CSI5126. Algorithms in bioinformatics

Essential **Cellular Biology**

Marcel Turcotte

uOttawa

School of Electrical Engineering and Computer Science (EECS)
University of Ottawa

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Summary

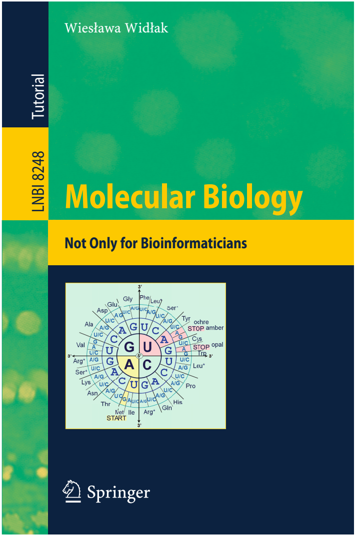
This lecture presents the **cell**, the **kinds of cells**, their **organization** and **composition**. Concepts from **molecular evolution** are introduced. It presents the **macromolecules** of the cell, with their basic organization. Throughout the presentation, we will highlight the importance of the notions for bioinformatics.

General objective

- **Describe** the organization of the cell and macromolecules

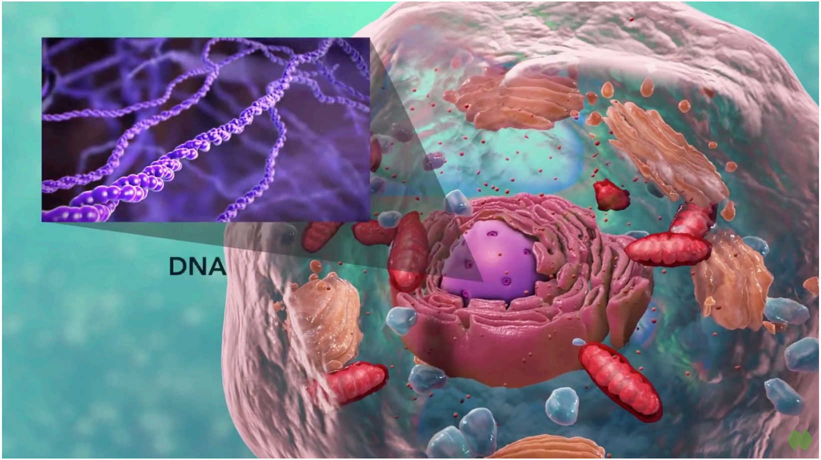
Reading

- Wiesława Widłak (2013). Molecular Biology: Not Only for Bioinformaticians (Vol. 8248). Springer. Chapters 1, 2, and 3.



link.springer.com/book/10.1007/978-3-642-45361-8

Cell Structure



https://www.youtube.com/watch?v=URUJD5NEXC8

Cells: building blocks of living organisms

Two **kinds** of cells (with and without nucleus)

Prokaryote (procaryote, prokaryotic cell, procaryotic organism):
Cell or organism **lacking** a membrane-bound, structurally **discrete nucleus** and other sub-cellular compartments. Bacteria are prokaryotes.

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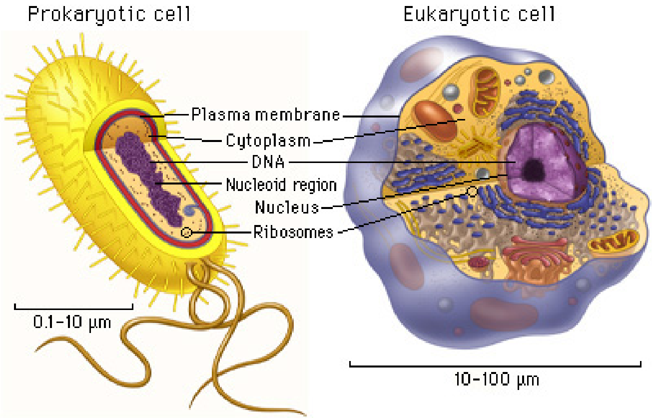
Eukaryote (eucaryote, eukaryotic cell, eucaryotic cell): Cell or organism **with** a membrane-bound, structurally **discrete nucleus** and other well-developed sub-cellular compartments. Eukaryotes include all organisms except viruses, bacteria, and cyanobacteria (blue-green algae).

