

グリッドシンポジウム in 関西 2003

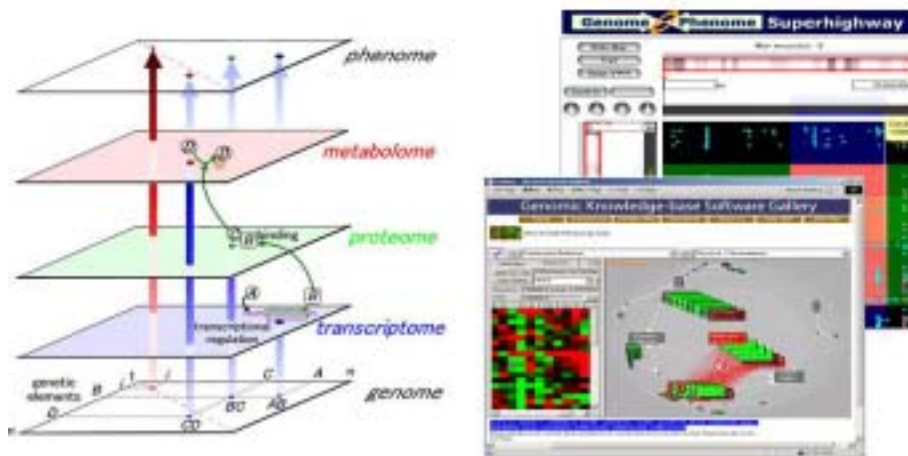
グリッドとライフサイエンス、 世界の状況

小長谷 明彦
理研GSCゲノム情報科学グループ
プロジェクトディレクター
東京工業大学
計算工学専攻客員教授

目次

- 自己紹介
- ポストゲノム時代
- 世界の生命グリッド研究動向
- Open Bioinformatics Grid (OBIGrid)
- 今後の展望

理研GSC



OMIC SPACE (Wada, 2003)

研究戦略

ゲノム⇔フェノーム
情報統合

モデル&シミュレーション

Grid

高性能計算技術

ポストゲノム時代

Bionetworks and Phenomics



RIKEN GSC シンポジウム

2003年6月20日(金)

10:00 - 17:30

交流棟ホール、横浜研究所

主催
理研GSCゲノム情報科学グループ
人工知能学会SIMBI研究会

ゲノムとフェノームを結ぶ バイオインフォマティクス技術

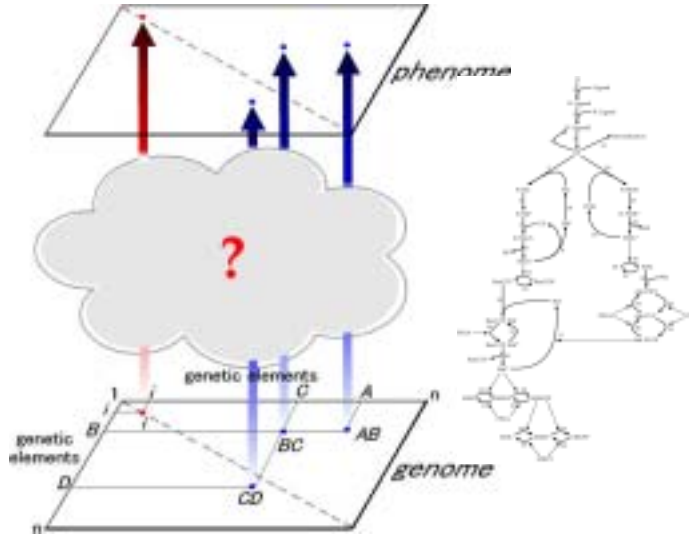
Phenome

Metabolome

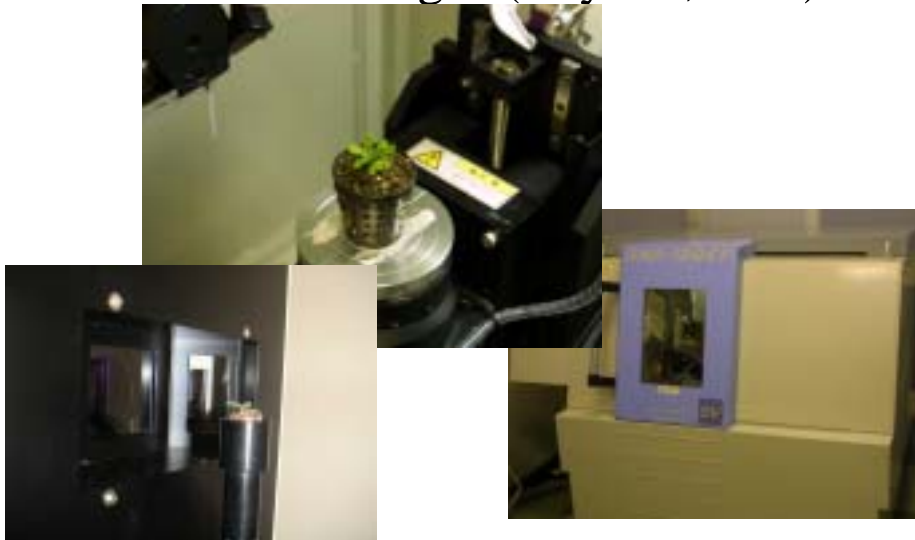
Proteome

Transcriptome

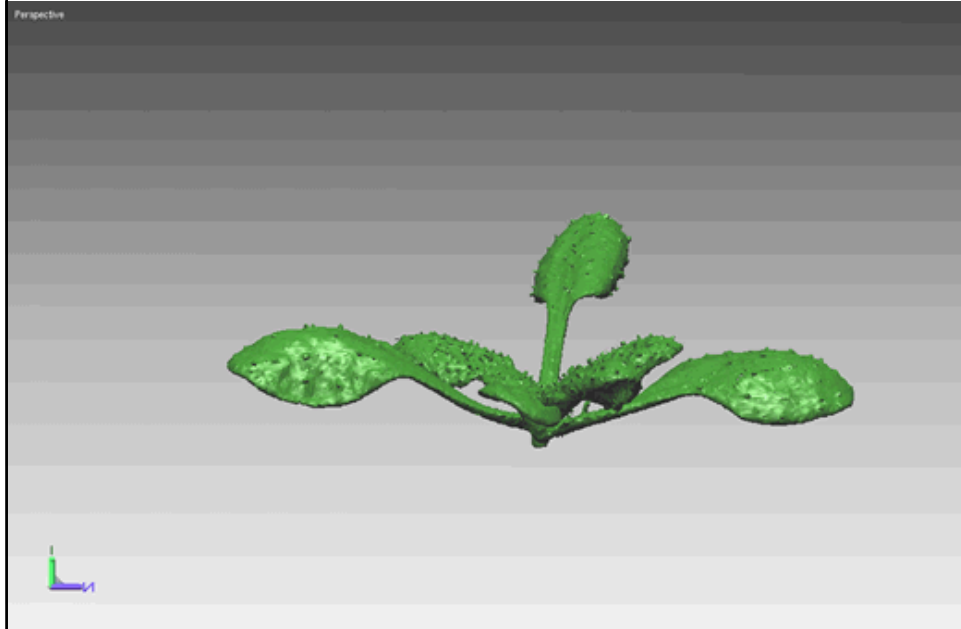
Genome



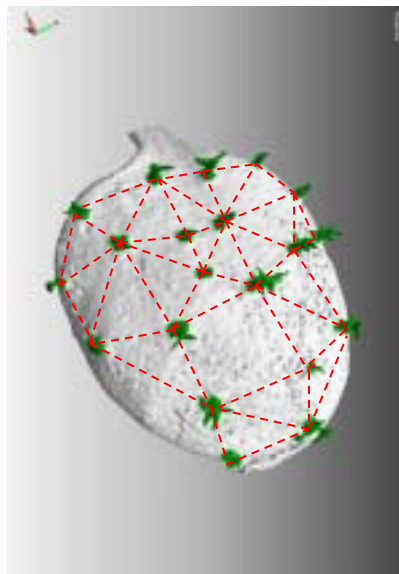
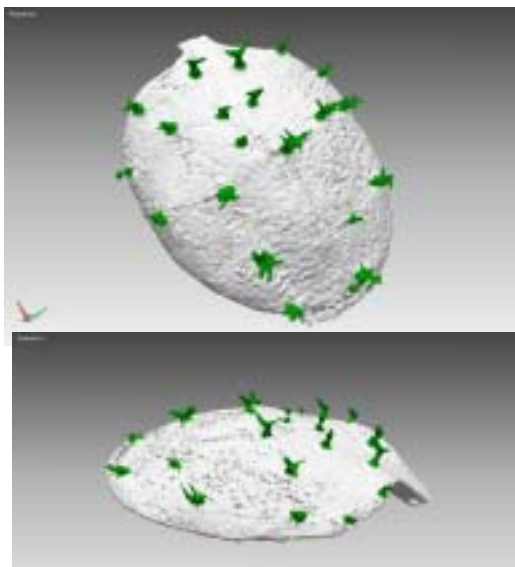
Precise 3D measurement with X-ray, Laser, and Color Images (Toyoda,2003)



Example : Morphological data of *A.thaliana*(JA17:Bla-14)

