



IBM Application Ready Solution for ANSYS

*An IBM Reference Architecture based on Flex System, System x, and
Platform Computing*

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Document history

Revision history

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Introduction

This document describes the reference architecture for the IBM Application Ready Solution for ANSYS. The IBM Application Ready Solution for ANSYS is a technical computing architecture supporting software products developed by ANSYS in the areas of computational fluid dynamics and structural mechanics.

ANSYS® computational fluid dynamics (CFD) software solutions (including ANSYS Fluent and ANSYS CFX) are used to predict fluid flow, heat and mass transfer, chemical reactions, and related phenomena by numerically solving a set of governing mathematical equations (conservation of mass, momentum, energy and others).

ANSYS structural mechanics software (including ANSYS Mechanical) offers a comprehensive solution for linear or nonlinear and dynamic analysis. It provides a complete set of elements behavior, material models and equation solvers for a wide range of engineering problems.

This document should be read in conjunction with the *IBM Application Ready Solutions: An IBM Reference Architecture* and other documents that detail the architecture and implementation of different components that are used to implement ANSYS application suite. For example, Desktop Cloud Visualization - 3D Remote (DCV) and Exceed on Demand (EOD) are used to implement remote rendering requirements of ANSYS application suite. Their use in implementing remote 3D visualization for ANSYS application suite is described here. However, the internal architecture and implementation of these components is not covered in this document. Similarly, detailed description and implementation of the following components is not covered in this document:

- IBM® Platform™ Products (LSF, PCM, PAC)
- Infiniband
- File System
- OS
- Networks and Security

IBM Technical Computing “ANSYS Application Ready Solution” gives an architecture overview, component model of the architecture to implement a variety of applications and then describes the deployment model of the architecture. IBM Application Ready Solutions for ANSYS makes use of this infrastructure to implement ANSYS applications. For completeness, the business problem, business value, and requirements are repeated here from the *IBM Technical Computing “IBM Application Ready Solutions”*.

The target audience of this document is:

- a. Architects in an IT or business organization who are responsible of deploying and operating a cluster to implement ANSYS applications.
- b. Technical users that are looking for an easy way to deploy and use High Performance Computing (HPC) or technical cluster that increases the performance and capabilities of ANSYS applications.
- c. ISV Architects and Business Partners using the building blocks described in this document to create customized reference architectures

Business problem and business value

Business problem

Technical computing users are often “technical” within their respective field (e.g., engineers designing automobile parts), but not experts in computer and software technology. Independent software vendors (ISVs) have made significant investments to increase their application’s performance and capability by enabling them to run in a distributed computing cluster environment. However, many users are unable to fully utilize the capabilities of these applications because they do not have the technical ability to efficiently deploy and manage a technical or HPC cluster. Consequently, they either struggle through sizing, building, integrating, provisioning and supporting a cluster infrastructure themselves or they compromise performance by running their applications on a single machine, a workstation, or a server.

Business value

IBM Application Ready Solution for ANSYS provides an expertly designed, tightly integrated and performance optimized architecture for ANSYS applications. This architecture defines

- (1) Complete cluster - A comprehensive, tightly integrated cluster designed for ease of procurement, deployment, and operation. It includes all required components for technical computing applications including servers, network, storage, operating system, management software, and run time libraries.
- (2) Application optimized configuration - The configuration of the cluster is carefully designed to optimize application performance and reduce total cost of ownership. The cluster is integrated with ANSYS application suite, enabling users to become productive more quickly.
- (3) Advanced technology for performance and robustness - The hardware and software components in the cluster are customizable to allow the best performance or the best price/performance ratio.
- (4) Commercial, solution-level support – The configurations are tested and supported for all hardware and software components.

Requirements

The following functional requirements provide a high level overview of the desired functionality to satisfy ANSYS users.

Functional requirements

Typical users of ANSYS applications perform the following tasks (see Figure 1).

- Preprocessing where the engineering model is created using graphics based applications,
- Solution Phase where a simulation of the model is carried out
- Post processing where the results are evaluated using graphics based applications.

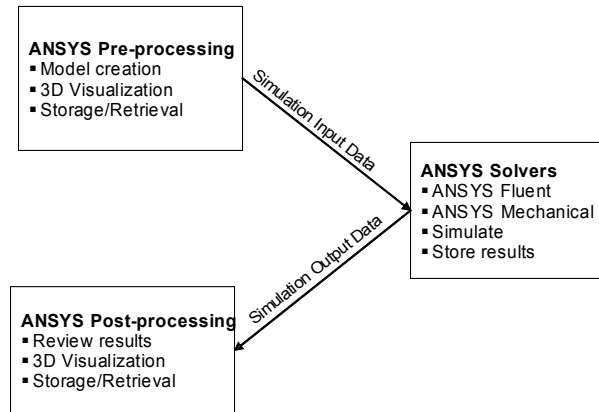


Figure 1: ANSYS Main Use Case

The resource allocation to address this use case scenario can be fully distributed, partially or fully centralized. The use case scenario where the resources are fully distributed such that each workstation is self contained to address all the three steps outlined above is not addressed in this architecture. In this architecture it is assumed one or more of the three steps are performed on a centralized resource. In practice, the main use case described in Figure 1 is realized in the following two ways to use centralized computing resources:

- (1) Workstations plus a cluster: Figure 2 demonstrates a typical use case for a back-end high performance cluster. In this case, an ANSYS user prepares data on the workstation using an application such as ANSYS Workbench, then submits a simulation job to leverage the performance and throughput of the cluster. After the simulation is completed, the results are downloaded and viewed on the client workstation. ANSYS simulation software such as ANSYS Fluent and ANSYS Mechanical, which are computationally intensive, run on the cluster.

The file system is shared across all workstations and the cluster so that the application running on the cluster can access any required data. If a shared file system is not provided then the input data is transferred from the client workstation and subsequent to the completion of the simulation, the results are downloaded from the cluster to the workstation for post processing.

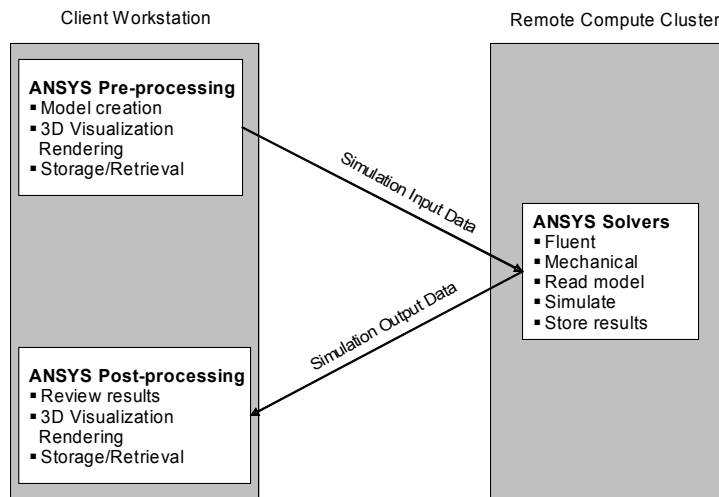


Figure 2: ANSYS Use Case 1

- (2) Thin clients with a cluster: As illustrated in Figure 3, both compute intensive simulation using ANSYS Fluent and ANSYS Mechanical and graphics intensive visualization run in the cluster environment. The client device can be a thin client with display capabilities instead of a powerful workstation. The only data that is transmitted between the client and the cluster are the keystrokes from the client and the rendered pixels from the cluster.

