BGGN 213

Foundations of Bioinformatics

Barry Grant

UC San Diego

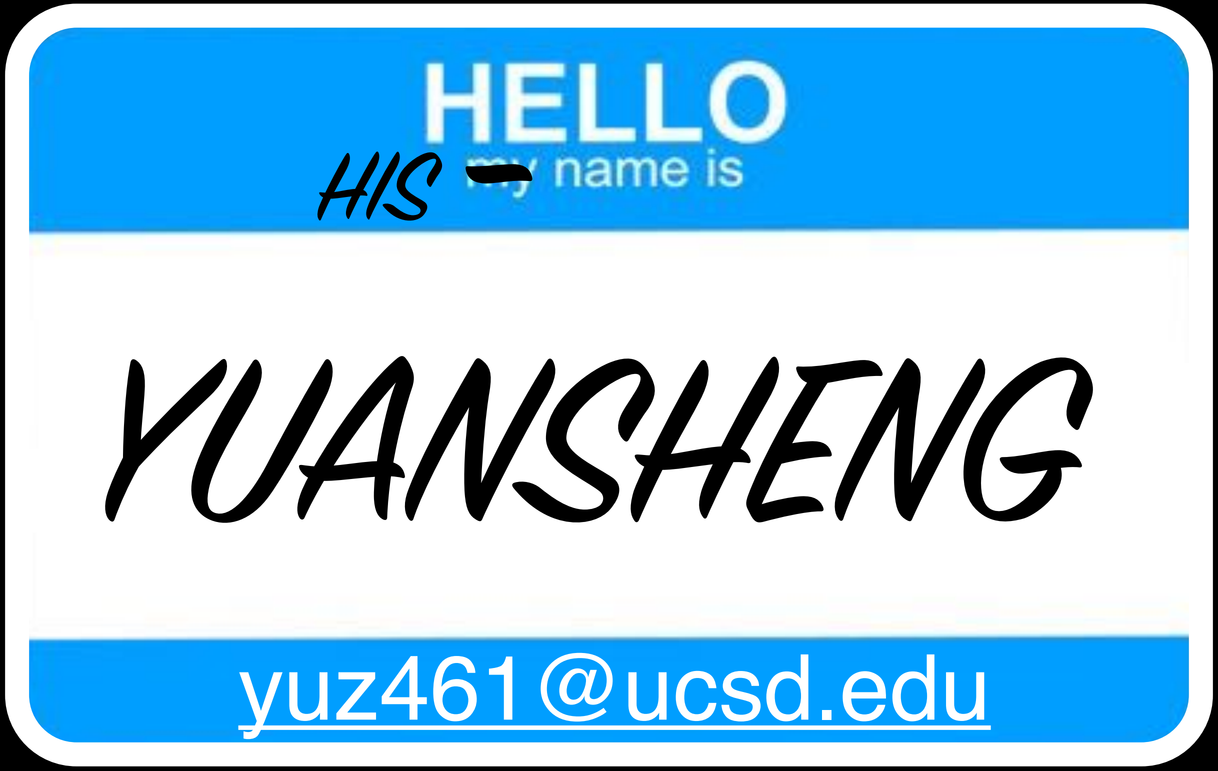
http://thegrantlab.org/bggn213

HELLO

my name is

BARRY

bjgrant@ucsd.edu



HELLO

HIS ~~my~~ name is

YUANSHENG

yuz461@ucsd.edu

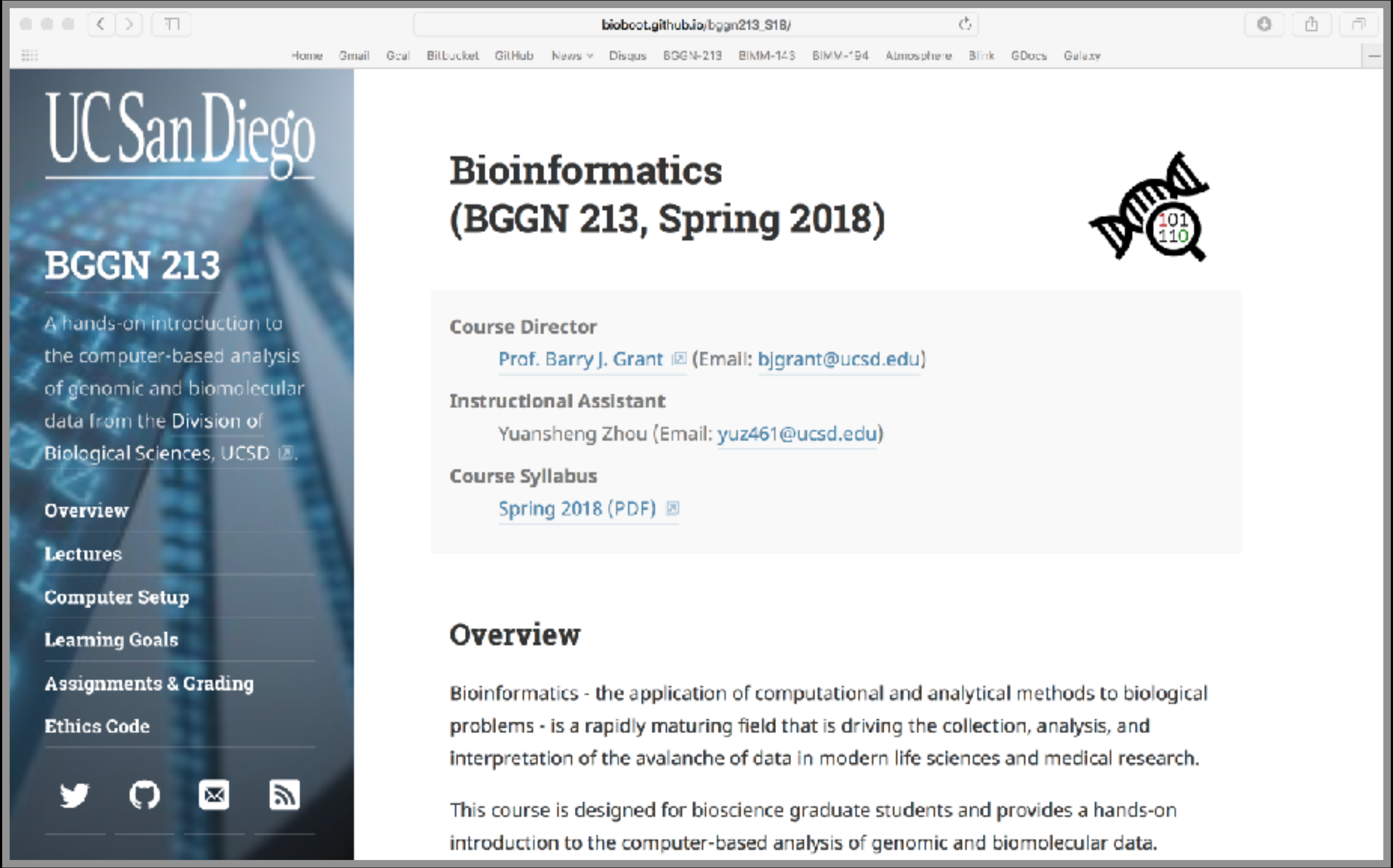
Introduce Yourself!

Your preferred name,
Place you identify with,
Major area of study/research,
Favorite joke (optional)!

Today’s Menu

Course Logistics	Website, screencasts, survey, ethics, assessment and grading.
Learning Objectives	What you need to learn to succeed in this course.
Course Structure	Major lecture topics and specific leaning goals.
Introduction to Bioinformatis	**Introducing the *what*, *why* and *how* of bioinformatics?**
Bioinformatics Database	**Hands-on** exploration of several major databases and their associated tools.

http://thegrantlab.org/bggn213/



BGGN 213

A hands-on introduction to the computer-based analysis of genomic and biomolecular data from the Division of Biological Sciences, UCSD.

- Overview
- Lectures
- Computer Setup
- Learning Goals
- Assignments & Grading
- Ethics Code

Bioinformatics
(BGGN 213, Spring 2018)

Course Director

Prof. Barry J. Grant (Email: bjgrant@ucsd.edu)

Instructional Assistant

Yuansheng Zhou (Email: yuz461@ucsd.edu)

Course Syllabus

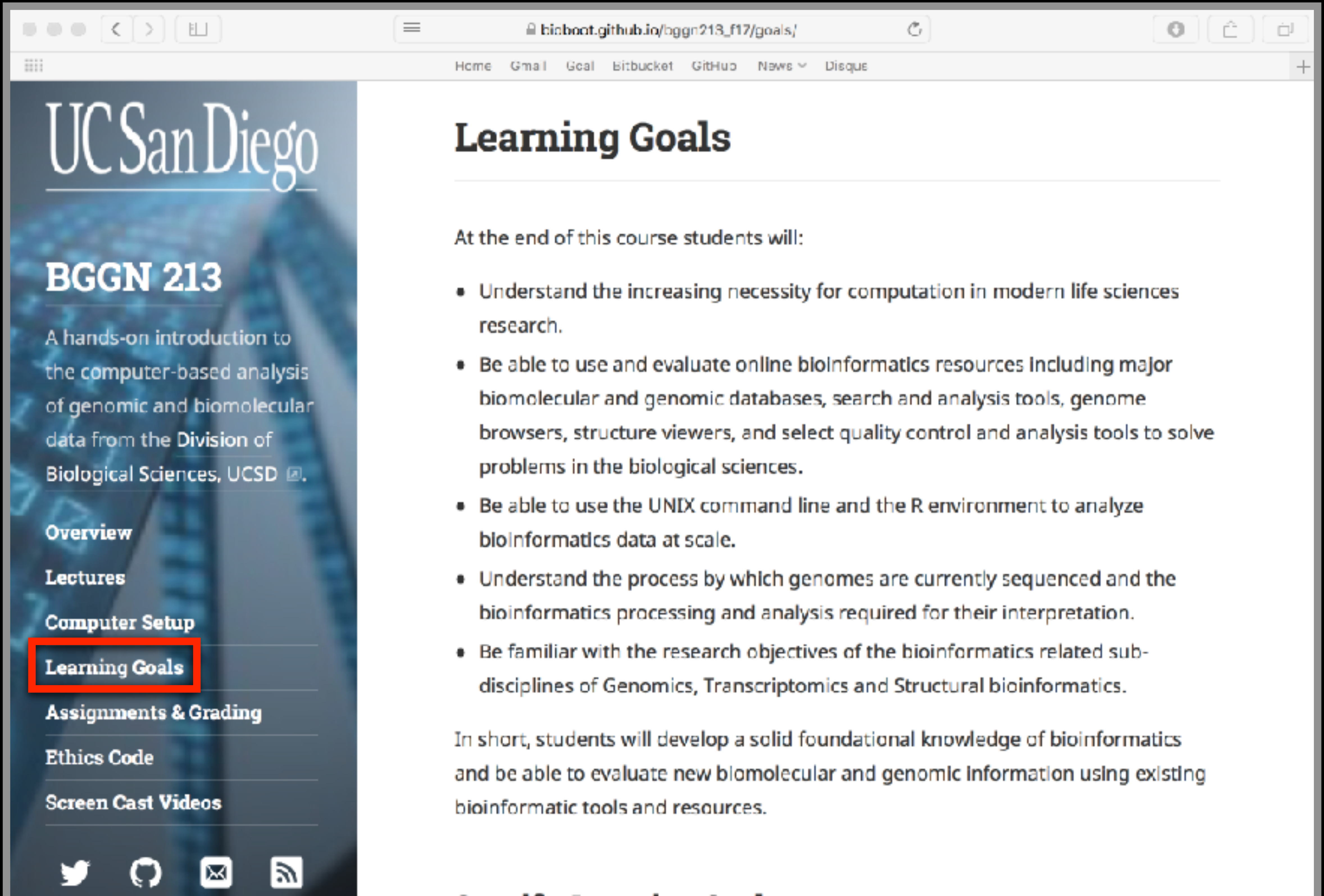
Spring 2018 (PDF)

Overview

Bioinformatics - the application of computational and analytical methods to biological problems - is a rapidly maturing field that is driving the collection, analysis, and interpretation of the avalanche of data in modern life sciences and medical research.

This course is designed for bioscience graduate students and provides a hands-on introduction to the computer-based analysis of genomic and biomolecular data.

What essential concepts and skills should YOU attain from this course?



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- **Overview**
- **Lectures**
- **Computer Setup**
- **Learning Goals**
- **Assignments & Grading**
- **Ethics Code**
- **Screen Cast Videos**

Learning Goals

At the end of this course students will:

- Understand the increasing necessity for computation in modern life sciences research.
- Be able to use and evaluate online bioinformatics resources including major biomolecular and genomic databases, search and analysis tools, genome browsers, structure viewers, and select quality control and analysis tools to solve problems in the biological sciences.
- Be able to use the UNIX command line and the R environment to analyze bioinformatics data at scale.
- Understand the process by which genomes are currently sequenced and the bioinformatics processing and analysis required for their interpretation.
- Be familiar with the research objectives of the bioinformatics related sub-disciplines of Genomics, Transcriptomics and Structural bioinformatics.

In short, students will develop a solid foundational knowledge of bioinformatics and be able to evaluate new biomolecular and genomic information using existing bioinformatic tools and resources.

At the end of this course students will:

- Understand the increasing necessity for computation in modern life sciences research.

- Be able to use and evaluate online bioinformatics resources and analysis tools to solve problems in the biological sciences.

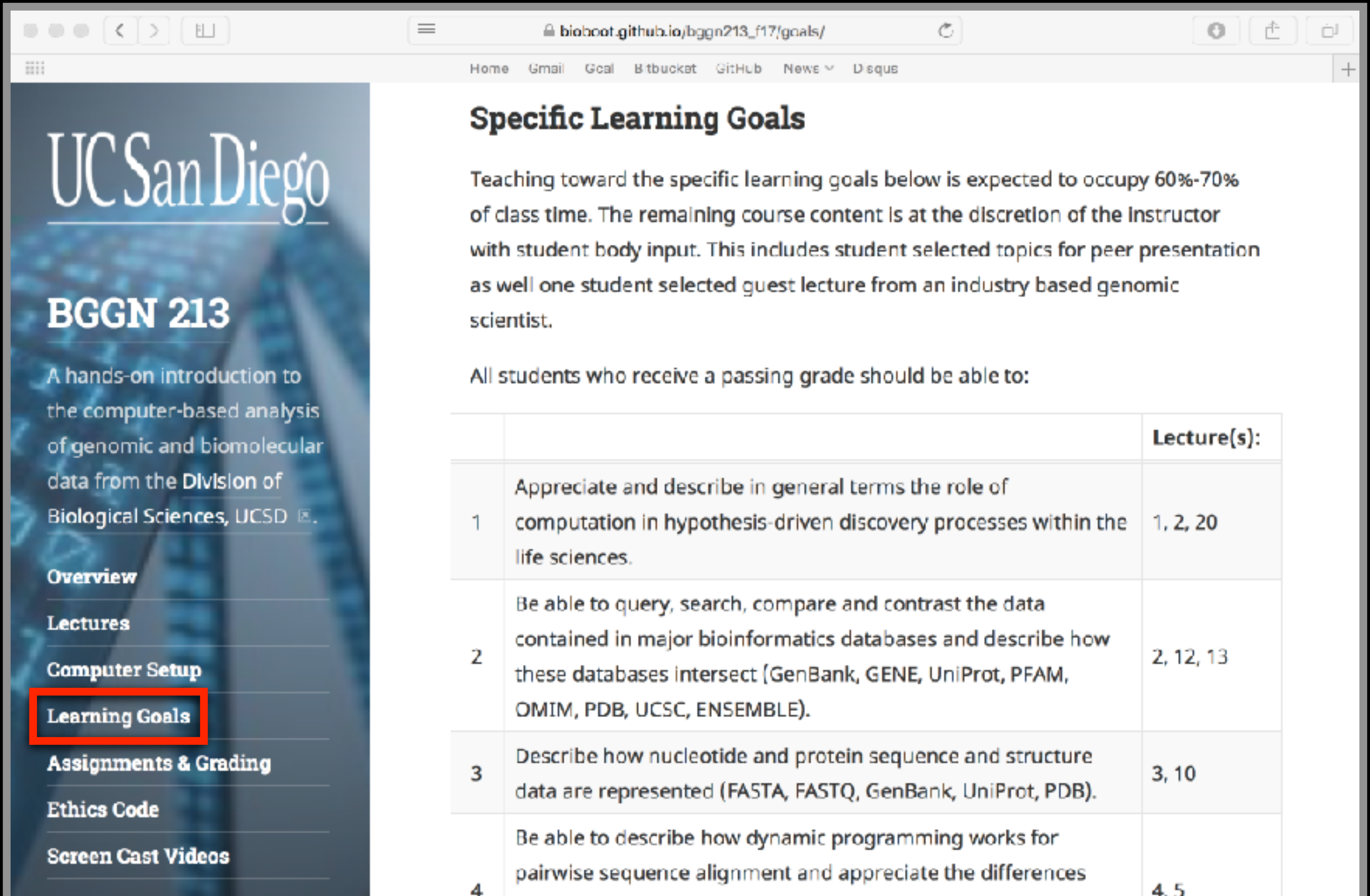
- Be able to use the R environment to analyze bioinformatics data at scale.

- Be familiar with the research objectives of the bioinformatics related sub-disciplines of Genome informatics, Transcriptomics and Structural informatics.

In short, you will develop a solid foundational knowledge of **bioinformatics** and be able to evaluate new biomolecular and genomic information using **existing bioinformatic tools and resources**.

Specific Learning Goals….

What I want you to know by course end!



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- **Learning Goals**
- Assignments & Grading
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Specific Learning Goals

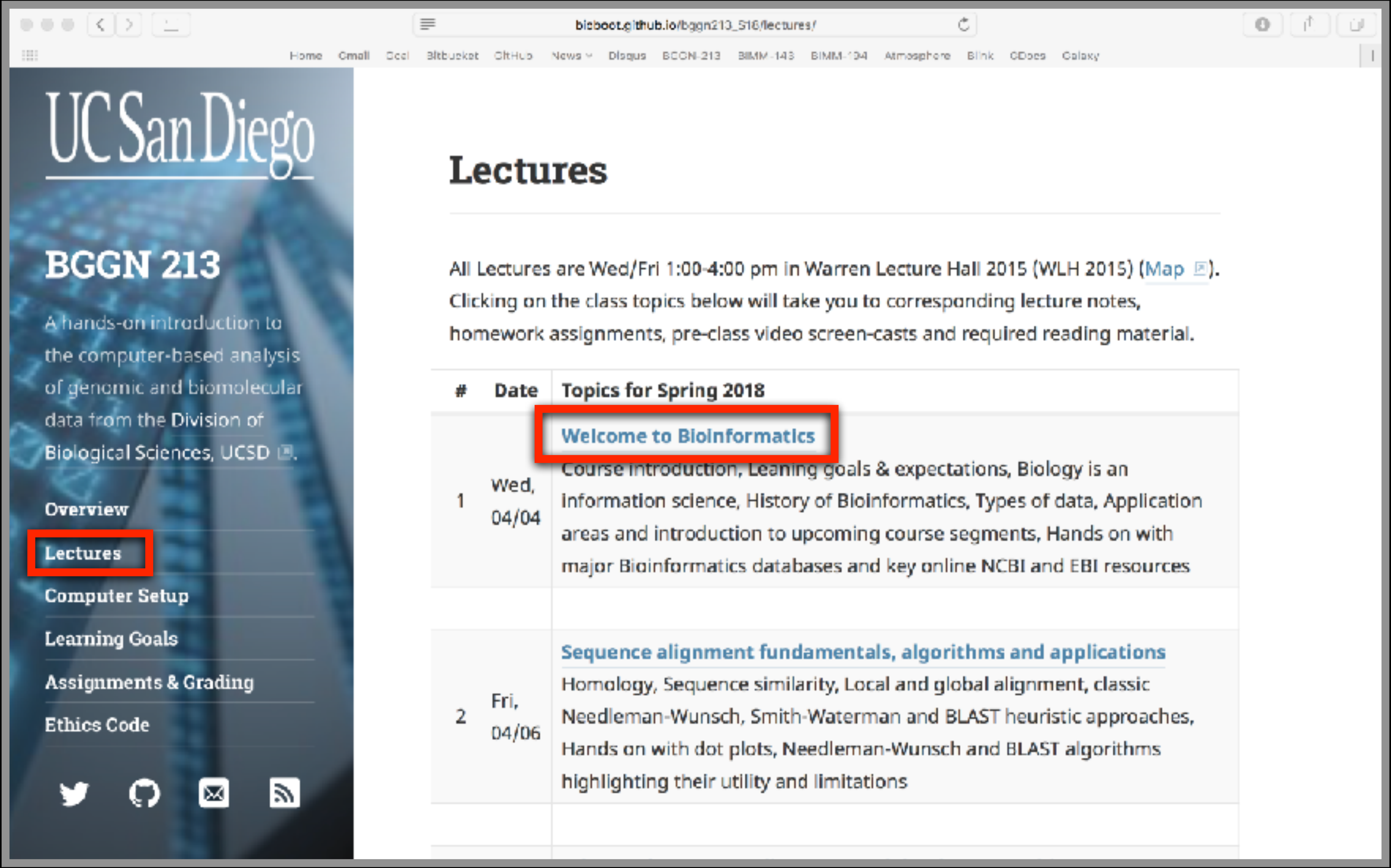
Teaching toward the specific learning goals below is expected to occupy 60%-70% of class time. The remaining course content is at the discretion of the instructor with student body input. This includes student selected topics for peer presentation as well one student selected guest lecture from an industry based genomic scientist.

All students who receive a passing grade should be able to:

		Lecture(s):
1	Appreciate and describe in general terms the role of computation in hypothesis-driven discovery processes within the life sciences.	1, 2, 20
2	Be able to query, search, compare and contrast the data contained in major bioinformatics databases and describe how these databases intersect (GenBank, GENE, UniProt, PFAM, OMIM, PDB, UCSC, ENSEMBLE).	2, 12, 13
3	Describe how nucleotide and protein sequence and structure data are represented (FASTA, FASTQ, GenBank, UniProt, PDB).	3, 10
4	Be able to describe how dynamic programming works for pairwise sequence alignment and appreciate the differences	4, 5

Course Structure

Derived from specific learning goals



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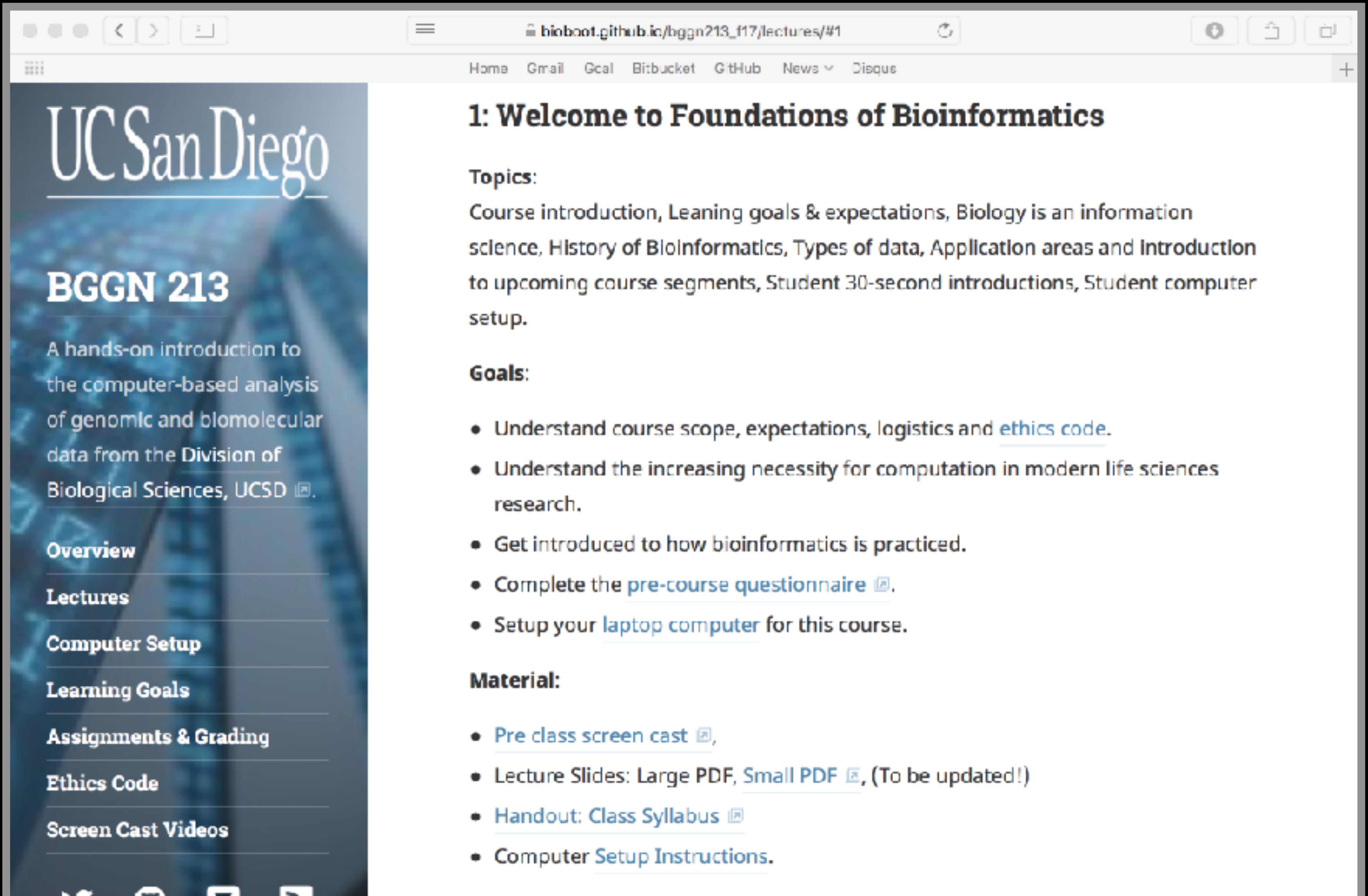
Lectures

All Lectures are Wed/Fri 1:00-4:00 pm in Warren Lecture Hall 2015 (WLH 2015) (Map). Clicking on the class topics below will take you to corresponding lecture notes, homework assignments, pre-class video screen-casts and required reading material.

