EMBnet.news

Volume 11 Nr. 3
September 2005

- eBiotools Sept. 1st 2005 (new release)
- BioX graphic interface
- The EBI resources in a Nutshell (part 4)
- Xgrid, a «just do it» solution for non IT's and more...

Editorial

The CBR and the HGMP/RFCGR hosting the Canadian and UK EMBnet node, respectively, have closed recently or will soon close. These two institutions were important members of the EMBnet community. These decisions mostly driven by funding concerns are symptomatic of the current trend in the Bioinformatics community. More and more universities and institutes create their own department of bioinformatics and do not want to rely on national centralized resources anymore. However the benefit of having multiple small centers with variable strength and interests is questionable, as compared to a multi-competent national center of excellence. Does it not sound like a waste of money and dispersion of talent? The evolution of Bioinformatics is still to be studied, but the current trend favors small reactive groups versus large, possibly slower, groups. Who will survive in the mid-to-long-term? Will a centralizing move force many small groups to join their efforts, recreating the good old center of excellence? Only the future will tell us the truth!

The editorial board: Erik Bongcam-Rudloff, Laurent Falquet, Pedro Fernandes, Oscar Grau, and Gonçalo Guimaraes Pereira.

proteinspotlight

> ONE MONTH, ONE PROTEIN <

Protein Spotlight (ISSN 1424-4721) is a periodical electronic review from the SWISS-PROT group of the Swiss Institute of Bioinformatics (SIB). It is published on a monthly basis and consists of articles focused on particular proteins of interest. Each issue is available, free of charge, in HTML or PDF format at
`http://www.expasy.org/spotlight`

We provide the EMBnet community with a printed version of issue 61. Please let us know if you like this inclusion.

Cover picture: Carolus Linnaeus (later, Carl von Linné) (1707-1778) inventor of the modern taxonomy, Uppsala [© Erik Bongcam-Rudloff]

Contents

Editorial 2
eBiotools Sept.1st 2005 3
BioX graphic interface 5
EBI resources in a Nutshell (4) 8
Xgrid, a "just do it" grid solution for non IT's 13
Protein spotlight 61 20
Node information 22

Editorial Board:

Publisher:

EMBnet Executive Board
c/o Erik Bongcam-Rudloff
Uppsala Biomedical Centre
The Linnaeus Centre for Bioinformatics, SLU/UU
Box 570 S-751 23 Uppsala, Sweden
Email: erik.bongcam@bmc.uu.se
Tel: +46-18-4716696

eBiotools Sept. 1st 2005 (new release)

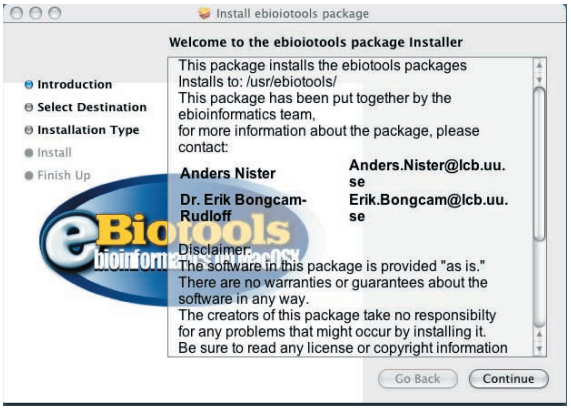
Anders Nister
Project Student

Erik Bongcam-Rudloff
Associate Professor

The Linnaeus Centre for Bioinformatics, SLU, UU, Uppsala, Sweden.

Introduction

After our previous release of eBiotools we started working on improvements and updated some of the existing packages. The size of the installation was also drastically reduced from 260 MB to 163.5MB.



Updates

In this release we updated the following packages/programs:

hmmer 2.3.2 from hmmer 2.1.3
`http://hmmer.wustl.edu/`

emboss.kaptain 0.97 from emboss.kaptain 0.95
`http://userpage.fu-berlin.de/~sgmd/`

Please note that this version of emboss.kaptain is our modified version and works with EMBOSS 3.0.0

ncbi-tools Jun-5-2005 from ncbi-tools Feb-2004
`ftp://ftp.ncbi.nih.gov/toolbox/`

primer3 1.0.0 from primer3 0.9
`http://frodo.wi.mit.edu/primer3/primer3_code.html`

Staden 1.53 from Staden 1.4
`http://staden.sourceforge.net/`
This release of Staden fixes many of the problems using the Staden-EMBOSS interface.

emboss 3.0.0 from emboss 2.8.0
`http://www.emboss.org`
The EMBOSS package also installs all current **embassy** extensions, namely:
DOMAINATRIX-0.1.0,
DOMALIGN-0.1.0,
DOMSEARCH-0.1.0,
EMNU-1.05,
ESIM4-1.0.0,
HMMER-2.1.1,
MEME-2.3.1,
MSE-1.0.0,
MYEMBOSS-3.0.0,
PHYLIP-3.6b,
SIGNATURE-0.1.0,
STRUCTURE-0.1.0,
TOPO-1.0.0

We have also added or updated the following databases needed by some EMBOSS programs:
aaindex 6.0, Rebase 508, Transfac 3.2, Prints 37_0, Cutg 148, Prosite 19.7.

New tools

Several new packages were added in this release:

ClustalX
This is our own AquaClustalX interface and installs in the directory `/Applications`. Clustal X provides a new Aqua-based user interface to the ClustalW multiple sequence alignment program.

Infernal 0.55
Infernal is a software package that allows you to make consensus RNA secondary structure profiles, and use them to search nucleic acid sequence databases for homologous RNAs,

or to create new structure-based multiple sequence alignments.
http://www.genetics.wustl.edu/eddy/infernal/

sim4 2003-09-21

sim4 is a similarity-based tool for aligning an expressed DNA sequence (EST, cDNA, mRNA) with a genomic sequence for the gene. It also detects end matches when the two input sequences overlap at one end (i.e., the start of one sequence overlaps the end of the other). If seqfile2 is a database of sequences, the sequence in seqfile1 will be aligned with each of the sequences in seqfile2.
http://globin.cse.psu.edu/html/docs/sim4.html

smile 1.47

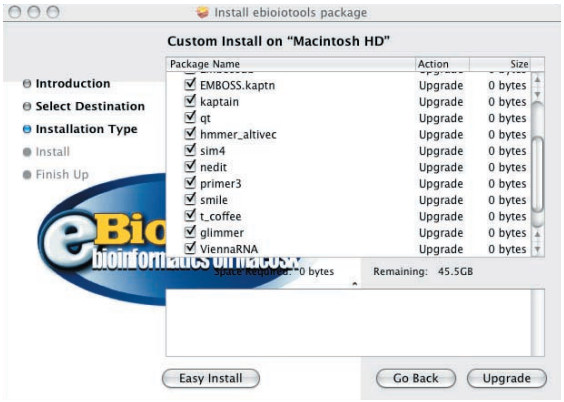
Structured Motifs Inference and Evaluation tool.
Marsan L, Sagot MF (2001). Algorithms for extracting structured motifs using a suffix-tree with application to promoter and regulatory site consensus identification. J. of Computational Biology, 7:345-360.
http://www-igm.univ-mlv.fr/~marsan/smile.html

Vienna RNA Package 1.5beta

The Vienna RNA Package consists of a C code library and several stand-alone programs for the prediction and comparison of RNA secondary structures.
http://www.tbi.univie.ac.at/~ivo/RNA/

meme 3.0.14

MEME is a tool for discovering motifs in a group of related DNA or protein sequences. MEME represents motifs as position-dependent letter-probability matrices which describe the probability of each possible letter at each position in the pattern. Individual MEME motifs do not contain gaps. Patterns with variable-length gaps are split by MEME into two or more separate motifs.
http://meme.sdsc.edu/meme/website/intro.html



Libraries

We added/updated new support packages with libraries or applications needed by some packages:
EMBOSS: **jpeg 6b, libpng1.2.8, gd 2.0.33**
Nedit: **openMotif 2.1.31**
Staden: **f2c 20030428**
Embosslauncher:**qt 3.3.4, kaptain 0.7, nedit 5.5,** with a **neditrc** file that makes it possible to see sequence alignments in full colour.

Removed

A major change in this release is that the **wwwblast** package has been removed from the default eBiotools installation. If needed, this package can be downloaded separately and installed as an extra package. It will install all necessary files to run your MacOSX machine as a BLAST server using your own sequences. You can read how to proceed with the installation descriptions in previous issues of EMBnet.news 9.2 & 10.4.
Please note that this package will be installed in the directory `/Library/WebServer/Documents`, and will overwrite any previous web-blast installation in this directory.

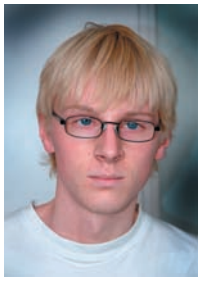
A new feature in this release is the addition of the files `/usr/ebiotools/profile` and `/usr/ebiotools/csh.login` containing all environment variables needed by eBiotools to work correctly and without any major manual editing by the users.

BioX

The biggest new addition to eBiotools is the creation of a native MacOSX graphic interface with a sequence editor: **BioX**. More about this interface in the following article.

For up to date information, bug reports and tutorials please go to:
www.ebioinformatics.org

BioX: a Graphic interface to eBiotools



Erik Lagercrantz
Project Student

Erik Bongcam-Rudloff
Associate Professor

The Linneaus Centre for Bioinformatics, SLU, UU, Uppsala, Sweden.

