CHEM 498Q / 630Q

Molecular modelling of proteins

Fall 2015 Term

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Syllabus:

http://faculty.concordia.ca/glamoure/pdfs/CHEM498Q_syllabus_2015.pdf

**Course material
(tutorials and overheads):**

http://faculty.concordia.ca/glamoure/teaching.html

Bioinformatics
versus Molecular modelling

Both disciplines are studying biology and biomolecules using computers but…

- **Molecular modelling** is based on "physics" (molecules & interaction)

- **Bioinformatics** is based on "information" (databases & statistical inference)

Sources of information

The (infamous) Wikipedia
- Do not use as your primary source of information
- Use only as a starting point to the original (peer-reviewed) articles

Google Scholar (http://scholar.google.com)

Web of Science (http://apps.webofknowledge.com)
- Indexes most scientific journals
- Better organized than Google Scholar

PubMed (http://www.ncbi.nlm.nih.gov/pubmed/)
- Comprehensive resource for biological and medical information
- Take some time to explore it: It will pay you back a thousand fold.

The… library!
- There still is nothing like reading textbooks to get an introduction to a new field.
- You may find that books nearby on the shelves are interesting as well.

Information overload !

Too many hits?
Learn how to use the advanced search features (e.g. Boolean operators).

Too much to read?
Start with review articles (the most recent ones) and work your way down.

Nothing relevant?
Try a different search approach:
- Use MeSH terms (http://www.ncbi.nlm.nih.gov/mesh) instead of your own keywords (start from the MeSh Browser: http://www.nlm.nih.gov/mesh/MBrowser.html).
- Look for the articles citing a "foundational" article.

"I had found a bunch of super-relevant articles, but I can't trace back the exact search that got me there!"
- In PubMed, save your searches.
- Keep the Digital Object Identifiers ("DOIs").
- Organize your references with Mendeley or Zotero.

Do you know your Subject Librarian ?

At Concordia University:
http://library.concordia.ca/about/staff/artscilib.php

At Université de Montréal:
http://www.bib.umontreal.ca/nous-joindre/bibliothecaires.htm

At McGill University:
http://www.mcgill.ca/library/contact/askus/liaison

Do you know what constitutes plagiarism ?

From Section 17 of the Concordia University Undergraduate calendar:

plagiarism – the presentation of the work of another person, in whatever form, as one's own or without proper acknowledgement

- If you can't write the introduction/discussion of a tutorial report in your own words, without including chunks of text from the articles you have consulted, you are not ready to write it yet. (Read more!)

- If you don't know the meaning of a technical term, don't use it.

- Writing takes time and effort. You should (temporarily) accept that your own words may not be as effective/concise/stylish as those from the world experts on the topic.

- In case of doubt about what constitutes plagiarism, or on how to cite a certain element of information, come see me.

Databases :
Primary *versus* Derived

Protein Data Bank (PDB)
- primary database of atomically resolved protein structures
- structures obtained from x-ray diffraction or NMR

How many structures?
What other experimental methods?

GenBank, **Ensembl**
- primary databases of DNA sequences
- contain taxonomic and functional information