#	Date	Topics for Spring 2018
1	Wed, 04/04	**Welcome to Bioinformatics** Course introduction, Leaning goals & expectations, Biology is an information science, History of Bioinformatics, Types of data, Application areas and introduction to upcoming course segments, Hands on with major Bioinformatics databases and key online NCBI and EBI resources
2	Fri, 04/06	**Sequence alignment fundamentals, algorithms and applications** Homology, Sequence similarity, Local and global alignment, classic Needleman-Wunsch, Smith-Waterman and BLAST heuristic approaches, Hands on with dot plots, Needleman-Wunsch and BLAST algorithms highlighting their utility and limitations

Class Details

Goals, Class material, Screencasts & **Homework**



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1: Welcome to Foundations of Bioinformatics

Topics:
Course introduction, Leaning goals & expectations, Biology is an information science, History of Bioinformatics, Types of data, Application areas and introduction to upcoming course segments, Student 30-second introductions, Student computer setup.

Goals:

- Understand course scope, expectations, logistics and ethics code.
- Understand the increasing necessity for computation in modern life sciences research.
- Get introduced to how bioinformatics is practiced.
- Complete the pre-course questionnaire.
- Setup your laptop computer for this course.

Material:

- Pre class screen cast,
- Lecture Slides: Large PDF, Small PDF, (To be updated!)
- Handout: Class Syllabus
- Computer Setup Instructions.

Homework

Goals, Class material, Screencasts & **Homework**

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Homework:

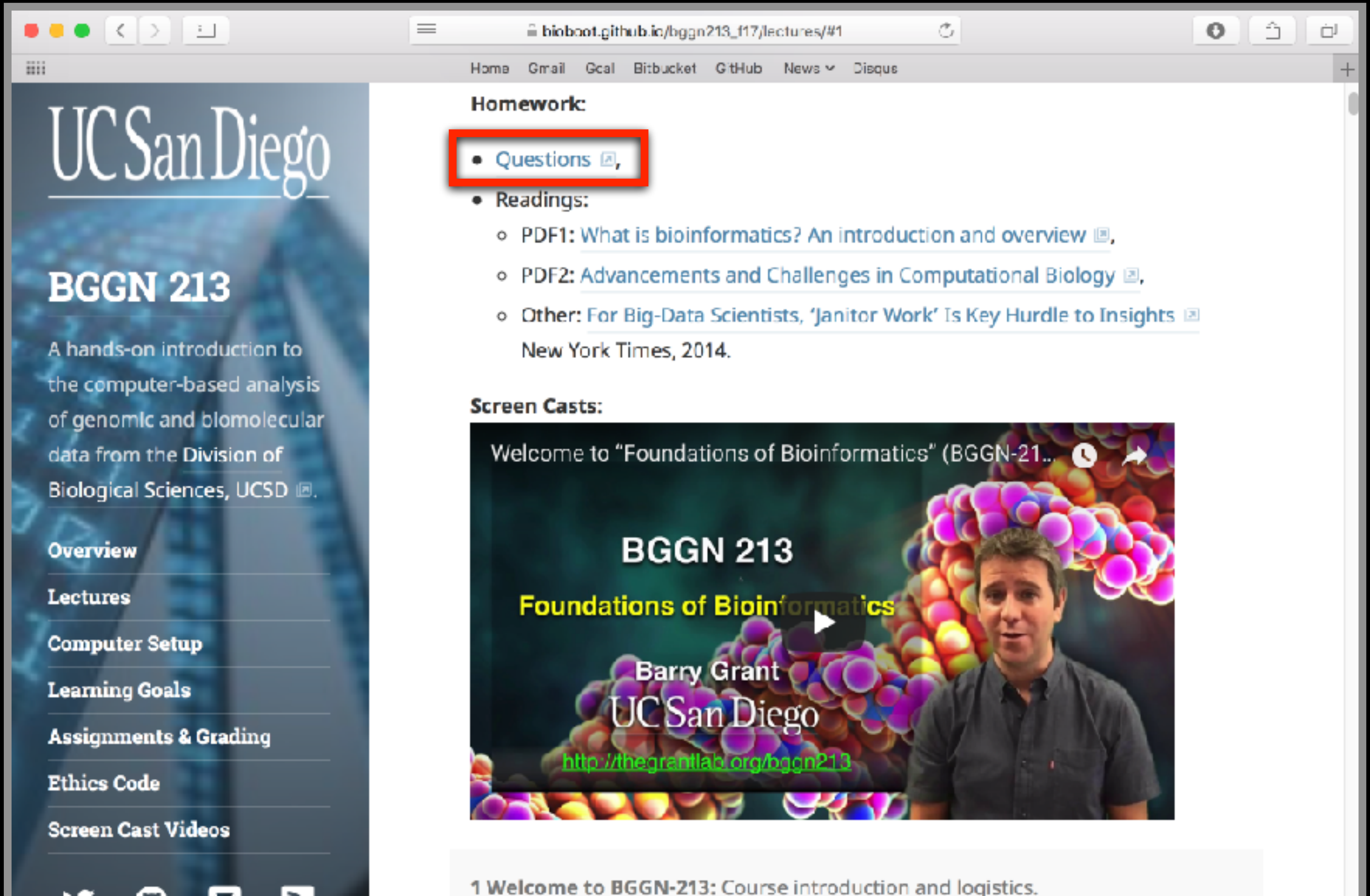
- Questions,
- Readings:
  - PDF1: What is bioinformatics? An introduction and overview,
  - PDF2: Advancements and Challenges in Computational Biology,
  - Other: For Big-Data Scientists, 'Janitor Work' Is Key Hurdle to Insights New York Times, 2014.

Screen Casts:

1 Welcome to BGGN-213: Course introduction and logistics.

Homework

Goals, Class material, Screencasts & **Homework**



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Homework:

- Questions,
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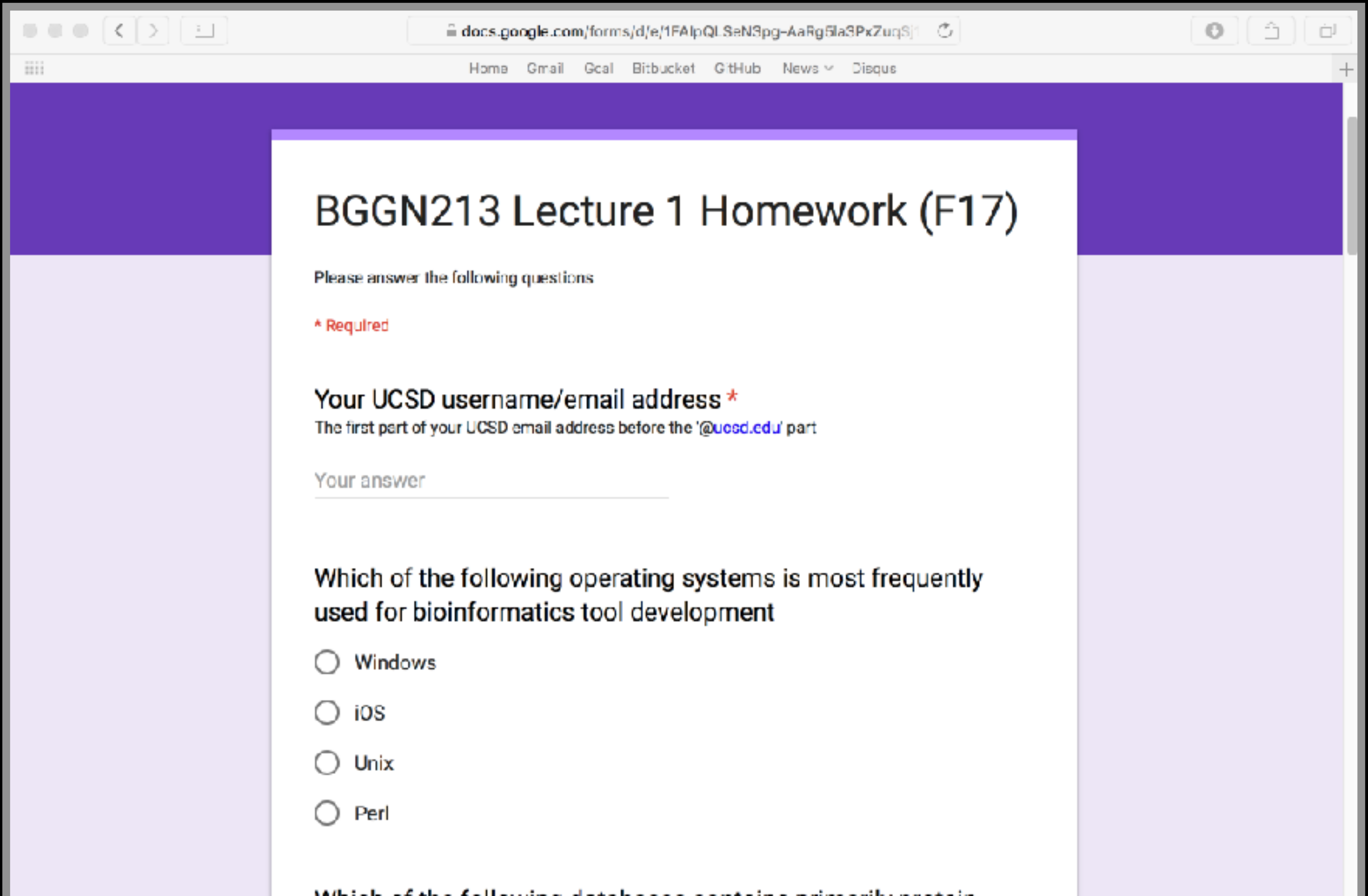
  - Other: For Big-Data Scientists, 'Janitor Work' Is Key Hurdle to Insights New York Times, 2014.

Screen Casts:

1 Welcome to BGGN-213: Course introduction and logistics.

Homework

Goals, Class material, Screencasts & **Homework**



BGGN213 Lecture 1 Homework (F17)

Please answer the following questions

* Required

Your UCSD username/email address *

The first part of your UCSD email address before the '@ucsd.edu' part

Your answer

Which of the following operating systems is most frequently used for bioinformatics tool development

○ Windows

○ iOS

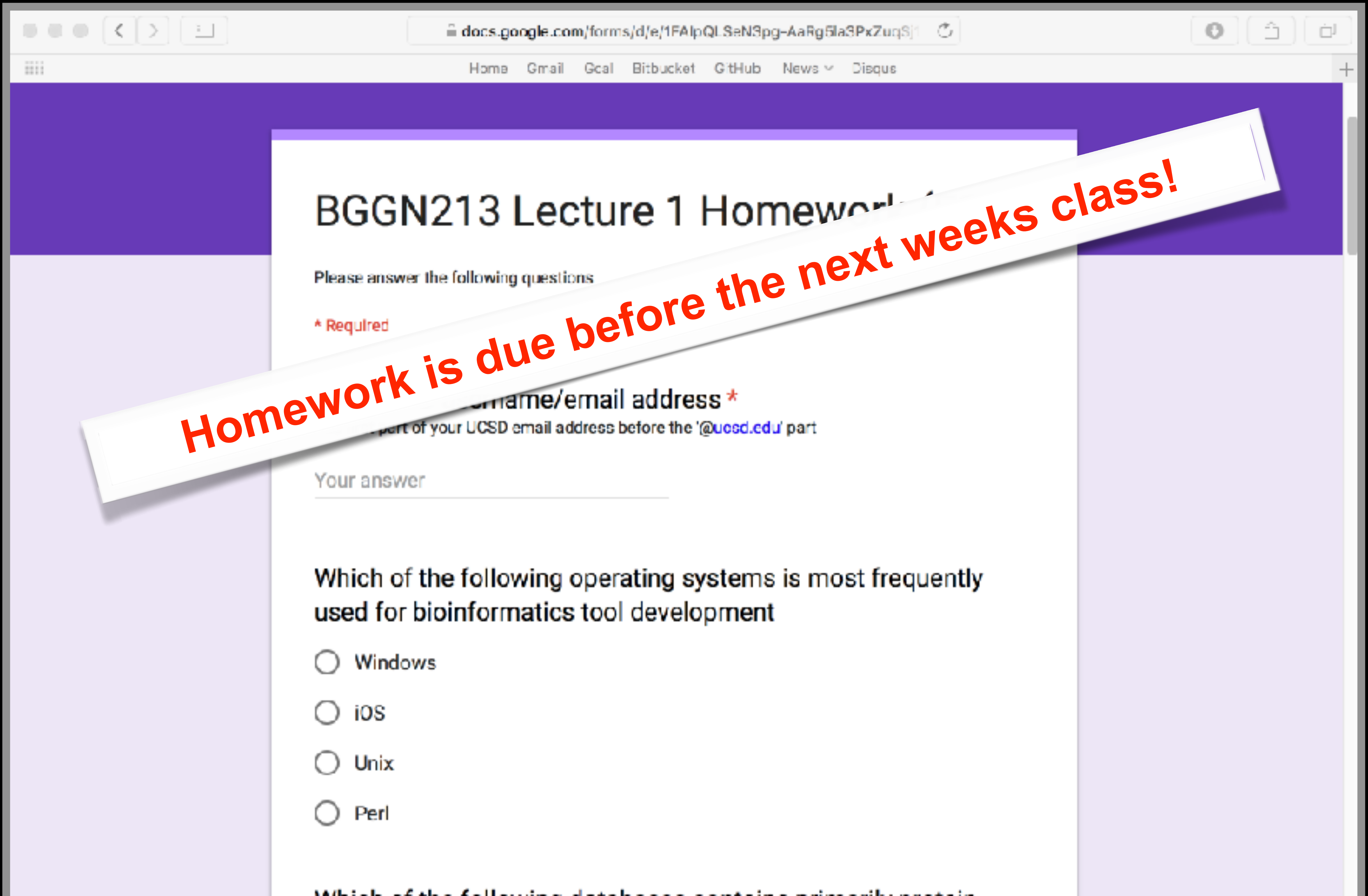
○ Unix

○ Perl

Which of the following databases contains primarily protein

Homework

Goals, Class material, Screencasts & **Homework**



Homework is due before the next weeks class!

BGGN213 Lecture 1 Homewor

Please answer the following questions

* Required

rname/email address *

part of your UCSD email address before the '@ucsd.edu' part

Your answer

Which of the following operating systems is most frequently used for bioinformatics tool development

○ Windows

○ iOS

○ Unix

○ Perl

Which of the following databases contains primarily protein

Side Note: **Why stick with this course?**

Provides a hands-on practical introduction to major bioinformatics concepts and resources.

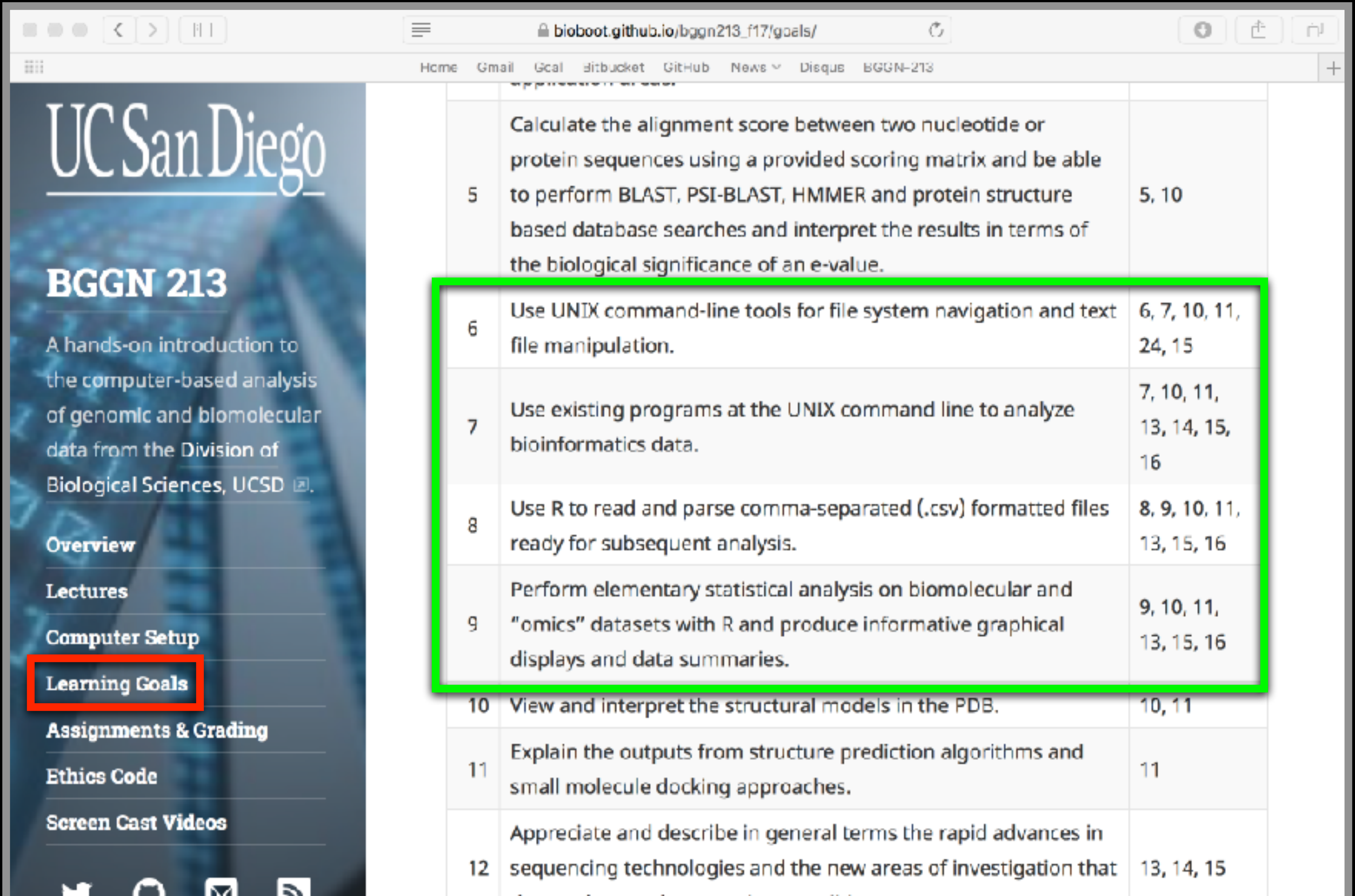
Covers modern hot topics and the intimate coupling of informatics with biology - highlighting the impact of computing advances and ‘big data’ on biology!

Designed for graduates in the biosciences with no programing experience or high level math skills.

Provides a hook for increasing computational and data science competencies in the biosciences - valuable high demand translational skills!

BGGN-213 Learning Goals….

Advanced UNIX and R based learning goals



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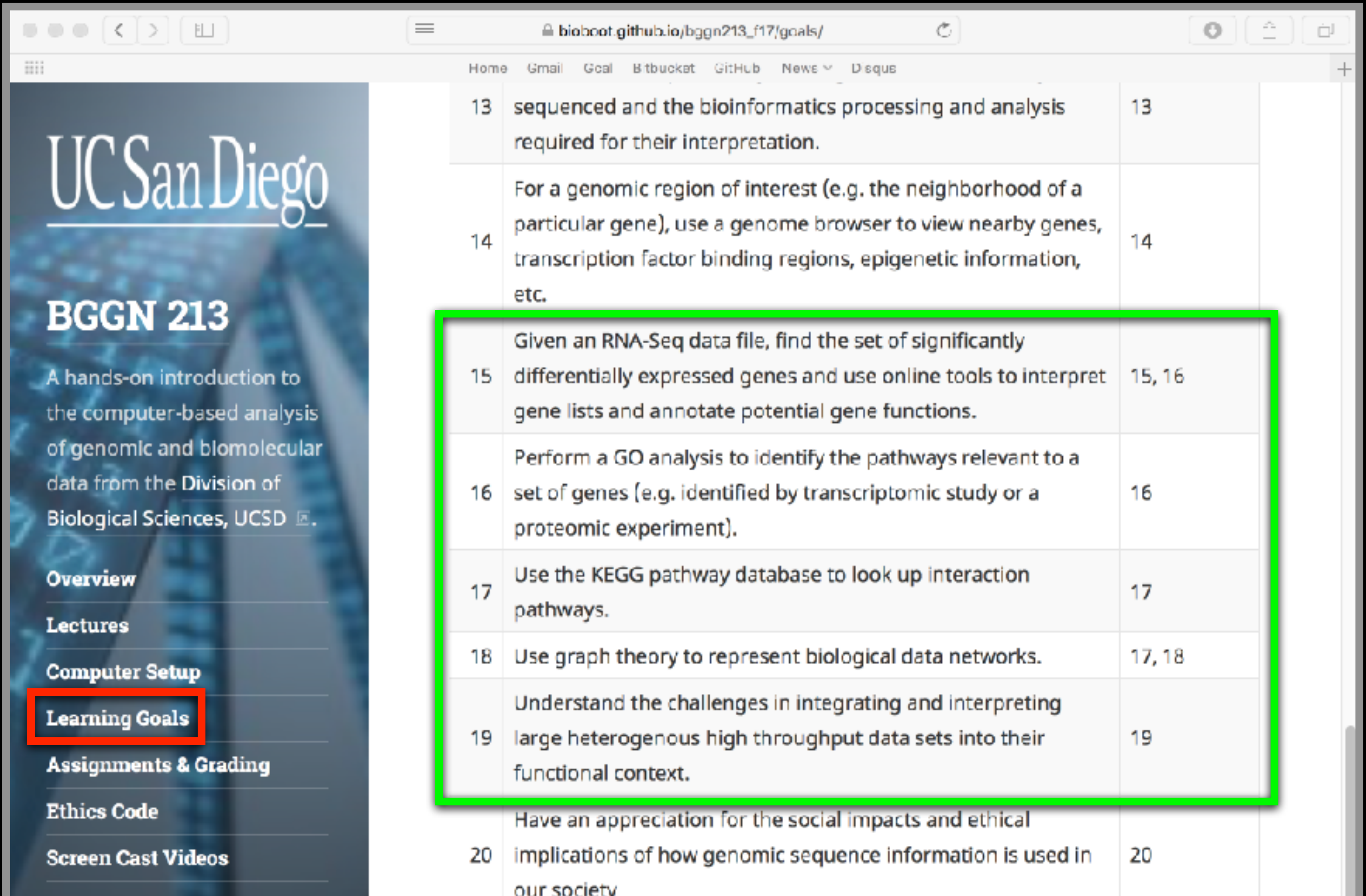
5	Calculate the alignment score between two nucleotide or protein sequences using a provided scoring matrix and be able to perform BLAST, PSI-BLAST, HMMER and protein structure based database searches and interpret the results in terms of the biological significance of an e-value.	5, 10
6	Use UNIX command-line tools for file system navigation and text file manipulation.	6, 7, 10, 11, 24, 15
7	Use existing programs at the UNIX command line to analyze bioinformatics data.	7, 10, 11, 13, 14, 15, 16
8	Use R to read and parse comma-separated (.csv) formatted files ready for subsequent analysis.	8, 9, 10, 11, 13, 15, 16
9	Perform elementary statistical analysis on biomolecular and "omics" datasets with R and produce informative graphical displays and data summaries.	9, 10, 11, 13, 15, 16
10	View and interpret the structural models in the PDB.	10, 11
11	Explain the outputs from structure prediction algorithms and small molecule docking approaches.	11
12	Appreciate and describe in general terms the rapid advances in sequencing technologies and the new areas of investigation that	13, 14, 15

BGGN-213 Learning Goals….

Delve deeper into “real-world” bioinformatics



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13	sequenced and the bioinformatics processing and analysis required for their interpretation.	13
14	For a genomic region of interest (e.g. the neighborhood of a particular gene), use a genome browser to view nearby genes, transcription factor binding regions, epigenetic information, etc.	14
15	Given an RNA-Seq data file, find the set of significantly differentially expressed genes and use online tools to interpret gene lists and annotate potential gene functions.	15, 16
16	Perform a GO analysis to identify the pathways relevant to a set of genes (e.g. identified by transcriptomic study or a proteomic experiment).	16
17	Use the KEGG pathway database to look up interaction pathways.	17
18	Use graph theory to represent biological data networks.	17, 18
19	Understand the challenges in integrating and interpreting large heterogenous high throughput data sets into their functional context.	19
20	Have an appreciation for the social impacts and ethical implications of how genomic sequence information is used in our society	20

These support a major learning objective

At the end of this course students will:

- Understand the increasing necessity for computation in modern life sciences research.
- Be able to use and evaluate online bioinformatics resources and analysis tools to solve problems in the biological sciences.
- Be able to use the R environment to analyze bioinformatics data at scale.
- Be familiar with the research objectives of the bioinformatics related sub-disciplines of Genome informatics, Transcriptomics and Structural informatics.