Prerequisites

- MacOSX 10.4.x (Tiger) + X11
- eBiotools Sept. 1st 2005

Introduction

BioX is a biological sequence editor and analysis program that can be used for creating multiple sequence alignments from nucleotide or amino acid sequences. This program is intended for the production of hand alignments and for preparing input for alignment programs like ClustalW and phylogeny reconstruction programs such as

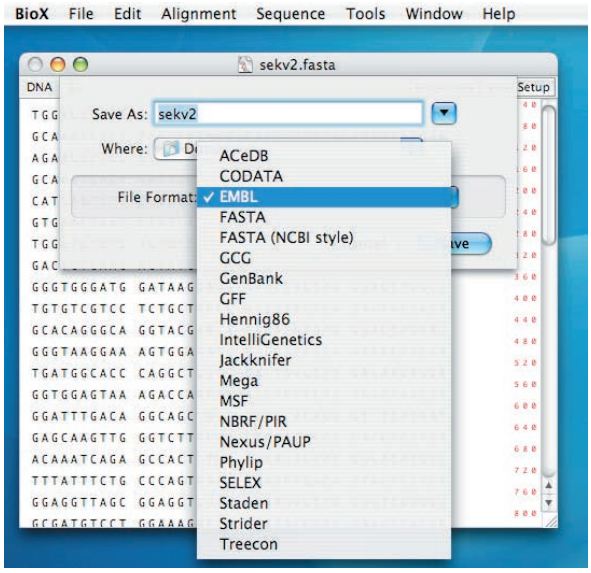
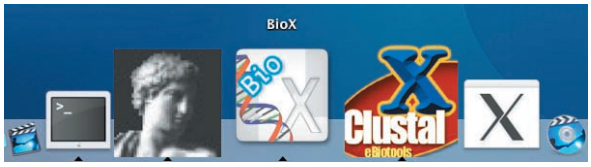


Figure 1. Sequence format menu



PHYLIP, all of them pre-installed by **eBiotools**. **BioX** is presently only available for Tiger (MacOSX 10.4 and above).

Features

• **BioX** can import and export sequences in the most commonly used sequence formats. BioX uses the EMBOSS **seqret** application to import and export sequences. BioX can also be used for sequence format conversions. See Figure 1.

• **Biox** can perform alignments using ClustalW (Figure 2a). The alignments can be moved by selecting a block of sequences and sliding them relative to the other sequences. Gaps will open up behind the block (Figure 2b).

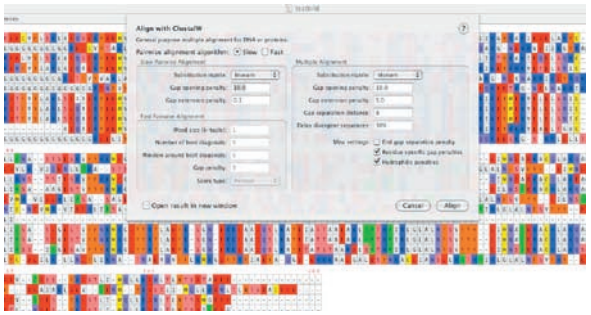


Figure 2a. Parameters window for ClustalW.

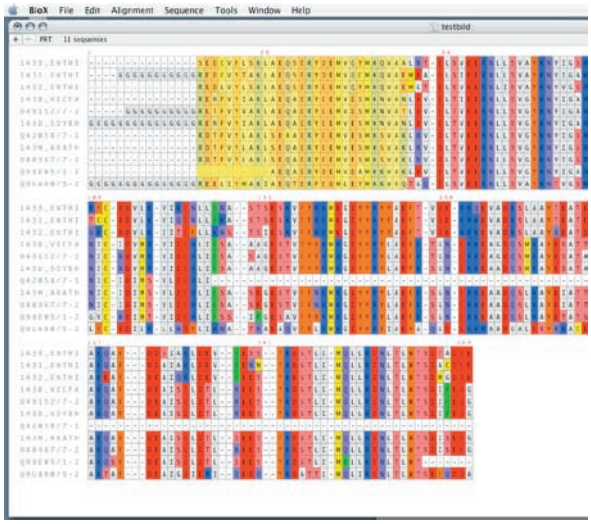


Figure 2b. Manual editing by moving blocks of sequences.

• Sequences and their names can be edited in a separate window (Figure 3, a & b). You do this by selecting the sequences you want to edit. The results of your editing are immediately reflected in the alignment window. Raw sequences can also be pasted from other sources into a new editor window. Spaces, formatting and non-sequence characters (e.g., numbers) will be removed automatically.

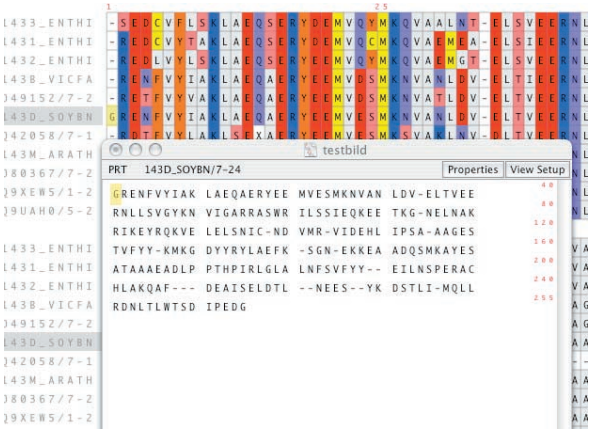


Figure 3a. Sequence editor window.

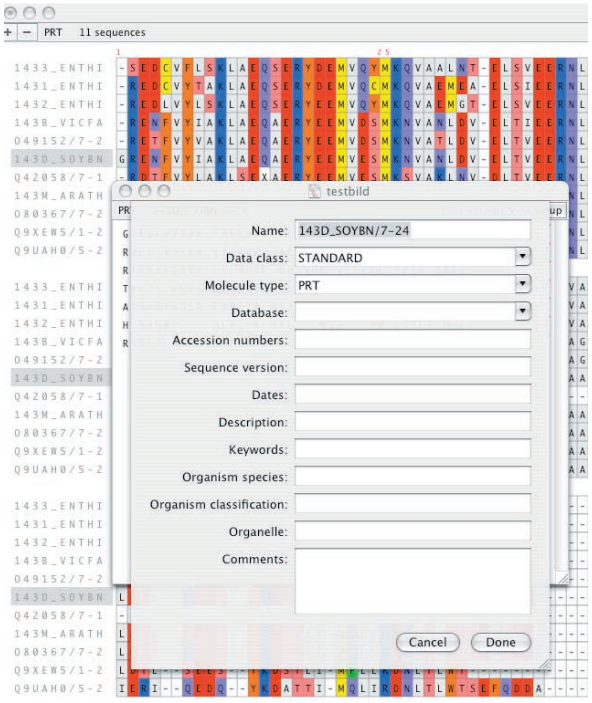


Figure 3b. Sequence name and data editor window.

• It is possible to Cut, Copy and Paste whole sequences or sections of alignments within and between alignment documents. Copy and paste between BioX and other applications is also possible (Figure 4).BioX supports also standard text editing functionality including undo/redo and find/replace.

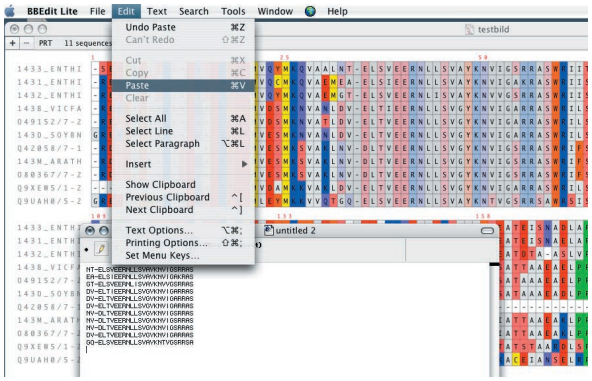


Figure 4. Cut&Paste menu.

• **BioX** uses all the power of the MacOSX graphic libraries and it is possible to zoom in and out with the help of keyboard commands.

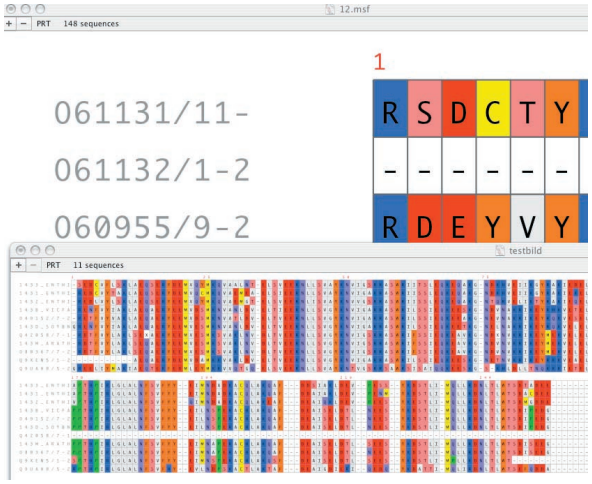


Figure 5. Zooming within an alignment.

• **BioX** can directly produce high quality printouts of your aligned protein or DNA sequences in many formats (e.g., PostScript, PDF). See Figure 6.

• To use the EMBOSS programs for which there is not yet a graphical interface in BioX, you can use the application **embosslauncher.kapt**, which is easily accessed from the Tools menu in BioX. Embosslauncher.kapt needs the X11 windows system and BioX launches X11 automatically (Figure 7) when you start X11-dependent programs (e.g., the Staden programs included).

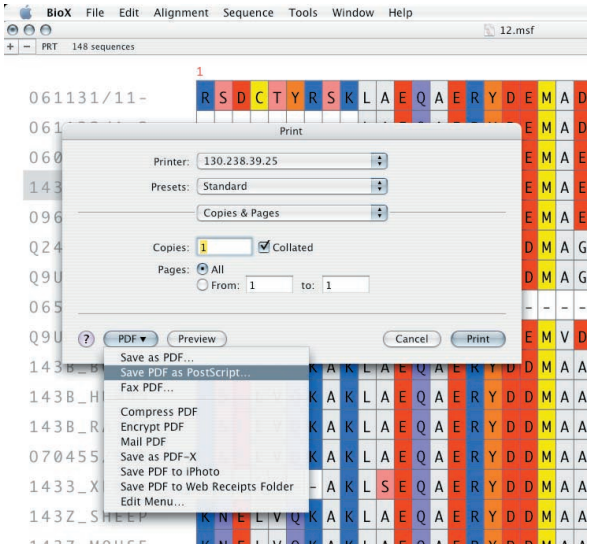


Figure 6. Printing window options.

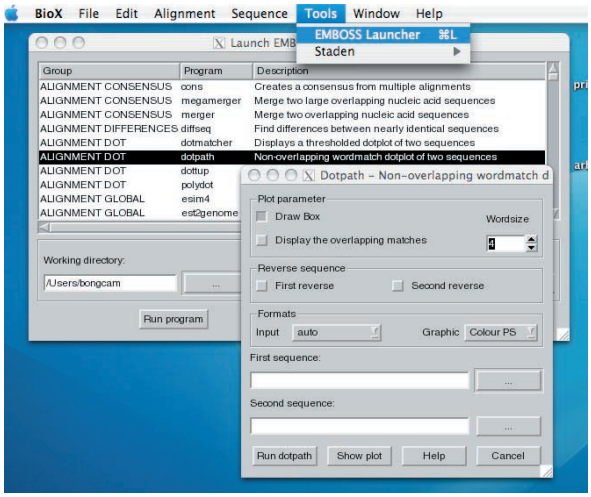


Figure 7. Launching external programs in X11 windows.

