# **Integrating Heterogeneous Biological Databases**

Russ B. Altman MIS 214/ CS 427

## An explosion of biological data

# **Biological data is usually stored in special purpose, focused collections of data:**

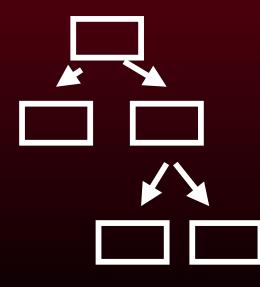
- DNA sequence
- Protein sequence
- Protein structure
- Mutations leading to disease
- Sequence motifs associated with function
- Biological literature
- Genome organization information

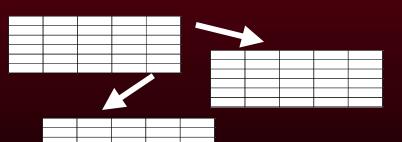
In addition, there are "virtual databases" created by application programs that associated data with other data.

## Methods for storing biological data

Biological data can be organized in many different manners:

Flat text files databases
 Relational databases
 Object oriented databases





LOCUS SYNWHLMG 507 bp DNA SYN 15-MAR-1989
DEFINITION Sperm whale synthetic myoglobin gene, complete cds.
ACCESSION 103666
NID #209563
KEYWORDS myoglobin.
SOURCE Synthetic DNA.
ORGANISM artificial sequence
artificial sequence.
REFERENCE 1 (bases 1 to 507)
AUTHORS Springer.B.A. and Sligar.S.G.
TITLE High-level expression of sperm whale myoglobin in Escherichia coli
JOURNAL Proc. Natl. Acad. Sci. U.S.A. 84, 8961-8965 (1987)
MEDLINE 88097408
FEATURES Location/Qualifiers
source 1.507
/organism="artificial sequence"
/db_sref="taxon:29278"
CDS 34498
/note="synthetic myoglobin"
/codon_start=1
/db_xref="PID g209564"
/transl_table=11
/translation="MVLSEGEWQLVLHVWAKVEADVAGHGQDILIRLFKSHPETLEKF
DRFKHLKTEAEMKASEDLKKHGVTVLTALGAILKKKGHHEAELKPLAQSHATKHKIPI
KYLEFISEAIIHVLHSRHPGNFGADAQGAMNKALELFRKDIAAKYKELGYQG"
BASE COUNT 155 a 108 c 115 g 129 t ORIGIN
l etgeagataa etaactaaag gagaacaaca acaatggtte tgtetgaagg tgaatggeag
61 etggttetge atgtttggge taaagttgaa getgaegteg etggteatgg teaggaeate
121 ttgattegae tgtteaaate teateeggaa aetetggaaa aattegateg ttteaaaeat
181 etgaaaaetg aagetgaaat gaaagettet gaagatetga aaaaaeatgg tgttacegtg
241 ttaactgeee taggtgetat eettaagaaa aaagggeate atgaagetga geteaaaeeg
301 ettgege aat egeatgetae taaacataag ateeegatea aataeetgga atteatetet

### **Flat Text File**

- Entries are stored in text.
- Text fields/attributes are labelled with identifiers
- May be standard vocabulary used for values of attributes (or not)
- Search by searching for text
- Can be indexed for faster search
- Easy to import/export
- Not platform dependent
- Ubiquitous
- Hard to do complicated queries

507 bp DNA LOCUS SYNWHLMG SYN 15-MAR-1989 Sperm whale synthetic myoglobin gene, complete cds. DEFINITION ACCESSION J03566 NID q209563 myoglobin. KEYWORDS Synthetic DNA. SOURCE ORGANISM artificial sequence artificial sequence. REFERENCE 1 (bases 1 to 507) AUTHORS Springer, B.A. and Sligar, S.G. High-level expression of sperm whale myoglobin in Escherichia coli TITLE Proc. Natl. Acad. Sci. U.S.A. 84, 8961-8965 (1987) JOURNAL MEDLINE 88097408 Location/Qualifiers FEATURES 1..507 source /organism="artificial sequence" /db xref="taxon:29278" CDS 34..498 /note="synthetic myoglobin" /codon start=1a /transl table=11 /db xref="PID:g209564" /translation="MVLSEGEWQLVLHVWAKVEADVAGHGQDILIRLFKSHPETLEKF DRFKHLKTEAEMKASEDLKKHGVTVLTALGAILKKKGHHEAELKPLAQSHATKHKIPI KYLEFISEAIIHVLHSRHPGNFGADAOGAMNKALELFRKDIAAKYKELGYOG" 115 g BASE COUNT 155 a 108 c 129 t 5 bp upstream of PstI site. ORIGIN 1 ctgcagataa ctaactaaag gagaacaaca acaatggttc tgtctgaagg tgaatggcag 61 ctggttctgc atgtttgggc taaagttgaa gctgacgtcg ctggtcatgg tcaggacatc 121 ttgattcgac tgttcaaatc tcatccggaa actctggaaa aattcgatcg tttcaaacat 181 ctgaaaactg aagctgaaat gaaagcttct gaagatctga aaaaacatgg tgttaccgtg 241 ttaactgccc taggtgctat ccttaagaaa aaagggcatc atgaagctga gctcaaaccg 301 cttgcgcaat cgcatgctac taaacataag atcccgatca aatacctgga attcatctct 361 gaagcgatca tccatgttct gcattctaga catccaggta acttcggtgc tgacgctcag 421 ggtgctatga acaaagctct cgagctgttc cgtaaagata tcgctgctaa gtacaaagaa 481 ctgggttacc agggttaatg aggtacc