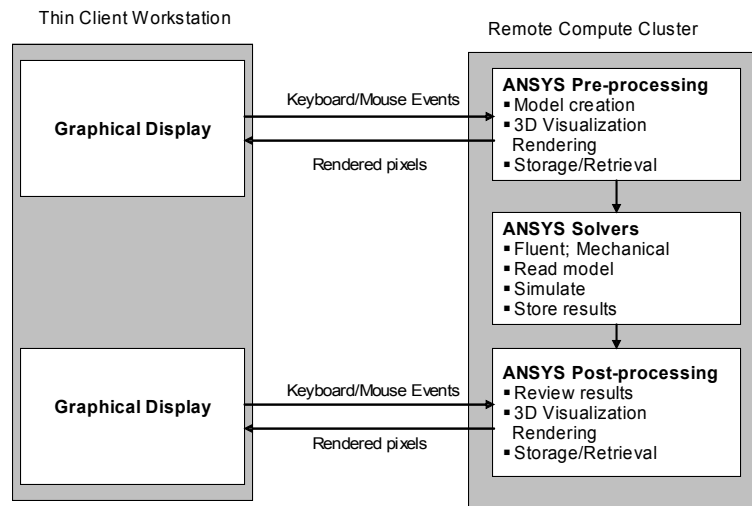


Figure 3: ANSYS Use Case 2

Additional functional requirements include:

Domain experts require technical or HPC clusters that can be quickly deployed without deep computer engineering skills. These clusters require the following attributes:

- The system is configured with an easy to use web management interface, which allows the system administrator to control all elements of the cluster.
- The cluster is easily integrated into an existing Ethernet or IB network and storage infrastructure. As part of the system configuration, the cluster manager will look for Lightweight Directory Access Protocol (LDAP) and Network Information Services (NIS) servers. In that environment, it supports a compute or data intensive application.
- The cluster has a built-in web interface to the target application that allows the user to submit jobs, review results and, start interactive sessions.
- Access to the cluster for job submission is provided by a web interface, however, remote terminal access via ssh to the management or compute nodes may be configured, if desired.
- The cluster must provide an option to support a high performance and reliable shared file system in addition to the Network File System (NFS).
- Support for a high-speed network is required. Although many technical applications work well with 10 Gigabit (Gb) Ethernet, others require larger bandwidth and lower latency. In these latter cases, Fourteen Data Rate (FDR) Infiniband (IB) is supported as an option.

Nonfunctional requirements

In addition to the functional characteristics, the cluster architecture requires the following non-functional characteristics:

- The hardware and software must be deployable by a competent UNIX administrator with cluster deployment experience. There must be an option to deploy the cluster without professional services.
- The head node (also referred to as the management node) of the cluster will be shipped with an installable operating system, management software, and run time libraries so that the entire application cluster can be deployed without requiring users to download additional software components. Whether or not this deployment includes the target application largely depends on the licensing of the application.
- If pre-installing the operating system is not possible due to licensing and legal issues, an easy to follow procedure needs to be developed for targeted users to easily deploy the head node.
- All of the compute nodes are deployed by IBM® Platform™ HPC to ensure that they all have the same software configuration.
- The cluster is high density (i.e. does not require a lot of floor space) and is also optimized for power and cooling.
- An average Linux administrator can operate and maintain the cluster without acquiring specific high performance computing skills.
- The cluster is usable by end users without extensive training, and is no more difficult to use than their own workstation.
- The latest technology is used for the compute servers to ensure either the best performance or best price/performance ratio.
- The Reference systems available worldwide through IBM or a Business Partner.

Architectural overview

Figures 4 and 5 describe the architecture of IBM Application Ready Solution for ANSYS to address the requirements of ANSYS Use Cases 1 and 2 respectively. This document does not address the issues of integration of the cluster within the client's data center, remote access and security. In addition, this document does not address the deployment of the client workstation beyond the specification of client software requirement on the thin client in the case of Use Case 2.

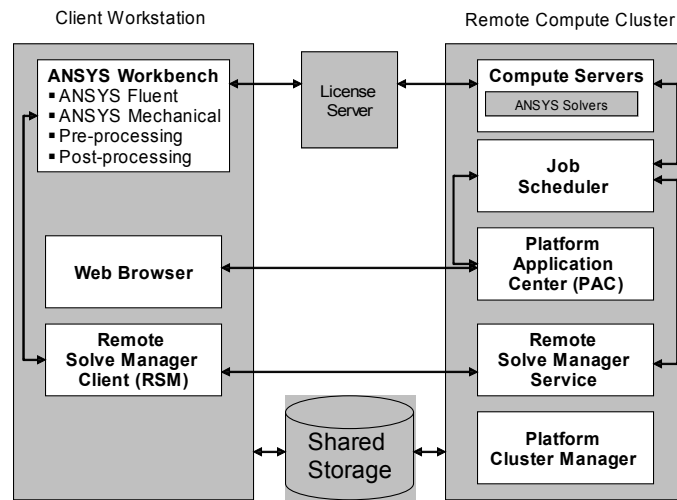


Figure 4: Overview of Architecture to support ANSYS Use Case 1

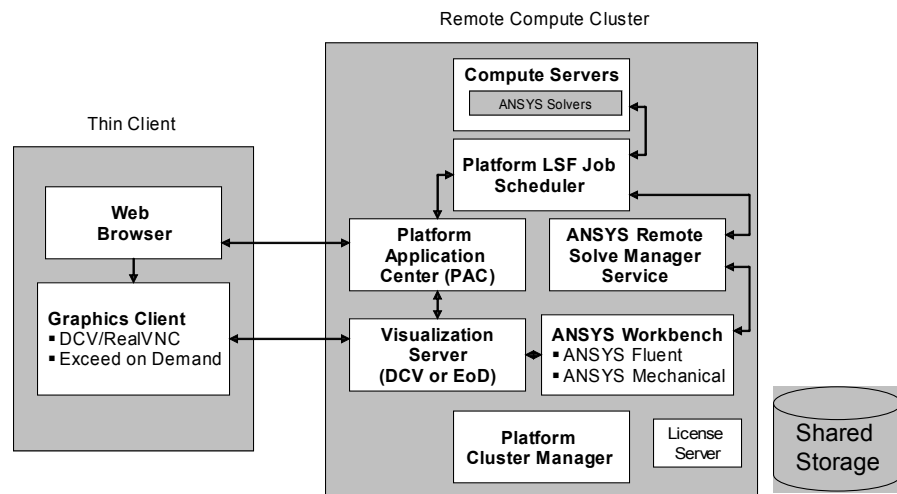


Figure 5: Overview of Architecture to support ANSYS Use Case 2

The two Use Case scenarios are similar, for both ANSYS Fluent and ANSYS Mechanical. However, each of these application areas has slightly different computing, graphics, network, and storage requirements. For example, in the case of ANSYS Mechanical, the memory requirements and data generated for post

processing during simulation can be significantly larger than it is for ANSYS Fluent. This may have some implications on the selection of cluster resources such as network bandwidth, memory size, storage subsystem etc.

Component model

In order to support the Use Cases for ANSYS Fluent and ANSYS Mechanical, the software components described in Figure 6 provide a number of services.