Cells: building blocks of living organisms

- Eukaryotic cells are generally larger than prokaryotic cells.
- The packaging of the genetic information (DNA) is much more **structured** and compact in **Eukaryotes** compared to **Prokaryotes**.

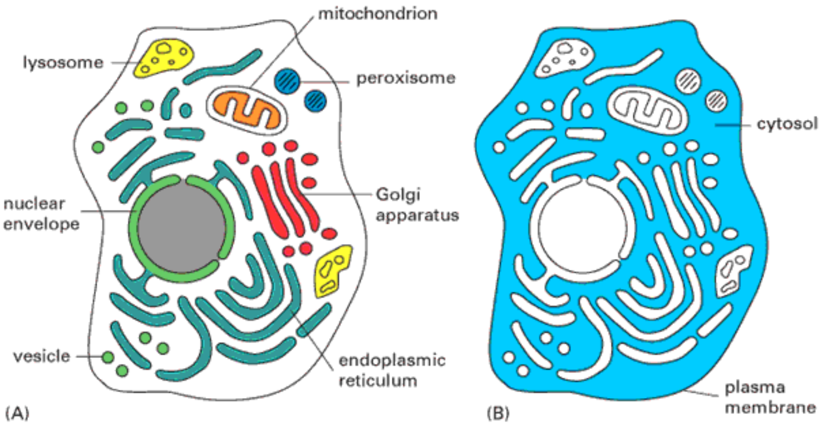
Cell theory: 1939 by Matthias Schleiden and Theodor Schwann.

Prokaryotic vs eukaryotic cell



www.phschool.com/science/biology_place/biocoach/cells/common.html

Organisation of an eukaryotic cell



Organelle genomes

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- Several organelles are believed to be engulfed prokaryotes (**endosymbiotic theory** made popular by Lynn Margulis)
- Mitochondrial genes are **inherited from the mother only**.

Bioinformaticist's point of view

- The **organization of genes** (genome structure) is quite different between the two kinds of cell.

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- Consequently the **gene-finding algorithms must be adapted**.
- Eukaryotic cells being more complex provide a richer set of problems:
  e.g. **protein sub-cellular localisation problem**.
- During the sequence assembly, one has to consider the possibility of contamination, mtDNA/nuclear DNA, bacterial DNA.

Resources

- Texas Education Agency
  Advanced Biotechnology Collection on iTunes U
  - https://itunes.apple.com/ca/itunes-u/tea-advanced-biotechnology/id876525204?mt=10
  - Specifically the **Cell Structure and Function** segment
- Help Me Understand **Genetics**
  - https://ghr.nlm.nih.gov/primer
- **BBC** The Cell The Hidden Kingdom
  - https://www.youtube.com/watch?v=aDuwkdQzb2g
- http://learn.genetics.utah.edu

(3) kingdoms of life

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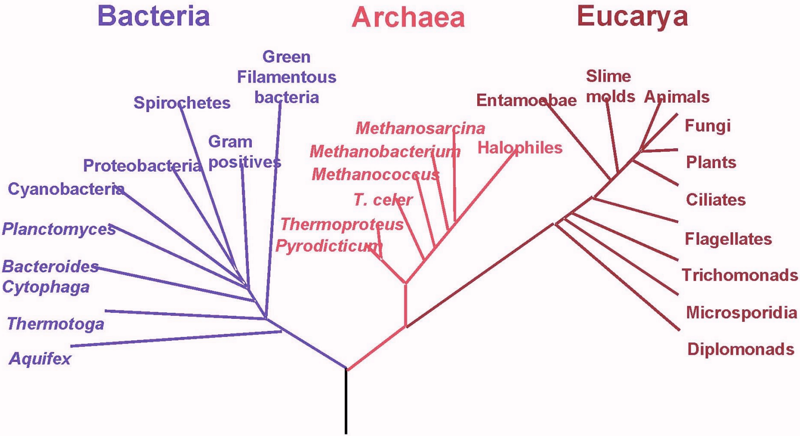
Archaea: (archaebacteria) like the prokaryotes **they lack the nuclear membrane** but have **transcription** and **translation mechanisms close to those of the eukaryotes**.