• **BioX** is currently a useful sequence editor but our goal is to create a more or less complete graphic interface to all the program packages installed by eBiotools. Some analysis functions are already implemented (most of which use EMBOSS programs for the actual calculations) - these can be accessed from the «Sequence» menu (Figure 8, a & b).

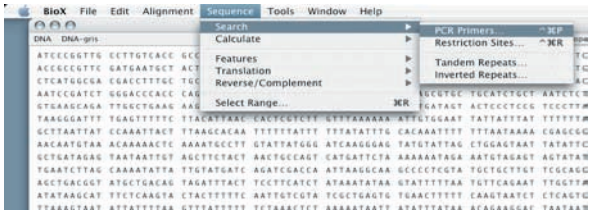


Figure 8a. Selecting integrated tools

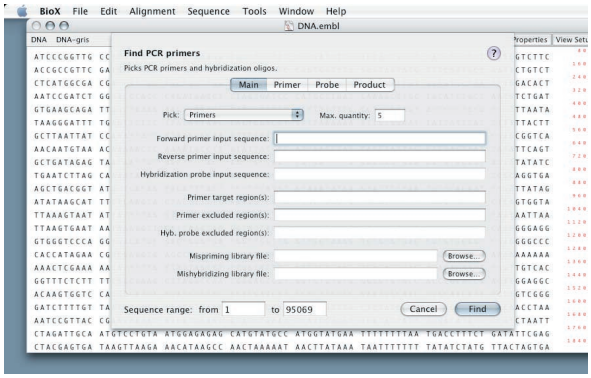


Figure 8b. PCR primer parameter window

Remarks

This application is a beta version and all comments as to how to improve it are most welcome! If there is demand for a particular function, we will try to include it in the development pipeline. If you would like to contribute to the development of BioX you can obtain all relevant information at:
`http://www.lagercrantz.name/projects/biox/`
You can download a pre-compiled version at `www.ebioinformatics.org`
A video tutorial will be available at the same URL and you will be able to see it using the free video client **DTV**. You can download it at `http://participatoryculture.org/download.php`

We plan to add a version for MacOSX on the Intel platform as soon as possible.

Other editor resources

CINEMA 5: `http://aig.cs.man.ac.uk/research/utopia/cinema/cinema.php`

Jalview 2: `http://www.jalview.org`

TXshade: `http://homepages.uni-tuebingen.de/beitz/txe.html`

Pfaat: `http://pfaat.sourceforge.net/`

STRAP: `http://www.charite.de/bioinf/strap/`

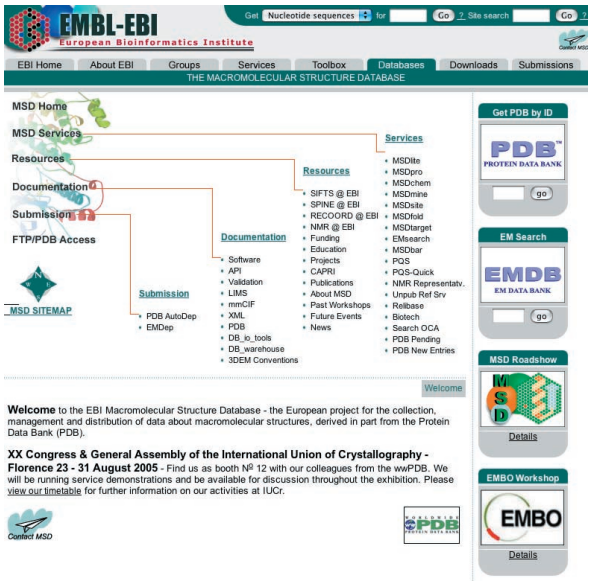
The EBI resources in a Nutshell (part 4)

Lisa Mullan
EMBL Outstation - Hinxton,
European Bioinformatics Institute, Wellcome Trust Genome Campus,
Hinxton,
Cambridge, CB10 1SD,
United Kingdom

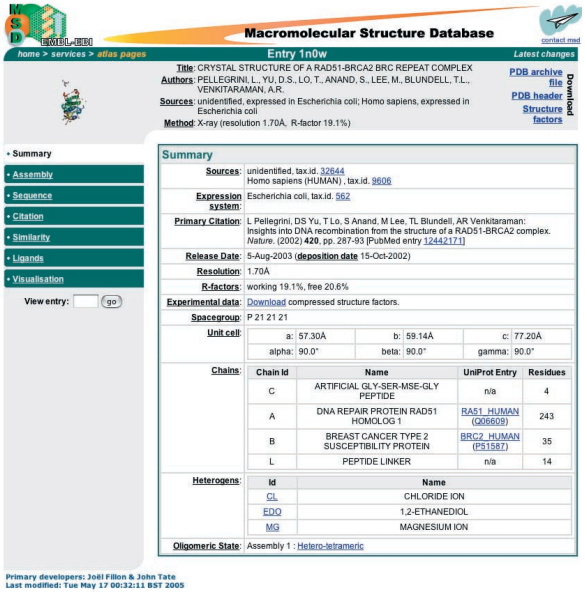
This practical was designed for the EBI's Small to Medium Sized Industry Programme and aims to offer a practical overview of some of what the EBI can offer in terms of bioinformatics resources in the form of web services (see Parts 1-3 in EMBnet.news issues 10.4, 11.1 & 11.2).

The MSD database

Enter the MSD using the homepage at `http://www.ebi.ac.uk/msd/` and using **MSDlite**, search for the PDB entry noted in

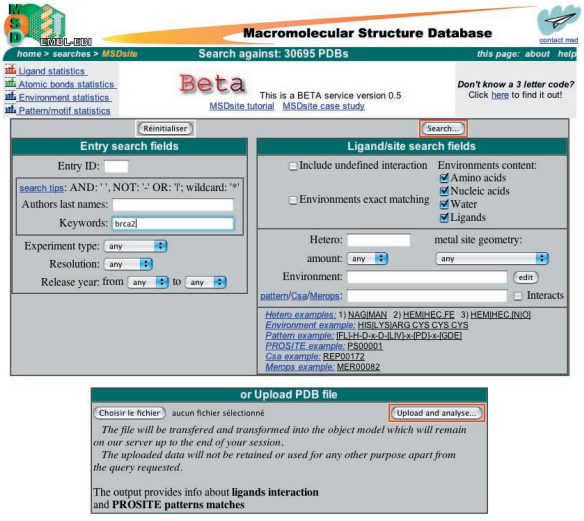


Reactome and in many cross references throughout the previous databases searches (i.e., UniProt:**P51587**).
Below is the MSD Atlas entry for **1n0w** and at the bottom the list of heterogens associated with this protein details Cl, EDO (1,2 ethanediol) and Mg as potential ligands bound to the structure.



Chloride and EDO may be dismissed straight away, as they are likely to be residuals of the crystallisation process. This may be the case with magnesium also, but before it is entirely dismissed, it warrants further investigation.

Return to the MSD services, either by going back to the home page, or by accessing the "services" link at the top of the page (in the green bar) and select MSDsite.

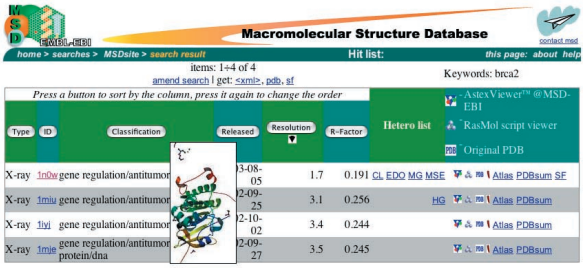


Citation:
Golovin A., Dimitropoulos D., Oldfield T., Rachedi A. and Henrick K. (2005)
MSDsite: A Database Search and Retrieval System for the Analysis and Viewing of Bound Ligands and Active Sites.
PROTEINS: Structure, Function, and Bioinformatics 58(1): 190-9.

Search using the keyword **brca2** and the results list four PDB entries. Only one contains all the ligands mentioned in the Atlas (**1n0w**).

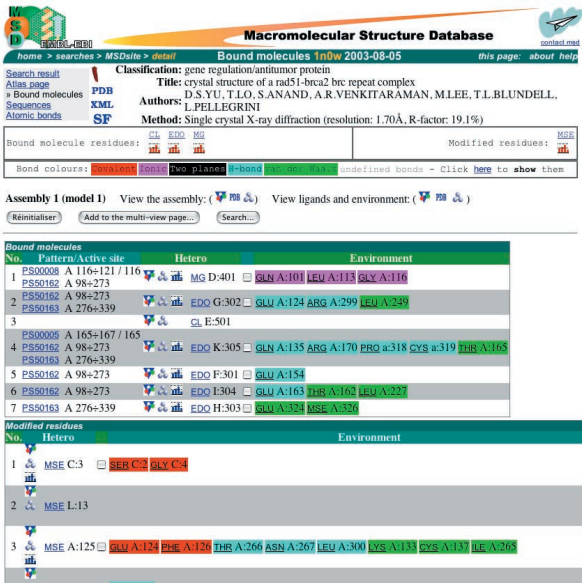
The additional "heterogen" in the list - MSE - is selenomethionine.

The second PDB entry in the table is **1miu**, which is cross referenced from the OB fold mentioned in Interpro (in a previous issue). It displays only Hg as its possible ligand. It is likely that this is an artefact arising from the insertion of a heavy metal for X-ray analysis of the structure.



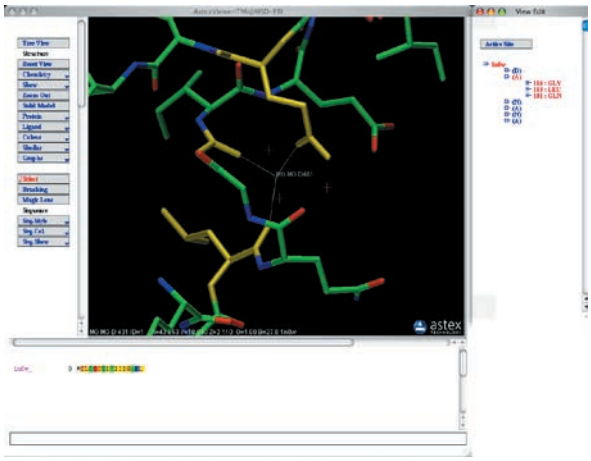
Mouse over the PDB IDs to see structural displays. To the right there are alternative view options and a link to the original information in the Atlas.