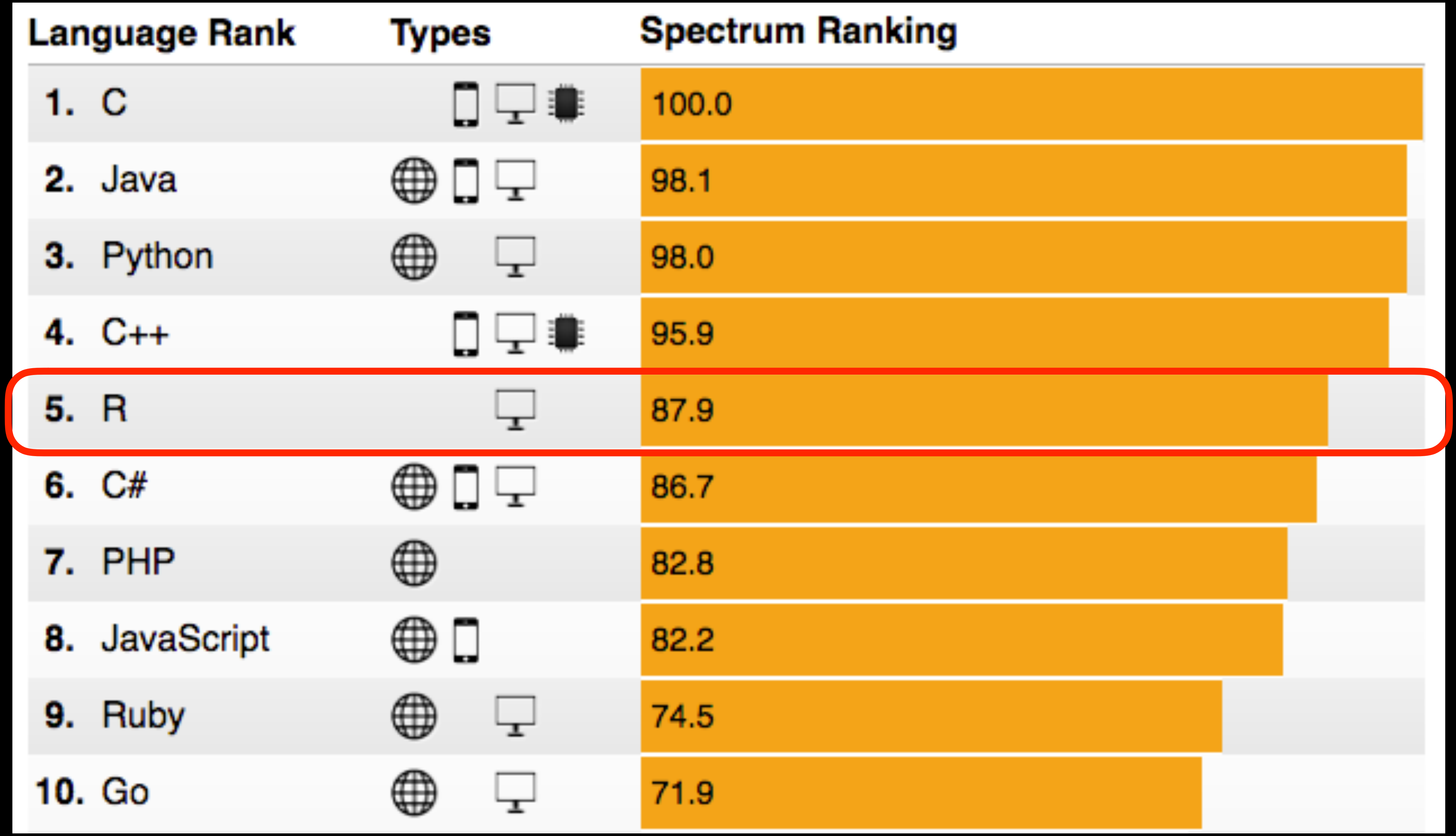
Why use R?

Productivity

Flexibility

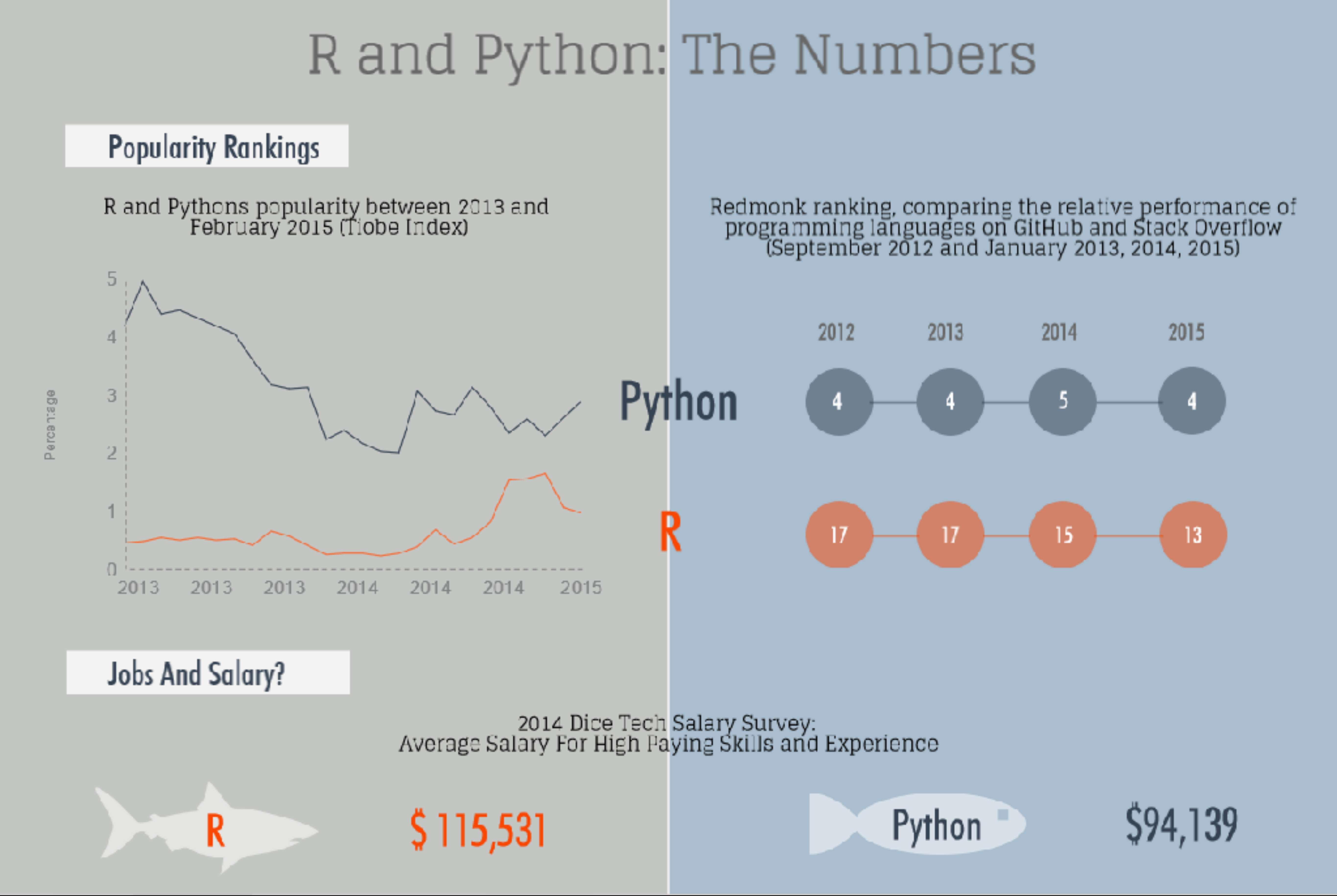
Designed for data analysis

IEEE 2016 Top Programming Languages



Language Rank	Types	Spectrum Ranking
1. C	📱 🖥 ▦	100.0
2. Java	🌐 📱 🖥	98.1
3. Python	🌐 🖥	98.0
4. C++	📱 🖥 ▦	95.9
5. R	🖥	87.9
6. C#	🌐 📱 🖥	86.7
7. PHP	🌐	82.8
8. JavaScript	🌐 📱	82.2
9. Ruby	🌐 🖥	74.5
10. Go	🌐 🖥	71.9

http://spectrum.ieee.org/computing/software/the-2016-top-programming-languages



R and Python: The Numbers

Popularity Rankings

R and Pythons popularity between 2013 and February 2015 (Tiobe Index)

Redmonk ranking, comparing the relative performance of programming languages on GitHub and Stack Overflow (September 2012 and January 2013, 2014, 2015)

	2012	2013	2014	2015
Python	4	4	5	4
R	17	17	15	13

Jobs And Salary?

2014 Dice Tech Salary Survey:
Average Salary For High Paying Skills and Experience

R	$ 115,531
Python	$94,139

http://www.kdnuggets.com/2015/05/r-vs-python-data-science.html?utm_medium=email&utm_source=flipboard

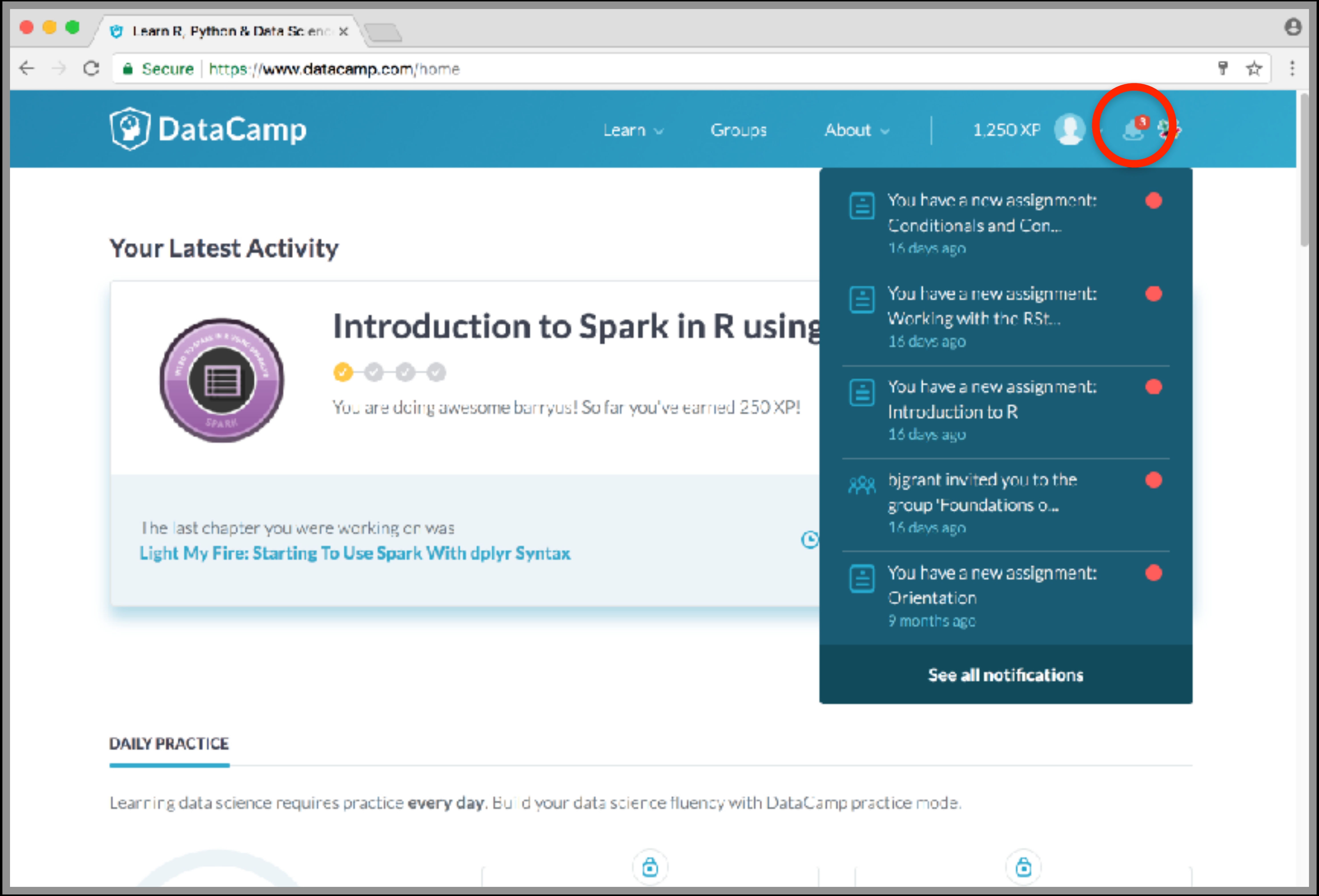
- R is the “lingua franca” of data science in industry and academia.

- Large user and developer community.
    - As of Jan 8th 2018 there are 12,039 add on **R packages** on **CRAN** and 1,473 on **Bioconductor** - more on these later!

- Virtually every statistical technique is either already built into R, or available as a free package.

- Unparalleled exploratory data analysis environment.

< https://www.datacamp.com/ >



Your Latest Activity

Introduction to Spark in R using

You are doing awesome barryus! So far you've earned 250 XP!

The last chapter you were working on was
Light My Fire: Starting To Use Spark With dplyr Syntax

You have a new assignment: Conditionals and Con...
16 days ago

You have a new assignment: Working with the RSt...
16 days ago

You have a new assignment: Introduction to R
16 days ago

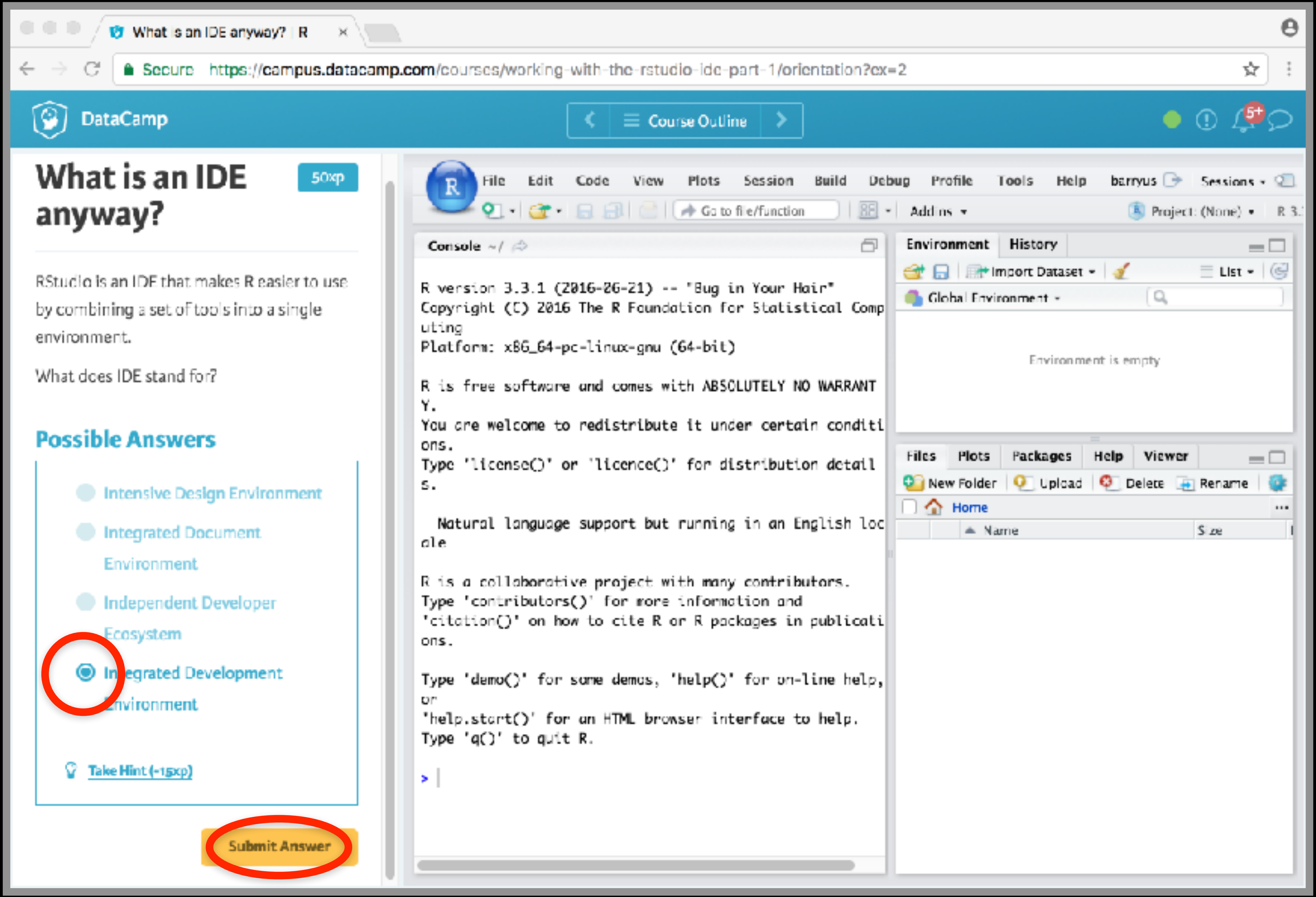
bjgrant invited you to the group 'Foundations o...
16 days ago

You have a new assignment: Orientation
9 months ago

DAILY PRACTICE

Learning data science requires practice **every day**. Build your data science fluency with DataCamp practice mode.

< https://www.datacamp.com/ >



What is an IDE anyway?

50xp

RStudio is an IDE that makes R easier to use by combining a set of tools into a single environment.

What does IDE stand for?

Possible Answers

○ Intensive Design Environment

○ Integrated Document Environment

○ Independent Developer Ecosystem

● Integrated Development Environment

Take Hint (-15xp)

Submit Answer

```
R version 3.3.1 (2016-06-21) -- "Bug in Your Hair"
Copyright (C) 2016 The R Foundation for Statistical Comp
uting
Platform: x86_64-pc-linux-gnu (64-bit)

R is free software and comes with ABSOLUTELY NO WARRANT
Y.
You are welcome to redistribute it under certain conditi
ons.
Type 'license()' or 'licence()' for distribution detail
s.

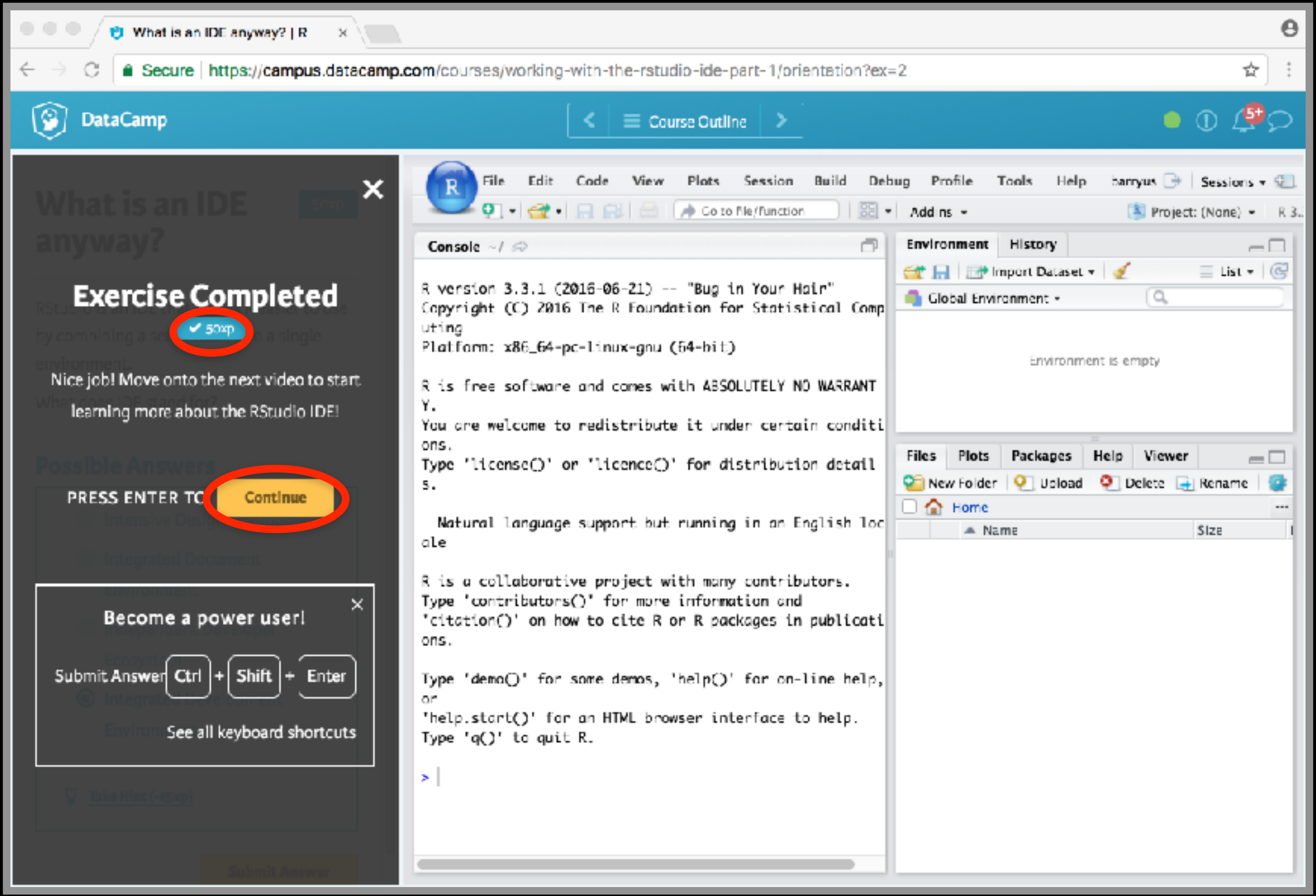
  Natural language support but running in an English loc
ale

R is a collaborative project with many contributors.
Type 'contributors()' for more information and
'citation()' on how to cite R or R packages in publicati
ons.

Type 'demo()' for some demos, 'help()' for on-line help,
or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.

> 
```

< https://www.datacamp.com/ >



Exercise Completed

✓ 50xp

Nice job! Move onto the next video to start learning more about the RStudio IDE!

PRESS ENTER TO Continue

Become a power user!