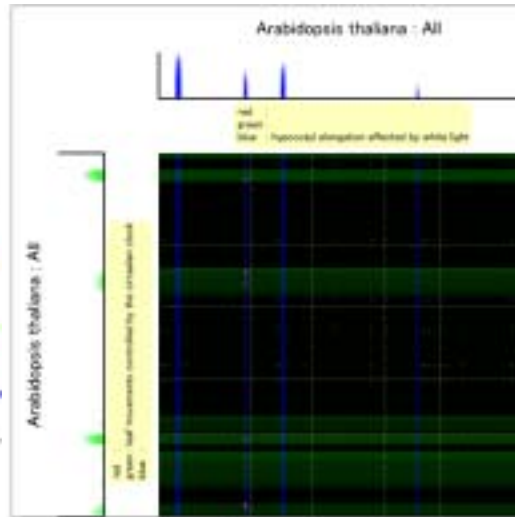
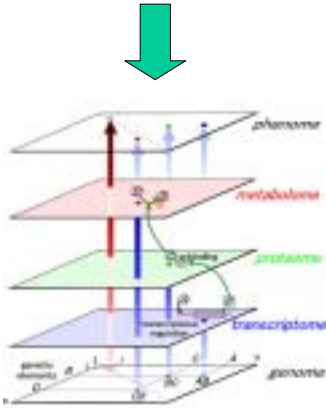


Example: 3D distribution of trichomes(Col-0)



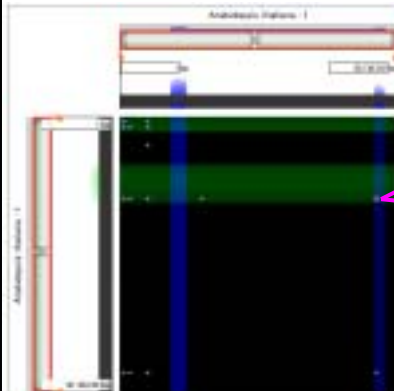
Omic space analysis

Search candidate pathways from QTL maps



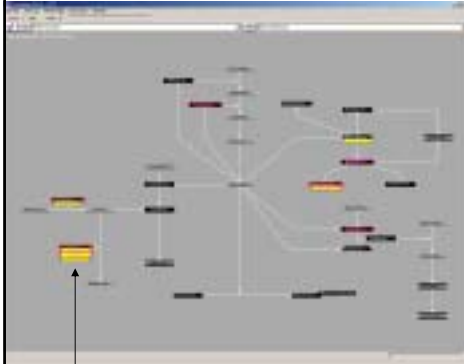
Candidate pathway compared with QTL results

QTLs shown in
Omic space



Brassinosteroid-related pathway

Phenome Metabolome Transcriptome inter-omic analysis



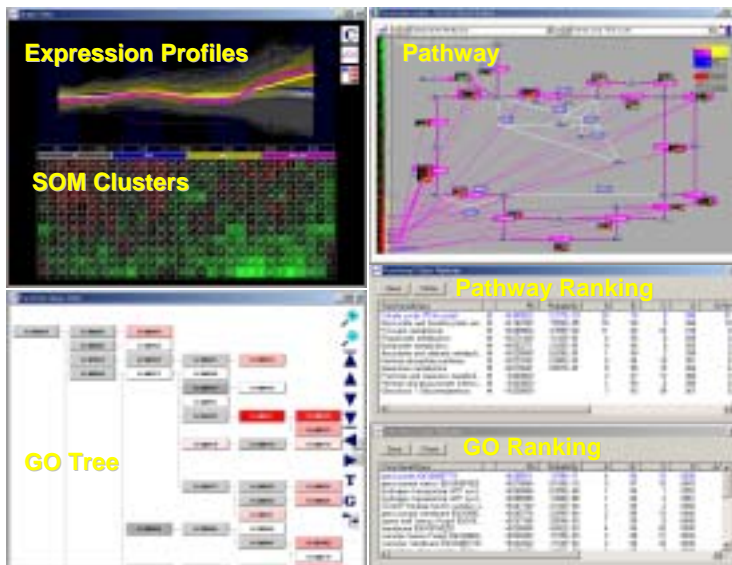
Existence of mutants is indicated by yellow rectangles



Time-course profiles of Gene expression induced by cold stress

Tools are available at <http://gscope.gsc.riken.go.jp>

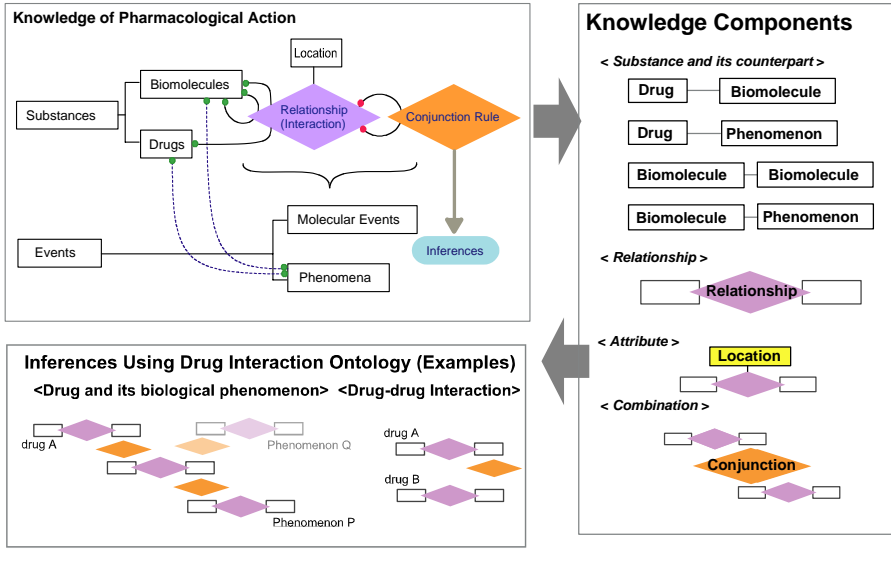
Pathway Ranking by GSCope2



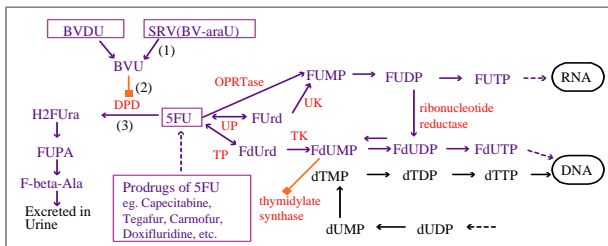
Academic Free

<http://gscope.gsc.riken.go.jp>

Drug Interaction Ontology (Yoshikawa, 2003)



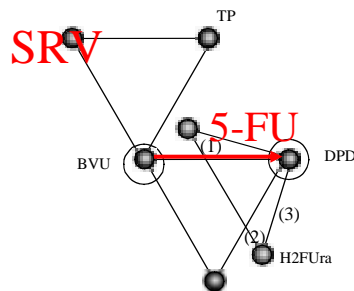
副作用の解析例 (ex. sorivudine & 5FU)



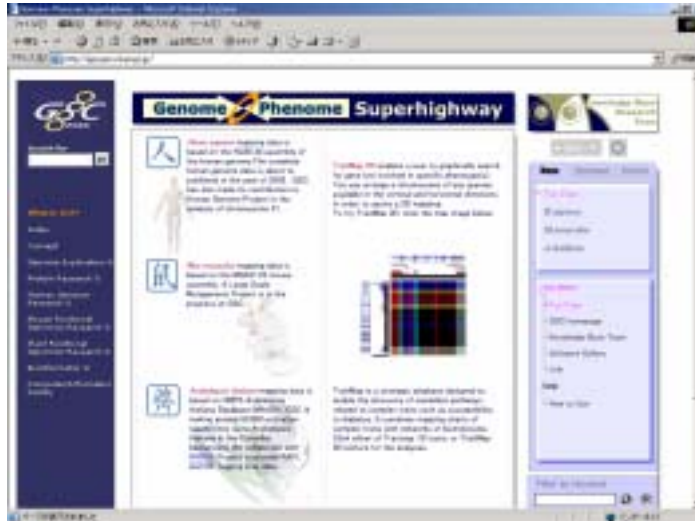
SRV (es) TP, BVU 酵素反応
 BVU (ei) DPD 酵素抑制
 5FU (es) DPD, H₂FUra 酵素反応

