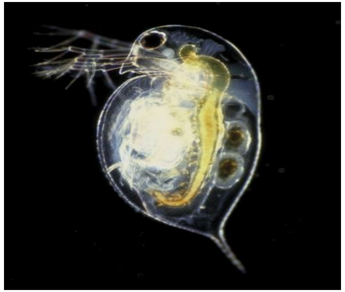


1 chromosome
4,000 genes
4.4 million nucleotides



23 chromosomes
+ mitochondrion
20,000 genes
3.1 billion nucleotides
(times two!)

Daphnia pulex

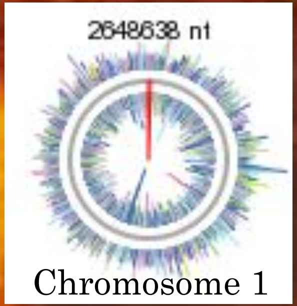


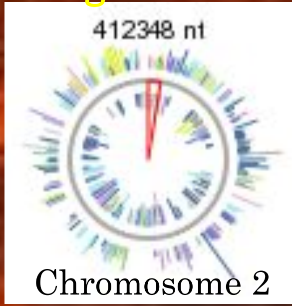
12 chromosomes
+ mitochondrion
<u>31,000</u> genes
200 million nucleotides

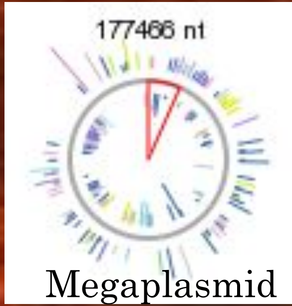
Paris japonica

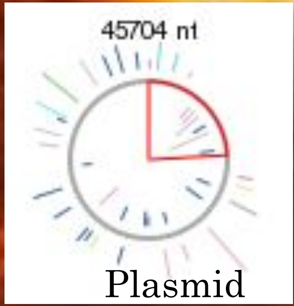
?? chromosomes
??? genes
<u>150 billion</u> nucleotides