Submit Answer Ctrl + Shift + Enter

See all keyboard shortcuts

```
R version 3.3.1 (2016-06-21) -- "Bug in Your Hair"
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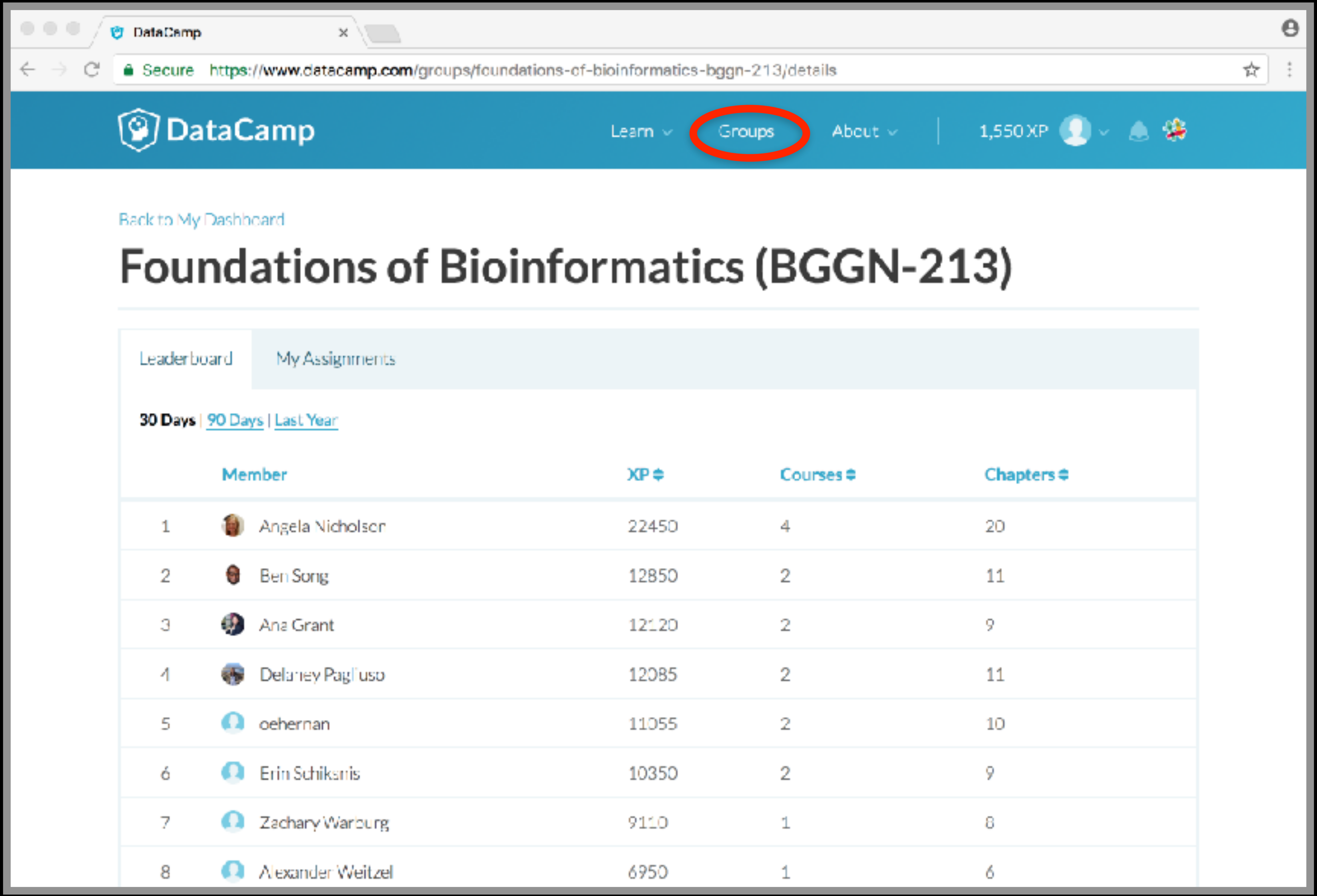


Back to My Dashboard

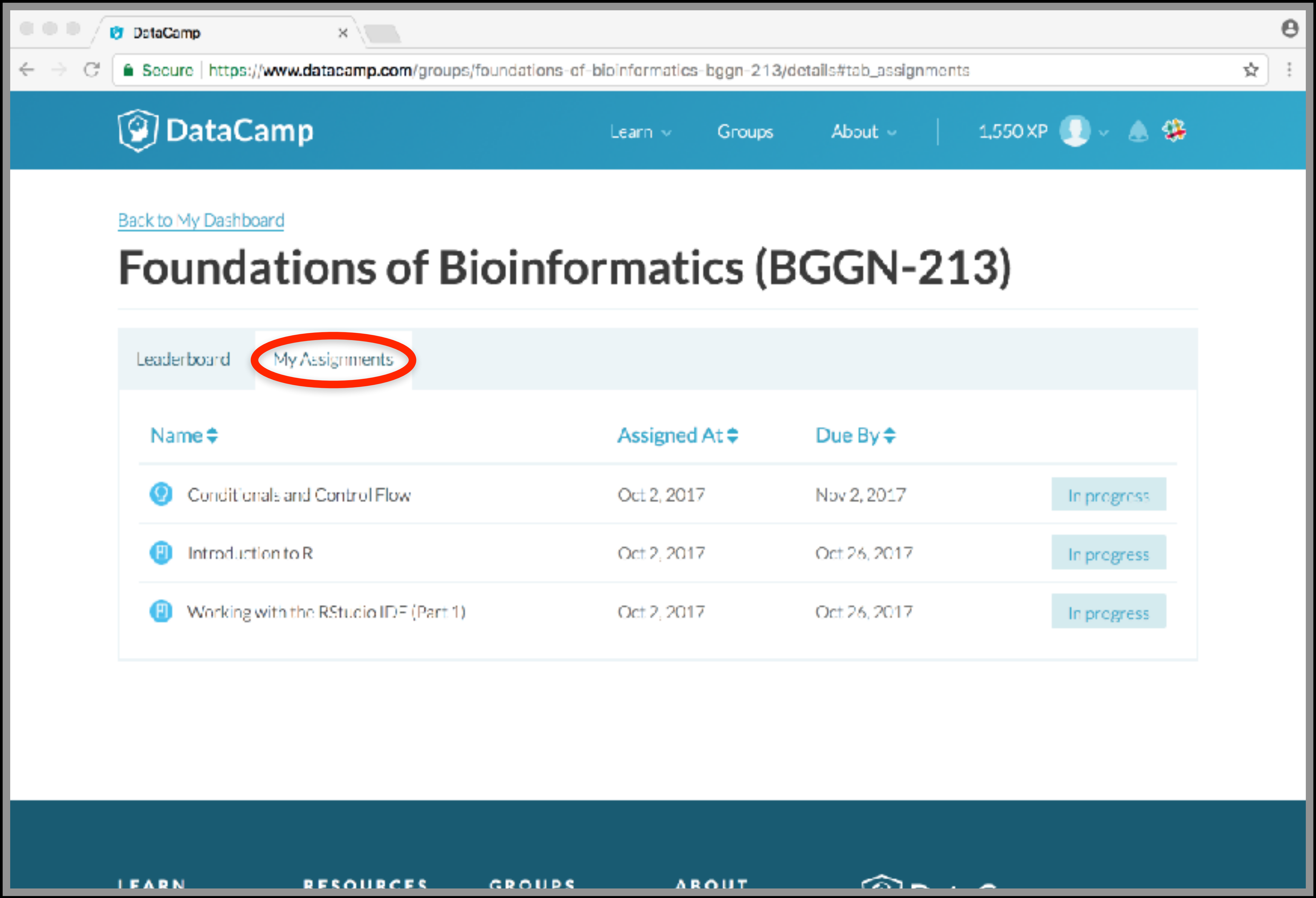
Foundations of Bioinformatics (BGGN-213)

Leaderboard | My Assignments

30 Days | 90 Days | Last Year

	Member	XP	Courses	Chapters
1	Angela Nicholson	22450	4	20
2	Ben Song	12850	2	11
3	Ana Grant	12120	2	9
4	Delaney Pagliuso	12085	2	11
5	oehernan	11055	2	10
6	Erin Schiksnis	10350	2	9
7	Zachary Warburg	9110	1	8
8	Alexander Weitzel	6950	1	6

< https://www.datacamp.com/ >



Back to My Dashboard

Foundations of Bioinformatics (BGGN-213)

Leaderboard | My Assignments

Name	Assigned At	Due By	
Conditionals and Control Flow	Oct 2, 2017	Nov 2, 2017	In progress
Introduction to R	Oct 2, 2017	Oct 26, 2017	In progress
Working with the RStudio IDE (Part 1)	Oct 2, 2017	Oct 26, 2017	In progress

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Learning Objectives	What you need to learn to succeed in this course.
Course Structure	Major lecture topics and specific leaning goals.
Introduction to Bioinformatis	Introducing the *what*, *why* and *how* of bioinformatics?
Computer Setup	Ensuring your laptop is all set for future sections of this course.

OUTLINE

Overview of bioinformatics

- The *what*, *why* and *how* of bioinformatics?
- Major bioinformatics research areas.
- Skepticism and common problems with bioinformatics.

Online databases and associated tools

- Primary, secondary and composite databases.
  - Nucleotide sequence databases (GenBank & RefSeq).
  - Protein sequence database (UniProt).
  - Composite databases (PFAM & OMIM).

Database usage vignette

- How-to productively navigate major databases.

Q. What is Bioinformatics?

"Bioinformatics is the application of computers to the collection, archiving, organization, and analysis of biological data."

… Bioinformatics is a hybrid of biology and computer science

Q. What is Bioinformatics?

“Bioinformatics is the application of computers to the collection, archiving, organization, and analysis of biological data.”

… Bioinformatics is a hybrid of biology and computer science

… **Bioinformatics is computer aided biology!**

Q. What is Bioinformatics?

"Bioinformatics is the application of computers to the collection, archiving, organization, and analysis of biological data."

… Bioinformatics is a hybrid of biology and computer science
… **Bioinformatics is computer aided biology!**

Computer based management and analysis of biological and biomedical data with useful applications in many disciplines, particularly genomics, proteomics, metabolomics, etc...

MORE DEFINITIONS

- “Bioinformatics is conceptualizing biology in terms of **macromolecules** and then applying **"informatics" techniques** (derived from disciplines such as applied maths, computer science, and statistics) to **understand** and **organize** the information associated with these molecules, on a **large-scale**.
  Luscombe NM, *et al.* Methods Inf Med. 2001;40:346.

- “Bioinformatics is research, development, or application of **computational approaches** for expanding the use of **biological**, **medical**, **behavioral** or **health data**, including those to **acquire**, **store**, **organize** and **analyze** such data.”
  National Institutes of Health (NIH) (http://tinyurl.com/l3gxr6b)

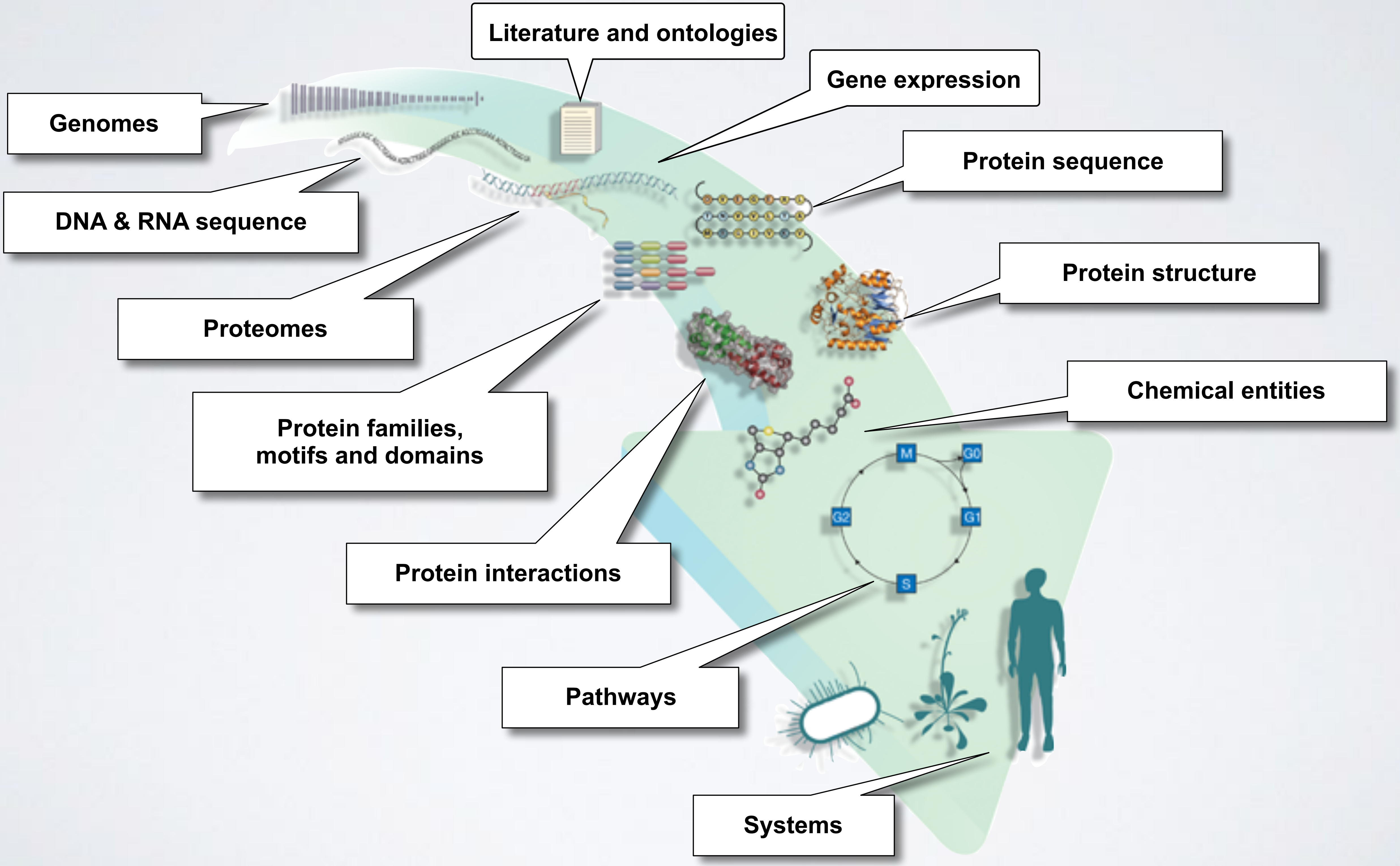
MORE DEFINITIONS

- “Bioinformatics is conceptualizing biology in terms of **macromolecules** and then applying **"informatics"** [illegible]**niques** (derived from disciplines such as applied mat[illegible]puter science, and statistics) to **understand** a[illegible]**ize** the information associated with these [illegible]s, on a **large-scale**.
  Luscombe NM, *et al.* Methods I[illegible]001;40:346.

- “Bioinformati[illegible]earch, development, or application of **compu**[illegible] **approaches** for expanding the use of **bi**[illegible], **medical**, **behavioral** or **health data**, including those to a[illegible]**quire**, **store**, **organize** and **analyze** such data.”
  National Institutes of Health (NIH) (http://tinyurl.com/l3gxr6b)

Key Point: Bioinformatics is Computer Aided Biology

Major types of Bioinformatics Data



Literature and ontologies

Genomes

Gene expression

DNA & RNA sequence

Protein sequence

Proteomes

Protein structure

Chemical entities

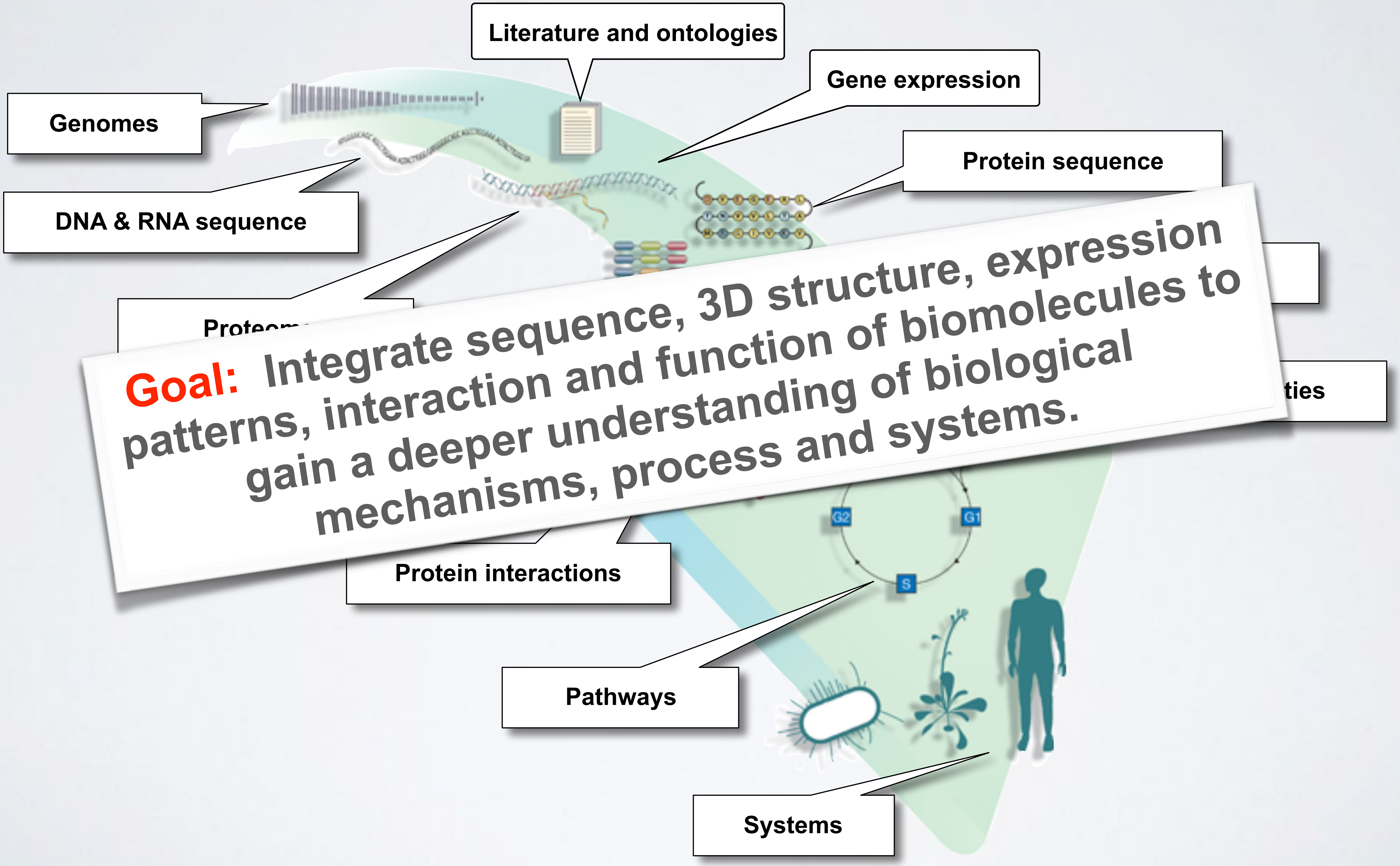
Protein families,
motifs and domains

Protein interactions

Pathways

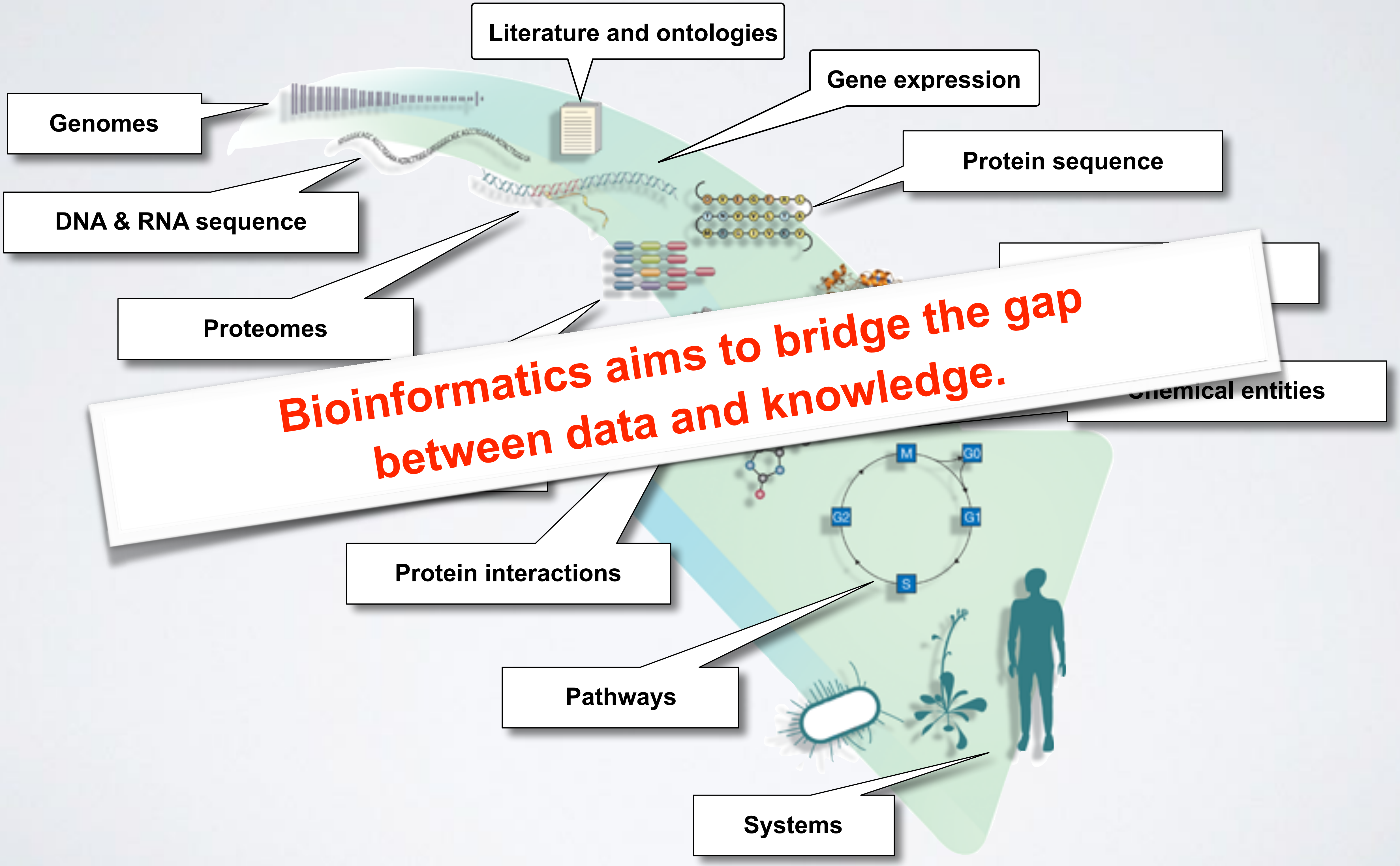
Systems

Major types of Bioinformatics Data



Goal: Integrate sequence, 3D structure, expression patterns, interaction and function of biomolecules to gain a deeper understanding of biological mechanisms, process and systems.

Major types of Bioinformatics Data



Literature and ontologies

Genomes

Gene expression

Protein sequence

DNA & RNA sequence

Proteomes

emical entities

Protein interactions

Pathways

Systems

Bioinformatics aims to bridge the gap between data and knowledge.

BIOINFORMATICS RESEARCH AREAS

Include but are not limited to:

- Organization, classification, dissemination and analysis of biological and biomedical data (particularly ‘-omics' data).
- Biological sequence analysis and phylogenetics.
- Genome organization and evolution.
- Regulation of gene expression and epigenetics.
- Biological pathways and networks in healthy & disease states.
- Protein structure prediction from sequence.
- Modeling and prediction of the biophysical properties of biomolecules for binding prediction and drug design.
- Design of biomolecular structure and function.

With applications to Biology, Medicine, Agriculture and Industry

Where did bioinformatics come from?

Bioinformatics arose as molecular biology began to be transformed by the emergence of molecular sequence and structural data

Recap: The key dogmas of molecular biology