(3) **kingdoms of life**: Archaea

Methanococcus jannaschii is an **methane producing archaebacterium** which had its complete genome sequenced in 1996. This organism was discovered in 1982 in white smoker of a hot spot at the bottom of the Pacific ocean: depth **2600 meters**, **temperature 48-94° C (thermophilic)**, optimum at 85° C, 1.66 Mega bases, 1738 genes. 56% of its genes are unlike any known eukaryote or prokaryote, one kind of DNA polymerase (other genomes have several).

Phylogenetic Tree of Life



Phylogenetic tree

- "The objectives of phylogenetic studies are (1) to reconstruct the correct **genealogical ties between organisms** and (2) to estimate the **time of divergence** between organisms since they last shared a common ancestor."

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- "The **nodes** represents the **taxonomic units**, and the **branches** define the **relationships** among the units in terms of descent and ancestry."
- "The **branch length** usually represents the **number of changes** that have occurred in that branch." (or some amount of time)

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Bioinformaticist's point of view

- **Bench-marking** (cross-validation) and **molecular evolution**
- **Molecular sequence alignment** : are the sequences evolutionary related?
- **Large phylogeny problem**: Reconstructing phylogenetic trees from molecular sequence data
- **Small phylogeny problem**: Reconstructing ancestral molecular sequences

Nothing in Biology Makes Sense Except in the Light of Evolution

Theodosius Dobzhansky

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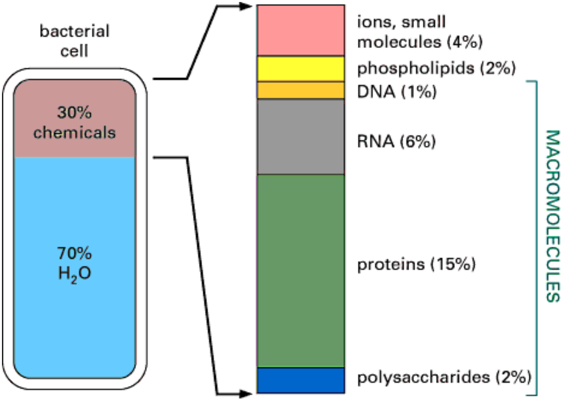
- Virus that infect bacteria are called phages or bacteriophages.
- Viroids don't even have a capsid – consists of a single-stranded RNA.

Composition of the Cell



⇒ **DNA**, **RNA** and **proteins** will be the main focus of the course.

Macromolecules: **DNA** (deoxyribonucleic acid), **RNA** (ribonucleic acid) and **Protein**

Bioinformatics is mainly concerned with three classes of molecules:

- **DNA**, **RNA** and **proteins** — collectively called **macromolecules** or **biomolecules**.

Macromolecules: **DNA** (deoxyribonucleic acid), **RNA** (ribonucleic acid) and **Protein**

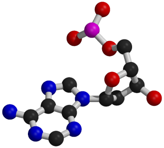
All three classes of macromolecules are **polymers**, that is they are composed of smaller units (molecules), called **monomers**, that are **linked sequentially** one to another forming **unbranched linear structures**.

Macromolecules: DNA (deoxyribonucleic acid), RNA (ribonucleic acid) and Protein

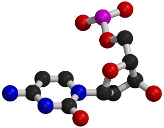
Generally speaking, the units (monomers) consits of two distinct parts, one that is **common** to all the monomers and defines the **backbone** of the molecule, and another part that confers the **identity** of the unit, and therefore its **properties**.

```
[ ]-[ ]-[ ]-[ ]-[ ]- ... -[ ]-[ ]
 |   |   |   |   |         |   |
 *   @   *   #   +         +   @
```

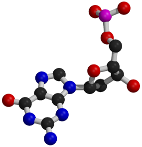
DNA's building blocks: ACGT



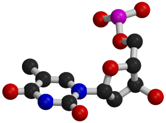
Adenine (A)



Cytosine (C)

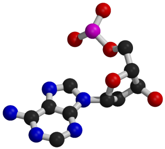


Guanine (G)



Thymine (T)

DNA's building blocks: ACGT



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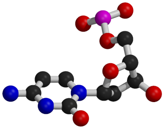

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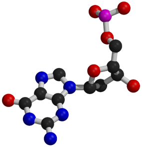
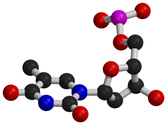


Guanine (G)



Thymine (T)

$\Rightarrow$ **Identify** the common and unique parts of each monomer.