Follow the PDB ID link to the top hit – this is the one that has been cross referenced in several databases. This page gives an overview of the bonding between the ligand and residues in the macromolecule.



The Mg entry is referenced to a PROSITE entry which is merely a myristylation site and as such of little analytical value. Follow the blue graph icon to the environment statistics which suggest that the combination of Gln-Leu-Gly is common in binding several ligands, although Mg is not mentioned.

Return to the Bound Molecules viewer and click on the coloured AstexViewer icon to display the region of protein molecule where the Magnesium is bound. Select the ligands and click on (**A**) to see those bound to the Mg ion in the display (the (A) symbol should turn red).

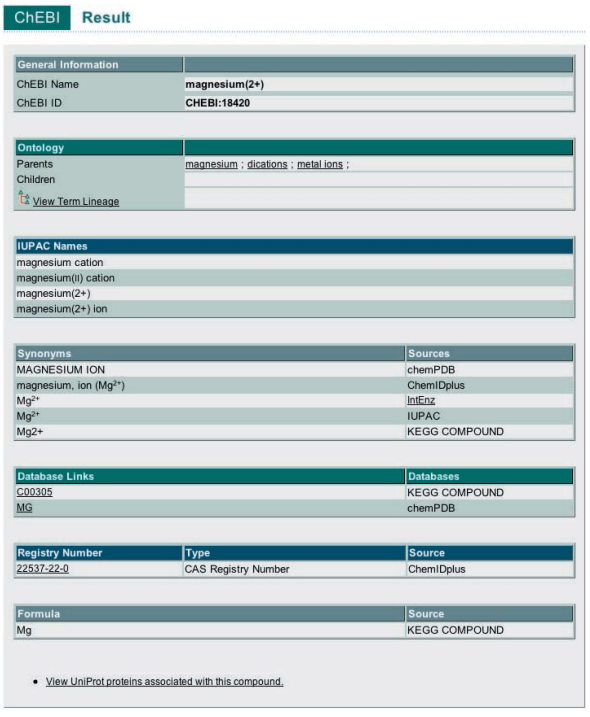


Click on one of the residues in the sequence below the display to zoom in on a particular region.

The ChEBI database

Access the Chemical Entities of Biological Interest (ChEBI) database at the EBI at `http://www.ebi.ac.uk/chebi/`. Type Mg in the Quick Search field on the left hand side and hit Search. Three results should appear for the search magnesium.

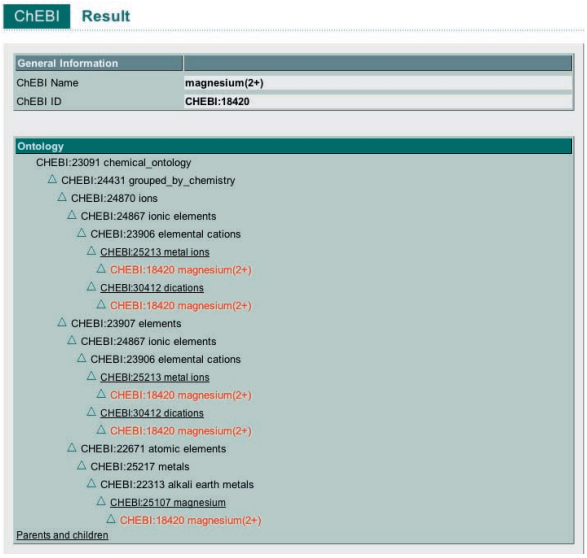
Follow the link for the **CHEBI:18420** entry.



ChEBI is a freely available dictionary of chemical entities, with IUPAC and NC-IUBMB endorsed terminology. It focuses on nomenclature and incorporates a chemical ontology and cross-references to UniProt. Compounds contained in ChEBI are either the natural products or are synthetic products used to intervene in the processes of living organisms. Molecules directly encoded by the genome, e.g. nucleic acids, proteins and peptides derived from proteins by cleavage, are excluded. ChEBI is a curated database where all entries are checked by a ChEBI curator and assigned an official ChEBI name. Relevant synonyms, CAS Registry Numbers and formulae are included.

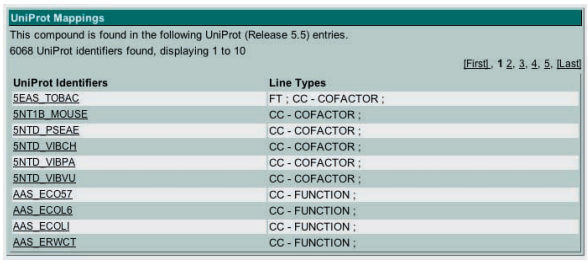
The data is non-proprietary and available in its entirety to download and use in-house.

Scroll to the Chemical Ontology and follow the "View Term Lineage" link. Magnesium is



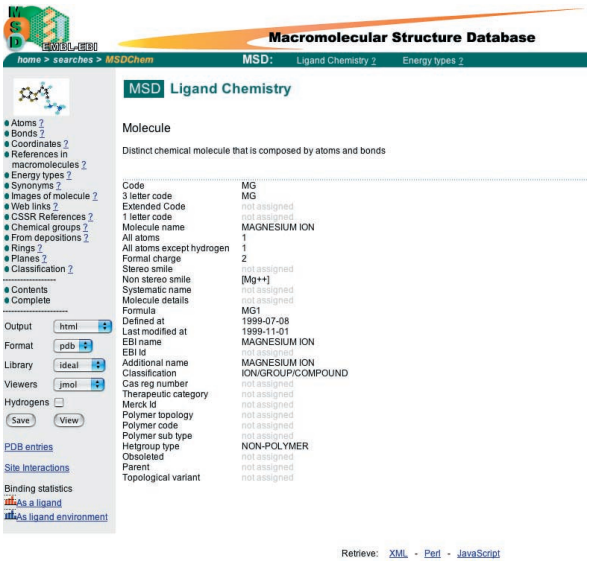
at the bottom of the compounds "grouped by chemistry". This is one of two main ontological hierarchies, the other being "grouped by functions" to explain those compounds grouped by biological functions. All the relevant groups in which Mg^{2+} appears are displayed.

Follow the link at the bottom of the page to view Uniprot proteins associated with this compound. The page will redraw and bring up a list of proteins with some connection to magnesium. It has currently been identified in 6068 proteins although this will change as the database is updated.



This information is taken from the Uniprot feature table.

The databases section reveals two links, one to the magnesium entry in the KEGG database, and the other to the MSD. Follow the MG link to the chemPDB.

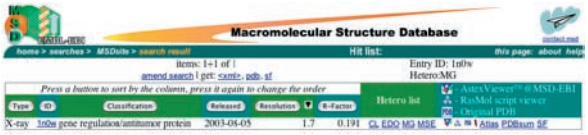


You are now in the MSDChem database accessing Ligand information for the magnesium ion. This information may be saved or viewed using the options in the various menus on the left hand side of the page.

Follow the links to the "Binding Statistics" on the left hand side of the page and note the most common environments for a magnesium ligand within a protein. Clicking on any of the bars in the statistics chart will link to information on that particular environment.

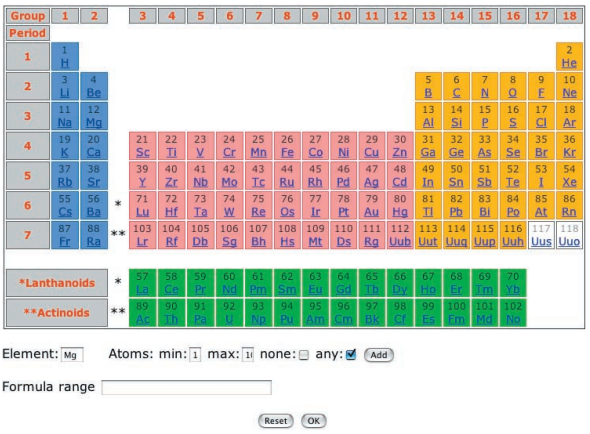
Follow the "Site Interactions" link on the left hand side to retrieve all the PDB entries with a magnesium ion in them. There are rather a

lot to look through – so a real search could be refined with the "amend search" link. Verify that the 1n0w protein is in the list.

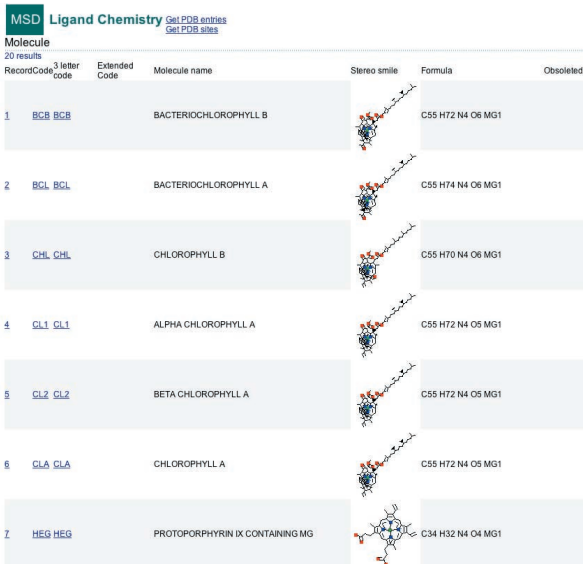


Return to the Mg information page and click the link "Complete" to retrieve data on all atoms and coordinates in the ligand (admittedly not many in this case!) and all PDB files containing magnesium. This information can be retrieved in XML, mmCIF, Perl or Javascript for further parsing by following the links in the middle of the page.

Follow the LigandChemistry link in the top green bar. This is the original search page for MSDChem. Putting Mg into the Code field would return us to the Magnesium ion information page. Instead, select the edit button from the "Formula" field and select Mg from the resulting periodic table. To allow for any number of Mg ions in the results, check the "any" box and then Add the information so it appears in the formula box below. Hit OK. This information has now been entered into the search page so hit the Search button. This lists all ligands which have a magnesium ion as part of their chemistry together with a visual representation of what the structure looks like.