### **Structured Flat File**

Use a standard syntax for facilitating automated reading of flat text files. Publications ={ [title: string, authors: { [[name: string, initial: string] ]], journal: <uncontrolled: string, controlled: <medline-jta: string, % Medline journal title abbreviation iso-jta: string, % ISO journal title abbreviation journal-title: string, % Full journal title issn: string>> % ISSN number volume: string. issue: string, year: int, pages: string, abstract: string. keywd: {string}]}

### **Relational Database**

All data represented in tables, representing relations within the data.

R1(A|B,C,D) R2(B|E,F) etc...

The collection of tables represents the information represented in the database.

Easy to perform basic operations, since structure is very constrained. sequences:

Column name, type, length, nulls? seq\_id , ddt\_int\_id , 4 , 0 seq\_lab\_symbol , varchar , 40 , 8 sequence , text , 16 , 0 sts\_flag , ddt\_flag\_tiny , 1 , 0

Primary key(s) seq\_id

seqd\_dict:

Column name, type, length, nulls? seqd\_code , ddt\_dict\_char\_code , 1 , 0 seqd\_desc , ddt\_dict\_desc , 255 , 0

Primary key(s) seqd\_code

### **Object oriented databases**

- Data organized into a hierarchy of concepts or *classes*.
- Each concept has a set of *attributes*, which can have typed values.
- Concepts can *inherit* values of attributes fromparents in the hierarchy.
- Can model richer set of relationships than the relational model...but queries are not as efficient for that reason.

Class: Molecule name: molecular-weight: type:

> Class: Polymer name: molecular-weight: type: length: sequence: basic subunit:

Class: DNA name: molecular-weight: type: nucleic-acid length: basic subunit: base sequence:

#### Class: Protein name: molecular-weight: type: polypeptide length: basic subunit: amino acid sequence:

# Problem: performing queries across databases

**Example:** *Find the DNA sequences associated with a 3D protein structure.* 

**Problem:** 3D protein structure stored in PDB DNA sequences stored in GENBANK

**Example:** Find the a mutation of a 3D protein structure known to cause disease.

**Problem:** 

**3D** protein structure stored in PDB DNA sequences stored in GENBANK Mutations in sequences stored in OMIM.

# Why is integration hard?

- vocabularies not shared different terms for same concept
- same term for different concepts different dependencies in the data
  - inheritance in object oriented systems implies relations
  - tables in relations imply logical connections
- queries are very different in the systems
  - text search
  - SQL
  - OOSQL
- different formats even when semantics are shared
- different semantics for basic concepts

# Creating integrated access to databases for performing queries.

**Two strategies:** 

- **1.** Consolidation
  - create single homogenous mega-DB
  - required DBs to use same tables, concepts
- 2. Federation
  - incorporate links from between DBs
  - couple the DBs loosely with common query language
  - construct a data warehouse

### **Fundamental data integration issues**

Integrating two databases fundamentally involves identifying information that is implicitly or explicitly shared, and can be used to create new relationships from existing ones.

Database X: R1(A|B,C) Database Y: R2(B|D,E)

Allows new relation R3(A,B,C,D,E) to be created.