(20) Amino Acids (Naturally Occuring)


A (Ala)


D (Asp)


E (Glu)


K (Lys)


P (Pro)


W (Trp)


V (Val)


R (Arg)


C (Cys)

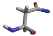

G (Gly)


I (Ile)


M (Met)


S (Ser)


Y (Tyr)


N (Asn)


Q (Gln)


H (His)


L (Leu)


F (Phe)


T (Thr)

⇒ Stick (licorice) representation.

Structure

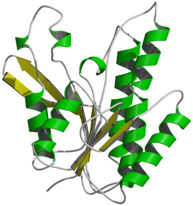
It's useful to distinguish between four **levels of abstraction** or **structure**: **primary**, **secondary**, **tertiary** and **quaternary** structure.

1, 2, 3, ...

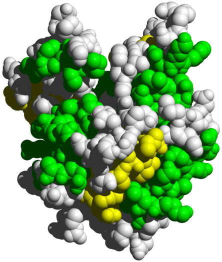
EARRVLVYGGRGALGSRCVQNW ...(236) ...

(a) primary structure

(b) secondary structure



(c) tertiary structure - ribbon



(d) tertiary structure - all atoms

Bioinformaticist's point of view

- A large number of computational problems are related to the **primary sequence**: sequence assembly, sequence alignment, phylogenetic tree inference, gene-finding, sequence motif discovery, etc.
- Predicting the **secondary, tertiary, and quaternary (docking) structure** are problems, on its own.
- These **abstractions** are allowing us to formulate efficient algorithms - understanding the implications is paramount.

Macromolecules: DNA (deoxyribonucleic acid), RNA (ribonucleic acid) and Protein

The primary structure or **sequence** is an ordered list of characters, from a given alphabet, written contiguously from left to right.
DNA : 4 letters alphabet,
$\Sigma = \{A, C, G, T\}$
RNA : 4 letters alphabet,
$\Sigma = \{A, C, G, U\}$
Proteins : 20 letters alphabet,
$\Sigma = \{A, C, D, E, F, G, H, I, K, L, M, N, P, Q, R, S, T, V, W, Y\}$

Examples

In the case of **nucleic acids** (DNA and RNA), the building blocks are called **nucleotides**, whilst in the case of **proteins** they are called **amino acids**.