上記の相互作用オントロジーから
 SRV > 5FU

すなわち、SRV存在下では5FU(毒性)の代謝が抑制されることが推論可能



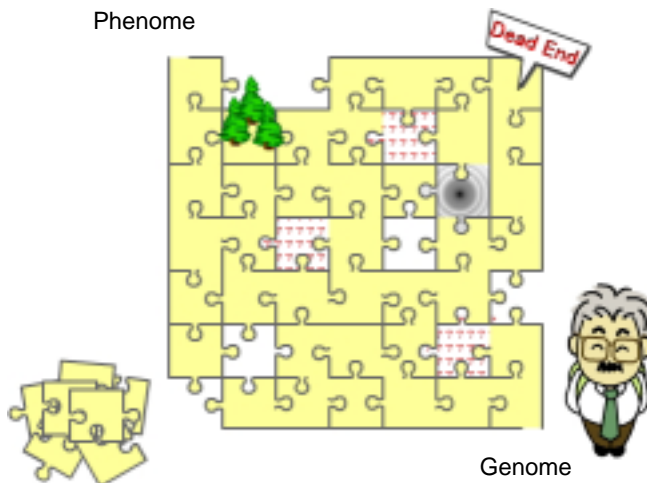
Genome Phenome Superhighway



Test site => <http://gps.gsc.riken.go.jp>

バイオネットワーク研究

Phenome



バイオネットワーク研究に必要な装備



生化学データ・ツール群



高性能計算機

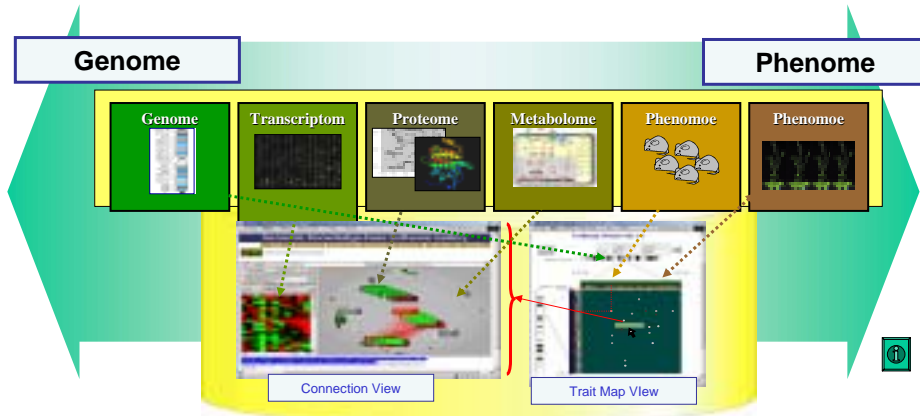


専門家の共同作業

Konagaya Akihiko, Bioinformatics Group, RIKEN GSC June 2003

生化学データ・ツール群

- 公共データベース (Unigene, TrEmbl,...)
- 実験データ (配列、遺伝子発現、質量分析、表現型)
- ホモロジー解析、アレイ解析、立体構造解析



Bio database mirror service

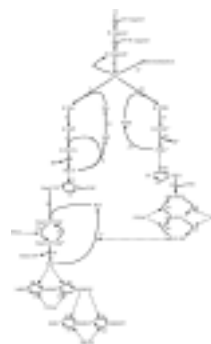
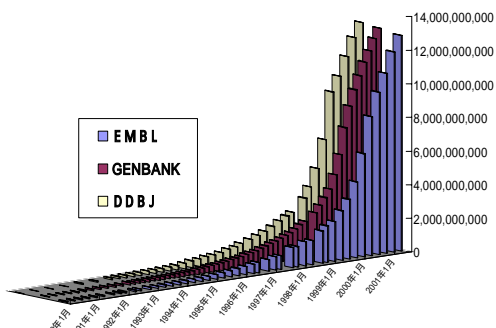
Local mirror	Description	Home site
Blast DB	Biosequence databases for BLAST searches	NCBI
Blocks	Highly conserved regions of proteins	NCBI
DDBJ	DNA Data Bank of Japan	NIG
EMBL	The EMBL Nucleotide Sequence Database	EBI
Ensembl	Automatic annotation on eukaryotic genomes	Ensembl
Enzyme	Enzyme nomenclature database	ExpASY
Genbank Genomes	Whole genome sequence section of GenBank	NCBI
Genbank	GenBank Sequence Database	NCBI
GeneOntology	Vocabularies of gene functions and roles	GeneOntology
InterPro	InterPro Protein databank	EBI
PDB	Protein Data Bank of 3-D macromolecular structures	RCSB
PIR	Protein Information Resource	NBRF
PIRNEW	PIR updates from NBRF, Georgetown	NBRF
Pfam	The Pfam database of protein domains and HMMs	WUSTL
Prosite	Database of protein families and domains	ExpASY
Rebase	The Restriction Enzyme Database	NEB
RefSeq	NCBI Reference Sequences	NCBI
SRS Databanks	List of active SRS databases around world	EBI
SWISS-PROT	Annotated protein sequence database	ExpASY
Taxonomy	Species names	NCBI, EBI
TreEMBL	A supplement to SWISS-PROT	EBI
Unigene	Unique Gene Sequence Collection for Human, Mouse, Rat, and Zebrafish	NCBI
euGenes	Eukaryote Genes Summary Databank	IUBio

Bio application service

Category	Program
Homology Search	fasta
	hmmcr
	ncbi-tools
	wise2
	wu-blast2
Repetitive Sequence Analysis	MaskerAid
	RepeatMasker
	phrap
Multiple Alignment	clstalw
	sam
Exon Finding	fgenes, fgenes+, fgenes-2, fgenes-c
	hmmgene
	genscan
Promoter Finding	tssg
	tssw
Splice Site Prediction	netgene2
Translation Initiation Site Prediction	netstat
Protein Localization Prediction	ChloroP

高性能計算機・ツール群

- 増えつづけるゲノム配列情報
- 探索空間の組み合わせ的増大
Genome * Transcriptome * Proteome * ... * Phenome
- 細胞シミュレーションにおけるパラメタ最適化

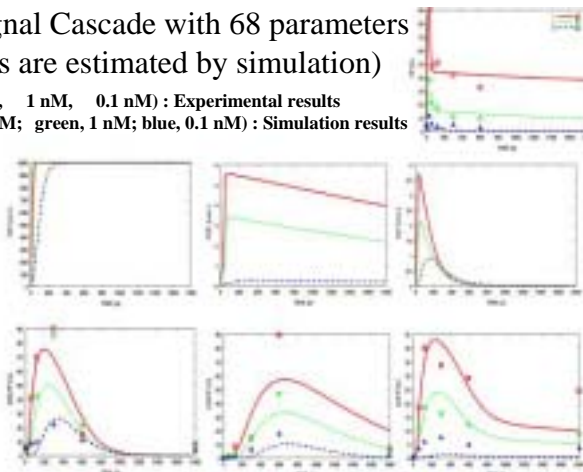
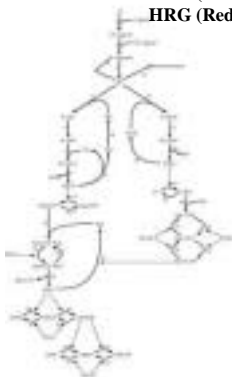


EGF Signal Transduction Pathway Simulation

Available at: <https://access.obigrid.org/yagns/>

Finding ErbB4 New Signal Cascade with 68 parameters
(43 unknown parameters are estimated by simulation)

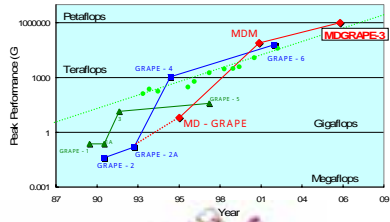
HRG (10 nM, 1 nM, 0.1 nM) : Experimental results
HRG (Red, 10 nM; green, 1 nM; blue, 0.1 nM) : Simulation results



Hatakeyama, M., Kimura, S. et al: A computational model on the modulation of MAPK and Akt pathways in heregulin induced ErbB signaling. **Biochem J.**, 373, 451-463, 2003. .

Petaflops Molecular Dynamics Machine

MDGRAPE3 (Will be the Fastest Computer for MD in 2005)



MDM-1a:
8 Tflops
(2003, GSC)



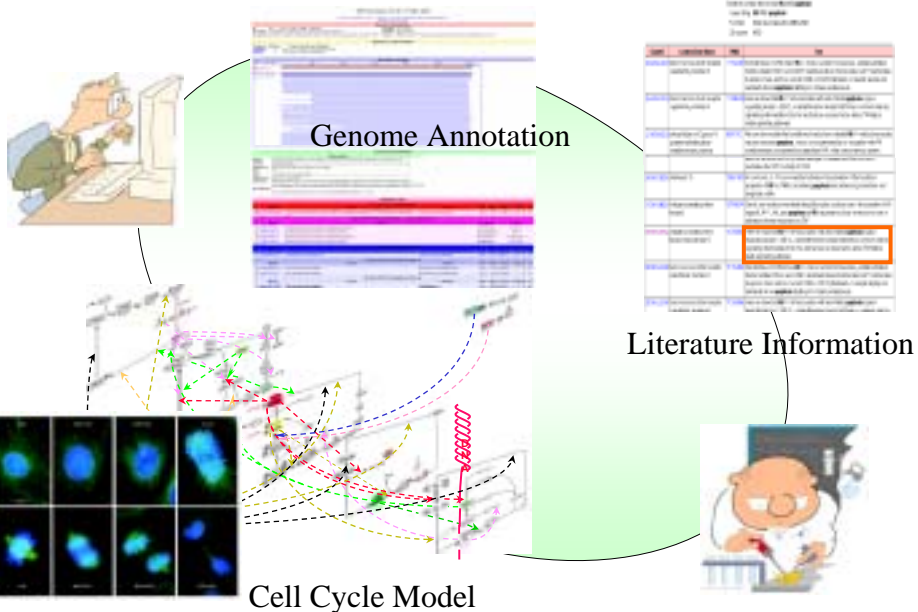
RNA Polymerase II
387,446 atoms



MDGRAPE-2s : 64 Gflops (2002)

Taiji, M., Narumi, T., Ohno, Y., Futatsugi, N., Suenaga, A., Takada, N., Konagaya, A. Protein Explorer: A Petaflops Special-Purpose Computer System for Molecular Dynamics Simulations. Proceedings of **Supercomputing 2003**, IEEE Computer Society, 2003.