# **Linking databases**

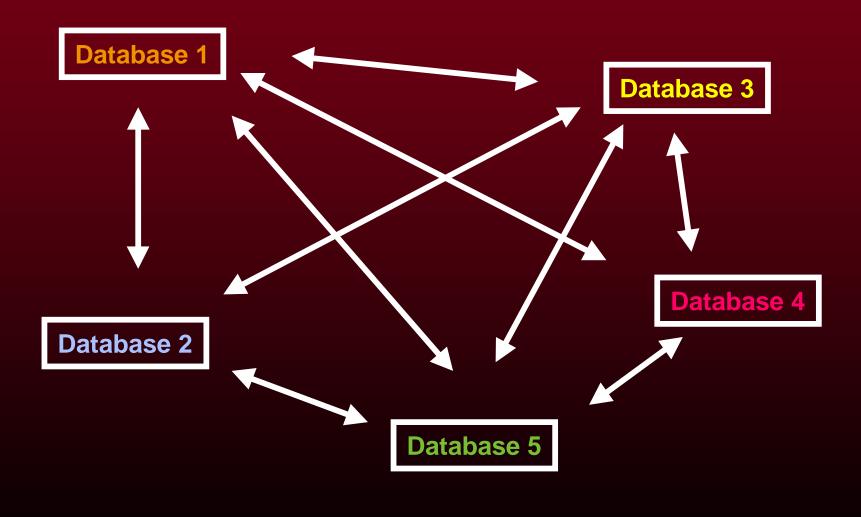
To link two databases, need to

- **1. Identify the critical shared data elements that allow relationships to be combined.**
- 2. Need to be sure that semantics of the shared data is similar.
- 3. Need to create theasaurus for corresponding concepts.

This creates a mapping from DB-1 to DB-2

For N databases  $O(N^2)$  mappings needed?

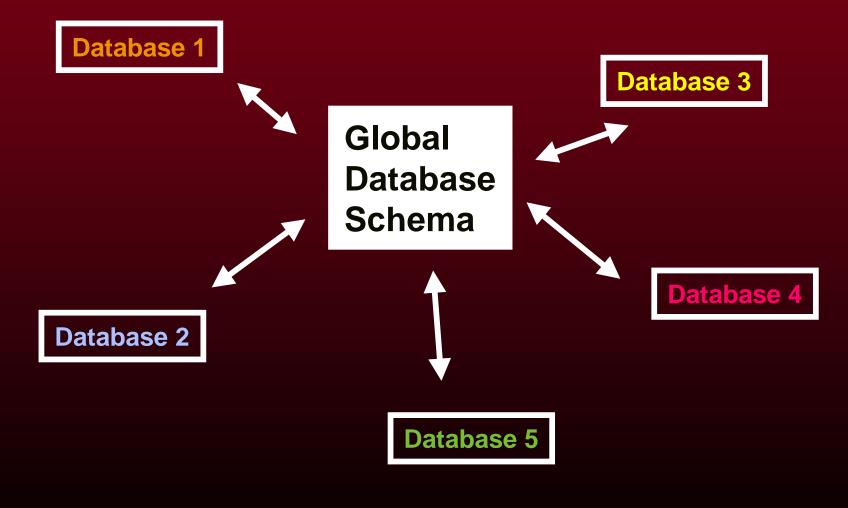
# Integration requiring lots of mappings



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### **Global Schema**

The  $O(N^2)$  problem can be avoided by defining a single GLOBAL schema to which all databases can be mapped--only O(N) mappings required.



## **Creating Global Schema**

Global schemas are very difficult to create, since they must be general enough to handle any type of data in the contributing databases.

Levels of "globality"

 Global query model
 -write queries in local language, but then combine queries as needed at global level (KLEISLI).

2. Global data model and query model
--write queries in global language, less knowledge of local structure required (OPM)

## Consolidation

- Gather together data of interest, and translate it once into common database structure, with all incompatibilities "scrubbed out."
- Remove the contributing legacy DBs once and for all.
- Rarely done--more likely in industry
- Nontrivial to resolve semantic incompatibilities
- Nontrivial to scrub data to match resolved semantics
- With rapidly growing data, one time translation is not adequate.

### **Federation 1: incorporate links** within databases to one another

- Often hypertext links from item in A to item in B.
- Data retrieval by traversal of links
- No other compatibility imposed on DBs
- Prone to missing or inconsistent links, especially in the setting of rapidly growing databases (are links static or dynamically computed?)
- No general purpose query facility to retrieve multiple records that satisfy some set of general requirements.
- Most commonly used technique: DBGET and SRS