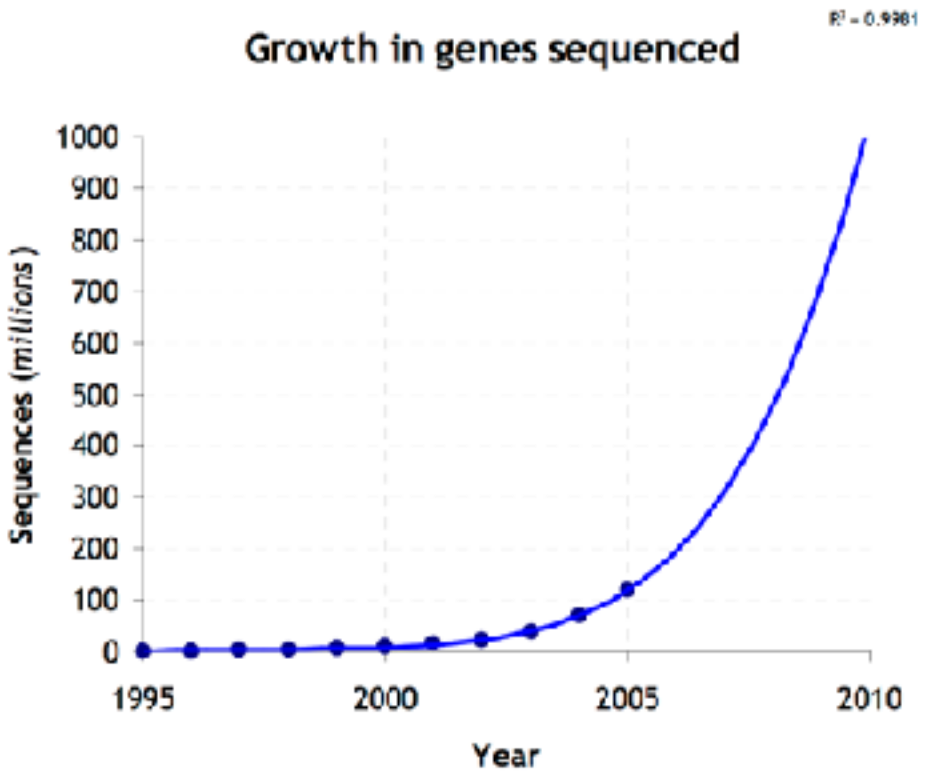
- *DNA sequence* determines *protein sequence.*
- *Protein sequence* determines *protein structure.*
- *Protein structure* determines *protein function.*
- *Regulatory mechanisms* (e.g. gene expression) determine the amount of a particular *function in space and time.*

Bioinformatics is *now* essential for the archiving, organization and analysis of data related to all these processes.

Why do we need Bioinformatics?

Bioinformatics is necessitated by the rapidly expanding quantities and complexity of biomolecular data

- Bioinformatics provides methods for the efficient:
  - **storage**
  - **annotation**
  - **search** and **retrieval**
  - data **integration**
  - data **mining** and **analysis**



E.G. data from sequencing, structural genomics, proteomics, new high throughput assays, *etc…*

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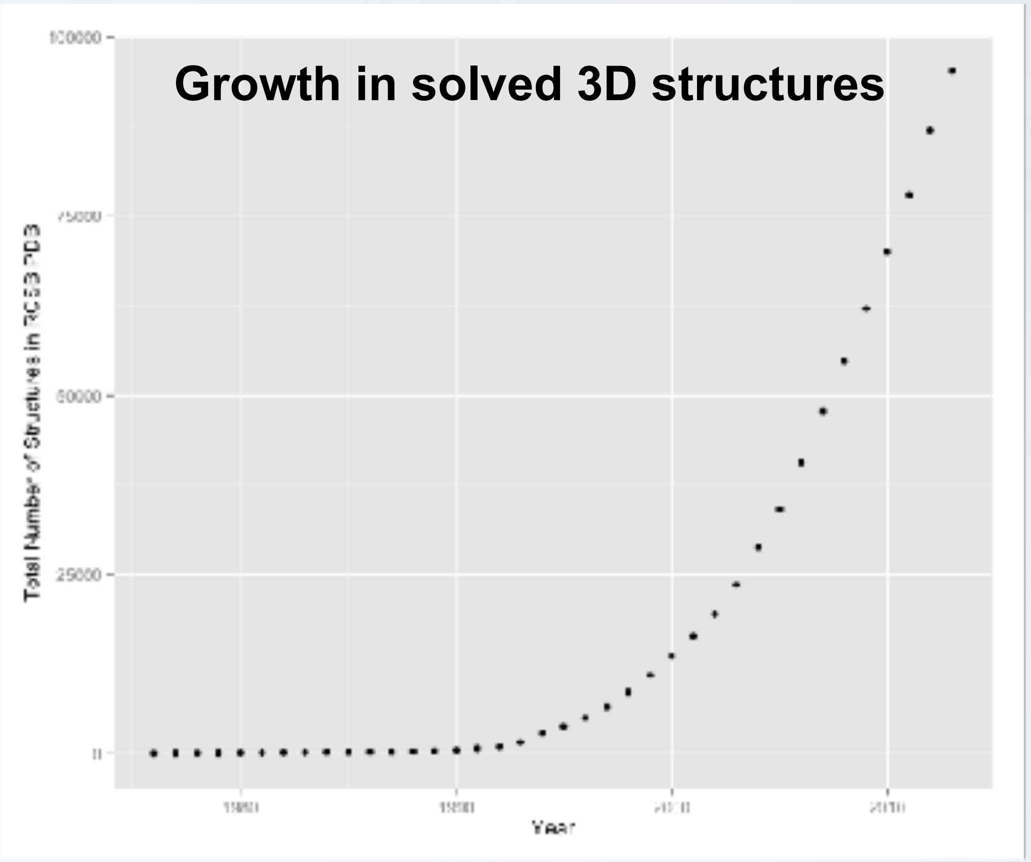

Growth in solved 3D structures

E.G. data from sequencing, structural genomics, proteomics, new high throughput assays, *etc…*

How do we do Bioinformatics?

- A “*bioinformatics approach*” involves the application of **computer algorithms**, **computer models** and **computer databases** with the broad goal of understanding the action of both individual genes, transcripts, proteins and large collections of these entities.

DNA → RNA → Protein

Genome → **Transcriptome** → **Proteome**

x 1,000

x 100,000

How do we *actually* do Bioinformatics?

Pre-packaged tools and databases

- Many online
- Most are free to use
- Time consuming methods require downloading…

Advanced tool application & development

- Mostly on a UNIX environment
- Knowledge of programing languages frequently required (*e.g.* **R**, Python, Perl, C, Java, Fortran)
- May require specialized high performance computing…

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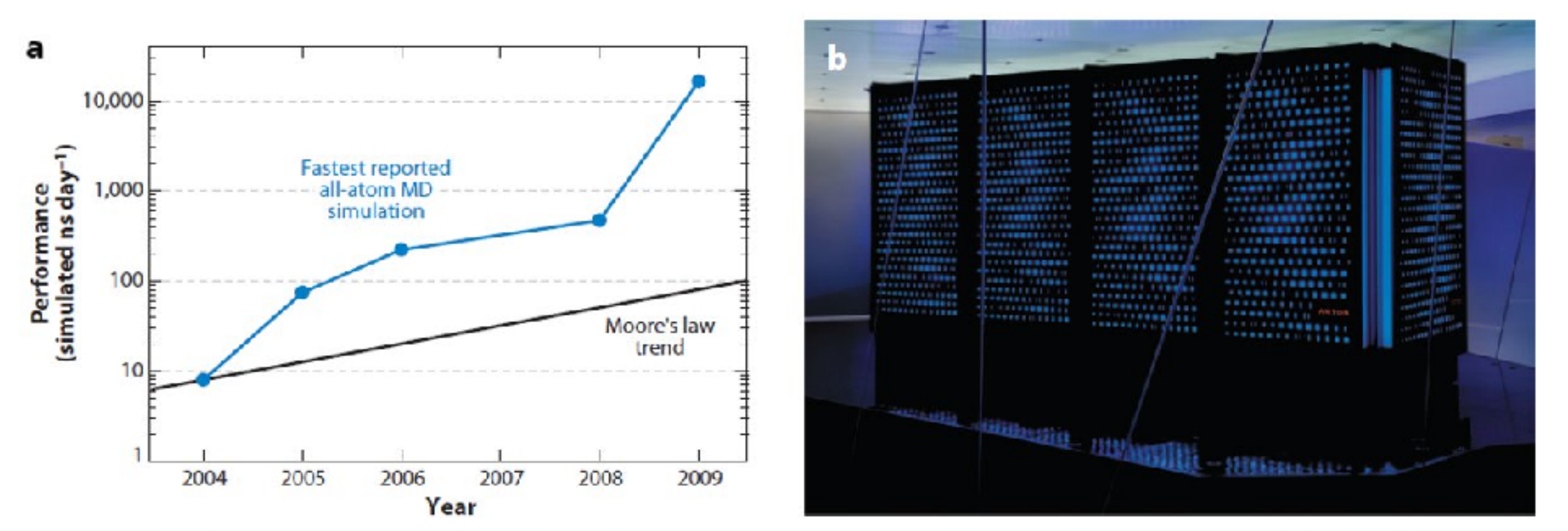
SIDE-NOTE: SUPERCOMPUTERS AND GPUS



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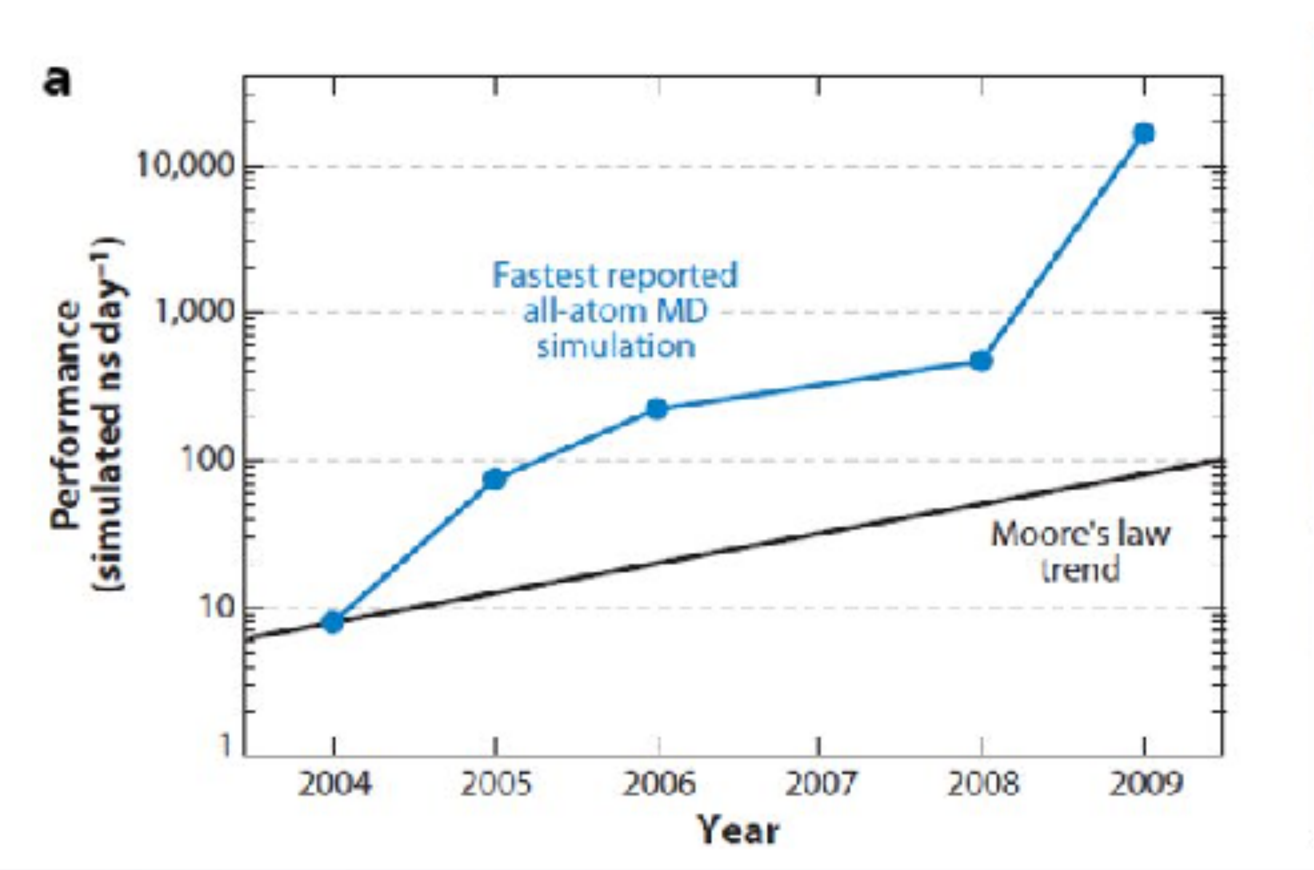
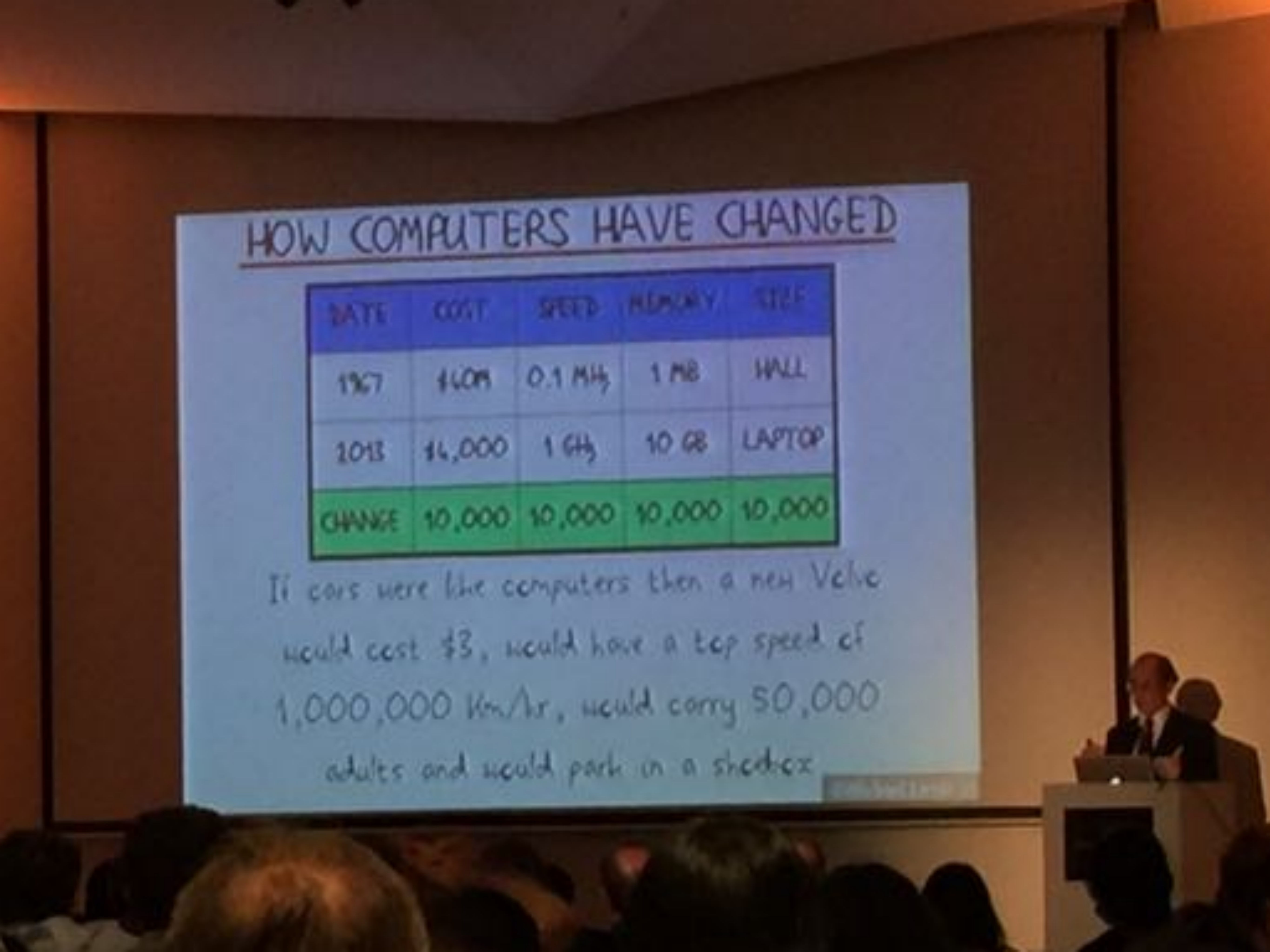


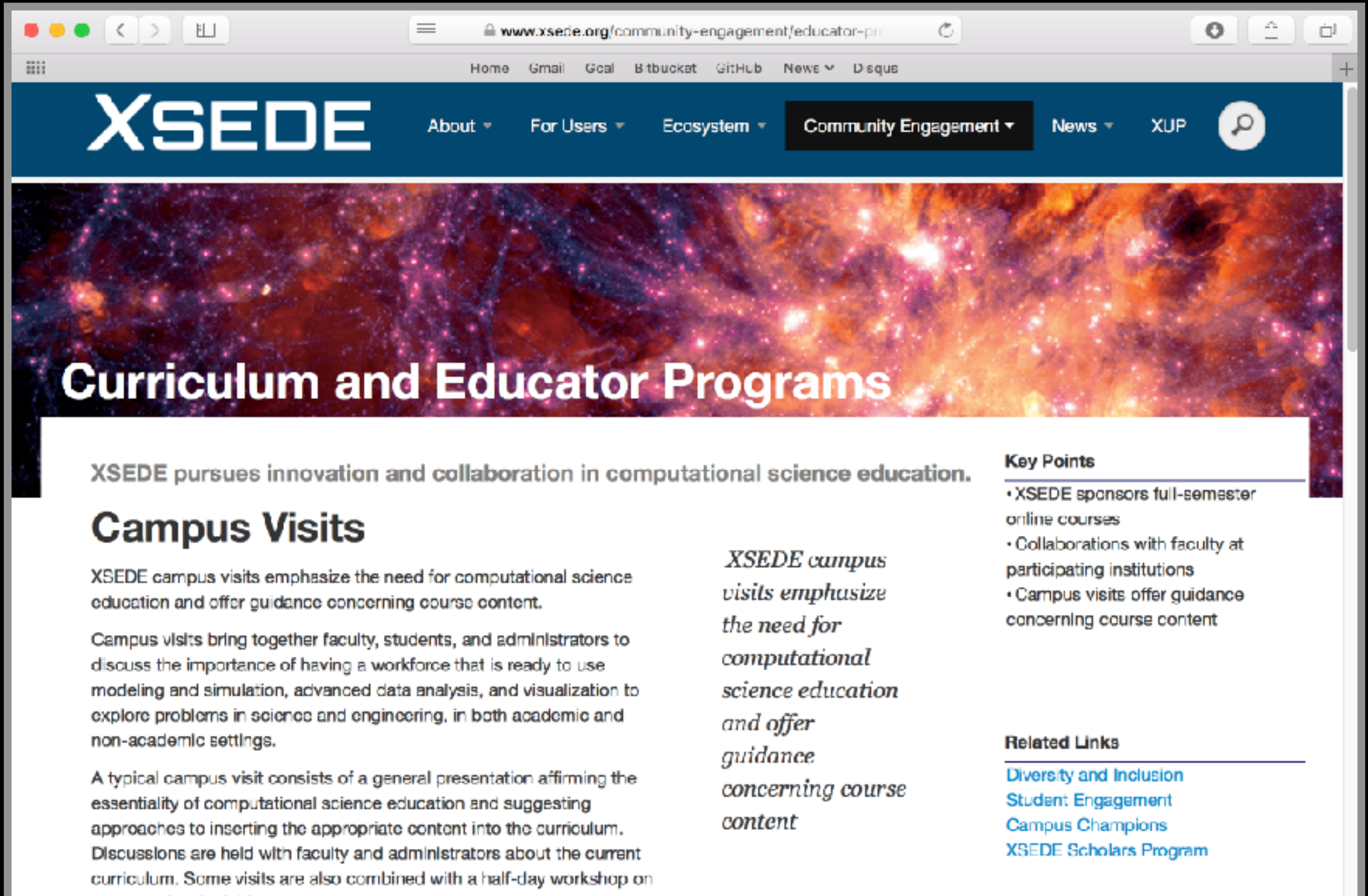


HOW COMPUTERS HAVE CHANGED

DATE	COST	SPEED	MEMORY	SIZE
1967	$60M	0.1 MHz	1 MB	HALL
2013	$6,000	1 GHz	10 GB	LAPTOP
CHANGE	10,000	10,000	10,000	10,000

If cars were like computers then a new Volvo would cost $3, would have a top speed of 1,000,000 Km/hr, would carry 50,000 adults and would park in a shoebox

NSF Extreme Science and Engineering Discovery Environment (XSEDE)



Curriculum and Educator Programs

XSEDE pursues innovation and collaboration in computational science education.

Campus Visits

XSEDE campus visits emphasize the need for computational science education and offer guidance concerning course content.

Campus visits bring together faculty, students, and administrators to discuss the importance of having a workforce that is ready to use modeling and simulation, advanced data analysis, and visualization to explore problems in science and engineering, in both academic and non-academic settings.

A typical campus visit consists of a general presentation affirming the essentiality of computational science education and suggesting approaches to inserting the appropriate content into the curriculum. Discussions are held with faculty and administrators about the current curriculum. Some visits are also combined with a half-day workshop on

XSEDE campus visits emphasize the need for computational science education and offer guidance concerning course content

Key Points

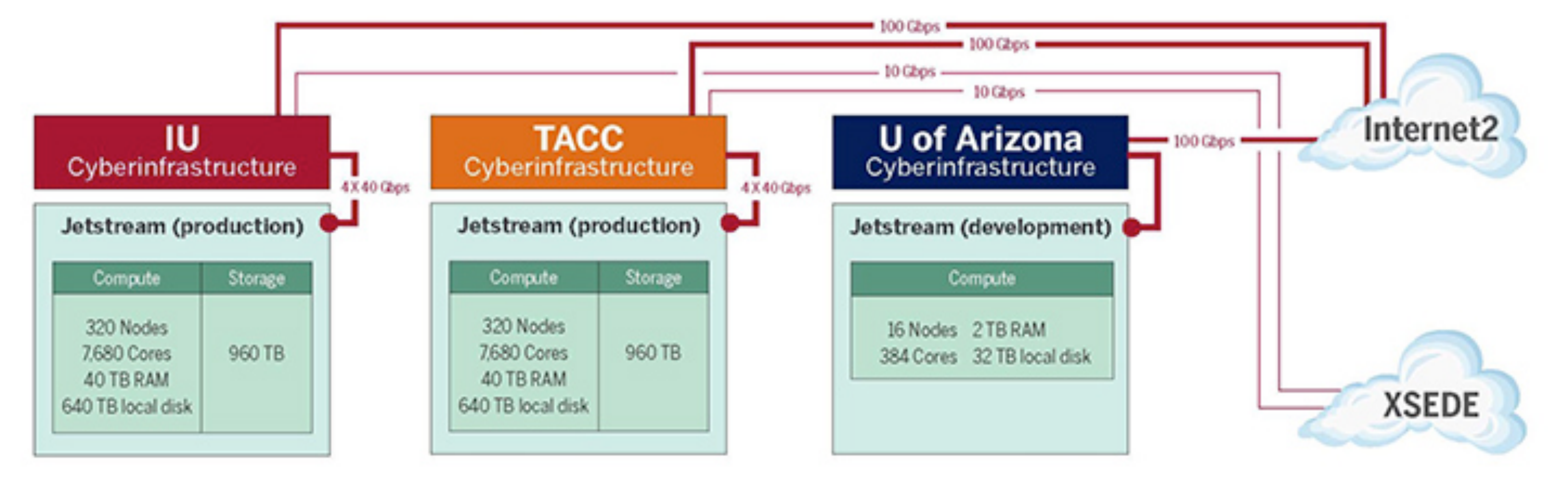
- XSEDE sponsors full-semester online courses
- Collaborations with faculty at participating institutions
- Campus visits offer guidance concerning course content

Related Links

Diversity and Inclusion
Student Engagement
Campus Champions
XSEDE Scholars Program

What is *Jetstream*?

- A new cloud computing environment based at Indiana University and the Texas Advanced Computing Center (TACC) providing on-demand access to interactive computing and data analysis resources.



Jetstream tutorials

Developed *user friendly* labs for Jetstream basics

BGGN 213

A hands-on introduction to the computer-based analysis of genomic and biomolecular data from the Division of Biological Sciences, UCSD.

Starting a Jetstream Computer Instance!

Here we describe the process of starting up and managing a Jetstream service virtual machine instance.

> **Note:** Jetstream is a cloud-based on-demand virtual machine system funded by the National Science Foundation. It will provide us with computers (what we call "virtual machine instances") that look and feel just like a regular Linux workstation but with thousands of times the computing power!

What we're going to do here is walk through starting up an running computer (an "instance") on the Jetstream service.

Below we walk through the process of starting up and accessing one of these instances. To begin with, just think of it like requesting and loging-in to a brand new remote computer. We have provided screenshots of the whole process that you can click on to see a larger version. The important areas to fill in are circled in red.

> **Note** Some of the details may vary – for example, if you have your own XSEDE account, you may want to log in with that – and the name of the operating system or "image" may also vary from "Ubuntu 16.04" depending

Jetstream tutorials

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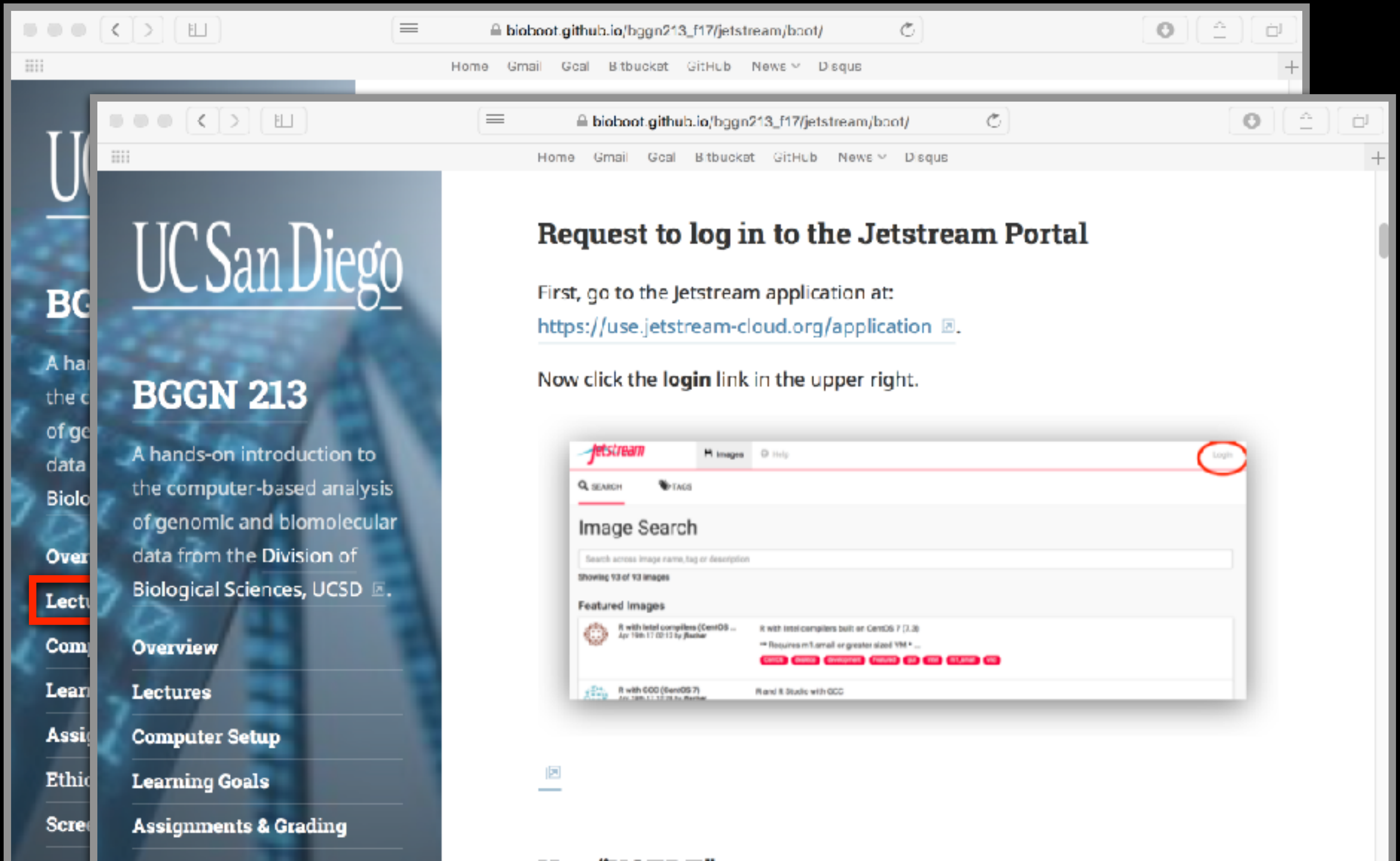

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- Overview
- Lectures
- Computer Setup
- Learning Goals
- Assignments & Grading

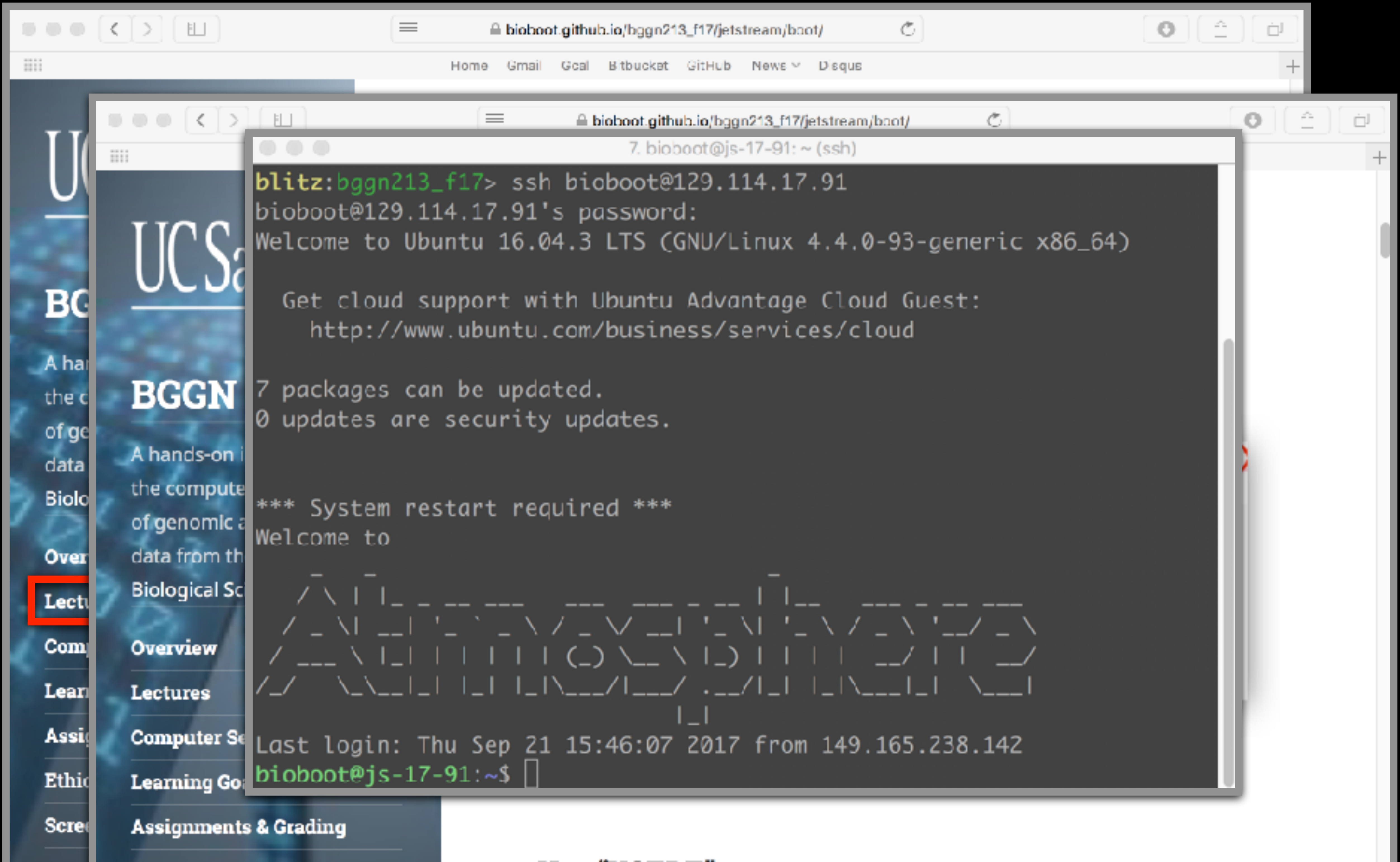
Request to log in to the Jetstream Portal

First, go to the Jetstream application at: https://use.jetstream-cloud.org/application.

Now click the **login** link in the upper right.

Jetstream tutorials

Developed *user friendly* labs for Jetstream basics