専門家の共同作業



何故Gridなのか?

- **“単純並列計算”に有効:**

- ホモロジー検索, 遺伝子アノテーション,
細胞シミュレーションにおける未知パラメタ探索
etc

- **組織間における“分散資源共有”を実現:**

- 計算資源, 二次記憶,
公的データベース, 生物実験データ,
アノテーションツール, シミュレーションツール,
etc

- **知識共有、知識創出のための“場”の実現:**

- 実験系と計算機系の協調
有識者グループ間での知識マネージメント

世界の生命グリッド研究動向

ApGrid	EOL	GBIF
PRAGMA	MyGRID	NVO
European Data Grid	BioGrid	OBI Grid
ESNW	BIRN	NASA IPG
EUROGRID	HealthGrid	TeraGrid
Bio-GRID	SARSGrid	APAN
NBCR	GRAB	GAMESS
NC BioGRID	Biodiversity	
		他多数

Life Science Grid Working Group

<https://forge.gridforum.org/projects/lsg-rg/>

年に3回、Global Grid Forum (GGF) で会合

Co-chairs: Dave Angulo (DePaul Univ.)
Abbas Farazdel (IBM)

主な活動

- World Wide LSG Survey (Piotr Bala, N. Copernicus Univ.)
- Open Life Science Grid Architecture (Rick Stevens, ANL)
- LSG Workflow (Carole Goble, U. of Manchester
and Virinder Batra, IBM)

主なイベント

- LSG Minisymposium (March, 2003, Tokyo)
- LSG Miniworkshop (Dec, 2003, Chicago)
- LSG Special Issue (Feb, 2004)
(Journal of New Generation Computing, vol. 22, no.2,
edited by Konagaya, A. etal.)

生命グリッドプロジェクトの動向 (Arzberger,P.他, NGC 2004)

多国間プロジェクト

PRAGMA, APGRID, European Data Grid,
REALISTE, EUROGRID, GRIP

地域グリッドプロジェクト

NBCR, North Carolina BioGRID, Tera Grid,
EOL, MyGRID, **BioGrid**, **OBIGrid**

特定応用向けプロジェクト

BIRN, HealthGrid, SARSGrid,
GRAB, Biodiversity World, GBIF

動向

- 国際グリッド活動の活発化
- 地域グリッドの増加
- 応用志向グリッドプロジェクトの台頭

PRAGMA

<http://www.pragma-grid.net>

PRAGMA has been founded as an open organization in which Pacific Rim institutions will collaborate more formally to develop grid-enabled applications and will deploy the needed infrastructure throughout the **Pacific Region** to allow **data, computing, and other resource sharing**. Based on current collaborations, PRAGMA will enhance these collaborations and connections among individual investigators by promoting visiting scholars' and engineers' programs, building new collaborations, formalizing resource-sharing agreements, and continuing trans-Pacific network deployment. PRAGMA provides an opportunity for member institutions to work together to address applications and infrastructure research of common interest. This website is a unique collaboration among webmasters from four different countries, to include **Japan, Korea, Singapore, and the U.S.**

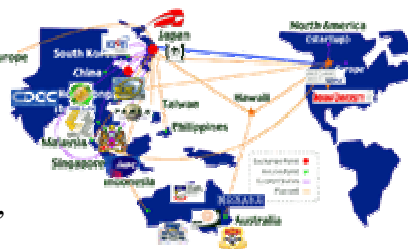
ApGrid

ApGrid is a partnership for Grid computing in the Asia Pacific region. ApGrid focuses on

<http://www.apgrid.org>

- (1) **sharing resources**
- (2) developing Grid technologies
- (3) helping the use of our technologies in **create new applications**
- (4) building on each other work, etc.,

and ApGrid is not restricted to just a few developed countries, neither to a specific network nor its related group of researchers.





<http://www.eurogrid.org>

The objectives of the EUROGRID project are

To establish a European GRID network of leading **High Performance Computing centres from different European countries.**

- To operate and support the EUROGRID software infrastructure. The EUROGRID software will use the existing Internet network and will offer seamless and secure access for the EUROGRID users.
- To develop important GRID software components and to integrate them into EUROGRID (fast file transfer, resource broker, interface for coupled applications and interactive access).
- To demonstrate **distributed simulation codes** from different application areas (Biomolecular simulations, Weather prediction, Coupled CAE simulations, Structural analysis, Real-time data processing).
- To contribute to the international GRID development and to liaise with the leading international GRID projects.
- To productise the EUROGRID software components. After project end the EUROGRID software will be available as supported product

myGrid - directly supporting the e-scientist

<http://www.mygrid.org.uk>

MyGrid aims to design, develop and demonstrate **higher level functionalities over an existing Grid infrastructure** that support scientists in making use of complex distributed resources myGrid is a research project that will extend the Grid framework of distributed computing, producing a **virtual laboratory workbench** that will serve the life sciences community. The integration environment will support patterns of scientific investigation that include:

- 1.accumulating evidence
- 2.assimilating results
- 3.accessing community information sources
- 4.collaborating with disparately located researchers via electronic forums

TeraGrid

<http://www.teragrid.org>

About the TeraGrid

TeraGrid is a multi-year effort to build and deploy the world's largest, fastest, distributed infrastructure for open scientific research. When completed, the TeraGrid will include **20 teraflops of computing power distributed at five sites**, facilities capable of managing and storing nearly **1 petabyte of data**, high-resolution visualization environments, and toolkits for grid computing. These components will be tightly integrated and connected through a network that will operate at **40 gigabits per second** — the fastest research network on the planet.

North Carolina BioGRID

<http://ncbiogrid.org/>

The NC BioGrid project was established in the **Fall of 2001** to research and implement new grid computing technologies that will enable researchers and educators throughout North Carolina to take full advantage of the genomic revolution.

The vision for the NC BioGrid was provided by the **High Performance Computing and Data Storage Focus Group** of the **NC Genomics and Bioinformatics Consortium** (NCGBC). The NCGBC is facilitated through the NC Biotech Center.

MCNC, a not-for-profit R&D company with a long history of collaboration with the North Carolina university community, seeded the NC BioGrid Testbed by providing the servers, software and IT expertise from the NC Supercomputing Center and the network infrastructure through NCREN.

BIRN

<http://www.nbirn.net>

The Biomedical Informatics Research Network (BIRN) is a

National Institutes of Health (NIH) – National Center for Research Resources (NCRR)-

sponsored initiative that fosters large-scale biomedical science collaborations by utilizing emerging **cyberinfrastructure** (high speed networks, distributed high-performance computing and the necessary software and data integration capabilities).

HealthGrid

<http://www.healthgrid.org>

A grid for health is a collaboration of companies and laboratories agreeing to **deploy biomedical services on a grid** made of mutualized storage and computing resources.

The services can be open source or proprietary. Computing and storage are also free or can be charged. The middleware infrastructure is shared by the participating entities.

The health grid works as a backbone where biomedical projects can be deployed and benefit of the services and resources made available on the grid.



SARSGrid

<http://antisars.nchc.gov.tw>

NCHC's SARS Combat Task Force is formed on **May 16th, 2003**. People have been working around the clock to assemble and test a Grid system, consisting systems of **Access Grid, H.323 VTC, medical information management, emergency dispatch and network monitoring**. Two sets of Access Grid and H.323 VTC systems are installed successfully in Sanchung Hospital and Chang Gung Memorial Hospital (CGMH) at Linkou in Taipei by May 20th. The third set is going to be established in Taiwan's Center of Disease Control by May 30 and the fourth in Taipei Municipal Jen-Ai Hospital by June 1; more are planned to be operational in 10 medical centers on the island. This blog will be updated frequently. The task force is formed for SARS Grid and hereby we take the expression "SARS Combat" from Teri Simas, Program Manager of PRAGMA, for the team. For more information please contact Grace Hong: gswhong@nchc.org.tw

GRID応用サーベイ (Arun,K., NGC 2004)

主要応用領域

- Genomics/ Proteomics
- Visualizations/ Simulation/ Imaging
- Database Applications
- Molecular Modeling/ Computational Chemistry

E O L : Encyclopedia of Life

<http://eol.sdsc.edu>

The Encyclopedia of Life (EOL) is a collaborative global project designed to catalog the **complete proteome of every living species** in a flexible reference system. It is an open collaboration led by the San Diego Supercomputer Center, and currently has three major development areas:

- Creating **protein sequence annotations using the integrated genome annotation pipeline (iGAP)**.
- Storage of these annotations in a data warehouse where they are integrated with other data sources
- A toolkit area that presents the data to users in the presence of useful annotation and visualization tools.