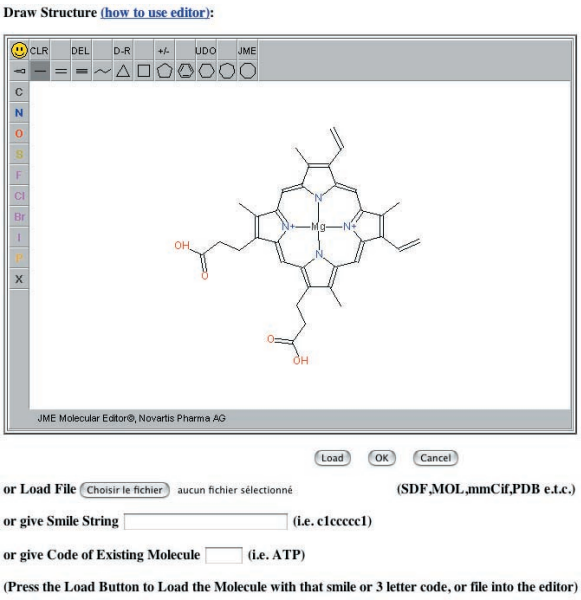


The magnesium ion is present together with a number of other compounds containing magnesium. It is unlikely at this stage that the Mg ion involved in our protein is little more than an experimental artefact, so this practical is designed more to display a further use for the MSD product.



Note the ligand with HEG as the three letter code. Return to the search page and hit the Edit button on the "Non stereo smile" field. Enter the code into the "Code of Existing Molecule" (this is case sensitive) and hit Load. The structure will pop up in the draw field.

Using the "DEL" button and by clicking on bonds with the mouse, delete everything except the Nitrogen bonds around the



magnesium. Hit OK and this formula will be loaded into the search page. By starting the search, all ligands containing this or similar formulas will appear.

This search can also be performed with chemical molecules drawn in the editor. Use the drawing tools in the top bar. Alternatively, existing molecules can be modified using these tools.

This is the end of the short tour of some of the resources available at the EBI. Perhaps you might like to try it again with a more relevant sequence. Remember that all this information is at your disposal and much of the data can be downloaded and installed in-house.

Xgrid, a "just do it" grid solution for non IT's

Hamid Hussain-Khan[1] **Olivier Michielin**[2]

1 Grid infrastructure development
University of Lausanne
Switzerland

2 Medical Faculty, University of Lausanne
Swiss Institute of Bioinformatics
Ludwig Institute for Cancer Research
Switzerland

The grid, an old idea becoming reality

Growing interest in grid solutions

Over the last few years, grid computing has aroused growing interest in scientific communities.

Due to the development of accurate modeling methods in a lot of different disciplines, numeric simulation has become a valuable tool to solve all kinds of challenging problems. Beside that, new fast experimental data collection procedures and exponential growth of storage capacity have lead to the accumulation of a gigantic amount of experimental data in a lot of different scientific fields. The generation of numeric models and the analysis of these large experimental data sets require growing amount of CPU power.

In early times large data centers provided scientists with the requested computing power. They had to share their financial resources to benefit from such centralized infrastructure. Then for years, following the Moore's Law, computing power grew exponentially and the price and the size per MFLOPS dropped proportionally. So universities, departments and even single institutes could afford their own IT infrastructure with the same amount of funding. Nowadays most scientists have at least one desktop computer and maybe one or several workstations at their disposal. Despite this virtual access to a large computing power, federating these resources in a useful way has been a cornerstone problem. In recent years, the focus has turned into developing the technology to achieve this goal; instead of sharing a budget to buy large centralized resources, development efforts are made to share CPU power or any other IT resources like storage, databases or any kind of data source over global networks. These networks of distributed and shared IT resources are known as grids. Among the various grid implementations, *data grids* that give access to large amount of distributed data and *computational grids* that harvest CPU powers from large amount of individual computers, are the most frequent. We will focus on computational grids for the rest of this discussion.

Definition and short history of Grid technologies

Although the concept of distributed computing appeared rapidly after the first personal computers, the term Grid was only introduced in 1996 in a proposal to the NSF by a consortium of institutions working on parallel and distributed computing related problems (1). It was formalized in 1998 for the first time by a definition in the book *The Grid: Blueprint for a New Computing Infrastructure* (2):

"A computational grid is a hardware and software infrastructure that provides dependable, consistent, pervasive, and inexpensive access to high-end computational capabilities."

The concept of grid computing is not new. As early as 1969 L. Kleinrock, the inventor of the packet switching technology and one of the fathers of the Internet declared in a 1969 UCLA press release (3):

"As now, computer networks are still in their infancy. But as they grow up and become more sophisticated, we will probably see the spread of computer utilities, which, like present electric and telephone utilities, will service individual homes and offices across the country."

This prediction has gradually been realized. In 1995 one of the first functional grids was publicly demonstrated at an IEEE/ACM computing conference in San Diego. Eleven computers were linked together over a network and ran a simulation of the Chesapeake Bay ecosystem.
Since then interest in grid technologies has always been growing in scientific communities. Over the last few years standards and middleware for global grid have been developed. One of the most widely used is the Globus toolkit. It is developed by the Globus Alliances (7) and is becoming a *de facto* standard.

Difference between massively scalar and parallel resources

Grid computing is generally more suited to loosely coupled or so called *embarrassingly parallel* computing tasks. In that computing model, a large computing task is divided into mutually independent subtasks. Each of these subtasks is distributed for computation through a network to local or distant scalar computing resources. Partial results are back collected and the final result of the initial task is computed. Common tasks like database processing, Monte-Carlo simulations, image processing or a lot of other digital signal processing tasks all fall in this category.
All the following research fields can benefit from massively scalar grid computing approaches and one or more large international grids are being developed to support them:

- Genomic and proteomic analysis (Bioinformatics)
- High-energy physics simulations
- Complex data mining
- Large-scale digital signal processing
- Experimental and symbolic mathematics
- Global climate, environmental or geological modeling
- Large-scale economic modeling

On the contrary, protein folding simulation and molecular nanotechnology modeling are generally not considered as embarrassingly parallel problem, as the data computed by one CPU needs to be available to the others very frequently. They are more suited for massively parallel computing resources. These types of computing resources are generally centralized and require a fast interconnect between CPUs. In such architectures, the price of the interconnect is typically much higher than that of the CPUs.

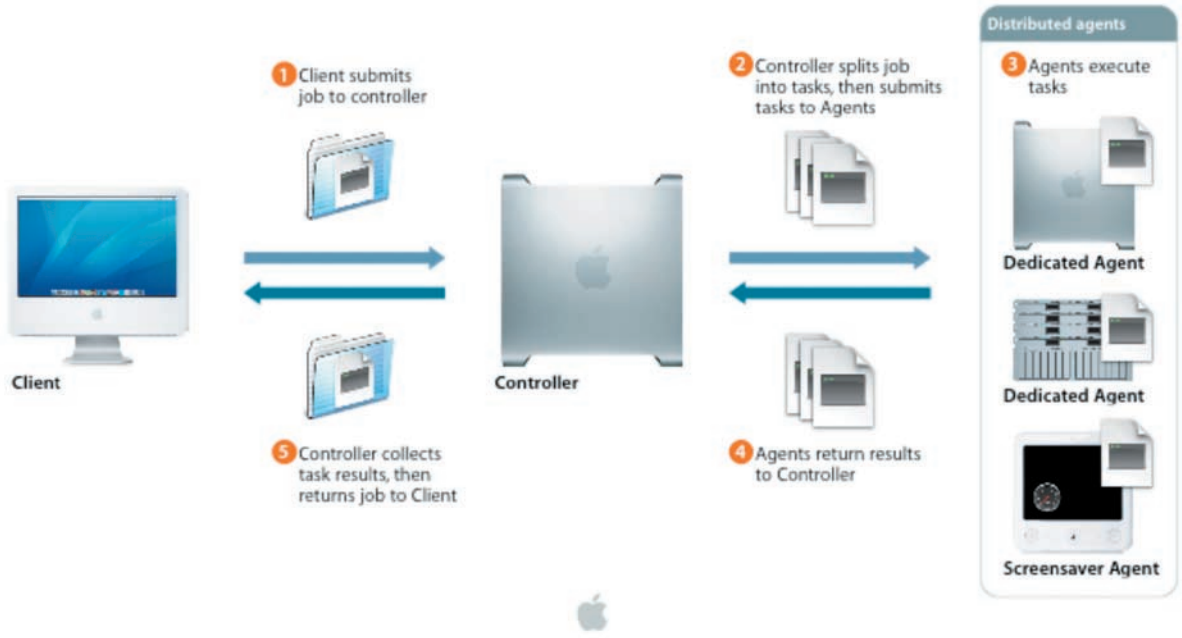


Figure 1. General overview of the Xgrid execution workflow.

Need for local (intradomain) grid solutions

Most global scale grid projects are extremely complex and cannot be realized individually by small organizations. They are relatively expensive and require large teams with a lot of different specialized IT skills. As an example, the actually not yet completed deployment of the LCG (LHC Computing Grid) at the CERN (5) which actually networked 10'000 CPUs all around the world and the development of its application layer totalize 389 FTE-years of human resources over a period of three and a half years (6). It is ultimately designed to scale to 1'000'000 CPUs serving a community of 5'000 scientists working on different aspects of the same challenging high energy physics problem.

Only research groups belonging to large international collaborations can directly benefit from such large infrastructure. They share their resources to solve challenging problems no research group could solve individually.

For smaller research groups, other grid technologies have been developed. Those are distributed computing systems, which harness idle CPU cycles on LANs or WANs and use these for grid computing. Condor (8), Entropia, United Devices and Apples's Xgrid are examples of such intradomain grid technologies. Some of them are commercial products and others are academic open source projects. All are based on the same principles but differ from each other as to the functionalities they offer and their deployment complexity.

The rest of this document will focus on Apple's Xgrid. It is by far the easiest way to start with grid technologies. No particular IT skills are required to buildup a small to medium sized functional grid.

Xgrid – the OS X grid solution

Xgrid concept

Xgrid is a grid technology implemented in Mac OS X server and Mac OS X client which allows the deployment and management of computational grids (9). It helps a network administrator to group computers in grids or computing dedicated clusters and allows clients to submit complex jobs to a group of configured computers.

General architecture

Xgrid is built on a three-tier architecture: clients, controllers and agents (Fig. 1). A *job* in the Xgrid context is a collection of computing tasks that may require data files, executables and parameters.

