

A Virtual Cluster Solution Using Overlay Network on Wide-Area Distributed Environment

Cybermedia Center, Osaka University, Japan

Applied Information System Division aims for the development of information technology useful for scientific users. For the purpose we have been researching elemental technology such as high-speed networking and Grid from a point of scientific application building view. A recent achievement in the Applied Information System Division is virtual cluster solution.

Concept and Architecture of our Virtual Cluster Solution

Grid technology has grown as a means to efficiently and effectively utilize computational resources among multiple organizations and it is highly required in scientific and business fields. However, the current Grid technology does not always provide the computational environment enough to satisfy users' requirements because users cannot setup or configure computational environment of the Grid as they like.

To solve this problem, we have been developing virtual cluster solution using overlay network. The virtual cluster is composed of virtual computational resources by Xen as a virtualization technology on top of an overlay network realized by PIAX as an overlay networking technology. With our solution, scientific users can build their own private virtual cluster, by dynamically aggregating computational resources on the Internet.

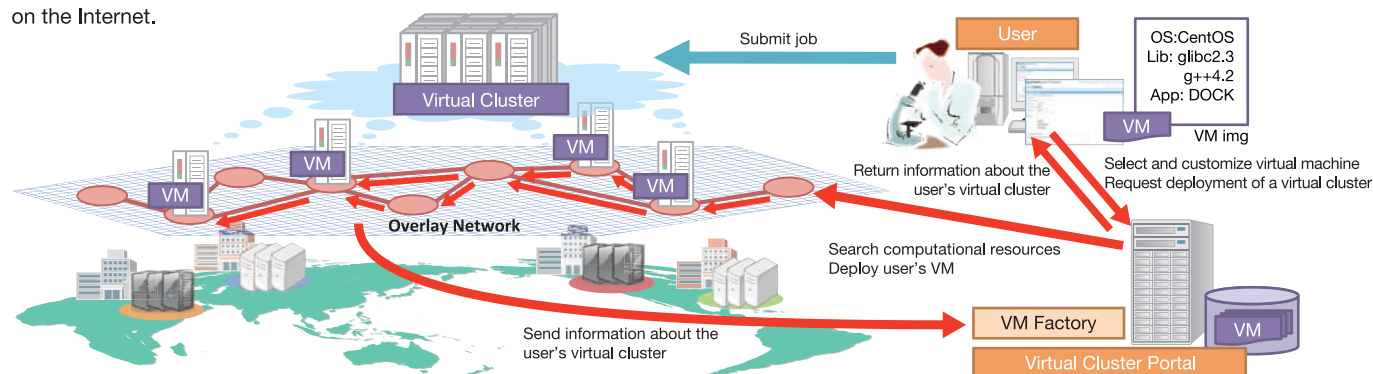


Fig.1 Concept of our virtual cluster solution

Our virtual cluster is built as follows. First, a user accesses to the Virtual Cluster portal and requests deployment of a virtual cluster. The request is sent to a resource discovery agent on the overlay network. The resource discovery agent finds appropriate computational resources which can host the requested virtual machines. After that, the virtual machines are deployed on selected computational resources and establish end-to-end IP communication among them and organize a virtual cluster. Finally, the portal returns the information necessary for access to the cluster.

The communication relay mechanism plays a role of relaying IP communication between virtual machines composing the virtual cluster on the overlay network. The mechanism performs this function by encapsulating IP packet into PIAX message frame exchanged on the overlay network. By leveraging this mechanism, scientific users can execute their own scientific applications without any modification on the virtual cluster.

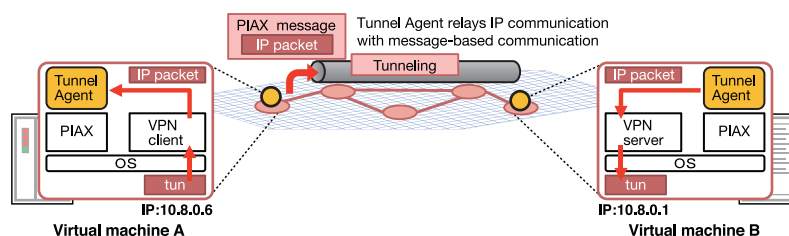


Fig.2 A Communication Relay Mechanism

Application Example: Docking Simulation

DOCK

DOCK is a simulation software for drug discovery. Bio scientists often use DOCK to investigate which chemical compound can bind to a target protein and so be a drug candidate. After simulation, the bio scientists experimentally test with the chemical compound ranked high of the chemical compounds. Usually, in the simulation, it is necessary to repeat multimillion combinations of chemical compounds and the target protein. For the reason, the recent high-performance computing technology such as PC cluster and Grid Computing is heavily required.

Performance

We measured the execution time of DOCK simulation on a physical cluster and a virtual cluster for investigating computational performance difference between them. In the measurement experiment, the total execution time of completing docking simulation between a target protein and 30 chemical compounds was measured on each cluster. The result shown in Fig. 4 indicates that the computational overhead on the virtual cluster is quite small compared with the physical cluster irrespective of the number of cluster node. Also, it shows our virtual cluster could be useful and effectively work for computationally intensive applications such as DOCK.

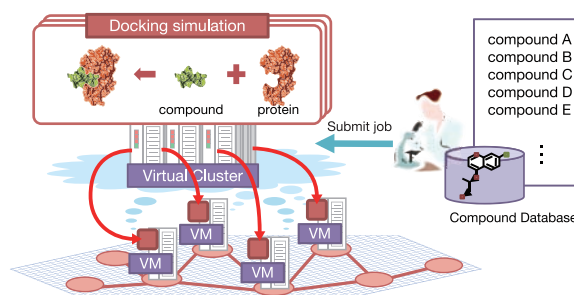


Fig.3 Execution of docking simulation on the virtual cluster

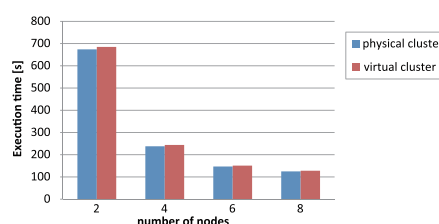


Fig.4 Execution time on physical cluster and virtual cluster