```
blitz:bggn213_f17> ssh bioboot@129.114.17.91
bioboot@129.114.17.91's password:
Welcome to Ubuntu 16.04.3 LTS (GNU/Linux 4.4.0-93-generic x86_64)

 Get cloud support with Ubuntu Advantage Cloud Guest:
   http://www.ubuntu.com/business/services/cloud

7 packages can be updated.
0 updates are security updates.


*** System restart required ***
Welcome to
    _   _                             _
   / \ | |_ _ __ ___   ___  ___ _ __ | |__   ___ _ __ ___
  / _ \| __| '_ ` _ \ / _ \/ __| '_ \| '_ \ / _ \ '__/ _ \
 / ___ \ |_| | | | | | (_) \__ \ |_) | | | |  __/ | |  __/
/_/   \_\__|_| |_| |_|\___/|___/ .__/|_| |_|\___|_|  \___|
                               |_|
Last login: Thu Sep 21 15:46:07 2017 from 149.165.238.142
bioboot@js-17-91:~$
```

Skepticism & Bioinformatics

We have to approach computational results the same way we do wet-lab results:

- Do they make sense?
- Is it what we expected?
- Do we have adequate controls, and how did they come out?
- Modeling is modeling, but biology is different...

  What does this model actually contribute?
- Avoid the miss-use of ‘black boxes’

Skepticism & Bioinformatics

Gunnar von Heijne in his old but quite readable treatise, *Sequence Analysis in Molecular Biology; Treasure Trove or Trivial Pursuit*, provides a very appropriate conclusion:

- "Think about what you're doing; use your knowledge of the molecular system involved to guide both your interpretation of results and your direction of inquiry; use as much information as possible; and do not blindly accept everything the computer offers you".
- Key-Point: **Avoid the miss-use of 'black boxes'!**

Common problems with Bioinformatics

Confusing multitude of tools available

- Each with many options and settable parameters

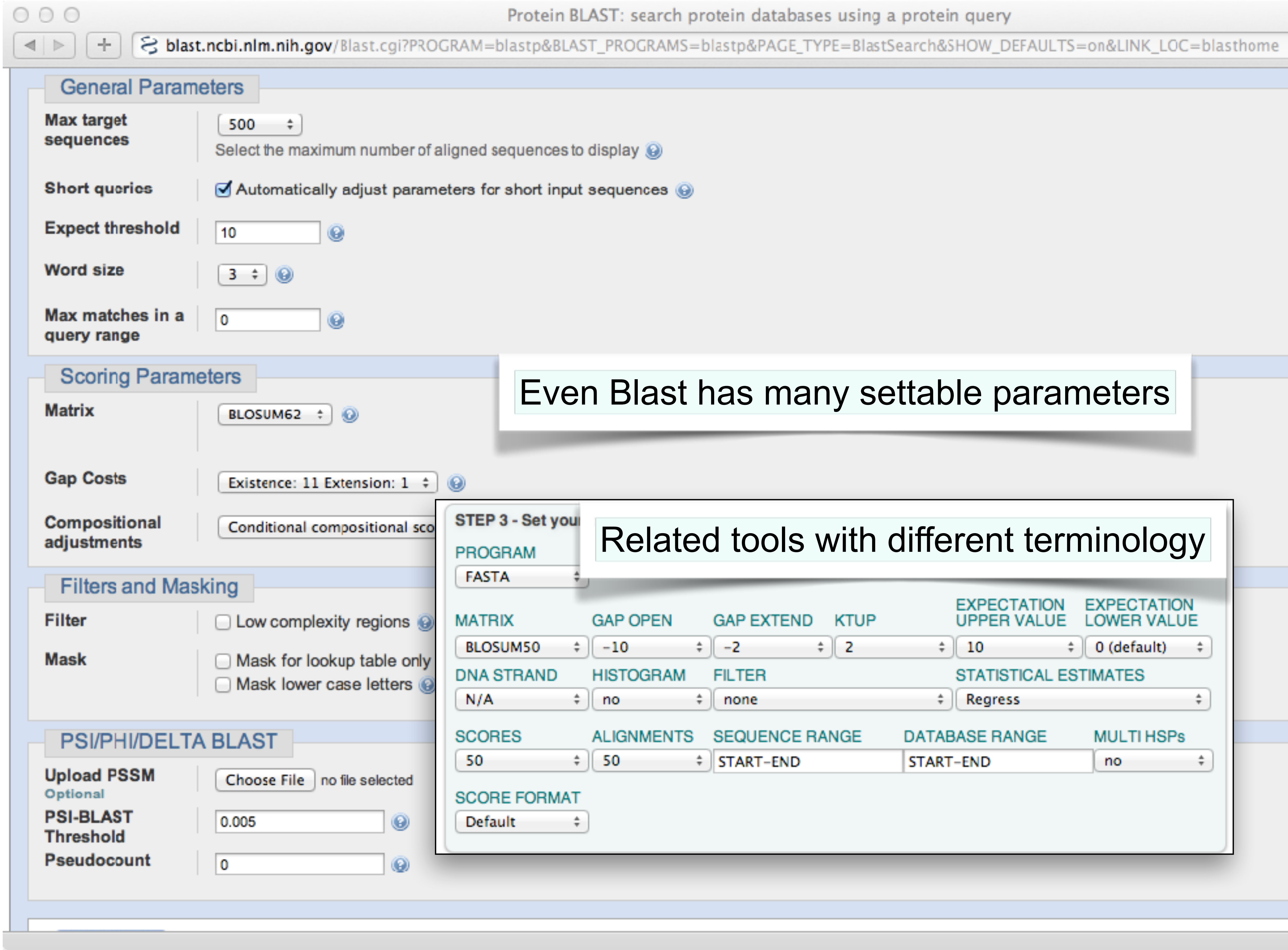
Most tools and databases are written by and for nerds

- Same is true of documentation - if any exists!

Most are developed independently

Notable exceptions are found at the:

- **EBI** (European Bioinformatics Institute) and
- **NCBI** (National Center for Biotechnology Information)



Protein BLAST: search protein databases using a protein query

blast.ncbi.nlm.nih.gov/Blast.cgi?PROGRAM=blastp&BLAST_PROGRAMS=blastp&PAGE_TYPE=BlastSearch&SHOW_DEFAULTS=on&LINK_LOC=blasthome

General Parameters

Max target sequences: 500 — Select the maximum number of aligned sequences to display

Short queries: ☑ Automatically adjust parameters for short input sequences

Expect threshold: 10

Word size: 3

Max matches in a query range: 0

Scoring Parameters

Matrix: BLOSUM62

Gap Costs: Existence: 11 Extension: 1

Compositional adjustments: Conditional compositional sco

Filters and Masking

Filter: ☐ Low complexity regions

Mask: ☐ Mask for lookup table only

☐ Mask lower case letters

PSI/PHI/DELTA BLAST

Upload PSSM Optional: Choose File — no file selected

PSI-BLAST Threshold: 0.005

Pseudocount: 0

Even Blast has many settable parameters

STEP 3 - Set you

PROGRAM: FASTA

MATRIX	GAP OPEN	GAP EXTEND	KTUP	EXPECTATION UPPER VALUE	EXPECTATION LOWER VALUE
BLOSUM50	-10	-2	2	10	0 (default)

DNA STRAND	HISTOGRAM	FILTER	STATISTICAL ESTIMATES
N/A	no	none	Regress

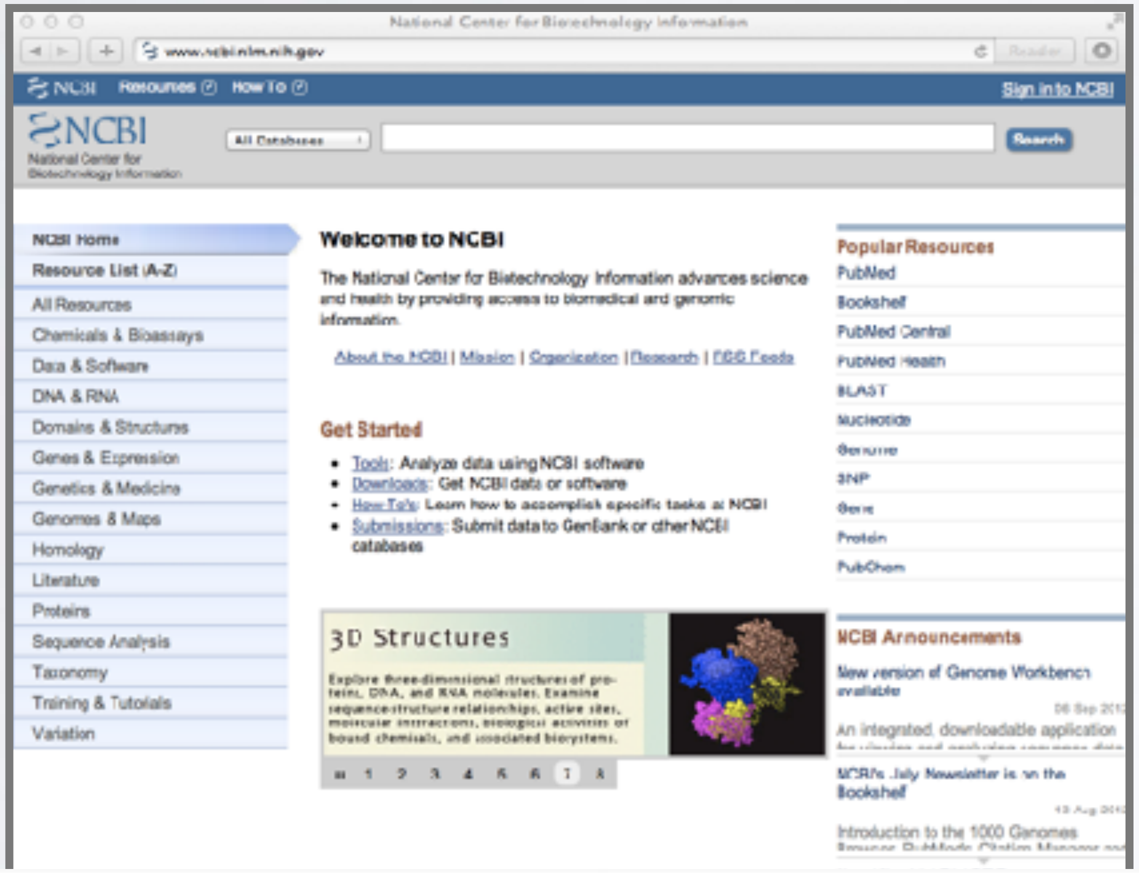
SCORES	ALIGNMENTS	SEQUENCE RANGE	DATABASE RANGE	MULTI HSPs
50	50	START-END	START-END	no

SCORE FORMAT: Default

Related tools with different terminology

Key Online Bioinformatics Resources: NCBI & EBI

The NCBI and EBI are invaluable, publicly available resources for biomedical research



Welcome to NCBI

The National Center for Biotechnology Information advances science and health by providing access to biomedical and genomic information.

About the NCBI | Mission | Organization | Research | RSS Feeds

Get Started

- Tools: Analyze data using NCBI software
- Downloads: Get NCBI data or software
- How-To's: Learn how to accomplish specific tasks at NCBI
- Submissions: Submit data to GenBank or other NCBI databases

Explore three-dimensional structures of proteins, DNA, and RNA molecules. Examine sequence-structure relationships, active sites, molecular interactions, biological activities of bound chemicals, and associated biosystems.

NCBI Announcements

New version of Genome Workbench available

An integrated, downloadable application

NCBI's July Newsletter is on the Bookshelf

Introduction to the 1000 Genomes

The European Bioinformatics Institute

Part of the European Molecular Biology Laboratory

EMBL-EBI provides freely available data from life science experiments, performs basic research in computational biology and offers an extensive user training programme, supporting researchers in academia and industry.

Find a gene, protein or chemical:

News from EMBL-EBI

Plant and Animal Genome conference (PAG XXIV)

http://www.ncbi.nlm.nih.gov

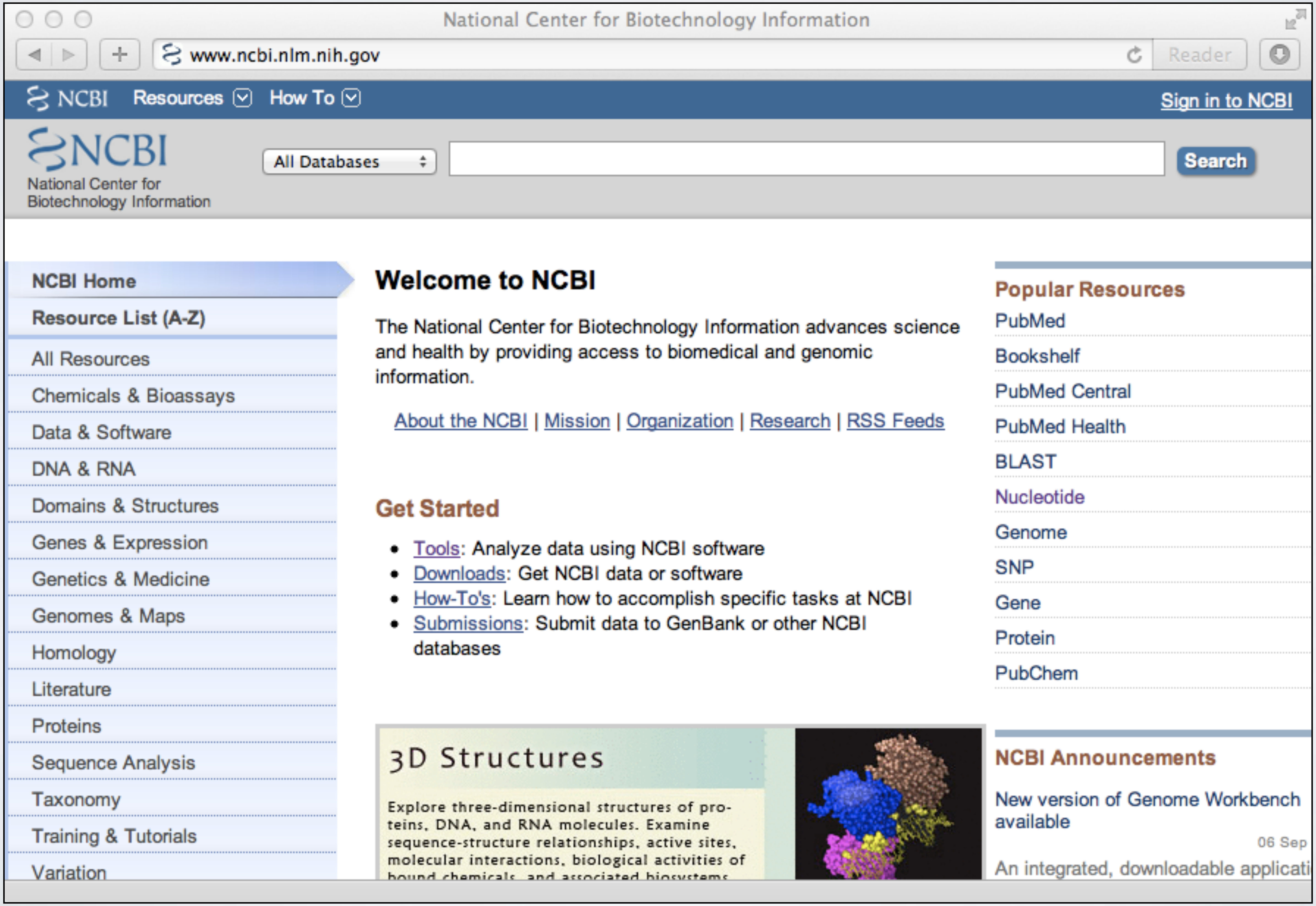
https://www.ebi.ac.uk

National Center for Biotechnology Information (NCBI)

- Created in 1988 as a part of the National Library of Medicine (NLM) at the National Institutes of Health
- NCBI’s mission includes:
  - Establish **public databases**
  - Develop **software tools**
  - **Education** on and dissemination of biomedical information

- We will cover a number of core NCBI databases and software tools in the lecture

http://www.ncbi.nlm.nih.gov



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- PubMed Central
- PubMed Health
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- Genome
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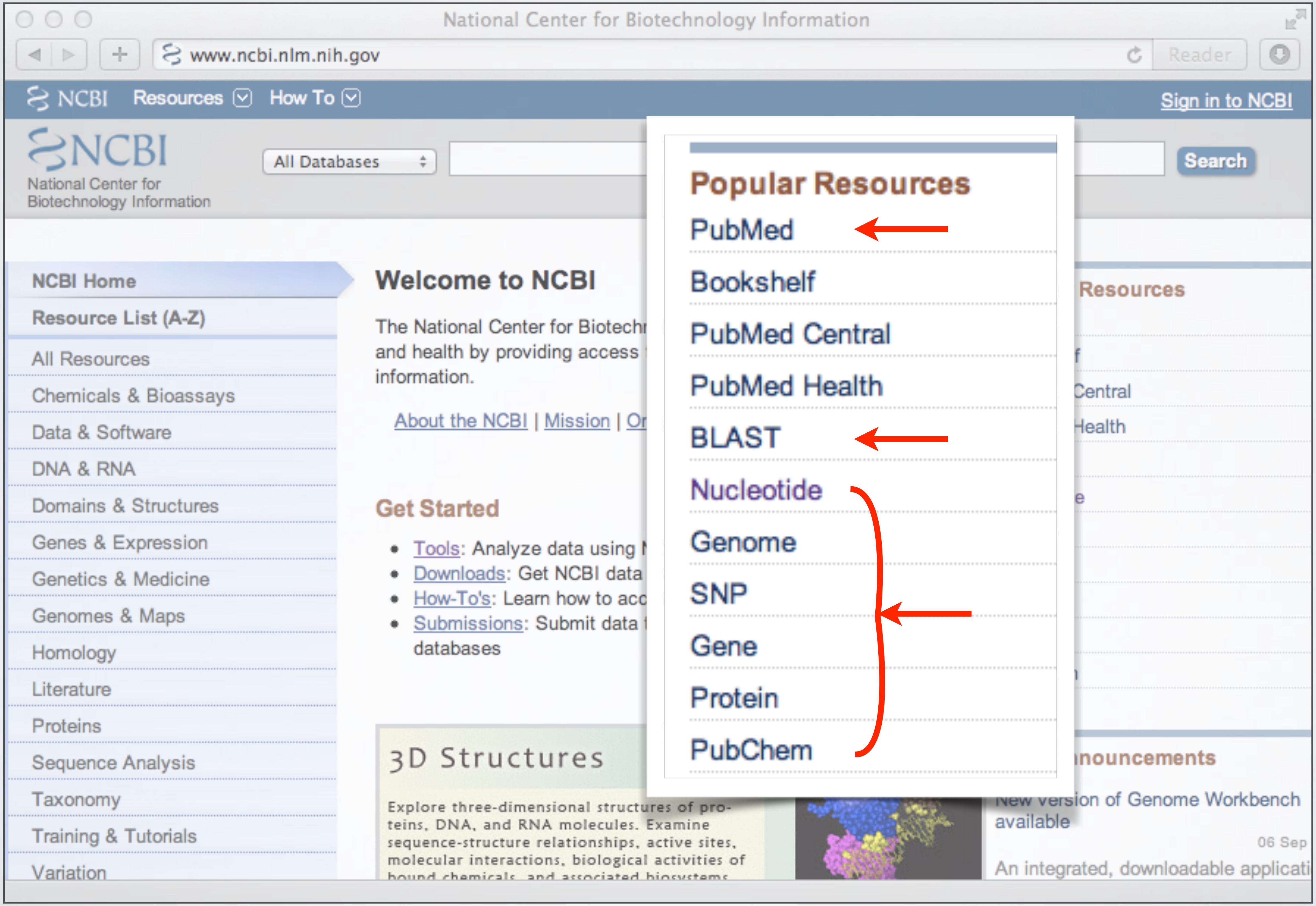

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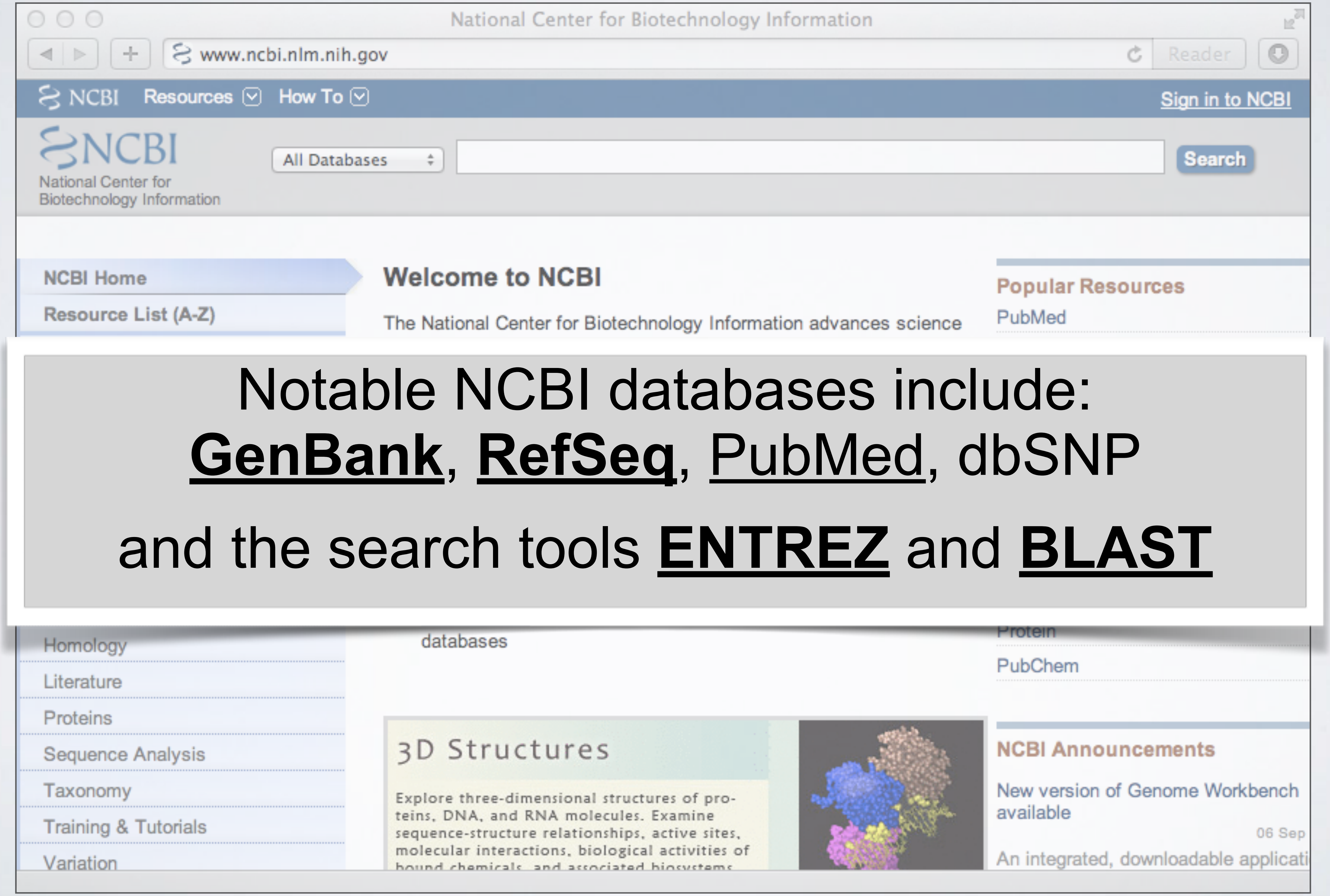

Welcome to NCBI

The National Center for Biotechnology Information advances science

databases

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06 Sep

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Notable NCBI databases include:
GenBank, **RefSeq**, PubMed, dbSNP

and the search tools **ENTREZ** and **BLAST**

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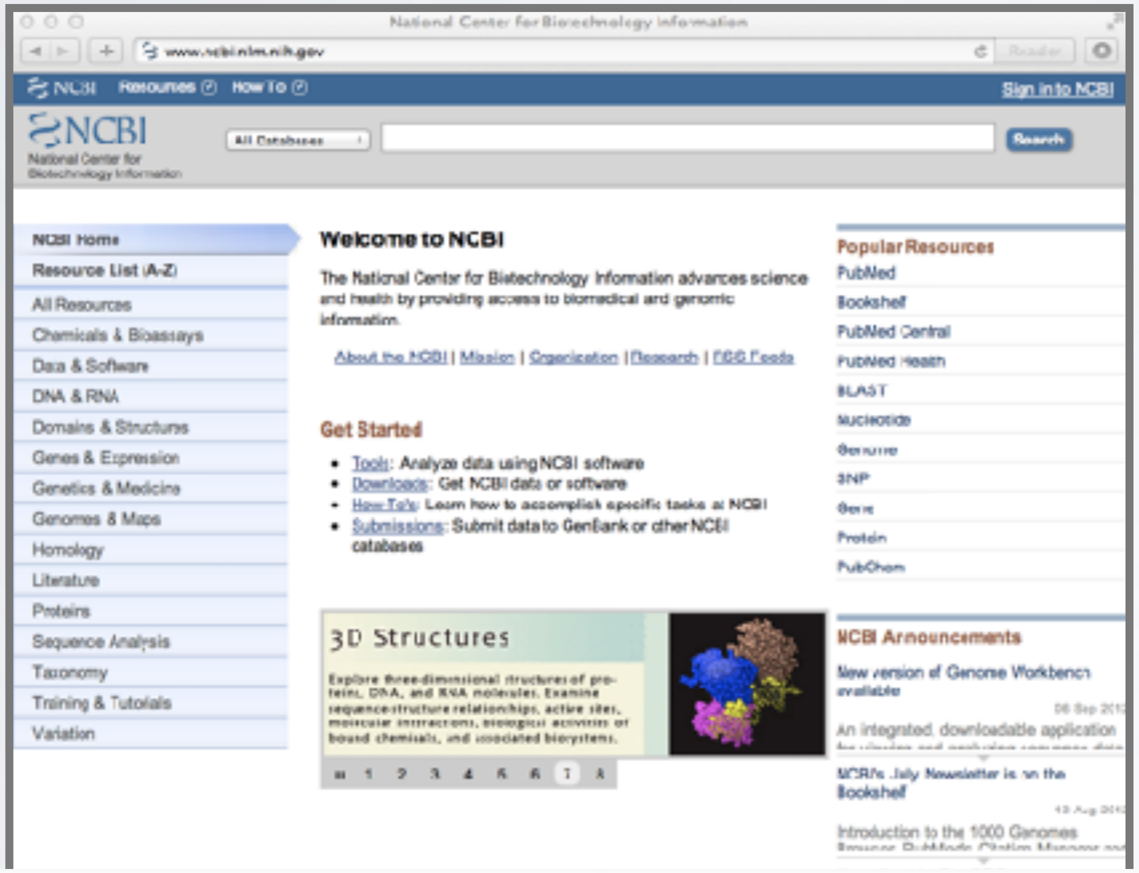

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Find a gene, protein or chemical:

News from EMBL-EBI

Upcoming events

Plant and Animal Genome conference (PAG XXIV)

SME Forum 2016

https://www.ebi.ac.uk

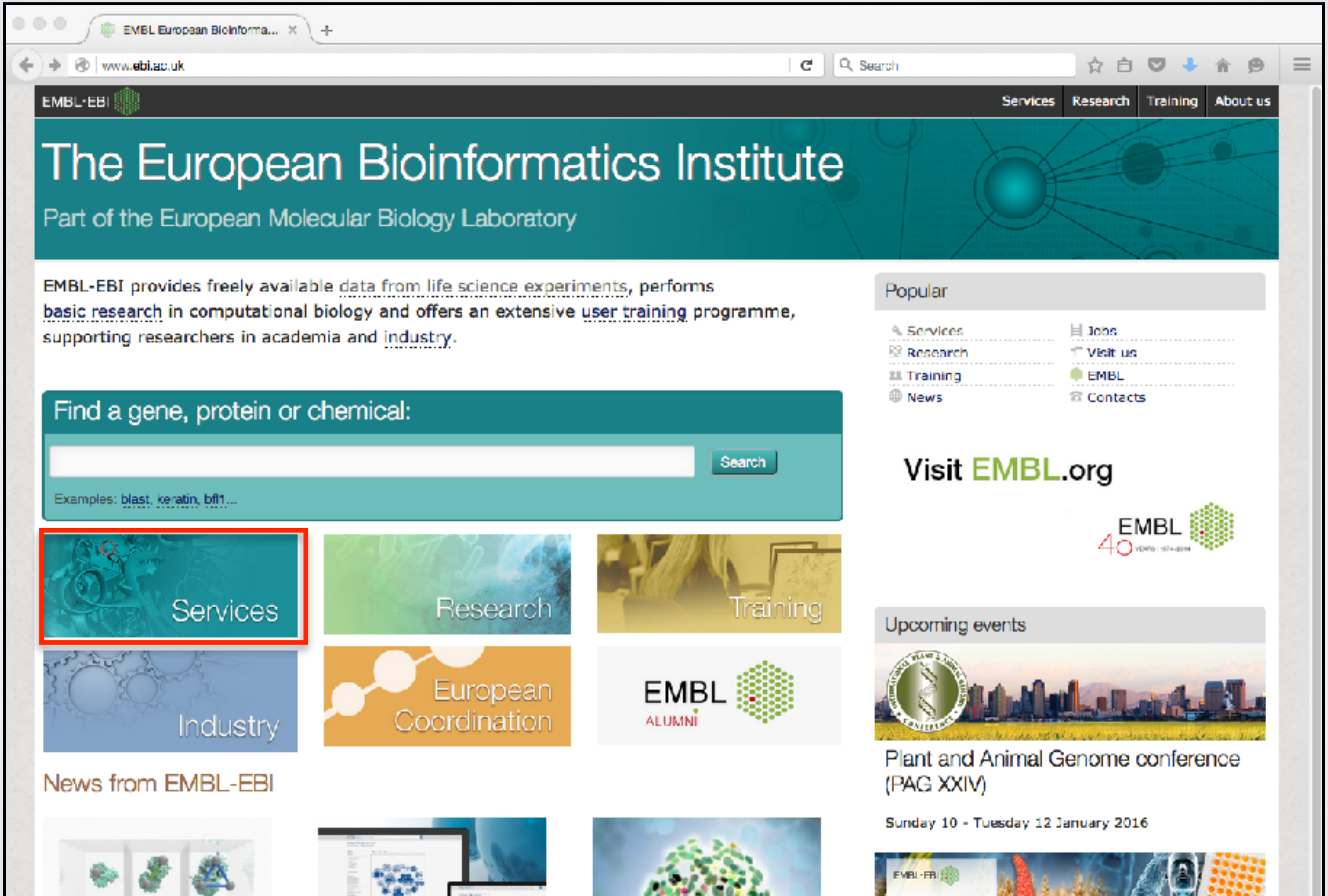
European Bioinformatics Institute (EBI)

- Created in 1997 as a part of the European Molecular Biology Laboratory (EMBL)
- EBI's mission includes:
  - providing freely available **data** and **bioinformatics services**
  - and providing advanced **bioinformatics training**

Hinxton,UK

- We will briefly cover several EBI databases and tools that have advantages over those offered at NCBI

The EBI maintains a number of high quality curated **secondary databases** and associated tools



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Sunday 10 - Tuesday 12 January 2016

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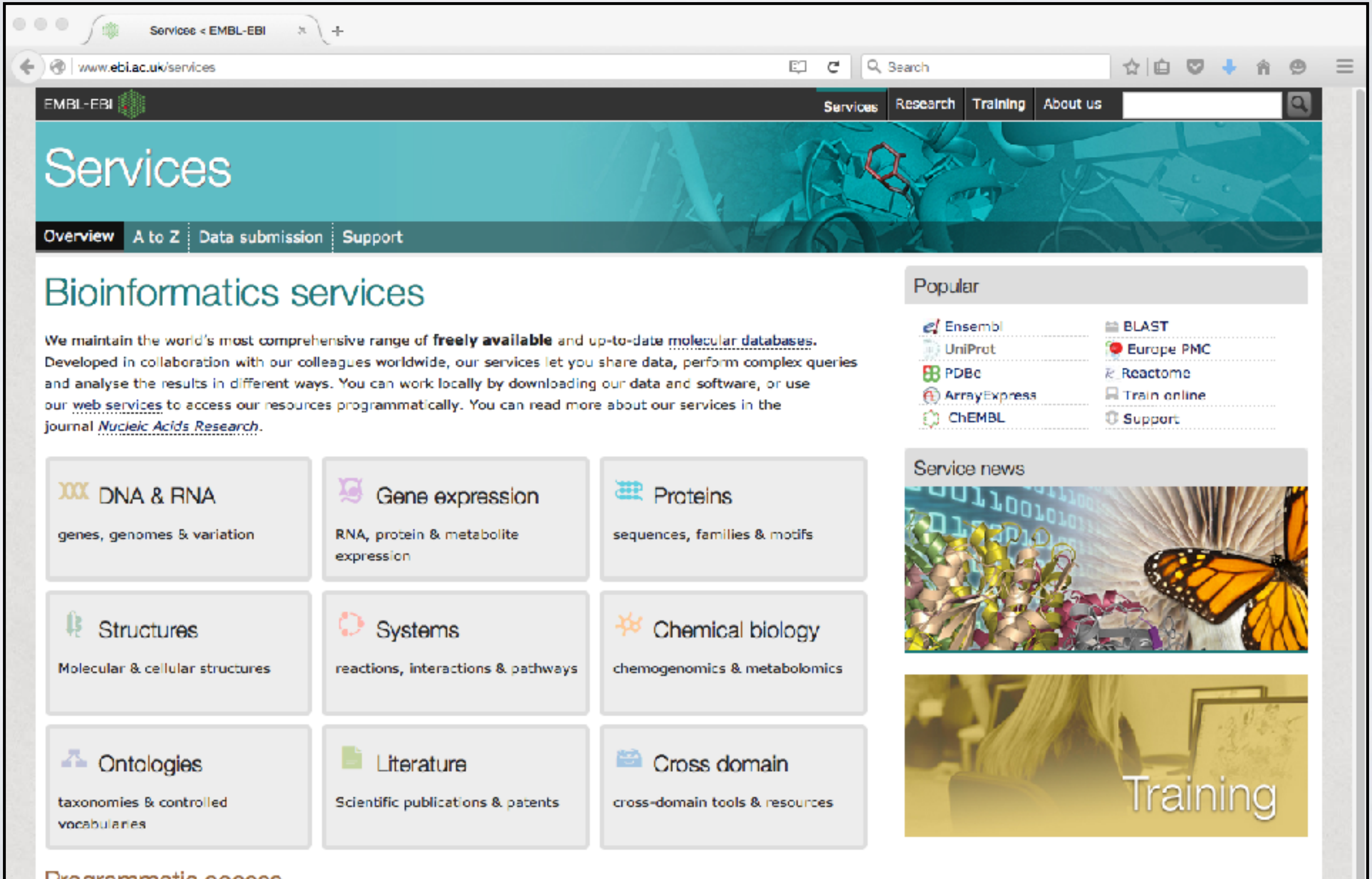

Services

Overview | A to Z | Data submission | Support

Bioinformatics services

We maintain the world's most comprehensive range of **freely available** and up-to-date molecular databases. Developed in collaboration with our colleagues worldwide, our services let you share data, perform complex queries and analyse the results in different ways. You can work locally by downloading our data and software, or use our web services to access our resources programmatically. You can read more about our services in the journal *Nucleic Acids Research*.

DNA & RNA genes, genomes & variation	**Gene expression** RNA, protein & metabolite expression	**Proteins** sequences, families & motifs
Structures Molecular & cellular structures	**Systems** reactions, interactions & pathways	**Chemical biology** chemogenomics & metabolomics
Ontologies taxonomies & controlled vocabularies	**Literature** Scientific publications & patents	**Cross domain** cross-domain tools & resources

Popular

- Ensembl
- UniProt
- PDBe
- ArrayExpress
- ChEMBL
- BLAST
- Europe PMC
- Reactome
- Train online
- Support

Service news

Programmatic access

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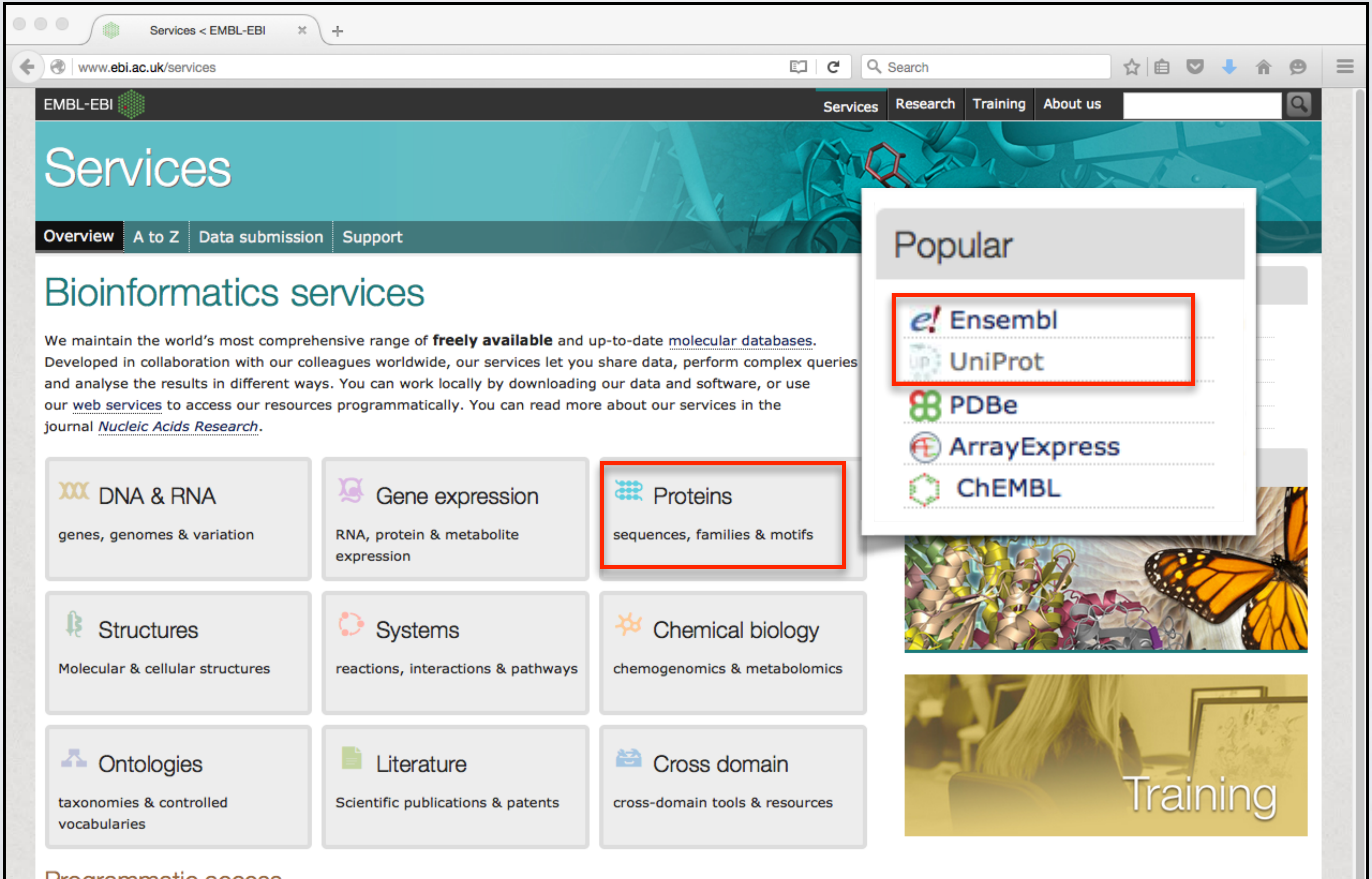

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genes, genomes & variation

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Cross domain
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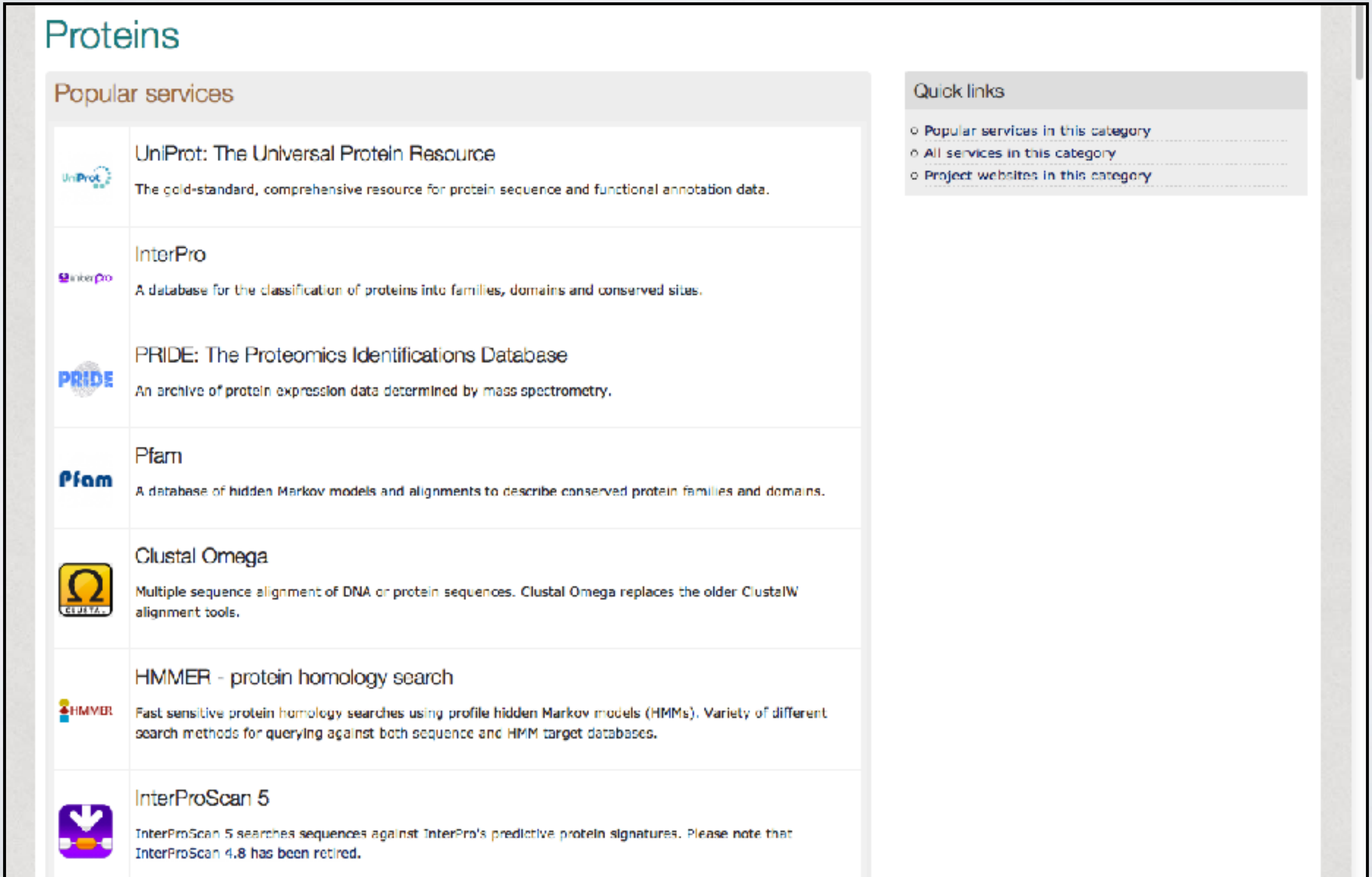
The EBI makes available a wider variety of **online tools** than NCBI



Proteins

Popular services

UniProt: The Universal Protein Resource

The gold-standard, comprehensive resource for protein sequence and functional annotation data.

InterPro

A database for the classification of proteins into families, domains and conserved sites.