The Xgrid agent is a system daemon that handles job execution on the behalf of the remote job submitter. By default agents are turned off on OSX 10.4. Once they are turned on, depending on their configuration, they contact a controller and signal that they are available for job execution. Once the controller sends a job they execute it and send back the result to the controller.

The client is a command line tool running within the terminal application. It contacts the controller and is used to describe, submit, monitor and retrieve jobs submitted to the grid.

The Xgrid controller manages the communication between clients and agents. It accepts connections from both entities. None of them can directly connect to each other. It receives job submissions from clients, breaks the jobs into tasks, and, if needed, stores them in a waiting queue and dispatches tasks to available agents. Once agents return results it forwards them back to the clients.

Xgrid – a short "How to start"

Installation

Xgrid is built in every copy of Mac OSX since version 10.4. This means that any new Mac comes with Xgrid preinstalled right out of the box. The client version of OSX contains the Xgrid client and the computing agent whereas the server version of OSX also provides the controller.

In case of OS reinstallation, the requested packages are automatically installed by the default OS installation procedure.

For those running on OSX 10.3, Apple provides on its website an install package containing a computing agent compatible with the controller included in the 10.4 version of the OS.

Configuration

If you are not concerned with strong authentication options present in Xgrid,

configuring a small grid on your local subnet is a straight forward procedure. Thanks to Bonjour, the Apple service detection and zero network configuration technology, Xgrid agents and controllers detect each other automatically and only minimum settings are required.
To configure the Xgrid agent, open the "Sharing" panel located in System Preferences. Then select the Xgrid service and press the configure button. An option panel similar to the one presented in Fig. 2 will appear.

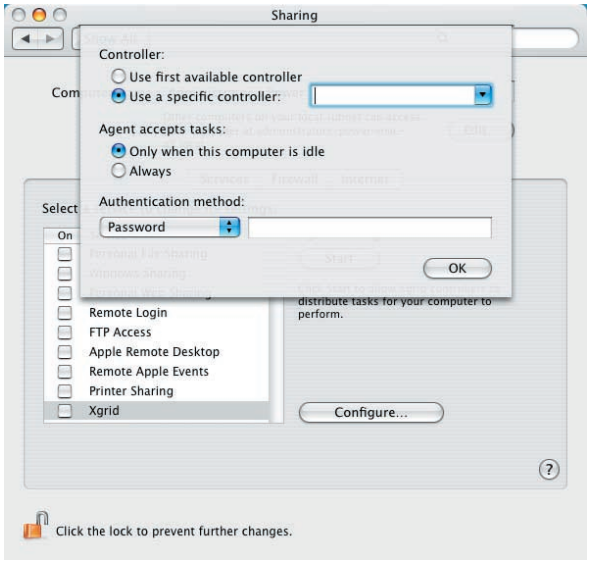


Figure 2. Agent configuration in System Preferences.

Three types of information should be provided:

i) Address or name of the controller serving this agent: if no information is entered, the agent automatically uses the first available controller found on the local subnet using Bonjour. Otherwise a controller can be specified by its IP address, URL or the machine name broadcasted by Bonjour on the local subnet.

ii) Task acceptance conditions: either always accept a computing task and run it in background with low CPU priority or accept a task only when the computer is idle, which means that there is no mouse/keyboard activity for at least 15 minutes.

iii) Authentication method of the controller to the agent. Three options are available. The "no password" option allows any controller to send jobs to the agent without authentication. This option should be used only if you are in a controlled local network environment. The second option requires the controller to authenticate using the password entered in the blank field. The third method is based on Kerberos single sign on authentication procedure (12). This last option is more involved; it requires previous deployment on your network of the necessary infrastructure to run a Kerberos kingdom. Although Apple provides wizards to help setting up Kerberos, it is beyond the scope of this article to detail that procedure. Such a solution allows one to build a completely secured Xgrid solution.

Finally click OK to save the settings and start the Xgrid agent service by pressing the Start button.

Repeat this configuration procedure on each computing node of your grid.

Configuration of the controller is also a fast procedure through a convenient GUI tool. On Mac OS X Server, launch the Server Admin tool. Locate and select the Xgrid service in the left side list. Click on the setting button at the bottom of the right panel. Two buttons appear on the top of the windows (Fig. 3). The first one configures an agent. If you want your server to also provide computing power to your grid, click on it and configure the options. They are identical to those previously presented for the Mac OS X client version of the agent. The second button opens the configuration panel for the controller. Two

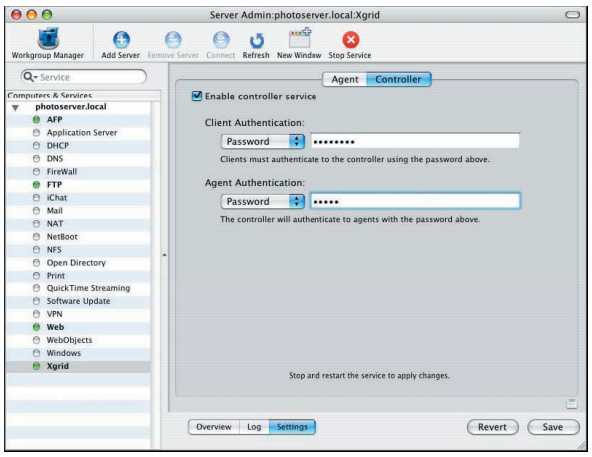


Figure 3. Controller configuration in Server Admin.

pairs of selectors and password text fields are present. The first one sets the password the clients have to provide to submit jobs on your grid through this controller. The second one sets the password the controller uses to authenticate when accessing the computing agents. This password should match the one set during the agent configuration procedure. Again, selectors let you choose authentication through password or single sign on based on Kerberos. Finally fill the check box to enable the Xgrid controller service on your server.

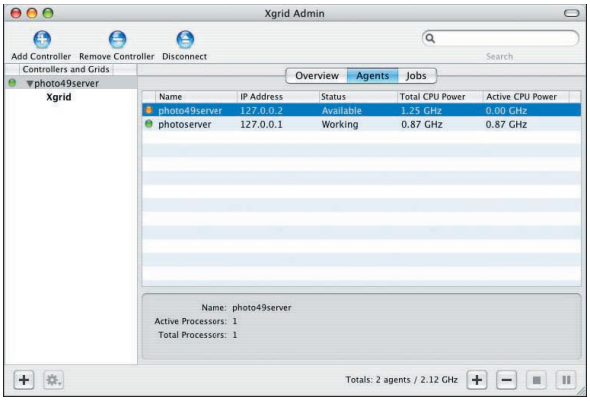


Figure 4. Agents management and monitoring.

Security aspects

By default, Xgrid uses single password authentication between clients and controller and between controller and agents. The process is based on a two-way random mutual authentication protocol including MD5 hashes. During the authentication procedure, no password is passed clear on the network. Once the two parties are authenticated, the rest of the communication and job transmission is done in clear. In the Xgrid context, the controller is the only device listening on the port 4111. This means that the only way to establish a connection for clients or agents is to initiate an outbound connection to the controller on the port 4111. This method facilitates firewall configuration and increase agent side security.

Once an agent accepts a job for execution, it runs it as an unprivileged user similar to the user nobody. In case of mutual authentication through Kerberos, the job runs with the identity of the user who submitted it and keeps all the privilege and authorizations of the job submitter. This means that the submitted jobs can securely use all the user's network reachable resources like a distributed file system or any other resources requiring authentication.

Management aspects

Xgrid Admin tool is a GUI based management utility that can handle multiple Xgrid controllers from the same interface.

Several functions are available in this tool. It can log onto one or several controllers and monitor their activities. Pressing the Overview button displays a summary of the total number of agents connected to the controller, the cumulated CPU power they provide and the total number of jobs they are running.

The Agents button (Fig. 4) displays a detailed list by name and IP addresses of all the agents registered to a controller, their availability status, the power of the CPU they run on and the total CPU power dedicated to the job they are running.

On each controller, the pool of registered agents can be redistributed in logical sub-pools, each with their own dedicated submission queue. These queues are basic FIFO (first in / first out) priority type. Sub-pools can be dynamically created and erased. The only limitation is that no agent can be moved or sub-pool deleted as long as jobs within it are running.

The Jobs button (Fig.5) displays the list of all jobs managed by each controller or sub-pools on a controller. Each job can be individually stopped, restarted or removed. The current status of each job is also displayed with the actual CPU power used, the job progression and the number of sub-tasks belonging to this job.

Jobs submission

Apple offers two solutions to submit jobs to Xgrid: a command line tool and a Cocoa API. The latter is dedicated to developers wanting to implement transparent distributed computing resources in their GUI based application (11).

The otherwise general submission client is the xgrid command line tool. It can be used to

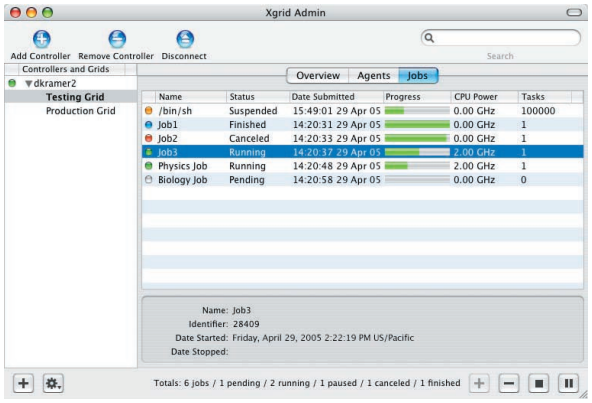


Figure 5. Jobs management and monitoring.

submit, monitor and retrieve submitted jobs. The advantage of the command line tool is its use within Perl or Shell scripts to submit or monitor jobs automatically.

A complete list of options can be found in the xgrid man pages.

The next lines are a submission procedure example issued from the Xgrid man pages

Submit myscript with the files in the input directory. Send email to somebody@apple.com on every job state change. Then retrieve the results and save the stdout and stderr streams in files instead of printing them out to the terminal and save the output files in the specified directory. Finally delete the job:

```
$ xgrid -job submit -in ~/data/working
-email   somebody@apple.com myscript
param1 param2

{ jobIdentifier = 27; }

$ xgrid -job results -id 27 -so job.
out -se job.err -out job-outdir

$ xgrid -job delete -id 27
```

For more complex submission pattern Xgrid supports an XML-based submission description language.

