Current Status of Biogrid Project

Shinji Shimojo
Osaka University

Current Network for Biogrid Project
Construction of a Supercomputer Network (BioGrid Project)

- BioGrid project is one of national R&D projects in IT-Program granted by Ministry of Education, Culture, Sports, Science and Technology.
- We desire to promote IT applied research specialized in medical science and biology in collaboration with Osaka University and other relevant institutions.
- Our goal is to develop necessary technology in grid as well as to develop exemplary applications in life science.

www.biogrid.jp
### Project Organization

**Advisory Committee**

**Project Leader**
Shinji Shimojo (Osaka University)

**Management Committee**

**Core Grid Group**
Leader: Susumu Date (Osaka University)
Osaka Univ., NEC System Technologies, Mitsui Knowledge Industry, Senri International Information Institute

**Data Grid Group**
Leader: Hideo Matsuda (Osaka University)
Osaka Univ., Kyoto Univ., Hitachi Software Engineering, Protein Research Foundation, Hewlett-Packard Japan, Fujitsu Kyushu System Engineering, Mitsubishi Space Software, Aztec System

**Computing Grid Group**
Leader: Haruki Nakamura (Osaka University)
Osaka Univ., NEC Fundamental Research Laboratories, Hitachi, Biomolecular Engineering Research Institute

**HTC Group**
Leader: Kazutoshi Fujikawa (Nara Institute of Science and Technology)
Osaka Univ., Kobe Univ., Nara Institute of Science and Technology, Japan Atomic Energy Research Institute

**Telescience Group**
Leader: Naoto Yagi (Japan Synchrotron Radiation Research Institute)
Osaka Univ., Japan Synchrotron Radiation Research Institute, National Institute of Advanced Industrial Science and Technology

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**Data Grid Technology Group**

PL: Hideo Matsuda

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**Pathway**

- **Drug**
- **Protein**
- **Genome**
- **Disease**

**OGSA-DAI**

**Web Service**

**Data Grid**

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**Osaka University**

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Japan
Outline of DataGrid

A large number of databases in Molecular Biology and Pharmaceutics exist on web. It is needed to integrate all these databases into one big database for analyzing the entire drug discovery process. However the cost of it would be too expensive and thus it is impractical to do so. We have developed a method for federating their databases using the Grid technology.

Development of Data Grid

Database federation using Grid technology.

Databases for each category are provided as Grid Services.
Application Scenario

1. **New Target Protein**
2. **Searching for new Ligand by using our Data Grid System**
3. **Homologous proteins with known compounds**
4. **In silico Drug Discovery**
   - New compounds possibly interacting with the target protein
   - Large query set of known compounds of homologous target proteins

**Data Grid Application View**
Computing Grid

PL: Haruki Nakamura
AMOSS Hartree Fock calculation

Hartree Fock

GSO-X DFT spin calculation

Hybrid Quantum Mechanics-Service

prestoX

Molecular Dynamics-Service

OSA Portal

SOAP BMSML

AMOSS

GSO-X

prestoX

User

Portal

Notification

BMSML

Hybrid Quantum Mechanics-Service

Data transfer of Grid-Service for QM/MM Calculation on BioPfuga

GT3: Globus Toolkit version 3.2 of OGSA-Open Grid Service Architecture

Osaka University
Japan

To Portal
or other Services

Site A

GT3 Grid-Service

I/F Adaptor

Application

prestoX/AMOSS

Disk

Memory

BMS-ML

Osaka University
Japan
HTC
High Throughput Computing

PL: Kazutoshi Fujikawa

Structure Prediction:
A key challenge in post-genome sequencing era

Given amino acid sequence:

Functional Annotation
Drug design
Sample workflow for ROKKY

ROKKY: Protein Structure Prediction Server
developed at Kobe Univ

For CM targets, use PDB-BLAST
For FR targets, use 3D-Jury, &
For NF targets, use SimFold
“Large scale folding simulation”
Full automation vs Human intervention

Answer  By full automation  By human intervention

Telescience

PL: Toyokazu Akiyama
Telescience Overview

- **Research goal**
  - Establish remote operation environments for high performance observation devices such as Ultra High Voltage Microscope, Spring-8 and MEG.

- **Research topics**
  - Remote operation
    - High resolution image transfer
    - Grid enabled remote operation environment
  - Data analysis
  - Visualization
  - Networking
    - QoS

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History and Relevant Background

- **June 1999**
  - Trans-Pacific Telemicroscopy controls the UHVEM at Osaka University from the NCMIR facilities at UCSD.

- **July 2003**
  - Memorandum of Understanding among UCSD/NCMIR, Osaka University, and KDDI Research Laboratories.

- **November 2003**
  - Telescience wins award for “Best Application” at the SC2003 Bandwidth Challenge.

- **June 2004**
  - PRIME 2004 sends three students to various programs through the Osaka University Cybermedia Center

- **November 2004**
  - New Demonstration on National Lambda Rail are shown in SC04. Courtesy by Stephen C. Geist, Ramsin Khoshabeh and Tomas Molina (UCSD)
Tele-science on Tomography

NCHC will host 5th PRAGMA in Oct. 2003

iGrid 02, joint demo, Sep. 2002
SC 02, HPC Challenge, Nov. 2002

Provided by Dr. Naoko Yamada (NCMIR)

Tomography Workflow (Courtesy by Tomas Molina)
Core Grid

PL: Susumu Date
GUIDE: A grid portal for bioinformatics

- Provides easy-to-use interface and enables efficient analyses in bioinformatics
  - Single sign-on (Globus GSI & MyProxy)
  - Interface for applications and job management
Summery

- Biogrid and NAREGI are Japanese flagship R&D project.
- In cooperation of Network R&D projects such as Super-sinet and JGN II, we could build AP grid infrastructure.
- Many national and international projects such as PRAGMA, APGRID in APAN, ASIA grid project in Japan have been promoting our collaboration.
- Life Science is one of a key application of Grid and Cooperation between science and IT is necessary.