

VIRTUAL WORKSPACE AS BASIS OF SUPERCOMPUTER CENTER

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Virtual workspace has recently become one of the ways to perform routine tasks in cloud environment, however, its use in scientific experiments is novel and offers a number of advantages compared to traditional grid-based approach. These are: universal access to all computational and storage resources from within single private virtual machine, easy workspace customization considering user's own needs and an ability to create virtual private cluster with desirable configuration. In such an environment network storage devices are connected both to computational nodes and to your virtual machine so that all the experiment input data and output results are automatically saved in one place and can be easily accessed from the workspace. Implementation of described approach is presented on the example of Resource Center Computational Center of Saint-Petersburg State University.

1 Introduction

Virtual workspace as the name suggests can be thought of as a desk of a scientist where all papers, referential materials and document's drafts are stored and developed, but it offers some advantages over such conventional desk. First of all, as more and more scientists rely in their research on software and hardware equipment they want universal access to storage, computational resources and software licenses. Moreover, as their research varies in scale and time constraints scientists want to dynamically extend their resource pool to the desired capacity. Last but not the least, scientists want to customize and convert their workspace into the problem solution environment by installing additional software and adapting architecture to the problem solved. Eventually, this is how advantages offered by a virtual workspace are characterized.

Virtual workspace alone is a powerful concept, however it is beneficial to review its implementation on the basis of university resource center. Such resource center should not only administer and support hardware and software equipment but also provide scientists with high performance computing services, offer distributed software licenses and also service unconventional large-scale scientific projects. In addition to this, HPC services should be readily accessible to users with a wide range of technical skills and easily customizable for advanced users. Resource Center Computational Center (RCCC) of Saint-Petersburg State University will be provided as an example of virtual workspace approach [1].

Conventional resource center often services many faculties and should be able to resolve conflicts between user's own preferences and problem requirements. An incomplete list of common problems includes human-machine interaction, cooperative usage of shared computational and storage resources, prioritized provisioning of software licenses, security of experiment's data. Using such resource center as an example it is easy to show advantages and disadvantages of virtual workspace approach and also demonstrate its practical implications. Resource center infrastructure is discussed in Section 2, implementation of virtual workspace is discussed in Section 3 and advantages and disadvantages as well as performance considerations are discussed in Section 4 and 5 respectively.

2 Resource center infrastructure

Typical resource center maintains a range of clusters with possibly different topologies, a range of special purpose computing machines (hybrid or SMP architecture) and some storage devices

all using high-speed interconnect. In case of RCCC these are: conventional T-Platform cluster, 3 SMP machines, hybrid cluster with GPU accelerators (Table 1) and HP X9300 storage system. Cluster nodes are managed by CentOS 5.6 and resources are exposed by PBS (Torque with Maui job scheduler) [2].

	T-Platform cluster T-EDGE96 HPC-0011828-001	SMP cluster, HP Proliant DL980	Hybrid cluster, HP SL390s G7
CPU	2x Intel E5335 2.0 GHz	8x Intel X7560 2.2 GHz	2x Intel X5650 2.67 GHz
GPU	–	–	3x (8x) NVIDIA Tesla M2050
RAM (Gb)	16	512-1024	96
HDD (Gb)	160	2000	120
Commutator	Infiniband 20 GB/s		
Total characteristics	768 TB RAM, 48 nodes, 384 cores	3 TB RAM, 3 nodes, 192 cores	2.3 TB RAM, 24 nodes, 288 cores, 112 GPUs
Peak performance (TFLOPS)	3.07	1.7	59.6

Table 1. RCCC infrastructure.

.Although traditional infrastructure has an advantage of being simple to configure and maintain, it also has the following disadvantages:

- (1) it offers no data consolidation, that is, user who obtained experiment results using special purpose machine should explicitly copy it to cluster access node for further analysis;
- (2) private resources are restricted only to special purpose machines and are accessed in a non-unified way;
- (3) there is no easy way to adapt machine architecture to problem solved.

The aim of virtual workspace is to solve these problems by borrowing some well-established principles of building private clouds. The key points are:

- (1) usage of single storage to improve data consolidation;
- (2) usage of single UNIX-based software repository;
- (3) usage of virtual machine as a basis of virtual workspace;
- (4) usage of private virtual clusters, conventional clusters and dedicated machines to extend virtual workspace resource capacity in a unified way.

The configuration of virtual workspace is not as easy as of traditional resource center infrastructure, however it is also superior to conventional setup in terms of flexibility and ease of customization.

3 Virtual workspace approach

Virtual machine is the main building block of a virtual workspace. In its simplest form a workspace consists of a single virtual machine connected to storage and licensed software repository. If desired, resource capacity can be extended naturally by replicating virtual machine to form a virtual cluster. Cluster can be owned exclusively by a single user or shared by members of a whole research group. Moreover, considering large scale problem one can acquire resources of dedicated high performance machine (SMP or hybrid) or conventional cluster. Resource capacity extension occurs dynamically and acquired resources can be accessed from within single virtual machine.