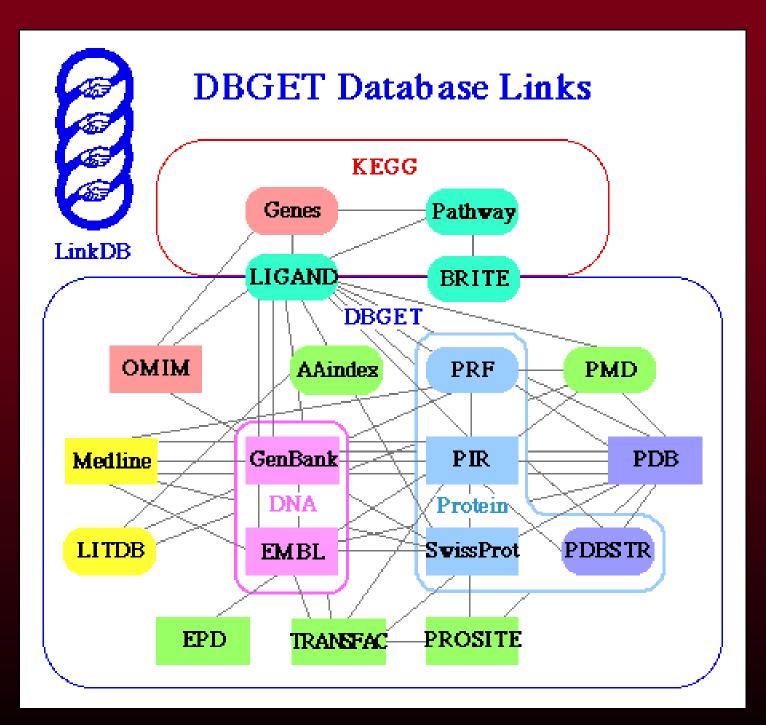
HEADER	OXYGEN STORAGE 05-APR-73 1MBN	1MBNH	1
COMPND	MYOGLOBIN (FERRIC IRON - METMYOGLOBIN)	1MBN	4
SOURCE	SPERM WHALE (PHYSETER CATODON)	1MBNM	1
AUTHOR	H.C.WATSON, J.C.KENDREW	1MBNG	1
REVDAT	20 27-OCT-83 1MBNS 1 REMARK	1MBNS	1
JRNL	AUTH H.C.WATSON	1MBNG	2
JRNL	TITL THE STEREOCHEMISTRY OF THE PROTEIN MYOGLOBIN	1MBNG	3
JRNL	REF PROG.STEREOCHEM. V. 4 299 1969	1MBNG	4
JRNL	REFN ASTM PRSTAP US ISSN 0079-6808 419	1MBNG	5
REMARK	1	1MBNG	б
REMARK	1 REFERENCE 1	1MBNQ	1
REMARK	1 AUTH J.C.KENDREW	1MBNQ	2
REMARK	1 TITL MYOGLOBIN AND THE STRUCTURE OF PROTEINS (NOBEL	1MBNQ	3
REMARK	1 TITL 2 LECTURE, DECEMBER 11, 1962)	1MBNQ	4
REMARK	1 REF PRIX NOBEL 103 1963	1MBNQ	5
REMARK	1 REFN ASTM PRIXAL SW ISSN 0546-8175 945	1MBNS	2
REMARK	10 CORRECTION. REORDER THE ATOMS OF THE HEME GROUP AND CHANGE	1MBNF	35
REMARK	10 THE CONECT RECORDS CORRESPONDINGLY. 23-AUG-77.	1MBNF	36
SEQRES	1 153 VAL LEU SER GLU GLY GLU TRP GLN LEU VAL LEU HIS VAL	1MBN	39
SEQRES	2 153 TRP ALA LYS VAL GLU ALA ASP VAL ALA GLY HIS GLY GLN	1MBN	40
HET	HEM 1 44 PROTOPORPHYRIN IX WITH FE(OH), FERRIC	1MBND	10
FORMUL	2 HEM C34 H32 N4 O4 FE1 +++ .	1MBNG	25
FORMUL	2 HEM H1 O1	1MBNG	26
HELIX	1 A SER 3 GLU 18 1 N=3.63,PHI=1.73,H=1.50	1MBN	52
HELIX	2 B ASP 20 SER 35 1 N=3.72,PHI=1.69,H=1.47	1MBN	53
HELIX	3 CHIS 36 LYS 42 1 SHORT IRREGULAR HELIX	1MBN	54
3			
SITE	1 HMB 9 PHE 43 ARG 45 HIS 64 VAL 68	1MBNN	4
CRYST1	64.500 30.900 34.700 90.00 106.00 90.00 P 21 2	1MBN	65
ORIGX1	1.00000 0.00000 0.00000 0.00000	1MBN	66
ORIGX2	0.00000 1.00000 0.00000 0.00000	1MBN	67
ORIGX3	0.00000 0.00000 1.00000 0.00000	1MBN	68
SCALE1	.01550 0.00000 .00445 0.00000	1MBN	69
SCALE2	0.00000 .03236 0.00000 0.00000	1MBN	70
SCALE3	0.00000 0.00000 .02998 0.00000	1MBN	71
ATOM	1 N VAL 1 -2.900 17.600 15.500 1.00 0.00 2	1MBN	72
ATOM	2 CA VAL 1 -3.600 16.400 15.300 1.00 0.00 2	1MBN (	C <b>7</b> 3yright R