SwissProt, **UniProt**
- primary databases of protein sequences
- richly annotated and connected to bibliographic databases
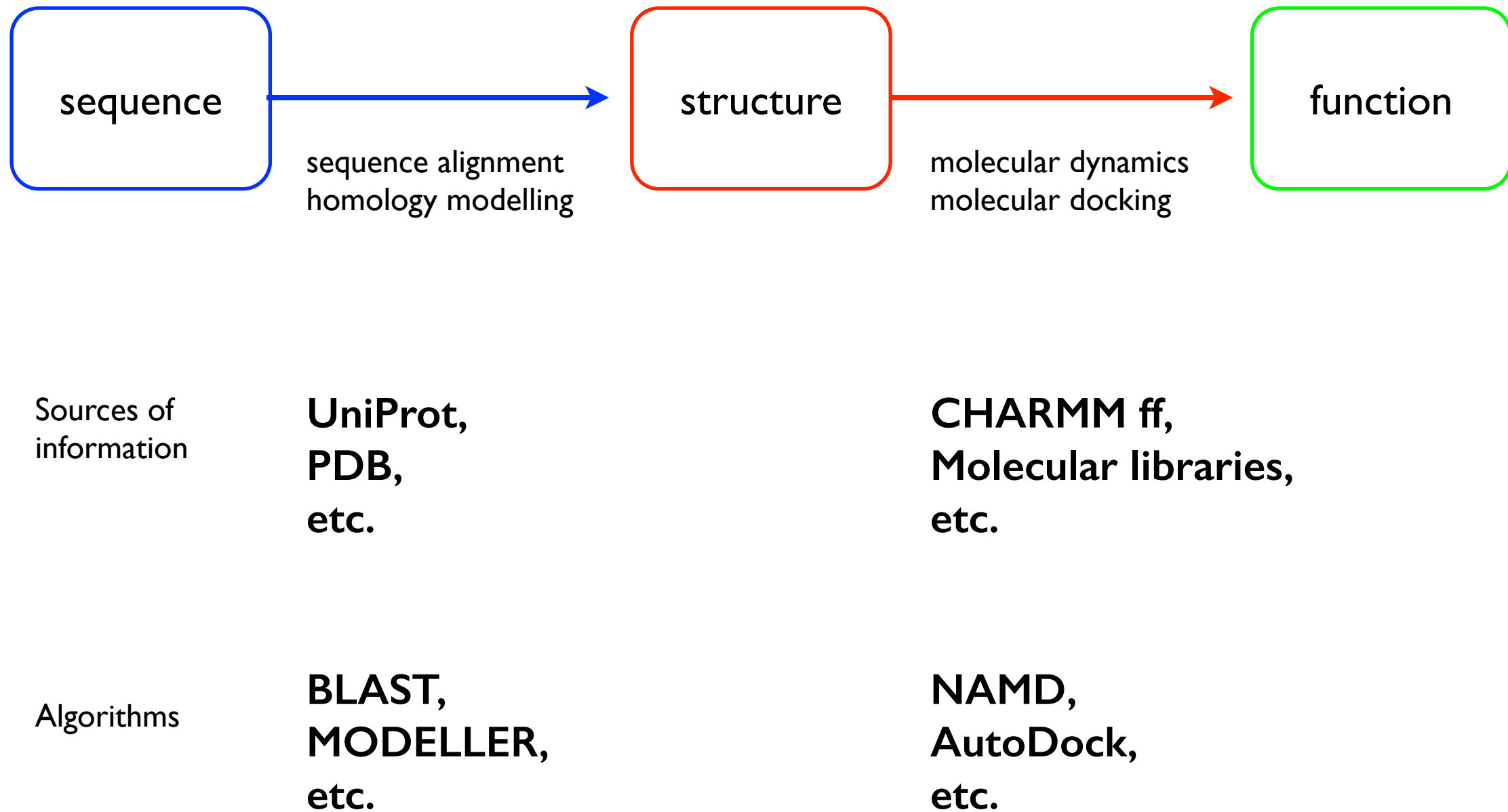
How many protein sequences?

SCOP, **CATH**, **Dali**
- classifications of proteins in terms of their structure
- derived from the PDB