Conclusions

The Xgrid approach presents a series of advantages over other more complex grid technologies: fast and easy grid configuration and deployment, automatic discovery of controllers by agents and clients, strong and secure authentication on both sides when run as a kerberized service, easy command line job submission, availability of a submission API for developers and finally usage of an XML-based open protocol for network communication.

All these features are built in the standard version of Mac OS X 10.4 client and server. This allows a non-IT specialist user to run a small grid in less than a few hours on regular hardware.

The command line tool can easily manage most of the embarrassingly parallel jobs run by research groups involved in different types of projects not requiring thousands or ten thousands CPUs. Even simple execution dependencies of the type job(n+1) dependent on the completion of the job(n) can be handled by Xgrid.

For more complex jobs with multiple execution dependencies or large multi-site projects requiring the collaboration of an important number of users, other grid middleware should be used. Condor or Globus are more suitable for these kinds of applications. Both are now officially supported on the OS X platform.

All in all, Xgrid on the Mac OS X platform is a smart solution for whoever wants to start using grid technologies in his scientific computing project. Depending on the number of CPUs at your disposal, this technology can dramatically improve your data production in a minimum amount of time.

References and links

1) G. von Laszewski "*The Grid-Idea and Its Evolution*"
http://www.mcs.anl.gov/~gregor/papers/vonLaszewski-grid-idea.pdf

2) I. Foster, C. Kesselman "*The Grid: Blueprint for a New Computing Infrastructure*" Morgan Kaufmann Publishers, July 1998.

3) L. Kleinrock "*UCLA to Build the First Station in Nation Wide Computer Network*"
http://www.lk.cs.ucla.edu/LK/Bib/REPORT/press.html

4) I. Foster "*What is the Grid? A Three Point Checklist*"
http://www-fp.mcs.anl.gov/~foster/Articles/WhatIsTheGrid.pdf

5) LCG web site
http://lcg.web.cern.ch/lcg/

6) LHC Computing Grid Project "*Quarterly Status and Progress Report - Second Quarter 2005*"
http://lcg.web.cern.ch/LCG/PEB/Documents/LCG-ProgressReport1-02Q05_02aug05.pdf
7) Globus Aliance web site
http://www.globus.org/
8) Condor web site
http://www.cs.wisc.edu/condor/
9) Xgrid administration manual
http://images.apple.com/server/pdfs/Xgrid_Admin_v10.4.pdf
10) Xgrid agent for Mac OS X 10.3
http://www.apple.com/support/downloads/xgridagentformacosx103.html
11) Xgrid Foundation API
http://developer.apple.com/documentation/Performance/Conceptual/XgridDeveloper/index.html
12) B. Clifford Neuman and Theodore Ts'o. *"Kerberos: An Authentication Service for Computer Networks"*, IEEE Communications, 32(9):33-38. September 1994
http://web.mit.edu/kerberos/www/

Announcements

Several important new software releases appeared recently.

EMBOSS 3.0.0

See changes here:
http://emboss.sourceforge.net/developers/changelog.html

wEMBOSS 1.5

See changes here:
http://www.wemboss.org/wemboss15

Jalview 2.05

See changes here:
http://www.jalview.org/releaseHistory.html

OSIRIX 2.00

See changes here:
http://homepage.mac.com/rossetantoine/osirix/Index2.html

Conferences

2005

Sept. 01 - 02 First Conference on Protein Imaging using Molecular Electron Tomography - Boston, US
Sept. 04 - 06 HUPO Proteomics Standards Initiative - Geneva, Switzerland
Sept. 06 - 10 2nd ESF Functional Genomics Conference - Oslo, Norway
Sept. 25 - 27 Computational Life Science - Konstanz, Germany
Oct. 03 - 06 5th Workshop on Algorithms in Bioinformatics - WABI 2005 - Eivissa, Spain
Oct. 05 - 07 NETTAB 2005 - Workflows management: new abilities for the biological information overflow - Naples, Italy
Oct. 05 - 07 German Conference on Bioinformatics 2005 - Hamburg, Germany
Oct. 05 - 07 Workflows management: new abilities for the biological information overflow - Naples, Italy
Oct. 10 International BCB-Workshop on Machine Learning in Bioinformatics - Berlin, Germany
Oct.28-Nov.01 4th European Conference on Computacional Biology and the 6th Meeting of Spanish Bioinformatics Network - Madrid, Spain
Nov. 14 - 18 European Conference on Complex Systems - Paris, France
Dec. 05 - 07 Algorithms and Computational Methods for Biochemical and Evolutionary Networks (CompBioNets'05) - Lyon, France

2006

Feb. 23 - 24 Annual Meeting of the Swiss Societies for Experimental Biology (USGEB 2006) - Geneva, Switzerland
Jul.30-Aug.04 In-Silico Analysis of Proteins - Celebrating the 20th anniversary of Swiss-Prot - Fortaleza, Brazil
Aug. 06 - 10 Annual International conference on Intelligent Systems for Molecular Biology (ISMB 2006) - Fortaleza, Brazil
Aug.27-Sep.01 17th International Mass Spectrometry Conference, Prague, Czech Republic

No one nose

Vivienne Baillie Gerritsen

Do we, or do we not, have a sixth sense? Yes say most. And it certainly does seem to be the case. Like many animals, we are capable of responding to sensory chemicals of which we are quite unaware – pheromones – and that can modify our behavior. We are, however, in the process of losing – though not all agree – the organ which may well have been used by our ancestors to perceive such an obscure sense: the vomeronasal organ which can be observed just in the inside of our nostrils. The intriguing part is that a subfamily of protein receptors, which suspiciously resemble known mammalian pheromone receptors, has been discovered in humans: the type 1 vomeronasal receptors. Could it be then that not only do we have a sixth sense but we also have an organ dedicated to it? Just like in the good old days?

Most living creatures depend upon a sense which we – for the most part – have lost: a sense that we can neither hear, see, taste, smell or feel. Such a sense is conveyed by molecules which were termed pheromones in the 1950s. Pheromones are chemical molecules of diverse and varied structure which are used in the animal world between a same species, to settle love affairs for the most part. In many of our mammalian counterparts, they are detected by a small organ – the vomeronasal organ (VNO) which is distinct from the main olfactory system but, like it, lines the nasal cavities. Though the way messages are conveyed from the outside world to the inside one and ultimately influence an individual's behavior is complex and demands a greater understanding, a general outline of the process is known. Neurons bathe within the VNO presenting specific pheromone receptors on their surface. A pheromone binds to its receptor and a signal is transmitted down the length of the neuron and ends up in the olfactory bulb which, in turn, will transmit its dispatch to the brain where some sense will be made out of the initial signal.

The existence of a VNO in humans has met with much controversial. It was first mentioned about 300 years ago but was only given full attention in 1877 by a German professor Rudolf Albert von Kölliker (1817-1905). It seems that though the organ is clearly present in the human fetus, not all adult humans have it, and when they do, it really is quite vestigial. Despite this, claims that pheromones can act on human VNOs have been made. Androstadienone is an androstene found under a man's arm, on the skin and the hair. According to some, if picogram quantities (quantities which could not stimulate the olfactory system) of androstadienone are presented to a woman's VNO – or where it is expected to be – she will experience a change of mood, i.e. a sense of well-being. As a result, it was not long before 'pheromone' perfumes boasting positive influences on those who wore them were put on the market…

Fig. 1 Professor Rudolf Albert von Kölliker (1817-1905). The man who had a nose.

Today, there is little doubt that human pheromones exist. Besides androstadienone, the most popular example of their existence is that of the synchronization of a woman's menstrual cycle and the regulation of her ovulation with fellow female colleagues due to molecules found under their armpits. What no one agrees upon is how these pheromones act upon us. Are they simply 'smelt' by the olfactory system and follow the classical transmission of a smell? Pheromone sensing does occur in this fashion in pigs and rabbits for instance. Or do we really have a VNO in which are lodged specific pheromone receptors as in many reptiles and other mammals?

Do humans sport pheromone receptors? Could be. They are few and far between though and no one knows whether they are functional either. However, they certainly are very similar in sequence to pheromone vomeronasal receptors found in other animals, of which there are two subfamilies in rodents; one of them, V1R, is found in human olfactory mucosa. Proteins of the V1R type are integral membrane proteins and belong to the very large G-protein coupled receptor family. Despite their hypothetical existence though, no one knows yet whether V1Rs are actually expressed in human VNO.

So, as far as human V1R goes, there seems to be very little certainty on anything at all really. What V1R has offered biology so far though is a window onto the sexual behavior of our ancestors and its evolution. And it is rather interesting. Scientists assumed that our higher primate ancestor – which is believed to have existed 23 million years ago – probably had as many functional pheromone receptors as the mouse does today. That is to say about 140. If reproduction based on pheromones existed in that ancestor and we lost that capacity over the 23 million years which separate us from it, statistics inform us that we should only have about 5 intact pheromone sequences today due to 'functional relaxation'. And such is the case… So the fact that adult VNO is vestigial is hardly surprising. More amazing yet is that our VNOs are a live – so to speak – incarnation of a behavior we had and which we are in the process of losing.

Why is it we discarded pheromones in the first place anyway? It is thought that primate vision may have become more and more acute so as to be able to distinguish the colors of fruit for feeding. As a result and with time, male primates may have been able to simply see when their female counterparts were ovulating because of changes in color of their genitalia. Consequently, reproductive behavior based on pheromones would have become less and less of an asset as primates counted more on vision to choose a mate. And slowly but surely, pheromone receptors such as V1Rs would have started to 'relax' since they were under less of a functional constraint. Such a theory gains strength when one is in the knowing that bird reproductive behavior is based solely on body color and that they do not have vomeronasal pheromone perception.

Besides not knowing what to think of what is left of the human VNO and its receptors, the fact that pheromones such as androstadienone can actually modify a human's behavior via the existing VNO has tickled scientists' fancies. Synthetic pheromones could have a therapeutic interest. Sprays have already been thought up which could free women from premenstrual mood shifts. The fight against prostrate cancer could perhaps be booted via a pheromone which could check testosterone production. And how about smearing gender-specific magazines with pheromones to lure men or women into buying them? Trials have been carried out already… Despite the obvious ethical issue, lab tests turned out to be quite conclusive but in a newsagent's, a potential buyer is submerged by so many cues that the emotional smear of a product would probably have no chance whatsoever. Pheromones certainly are mysterious molecules for the rational human and make us wonder yet again whether we really have been granted the power of free will or not (Protein Spotlight issue 52).