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- ID AGP1\_YEAST STANDARD; PRT; 633 AA.
- AC P25376;
- DT 01-MAY-1992 (REL. 22, CREATED)
- DT 01-MAY-1992 (REL. 22, LAST SEQUENCE UPDATE)
- DT 01-NOV-1997 (REL. 35, LAST ANNOTATION UPDATE)
- DE ASPARAGINE/GLUTAMINE PERMEASE.
- GN AGP1 OR YCL25C.
- OS SACCHAROMYCES CEREVISIAE (BAKER'S YEAST).
- OC EUKARYOTA; FUNGI; ASCOMYCOTINA; HEMIASCOMYCETES.
- RN [1]
- RP SEQUENCE FROM N.A.
- RA HOLLENBERG C.P., KLEINHANS U., LUETZENKIRCHEN K., RAD M.R., XU G.;
- RL SUBMITTED (MAR-1992) TO EMBL/GENBANK/DDBJ DATA BANKS.
- RN [2]
- **RP** CHARACTERIZATION.
- RA SCHREVE J.L., SIN J., GARRETT J.M.;
- RL UNPUBLISHED OBSERVATIONS (JUL-1997).
- CC -!- FUNCTION: BROAD SUBSTRATE RANGE PERMEASE WHICH TRANSPORTS CC ASPARAGINE AND GLUTAMINE WITH INTERMEDIATE SPECIFICITY.
- CC -!- SUBCELLULAR LOCATION: INTEGRAL MEMBRANE PROTEIN (PROBABLE).
- CC -!- SIMILARITY: BELONGS TO A FAMILY THAT GROUPS MANY AMINO ACID CC PERMEASES.
- DR EMBL; X59720; E264437; -.
- DR PIR; S19352; S19352.
- DR SGD; L0003271; AGP1.
- DR PROSITE; PS00218; AMINO\_ACID\_PERMEASE; 1.
- KW TRANSPORT; AMINO-ACID TRANSPORT; TRANSMEMBRANE.
- FT TRANSMEM 125 141 POTENTIAL.
- FT TRANSMEM 152 169 POTENTIAL.
- FT TRANSMEM 191 214 POTENTIAL.

### **Swiss-Prot**



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### LinkDB Search Result

#### Database: LinkDB

Database of Link Information Release 98-05-14, May 98 Institute for Chemical Research, Kyoto University 5,131,470 entries

#### PDB : 1mbn - related entries

Factual Links (9 hits from 5 databases)

- 1. SWISS-PROT (1)
- 2. PIR (2)

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- 3. PDBSTR (1)
- 4. PROSITE (1)
- 5. MEDLINE (4)
- 6. All databases (9)

Link table for PDB

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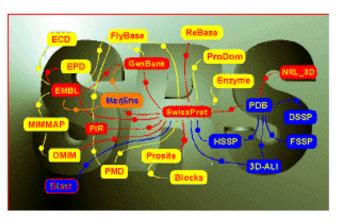
#### SRSWWW at EMBL-EBI, Hinxton, UK - Netscape

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### Sequence Retrieval System

Network Browser for Databanks in Molecular Biology





Start a new SRS session



The SRS Manual



SRS World Wide



The SRS newsgroup



- A.

SRS Developers

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#### http://www.pdb.bnl.gov/

#### Data-fields in SRS

Name	Short Name	Туре	No of Keys	No of Entry References	Indexing Date	Status
ID	id	ID	7596	7596	5/14/98	ok
Date	dat	int	2086	7596	5/14/98	ok
Supersedes	spr	string	299	304	5/14/98	ok
Compound	com	string	8107	126425	5/14/98	ok
Source	src	string	5192	86294	5/14/98	ok
<b>EntryAuthors</b>	eat	string	7293	26243	5/14/98	ok
Authors	aut	string	15149	66912	5/14/98	ok
Title	tit	string	8107	126425	5/14/98	ok
JournalName	jnl	string	757	19601	5/14/98	ok
<u>Remark</u>	rem	string	51338	1741048	5/14/98	ok
CRYST1	er1	show				not indexed
<u>ORIGXn</u>	ori	show				not indexed
SCALEn	sca	show				not indexed
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TVECT	tve	show				not indexed
MODEL	mod	show				not indexed