Virtual machine is customized by changing its hardware characteristics and by selecting

desired operating system and software packages. Hardware characteristics include CPU cores, RAM and virtual storage capacity and operating system can be UNIX-like or Windows (Table 2). User is provided with restricted administrative access to update and configure operating system. Furthermore, user can choose between command line (SSH) and GUI-based (VNC, FreeNX or RDP) access and also select OpenVPN or announced IP option. Possibility of such flexible configuration improves usability without interfering with virtual machine management.

Intended virtual machine usage is summarized as follows:

- solve scientific problems that fit into single virtual machine resources;
- access to computational resources, both clusters and dedicated machines;
- store experiment's data;
- develop applications (programming using commercial and open source compilers);
- perform other routine tasks.

Unified access to the workspace resources is essential to achieve usability and data coherence. Although computational resources are distributed, experiment's data remains in one place due to automatic mounting of file system from virtual machine. Applications are launched in a unified way by using package specific scripts taking cluster host name and job queue as arguments. In addition to this LDAP single sign-on [3] is used to simplify user login to multiple machines and to restrict cluster access. Organizing services in that way provides users with easy access to both research data and computational resources.

Backup process is simplified with data residing in one place and user have an option to backup only selected directories or the whole virtual machine. The first option is sufficient for experienced user processing arrays of data on a regular basis and has a short backup period. The second option is suitable for normal user who accidentally put system out of order and it also has a long backup period. Finally, using any backup approach increases overall system ability to recover from unexpected failure.

Virtual machine is a lively entity with constantly varying resource consumption, however it does not implies wasting resources of low-loaded virtual machine. In such case hypervisor (VMware in case of RCCC) dynamically migrate active virtual machines to available low-loaded physical machines to balance overall workload [4]. Moreover, in most cases virtual machine is acquired on a finite period of time until the research is complete, so unused virtual machines are eventually destroyed and resources are reclaimed by hypervisor. All in all, efficiency of using virtual machines is totally defined by operating hypervisor.

	Default	Maximum
CPU	Intel Xeon X5760 2.93Ghz	
CPU cores	4	12
RAM	4 Gb	24 Gb
HDD	50 Gb	~1 Tb
OS	CentOS 5.6	

Table 2. Virtual machine characteristics.

To sum up, virtual workspace allows dynamic control over resource consumption adapting to the problem solved and provides coherent interface to the extended resources. If the problem is small enough to fit resources of a single virtual machine there is no need to use clusters and problem can be solved «in-place». If the problem is solved on the daily basis and does not fit into single virtual machine, then private virtual cluster is the best option. Finally, if the problem is so large that it consumes significant part of a cluster resource pool, then dedicated high performance machine is the right way to go. This approach leaves medium-sized problems to conventional clusters.

4 Advantages and disadvantages of virtual workspace

Virtual workspace advantages and disadvantages are summarized and validated as follows.

Advantages:

- (1) Universal access to high performance resources over internet (SSH, VNC, RDP)
- (2) Unified access to both computational and storage resources from within single virtual machine (PBS, file system auto mounting)
- (3) Customizability with restricted administrative rights
- (4) Improved security: all data is accessed only from a private virtual machine
- (5) Easy selective backup of meaningful data
- (6) Resilience to unexpected failures: virtual machine can be restored from regular backup snapshots
- (7) Easy configuration of virtual machine characteristics by means of hypervisor
- (8) Natural extension of resources by creating virtual private cluster adapted to problem being solved

Disadvantages:

- (1) Load balancing efficiency and resource consumption control are totally dependent on a hypervisor
- (2) Complex virtual machine configuration: creating virtual machine templates and performing initial machine configuration consumes time when done manually and should be automated
- (3) Virtual cluster interconnect performance is degraded when multiple virtual nodes reside on a single physical host thus limiting flexibility of cluster topology configuration (Table 3)

Total cores	T-Platform cluster	SMP machine	Virtual cluster
32	84	42	35
64	66	36	48

Table 3. Crystal09 SrTiO3 test case wall clock time in minutes showing virtual cluster performance degradation. Virtual cluster characteristics: 16 virtual machines on 4x BL460c G7, 2x Intel X5675 CPUs and 96 Gb RAM on one node, 64 cores total.

5 Scientific application examples

Each method of resource capacity extension found efficient application area, but with different kinds of software. First, private virtual cluster approach proved to be beneficial when using interactive resource-hungry software like Materials Studio [5] or ADF [6]. In that case computational resources of a single host exposed as a virtual machine are not enough for application to run smoothly, and virtual cluster boosts its performance. Second, dedicated high performance machine approach is known to be successful in solving large-scale problems in Crystal09 [7] (Figure 1). In that case a single application run takes more than 1 month to complete even on multi-core SMP system with OpenMPI [8] shared memory interconnect, so running application on conventional cluster takes even more time due to slower link or will put heavy burden on network throughput in case of a virtual cluster. So private virtual cluster can be recommended for interactive applications used on the daily basis and dedicated machine is the most suitable to large-scale problems and long-term simulations.

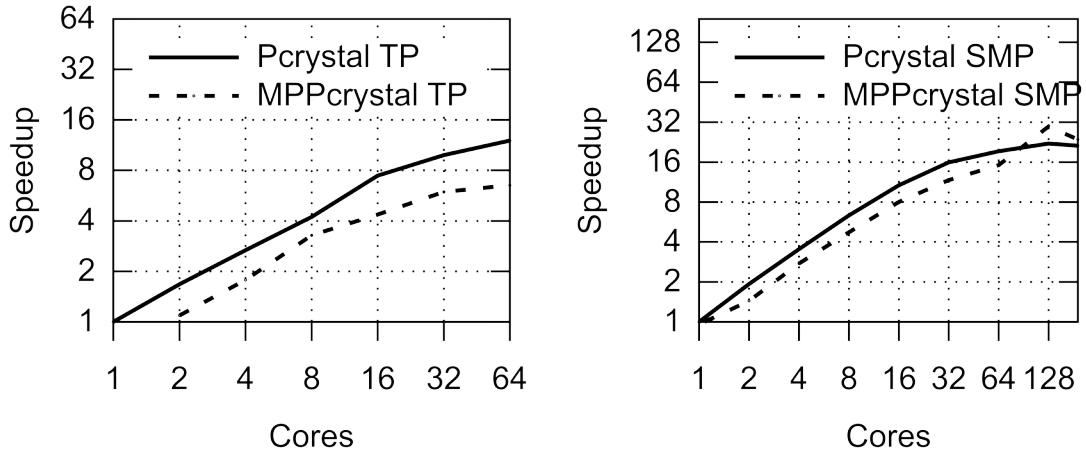


Fig. 1: Speedup of Crystal09 SrTiO3 test case running on conventional public cluster (left) and dedicated SMP machine (right). SMP machine has better speedup (see 16 cores mark).

Performance degradation may occur when using single storage and mounted directories, however only a simple fix is required to restore it. Degradation occurs when multiple parallel processes of a single job simultaneously write to a mounted directory thus inevitably creating performance bottleneck. One demonstrative example of such application is OpenFOAM [9] running simple cavity case in parallel having each process writing multiple files into separate directories of mounted file system (Figure 2). As was mentioned before, this bottleneck is easy to fix by modifying PBS job script to use temporary directory of each node as a working directory and copying results back from each node to mounted file system after computation is over.

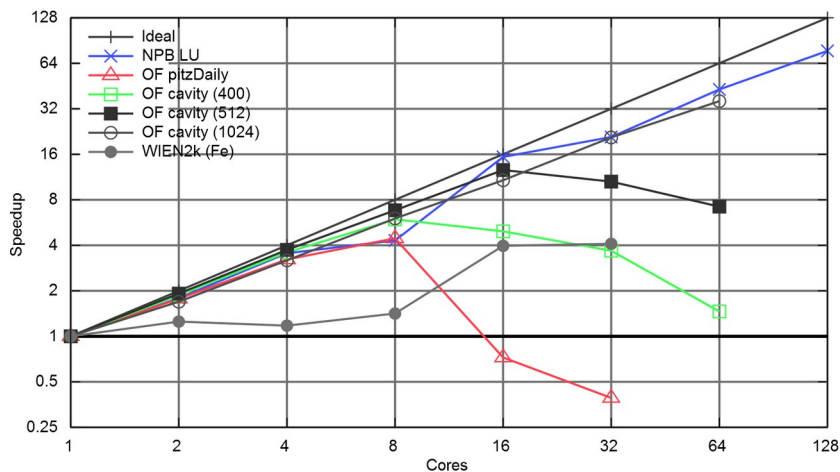


Fig. 2: Speedup of different applications on hybrid cluster. Performance degradation occurs when multiple processes write simultaneously to single mounted directory.

6 Conclusion

Virtual workspace hides intricacies of distributed computing behind a virtual machine to streamline and boost scientific research work flow. It provides a convenient way of accessing hardware and software resources using unified tools, consolidates experiment's data and offers options to dynamically extend available resources using either private virtual cluster or high performance dedicated machines and also public university cluster. Resources are accessed universally and in a unified way.

Virtual workspace is a novel approach of conducting scientific experiments which

harmonically combines ideas of building private clouds with scientific software requirements and specifics of resource center operation. Although, virtual workspace configuration requires more human resources than configuration of conventional cluster do, it gives convenience of flexible, easily extensible and coherent system. Finally, the problems mentioned in the paper that occurred during workspace integration were solved thus showing RCCC as a demonstrative example of exploiting virtualization benefits for scientific needs.

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