Examples of DNA, RNA and protein sequences.

```
> Chimpanzee Chromosome 1; A DNA sequence (size = 245,522,847 nt)
TAACCCTAACCCTAACCCTAACCCTAACC ... TCTCATGACAGTGAGTGAGTTCTCATGATC
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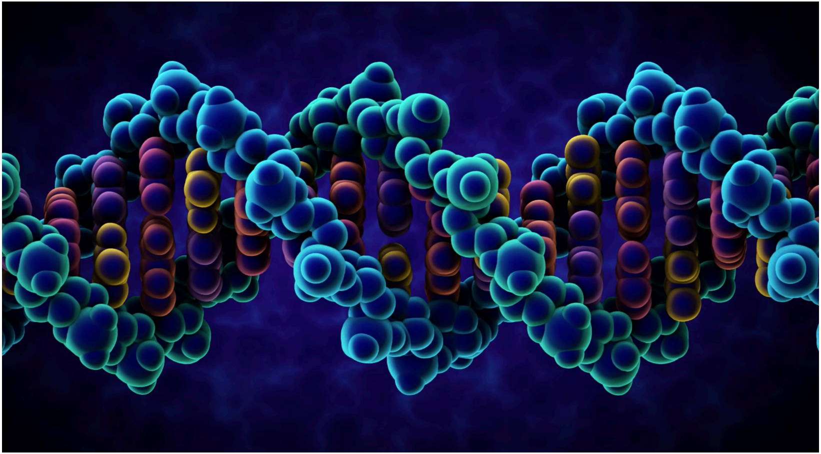
```
> Beta Globin; A protein sequence (size = 147 aa)
MVHLTPEEKSAVTALWGKVNVDEVGGEAL ... FFESFGDLSTPDAVMGNPKVKAHGKKVLGA
```

Bioinformaticist's point of view

- **Exact string** (sequence) comparison, **approximate matching** ($k-$mismatches), comparison under the **edit-distance**, **significance** of match, **multi-way** sequence comparison
- Finding **repeats**, **approximate repeats**, finding interesting **patterns**
- Secondary, tertiary and quaternary structure inference

DNA

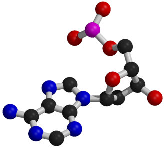


https://www.youtube.com/watch?v=o_-6JXLYS-k

Deoxyribonucleic acids (**DNA**)

- **DNA** was discovered by **Johann Friedrich Miescher** in **1869**. Who discarded the possibility that DNA might be related to heredity!
- The **double-helical structure** of DNA was proposed in **1953** by James Watson and Francis Crick (who died on July 28, 2004).
- This discovery is often referred to as the **most important breakthrough in biology of the 20th century**.
- The proposed model finally explained Chargaff's rule (same amount of adenine and thymine, same amount of guanine and cytosine).
- More importantly, the model finally explains **how DNA and heredity are linked!** (replication)

DNA's building blocks: ACGT



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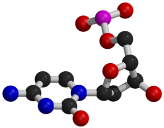

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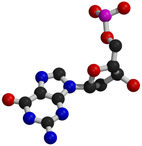
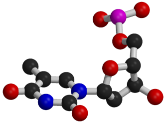


Guanine (G)



Thymine (T)

DNA/RNA's building blocks

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- In the case of **RNA**, the bases are Adenine (**A**), Cytosine (**C**), Guanine (**G**) and Uracil (**U**).

DNA/RNA's building blocks

- The length of a DNA/RNA molecule is often expressed in **bases**, e.g. a 10 **mega base** long region.
- Or, since nucleic acids molecules **hybridize** (bind together) to form a duplex (double helical) structure, the length of a molecule is often expression is base pairs to avoid confusion, e.g. a 10 **mega base** pairs region.

DNA/RNA's building blocks

- **DNA** stands for deoxyribonucleic acid, and **deoxy** comes from the fact that the **C2' carbon of the sugar has no oxygen**; while RNA has one. **RNA**'s O2' oxygen is key to its **functional versatility**!
- The other difference is the use of **T** (thymine) in the case of **DNA** vs **U** (uracil) in the case of **RNA**.