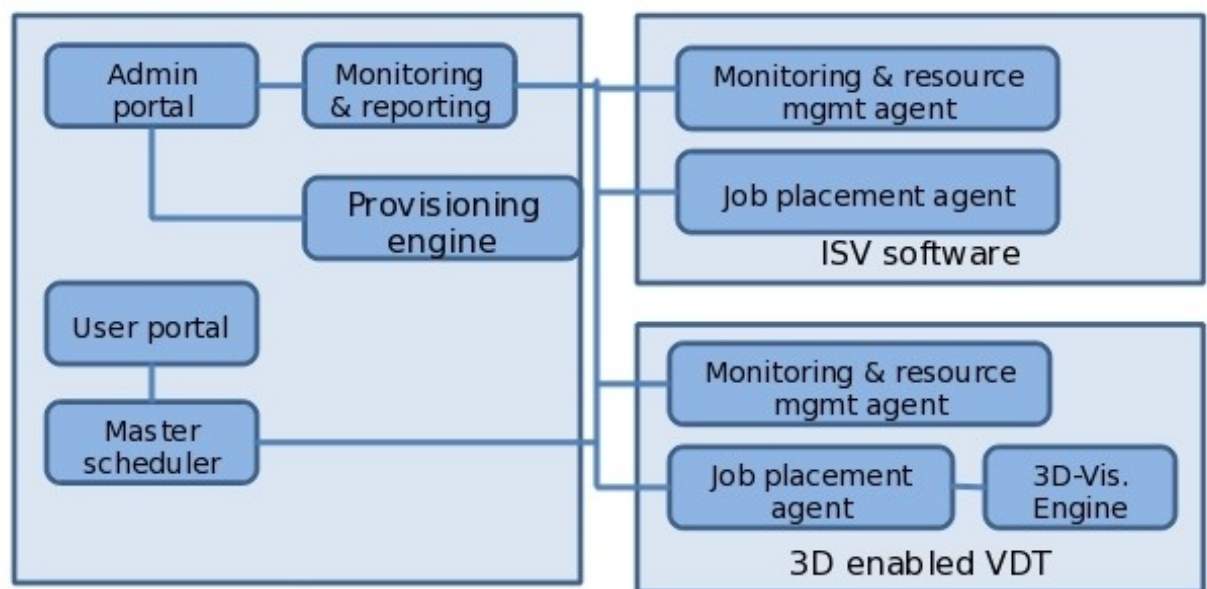


Figure 6: Software Components Diagram

Prior to starting any application software, all of the nodes must be installed with the OS and any application specific software. This function is provided by the provisioning engine. Here the user creates or uses a predefined template that describes the desired characteristics of the compute node software. This provisioning engine listens for boot requests over a selected network and installs the system with the desired operating system and application software. After the installation is complete, the target systems are eligible to execute applications.

Although the compute images are able to run application software, normally access to these images is controlled by the master scheduler. This scheduler function ensures that computational resources on the compute engines are not overused by serializing access to them. The properties of the master scheduler are normally defined at installation. The scheduler may be configured to allocate different workloads to be submitted to a subset of the job placement agents. There is a job placement agent on every operating system image where the master scheduler requests task execution.

The monitoring and resource agent reports back to the provisioning agent and master scheduler the state of the system on every operating system image. This provides a mechanism to provide alerts when there is a problem and to ensure jobs are only scheduled on OS images that are available and have resources.

The administration portal provides an easy to use mechanism to control and monitor the overall cluster, while the user portal provides easy to use access to the system.

Operational model

The software components described in the previous section are implemented on the following hardware components. Each of the components shown is described in detail in the subsequent sections.

Deployment / management node with local storage

The management node functions as a deployment node at the user site and contains all software components required for running the application in the cluster. After the management node is connected to a cluster of nodes it provisions and deploys the compute nodes with client software. The software installed on the management node includes:

- (1) Operating system: Red Hat Enterprise Linux (RHEL) Server
- (2) Operating system repository: RHEL repository for deploying the cluster nodes, including all required device drivers (e.g. OFED for InfiniBand)
- (3) Cluster management and monitoring software: IBM® Platform™ HPC
- (4) Web interface for both cluster administrators and users: IBM® Platform™ Application Center - Standard Edition
- (5) Workload management for scheduling jobs and tasks in the cluster environment: IBM® Platform™ HPC
- (6) Optionally includes an application runtime environment: IBM® Platform™ MPI, packaged in IBM® Platform™ HPC
- (7) Optionally includes an InfiniBand subnet manager if an InfiniBand network is used. The Open Subnet Manager (OpenSM) package can be downloaded directly from the Openfabrics web site (www.openfabrics.org) as the manager. Alternatively, the Unified Fabric Manager (UFM) may be purchased with support from Mellanox (www.mellanox.com). Since the network size is small and there are at most three route hops with dedicated links between any two pairs of nodes, the OpenSM is sufficient for these configurations.

It should be noted that the IBM® Platform™ HPC product provides cluster and workload management functions. References to Platform Cluster Manager Standard Edition may refer either to the stand alone product or to the equivalent function packaged with IBM® Platform™ HPC. References to IBM®

Platform™ LSF may refer to IBM® Platform™ LSF – Standard Edition or equivalent function packaged with IBM® Platform™ HPC , each of which provide the required functionality for this architecture.

After the cluster is deployed, this node provides the following functions:

- (1) Management function, which enables cluster administrators to manage and monitor the entire cluster.
- (2) Master scheduler for workload management
- (3) Web interface enabling users to access the cluster and run their applications which is provided by Platform Application Center (PAC)
- (4) Optional NFS server. If there is no external shared storage for the cluster, the local storage on the management server, including SAS attached disk arrays, provides the shared file system. The management node is configured with enough resources to simultaneously allow file serving and other management functions.

The head or management node is the base of a clustered system using the architecture defined in this document and is supported in both single and high availability (HA) configurations. All of the software is installed on this node and scripts are provided to configure the rest of the system. The script also creates LSF queues to support OpenText Exceed onDemand or RealVNC/DCV, if they have been separately procured. The head node is sized so that it has enough capacity to serve both as a management node, a IB subnet manager and a file server. The head node configurability is limited to ensure that each possible variation has been well tested. Although the DS3524 is the only storage option that is part of this architecture, customer-supplied NFS servers may also be integrated into the cluster. For many use cases, NFS access is sufficiently fast to support the workload. Although it is not part of the architecture, a fiber channel adapter can be added to the head node to attach it directly to a SAN switch on a fiber channel network.

Compute Node

The compute nodes are architected for computationally intensive applications. They are required to satisfy the computational requirements of both Use Cases. They have some local disk for the OS and temporary storage that is used by running applications. The compute nodes also mount NFS for shared storage. These compute nodes can cooperate in solving a single ANSYS Fluent and ANSYS Mechanical problem. This is facilitated by connectivity to a high-speed network. ANSYS Fluent does not require large disk storage on each compute node during simulation. However, very large models in ANSYS Mechanical may not fit in the available memory and need to be solved out-of-core and can benefit from robust local storage.

In addition to the operating system, the application and run time libraries are installed on all compute nodes. The monitoring and resource management agents are connected to the cluster management software and the workload management software is installed.

Visualization node

A Visualization node is required to support the Use Case 2 only. A pool of nodes is designated as visualization nodes which are excluded from the computational work queues. These nodes are equipped with Graphical Processing Units (GPU) which are officially supported by ANSYS. Each visualization node is equipped with two GPUS. Each GPU can support two simultaneous interactive login sessions. A single visualization node can support four simultaneous interactive sessions. Platform LSF keeps track of the allocation of these interactive sessions. When a user requests an interactive login session through the Platform Application Center web portal, a free session is allocated to the user. Through remote visualization, the rendering of a graphics application is done on the graphics adapter. The rendered graphics are compressed and transferred to the thin client. Two remote visualization software engines are supported on the visualization node. These are Nice Desktop Cloud Visualization (DCV) produced by Nice Corporation and OpenText Exceed onDemand (EOD) produced by OpenText Corporation.