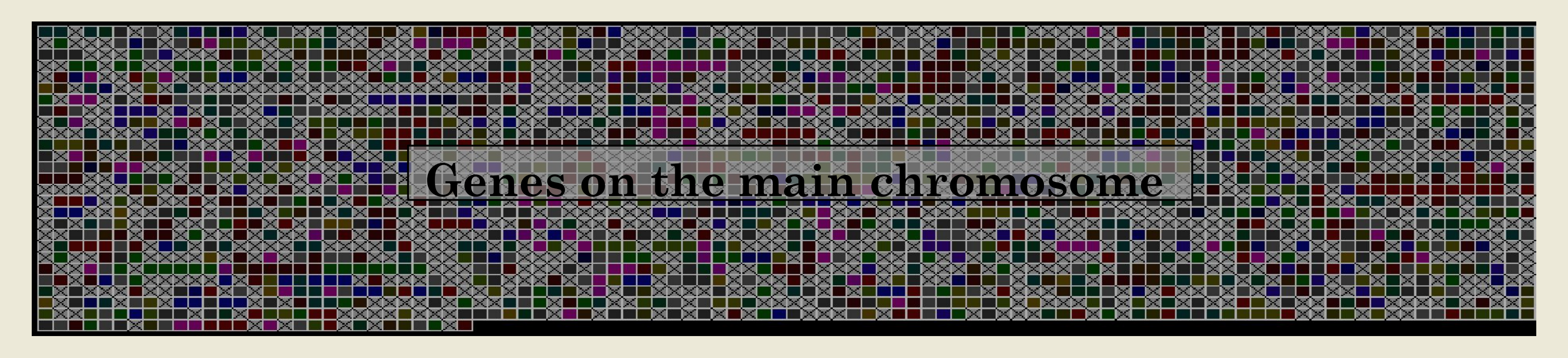
The genome of *Deinococcus radiodurans*

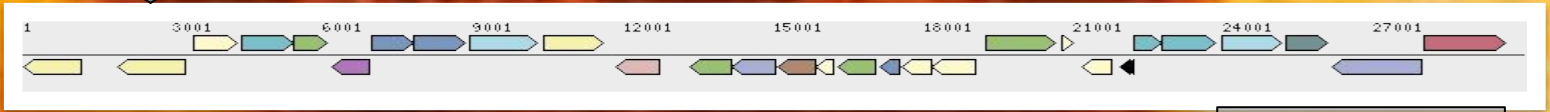








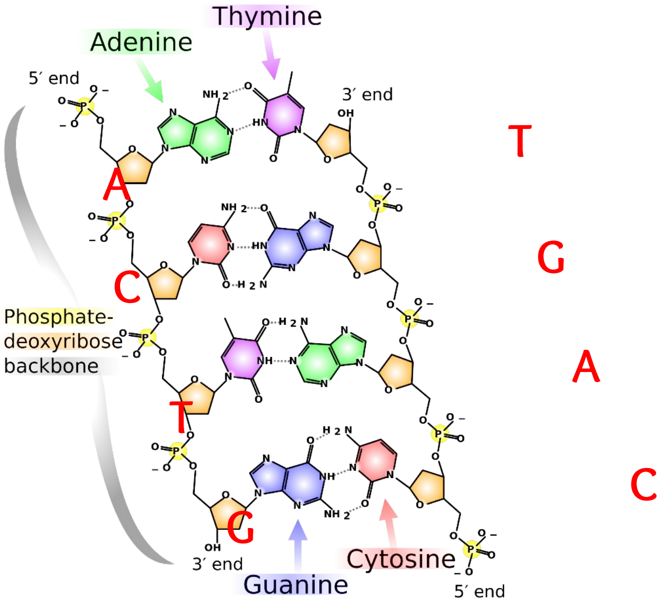




Gene order

Michael Daly
http://www.genomenewsnetwork.org/articles/07_02/deinococcus.shtml

The DNA sequence of a gene



5´ - ATGCGTTACTTCGAAATGGCAACCCACTCGGGGACTTCCTCCAACGGTTGA- 3´
3´ - TACGCAATGAAGCTTTACCGTTGGGTGAGCCCCTGAAGGAGGTTGCCAACT- 5´

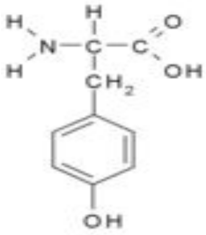
http://en.wikipedia.org/wiki/File:DNA_chemical_structure.svg (Madeleine Price Ball)