- Nucleotides are **always attached one to another in the same way** (well, almost always): the **C3' atom** of the nucleotide i is covalently linked to the **phosphate group** of the nucleotide $i + 1$.

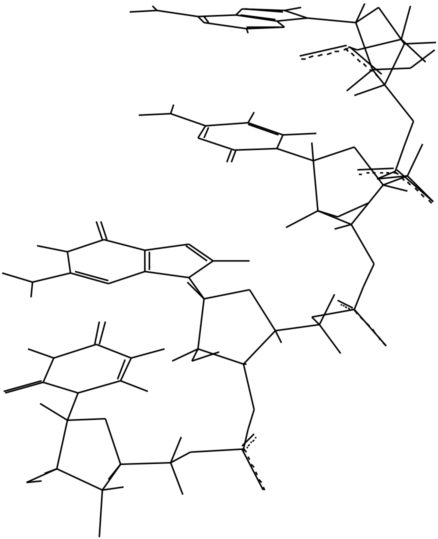
DNA/RNA's building blocks

- The **orientation of a DNA molecule** is important; just like the orientation of words are important in natural languages.

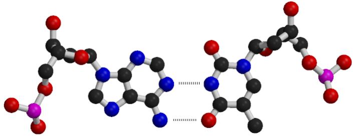
DNA/RNA's building blocks

- The **orientation of a DNA molecule** is important; just like the orientation of words are important in natural languages.
- The convention is to enumerate the string from its **5' end**; this correspond to the order into which information is process for certain key steps, to be described later. The features that are occurring **before the 5'** are said to be **upstream** while those occurring after the **3'** end are **downstream**, upstream and downstream signals.

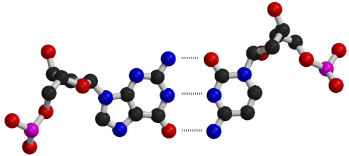
DNA strand



Watson-Crick (Canonical) **base pairs**



(Adenosine) A : T (Thymine)



(Guanine) G : C (Cytosine)

⇒ One of the two base pairs is stronger that the other, which one?

Watson-Crick (Canonical) **base pairs**

In the case of **DNA**, bases interact, i.e. form hydrogen bonds, primarily through the following set of rules:

- **A** interacts with **T** (and vice versa)
- **G** interacts with **C** (and vice versa)

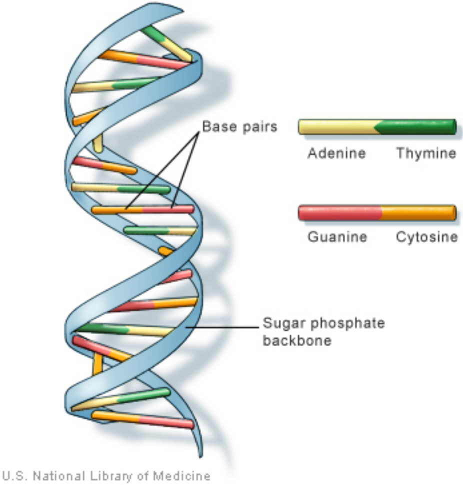
Watson-Crick (Canonical) **base pairs**

In the case of **DNA**, bases interact, i.e. form hydrogen bonds, primarily through the following set of rules:

- **A** interacts with **T** (and vice versa)
- **G** interacts with **C** (and vice versa)

Those rules are the consequence of the fact that A:T and G:C pairs position the backbone atoms roughly at the same three-dimensional location and therefore both produces the same double helical structure; isosteric base pairs.

- **DNA** molecules generally form **right-hand** side helices in **B form**, while **RNA** are **A form**, also right-hand side. A left-hand side helix exists that is called **Z DNA**.
- **DNA** molecules **cannot exist as a single strand**, they are degraded, i.e. cut into pieces.
- A **DNA** molecule is made of **two complementary strands running in opposite directions**.


Base pairs
Adenine
Thymine
Guanine
Cytosine
Sugar phosphate backbone
U.S. National Library of Medicine

DNA and Heredity

- **DNA structure explains how information can be copied from one generation to the next**, or simply from one parent cell to its daughter cells during replication.

Before replication