When an interactive session is allocated, it is associated with one of these two visualization products and PAC downloads session related information associated with the visualization software to the client workstation requesting the session. The client component of the visualization software, which resides on the client workstation uses this session information and connects with the visualization node on which Platform LSF had allocated the session. The client part of the visualization prompts the user for credentials for authentication and if the login is successful, the interactive session is established to launch graphic oriented applications such as ANSYS Workbench. ANSYS Workbench provides a uniform user interface on both Windows and LINUX. For users who simply want to use ANSYS Workbench and do not have to deal with the underlying platform the ANSYS Workbench is automatically launched. For users who need direct access to the underlying platform, a desktop is provided.

As in the case of compute nodes, in addition to the operating system, the application and run time libraries are installed on all visualization nodes. The monitoring and resource management agents are connected to the cluster management software and the workload management software is installed.

The visualization nodes have some local disk for the OS and temporary storage which can be used by running applications. The visualization nodes also mount NFS systems for shared storage.

Network connections

Networks are used to accomplish several functions in the cluster. Each of these functions may have a dedicated network or share a common network with others.

- (1) Management network: This is the network connected to CMM (chassis management module) on each [IBM Flex System](#)™ node. This network allows the management software to manage and monitor the hardware without the operating system on a 1 Gigabit Ethernet interconnect. Typical hardware-level management includes power cycling the node, hardware status monitoring, firmware configuration, hardware console access, etc.
- (2) Provisioning network: This is the network that is used for provisioning the operating system and deploying software components and applications. This network is also used for monitoring and workload management and may either use a 1 or 10 Gigabit Ethernet interconnect.

- (3) Application network: This network is mainly used by applications, particularly communications among different tasks within an ANSYS application across multiple nodes. This network is often used as a data path for applications to access the shared storage. The application network uses a high speed interconnect such as 10 Gigabit Ethernet and FDR InfiniBand.

The above networks may be combined into a single physical network to minimize the network cost and cabling in some configurations.

A typical deployment would be:

- Combined management network and provisioning network, plus a dedicated high speed interconnect for applications. This is often the case if the high speed interconnect is InfiniBand.
- Combined provisioning network and application network by using 10 Gigabit Ethernet, plus a dedicated management network. This network architecture can be implemented when management work has a dedicated switch on the chassis.

Storage and file system

A shared file system is considered as optional and if configured, is used by ANSYS application suite for long-term storage of engineering models. The storage is connected to the management node which acts as a file server. Data is transferred between the file server and the client nodes using a 10 Gigabit Ethernet.

If an already existing shared storage at the customer site is used, the customer file server is connected with the nodes specified in this architecture using a 10 Gigabit Ethernet.

Configuration

The components that comprise of configurations that support ANSYS Fluent and ANSYS structural mechanics are outlined as follows. Several recommended configurations and sizing guidelines which use these components for ANSYS Fluent and ANSYS structural mechanics are described in the Application Considerations section.

Table 1 lists the features included in this architecture and their applicability to ANSYS Fluent and ANSYS structural mechanics. Sample configurations are provided in the Applications Considerations section. These specifications can be customized for individual situations.

Cluster Component	ANSYS Fluent	ANSYS Mechanical
Head Node	Required	Required
Visualization Node/ Visualization Software	Depends on Customer Requirements	Depends on Customer Requirements
Compute Node	Required	Required

High Speed Network (Infiniband)	For small networks optional For large networks required	For small networks optional For large networks required
File System	Optional	Optional
Job Scheduler	Required	Required
Cluster Management	Required	Required
Frames/Chassis	Required	Required

Table 1: Cluster Components for ANSYS Fluent and ANSYS Mechanical workloads

An application-specific guideline will translate workload requirements into number of cores, memory. These rules are given to help choose the optional features needed for specific application clusters. Although a feature may be optional as part of the overall architecture, application requirements for specific use cases may dictate the inclusion of that feature. For example,

- The use of MPI merits the inclusion of an InfiniBand network in the case of large networks.
- If InfiniBand is not used, unless the file system usage is very light, a 10GigE network should be configured.
- If network storage is not provided by a server outside of the cluster, include the DS3524 storage controller
- In cases where there is a requirement for fast scratch, use the System x3550 M4 as a compute node.

Compute Node

ANSYS Fluent

The compute node is a Flex System x240 ITE. For the non-parallel scale out case, where access to shared storage is less important than access to fast local disk, this node may be the best option.

The compute node processor is an Intel Xeon E5-2670 processor in the default configurations, which has eight cores per socket in a two socket configuration. A node in each of these configurations is configured with 32 GB of memory using 8 GB DIMMs, which also provides a very good price/upgrade path. This works out at 2 GB per core, which is adequate for most ANSYS Fluent applications.

ANSYS Mechanical

The compute node is x3550 M4 server. The compute node processor is an Intel Xeon E5-2670 processor in the default configurations, which has eight cores per socket in a two socket configuration. A node in each of these configurations is configured with 64 GB of memory using 8 GB DIMMs, which also provides a very good price/upgrade path. For ANSYS mechanical, it is important to have robust local storage for scratch space since very large problems are solved out-of-core due to insufficient memory.

If the model is solved out-of-core due to insufficient memory resulting from cost/configuration restrictions, consider:



- Adding 2 to 4 500GB SSD disks with RAID0 level to each node, or
- Adding 8 15K RPM 300GB SAS disks with RAID0 level to each node

For better performance, use a local file system for I/O during the solver phase.

Visualization Node

The visualization node is the dx360 M4. The visualization node processor is an Intel Xeon E5-2670 processor in the default configurations, which has eight cores per socket in a two socket configuration. Since, the pre/post processing applications require large amounts of memory, 256GB memory is recommended. If the customer requirements exceed the 256GB memory larger memory of memory can be configured in the dx360 M4 node. It should be noted that 256GB is the maximum memory at the maximum rated speed of 1600 MHz; 512GB is the maximum which can operate at the speed of 1333 MHz; and 768GB in the maximum which can operate at 1066MHz.

Since the graphics rendering is done on the Visualization node, each node is equipped with 2 GPUs. Each GPU can support 2 simultaneous interactive sessions. Each visualization node can accommodate 4 simultaneous interactive sessions. The pre/post processing applications in ANSYS are mostly serial and hence the processor resources in the node should be sufficient to handle their computation requirements. The GPUs recommended in this architecture are NVIDIA Quadro 5000.

Remote 3D Visualization

Two software products are supported for remote 3D visualization for ANSYS. These are Nice Desktop Cloud Visualization (DCV) and OpenText Exceed onDemand (EOD).

The following versions of these two products are recommended in this architecture:

Visualization Software	Version Supported
NICE DCV	Version 2012.2-7878
Exceed onDemand	Version 8

File System

The file system is optional in this architecture. The IBM System Storage DS3524 provides the best value, More than 100 TB of disk may be configured when using the expansion frames. An NFS configuration may be chosen with this storage option. In the NFS configuration, redundancy is optional.

Network

The network is used to transfer data between the application and file system and also for inter-process communication during the simulation. Application requirements in each of these situations will determine whether there needs to be a separate high speed compute network. The 10 GigE network is sufficient for

network data access for the smaller cluster sizes proposed in this architecture. During the simulation, if each job can run within a single node, then a high-speed interconnect such as Infiniband is not required. Serial jobs and parallel jobs which require less than the number of cores available in a single node fit into this category. In the case of ANSYS Mechanical, even small clusters can benefit from a high-speed network. In the case of simulations which require a large number of nodes, for example in ANSYS Fluent, there is a requirement for a low latency network. In these cases, the network of choice is FDR InfiniBand.