Visualization/ Simulation/ Imaging

- Electron Microscope Tomography (Fernandez et al)
- Telescience for Tomography (Ellisman et al)
- Monte Carlo Simulator (MCell)
- MRI Simulation (Benoit et al)
- Medical Image Indexing (Montagnat et al)

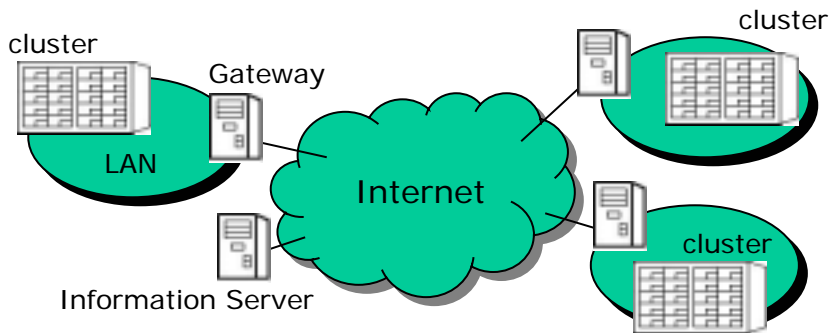
Grid-Oriented Genetic Algorithm Framework for Bioinformatics

Tokushima Univ., Kyushu Univ.

General purpose parallel GA framework

over the Internet scalable more than 100 nodes

- Multiple population, UNDX+MGG, S-system for Genenetwork



Database

- Distributed Medical Data Manager (DM2, Duque etal)
- Heterogeneous Distributed Data Management (SRB)
- Scalable Genome Database for DDBJ XML (OBISgd)
- Heterogeneous Database Federation (BioGrid)

GRAB (GRid And Biodiversity)

<http://www.gridoutreach.org.uk/docs/pilots/grab.htm>

Biodiversity Benefits from Grid Technology

Federations of heterogeneous databases can be exploited through the Grid to solve complex questions about global issues such as biodiversity.”

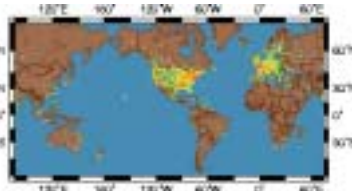
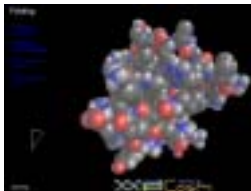


Molecular Modeling

- Folding@Home
- Virtual Lab for Molecular Docking (Buyya et al)
- Molecular Docking (Tantoso et al)
- BioPfuga (BioGrid)
- Evolve/G (Tanimura et al)
- GAMESS

Folding@home Distributed Computing

タンパク質折り畳みをシミュレートする。



UNFOLDING OF THE DNA BINDING DOMAIN OF HIV INTEGRASE

HIV uses proteins to insert its genetic code into our DNA. The DNA binding domain of HIV integrase (below) is the protein which HIV uses to grab onto our DNA such that it can then connect its genetic code into ours.

Number CPUs	Number Active CPUs	Number Users	Number Teams	Last Update
486010	81683	234182	26865	2003-07-26 01:03:06

<http://www.stanford.edu/group/pandegroup/folding/>

GAMESS

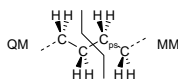
<http://www.msg.ameslab.gov/GAMESS/GAMESS.html>

GAMESS is a program for *ab initio* quantum chemistry. Briefly, GAMESS can compute SCF wavefunctions ranging from RHF, ROHF, UHF, GVB, and MCSCF. Correlation corrections to these SCF wavefunctions include Configuration Interaction, second order perturbation theory, and Coupled-Cluster approaches, as well as the Density Functional Theory approximation.

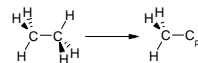
(a)



(b)



(c)



(a) Concept of the QM/MM approach. (b) Partitioning of a QM/MM system with the pseudobond method. (c) Parameterization of the pseudobond with ethane (Cps = F with pseudopotential)

世界のグリッドのまとめ

- 研究基本インフラとして定着

資源・データ・知識の共有 (BIRN, GRAB, OBITco)
計算パワーの共有 (EuroGrid, OBIGrid)
拠点間から国際協調へ (PRAGMA, APGrid, DataGrid)

- 計算モデルは単純並列計算、データ並列、
またはマスタークライアント

- 巨大データの取り扱いが鍵

小規模データに分割 (TurboGrid)
事前に転送 (OBIEEnv)

Open Bioinformatics Grid
(OBIGrid)

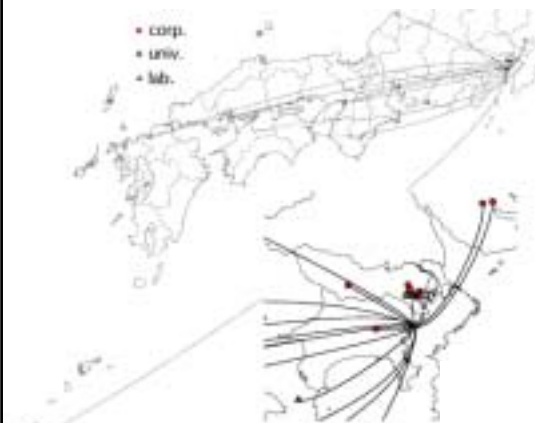
OBIGrid Web Site



<http://www.obigrid.org>



Overview of OBIGrid



2002年4月より開始

目標:

グリッド上でのバイオインフォマティクス環境の構築

技術:

Virtual Private Net (VPN)
Globus Tool Kit
Bioinformatics Frameworks

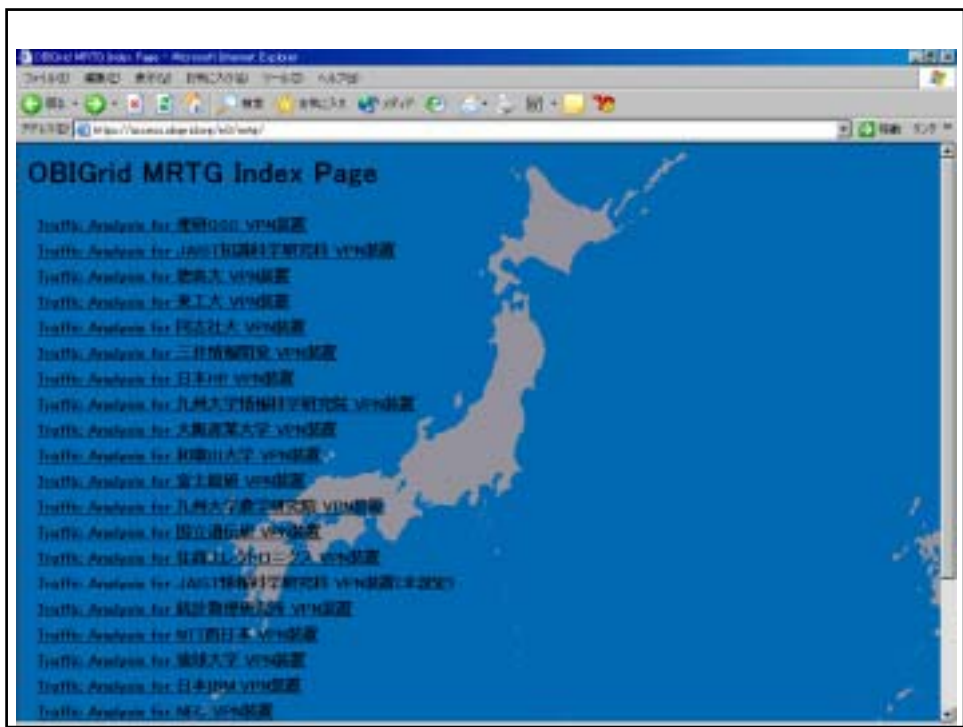
組織母体:

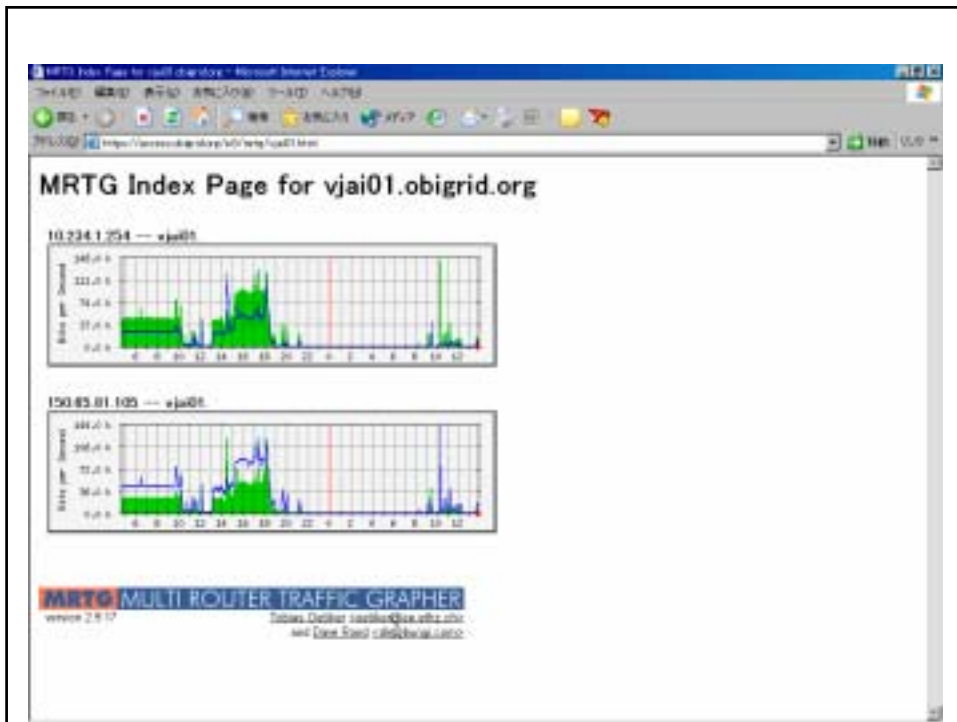
現状:


Aca. 13 Ent. 9 Nat.Res. 5
Nodes 290 CPUs 482
Registered Users 154

・並列生物情報処理イニシアティブ (IPAB)
・文科省特定領域研究ゲノム情報科学
ソフトウェア共有化および高速化委員会

OBIGrid partners







バイオインフォマティクス応用

OBISgd: Distributed XML DB Search

XML DBs → Distributed Index Search Servers → Web portal (JAVA API, Perl API)

- Scalability
- Quick Response
- High reliability

OBİYagns: Cell Simulation Environment

Signal Transduction → Cell Cycle → Mathematical Modeling → Solver

- ODE Solver for Stiff Problems
- Unknown Parameter Estimator

Web portal, JAVA API, Perl API

OBITco: Thermus Thermophilus Cyber Outlet

Access Manager → SSL connection → OBI Grid network

Secure remote annotation by biologists using SSL on Web Browser

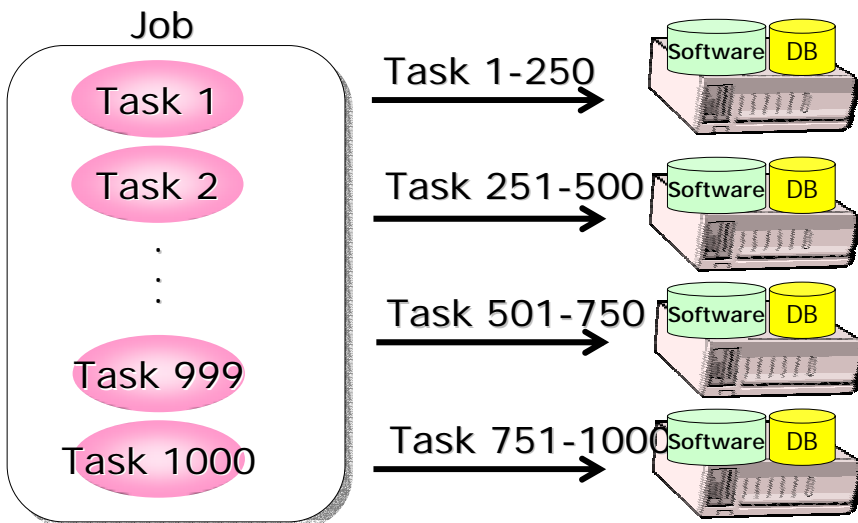
OBIEnv: Bioinformatics Environment

Resource Searcher → Job Dispatcher → Resource Manager → Job Execution Workers

- Single Account
- Script Prog. Env.
- Parallel BLAST/DB

スケーラブルコンピューティング

バイオインフォマティクスにおける典型的計算



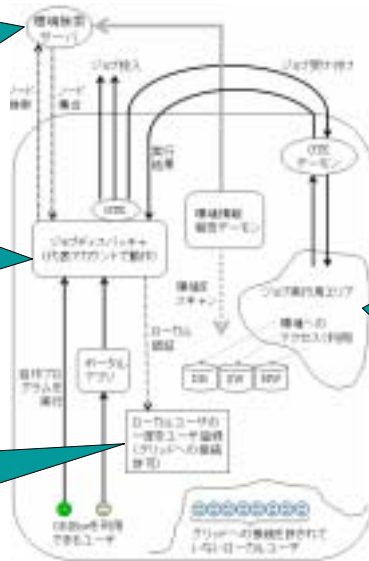
独立した極めて多数のタスクを大量に発行

OBIEnvの概略図

環境検索サーバに各ノードの情報を集中させる(データ、ソフト、ハード)

計算に適した環境を検索し、各ノードにジョブを投入する

各ノードにおけるユーザ登録の手間を省くため、OBIEnvでは代表アカウントだけを使う

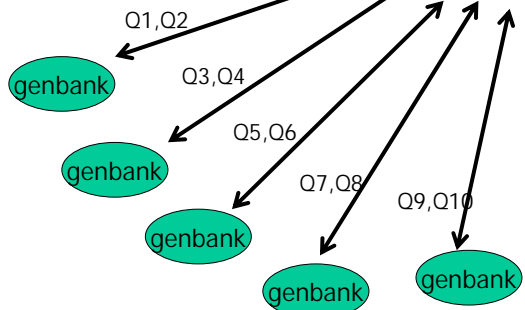


投入されたジョブごとに動的に作業領域が作成され、計算が行われる

OBIEnvでジョブを実行

ジョブ(タスクリスト)

- blast Q1 genbank
- blast Q2 genbank
- ...
- blast Q10 genbank



ノード集合 ↑ ↓ GenBankとBLASTを持っているノードは?
環境情報検索サーバ

各タスクは独立(互いに依存しない)

ユーザからジョブディスパッチャへの指示

必須条件として指定したい場合

- 例) BLAST2.0 ~ および最新版のGenBank
- 例) Linux 2.4.X および Perl 5.6.X
- 例) PentiumIII 800MHz ~

Preferenceとして指定したい場合

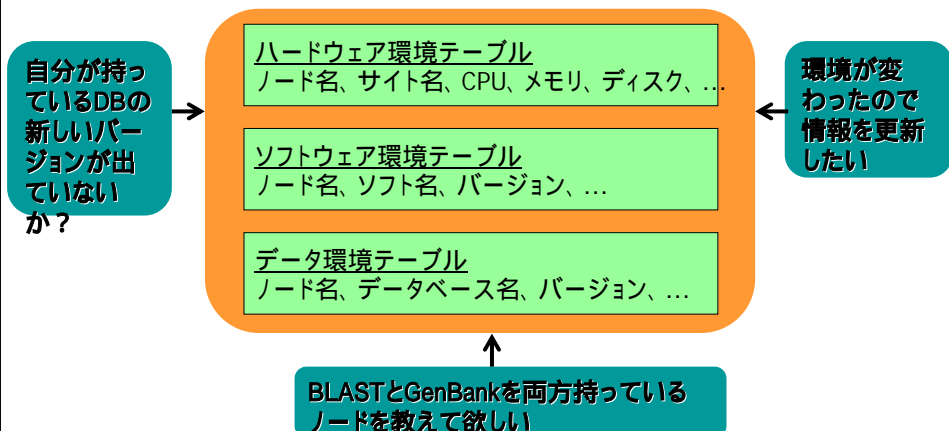
- 例) できるだけ分散して実行して欲しい
- 例) できるだけ同じ環境で実行して欲しい
- 例) できるだけ速そうなCPUで実行して欲しい



これらの指示に応じてジョブディスパッチャが
ノードの検索と選択を行う

環境情報検索サーバ

各ノードの環境情報を集積し、検索要求に応える (PostgreSQLを使用)。



登録情報の例(一部)

マシン情報テーブル

ホスト名	メモリ(MB)	ディスク(GB)	CPU数	ジョブ実行数	ジョブ最大数	VPNのパス	最終更新
crobi01	1000	80	2	1			
4					

CPU情報テーブル

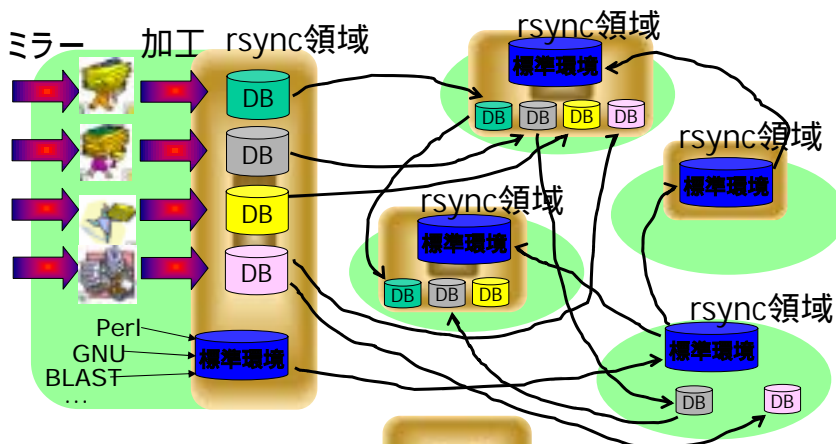
ホスト名	CPUID	CPU種別	CPU速度(Mhz)	最終更新
crobi01	1	PenIII	1130	...

データベース情報テーブル

ホスト名	DB名	バージョン	サイズ	rsync利用者数	最終更新
crobi01	trembl	2002:11:20	...	1	...
crobi01	trembl	2002:11:14	...	0	...

