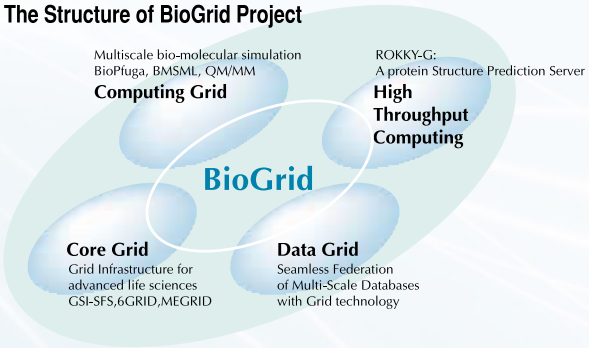
BioGrid Project

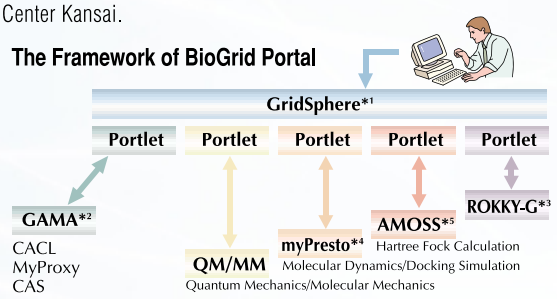
Construction of a Supercomputer Network

The Cybermedia Center, Osaka University has been promoting the BioGrid Project since 2002 with other relevant research institutions and private sectors. Funded by MEXT, this project has been entrusted with the mission of attaining the following three goals: 1) A series of analyzers deployed on a supercomputer network, 2) "Computing Grid technology", which may facilitate a truly systematic linkage among the databases and data processing requiring ultra high-speed computing resources and 3) "Data Grid technology", which will allow total and safe linkage and manipulation among various types of huge databases.
We have accomplished our initial mission and made much progress in the biological grid technologies. We have gridified our original simulation programs based on our own algorithms in the field of biological simulation. We have also proposed several fundamental technologies to make full use of biological information through the seamless federation of multi-scale databases with the Grid technology and have created several grid tools to establish a useful research infrastructure.
Now, we are constructing a BioGrid Portal that allows scientists to perform their analyses in the life sciences. This portal system is based on the recent frameworks such as GridSphere*1 and GAMA*2 in association with NBCR and SDSC. We will provide this grid portal service for various users in collaboration with the NPO BioGrid Center Kansai.

The Structure of BioGrid Project



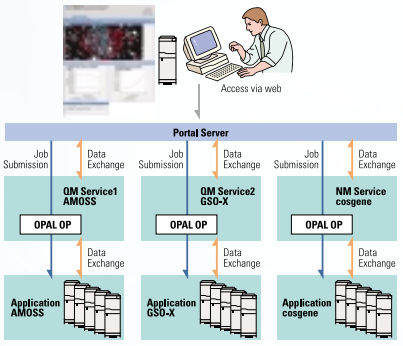
The Framework of BioGrid Portal



(*1) GridSphere : Copyright 2002-2006 Team GridSphere.
(*2) GAMA is developed by the San Diego Supercomputer Center and its contributors.
(*3) ROKKY has been developed by Takada Lab. at Kobe University.
(*4) myPresto is developed by JBiC, AIST, FUJITSU, Hitachi and its contributors.
(*5) ab initio molecular orbital program developed by NEC

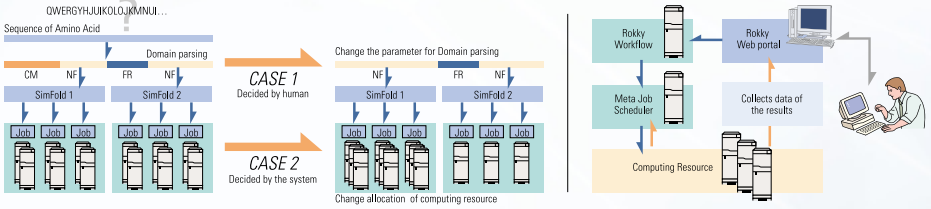
The Opal Operation Provider and an Application of BioPfuga for Hybrid-QM/MM Simulation

In order to construct a grid system rapidly for highly-sophisticated science problems, it is essential to utilize existing applications effectively. For this purpose, existing technologies and cutting-edge technologies of the grid must be merged rapidly. However, such a method has not been well defined.
The Opal Operation Provider (Opal OP) is one possible way to gridify existing applications easily. Opal has been developed in the National Biomedical Computation Resource (NBCR) Project. Opal manages job submission and wraps up existing applications as Web services. Our project has developed Opal OP as an operation provider using Opal in the Globus Toolkit4 (GT4). The Opal OP enables the creation of WSRF based services wrapping existing applications easily. Also, the Opal OP provides application developers the opportunity to modify the generated WSRF services. Application developers then can develop flexible services to meet their specific problems using the Opal OP.
We are now using this OPAL Operation Provider to construct a grid system for bio-molecular simulation in a hybrid-QM/MM simulation system. This system consists of different simulation components developed by different organizations. Each component needs large computational resources. In order to integrate these components, we have developed WSRF services for each component by using Opal OP.



ROKKY-G : A Gridified Protein Structure Prediction System

In the scientific simulations, users want to obtain highly reliable results using limited computational resources. If users cannot decide the optimal values of input parameters of jobs beforehand, the results of job execution are sometimes unreliable. In this case, the computational resources for the job execution have gone to waste. To deal with this problem, ROKKY-G, which is a Gridified protein structure prediction system, provides a trial-and-error job management mechanism for users.



In Cases 1 and 2, we show two examples of the trial-and-error job execution on ROKKY-G.
In CASE 1, a user divides a protein's amino-acid sequence into several domains and submits jobs for structure prediction of each domain. The user can check the results during job execution at any time. If the user finds some results are unreliable, he/she can dynamically change the domain division.
In CASE 2, ROKKY-G can automatically and dynamically change the assignment of the computational resource for the job execution of each domain, depending on trial-and-error of the user's job execution and the user's intention.

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