Software

The software choice is dictated by the application requirements. The IBM Platform Cluster Manager Standard Edition software is required in all cases either as a stand alone product or as part of IBM Platform HPC. This, as described elsewhere, supports installation and management of the cluster. Platform HPC is required in all cases where MPI is used.

Deployment model

After it is deployed and functioning, the cluster operates as a single system. System administrators use the Platform Cluster Manager Standard Edition web-based interface (see Figure 7) as the management console for performing daily management and monitoring of the cluster. This eliminates the need for a full time system administrator with extensive technical or HPC expertise for managing the cluster. However, a part time Linux administrator or end user with Linux administration experience is expected to have the skills to ensure the cluster remains operational.

The console dashboard provides status on:

- (1) Cluster health
- (2) Application license usage
- (3) Jobs
- (4) Hardware status
- (5) Alerts

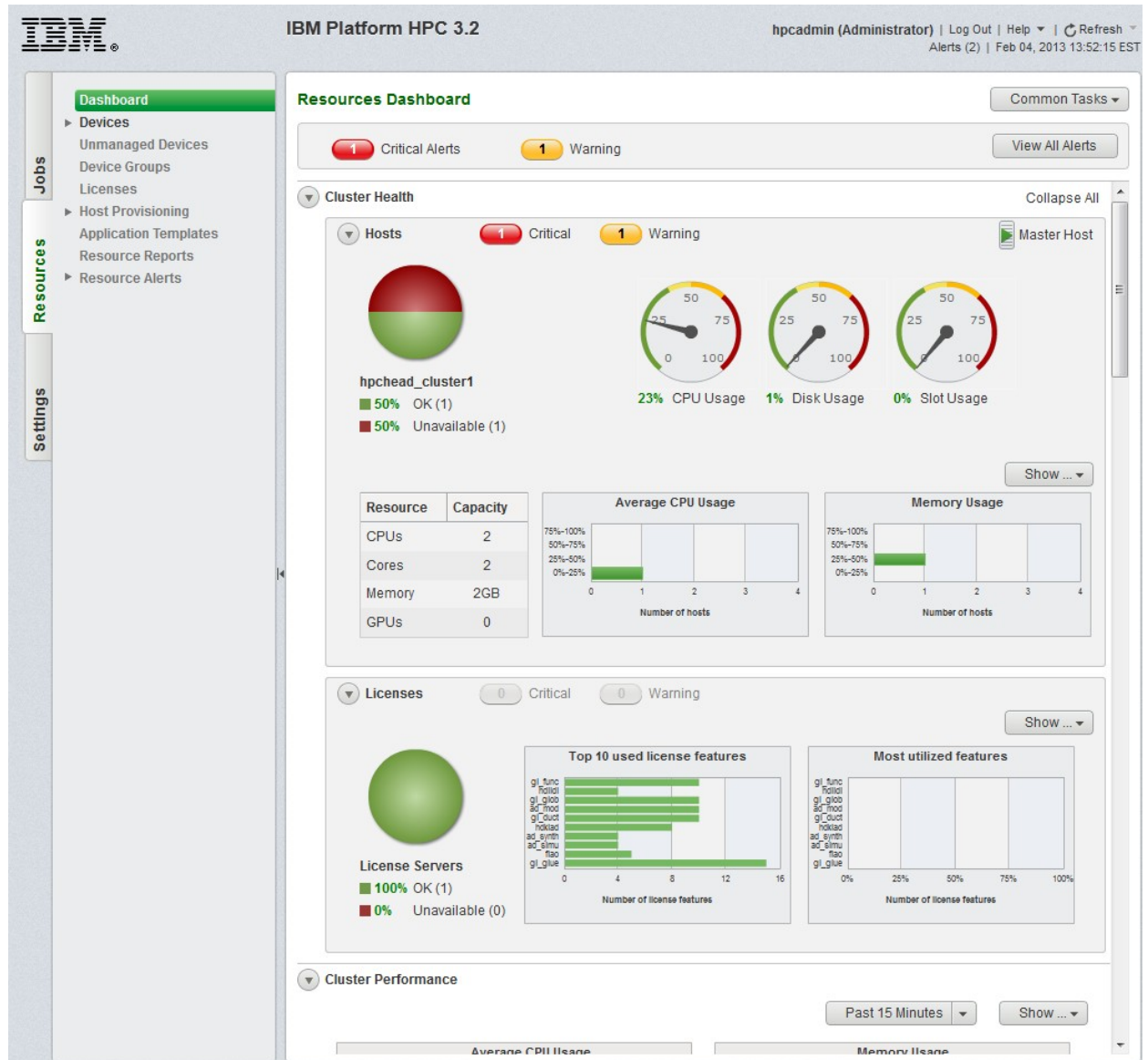


Figure 7: Cluster management dashboard

Users have the following options for accessing the cluster:

- (1) *Using the application front-end that is integrated with Platform LSF or Platform HPC.* To users, a cluster is transparent. In other words, users experience performance improvements without the need to deal with a complex cluster environment. ANSYS provides several methods to submit jobs to the cluster:
 - a. ANSYS Fluent can be used to submit jobs to the backend LSF cluster
 - b. ANSYS Workbench and ANSYS Remote Simulation Manager (RSM) can be used to submit ANSYS Fluent and ANSYS Mechanical jobs to the backend cluster

If Graphical User Interface (GUI) based tools such as ANSYS Workbench are used, they can either reside on the user workstation which has graphics capabilities or on the cluster itself if remote visualization facilities are provided.

- (2) *Using the Web Interface on the cluster for submitting and managing jobs, as well as using the interface to manage application data.* As Figure 8 illustrates, users can easily manage jobs and job related files through the user interface.