Cross-references to Swiss-Prot

Type 1 vomeronasal receptors 1-5, *Homo sapiens* (human) : Q9GZP7, Q8NFZ6, Q9BXE9, Q7Z5H5, Q7Z5H4

References

1. Rodriguez I., Mombaerts P.
Novel human vomeronasal receptor-like genes reveal species-specific families
Curr. Biol. 12:R409-R411(2002)
PMID: 12123587

2. Zhang J., Webb D.M.
Evolutionary deterioration of the vomeronasal pheromone transduction pathway in catarrhine primates
PNAS 100:8337-8341(2003)
PMID: 12826614

3. Taylor R.
The sixth sense
The New Scientist magazine, January 25th 1997, Issue 2066

National Nodes

Argentina
Oscar Grau
IBBM, Facultad de Cs. Exactas, Universidad Nacional de La Plata
Email: grau@biol.unlp.edu.ar
Tel: +54-221-4259223 Fax: +54-221-4259223
http://www.ar.embnet.org

Australia
Sonia Cattley
RMC Gunn Building B19, University of Sydney,NSW, 2006
Email: scattley@angis.org.au
Tel: +61-2-9531 2948
http://www.au.embnet.org

Austria
Martin Grabner
Vienna Bio Center, University of Vienna
Email: martin.grabner@univie.ac.at
Tel: +43-1-4277/14141
http://www.at.embnet.org

Belgium
Robert Herzog, Marc Colet
BEN ULB Campus Plaine CP 257
Email: rherzog@ulb.ac.be mcolet@ulb.ac.be
Tel: +32 2 6505146 Fax: +32 2 6505124
http://www.be.embnet.org

Brazil
Gonçalo Guimaraes Pereira
Laboratório de Genômica e Expressão - IB
UNICAMP-CP 6109
13083-970 Campinas-SP, BRASIL
Tel: 0055-19-37886237/6238
Fax: 0055-19-37886235
Email: goncalo@unicamp.br
http://www.br.embnet.org

Canada
Canadian Bioinformatics Resource, National Research Council Canada, Institute for Marine Biosciences,
Email: manager@cbr.nrc.ca
Tel: +1-902-426 7310 Fax: +1-902-426 9413
http://www.ca.embnet.org

Chile
Ricardo Baeza-Yates
Dept. of Computer Science, Santiago,
Email: rbaeza@dcc.uchile.cl
Tel: N/A
http://www.embnet.cl

China
Jingchu Luo
Centre of Bioinformatics
Peking University
Beijing 100871, China
Tel: 86-10-6275-7281
Fax: 86-10-6275-9001
Email: luojc@pku.edu.cn
http://www.cn.embnet.org

Colombia
Emiliano Barreto Hernández
Instituto de Biotecnología
Universidad Nacional de Colombia
Edificio Manuel Ancizar
Bogota - Colombia
Tel: +571 3165027 Fax: +571 3165415
Email : ebarreto@ibun.unal.edu.co
http://www.co.embnet.org

Cuba
Ricardo Bringas
Centro de Ingeniería Genética y Biotecnolgía,
La Habana, Cuba
Email: bringas@cigb.edu.cu
Tel: +53 7 218200
http://www.cu.embnet.org

Finland
Eija Korpelainen
CSC, Espoo
Email: eija.korpelainen@csc.fi
Tel: +358 9 457 2030
http://www.fi.embnet.org

France
Jean-Marc Plaza
INFOBIOGEN, Evry
Email: plaza@infobiogen.fr
Tel: +33 1 60 87 37 11 Fax: +33 1 60 87 37 96
http://www.fr.embnet.org

Germany
Sandor Suhai
EMBnet node at the German Cancer Research Center
Department of Molecular Biophysics (H0200)
Email: genome@dkfz.de
Tel: +49-6221-422 342 Fax: +49-6221-422 333
http://www.de.embnet.org

Hungary
Endre Barta
Agricultural Biotechnology Center
Szent-Gyorgyi A. ut 4. Godollo,
Email: barta@abc.hu
Tel: +36 30-2101795
http://www.hu.embnet.org

India
Akash Ranjan
Laboratory of Computational Biology & Bioinformatics facility, Centre for DNA Fingerprinting and Diagnostics (CDFD), Hyderabad
Email: akash@cdfd.org.in
Tel: +91 40 7155607 / 7151344 ext:1206
Fax : +9140 7155479
http://www.in.embnet.org

Israel
Leon Esterman
INN (Israeli National Node) Weizmann Institute of Science
Department of Biological Services, Biological Computing Unit, Rehovot
Email: Leon.Esterman@weizmann.ac.il
Tel: +972- 8-934 3456
http://www.il.embnet.org

Italy
Cecilia Saccone
CNR - Institute of Biomedical Technologies
Bioinformatics and Genomic Group
Via Amendola 168/5 - 70126 Bari (Italy)
Email: saccone@area.ba.cnr.it
Tel. +39-80-5482100 - Fax. +39-80-5482607
http://www.it.embnet.org

Mexico
Cesar Bonavides
Nodo Nacional EMBnet, Centro de Investigación sobre Fijación de Nitrógeno, Cuernavaca, Morelos
Email: embnetmx@cifn.unam.mx
Tel: +52 (7) 3 132063
http://embnet.cifn.unam.mx

The Netherlands
Jack A.M. Leunissen
Dept. of Genome Informatics
Wageningen UR, Dreijenlaan 3
6703 HA Wageningen, NL
Email: Jack.Leunissen@wur.nl
Tel: +31 317 484074
http://www.nl.embnet.org

Norway
George Magklaras
The Norwegian EMBnet Node
The Biotechnology Centre of Oslo
Email: admin@embnet.uio.no
Tel: +47 22 84 0535
http://www.no.embnet.org

Poland
Piotr Zielenkiwicz
Institute of Biochemistry and Biophysics
Polish Academy of Sciences Warszawa
Email: piotr@pl.embnet.org
Tel: +48-22 86584703
http://www.pl.embnet.org

Portugal
Pedro Fernandes
Instituto Gulbenkian de Ciencia
Unidade de Bioinformatica
2781-901 OEIRAS
Email: pfern@igc.gulbenkian.pt
Tel: +351 214407912 Fax: +351 2144079070
http://www.pt.embnet.org

Russia
Sergei Spirin
Biocomputing Group, Belozersky Institute Moscow
Email: sas@belozersky.msu.ru
Tel: +7-095-9395414
http://www.genebee.msu.ru

Slovakia
Lubos Klucar
Institute of Molecular Biology SAS Bratislava
Email: klucar@embnet.sk
Tel: +421 7 5941 2284
http://www.sk.embnet.org

South Africa
Ruediger Braeuning
SANBI, University of the Western Cape, Bellville
Email: ruediger@sanbi.ac.za
Tel: +27 (0)21 9593645
http://www.za.embnet.org

Spain
José M. Carazo, José R. Valverde
EMBnet/CNB, Centro Nacional de Biotecnología, Madrid
Email: carazo@es.embnet.org, jrvalverde@es.embnet.org
Tel: +34 915 854 505 Fax: +34 915 854 506
http://www.es.embnet.org

Sweden
Nils-Einar Eriksson, Erik Bongcam-Rudloff
Uppsala Biomedical Centre, Computing Department, Uppsala, Sweden
Email: nils-einar.eriksson@bmc.uu.se
erik.bongcam@bmc.uu.se
Tel: +46-(0)18-4714017, +46-(0)18-4714525
http://www.embnet.se

Switzerland
Laurent Falquet
Swiss Institute of Bioinformatics, CH-1066 Epalinges
Email: Laurent.Falquet@isb-sib.ch
Tel: +41 (21) 692 5954 Fax: +41 (21) 692 5945
http://www.ch.embnet.org

United Kingdom
Alan Bleasby
UK MRC HGMP Resource Centre, Hinxton, Cambridge
Email: ableasby@embnet.org
Tel: +44 (0) 1223 494535
http://www.uk.embnet.org

Specialist Nodes

EBI
Rodrigo López
EBI Embl Outstation, Wellcome trust Genome Campus, Hinxton Hall, Hinxton, Cambridge, United Kingdom
Email: rls@ebi.ac.uk
Phone: +44 (0)1223 494423
http://www.ebi.ac.uk

ETI
P.O. Box 94766
NL-1090 GT Amsterdam, The Netherlands
Email: wouter@eti.uva.nl
Phone: +31-20-5257239
Fax: +31-20-5257238
http://www.eti.uva.nl

ICGEB
Sándor Pongor
International Centre for Genetic Engineering and Biotechnology
AREA Science Park, Trieste, ITALY
Email: pongor@icgeb.trieste.it
Phone: +39 040 3757300
http://www.icgeb.trieste.it

LION Bioscience
Thure Etzold
LION Bioscience AG, Heidelberg, Germany
Email: Thure.Etzold@uk.lionbioscience.com
Phone: +44 1223 224700
http://www.lionbioscience.com

MIPS
H. Werner Mewes
Email: mewes@mips.embnet.org
Phone: +49-89-8578 2656
Fax: +49-89-8578 2655
http://www.mips.biochem.mpg.de

UMBER
Terri Attwood
School of Biological Sciences, The University of Manchester, Oxford Road, Manchester M13 9PT, UK
Email: attwood@bioinf.man.ac.uk
Phone: +44 (0)61 275 5766
Fax: +44 (0) 61 275 5082
http://www.bioinf.man.ac.uk/dbbrowser

TECH-MGR
Email: tech-mgr@embnet.org
The team gives support to EMBnet nodes and helps them with maintenance and troubleshooting.
The team consists of experienced system administrators and programmers who ensure the availability of local services for all EMBnet users.

EMBnet.news

ISSN 1023-4144

Dear reader,

If you have any comments or suggestions regarding this newsletter we would be very glad to hear from you. If you have a tip you feel we can print then please let us know. Please send your contributions to one of the editors. You may also submit material by e-mail.

Past issues of embnet.news are available as PostScript or PDF files (ISSN 1023-4144). You can get them by anonymous ftp from:
the EMBnet organisation Web site
`http://www.embnet.org/download/embnetnews`
the Belgian EMBnet node
`ftp://ftp.be.embnet.org/pub/embnet.news`
the UK EMBnet node
`ftp://ftp.uk.embnet.org/pub/embnet.news`
the EBI EMBnet node
`ftp://ftp.ebi.ac.uk/pub/embnet.news`

Submission deadline for the next issue:
October 31, 2005