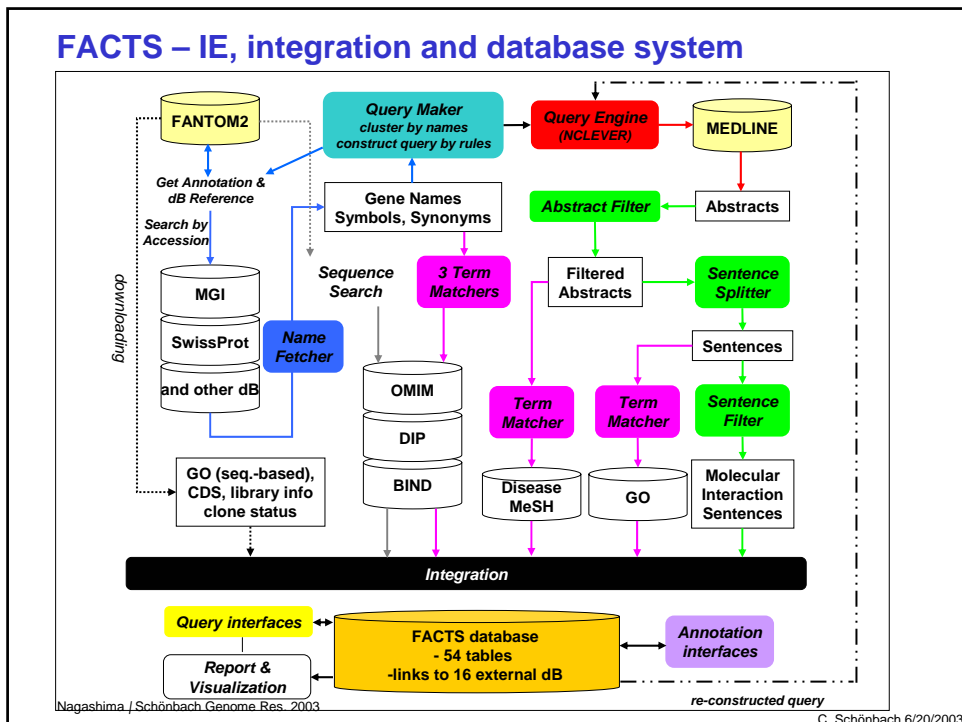
他にもソフトウェア情報などがある

DBと標準環境は自動転送(選択可能)



配布元のサイトはグリッド内で1つとは限らない(DBやソフトごとに分散可能)

分散資源共有



FREP Functional Repeat Database

The screenshot displays the FREP search and extraction results for accession number AC060008.060 (p4046457). It includes a search window, a table of repeat elements with columns for Name, Repeat, Repeat Summary, and Repeat Class, and a detailed classification table with columns for Repeat, Int, Pub, LTR, and various structural and functional attributes.

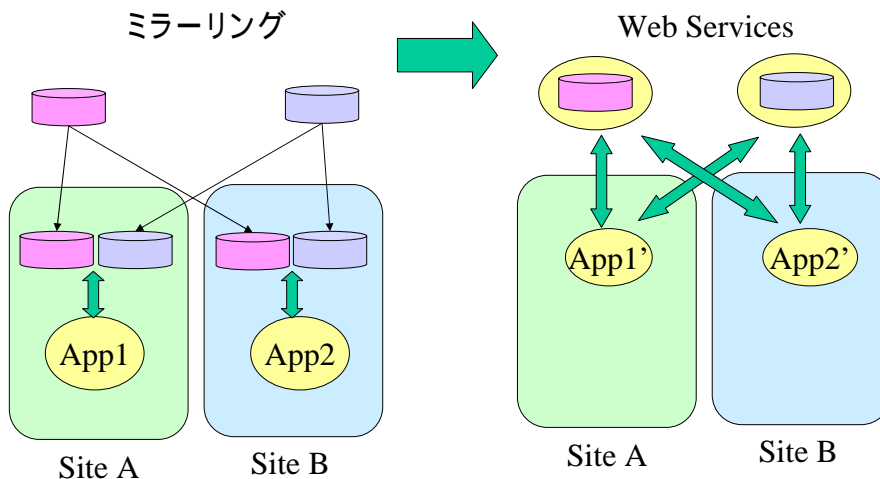
Details of FREP Classification

Repeat	Int	Pub	LTR	Quality	Structure	Function	Repeat	Repeat	Repeat	Repeat	Repeat	Repeat	Repeat
L1	1	1	1	1	1	1	1	1	1	1	1	1	1
L2	1	1	1	1	1	1	1	1	1	1	1	1	1
L3	1	1	1	1	1	1	1	1	1	1	1	1	1
L4	1	1	1	1	1	1	1	1	1	1	1	1	1
L5	1	1	1	1	1	1	1	1	1	1	1	1	1
L6	1	1	1	1	1	1	1	1	1	1	1	1	1
L7	1	1	1	1	1	1	1	1	1	1	1	1	1
L8	1	1	1	1	1	1	1	1	1	1	1	1	1
L9	1	1	1	1	1	1	1	1	1	1	1	1	1
L10	1	1	1	1	1	1	1	1	1	1	1	1	1
L11	1	1	1	1	1	1	1	1	1	1	1	1	1
L12	1	1	1	1	1	1	1	1	1	1	1	1	1
L13	1	1	1	1	1	1	1	1	1	1	1	1	1
L14	1	1	1	1	1	1	1	1	1	1	1	1	1
L15	1	1	1	1	1	1	1	1	1	1	1	1	1
L16	1	1	1	1	1	1	1	1	1	1	1	1	1
L17	1	1	1	1	1	1	1	1	1	1	1	1	1
L18	1	1	1	1	1	1	1	1	1	1	1	1	1
L19	1	1	1	1	1	1	1	1	1	1	1	1	1
L20	1	1	1	1	1	1	1	1	1	1	1	1	1

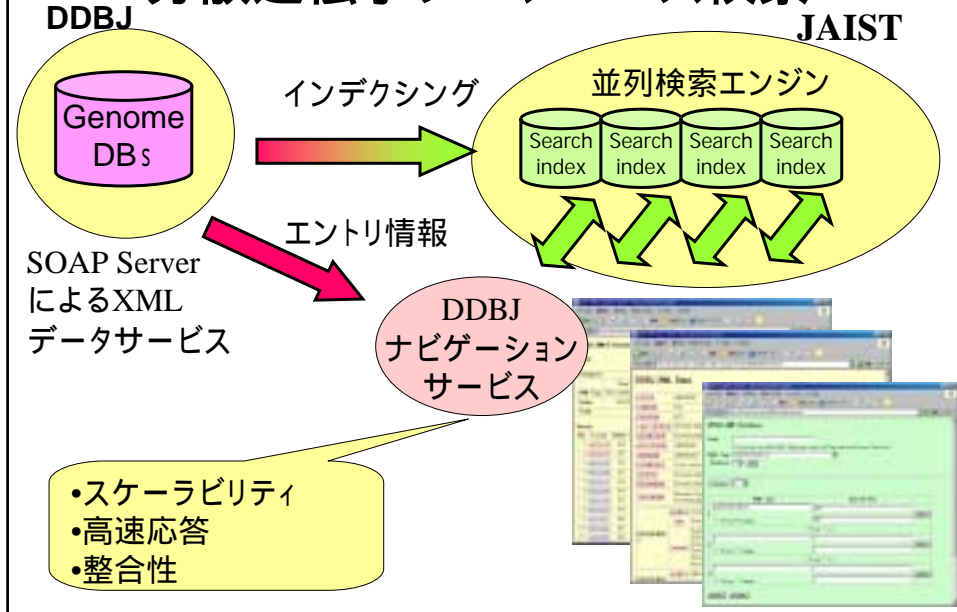
Collation of repeat elements with transcriptional variation, regulation and disease etiology (available in *January 2004*)