Pfam, **CDD**, **PROSITE**
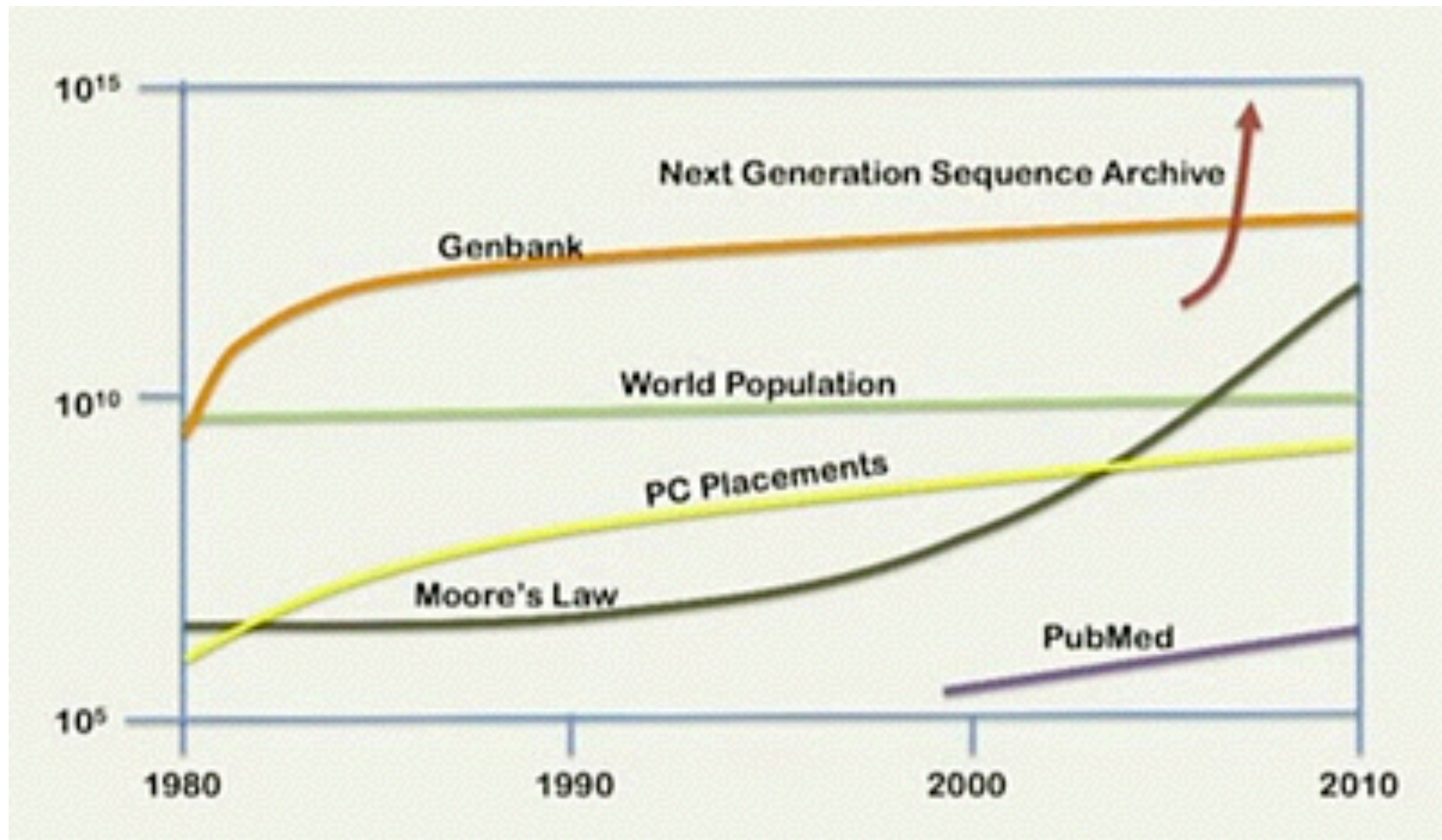- classification based on protein sequence patterns
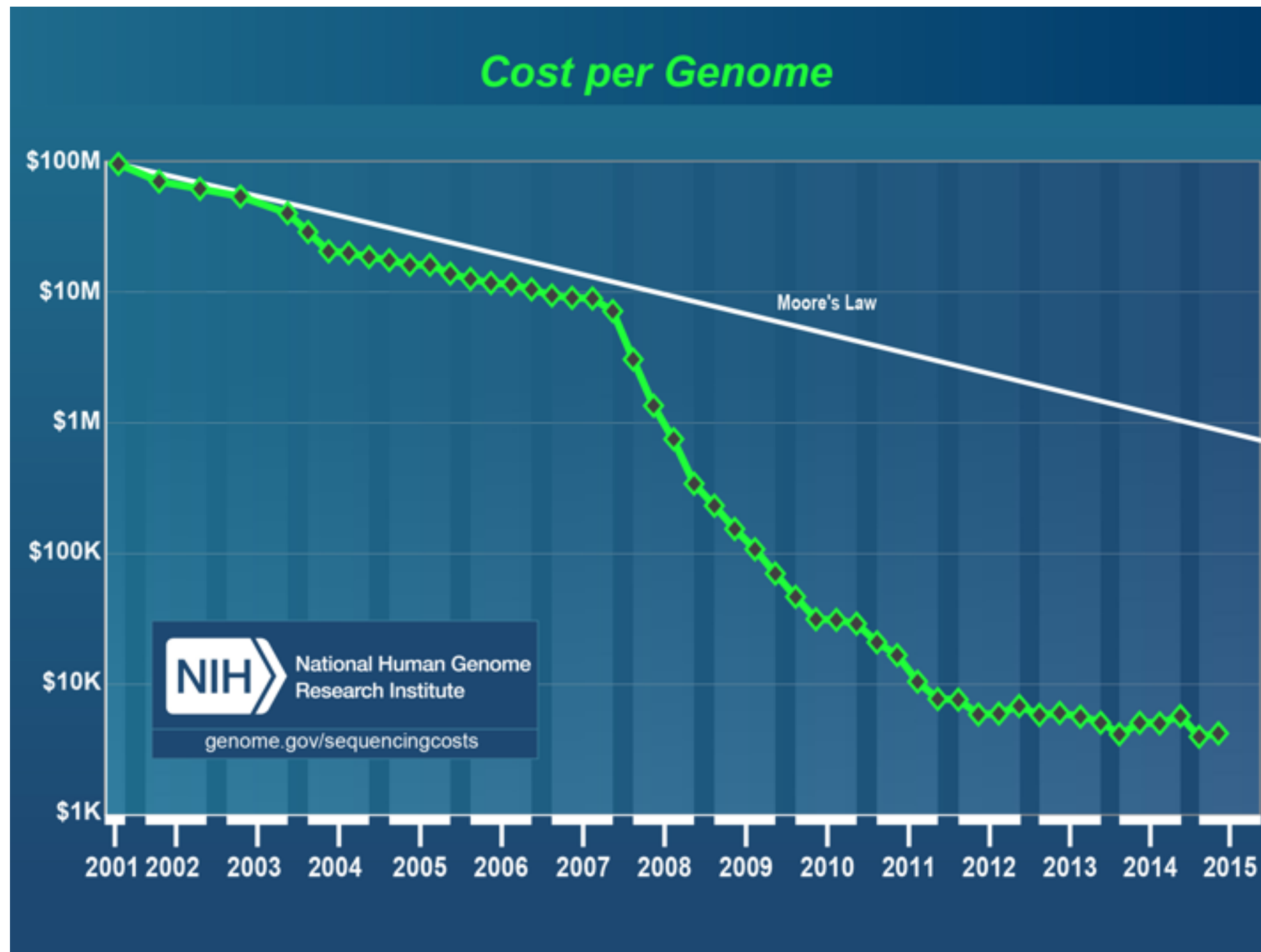- derived from protein sequence databases

Overview of the course

sequence → structure → function

sequence alignment
homology modelling

molecular dynamics
molecular docking

Sources of information

Sources of information	**UniProt, PDB, etc.**	**CHARMM ff, Molecular libraries, etc.**
Algorithms	**BLAST, MODELLER, etc.**	**NAMD, AutoDock, etc.**

Why computer modelling ?

Towards personalized biology and medicine ?