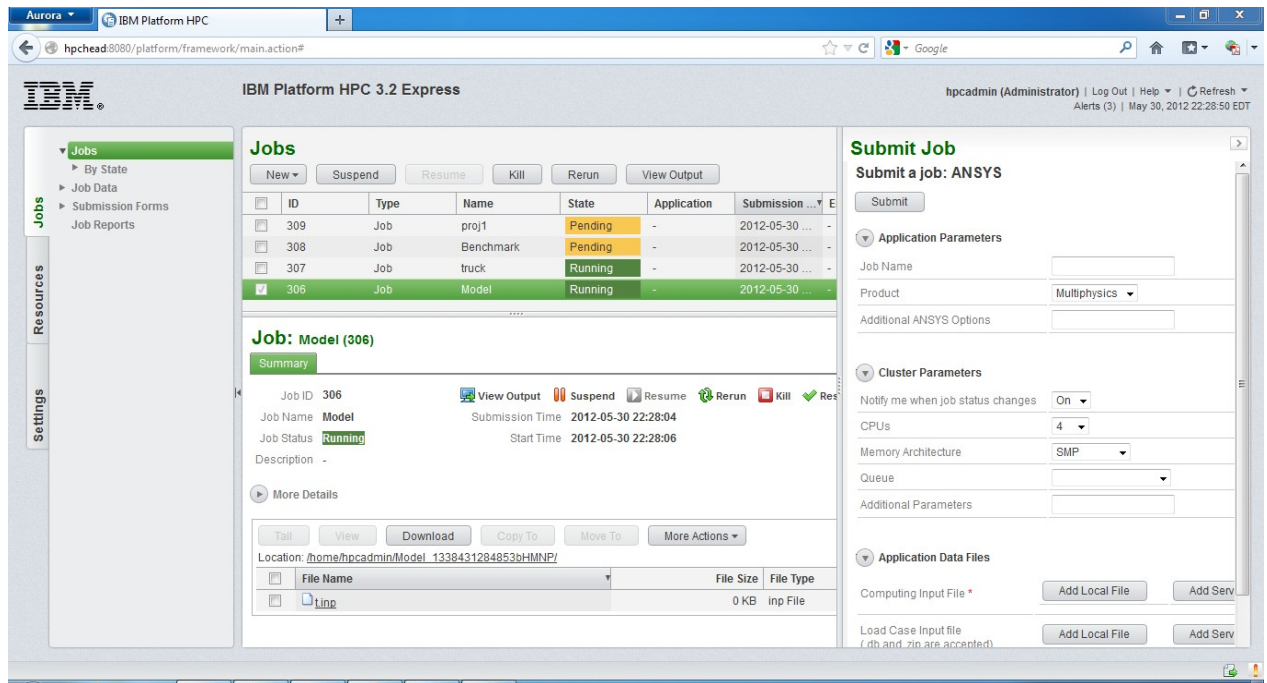


Figure 8: User job submission and management interface

- (3) *Remote visualization.* After a user has been allocated a virtual desktop, the user interacts with an application specific graphics intensive modeling tool such as ANSYS Workbench running on the cluster. Remote visualization is enabled by intercepting GL calls, rendering them on the server machine and sending the rendered output to the client using the X protocol. This is supported by either a combination of Exceed onDemand, or RealVNC and Nice DCV, where a vnc viewer for local display is provided by all options. The configuration script provided will support any of these options. The DCV support for 3D rendering is more tightly integrated into the viewer. Both the DCV and Exceed onDemand support network security and have similar functionality. In both cases, the appropriate optimized graphics device driver is installed on the cluster.

Deployment considerations

Because the architecture is optimized for a specific application, and most software deployments are fully automated, a cluster can be deployed in a day or two. Users are able to take advantage of the performance and capability that the cluster delivers with minimal training.

Platform deployment

The management node comes with a bootable software medium that allows one step installation of all the software from the bare metal at the customer site. After the management node is up and running, it can be connected to the corporate network with a number of simple steps:

- (1) Change the host name and IP address
- (2) Set up users by using either local users or connecting to corporate user account management systems like LDAP, NIS, etc.
- (3) Connect to external shared storage or use the script provided as part of the solution to configure the cluster storage

Applications should be installed to the repository on the management node as part of the management node installation.

Device drivers are also deployed as part of the cluster deployment. Examples are OFED for InfiniBand, VNC server and DCV or Exceed onDemand for 3D visualization.

After the management node is fully connected and running, the administrator can go to the management interface to deploy the entire cluster. The auto discovery feature supports a single step cluster deployment with a fully automated deployment process.

The IBM Platform Cluster Manager supports what are called kits which provide a framework that allow third party packages to be configured with the system. IBM Platform Cluster Manager ships a kit for Nagios, a popular tool for monitoring the system including the file system.

Application Deployment

All applications are deployed together with the operating system to all compute nodes. The application is ready to use with one more step after the cluster is deployed: enabling the application licenses. Enabling the application licenses typically involves installing the license management tool manually on the management node and applying the license file.

Installation of ANSYS Application Suite and ANSYS License Server

The installation of ANSYS software is a very simple process. ANSYS provides a simplified installation of FlexLM license management. Instead of directly installing FLM, users are advised to download the license management software from ANSYS and install the license server using ANSYS license management software. For detailed instructions about installation of ANSYS application suite, please refer to *ANSYS Installation and Licensing Documentation*, 2012. The installation ANSYS software should be performed on all compute nodes.

Before ANSYS software is launched on client nodes, the following environment variables need to be set in the user environment:

- ANSYSLMD_LICENSE_FILE
- ANSYSLI_SERVERS

These variables can be part of user environment or embedded into Platform Application Center's (PAC) ANSYS templates. If this information is embedded in the ANSYS template in PAC, it is important that when changes are made to the installation of the ANSYS application suite those changes are propagated to ANSYS application templates in PAC.

PAC Templates

The primary interface to the ANSYS Fluent and ANSYS Mechanical is Platform Application Center (PAC). In PAC, this interface is provided through the Application Templates.

Use Case 1:

Use Case 1 requires a facility to submit a batch job to the cluster by providing input datasets which are located either locally on their workstation or the cluster itself. In order to address the requirements of Use Case 1, the following two application templates are provided in PAC:

- ANSYS-Fluent
- ANSYS-Mechanical

Each of these templates has the following information embedded in them by the system administrator so that it will be transparent to the user where these resources are located on the cluster:

- PATH to the application executable
- License server information

When a new version of ANSYS application is installed, the ANSYS application in PAC should be updated either automatically or by the system administrator.

ANSYS Fluent

When the users click on the ANSYS-Fluent template, a Web based form is presented requesting the following information:

Application Parameters

Job Name: MYFLuent

Version: 3d

Console Support*: Yes

Additional FLUENT Options: -g -pinfiniband -ssh

Cluster Parameters

Queue: normal

Memory Architecture: DMP

CPUs: 4

MPI Type: pcmpi

Additional Parameters:

Application Data Files

FLUENT Journal File *	Add Local File	Add Server File		
	in.tu...k.jou	Server	/gpfs/gpfs2/home/har...s/fluent/	142B Remove
CAS Input File (.cas .dat)	Add Local File	Add Server File		
	turbo_500k.cas	Server	/gpfs/gpfs2/home/har...s/fluent/	46MB Remove

Figure 9A: PAC Template for ANSYS Fluent

The input datasets can either be located locally on the workstation or on the server.

Once the users provide the information and press the submit button, PAC constructs an LSF command which includes all the information needed and submits the ANSYS Fluent job to LSF. Optionally, for each job a temporary working directory is created. If the datasets are on the workstation, they are transferred to a working directory on the cluster and all the output that is generated, if any, is stored in the same directory. The users can retrieve the information and delete that directory. The progress of these jobs can be monitored by pressing the jobs tab on the left side of the screen.