PRIDE: The Proteomics Identifications Database

An archive of protein expression data determined by mass spectrometry.

Pfam

A database of hidden Markov models and alignments to describe conserved protein families and domains.

Clustal Omega

Multiple sequence alignment of DNA or protein sequences. Clustal Omega replaces the older ClustalW alignment tools.

HMMER - protein homology search

Fast sensitive protein homology searches using profile hidden Markov models (HMMs). Variety of different search methods for querying against both sequence and HMM target databases.

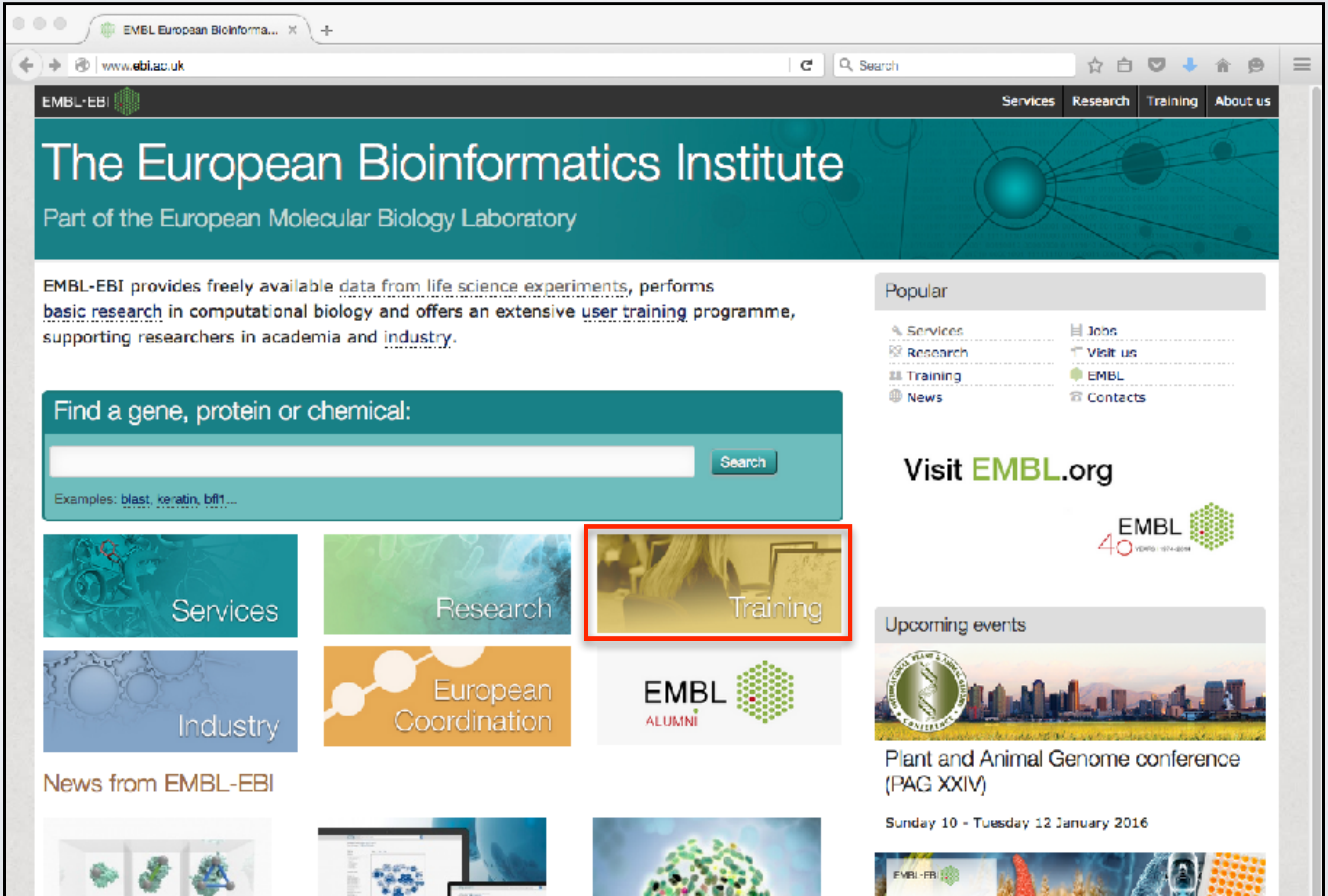
InterProScan 5

InterProScan 5 searches sequences against InterPro's predictive protein signatures. Please note that InterProScan 4.8 has been retired.

Quick links

- Popular services in this category
- All services in this category
- Project websites in this category

The EBI also provides a growing selection of **online tutorials** on EBI databases and tools



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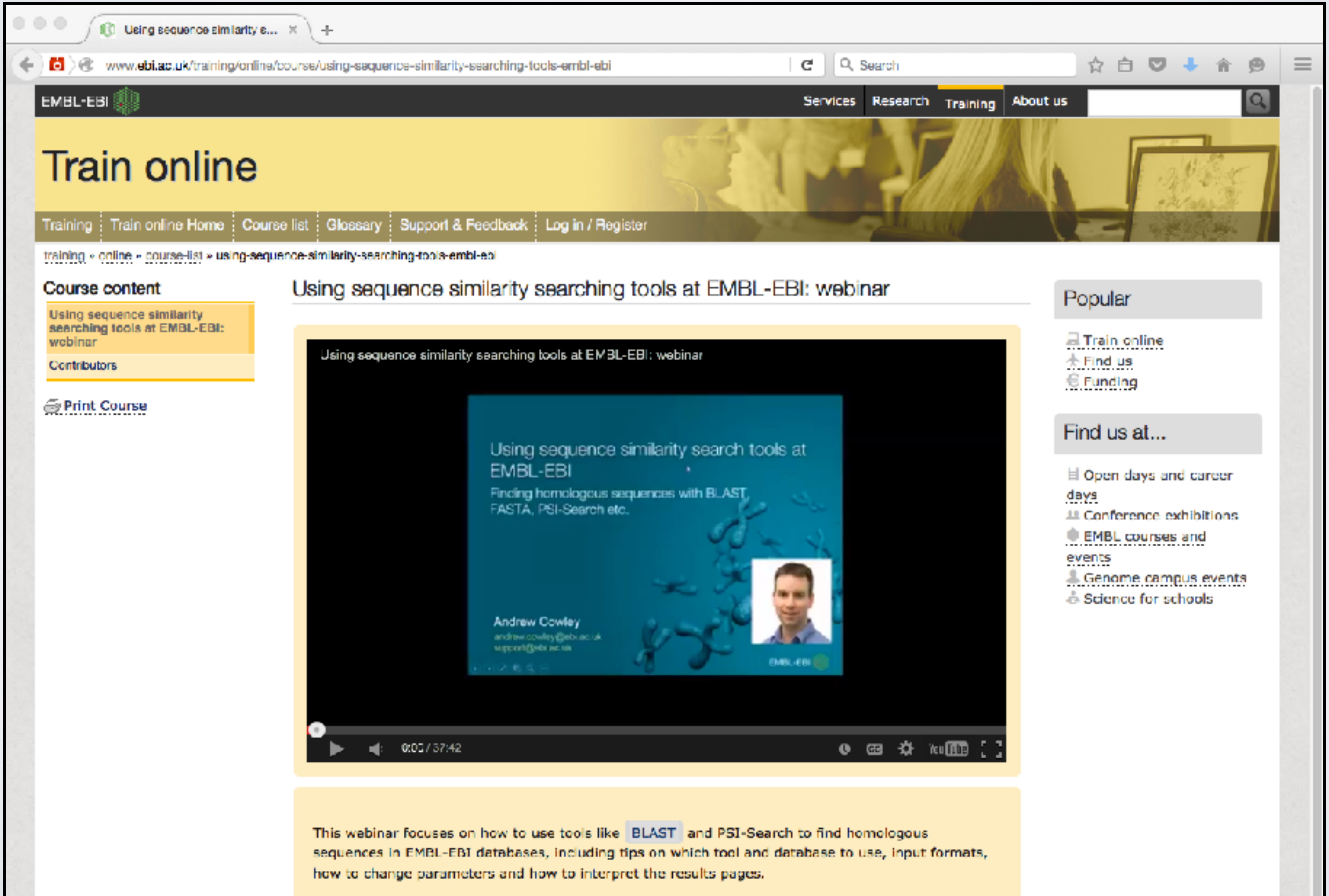


Train online

Course content

- Using sequence similarity searching tools at EMBL-EBI: webinar
- Contributors

Print Course

Using sequence similarity searching tools at EMBL-EBI: webinar

Using sequence similarity searching tools at EMBL-EBI: webinar

Using sequence similarity search tools at EMBL-EBI

Finding homologous sequences with BLAST, FASTA, PSI-Search etc.

Andrew Cowley

andrew.cowley@ebi.ac.uk

This webinar focuses on how to use tools like BLAST and PSI-Search to find homologous sequences in EMBL-EBI databases, including tips on which tool and database to use, input formats, how to change parameters and how to interpret the results pages.

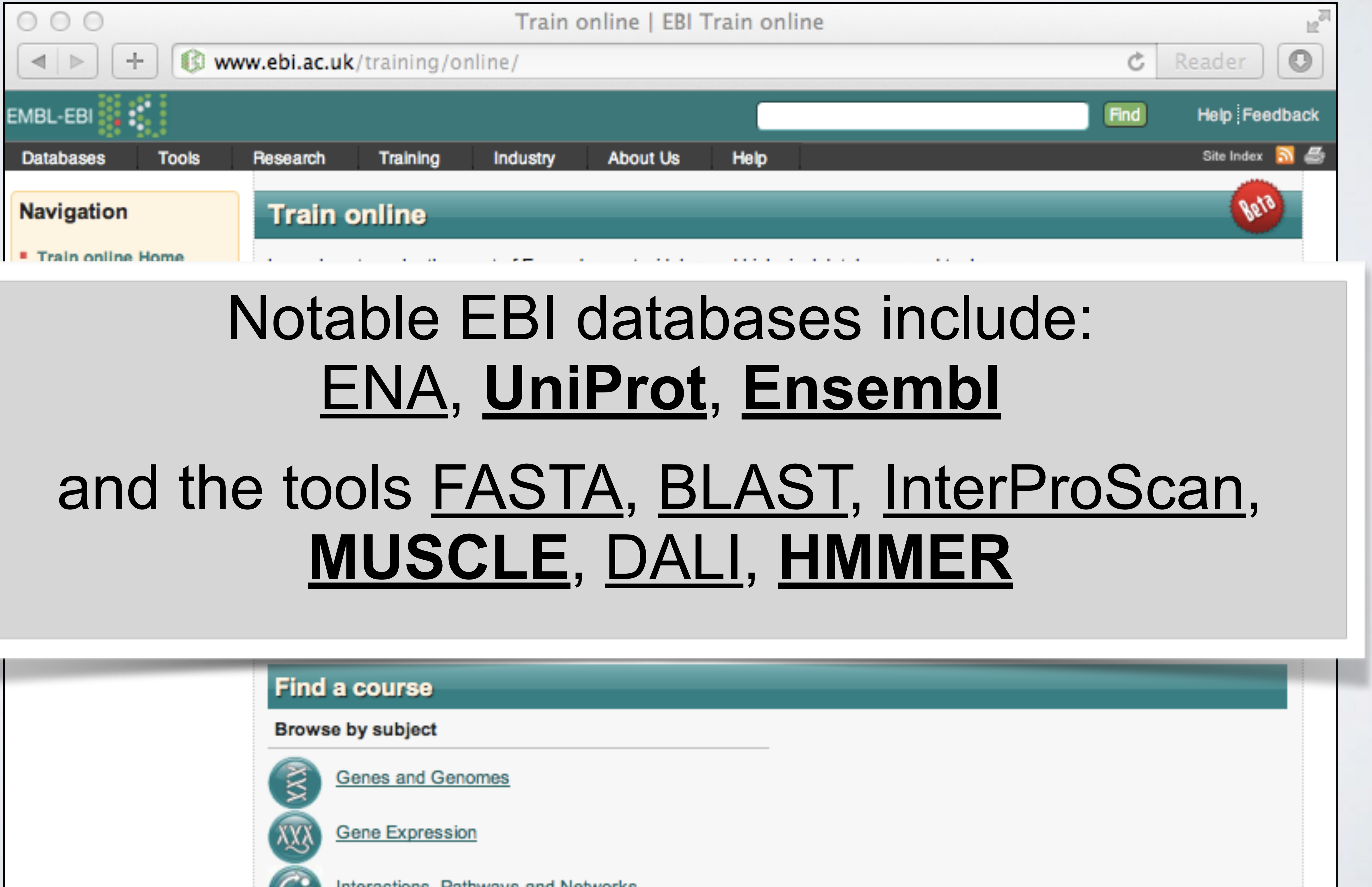
Popular

- Train online
- Find us
- Funding

Find us at...

- Open days and career days
- Conference exhibitions
- EMBL courses and events
- Genome campus events
- Science for schools

The EBI also provides a growing selection of **online tutorials** on EBI databases and tools



Notable EBI databases include:
<u>ENA</u>, **<u>UniProt</u>**, **<u>Ensembl</u>**

and the tools <u>FASTA</u>, <u>BLAST</u>, <u>InterProScan</u>, **<u>MUSCLE</u>**, <u>DALI</u>, **<u>HMMER</u>**

Next Class…

MAJOR BIOINFORMATICS DATABASES AND ASSOCIATED ONLINE TOOLS

Bioinformatics Databases

AATDB, AceDb, ACUTS, ADB, AFDB, AGIS, AMSdb, ARR, AsDb,BBDB, BCGD, Beanref, BioImage, BioMagResBank, BIOMDB, BLOCKS, BovGBASE, BOVMAP, BSORF, BTKbase, CANSITE, CarbBank, CARBHYD, CATH, CAZY, CCDC, CD4OLbase, CGAP, ChickGBASE, Colibri, COPE, CottonDB, CSNDB, CUTG, CyanoBase, dbCFC, dbEST, dbSTS, DDBJ, DGP, DictyDb, Picty_cDB, DIP, DOGS, DOMO, DPD, DPInteract, ECDC, ECGC, EC02DBASE, EcoCyc, EcoGene, EMBL, EMD db, ENZYME, EPD, EpoDB, ESTHER, FlyBase, FlyView, GCRDB, GDB, GENATLAS, Genbank, GeneCards, Genlilesne, GenLink, GENOTK, GenProtEC, GIFTS, GPCRDB, GRAP, GRBase, gRNAsdb, GRR, GSDB, HAEMB, HAMSTERS, HEART-2DPAGE, HEXAdb, HGMD, HIDB, HIDC, HIVdb, HotMolecBase, HOVERGEN, HPDB, HSC-2DPAGE, ICN, ICTVDB, IL2RGbase, IMGT, Kabat, KDNA, KEGG, Klotho, LGIC, MAD, MaizeDb, MDB, Medline, Mendel, MEROPS, MGDB, MGI, MHCPEP5 Micado, MitoDat, MITOMAP, MJDB, MmtDB, Mol-R-Us, MPDB, MRR, MutBase, MycDB, NDB, NRSub, 0-lycBase, OMIA, OMIM, OPD, ORDB, OWL, PAHdb, PatBase, PDB, PDD, Pfam, PhosphoBase, PigBASE, PIR, PKR, PMD, PPDB, PRESAGE, PRINTS, ProDom, Prolysis, PROSITE, PROTOMAP, RatMAP, RDP, REBASE, RGP, SBASE, SCOP, SeqAnaiRef, SGD, SGP, SheepMap, Soybase, SPAD, SRNA db, SRPDB, STACK, StyGene,Sub2D, SubtiList, SWISS-2DPAGE, SWISS-3DIMAGE, SWISS- MODEL Repository, SWISS-PROT, TelDB, TGN, tmRDB, TOPS, TRANSFAC, TRR, UniGene, URNADB, V BASE, VDRR, VectorDB, WDCM, WIT, WormPep, etc .... !!!!

Bioinformatics Databases

There are lots of Bioinformatics Databases

For a annotated listing of major bioinformatics databases please see the online handout

< Major_Databases.pdf >

AATDB, AceDb, ACUTS, ADB, AFDB, AGIS, AMSdb, ARR, AsDb,BBDB, BC Beanref,
BioImage, BioMagResBank, BIOMDB, BLOCKS, BovGBASE, BOV TKbase,
CANSITE, CarbBank, CARBHYD, CATH, CAZY AP,
ChickGBASE, Colibri, COPE, CottonD bEST,
dbSTS, DDBJ, DGP, DictyDb CDC,
ECGC, EC02DBASE THER,
FlyBase Link,
G DB, HAEMB,
H Vdb, HotMolecBase,
H 2RGbase, IMGT, Kabat, KDNA,
K DB, Medline, Mendel, MEROPS, MGDB, MGI,
MHC OMAP, MJDB, MmtDB, Mol-R-Us, MPDB, MRR, MutBase,
Myc db, 0-lycBase, OMIA, OMIM, OPD, ORDB, OWL, PAHdb, PatBase,
PD Pfam, PhosphoBase, PigBASE, PIR, PKR, PMD, PPDB, PRESAGE, PRINTS,
ProDom, Prolysis, PROSITE, PROTOMAP, RatMAP, RDP, REBASE, RGP, SBASE, SCOP,
SeqAnaiRef, SGD, SGP, SheepMap, Soybase, SPAD, SRNA db, SRPDB, STACK,
StyGene,Sub2D, SubtiList, SWISS-2DPAGE, SWISS-3DIMAGE, SWISS- MODEL
Repository, SWISS-PROT, TelDB, TGN, tmRDB, TOPS, TRANSFAC, TRR, UniGene,
URNADB, V BASE, VDRR, VectorDB, WDCM, WIT, WormPep, etc .... !!!!

Side-note: Databases come in all shapes and sizes

Databases can be of variable quality and often there are multiple databases with overlapping content.

Primary, secondary & composite databases

Bioinformatics databases can be usefully classified into *primary*, *secondary* and *composite* according to their data source.

- **Primary databases** (or *archival databases*) consist of data derived experimentally.
  - **GenBank**: NCBI's primary nucleotide sequence database.
  - **PDB:** Protein X-ray crystal and NMR structures.

- **Secondary databases** (or *derived databases*) contain information derived from a primary database.
  - **RefSeq**: non redundant set of curated reference sequences primarily from GenBank
  - **PFAM**: protein sequence families primarily from UniProt and PDB

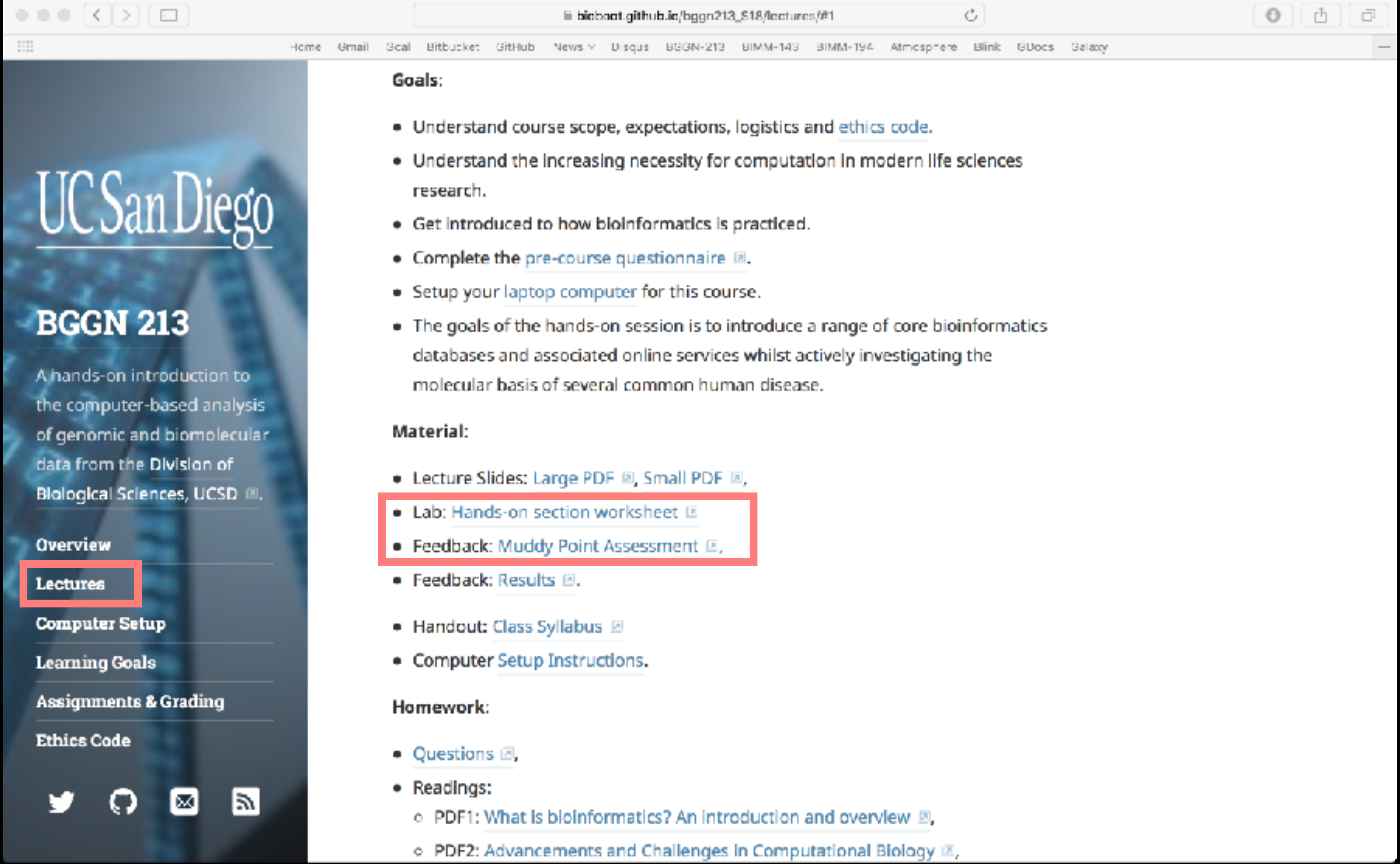
- **Composite databases** (or *metadatabases*) join a variety of different primary and secondary database sources.
  - **OMIM**: catalog of human genes, genetic disorders and related literature
  - **GENE**: molecular data and literature related to genes with extensive links to other databases.

Today's Menu

Course Logistics	Website, screencasts, survey, ethics, assessment and grading.
Learning Objectives	What you need to learn to succeed in this course.
Course Structure	Major lecture topics and specific leaning goals.
Introduction to Bioinformatis	Introducing the *what*, *why* and *how* of bioinformatics?
Bioinformatics Database	**Hands-on** exploration of several major databases and their associated tools.

Your Turn!

https://bioboot.github.io/bggn213_S18/lectures/#1



BGGN 213

A hands-on introduction to the computer-based analysis of genomic and biomolecular data from the Division of Biological Sciences, UCSD.

Goals:

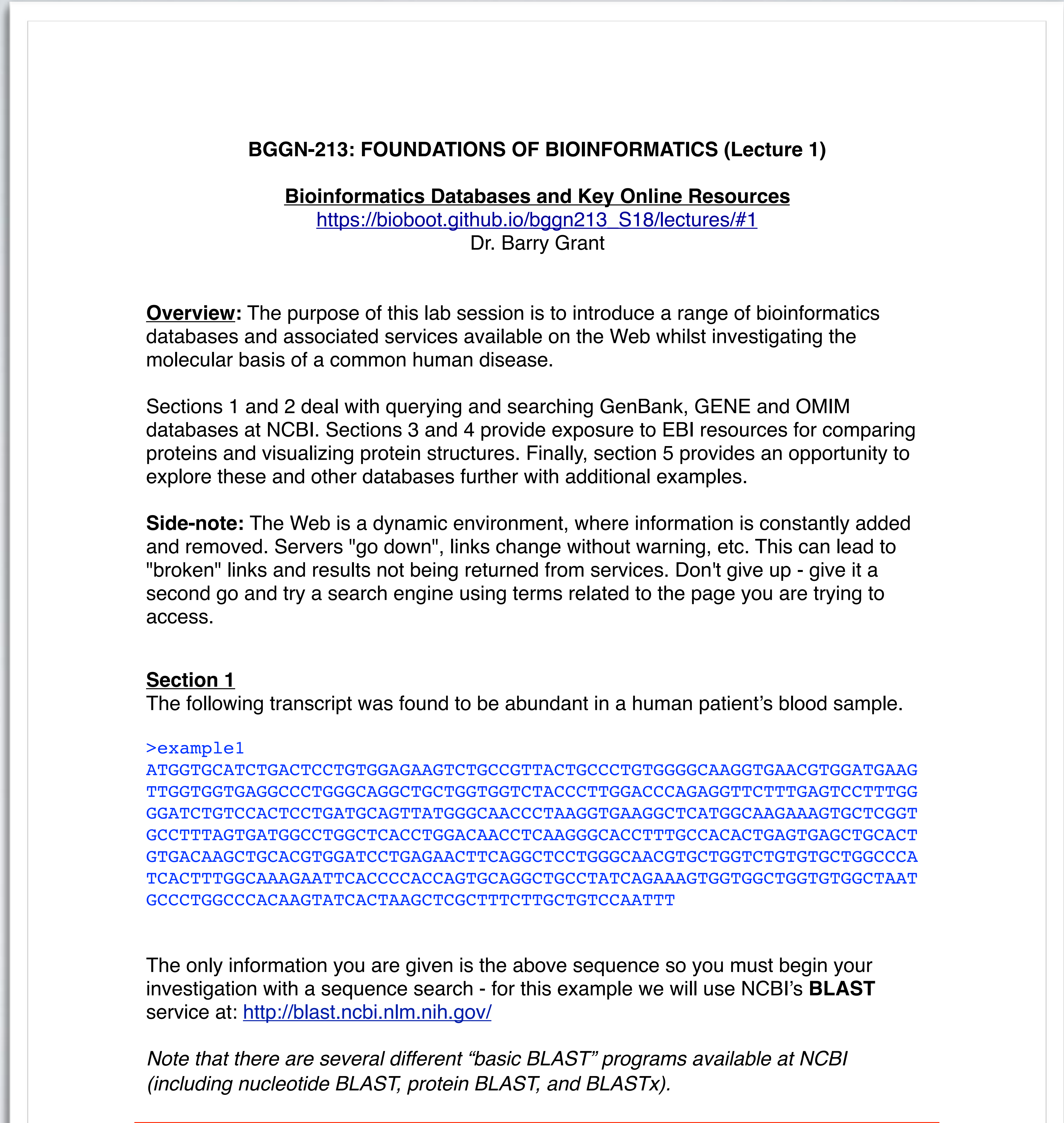
- Understand course scope, expectations, logistics and ethics code.
- Understand the increasing necessity for computation in modern life sciences research.
- Get introduced to how bioinformatics is practiced.
- Complete the pre-course questionnaire.
- Setup your laptop computer for this course.
- The goals of the hands-on session is to introduce a range of core bioinformatics databases and associated online services whilst actively investigating the molecular basis of several common human disease.

Material:

- Lecture Slides: Large PDF, Small PDF,
- Lab: Hands-on section worksheet
- Feedback: Muddy Point Assessment,
- Feedback: Results.
- Handout: Class Syllabus
- Computer Setup Instructions.

Homework:

- Questions,
- Readings:
  - PDF1: What is bioinformatics? An introduction and overview,
  - PDF2: Advancements and Challenges in Computational Biology,



BGGN-213: FOUNDATIONS OF BIOINFORMATICS (Lecture 1)

Bioinformatics Databases and Key Online Resources

https://bioboot.github.io/bggn213_S18/lectures/#1
Dr. Barry Grant

Overview: The purpose of this lab session is to introduce a range of bioinformatics databases and associated services available on the Web whilst investigating the molecular basis of a common human disease.

Sections 1 and 2 deal with querying and searching GenBank, GENE and OMIM databases at NCBI. Sections 3 and 4 provide exposure to EBI resources for comparing proteins and visualizing protein structures. Finally, section 5 provides an opportunity to explore these and other databases further with additional examples.

Side-note: The Web is a dynamic environment, where information is constantly added and removed. Servers "go down", links change without warning, etc. This can lead to "broken" links and results not being returned from services. Don't give up - give it a second go and try a search engine using terms related to the page you are trying to access.

Section 1

The following transcript was found to be abundant in a human patient's blood sample.