Links To

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none

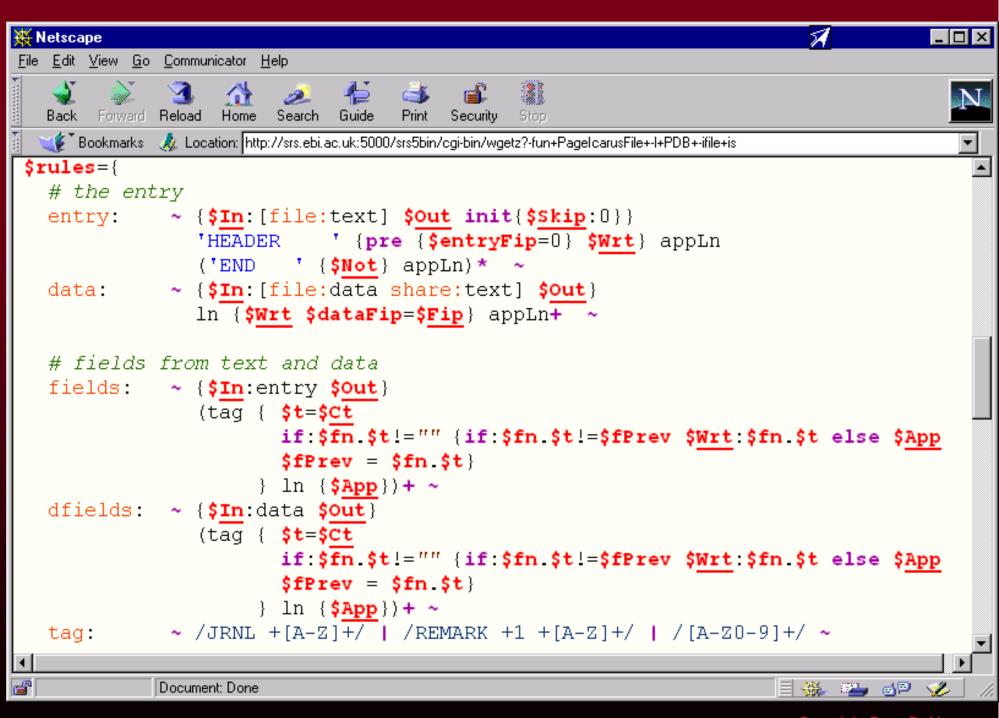
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<pre>format:@PDB_FORMAT maxNameLen:30 ifiles:{"pdb.i" "pdb.is"}</pre>	
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\$field:@DF ALL	
<b>field</b> : [@DF HeaderField name: 'Title Section']	
<b>field</b> : [@DF ID code:header index:id indexToken:id]	
<pre>\$field:[@DF Date code:header index:int indexToken:date]</pre>	
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tableToken:'t_fields compnd']	
<pre>\$field:[@DF_Source code:source index:str indexToken:'wordX source'</pre>	
tableToken:'t_fields source']	
<pre>\$field:[@DF_EntryAuthors code:author index:str indexToken:author]</pre>	
<pre>\$field:[@DF_Authors code:auth index:str indexToken:auth]</pre>	
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### **Federation 2: couple DBs loosely**

- Construct queries over multiple DBs without touching the DBs themselves
- Create query processor which can map query to individual search capabilities of DBs and integrate answer together
- Kleisli: uses common query language, with queries mapped directly into valid searches in the local DB.
  OPM: uses common data model, and maps local DBs onto the common model, and then queries the model (with translation into local DB)

#### Net External Data Drivers shell Servers ML<-Queries Data -> GenBank ASN.1 С ASN.1 Ю Kleisli CFLSybase Library perl5 GDB Sybase BLAST prolog Optimizer AceDB HTML Chr224b Sybase Key Open Local Socket NCBI Data AceDB Stream BLAST (pipe)

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### Sample Kleisli Syntax

For relational database like GDB, define query to determine whether entry is part of chromosome 22:

```
define GDB == Open-Sybase([server="GDB",
    user="guest", password="smith@stanford"]);
define Loci22 == GDB([query=
        "select locus_symbol, genbank_ref
        from locus
        where loc_cyto_chrom_num = `22'"])
For flat text file database Genbank, find accession number:
define Genbank==Open-ASN([server="NCBI",
    user="guest", password = "")];
define ASN-IDs==\accession =>
Genbank([db="na", select="accession" ^ accession,
        path = "Seq-entry.seq.id..giim",args=[]]);
```

Query for all genbank entries that occur on chromosome 22: {[locus=locus]| \locus <- Loci22, \uid<- ASN-IDs(locus.genbank\_ref)}

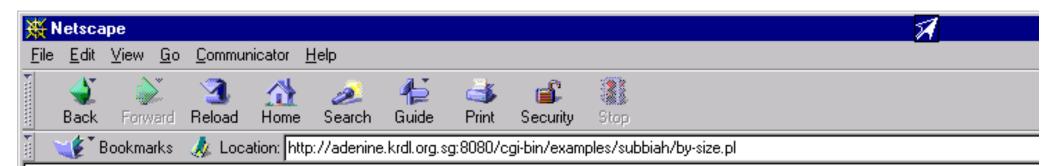


Determine which sequences of unknown structure should be prioritized for structure determination.

Insight: Find sequences that are referred to in literature at high rate, but which don't have a structure.

### Query plan:

- 1. Extract all sequences of known structures from SCOP
- 2. Extract all sequences of proteins from Swiss-Prot
- **3.** Remove from (2) all homologous to (1)
- 4. Cluster remaining sequences with BLAST
- 5. Rank clusters based on number of MEDLINE references to members of the cluster



### **Proteins of Unknown Structure**

Clusters that have at least 3 members and at least Medline references. Members of these clusters does not have any BLAST-relationship at a pscore better than 1.0E-4 to any protein of known structure. Members of the same cluster are BLAST-related at a pscore no more than 1.0E-4. The clusters are sorted by Medline count.

- cluster-rep <u>mus musculus (mouse). kappa-type opioid receptor (kor-1) (msl-1). 10/96</u> cluster-size <u>8942</u> medline-count <u>8058</u>
- cluster-rep bacillus subtilis, probable aldehyde dehydrogenase ycbd (ec 1.2.1.3), 10/96 cluster-size <u>192</u> medline-count <u>195</u>
- 3. cluster-rep sulfolobus solfataricus, aspartate aminotransferase (ec 2.6.1.1) (transaminase a) (aspat), 11/95 cluster-size <u>170</u> medline-count <u>179</u>
- cluster-rep bos taurus (bovine). acetylcholine receptor protein, delta chain precursor. 10/96 cluster-size <u>144</u> medline-count <u>173</u>

# **Sample OPM query**

Find name and annotation in GSDB of Gene called ACHE in GDB.

SELECT Name = GSDB:gene.name, Annotation = GDB:Gene.annotation FROM GSDB:Gene, GDB:Gene WHERE GDB:Gene.accessionID = GSDB.Gene.gdb\_xref AND GSDB:Gene.name = "ACHE"

#### 💥 The Genome Database - Netscape

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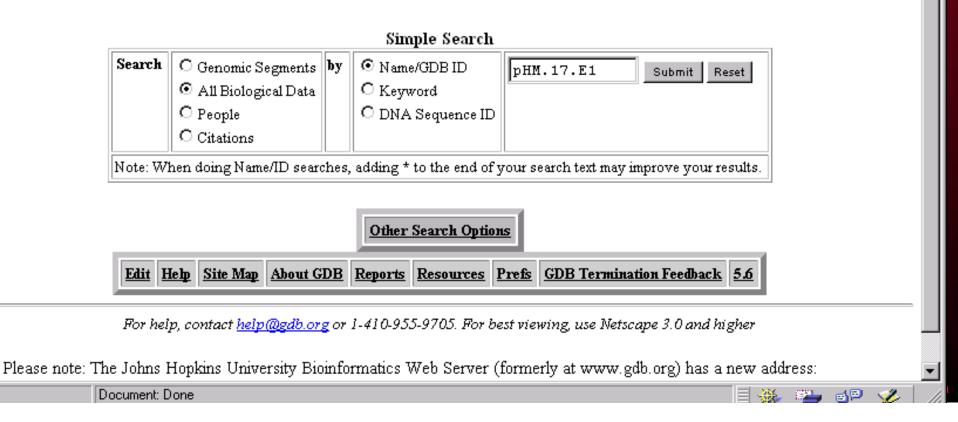
### The Genome Database

An international collaboration in support of the Human Genome Project.

Hosted by The Johns Hopkins University School of Medicine, Baltimore, Maryland USA and available at <u>mirror sites</u> <u>worldwide</u> What's New (9-Mar-98):

- GDB 6.4 released (includes Mapview 2.4)
- New Mirror Site in Taiwan
- Bioinformatics Seminar Series
- GDB Termination Announcement

#### GDB Termination Announcement

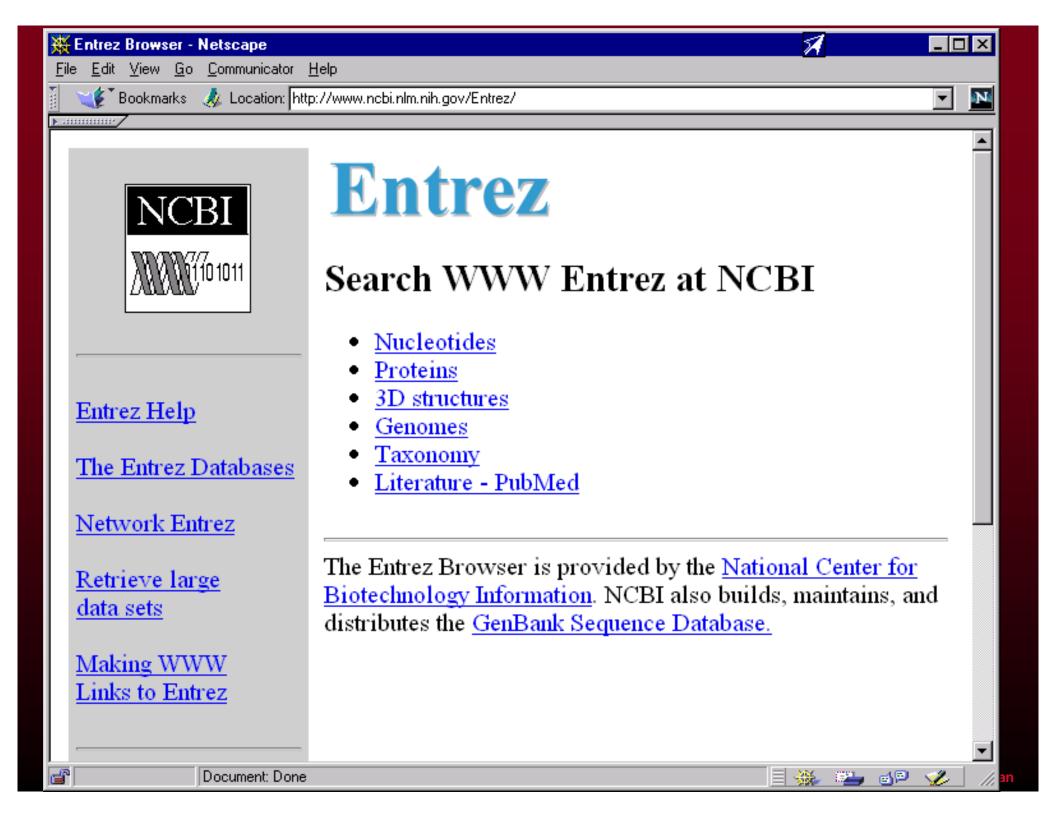


### **Federation 3: Data warehouse**

- Develop a global schema for all the data in the DBs
- Data are tranformed into this common schema and loaded in central repository on a regular basis
- Query facilities provided by central repository
- Need to update global schema if/when local DBs change their data formats/schemas
- Similar to consolidation strategy, but local DBs remain and are synchronized in the global DB.

### ENTREZ system from NCBI http://www.ncbi.nlm.nih.gov/Entrez/

- 1. All data is translated into Abstract Syntax Notation (ASN.1) structured files.
- 2. Most links to other parts of database are determined at the time of translation into ASN.1
- **3.** Some dditional links can be computed on the fly using keyword searches, sequence similarity searches, or any other comparison metrics over the entire DB.
- 4. Updates are performed at regular interval.



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<u>link</u> , or <u>1528 protein neighbors</u> )						
□ P02185						
MYOGLOBIN						
gi 127687 sp P02185 MYG_PHYCA [127687]	7					
(View <u>GenPept Report, FASTA report,ASN.1 report,Graphical view,4 MEDLIN</u> links, or 987 protein neighbors )	2					
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### **ASN.1 version of data record**

```
Seq-entry ::= seq {
  id {
   pdb {
     mol "1MBN" ,
     rel
        std {
         year 1994 ,
         month 1 \} \}
   gi 230152 } ,
 descr {
   pdb {
      deposition
        std {
          year 1973 ,
         month 4,
          day 5 },
      class "Oxygen Storage" ,
      compound {
        "Myoglobin (Ferric Iron - Metmyoglobin)" } ,
      source {
        "Sperm Whale (Physeter Catodon)" } ,
      exp-method "X-Ray Diffraction" },
AND MORE...
```