C. Schönbach 10/11/2003

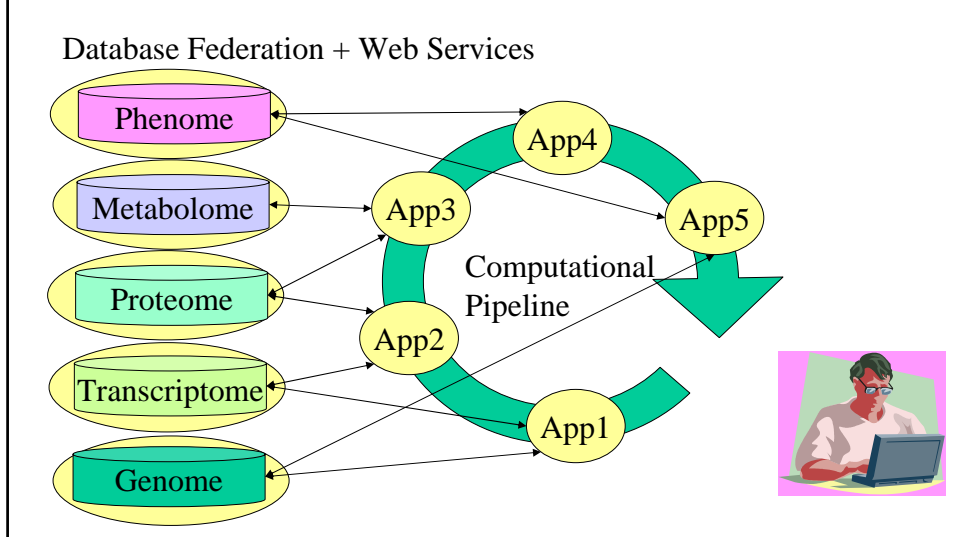
データベースアクセス形態



分散遺伝子データベース検索

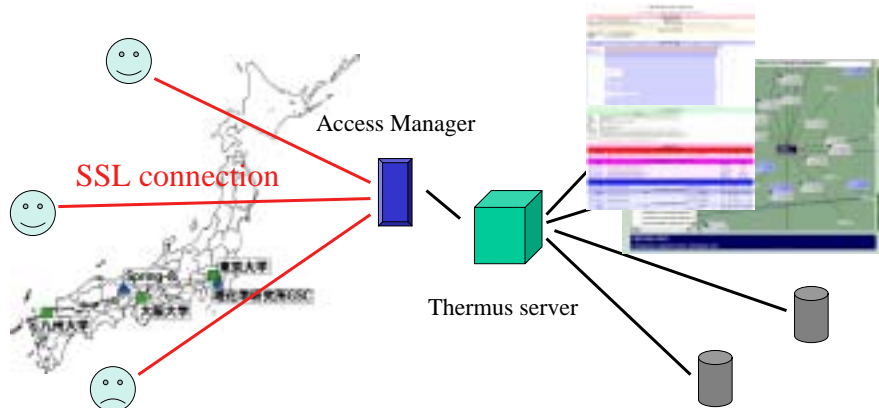


分散資源サービスを用いた応用開発



コミュニティ (スーパーストラクチャ)

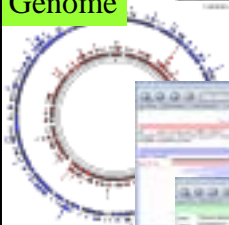
OBITco:高度好熱菌知識ベース



Webブラウザ・よりSSLで全国からThermus serverに接続
遠隔地の研究者と共同でアノテーション作業が安全に行える

Thermus thermophilus Whole cell simulation

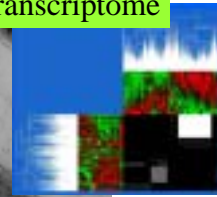
Genome



Structurome



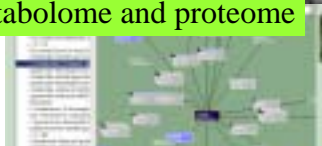
Transcriptome



Simulation



Metabolome and proteome

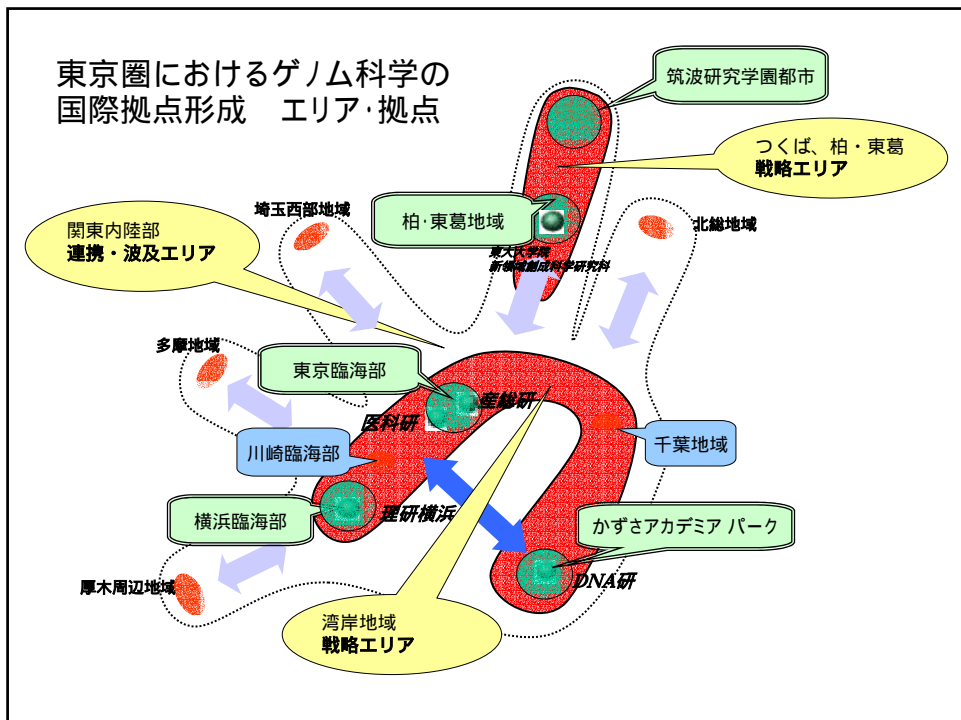


福崎、長嶋、井出、小西、畠山、横山、倉光、小長谷: *Thermus thermophilus* ORFアノテーションシステムへのグリッド技術利用について、高度好熱菌丸ごと一匹プロジェクト第2回ストラクチュローム連携研究会, (2003年8月)

今後の展望

グリッド実用化への課題

- 基幹インフラとしてのグリッド網の構築
- ビジネスモデル(課金制度)の確立
- 参加者の信頼性の確保(トラストの確立)

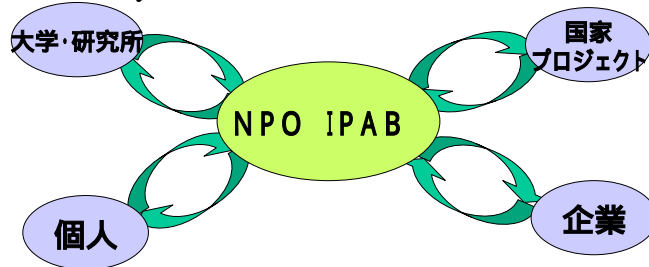


NPO IPABを核とした OBIGridの運用

<http://www.ipab.org> 法人会員 25万円/年
個人会員 1万円/年 (予定)

12月22日(月) GRID WG@理研 GSC 鶴見

International Workshop on Life Science Grid (LSGRID2004)
Kanazawa, May 31- June 1



まとめ

- ゲノム配列からバイオネットワークへ
- データ集約から知識集約
(ヒューマンネットワーク)へ
- グリッドを核としたバイオインフォマティクス
環境の構築

謝辞

敬称略

代表 小長谷(GSC, 東工大)
事務局 古野, 遠藤(GSC)
VPN/Globus網 梅田(IBM)、大木、梅津(GSC)、浜野(ベストシステム)
OBIEEnv/OBISgd 佐藤(JAIST)、辻、中島(HNES)
OBIMde 泰地、成見、二木、高田(GSC)、山本(JAIST)
OBITco 小西、福崎、島山、井出(GSC)、
倉光、横山、増井、中井(ストラクチュアーム)
木村(GSC)、川崎(富士総研)
OBiYagms

科研特定領域研究ゲノム情報科学
ソフトウェア共有化および高速化委員会

小坂(大阪産業大)、松田(阪大)、田中(JST)、岡本、中西、福田(九大)、宮崎(遺伝研)、藤山(NII)、秋山、中田(産総研)、丸山(筑波大)、遠藤(東京医科歯科大)、松岡(東工大)、山村(東工大)、森下、高木、矢田(東大)、染谷(統数研)、廣安(同志社大)、小野(徳島)、佐藤、デファコ、林(JAIST)、山本(JAIST)、小長谷、小西(GSC)、名嘉村(琉球大)、斉藤(和歌山)

並列生物情報処理イニシアティブ(IPAB)グリッド構築ワーキンググループ

株式会社 NTTデータ	日本アイ・ピー・エム 株式会社	株式会社 三菱総合研究所
コグニティブリサーチラボ 株式会社	日本新薬 株式会社	理化学研究所 横浜研究所(GSC)
コンバックコンピュータ 株式会社	日本電気 株式会社	株式会社 理経
独立行政法人 産業技術総合研究所	株式会社 富士総合研究所	有限会社 エスカ
株式会社 数理技研	富士通 株式会社	インテック・ウェブ・アソシエーツ・ゲノム・インフォマティクス(株)
住商エレクトロニクス 株式会社	株式会社 ベストシステムズ	CTCラボラトリーシステムズ 株式会社
北陸日本電気ソフトウェア 株式会社		

International Workshop on Life Science Grid (LSG2004) Kanazawa, May 31- June 1, 2004

Place: Kanazawa Kosei Nenkin Kaikan, 4-17-1 Ishibiki, Kanazawa-city, Ishikawa, Japan

Co-organizers:

JSAI SIGMBI (Japanese Society of Artificial Intelligence)

RIKEN GSC

IPAB (Initiative for Parallel Bioinformatics) under consideration

JHPB (Japan Committee of High Performance Biocomputing)

(more)

Area and Scope:

Researchers in the field of Life Sciences rely increasingly on information technology to extract and manage relevant knowledge. The complex computational and data managements needs of life sciences research make Grid technologies an attractive support solution. However, many important issues must be addressed before the Life Sciences Grid becomes common place. The scope of this workshop focuses on life science application of grid systems especially for bionetwork research and systems biology which require heterogeneous data integration from genome to phenome, mathematical modeling and simulation from molecular to population levels, and high performance computing including parallel processing, special hardware and grid computing.