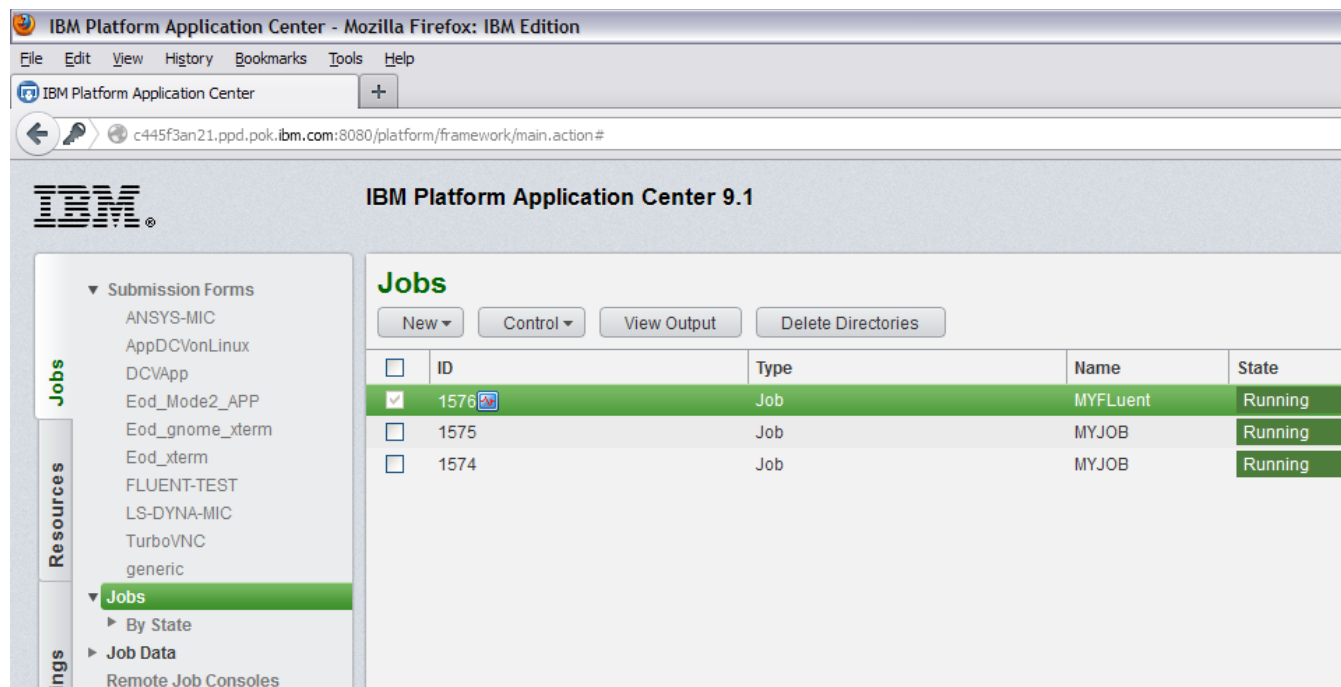


Figure 9B: LSF job queue showing the ANSYS Fluent job waiting for resources

ANSYS Mechanical

The process of launching ANSYS Mechanical is similar to that of ANSYS Fluent. Special consideration should be given to the amount of data that is generated for post processing while offloading ANSYS Mechanical jobs to the cluster from a remote workstation. These datasets can be very large making it infeasible to transfer them over slow networks. For these use cases the options are either remote visualization or high-speed connectivity to the user workstation.

Use Case 2:

The Use Case 2 requires an interactive session where the users can launch applications which use OpenGL based graphics. Two visualization engines are supported in this architecture. These are Desktop Cloud Visualization (DCV) and Exceed onDemand (EOD). PAC templates for DCV and EOD are created to allow the users to submit a request for a visualization session.

ANSYS-DCV

When the user clicks on ANSYS-DCV template from the list under job submission forms, the following form is presented (Figure 9A). The command to launch ANSYS Workbench command is embedded into this form so that users do not have to remember the platform or application installation specific details. For power users, who are familiar with the specific OS platform and require command line facilities, a generic DCV template is provided to open an xterm window to perform those operations. Providing a desktop facility allows the users to manage their datasets locally on the cluster.

IBM Platform Application Center 9.1

Submit a job: AppDCVonLinux

Submit

Save As

Delete

Session Parameters

Note: DCV and RealVNC VE server software must be installed on all LSF server hosts. RealVNC client must be installed on your browser host (the host you are using to access PAC). The purpose of this form is to submit a job on linux that can be managed through PAC.

Job Name

MYJOB

Application Command *

/home/hari/run.cmd1

Display Resolution

1024x768

Queue

dcv

Submit

Revert

Figure 9A: DCV Template to request a visualization session

IBM Platform Application Center 9.1

Rerun

Kill

Resubmit

Job ID

1614

Job Name

MYJOB

Job Status

Pending

Pending Reasons

New job is waiting for scheduling;

More Details

Figure 9B: Job status showing that job is waiting for the interactive session

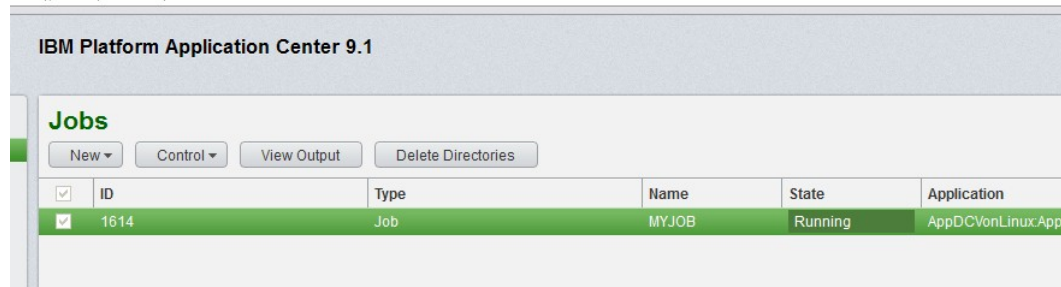


Figure 9C: LSF job queue showing an interactive session is allocated to the job

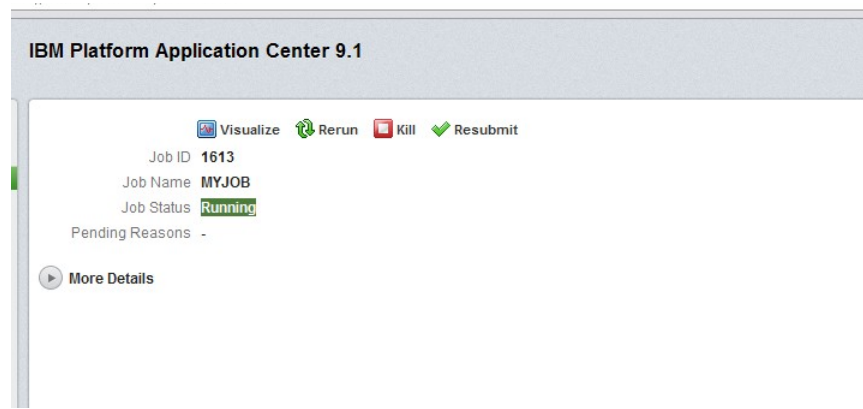


Figure 9D: Clicking on "Visualize" activates the interactive session

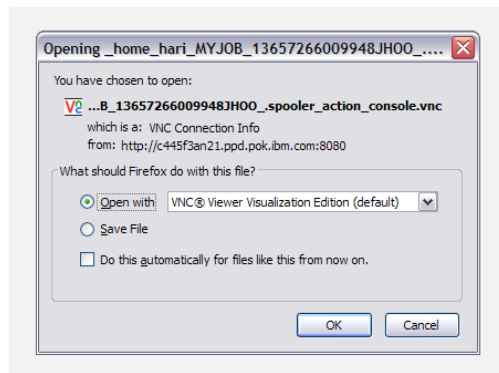


Figure 9E: Session downloads session information and performs user authentication