```
>example1
ATGGTGCATCTGACTCCTGTGGAGAAGTCTGCCGTTACTGCCCTGTGGGGCAAGGTGAACGTGGATGAAG
TTGGTGGTGAGGCCCTGGGCAGGCTGCTGGTGGTCTACCCTTGGACCCAGAGGTTCTTTGAGTCCTTTGG
GGATCTGTCCACTCCTGATGCAGTTATGGGCAACCCTAAGGTGAAGGCTCATGGCAAGAAAGTGCTCGGT
GCCTTTAGTGATGGCCTGGCTCACCTGGACAACCTCAAGGGCACCTTTGCCACACTGAGTGAGCTGCACT
GTGACAAGCTGCACGTGGATCCTGAGAACTTCAGGCTCCTGGGCAACGTGCTGGTCTGTGTGCTGGCCCA
TCACTTTGGCAAAGAATTCACCCCACCAGTGCAGGCTGCCTATCAGAAAGTGGTGGCTGGTGTGGCTAAT
GCCCTGGCCCACAAGTATCACTAAGCTCGCTTTCTTGCTGTCCAATTT
```

The only information you are given is the above sequence so you must begin your investigation with a sequence search - for this example we will use NCBI's **BLAST** service at: http://blast.ncbi.nlm.nih.gov/

Note that there are several different "basic BLAST" programs available at NCBI (including nucleotide BLAST, protein BLAST, and BLASTx).

YOUR TURN!

- There are five major hands-on sections including:

1. BLAST, GenBank and OMIM @ **NCBI** [~35 mins]
2. GENE database @ **NCBI** [~15 mins]

— BREAK —

3. UniProt & Muscle @ **EBI** [~25 mins]
4. PFAM, PDB & NGL [~30 mins]

— BREAK —

5. Extension exercises [~30 mins]

- Please do answer the last review question (**Q19**).
- We encourage discussion and exploration!

YOUR TURN!

- There are five major hands-on sections including:

	End times:
1. BLAST, GenBank and OMIM @ **NCBI**	[10:45 am]
2. GENE database @ **NCBI**	[11:00 am]
— BREAK —	— 11:10 am —
3. UniProt & Muscle @ **EBI**	[11:35 am]
4. PFAM, PDB & NGL	[12:05 pm]
— BREAK —	— 12:15 am —
5. Extension exercises	[12:45 pm]

- Please do answer the last review question (**Q19**).
- We encourage discussion and exploration!

SUMMARY

- Bioinformatics is computer aided biology.
- Bioinformatics deals with the collection, archiving, organization, and interpretation of a wide range of biological data.
- There are a large number of primary, secondary and tertiary bioinformatics databases.
- The NCBI and EBI are major online bioinformatics service providers.
- Introduced Gene, UniProt, PDB databases as well as a number of ‘boutique’ databases including PFAM and OMIM.

HOMEWORK

https://bioboot.github.io/bggn213_S18/lectures/#1

- ☑ Complete the **initial course questionnaire**:
- ☑ Check out the “**Background Reading**” material online:
- ☑ Complete the **lecture 1 homework questions**: