

PERSPECTIVES OF DATABASES AND PROGRAM TOOLS DEVELOPMENT IN BIOINFORMATICS

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Outline of talk



Biological data growth in post-genomic era Bioinformatics resources development

New IT solutions for bioinformatics



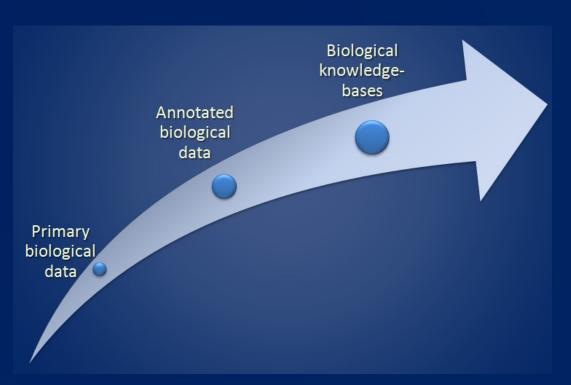
"Bioinformatics is the science of managing, mining, and interpreting information from biological data" *

*- http://bio.informatics.iupui.edu/biokdd10/

BIOLOGICAL DATA GROWTH IN POST-GENOMIC ERA

Biological data growth in post-genomic era

- Information flow
- New 'omics' era
- Worldwide projects

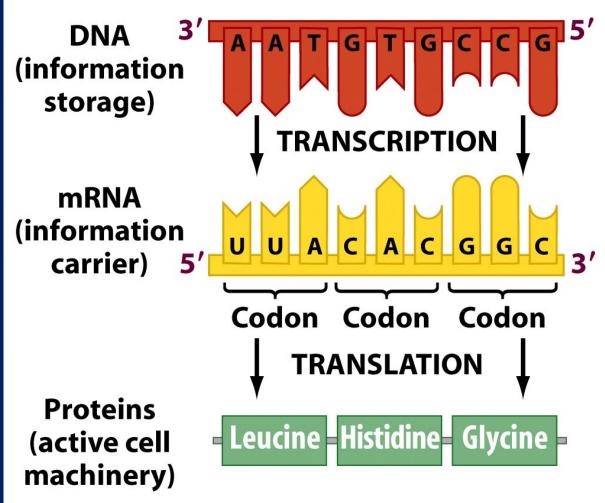


Biological information carriers

| Object | Polymer | Monomers | Types of mono- mers | Approx. length (nbases) | Biological function | Template for synthesis |
|------------|-------------------------------|-----------------------------|---------------------------|-------------------------------|---|--|
| Gene | DNA | (deoxyribo)- nucleotides | 4 (AGCT) | 10,000 - 100,000 | Information storage | Compleme ntary DNA strand |
| Transcript | RNA | (ribo)- nucleotides | 4 (AGCU) | ?<50 - 10,000 | Information messenger, catalysis, regulation | Gene (1 strand of DNA region) |
| Protein | Protein = poly- peptide | Amino acids | 20 + modified | 50-1,000 or more | Catalysis, transport, regulation, movement, cytoskeleton, etc. | mRNA (processed transcript) |

http://www.uic.edu/classes/bios/bios100/lectures/proteins.htm

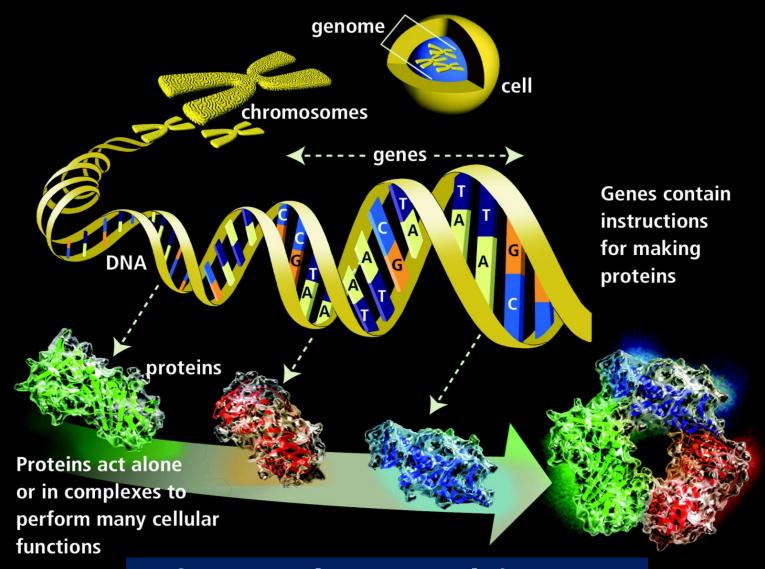
Information flows from DNA to RNA to proteins.



4³ types of triplets (codons)= 61 coding (for 20 types of AAs)+ 3 stops

Figure 15-10a Biological Science, 2/e

http://www.stanford.edu/group/pandegroup/folding/education/GAH/mol_mach.html



Sequence \rightarrow structure \rightarrow function

>chromosome:GRCh37:11:6451679:6462894:-1

CCTCATTACTGTCAACCCTTCACTTCCAGGCACTTTTTGCAAAGCCCTTTGCCAGTCAGG GAAGGCGAGAGGCTGGGCATGGGGCTTGGACATTTGACAACAGTGAGACATTATTGTCCC CAGACTCACTAGCCCAAGGGTAAAGCTGAAGAGGCTTGGGCATGCCCCAGAAAGGCCCCT GTTACTAAAAGTAGTAAGTATTGCTGTCTCTAGCTGCCTTAGAGCAGGGCTTGACACAGT ACACAGCAATATTAGTTCCCCTCCTTTTCTCACCTCCCCCATTGTGGAGATAAACTCAATC ACAAAAGGTGATCCTCAGTCTACTCACTTCCCTGACTTATGGATGCCTGGACCCATTGCC AGTGTGAGAGTCACAGCTGGACGTCAGCAGTGTAGCCCAGTTACTGCTTGAAAATTGCTG AAGGGGGTTGGGGGGGCAGCTGCCGGGAAAAAGGAGTCTTGGATTCAGATTTCTGTCCAGA CCCTGACCTTATTTGCAGTGATGTAATCAGCCAATATTGGCTTAGTCCTGGGAGACAGCA ACTGGTCACCCAGAGCTGTCCTGTGGCCTCTGCAGCTCAGCATGGCTAGGGTACTGGGAG CACCCGTTGCACTGGGGGTTGTGGAGCCTATGCTGGTCTCTGGCCATTGCCACCCCTCTTC CTCCGTGAGTAAAGCTGGGACTAGAAGCGAAGGATTGAGTTCTGGGCTAGGGTAAGGTAG GGCCAGTTTTTAGGCCTCGGTCAAATTTGGGGGTCAGGGGCTATGGGAAAGGGATCGGTCC CAATGGATCAAGATATCTATTTTGTTCTCCCCTAGGACTAGTGCCCATGGGAATGTTGCTG AAGGCGAGACCAAGCCAGACCCAGACGTGACTGGGGCCCTGACTCCCTAAGTCTGTC TTTTTTTTTTTTTTTTACTTTGCCATCTCCCTACCTCCACCCCAGAACGCTGCTCAGAT GGCTGGAGCTTTGATGCTACCACCCTGGATGACAATGGAACCATGCTGTTTTTTAAAGGT AGGAGGGACTGAGGTTAGGGCGTTTAGGACCTTAGACTTACTCCTCCCTTCACAAAGGGTGT CCCTGTCTGTGGGGAGGTCTTAGGAATTATCTGATGGTATCACTGACAGCTTCTCTCAAGC GAGTTTGTGTGGAAGAGTCACAAATGGGACCGGGAGTTAATCTCAGAGAGATGGAAGAAT TTCCCCAGCCCTGTGGATGCTGCATTCCGTCAAGGTCACAACAGTGTCTTTCTGATCAAG GTACTGCTGGGCCAAAATCAGGGCCAGGCTGGAAAGGGCTGGAATCGACACTGGGGACCC TGCCCTCCTTTCCTGTAAAAGCTTGGGCTAAGGGAGTGTGCATGCGTGTGGGCCTGGCAG GTGCACCATCCAGTGGCTGTTCTTCAGTCCTAGTCTTAGTTCTACACCGCTCTGCTGTAC

1D biological Information : sequences

> Gene of hemopexin (about 11,000 nb)

mRNA (1652 nb)

Protein (462 aa)

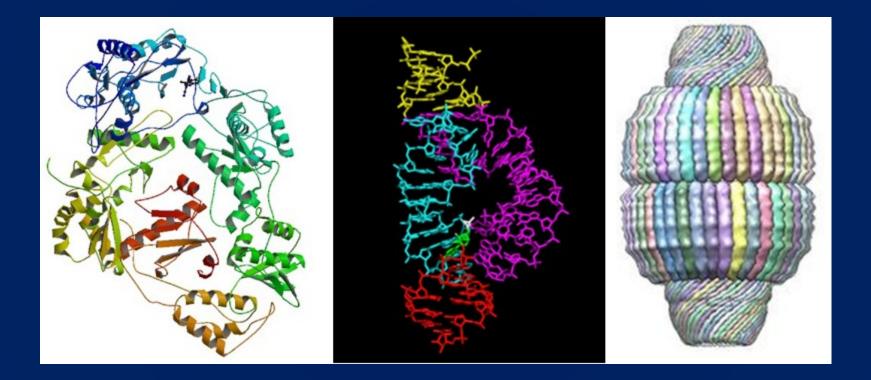
TGTATCAAGTCCTCTTCATAGGGCAAGGCAAGTTGTTCCCCAACACAATGGCACCTGGCT GAAGAGCATGTGGGAGCATGAAATCCAGTCTGC GCTGTGTCTGCTCAGAGGGAAGGGGTGCCTTTT GGGGGAAGTCCTGACTGTCGGCTTTGTTTTCCC TGTCTCATTCTATCTCAACCAGTTCCCTAATG ATATACCTTCCCTCAGTGATCTCAACCATCAC GACACTGGATCTAGATCTACTTTCTGAGCTCC CAGGCACCTAAAATTCAGCATCCCCCAAACTA TTTCCTCCTGTGTTTCCTGTTTCAGTAAATGA CAAGTGCACACAGGGTCTCATGATCTGGGCCT CCTGCCACATTCACTGTGTGCCAGCCATACGA CCTCATGTTTGGGCTCTGCATGCTGCCCCCC

>gi|11321561|ref|NP_000604.1| hemopexin precursor [Homo sapiens] MARVLGAPVALGLWSLCWSLAIATPLPPTSAHGNVAEGETKPDPDVTERCSDGWSFDATTLDDNGTMLFF KGEFVWKSHKWDRELISERWKNFPSPVDAAFRQGHNSVFLIKGDKVWVYPPEKKEKGYPKLLQDEFPGIP SPLDAAVECHRGECQAEGVLFFQGDREWFWDLATGTMKERSWPAVGNCSSALRWLGRYYCFQGNQFLRFD PVRGEVPPRYPRDVRDYFMPCPGRGHGHRNGTGHGNSTHHGPEYMRCSPHLVLSALTSDNHGATYAFSGT HYWRLDTSRDGWHSWPIAHQWPQGPSAVDAAFSWEEKLYLVQGTQVYVFLTKGGYTLVSGYPKRLEKEVG TPHGIILDSVDAAFICPGSSRLHIMAGRRLWWLDLKSGAQATWTELPWPHEKVDGALCMEKSLGPNSCSA NGPGLYLIHGPNLYCYSDVEKLNAAKALPOPONVTSLLGCTH

AACCTTGGAAAATTCCTGCTGATTTTTCAGCTCTTGGGCCCCAATGCTTCCTCTTTGGTGTG AAACCTTCCACAACTTCTCTGGGCAGACTTAGGCACTCTGTCTATATTCTCAGTGCACTC

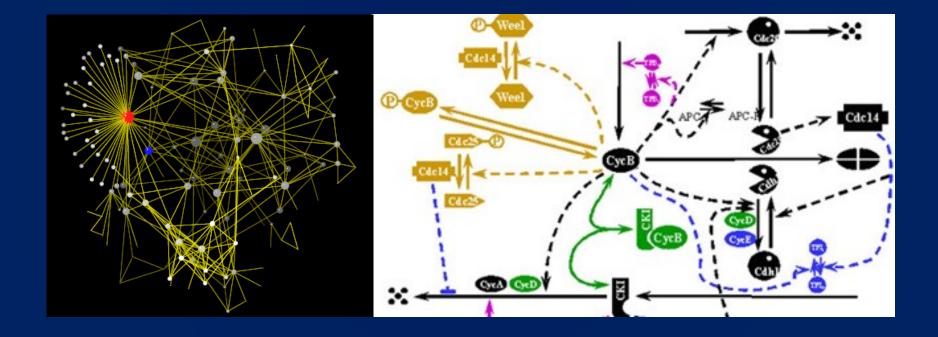
CTCACACTGCTGGCCATCCTTTTTTTCTCTGGCAATTGCTTCCCTTGCCTTCCATGACCC

3D biological Information : structure



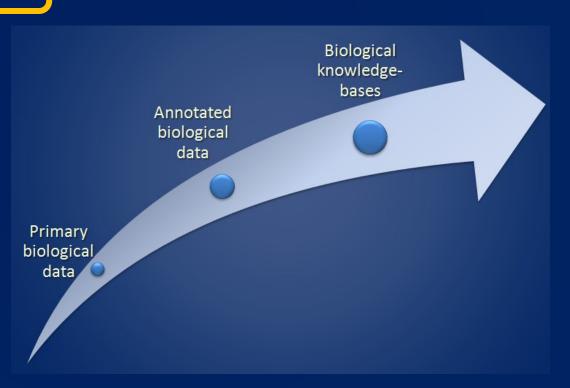
Proteins and RNAs Sequence determines structure

4D biological Information : networks, metabolites flows

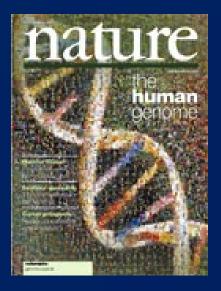


Biological data growth in post-genomic era

- Information flow
- New 'omics' era
- Worldwide projects



2001: publication of human genome





Nature **409**, 745 (15 February 2001)

Science 16 February 2001: Vol. 291, pp. 1304 - 1351

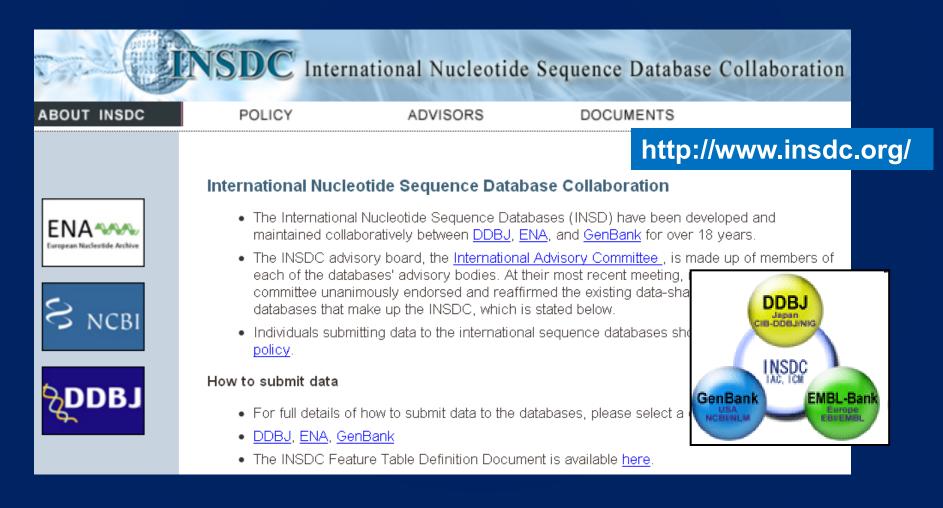
Pre-genomic \rightarrow Post-genomic era

Bioinformatics analysis for 'omics' era in biology

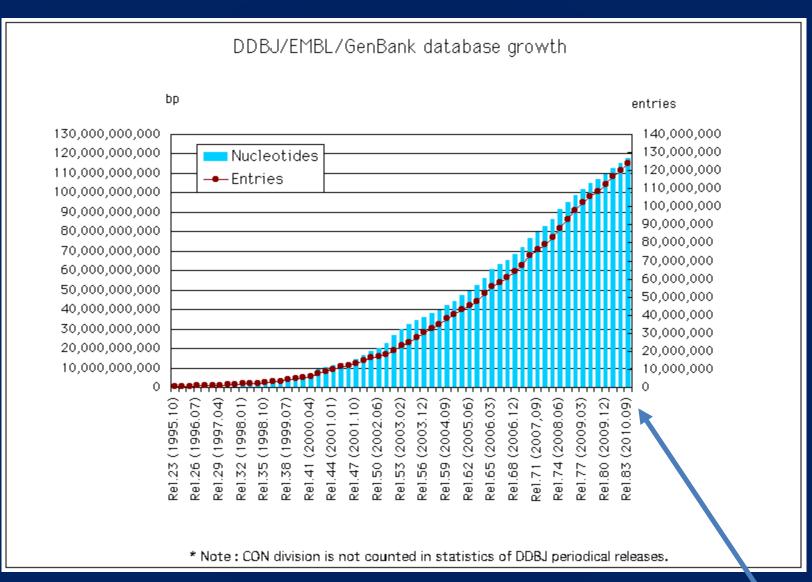
| 'omics' | Object for study | Types of analysis |
|-----------------|--|---|
| Genomics | Genome (full set of genes) | Genome assembly, gene finding, gene structure analysis, regulators identification, finding of sites of regulators binding with DNA |
| Transcriptomics | Transcriptome (full set of transcripts: mRNAs, rRNAs, tRNAs, ncRNAs) | Analysis of gene expression, RNA processing, splicing isoforms , RNA structure, ncRNAs functions |
| Proteomics | Proteome (entirety of proteins) | Proteome analysis, identification of proteins, analysis and prediction of protein structure and interactions |
| Metabolomics | Metabolome (set of metabolites, regulators) | Small molecules identification, analysis of their transformations |

International Nucleotide Sequence Database Collaboration

- •GenBank (USA)
- •EMBL-Bank (Europe)
- •DDBJ (DNA Databank of Japan)



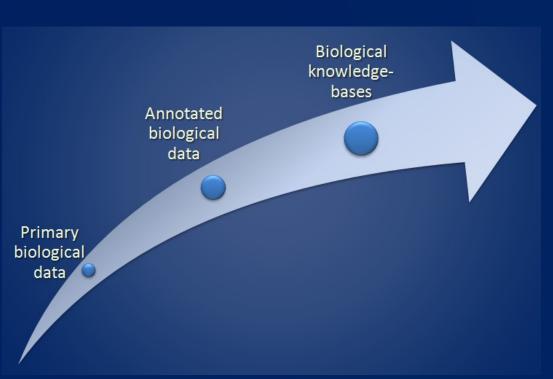
http://www.ddbj.nig.ac.jp/images/breakdown_stats/DBGrowth-e.gif





Biological data growth in post-genomic era

- Information flow
- New 'omics' era
- Worldwide projects



http://www.1000genomes.org/page.php

1000 Genomes

A Deep Catalog of Human Genetic Variation



| Home About Data Analysis Participants Contact Browser Wiki | | | | | | |
|--|-----------------------------|--|--|--|--|--|
| | LOG IN | | | | | |
| LATEST ANNOUNCEMENTS | Username: | | | | | |
| July 2010 Data Release | Password: | | | | | |
| 20 JULY 2010 | Login (Send me my password) | | | | | |
| Pilot Project Variant call release | LINKS | | | | | |
| Variant Calls from the three pilot projects are now available in VCF 4.0 format. This release includes SNPs, short indels and large scale structural variants. All 1000 genomes pilot project files reference the NCBI build 36 assembly of the human genome | | | | | | |
| Data access links: EBI / NCBI | | | | | | |
| Link to additional information: README file | | | | | | |
| Recent project announcements | Sample and Project | | | | | |
| 4 AUGUST 2010 New sequence data is available The latest release of sequence data from the 1000 Genomes full project is now available. The new sequence index file can be found at: 20100804.sequence.index | Media Archive | | | | | |
| Data access links: EBI / NCBI / Instructions for data download and Aspera | | | | | | |

Links to additional information: List of new index and statistics files / Sequence index file format

http://www.sanger.ac.uk/genetics/CGP/

| | ellcome trust Sanger stitute | | | 2 | 73.0 35 | - | |
|----------------------------|------------------------------------|---------------|---------------------------|--|---|--|--|
| ⊠ ⊟ c Cancer Project | Genome | The | Cancer | Genome | Project | | |
| Genomic | s & Genetics | _ | | | Summary | | Data Resources |
| | | | | abnormalities Throughout li cells of the hu mutagens an | fe, the genome iman body is exp d suffers mista | quence. within osed to kes in | Cancer Gene Census: Mutated genes causally implicated in human cancer. |
| | | | Desiseda | | ese corrosive inf essive subtle dive | | COSMIC: Catalogue Of Somatic Mutations In Cancer |
| 1. t- 001 | | N de alta alt | Projects ion detection | | | i the | |
| <u>AutoCSA</u> DbCon | Database po | | outed config | uration and SQL | Libraries for | ne of s the ovidina | CGP Resequencing Studies: Somatic mutations from systematic large scale |
| | | | Java | | | hich it | resequencing of genes in human |
| PICNIC | | | | gmentation Tool | | n the | cancers. |
| <u>GRAFT</u> | | Rearrar | igement Phy | waves of clona evolution of f | ations, and con al expansion resu the mutinous ce | lt in the | CGP Cancer Cell Line Project: Resequencing of known cancer genes and other analyses of human cancer cell lines. |
| | | | | metastasise. C Western world in five die of | ounding tissues one in three peopl I develop cancer a the disease. Ca e commonest | e in the and one | CGP Copy Number Analysis in Cancer: Analysis of copy number and loss of heterozygosity in cancer cell lines and primary tumours. |
| | | | | uisedse. | | | |

http://www.hupo.org/



Human Proteome Organisation

Home | Search | Contact Us | Login

| Overview | HUPO Initiatives | O Meetings | C Educational Programs | News & Highlights | O HUPO Journals |
|------------------|------------------|--|---|--|---|
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| | | ir | ostering inter nitiatives to k uman disease | etter under | teomic rstand |
| Human Prote | INFORMATION | come to the Hu | man Proteome Organisa | tion's (HUPO) website | е |
| Register for our | Newsletter promo | oting proteomics thr technologies, techni | ganisation (HUPO) is an internation ough international cooperation a iques and training. Should you ha I in our organization, please click | nd collaborations by fosterin ave any questions regarding | g the development of our activities or how |

and the HUPO Secretariat, based in Montreal Canada, would be happy to assist you.

First name

http://www.metabolomics.ca/

Metabolomics Toolbox

| Contact About Person | nnel Publications | SOPs Jobs | Partners | News & Links | MetaboDatabase | MetaboLibrary | DrugBank |
|--|-------------------|-----------|----------|--------------|----------------|------------------------|----------|
| | | | | | | | |
| Home | | | | | | | |
| Welcome | | | | | | | |
| Welcome to the official | | | | | / | hm | n |
| Welcome to the official website of the Human Metabolome Project. | The Humar | n Metabol | ome P | roject | hur | nan metabolome project | r |

Our goal is to be the first group in the world to complete the human metabolome.

This large-scale and integrated effort will involve identifying and quantifying several hundred unknown metabolites in both Metabolomics is a newborn cousin to genomics and proteomics. Specifically, metabolomics involves the rapid, high throughput found in an organism. Since the metabolome is closely tied to the genotype of an organism, its physiology and its environment offers a unique opportunity to look at genotype-phenotype as well as genotype-envirotype relationships. Metabolomics is increating pharmacology, pre-clinical drug trials, toxicology, transplant monitoring, newborn screening and clinical chemistry. How the human metabolome is not at all well characterized.

Unlike the situation in genomics, where the human genome is now fully sequenced and freely accessible, metabolomics is not endogenous or common metabolites that are detectable in the human body. Not all of these metabolites can be found in an tissues/biofluids serve different functions or have different metabolic roles. To date, the HMP has identified and quantified (i.e. of metabolites in CSF, 1122 metabolites in serum, 458 metabolites in urine and approximately 300 metabolites in other tissues and desirable and this is one of the long term goals of the HMP and other affiliated metabolomic projects around the world.

Computational Biology needs HPC

Problems of scale

- Genomes with millions to billions of nucleotides
- Profiling experiments with tens of thousands of data points measured on hundreds or thousands of samples
- Thousands of protein mass spectra representing GigaBytes of data/experiment

Problems of complexity

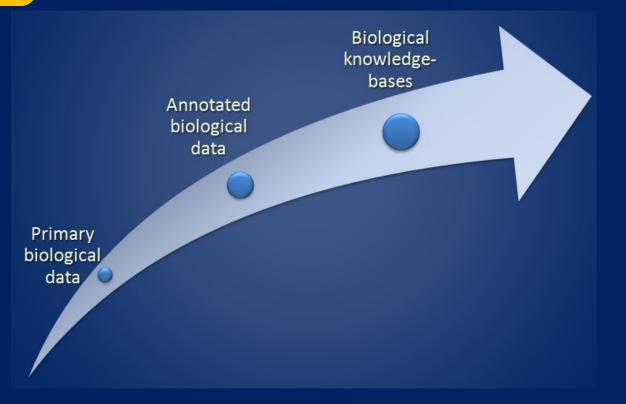
- Combinatorial: >3 10⁴ interacting gene products can create more functions than there are atoms in the Universe
- Structural: >10⁵ dynamically interacting atoms make up the smallest of molecular machines

http://www.opengridforum.org/gf/event_schedule/materials.php?event_id=15

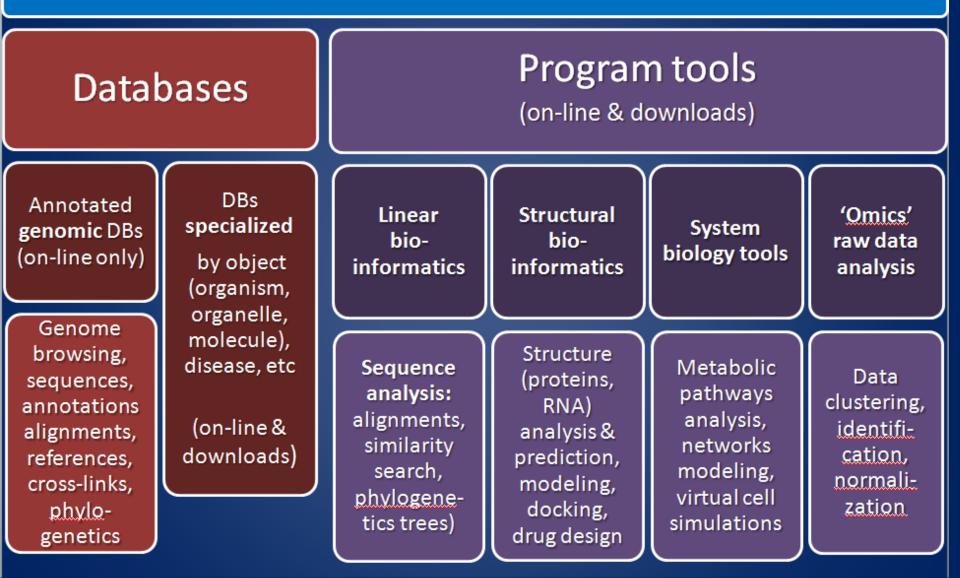
BIOINFORMATICS RESOURCES DEVELOPMENT

Bioinformatics resources development

- Resources variety
- Databases
- Program tools
- Search and workflows
- Towards knowledgebases



Bioinformatics resources



Thematic collections of DB and tools http://www.expasy.org/



ExPASy Proteomics Server

You are here: ExPASy CH

The ExPASy (Expert Protein Analysis System) proteomics server of the Swiss Institute of Bioinformatics (SIB) is dedicated to the analysis of protein sequences and s ExPASy).

Databases

UniProtKB, PROSITE, HAMAP, SwissVar, ViralZone, SWISS-MODEL Repository, SWISS-2DPAGE, World-2DPAGE Repository, MIAPEGeIDB, ENZYME, GlycoSuiteDB, UniPathway [details] [full list]

Education & services

Downloads, Protein Spotlight, Protéines à la «Une», e-proxemis, Bioinformatics core facility for Proteomics, Click2Drug - in silico Drug Design tools [full list]

Tools & Software

Proteomics tools, Blast, ScanProsite, Melanie, MSight, Make2D-DB, SWISS-MODEL, Swiss-PdbViewer, SwissDock, SwissParam [full list]

Documentation

What's New?, E-mail alerts, UniProtKB documentation, How to link to ExPASy, Advanced search [full list]

Web servers annual collection http://nar.oxfordjournals.org/content/38/suppl_2

Contents

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Volume 38, Web Server issue, July 1, 2010

W1-W2

Editorial: *Nucleic Acids Research* Annual Web Server Issue in 2010

Providing web servers and training in Bioinformatics: 2010 update on the Bioinformatics Links Directory

- TranslatorX: multiple alignment of nucleotide sequences guided by amino acid translations
- ALTER: program-oriented conversion of DNA and protein alignments

DIALIGN-TX and multiple protein alignment using secondary structure information at GOBICS

GUIDANCE: a web server for assessing alignment confidence scores

SATCHMO-JS: a webserver for simultaneous protein multiple sequence alignment and phylogenetic tree construction

Multi-Harmony: detecting functional specificity from sequence alignment

G.Benson

NEW IMPACT FACTOR OF Research 7.479

| D.Glez-Peña, D.Gómez-Blanco, M.Rebo F.Fdez-Riverola and D.Posada | piro-Jato, W | 14–W18 |
|--|--|-------------|
| A.R.Subramanian, S.Hiran, R.Steinkamp P.Meinicke, E.Corel and B.Morgenstern | Nucleic Acids Research | -W22 |
| O.Penn, E.Privman, H.Ashkenazy, G.La D.Graur and T.Pupko | Manderay | -W28 |
| R.Hagopian, J.R.Davidson, R.S.Datta, I G.R.Jarvis and K.Sjölander | 2012 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 | -W34 |
| B.W.Brandt, K.A.Feenstra and J.Hering | Alting Ming and Ming Alting and | W 40 |
| | | |

ALADYN: a web server for aligning proteins by

R.Potestio, T.Aleksiev, F.Pontiggia, S.Cozzini and W41–W45

Annual bioinformatics links collections: http://bioinformatics.ca/links_directory/

bioinformatics.ca

Bioinformatics Links Directory

The Bioinformatics Links Directory features curated links to molecular resources, tools and databases. The links listed in this directory are selected on the basis of recommendations from bioinformatics experts in the field. We also rely on input from our community of bioinformatics users for suggestions. Starting in 2003, we have also started listing all links contained in the NAR Webserver issue.

Search Directory

Bioinformatics Links Directory

Computer Related (76)

This category contains links to resources relating to programming languages often used in bioinformatics. Other tools of the trade, such as web development and database resources, are also included here.

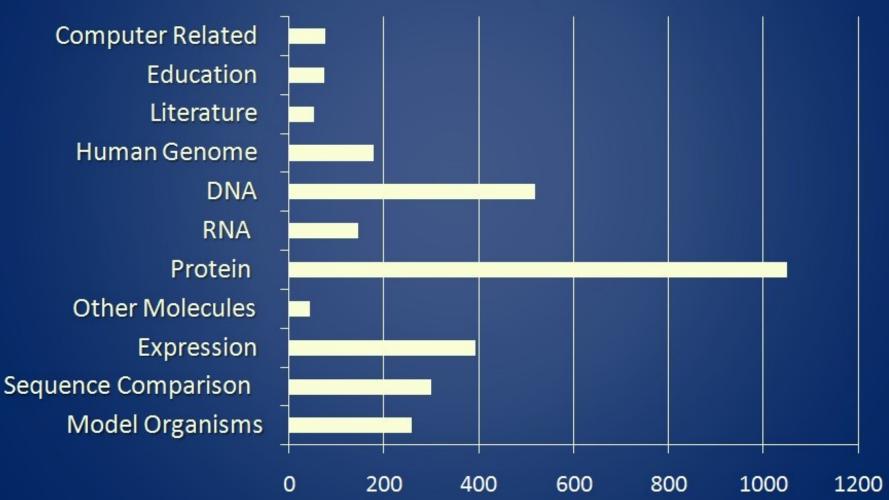
DNA (520)

This category contains links to useful resources for DNA sequence analyses such as tools for comparative sequence analysis and sequence assembly. Links to programs for sequence manipulation, primer design, and sequence retrieval and submission are also listed here.

Education (74)

Expression (394)

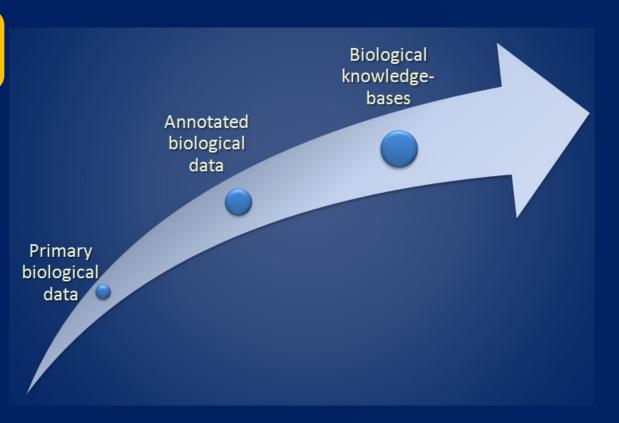
Thematic analysis of 2010 resources collection on Bioinformatics links directory



number of resources (links)

Bioinformatics resources development

- Resources variety
- Databases
- Program tools
- Search and workflows
- Towards knowledgebases

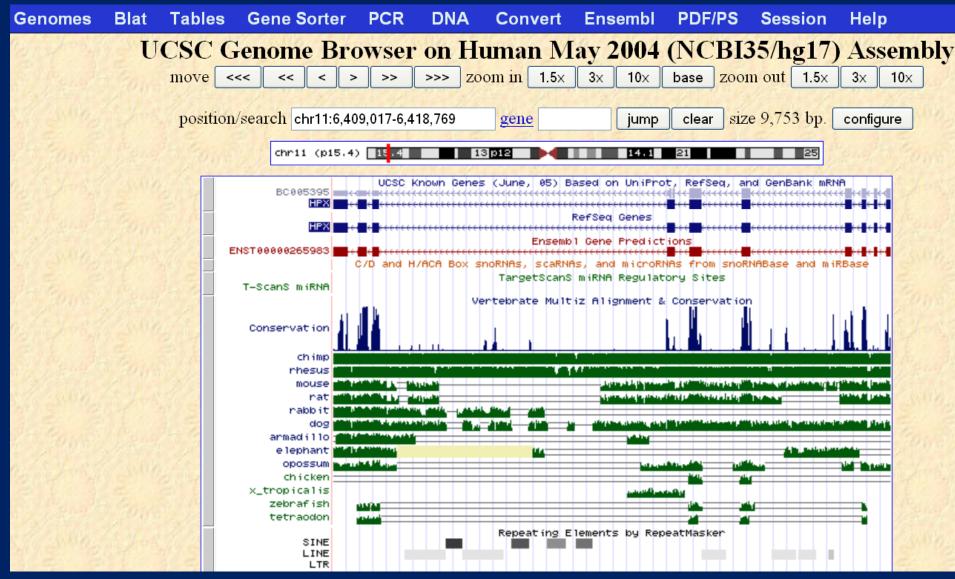


Annotated genomic databases: http://www.ensembl.org/

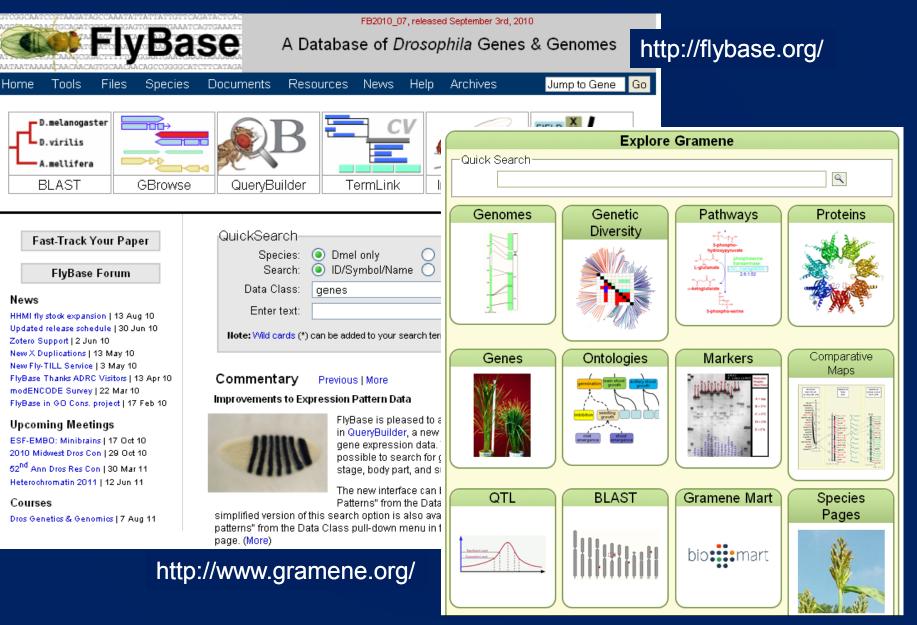
| Human (GRCh37) Location | n: 11:6,452,279-6,462,294 Ge | ne: HPX Transcript: HPX-00 | 1 | | | |
|---|------------------------------|---|--|---|---|---|
| Location-based displays | Chromosome 11: 6,452,27 | 9-6,462,294 | | | | |
| Whole genome Chromosome summary Region overview | | | chromosome 11 | p12 | q14.1 | |
| ⊢ Region in detail ⊡ Comparative Genomics | | | | | | Export Image |
| Alignments (image) (51) Alignments (text) (51) Multi-species view (47) | « Region overview | | | Region in | detail he!p | |
| Synteny (13) Genetic Variation Resequencing (2) Linkage Data Markers Other genome browsers UCSC NCBI Vega Configure this page | | | Chromo some bands Contigs Ensembl/Havana g | AC111177.15 TRIM5 COR56A1 C11orfi COR56A3 COR52L2P FAM16 AC025016.1 CCC COR52L1 COR56B4 COR52L1 COR56B4 COR56A4 AC111177.2 AC022762.1 | P13.4 42 60A2 CKBR PRKCDBP FXC1 SMPD1 | Forward strand 6.60 Mb 6.70 Mb 6.80 Mb 6.90 M AC091564.12 > AC091564.12 > AC091564.12 > 1 'LIK 'MRPL17 'OR2AG1 'OR2 'TAF10 'OR2AG2 'OR10 'TPP1 'OR6A2 'OR10 'DCHS1 'OR10AS 'RRP8 'OR104 'RP11-732A19.1 'Z |
| 🕞 Manage your data | | | | LOR52B2 LOR52X1P LOR52W | - | |
| Bookmark this page | | | ncRNA gene All Structural varia | 5S rRNA 6.00 Mb 6.10 Mb 6.20 Mb 6 Ensembl Homo sapiensversion | | osome 11: 5,957,287 - 6,957,286 |
| elen Human (GR | Ch37) Location: 1 | n Register BL/ 1:6,452,279-6,462,2 | | BioMart Tools | | Help |
| Gene-base | | Gene: HPX (ENS | | | | |

Annotated genomic databases:

http://www.genome.ucsc.edu/



Specialized databases: organism-specific



On-line collections of databases: http://www.oxfordjournals.org/nar/database/c/

OXFORD JOURNALS

Nucleic Acids Research

ABOUT THIS JOURNAL CONTACT THIS JOURNAL SUBSCRIPTIONS

Oxford Journals > Life Sciences > Nucleic Acids Research > Database Summary Paper

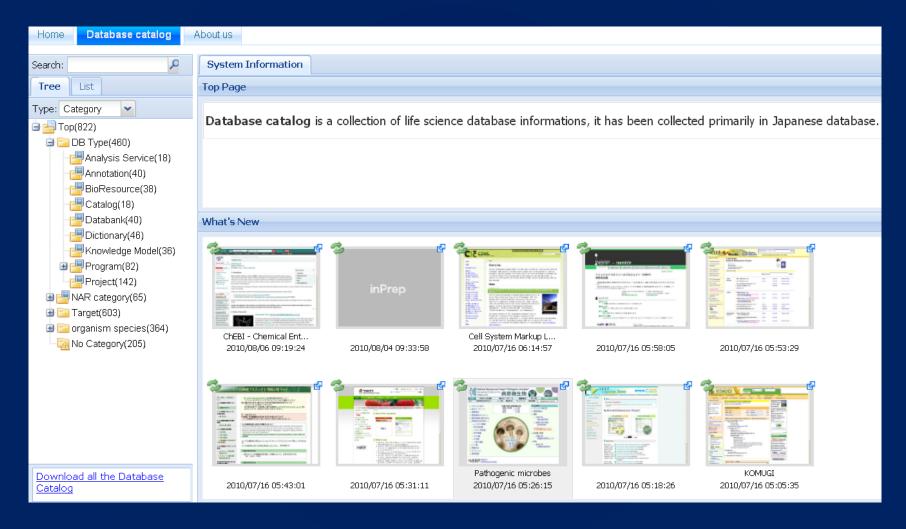
2010 NAR Database Summary Paper Category List

Nucleotide Sequence Databases RNA sequence databases Protein sequence databases Structure Databases Genomics Databases (non-vertebrate) Metabolic and Signaling Pathways <u>Human and other Vertebrate Genomes</u> Human Genes and Diseases Microarray Data and other Gene Expression Databases Proteomics Resources Other Molecular Biology Databases Organelle databases Plant databases 1230 selected databases

C



Database catalogue http://lifesciencedb.jp/?lng=en&pg=1



DBs standardization http://casimir1.pdn.cam.ac.uk/casimir_ddf/



CASIMIR Database Description Framework

Apply

Navigation

- DDF summary
- Download
- Web services

User login



-CAPTCHA

This question is for testing whether you are a human visitor and to prevent automated spam submissions.



What code is in the image?: *

Enter the characters (without spaces) shown in the image.



- Create new account
- Request new password
- 2 Old versions available but no tracking between versions
 - 3 Old versions available and tracking between versions

The CASIMIR Database Description Framework (DDF) allows resources to describe key technical metadata in a formalised way. The aim of the DDF is to support the standards and interfaces they require. This is a vital component for the online registries of resources currently being developed for many of this deployment displays the DDF annotation performed by resources as part of the MRB project. Other communities can follow the **Download** link in the instruction to install this site for their own curation requirements. The DDF annotation is also available through RESTful **Web services**.

Please feel free to create an account and try out annotating your own resource using the Add a new resource link.

Legend

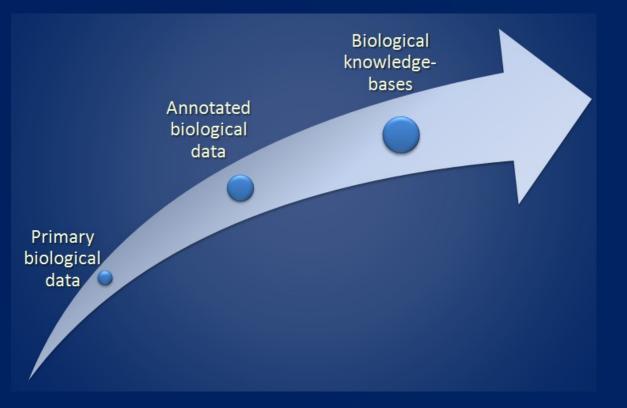
Yellow blocks represent resources assessed as being at level 1 of the DDF category Light blue blocks represent resources assessed as being at level 2 of the DDF category Dark blue blocks represent resources assessed as being at level 3 of the DDF category

Click on individual blocks to see full descriptions of each level per category

| Accessibility | Currency | | | | |
|--|---|--|--|--|--|
| 1 - Access via browser only | 1 - Closed legacy database | | | | |
| 2 - Access via browser + database reports or dumps | Updates or versions more than once a year | | | | |
| 3 - Access via browser + API, SQL access or web services) | 3 - Updates or versions more than once a month | | | | |
| Data representation standards | Data structure standards | | | | |
| 1 - Data coded by local formalism only | 1 - Data structured with local model only | | | | |
| 2 - Some use of controlled vocabs, ontologies or MIBBI | 2 - Data structured with formal model e.g. an XML schema | | | | |
| 3 - General use of controlled vocabs, ontologies or MIBBI | 3 - Use of recognised standard model e.g. FUGE | | | | |
| Output | Quality and Consistency | | | | |
| 1 - HTML or similar to browser only | 1 - No explicit process for assuring consistency | | | | |
| 2 - HTML + sparse standard file formats e.g. FASTA | Process for assuring consistency, automatic curation only | | | | |
| 3 - HTML + rich standard file formats e.g. XML, SBML | 3 - Process for assuring consistency with manual curation | | | | |
| Technical documentation | User support | | | | |
| 1 - Written text only | 1 - User docs only | | | | |
| 2 - Written text + formal docs (API docs, schema, UML etc) | 2 - User docs + Email/web form help desk function | | | | |
| 3 - Written text + formal docs + tutorials/demos | 3 - User docs + personal contact help desk function/training | | | | |
| Versioning | Resource name contains | | | | |
| 1 - No provision | | | | | |

Bioinformatics resources development

- Resources variety
- Databases
- Program tools
- Search and workflows
- Towards knowledgebases



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

S NCBI Tools for Data Mining

| PubMed | Entrez | BLAST | OMIM | Book | s | TaxBrowse | er Structure |
|--------------|-------------------|----------------|--------------|------------|-------|-------------|-----------------|
| Search | Entrez | 🖌 for | | | Go | | |
| Nucleotide S | Sequence Analysis | Protein Sequer | nce Analysis | Structures | Genom | ie Analysis | Gene Expression |

NCBI

Site Map Guide to NCBI resources

Tools for Programmers

Tools - Nucleotide Sequence Analysis

BLAST The **Basic Local Alignment Search Tool** (BLAST) for comparing gene and protein sequences against others in public databases, now comes in several types including PSI-BLAST, PHI-BLAST, and BLAST 2 sequences. Specialized BLASTs are also available for human, microbial, malaria, and other genomes, as well as for vector contamination, immunoglobulins, and tentative human consensus sequences.

electronic PCR sequence tagged sites (STSs) that have been used as landmarks in various types of genomic maps. It compares the query sequence against data in NCBI's UniSTS, a unified, non-redundant view of STSs from a wide range of sources.

http://pbil.univ-lyon1.fr/alignment.html

Tools for Multiple Alignments

$^{m k}$ Search for sequence similarities in databases

- <u>WU-BLAST at ISREC</u> (Lausanne, Switzerland)
- BLAST2 Search at EMBL (Heidelberg, Germany) Performs multiple alignment on homologous sequences detected by BLAST.
- FASTA at EBI (Hinxton, UK)
- Smith-Waterman search at EBI (Hinxton, UK)
- <u>BCM search launcher</u> (Houston, USA)
- o GeneStream at CRBM (Montpellier, France)
- BLAST search at PBIL (Lyon, France) Possibility to select BLAST output results by taxa or keyword.

Web Sites for Pairwise Alignments

- LFASTA Local alignment tool at PBIL (Lyon, France)
- SIM4 align cDNA and genomic DNA at PBIL (Lyon, France)
- WISE align protein and genomic DNA at Pasteur (Paris, France)
- o SIM Alignment Tool at ExPASy (Geneva, Switzerland)
- <u>BLAST two sequences at NCBI</u> (Bethesda, USA)
- LALIGN at CRBM (Montpellier, France)
- o SIM, GAP, NAP, LAP (Michigan Tech. Univ., USA)
- <u>JAligner: open source Java implementation of the Smith-Waterman algorithm</u> (Alexandria, Egypt)

Toolkits

http://toolkit.tuebingen.mpg.de/

| HOME | | | Login | PDBalert | Personal I | | | | |
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| | Bioinformatics Toolk Max-Planck Institute for Develo | opmental Biology | | | | | | | |
| IAX-PLANCK-GESELLSCHAFT Show results of job: | Search Alignment Sequence Ana | lysis 2ary Structure 3ary Structure Classificatio | on Utils | | | | | | |
| | | | | | | | | | |
| Show results | Welcome to the Bioinforn | natics Toolkit | | | | | | | |
| Recent jobs: Select all Deselect all | Many tools are developed in-house, and serveral public tools are offered with extended functionality. | | | | | | | | |
| Clear sel. Jobs | The toolkit includes, among others: NucleotideBLAST, ProteinBLAST, PSI-BLAST, fastHMMER, HHsenser; ClustalW, MUSCLE, Mafft, ProbCons; HHrep, PCOILS, REPPER; Quick2D; HHpred, Modeller; CLANS, ANCESCON, PHYLIP; Reformat, RetrieveSeg, gi2promoter. For a short descrition of the tools, click the section tabs. | | | | | | | | |
| queued running | Reformat, Retrieveded, gizpiomoter | . For a short descrition of the tools, click the section | r taba. | | | | | | |
| done error | Job submission | Each tool has a separate input page with a web forr sequence data, upload sequence files, and specify alignments as input accept the most widely used | options formats (| All tools that (FASTA, CLU | take STAL, | | | | |
| | | Stockholm and A3M). You may also choose your | own job-r | names to org | anize | | | | |

your work. Snail symbols inside the submit buttons inform you about tools that

typically run for more than 10 minutes.

Analysis systems

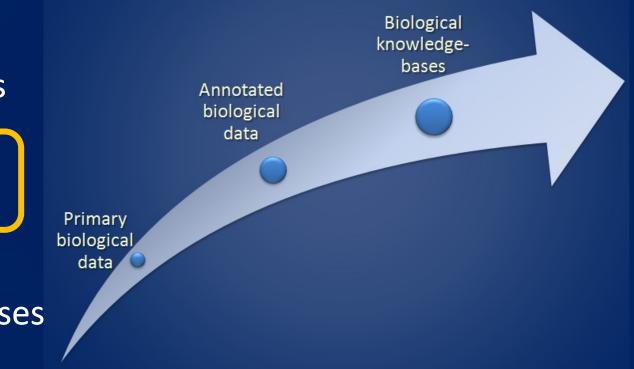
www.migenas.mpg.de



| | MIGENAS | |
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| Con the second s | | Max-Planck Integ |
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| Номе | | |
| • Авоит | | |
| News | Welcome to the Integrated Gene Analysis System MIGenAS of the Max-Planck-Society | 5 |
| CONTACT | MIGenAS (Max-Planck Integrated Gene Analysis System) provides an integrated software environment for bio | informatics applications |
| | MIGenAS workflow engine: Integrated bioinformatics toolkit for web-based sequence analysis | |
| START TOOLKIT GENDB 2.2 GENOMES HALOLEX | facilitates similarity searches in public or user-supplied sequence databases, computation and validation of multiple sequence alignments, phylogenetic analysis, protein structure prediction. allows seamless chaining of different tools into pipelines. no need for format conversions or parsing of intermediate results. supports efficient processing of predefined workflows. offers programmatic access via webservices. | |
| HALOLEX | GenDB: Annotation system for prokaryotic genomes (provided by University of Bielefeld) | |
| | Software system for automatic identification, classification and annotation of genes. Web interface allows manual annotation with geographically dispersed teams of experts. Local installation of GenDB 2.2 available at RZG with connection to dedicated computing facilities. | |
| | HaloLex: Genome information system for archaea and other prokaryotic genomes | |
| | Data management and analysis platform for microbial genomes and related <i>omics</i> data. Web interface supports browsing and versatile searches in annotated (public) microbial genomes. Provides access to high-quality, expert-curated annotations of a number of halophilic archaea. | |

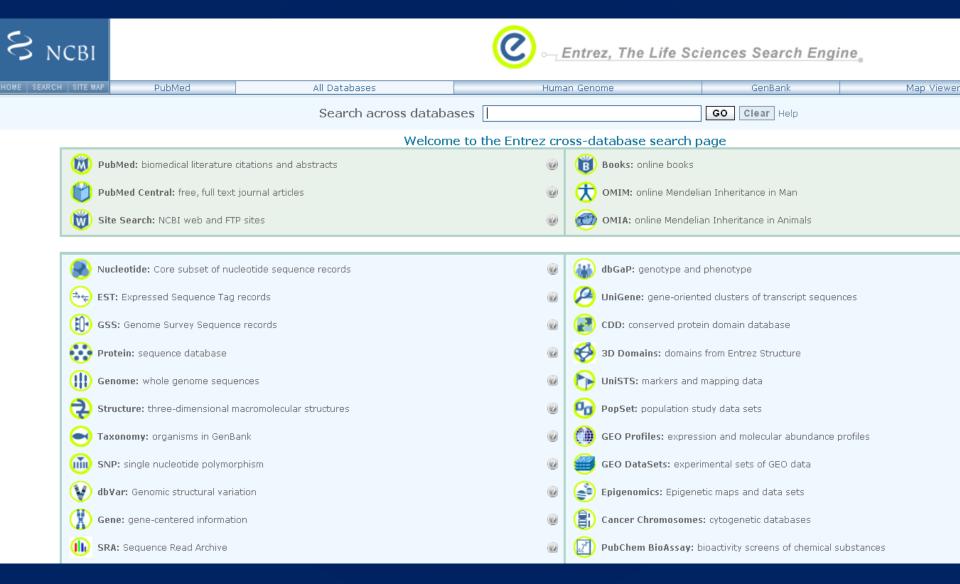
Bioinformatics resources development

- Resources variety
- Databases
- Program tools
- Search and workflows
- Towards knowledgebases



Cross-search

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



Links **Cross-links and references** Order cDNA clone Entrez-gene: http://www.ncbi.nlm.nih.gov/gene/ BioAssay, by Gene target CCDS Conserved Domains 🗧 NCBI Resources 🗹 How To 🗹 EST Limits Advanced search Help Entrez Gene Search: Gene ~ Full text in PMC Genes and mapped Search Clear phenotypes GEO Profiles Display Settings: 🕞 Full Report Send to: 🖂 Table of cont Genome Summary HPX hemopexin [Homo sapiens] Genomic regio Gene ID: 3263, updated on 19-Sep-2010 HomoloGene Genomic cont Bibliography Summary Map Viewer General gen info Official Symbol HPX provided by HGNC ein info General nr Official Full Name hemopexin provided by HGNC Nucleotide Reference sequend Primary source HGNC:5171 Related equences See related Ensembl:ENSG00000110169; HPRD:00793; MIM:142290 OMIM Addition al links Gene type protein coding RefSeq status REVIEWED Peptidome Organism Homo sapiens Links Lineage Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi; Mammalia; Eutheria; Euarchontoglires; Primates; Haplorrhini; Ca Related sites Order cDNA Also known as HX: FLJ56652; HPX Probe. Summary This gene encodes a plasma glycoprotein that binds heme with high affinity. The encoded protein is an acute phase protein that tran BioAssay, by Gene be involved in protecting cells from oxidative stress. [provided by RefSeq] BLAST CCDS Protein Conserved Domain: Links to external resources Genomic regions, transcripts, and products Entrez Genome EST PubChem Compound (minus strand) Go to reference sequence details Full text in PMC HGNC Genome Project GEO Profiles PubChem Substance -6,455 K -6,461 K -6,460 K -6.462 K Genome io sapiens c primary reference assembly Ensembl Genomic Biology PubMed HPRD GEO PubMed (GeneRIF) Evidence Viewer HomoloGene PubMed (OMIM) ModelMaker Map Viewer **RefSeq Proteins** AceView OMIM RefSeq RNAs UCSC Probe. SNP MGC RefSeq SNP: GeneView HuGE Navigator UniGene SNP: Genotype KEGG UniSTS Taxonomy

DBs/tools **cross-search** http://www.hsls.pitt.edu/guides/genetics/obrc/

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| Jourr | nals & Articles • Books • More Resources • Lil | brary Services • How Do I? |
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| OBRC: Online | Bioinformatics Resources Collectio | n |
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| OBRC | search.HSLS.OBRC | About search.HSLS.OBRC |
| Email Suggestions | | |
| Recommend a New Resource | Databases/Tools Articles on Databases/Tools Web | |
| Resource | Databases/Tools | |
| | Find molecular databases & software tools with a combined s | |
| | Online Bioinformatics Resource Collection (OBRC) & the | BioMed Central Databases collection. |
| | | Search |
| | | |
| | Search Examples: keyword (<u>HapMap</u> , <u>SNP</u>); phrase (prote | in structure prediction) |
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| | The Online Bioinformatics Resources Collection (OBRC) contai | ins annotations and |
| | links for 2724 bioinformatics databases and software tools. | |
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| 0701 linka | Diowse. | |
| 2724 links | <u>DNA Sequence Databases and Analysis Tools</u> (493) | |
| | • Enzymes and Pathways (266) | |
| | Gene Mutations, Genetic Variations and Diseases (246 | δ) |
| | Genomics Databases and Analysis Tools (674) | |
| | Immunological Databases and Tools (61) | |

Harvesting engines http://harvester.fzk.de/harvester/



Harvester crawls and crosslinks the following bioinformatic sites:

<u>4DXp</u> - <u>AceView</u> - <u>BLAST</u> - <u>BLINK</u> - <u>Biocompare</u> - <u>CDART</u> - <u>CDD</u> - <u>EB-eye</u> - <u>ensEMBL</u> - <u>Entrez</u> -<u>FishMap</u> - <u>Galaxy</u> - <u>GeneSorter</u> - <u>UCSC</u> <u>GenomeBrowser</u> - <u>gfp-cDNA</u> - <u>Google-Scholar</u> - <u>gopubmed</u> -<u>Harvester42</u> - <u>H-Inv</u> - <u>HomoloGene</u> - <u>iHOP</u> - <u>IPI</u> - <u>LOCATE</u> - <u>MapView</u> - <u>MGI</u> - <u>MINT</u> - <u>Mitocheck</u> -<u>OMIM</u> - <u>PolyMeta</u> - <u>Proteinatlas</u> - <u>PSORT II</u> - <u>RGD</u> - <u>SMART</u> - <u>SOSUI</u> - <u>STTTCH</u> - <u>STRING</u> - <u>TAIR</u> - <u>Unigene</u> - <u>UniprotKB</u> - <u>Wikipedia</u> - <u>WikiProtein</u> - <u>YIF</u> - <u>ZFIN</u> <u>Harvester Sequence Search</u> device - <u>YaCy-Sciencenet p2p search engine</u> See our <u>H-Wiki</u> for latest activities...<u>Try YaCy Harvester Search (all genomes)</u> - Have fun...

Bioinformatic Harvester IV

...serving 10.000s of pages every day - Note that '*' and '?' wildcards are supported.

| Search human |
|--------------------|
| Search mouse |
| Search rat |
| Search zebrafish |
| |
| Search arabidopsis |

Organization of frameworks https://projets.pasteur.fr/wiki/mobyle

| Mobyle | | | | | | |
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| Просмотр Активность Оперативный план Задачи Новости Документы <mark>Wiki</mark> Download Файлы Хранилищ | e | | | | | |
| Welcome to the Mobyle Project Website! | | | | | | |
| Mobyle is a framework and web portal specifically aimed at the integration of bioinformatics software and databanks. | | | | | | |
| Mobyle is the successor of Pise and the RPBS server , previous systems that provided web environments to define and execute Users bioinformatics analyses. | | | | | | |
| Functionalities: | Administrators and Learn more | | | | | |
| data reusability: the tagging of the user data facilitates the reuse of input values or results between different programs. automatic data validation and format conversion: the description of the expected data and their format allows to verify and convert input values if necessary. service discovery and workflow authoring assistance: services are provided through a searchable menu; furthermore, type compati and potential program inputs let users either interactively pipe tasks or build complete workflows before to run them. | | | | | | |
| Based on extensive user studies, we developed the end-user interface as a Web Portal that provides a global and integrated view of all the elem such as the available programs, the submitted jobs and the data of interest. | ents needed to perform | | | | | |

| U | sers |
|---|----------------|
| L | ife scientists |

B.Néron, H.Ménager, C.Maufrais et al. **Mobyle: a new full web bioinformatics framework** *Bioinformatics (2009) 25(22): 3005-3011*

tics prog

Want to run bioanalyses through a web interface without ins

See our User guide - Mobyle Public Servers

Administrators and developers

1.1

Mobyle@pasteur

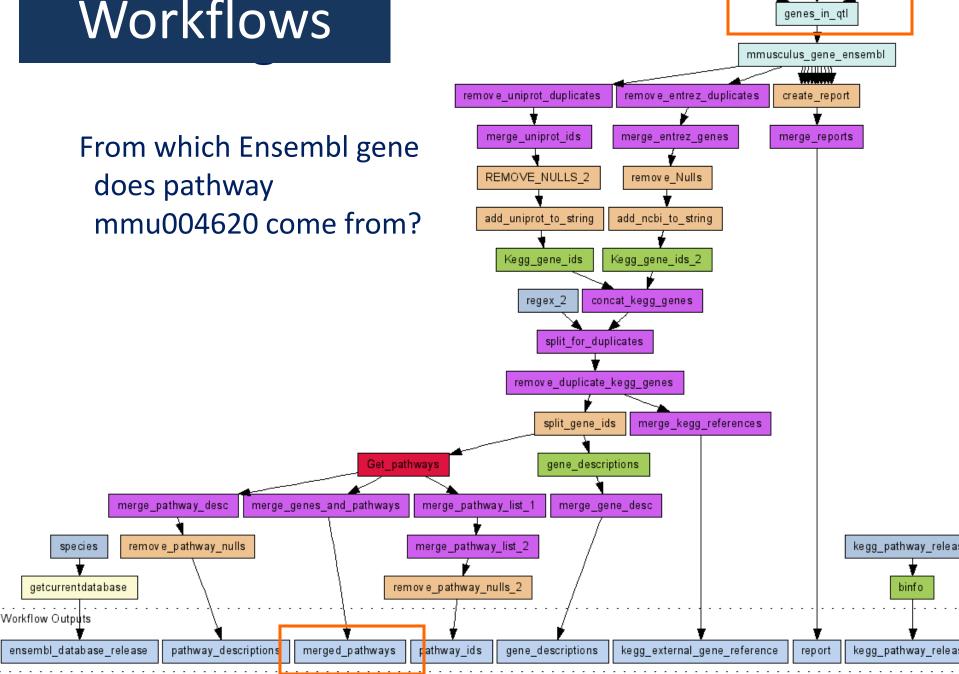
http://mobyle.pasteur.fr/

Institut Pasteur

| Programs | Welcome | Programs | Data Bookmarks | Jobs | Tutorials |
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| Search > | | | w | elcome | to Mobyle, |
| alignment assembly database display genetics | \leftarrow | Select an a | analysis in the Progra | ms <u>menu</u> . | |
| hmm nucleic phylogeny protein sequence structure | | | | | |
| ▶ LIPM ▶ RPBS | | | | | |
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| Jobs refresh Tutorials How to use Mobyle? A step | \leftarrow | Tutorials | are available. See our | interactive | <u>guided tour</u> . |
| <u>by step tutorial</u> <u>Registration information</u> <u>Sequence formats</u> <u>Alignment formats</u> | | | ped jointly by the <u>Insti</u> project can be found | | <u>r</u> "Logiciels et |

The end-user interface as a Web Portal provides a global and integrated view of all the elements needed to perform analysis, such as the available programs, the submitted jobs and the data of interest.

Workflows

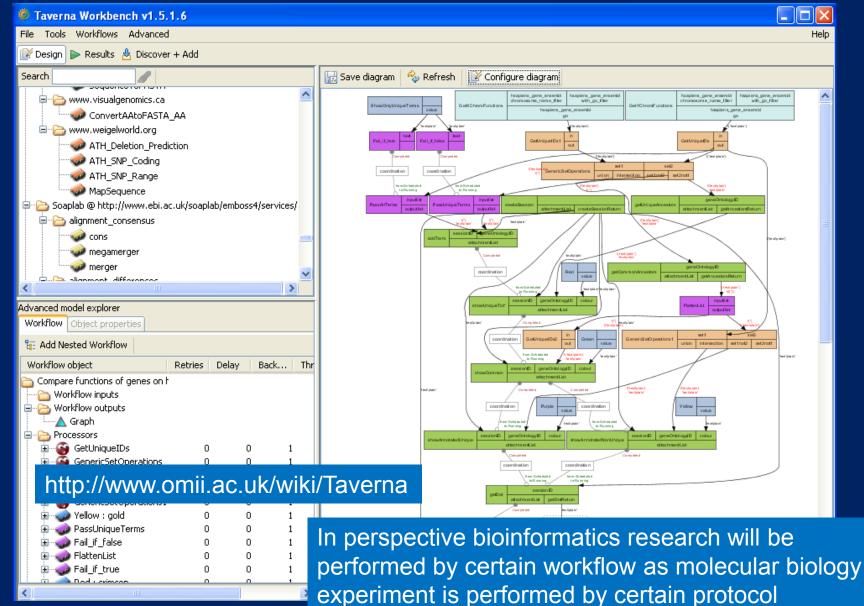


end_position

start_position

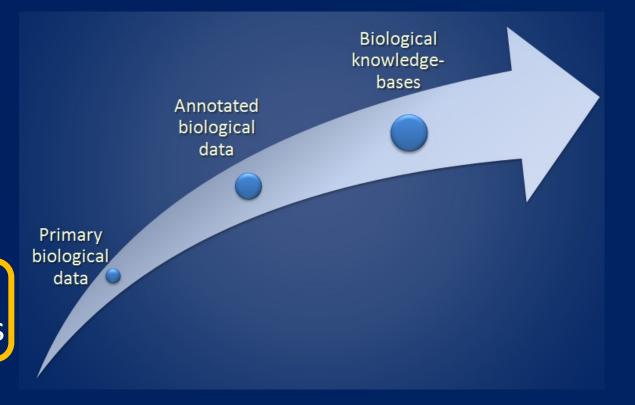
chromosome

Taverna Workflow Workbench



Bioinformatics resources development

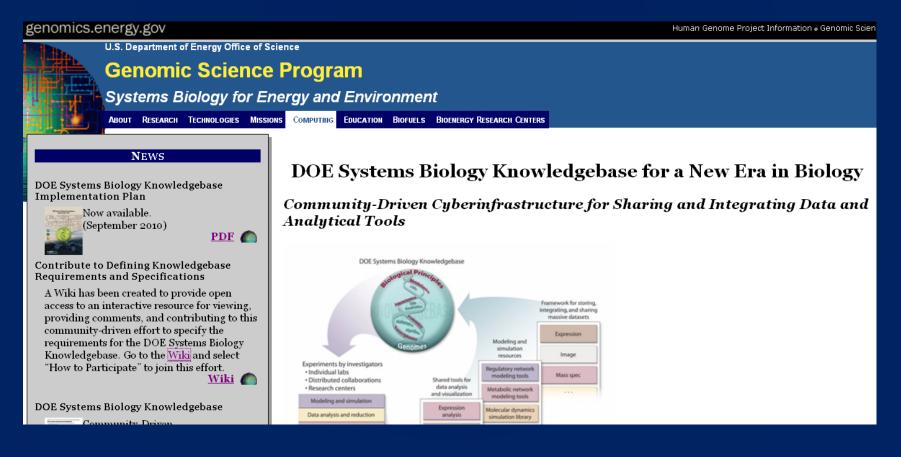
- Resources variety
- Databases
- Program tools
- Search and workflows
- Towards knowledgebases



Integrated Knowledgebases as Web environment

http://genomicscience.energy.gov/compbio/

The Systems Biology Knowledgebase is **a cyberinfrastructure** to facilitate a new level of scientific inquiry by serving as a central component for the integration of modeling, simulation, experimentation, and bioinformatic approaches.



Data generators



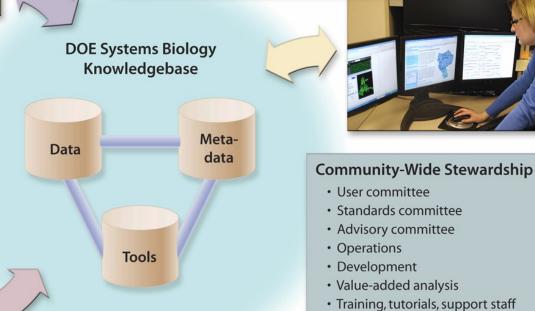
Seamless Submission and Incorporation of Diverse Data

- Standards for data and metadata representation
- Quality control and assurance capabilities
- Automated systems for depositing and updating bulk data
- Tracking and evaluation of data use

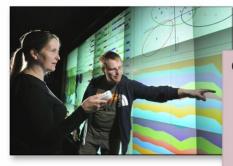
Open-Access Data and Information Exchange

- · Access through several flexible interfaces
- Retrieval of experimental data and products of modeling and simulation
- Working environment for testing hypotheses by *in silico* experimentation
- Provision and sharing of user feedback

Data users



Software and tool developers



Open Development of Open-Source Software and Tools

- Data analysis and visualization tools
- Resources for in silico experimentation
- · Modeling and simulation tools
- · Customizable tools with layers of functionality
- Tracking and evaluation of tool use

The Systems Biology Knowledgebase (Kbase)

In addition to supporting data storage, retrieval, and management capabilities, Kbase also would enable *new knowledge acquisition and management*, through *free and open access* to data, analysis tools, and information for the scientific research community.

Kbase, therefore, must serve multiple roles, *including*:

- A repository of data and results from high-throughput experiments.
- A collection of tools to derive new insights through data synthesis, analysis, and comparison.
- A foundation for prediction, design, manipulation, and ultimately, engineering of biological systems.

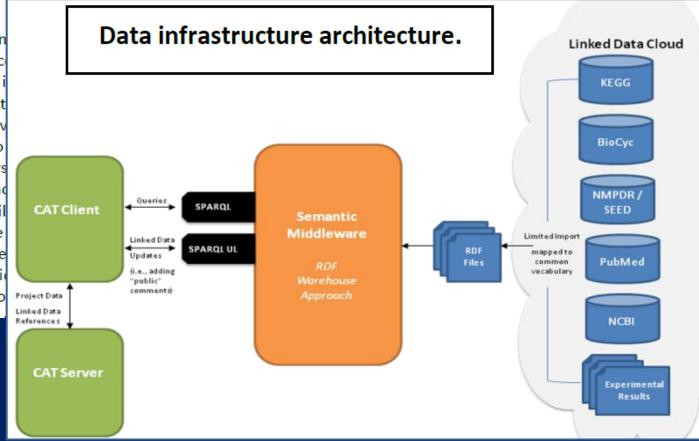
Pilot projects

Semantic Driven Knowledge Discovery and Integration in the System Biology Knowledgebase Project

Kerstin Kleese van Dam, Cliff Joslyn, Lee Ann McCue, Bill Cannon, Carina Lansing, Zoe Guillen, Margaret Romine, Gordon Anderson, Abigail Corrigan

Pacific Northwest National Laboratory

It is the goal of the DOE Systen Knowledgebase to become a confrastructure for sharing and i Analysis tools. This new infrast the science community to mov Biology, where it is possible to understanding of biological sys address core DOE Missions and the community wide accessibil and the capability to integrate within its environmental conte technical functionalities the Bio enable. The ultimate success o



Database Management Systems Technologies for Computational Biology & Bioinformatics Applications Knowledgebase R&D Pilot Project

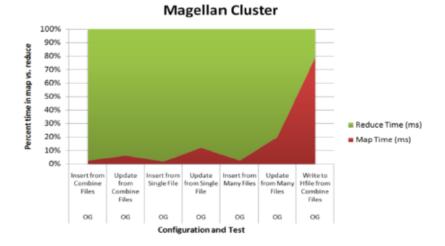
Victor Markowitz, Keith Jackson, Ernest Szeto, Konstantinos Mavrommatis Lawrence Berkeley National Laboratory (LBNL)

The aim of this project was to examine new database management system technologies for supporting efficient analysis of very large genome and metagenome sequence datasets.

ms for Bioinformatics

Pilot projects

Comparative analysis of genomic and metagenomic datasets is usually based on integrating these datasets in the context of databases implemented using relational commercial database management systems (DBMS) such as Oracle or open



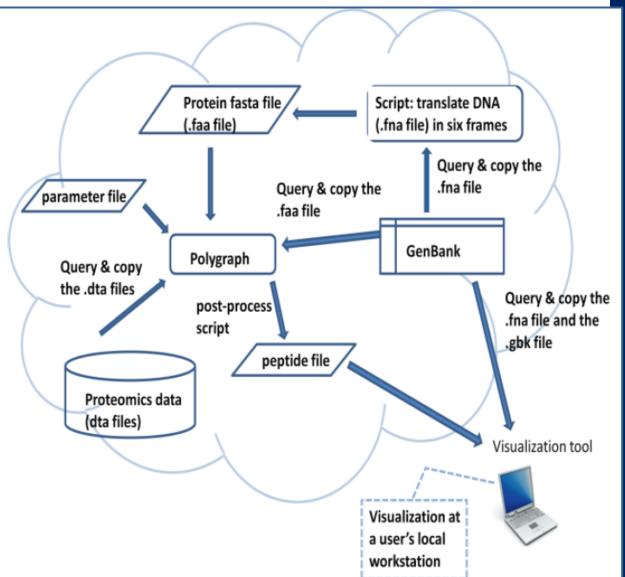
source DBMS such as MySQL. The rapid increase in the number and size of these datasets results in a decrease in performance of typical comparative analysis tools, such as examining putative operons across microbial genomes. A recent benchmark of relational DBMS¹ indicates that new database management technologies are better suited for scientific data management applications. We set out to evaluate the usage of cloud based data management technologies for handling large genome and metagenome datasets, in particular Hadoop data management components for data storage and querying. Hbase² is a distributed, column-oriented data store that supports real-time access to extremely large data.

Exploring Architecture Options for Workflows in a Federated, Cloudbased Systems Biology Knowledgebase

Ian Gorton, Yan Liu, Jian Yin, Leeann McCue, Bill Cannon, Gordon Anderson

Systems biology is characterized by a large who use a wide variety of fragmented an computational tools of all scales to supp to provide a more coherent computationa biology, we are working as part of th Systems Biology Knowledgebase (Kba federated cloud-based system archite eventually host massive amounts of bio performance and scalable computational large user community with tools and se utilize the Kbase resources. We invest workflow infrastructure suitable for use it utilizes standards-based workflow desc integration technologies, and incorporate execution layer for exploiting data architecture.

Pilot projects

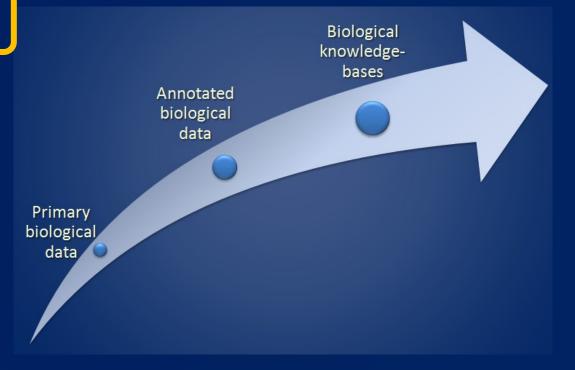


NEW IT SOLUTIONS FOR BIOINFORMATICS

New IT Solutions for bioinformatics

• Data compression

- Web semantics
- Web services
- Gridification
- Biocomputing



Textual data compression in post-genomics era

- DNAzip: DNA sequence compression using a reference genome [Christley S., Lu Y., Li C., and Xie X. Human genomes as email attachments //Bioinformatics (2009) 25:274-5] http://silver.ics.uci.edu/~dnazip/index.html
- **G-SQZ: compact encoding of genomic sequence and quality data** [W.Tembe, J.Lowey, and E.Suh // Bioinformatics (2010) 26(17): 2192-2194]
- Compression of whole genome alignments [P.Hanus, J.Dingel, G.Chalkidis, J.Hagenauer//IEEE Transactions on Information Theory.- Vol.56, No.2 (Feb2010) Special issue on information theory in molecular biology and neuroscience. P.696-705

| HIT000291102_Homo. | 35 | VAEGETKPDPDVTERCSDGWSFDATTLDDNGTMLFFK-GEFVWKSHKW 81 |
|-----------------------------|----|---|
| ENSPTRT0000006246_Pan. | | VAEGETKPDPDVTERCSDGWSFDATTLDDNGTMLFFK-GEFVWKSHKW |
| XM_001109797_Macaca. | | VAEGETKPDPDVTERCSDGWSFDATTLDDNGTMLFFK-GEFVWKSHKW |
| AK145928_Mus. | | VAEVENGTKPDSDVPEHCLDTWSFDAATMDHNGTMLFFK-GEFVWRGHSG |
| BC091137_Rattus. | | VAKGENGTKPDSDVIEHCSDAWSFDATTMDHNGTMLFFK-GEFVWRGHSG |
| ENSCAFT00000010394_Canis. | | GTEGGSGARVKPDVTELCLDGWSFDATTLDEHGAMLFFK-GEFVWKSHRW |
| XM_001504590_Equus. | | GAEGGNGVKQDPDVIERCSDGWSSDATTLDEHGAMVFFK-GEFMWKSPNW |
| BC102687_Bos. | | GVEGGNVAKPDPEVTERCSDGWGFDATTLDEHGNMLFLK-GEFVWKGHAW |
| ENSDARTOOOOOO73621_Danio. | | MLKDAPEDHHEDRCKG-IEFDAIAPDEKGNTFFFKVGDRLWKGLTG |
| ENSORLTO0000004740_Oryzias. | | SVILISHPDGDSALPDRCAG-IEFDAITPDDKGQTFFFK-GDHVWKGFDG |
| AB075198_Oryzias. | | HHEHRRKGAVRDRCKG-IEMDAVAVNEEGIPYFFK-EDHLFKGFHG |
| CR647288_Tetraodon. | | NVSEMRDEDSGPALPDRCAG-IEFDAITPDEKGKTFFFK-GAYMWKGFQW |
| CR635722_Tetraodon. | | GDSHGLAKLDRCQG-LEMDAVAVNEIGIPYFFK-GDHLFKGFHG |
| AB125933_Takifugu. | | NISEVKEEDSGPALPDRCAG-IEFDAITPDEKGKTLFFK-GAYMWKDFHG |
| | | . * ** * . * |

http://www.tgen.org/research/gsqueez.cfm

THE TRANSLATIONAL GENOMICS RESEARCH INSTITUTE A Non-profit Biomedical Research Institute

October 2, 2010

Genomic Sequence-Quality Data Encoding & Compression

G-SQueeZ offers indexed, order preserving, compressed format for genomic sequence reads.

WHAT IS G-SQUEEZ™?

Genomic Squeeze (G-SQueeZ™) is a technique to encode genomic sequence-quality data into an indexed, compact binary format, and that can result in substantial savings in storage and processing over conventional plain text formats (such as FASTQ, CSFASTA/QUAL formats).

In G-SQueeZ™ encoding, order of the data is preserved and the indexed structure directly allows selective access to various parts of the file. In addition, resulting binary files can be queried to obtain useful information about the file, such as number of reads, base composition, platform, etc.

For an in-depth description, please read the manuscript [<u>Link to the paper on the Bioinformatics Journal</u> <u>Website</u>]



W.Tembe, J.Lowey, and E.Suh G-SQZ: compact encoding of genomic sequence and quality data *Bioinformatics (2010) 26(17): 2192-2194*

CONTACT INFORMATION

Questions, comments and usage inquiries should be directed to: <u>gsgz-admin@tgen.org</u>.

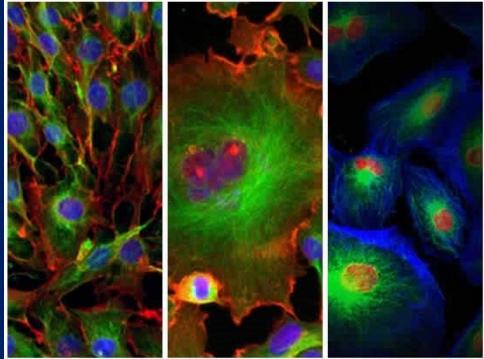
F.A.Q.

Which platforms are supported? G-SQueeZ™ version 0.5 supports SOLEXA

AVAILABILITY

Compression techniques for images processing

- CATMAID: collaborative annotation toolkit for massive amounts of image data [S.Saalfeld, A.Cardona, V.Hartenstein, and P.Tomančák// Bioinformatics (2009) 25(15): 1984-1986]
- **Bisque: a platform for bioimage analysis and management** [K.Kvilekval, D.Fedorov, B.Obara et al. //Bioinformatics (2010) 26(4): 544-552]
 - Bioimage informatics: a new area of engineering biology [H.Peng//Bioinformatics (2008) 24(17): 1827-1836]



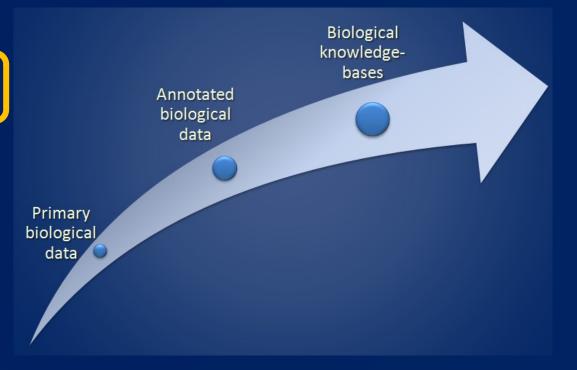
http://www.jatit.org/volumes.php Journal of Theoretical and Applied Information Technology

P.R.Rajeswari & A.Apparao Genbit compress – algorithm for repetitive and non-repetitive DNA sequences// 2010, vol 11, no. 1

- P.R.Rajeswari, A.Apparao, R.K.Kumar **Huffbit compress algorithm to compress DNA sequences using extended binary trees**// 2010, vol 13, no.2.
- J.H. Pujar, I.M. Kadlaskar **A new lossless method of image compression and** decompression using Huffman coding techniques//2010, vol 15, no.1
- G.Bhopale Image noise reduction using mathematical morphology size distributions. A new image noise reduction and compression algorithm for grayscale images //2010, vol 16. No. 1

New IT Solutions for bioinformatics

- Data compression
- Web semantics
- Web services
- Gridification
- Biocomputing



http://hackathon3.dbcls.jp/



| /iki | Timeline | F |
|------|----------|---|
| | | |

DBCLS BioHackathon 2010

The 3rd DBCLS BioHackathon for interpreting biological knowledge with Semantic Web technologies will be held during 2010/2/ 8-12 in Japan.

- Participants
- Schedule
- Symposium
- PosterSession
- OpenSpace
- Hackathon
- MeetingReport

Objectives

DBCLS is working on the integration of biological resources. To achieve this goal, we have been organizing BioHackathons since 2008 to surve environments with open source software and public services. Themes of the hackathons evolved year by year, and we are continuously providi gather for utilizing state of the art technologies to emerging demands in life sciences.

DBCLS BioHackathon for interpreting biological knowledge with Semantic Web technologies is working on the integration of biological resources. To achieve this goal, we have been organizing BioHackathons since 2008 to survey existing efforts and develop integrated environments with open source software and public services.

Semantic Web technologies http://rewerse.net/A2/Overview.htm

Rewerse Working group A2: Adding Semantics to the Bioinformatics Web

Sections

Overview Demos Deliverables Participants Publications

reasoning on the web

Overview

Objectives

The objective of the WG is to create the core of a Bioinformatics Semantic Web populated by a number of sa Bioinformatics and to demonstrate novel, reasoning-based solutions dealing with the following problems:

- Rules for mediation and to formulate complex queries
- · Consistent integration of Bioinformatics data
- Adaptive portals for molecular biologists

Bioinformatics is an ideal field for testing Semantic Web technologies for three reasons: First, Web-based systems and Web databases have been applied very early i dramatic increase of data produced in the field calls for novel processing methods, third, the high heterogeneity of Bioinformatics data require semantic-based integratic

A2: Bioinformatics

rewerse.net

Consider the following scenario: a biologist obtains a novel DNA sequences nothing is known about. He or she wants to run an alignment, but has specific requirements are captured as rules and constraints, which are taken into account by the online accessible semantic. Web enabled sequence comparison service

The objective of the WG is to create the core of a Bioinformatics Semantic Web populated by a number of sample data sources and applications representative of the use of the Web in Bioinformatics and to demonstrate novel, reasoning-based solutions dealing with the following problems:

Rules for mediation and to formulate complex queries Consistent integration of Bioinformatics data Adaptive portals for molecular biologists

http://www.ida.liu.se/~iislab/projects/ SAMBO (System for Aligning and Merging Biomedical Ontologies)



KitAMO (a ToolKit for Aligning and Merging Ontologies)



Gene onthologies http://bioportal.bioontology.org/

| O BioPortal | Browse | Search | Projects | Annotate | All Mappings | All Resources Alpha | <u>Sign In</u> <u>Register</u> <u>Help</u> |
|--|--|--|---|---|--|--|---|
| | | | | | | | |
| Welcome to the I | ICBO Bioportal | | | | | | |
| column), browse a l (try typing "Melanon <u>ontologies , find an</u> c | ist of ontologies in E na" in the "Search re I create relations be | BioPortal (type "NCI T sources" box in the r stween terms in diffe | Thesaurus" in the "Fir right column). You ca | nd an ontology" box i in <u>create ontology-ba</u> iew and comment on | n the middle column) used annotations for y |), search biomedical i your own text , link y | ping "Melanoma" in the "Search all ontologie resources that we automatically annotated your own project that uses ontologies to the prowse them. <u>Sign in to BioPortal</u> to submit |
| Search all ontolog | gies — | | Find a | an ontology ——— | | 1 | Search resources |

| Search all ontologies | | Find an ontology | | Search resources |
|---------------------------|--------|---|---|-----------------------------|
| Enter term, e.g. Melanoma | Search | Enter ontology name, e.g. NCI Thesaurus Explore | | Enter a term, e.g. Melanoma |
| Advanced Search | | Browse Ontologies > | | Advanced Resource Search |
| | | | _ | |

| — Most Viewed Ontologies (August, 2010) — | |
|---|-------|
| Ontology | Views |
| SNOMED Clinical Terms | 2044 |
| NCI Thesaurus | 1294 |
| NCBI organismal classification | 1177 |
| RadLex | 738 |
| MedDRA | 639 |

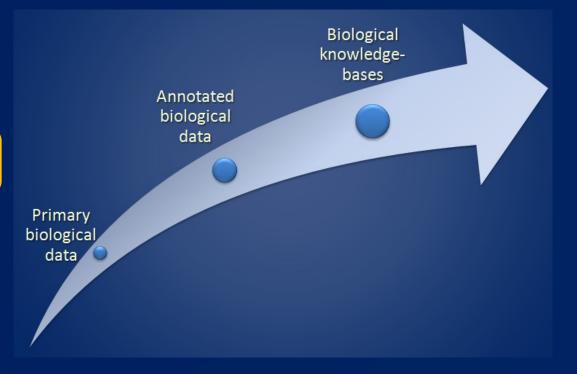
| Latest Notes | Latest Mappings |
|--|--|
| Order Chiroptera has been included (Malaria Ontology) 15 days ago by topalis Bats are now correctly appearing as members of Chiroptera. | Patient (Health Level Seven) => Interve (SNOMED Clinical Terms) 08/06/10 nigam |
| <u>New Relationship Proposal: is_a (Malaria</u> | <u>Melanoma (NCI Thesaurus) => Maligna</u> <u>melanoma (SNOMED Clinical Terms)</u> 08/02/10 nigam |
| <u>Ontology)</u> 24 days ago by slozano | Malignant melanoma (SNOMED Clinical => Melanoma (NCI Thesaurus) |

08/02/10 nigam

New Term Proposal: ventral fin lepidotrichium

New IT Solutions for bioinformatics

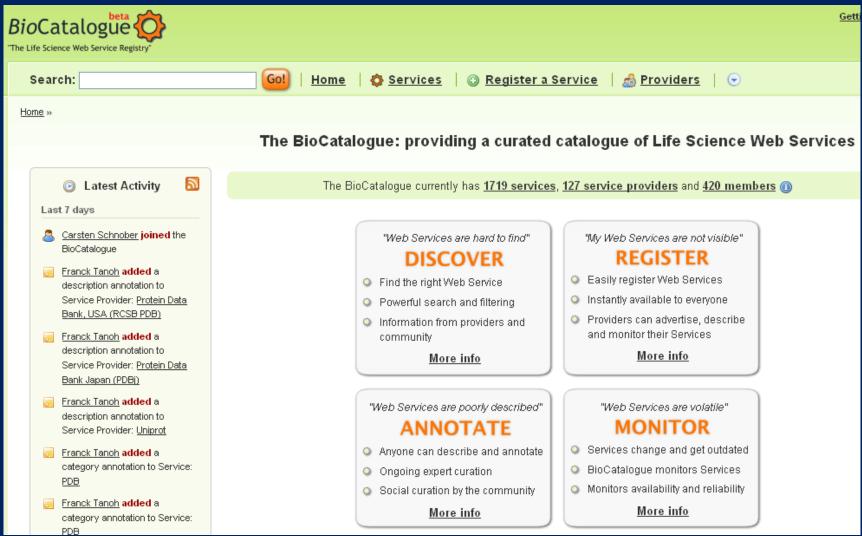
- Data compression
- Web semantics
- Web services
- Gridification
- Biocomputing



Recent publications on Web services for bioinformatics

- Kalas M, Puntervoll P, Joseph A et al. BioXSD: the common data-exchange format for everyday bioinformatics web services// Bioinformatics. 2010 Sep 15;26(18):i540-6.
- Zappa A, Miele M, Romano P. IBWS: IST Bioinformatics Web Services// Nucleic Acids Res. 2010 Jul 1;38 Suppl:W712-8
- Katayama T, Nakao M, Takagi T. TogoWS: integrated SOAP and REST APIs for interoperable bioinformatics Web services// Nucleic Acids Res. 2010 Jul 1;38 Suppl:W706-11
- Smedley D, Schofield P, Chen CK et al Finding and sharing: new approaches to registries of databases and services for the biomedical sciences // Database (Oxford). 2010 Jul 6;2010: baq014.
- Ramírez S, Muñoz-Mérida A, Karlsson J et al. MOWServ: a web client for integration of bioinformatic resources// Nucleic Acids Res. 2010 Jul 1;38 Suppl:W671-6.

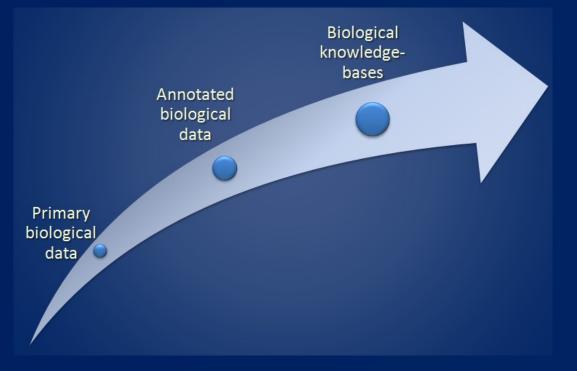
http://www.biocatalogue.org/



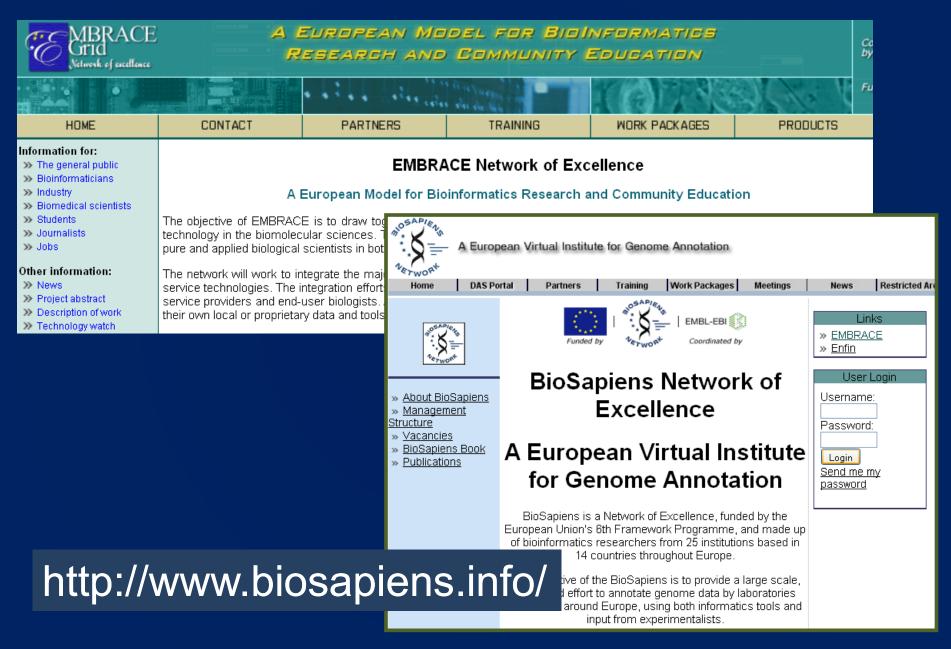
BioCatalogue: a universal catalogue of web services for the life sciences// NAR, Web servers issue, 2010

New IT Solutions for bioinformatics

- Data compression
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http://www.embracegrid.info/



https://cabig.nci.nih.gov/



National Cancer Institute

CaBIG[®] Cancer

Home

Getting Connected

Setting the Stage

Finding caBIG® Tools

caBIG® Compatibility

caCORE

caGrid

Data Sharing

Getting Support

Knowledge Centers

Service Providers

Training Portal

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Communications Resources

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News Articles

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главная » concepts » cancer common ontologic representation environment (cacore) Cancer Common Ontologic Representation Environment (caCORE)

🖝 caCORE 3.x APIs and Grid Services Decommissioned August 7, 2009. Announcement posted 🖄

Key to achieving interoperability and compatibility, caCORE tools and APIs are developed by the National Cancer Institute Center for Bioinformatics and Information Technology (NCI CBIIT) to provide the building blocks for development of interoperable information management systems. This ultimately enables interoperability and data sharing from the scientific bench to the clinical bedside and back.

caCORE includes the following key components:

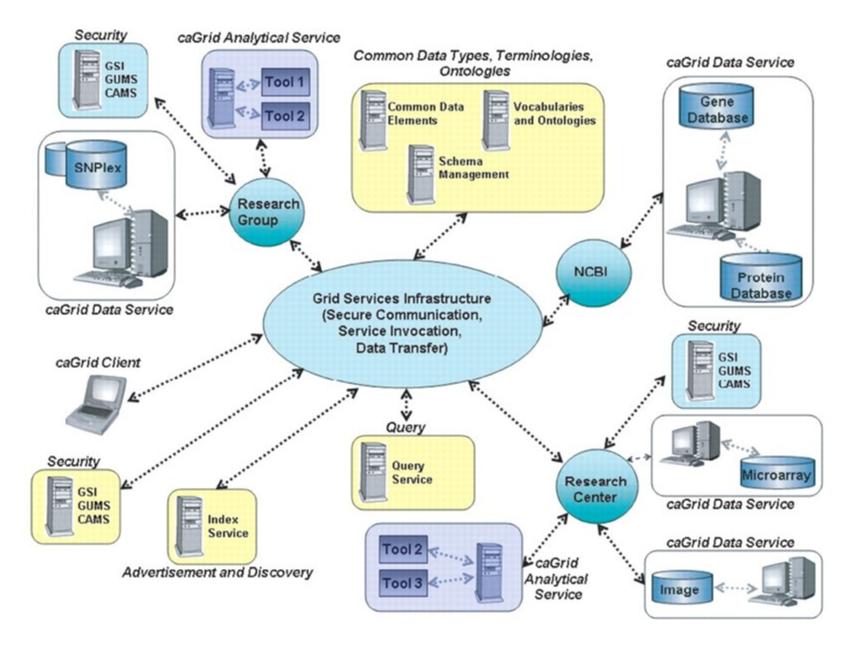
- EVS (Enterprise Vocabulary Services) for hosting and managing vocabulary.
- <u>caDSR</u> (Cancer Data Standards Registry and Repository) for hosting and managing metadata.
- <u>caCORE SDK</u>, the GUI-based <u>caCORE Workbench</u>, and associated tools for model-driven software engineering of systems which can be easily integrated with <u>caGrid</u>.

<u>EVS</u> and the <u>caDSR database and tools</u> are the basis of the semantic foundation for interoperable data and analytical services.

Developers use caCORE components to create "caCORE-like" systems. By definition these systems have object-oriented information models registered in caDSR whose meaning is linked to EVS vocabularies, and have

p. The <u>caBIO data service</u> 🗹 is an example of a

caBIG (Cancer Biomedical Informatics Grid)



http://dockinggrid.gforge.inria.fr/

Objectives and Project Outlines Project Coordinators and Partners Project Project Organization Softwares **Download** Meetings Publications Related links Deliverables

ANR DOCK Molecular Docking on Grids

Objectives and Project Outlines

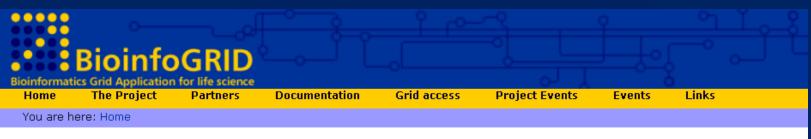
Finance par

Acronym of the project: Docking@Grid Title of the project: Conformational Sampling and Docking on Grids

Goals and Summary

Molecular modelling – and notably the conformational sampling and docking procedures for understanding the interaction mechanisms between (macro)molecules involved in pł obvious interest in computationally predicting the binding modes of partners involved in participating in regulatory processes within the living cell, such approach may equally be means to interfere with the normal or pathological process (rational drug design). Howe combinatorial complexity (molecule size, number of degrees of freedom) that represent currently available computing power, hence the three imperative research directions in the search for mathematical models of maximum simplicity that nevertheless provide a

http://www.bioinfogrid.eu/



Navigation

- The Project
- Partners
- Documentation
- Grid access
- Project Events
- Events
- Links



The BioinfoGRID Project



The European Commission promotes the Bioinformatics Grid Application for life science (Bioin centres in order to carry out Bioinformatics research and to develop new applications in the technology that represents the natural evolution of the Web.

Grid networking promises to be a very important step forward in the Information Technolog of thousands of interconnected computers possible, allowing the shared use of calculating power, data storag communication between computers and aims instead to transform the global network of computers into a vas

The BioinfoGRID White Paper



The BioinfoGRID White paper outlines guidelines and recommendations for the scientific co BioinfoGRID project.

The BioinfoGRID European project aims to promote the Bioinformatics applications for life s technology. More specifically the BioinfoGRID project evaluates applications in the fields or data calculation times by distributing the calculation on thousands of computers using the Framework Program). The massive potential of Grid technology is indispensable when deali data, for example, in searching the human genome or when carrying out docking simulation Organisations related to the BioinfoGRID project are able to run Bioinformatics challenges o biology.

The BioinfoGRID white paper provides guidelines and recommendations that have been drawn from our experie findings we give advice to different user communities on how to take advantage of the power of the GRID.

📆 Download the BioinfoGRID White Paper in pdf format (3.2MB)



Мониторинг УАГ

Контакты

О Гриде

- » Что такое Грид?
- » Проекты Грид
- » Грид в Украине
- » Литература
- » Ресурсы

Проекты EGEE и EGI

- » Что такое EGEE?
- » EGEE Activities
- » Партнеры EGEE
- » События EGEE
- » Грид-приложения
- » Что такое EGI?
 - Полезные ссылки



Главная

Карта сайта

Новости

http://uag.bitp.kiev.ua/

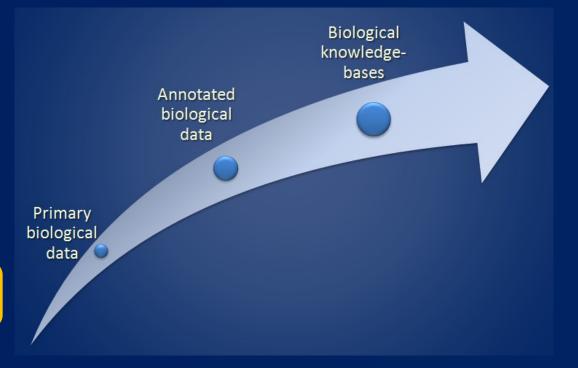
(o)IID wm(Gi Virtual Lab





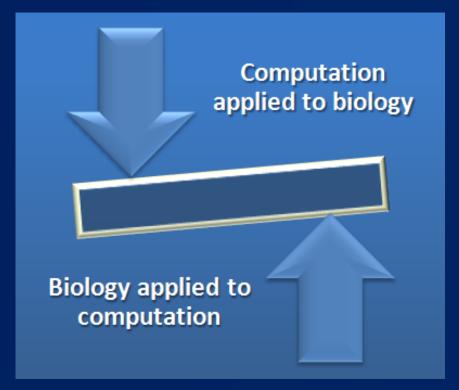
New IT Solutions for bioinformatics

- Data compression
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Two Kinds of Computation Motivated by Biology

- Computation applied to biology
 - Bioinformatics
 - computational biology
 - modeling DNA, cells, organs, populations, etc.
- Biology applied to computation
 - biologically-inspired computation
 - neural networks
 - artificial life, etc.



http://www.cs.utk.edu/~mclennan/Classes/420



Bioinformatics vs biocomputing

Bioinformatics: the application of computer technology to the management of biological information. Is associated with knowledge extraction and interpretation of data

Biomolecular computing: the use of biological and chemical processes to perform computations

Bio-inspired computing: the use of biological paradigms (e.g., neural nets, genetic algorithms) in the design of computational algorithms. Algorithms may be implemented in *any* appropriate technology.

Useful links

http://www.biochem.oulu.fi/Biocomputing/juffer/Teaching/Biocomputing/ http://www.cs.utk.edu/~mclennan/Classes/420

IT solutions from biology data

BIO-INSPIRED COMPUTING (BIOCOMPUTING)

- Genetic Programming
- Evolutionary algorithms
- Swarm Intelligence
- Cellular Automata
- Neural Computing / Pattern recognition using *neural networks* (the most widely used form of BIC in industry and science)
- Artificial Immune System methods
- etc

http://www.macs.hw.ac.uk/~dwcorne/Teaching/bic.html

IT solutions from biology data

DATA COMPRESSION-BASED APPROACHES TO ANALYSIS OF BIOLOGICAL NETWORKS

Tatsuya Akutsu (Kyoto University)

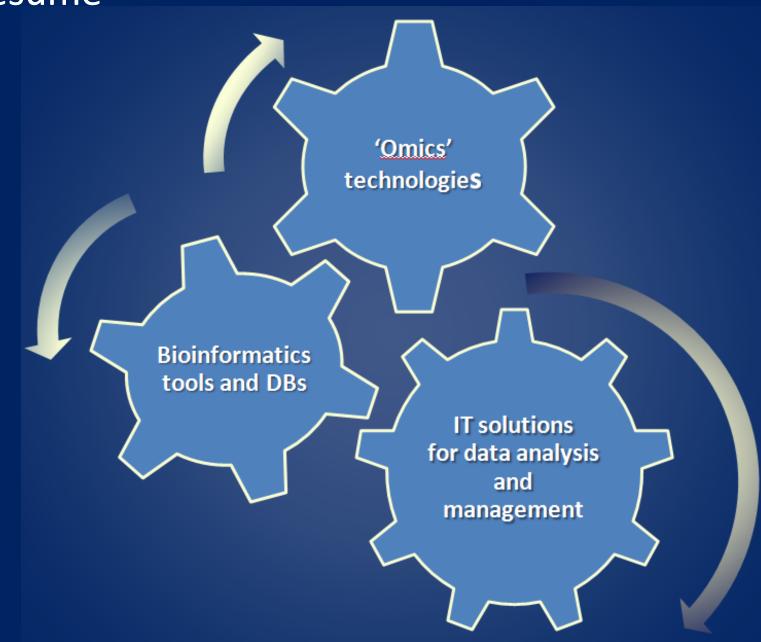
From Plenary talk on **The Fourth International Conference on Computational Systems Biology (ISB2010)** Suzhou, China, September 9-11, 2010

The human genome consists of around 3 billion base pairs whereas the number of cells in the human body is estimated to be 60 trillion. Therefore, it is considered that information on the human body consisting of 60 trillion cells is compressed into 3 billion base pairs. *Deciphering this data compression mechanism* is one of major goals of systems biology.

Lecture Notes in Operations Research 13

Series Editors: Ding-Zhu Du and Xiang-Sun Zhang Computational Systems Biology

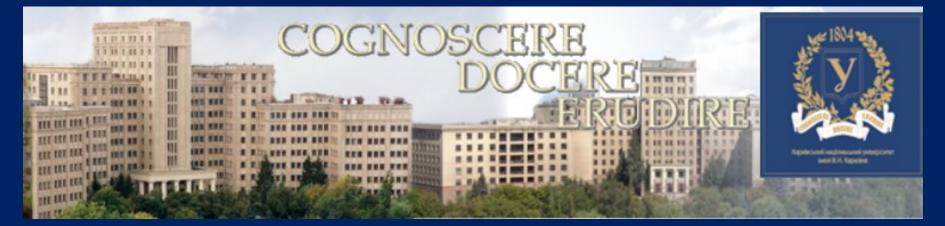
Resume



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