DNA to protein

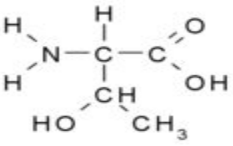
DNA is read in triplets

ATG CGT TAC TTC GAA ATG GCA ACC CAC TCG GGG ACT TCC TCC AAC GGT TGA

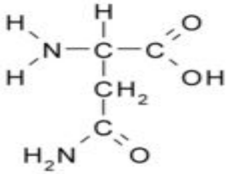
M A Y F E M A T H S G T S S N G *



Tyrosine



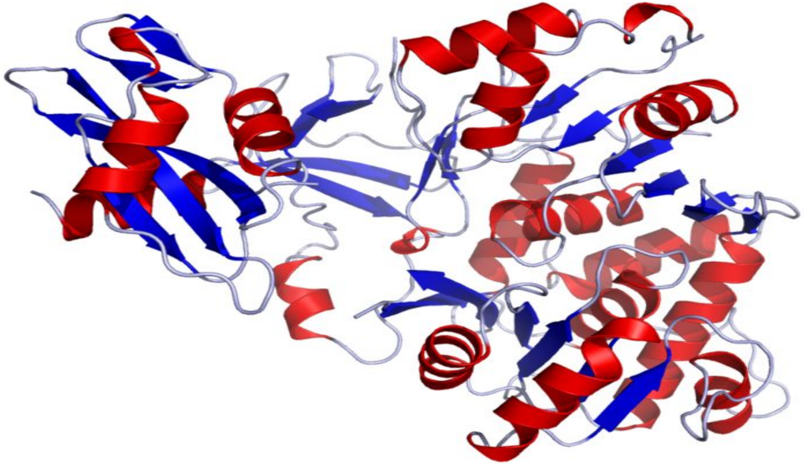
Threonine



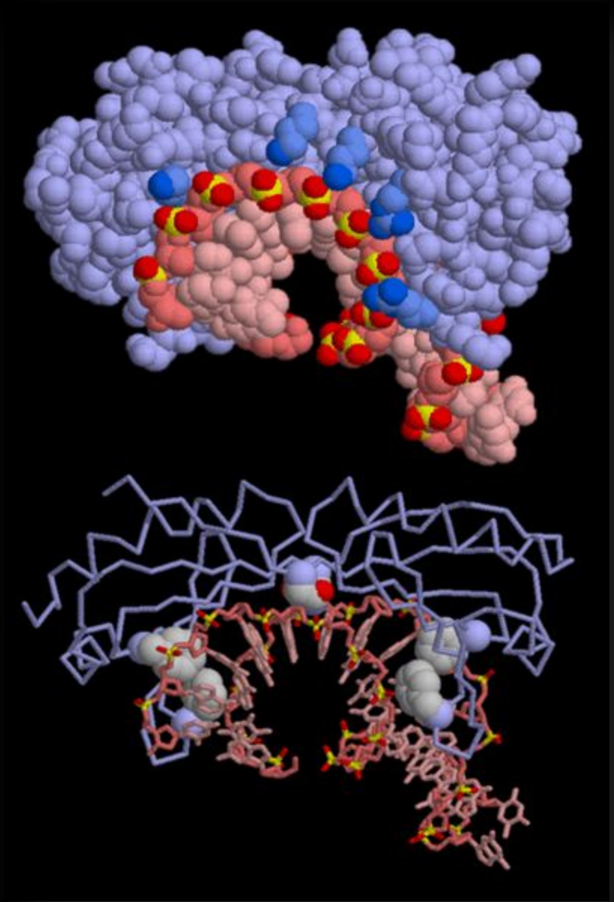
Asparagine

Protein sequence and structure

M A Y F E M A T H S G T S S N G *



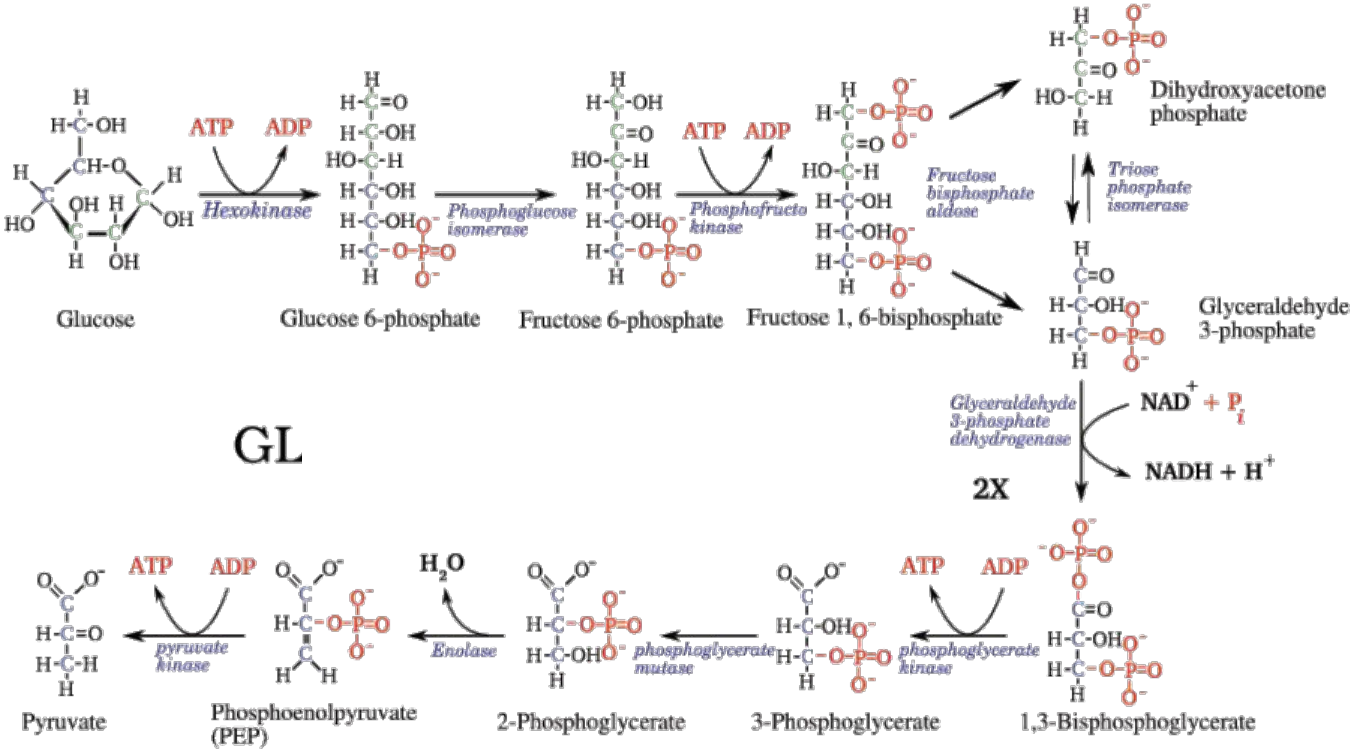
A DNA-protein complex



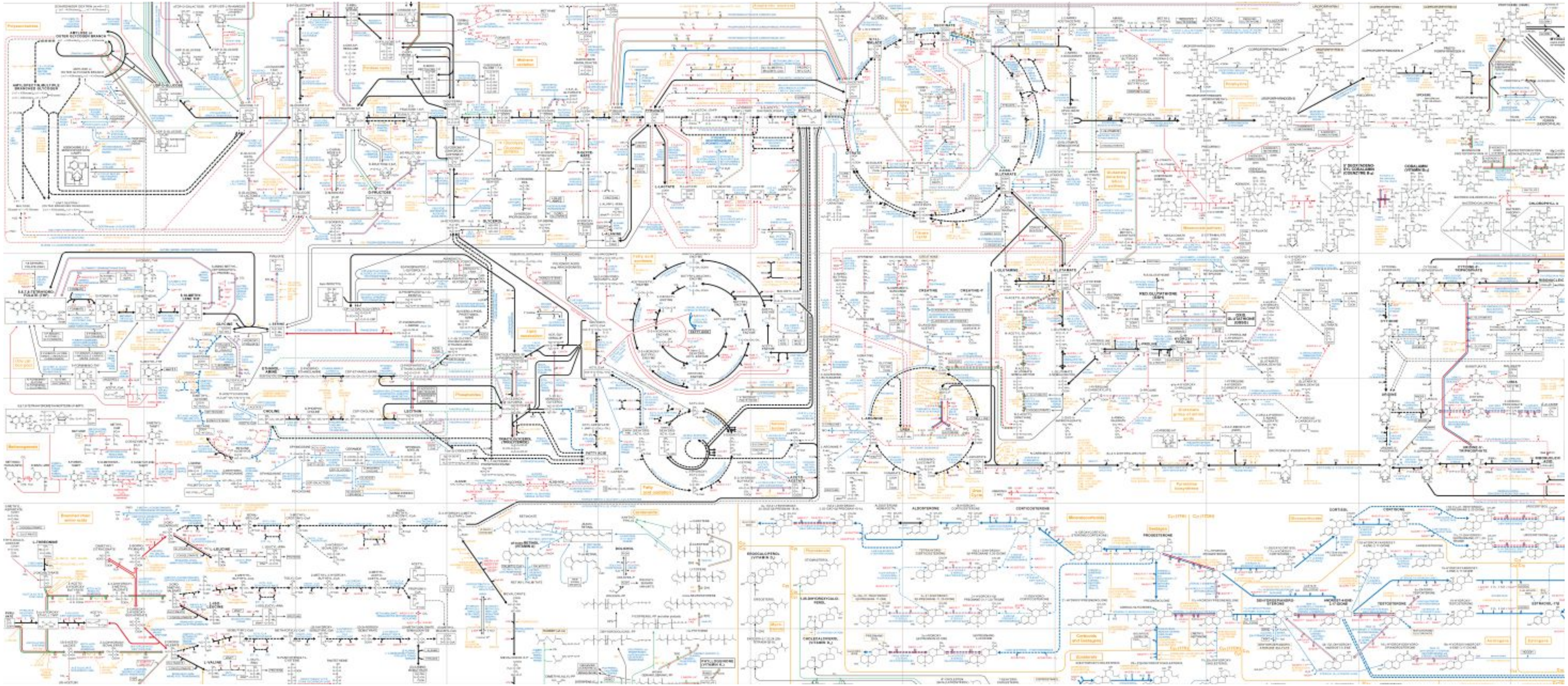
DNA-binding protein
("TATA-box binding protein")

DNA (note the recurring pattern;
yellow = phosphate)

Metabolism – Proteins working together

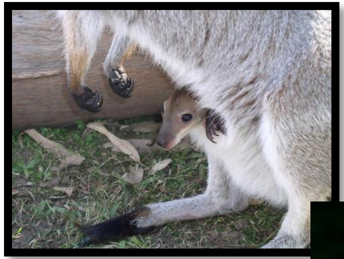


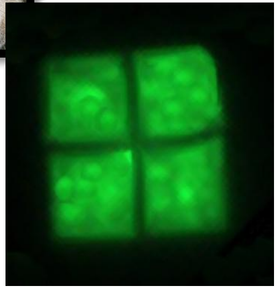
http://www.opencurriculum.org/5363/powering-the-cell-cellular-respiration-and-glycolysis/



Pathways (metabolism
+ self-replication
+ signalling)

=





Populations

http://commons.wikimedia.org/wiki/File:Herd_Of_Goats.jpg

Communities and Ecosystems

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