```
5'  - GATACA -> 3' A
      ||||||
3' <- CTATGT -  5' B
```

$\Rightarrow$

A is as a template to produce **B'**

```
5'  - GATACA -> 3' A


5'  - GATACA -> 3' A
      ||||||
3' <- CTATGT -  5' B'
```

DNA and Heredity

Before replication

```
5'  - GATACA -> 3' A
      ||||||
3' <- CTATGT -   5' B
```

$\Rightarrow$

B is as a template to produce **A'**

```
5' -  TGTATC -> 3' B


5' -  TGTATC -> 3' B
      ||||||
3' <- ACATAG -> 5' A'
```

DNA and Heredity

Parent cell (AB)

```
5'  - GATACA -> 3' A
      ||||||
3' <- CTATGT -  5' B
```

Daughter cell AB'

```
5'  - GATACA -> 3' A
      ||||||
3' <- CTATGT -  5' B'
```

Daughter cell A'B

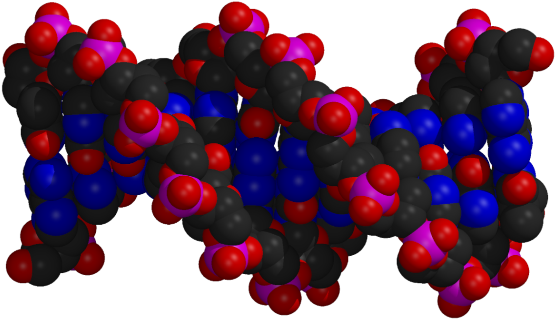
```
5' -  TGTATC -> 3' B
      ||||||
3' <- ACATAG -> 5' A'
```

Two daughter cells, identical to their parent.
(semi-conservative process)

Remarks

- Complex organisms are growing from a single cell to billions of cells. Each cell contains an **exact copy** of the **DNA** of its **parent cell**.
- The information is redundant, the information on the second strand can be inferred from the information on the first strand. This is the basis of **DNA repair mechanisms**. A base that is deleted can be replaced. A mismatch can be detected.

CPK representation of a fragment of a **DNA helix** (B form)

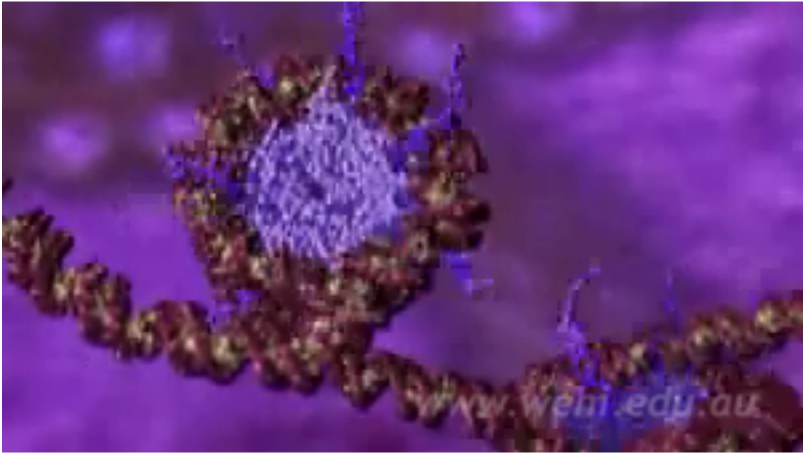


```
TAAGTTATTA                                AAAAAAATAC
||||||||||  ...  (580,074 bp)  ...  ||||||||||
ATTCAATAAT                                TTTTTTTATG
```

About CPK

CPK stands for **Corey-Pauling-Koltun** representation. **Every atom** is represented as a sphere, with **radius proportional to its van der Walls radius**. The usual color scheme is to represent carbon atoms in black, nitrogen in blue, oxygen in red and phosphorus atoms in pink.

Chromosome



https://youtu.be/0jPcT1uUZiE?list=PLD0444BD542B4D7D9

About the animation

- **Histone proteins** attach to the **DNA**.
- **Histones interact one with another** to form a complex called **nucleosome**, but also forcing the DNA to wrap around it.
- The histone, nucleosome and DNA models were derived from their PDB (http://www.rcsb.org/pdb/) structures and other published data.

About the animation

- **Histone proteins** attach to the **DNA**.
- **Histones interact one with another** to form a complex called **nucleosome**, but also forcing the DNA to wrap around it.
- The histone, nucleosome and DNA models were derived from their PDB (http://www.rcsb.org/pdb/) structures and other published data.
- Macromolecular structures cannot be directly oberserved. A molecular bond is between 1 and 2 Å (angstrom – 10^{-10} m) long, wave length in the visible spectrum are 400 to 700 nm (10^{-9} m).

Bioinformaticist's point of view

- Given DNA sequence information alone, **predict the locations where the histones will be binding**.
- Knowing the location of the histones might help predicting the **location of genes** as well as the **location of regulatory elements**.
- The **three-dimensional organization of the genome** is a hot topic.

Summary

- Two kinds of cells: **prokaryotic** and **eukaryotic**.
- **Eukaryotic cells have organelles**, and some organelles, such as the mitochondria, contain DNA.
- Three Kingdom of life: **Prokarya**, **Eukarya**, and **Archea**
- A **phylogeny** specifies the relationships between organisms and time of divergence.
- Three kinds of macromolecules: **DNA**, **RNA**, and **proteins**.
- **Macromolecules are linear (unbranched) polymers**, such that all the monomers have a common and a specific part (remember the analogy with the linked nodes).

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Pensez-y!

L'impression de ces notes n'est probablement pas nécessaire!