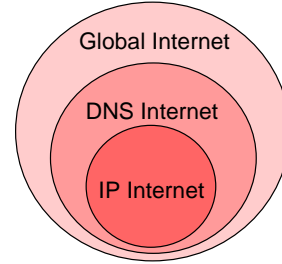


BINF 630: Introduction to Bioinformatics

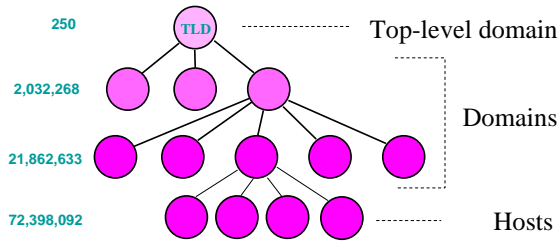
Iosif Vaisman

Email: ivaisman@gmu.edu

What is Internet



Domain Name System

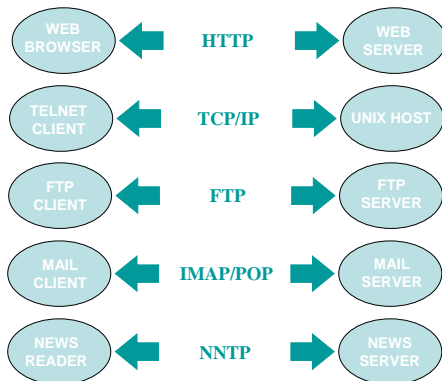


Data from ISC
(January 2000)

Client - Server Model



Client - Server Model



Uniform Resource Locator (URL)

protocol://host.domain[:port]/path/filename

ftp - an anonymous FTP server (<ftp://ftp.pdb.pdb.gov>)
http - a World Wide Web server (<http://mmlin4.pha.unc.edu/~cmb96>)
telnet - a telnet session (<telnet://nun.oit.unc.edu>)

Network applications in science

- Virtual Laboratory
- Virtual Library
- Virtual Conference
- Virtual Classroom

Network collaboration

Real-time data sharing -- exchange of information between remote participants in the project

Resources sharing -- remote access to the instruments and computers

Resources integration -- simultaneous use of remote instruments and computers

Bioinformatics servers

Remote data access -- database search, cross-links between the databases

Remote computing -- use of server's processing capabilities (sequence alignment, structure prediction, homology modeling)

Infospace navigation -- pointers to the available resources

Bioinformatics servers

Real-time

Asynchronous

Digital information cycle

Creation and capture
Storage and management
Rights management
Search and access
Distribution

Electronic publishing

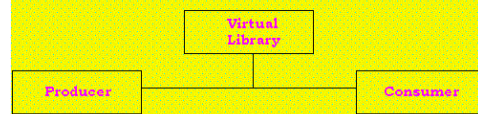
Quality (peer review, retrospective evaluation)
Reliability (stability of servers, control over alterations, proper archiving and mirroring)

Organizational models of the electronic publishing:

- Centralized (similar to the conventional information chain)



- Distributed (with no intermediaries)



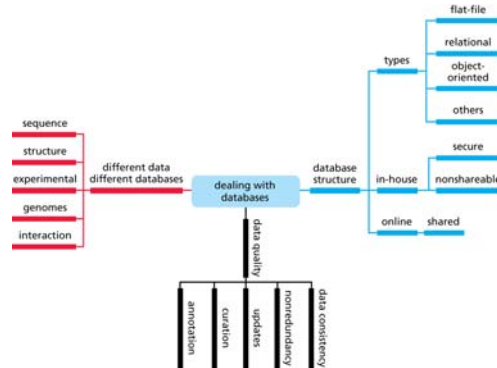
Hypertext Functionality in Scientific Literature

Active references
Forwarding references
Dynamic publishing

Ethical, Legal, and Economical Issues of Electronic Publishing

Intellectual property rights
Ownership of information
Information as a commodity

Databases in Bioinformatics



Molecular Databases

Nucleic acid sequences: GenBank, DNA Data Bank of Japan, EMBL Nucleotide Sequence Database

Nucleic acid structures: NDB - Nucleic Acid Database

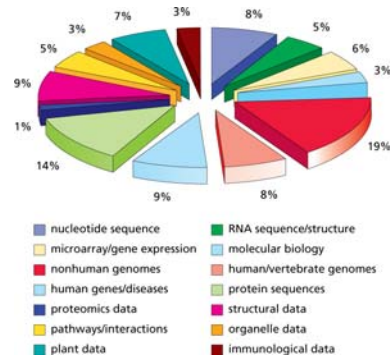
Protein sequences: PIR - Protein Information Resource, SWISS-PROT

Protein structures: PDB - Protein Data Bank, NRL_3D

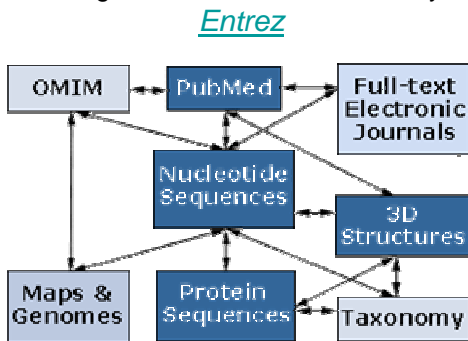
Physical properties: Biological Macromolecule Crystallization Database, BioMagResBank

Molecular images: SWISS-3DIMAGE, Molecules R US

Molecular Databases



NCBI integrated search and retrieval system



NCBI Databases

- **nr** - All non-redundant GenBank CDS translations+PDB+SwissProt+PIR
- **month** - All new or revised GenBank CDS released in the last 30 days
- **swissprot** - the last major release of the SWISS-PROT protein sequence database (no updates)
- **yeast** - Yeast (*Saccharomyces cerevisiae*) protein sequences.
- **E. coli** - *E. coli* genomic CDS translations
- **pdb** - Sequences derived from the 3-dimensional structure Brookhaven Protein Data Bank
- **kabat** - Kabat's database of sequences of immunological interest

Database



Database

database	a collection of related structured information about entities
file	a collection of records
record	a set of fields
field	a single characteristic of an entity
character	a symbol used in data field

Example of a Genbank entry

```

LOCUS      VIBHALUXA 3141 bp DNA BCT 15-FEB-1996
DEFINITION V.harveyi luciferase alpha and beta subunit (luxA and luxB) genes,
            complete cds.
ACCESSION  M10961, M13494
NID        g155174
KEYWORDS   luciferase.
SOURCE     Vibrio harveyi DNA.
ORGANISM   Vibrio harveyi
            Eubacteria; Proteobacteria; gamma subdivision; Vibrionaceae;
            Vibrio.
REFERENCE  1 (bases 1 to 1838)
AUTHORS    Cohn,D.H., Milcham,A.J., Simon,M.I., Nealson,K.H., Rausch,S.K.,
            Bonam,D. and Baldwin,T.O.
TITLE      Nucleotide sequence of the luxA gene of Vibrio harveyi and the
            complete amino acid sequence of the alpha subunit of bacterial
            luciferase
JOURNAL    J. Biol. Chem. 260 (10), 6139-6146 (1985)
MEDLINE    85207595
REFERENCE  2 (bases 1745 to 3141)
AUTHORS    Johnston,T.C., Thompson,R.B. and Baldwin,T.O.
TITLE      Nucleotide sequence of the luxB gene of Vibrio harveyi and the
            complete amino acid sequence of the beta subunit of bacterial
            luciferase
JOURNAL    J. Biol. Chem. 261 (11), 4805-4811 (1986)
MEDLINE    86168191
    
```

Example of a Genbank entry

```

FEATURES             Location/Qualifiers
     gene             707..1774
                     /gene="luxA"
     CDS              707..1774
                     /gene="luxA"
                     /codon_start=1
                     /product="luciferase alpha subunit"
                     /db_xref="PID:g155175"
                     /transl_table=11
                     /translation="MHPGNPFLTYQPPELSQTEVMKRLVNLGKASEGCGFDTVLLEH
                     HPTFGLLGNPVVAAHLGATETLVGTAAIVLPTAHFVQAEDEVNLLDQMSKGRFR
                     FGCICRGLYKDFRVFVTMDNSRALMDCWYDLMKEGFNEGYIAADNEHLKFPKIQLNP
                     SAYTQGGAPVYVVAESASTTEWAAERGLPMLSWINTHEKKAQLDLNVEVATEHGVD
                     VTKIDHCLSVITSDVHDSNRKADICRNLFLGHVYDSVYVNAATKLPFDDSDQTKGYDFNKGQ
                     WRDFVLKGHKDTNRRIDYSYEINPVGTPEECIAIQDDIDATGIDNICGFEANGSEE
                     EIIASMKLFQSDVMPYLKERQ"
BASE COUNT          883 a      665 c      741 g      852 t
ORIGIN              1 bp upstream of EcoRI site.
     1  gaattcacca  tgacgacggy  caaaaatagt  ttgtgcactg  ttatcactg  gctgcagacc
     61  aagggcacac  aaacatggy  ctgattgcy  gcaagtctct  cagctcgtg  cgccatgaa
    121  gttatctctg  atctggagct  gtctttctg  attactcgy  ttggttgyt  gaacttgcgt
    181  gacacactag  aaaaagcgt  tggtttgat  tacctcagtt  tgccatcga  tgagctacca
     ....
    
```