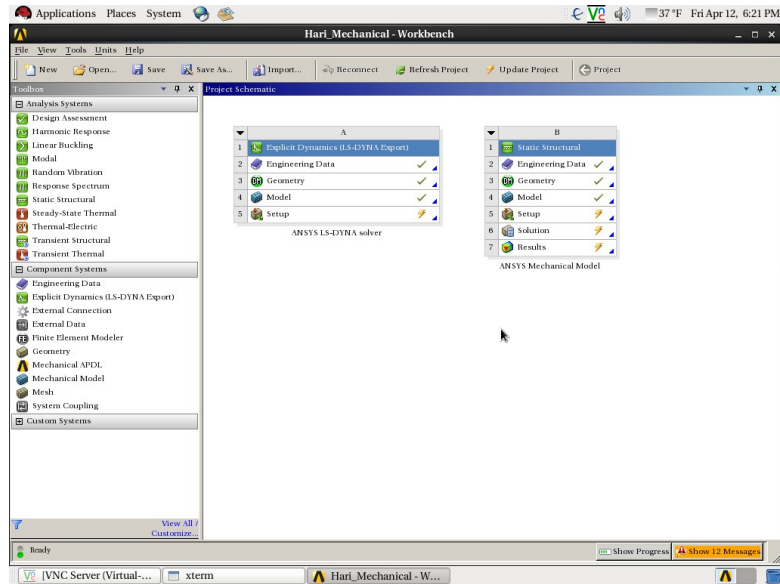


Figure 9F: PAC automatically launches the ANSYS Workbench

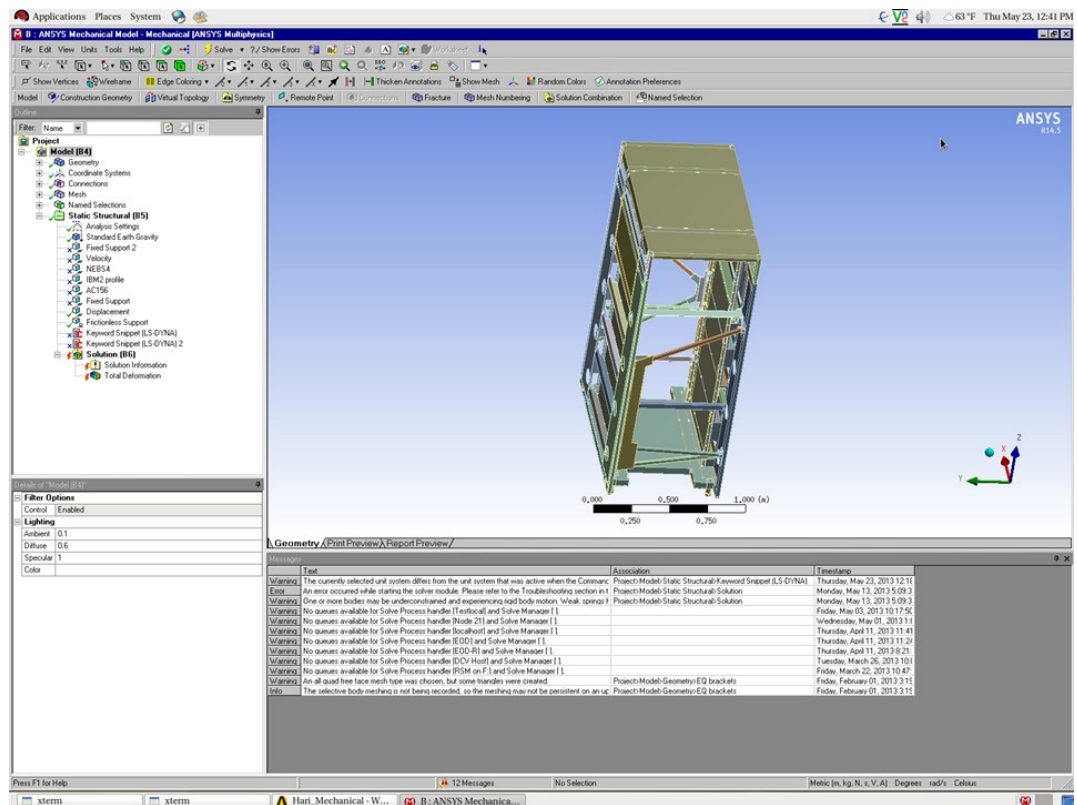


Figure 9G: User interacts with ANSYS Fluent and ANSYS Mechanical through Workbench

Once the user submits the form, PAC requests LSF to allocate an interactive session to use DCV. Initially, the job is assigned status "PENDING" if a free interactive session is not available (Figure 9B). The progress of these requests can be monitored by pressing jobs tab on the left side of the screen (Figure 9C). When the interactive session is allocated, a new status icon "Visualize" appears (Figure 9D). When the user clicks on this button, session information is downloaded to the workstation and the user is prompted to start up a real-VNC session and provide credentials for authentication (Figure 9E). Once the user session is authenticated, PAC starts up ANSYS Workbench (Figure 9F). From that point, ANSYS users can work with ANSYS Fluent and ANSYS Mechanical (Figure 9G). Since both ANSYS Fluent and ANSYS Mechanical use OpenGL calls for graphics, DCV intercepts these calls and performs rendering operations on the server and compresses the bit maps and transfers to the real-VNC client on the user workstation. If the session disconnects, PAC does not terminate the session. The session can be reconnected starting from the step in Figure 9C by selecting the job in progress and clicking on the "Visualize" button and the user will be reconnected to the application in progress.

Once the user completes the graphics operations manipulating the 3D models, the next step is to submit the solver jobs in batch mode to LSF to be scheduled on the back-end cluster. There are two ways this can be accomplished:

- ANSYS Workbench uses a tool called Remote Simulation Manager (RSM) through which ANSYS Fluent and ANSYS Mechanical jobs can be submitted to an LSF cluster
- Alternatively, once the input datasets are prepared, the two Application templates, ANSYS Fluent and ANSYS Mechanical described under Use Case 1 can be used to submit the batch jobs outside ANSYS Workbench.

ANSYS-EOD

The process of submitting a request for interactive session which uses Exceed onDemand for remote visualization is similar to that of DCV.

Storage Integration

If there is an external storage system that contains data required by the application, there are two supported access methods:

- (1) *Connect the storage to the cluster private network (i.e. the application network).* This method allows applications running on compute nodes to access the storage and should be the only option if application requires constant change to the files and the application performance is heavily dependent on the performance of accessing those files. If the data is stored in a database, this option should also be used.
- (2) *Connect the storage to the management node.* Every time a job requires access to certain files, these files need to be explicitly named during the job submission time. These required files are copied automatically to the compute nodes as part of the job scheduling process before the job

starts. This is a viable option if the file size is small (< 100MB) and the data is not stored in a database. Similarly, the output files the job creates can be automatically transferred back to the management node after the job is completed.

ANSYS Application considerations

Scaling up high-performance computing resources allows engineering teams to dramatically increase the value of engineering simulation, enabling more detailed and accurate simulations and more design exploration within the time constraints of project deadlines. Choosing the right HPC resources, however, requires an understanding of how key technologies determine application performance. In this section, guidelines to size cluster resource that satisfies ANSYS Fluent and ANSYS structural mechanics are described. In addition, three sample configurations for ANSYS Fluent, two for ANSYS structural mechanics and one for mixed ANSYS Fluent and ANSYS structural mechanics workloads are provided. These are available through the IBM fulfillment process and can be used as a starting point and adjusted, if necessary, to further accommodate individual customer requirements.

ANSYS Fluent

In ANSYS Fluent, the problem size is measured in the number of cells. ANSYS Fluent scales very well into large number of cores even for a small problem of a few hundred thousand cells. For example, recent benchmark results indicate that the solvers in ANSYS Fluent are capable of delivering efficient scalability even when per core allocation is as low as 10,000 cells. As illustrated in the following Table, for a given problem size, this allows users to choose from a wide range of hardware configurations to fit their budget and productivity requirements.

System Sizing Guidelines For ANSYS CFD Applications (medium size models)			
	Extreme Performance	Balanced	Extreme Price Sensitive
Cells/core	10,000	150,000	250,000
Average model size	14M cells	14M cells	14M cells
Cores/job	1400	94	56
Memory per job	21 GB	21 GB	21 GB
Node configuration	E5-26XX 2P 8C32GB	E5-26XX 2P 8C32GB	E5-26XX 2P 32GB
Number of nodes/job	88	6	4
Simultaneous jobs	3	3	3
Total number of nodes	264	18	12
Network Config (2:1 blocking where applicable)	FDR Infiniband	FDR Infiniband	10 GbE

For high-end clusters, total cost rises linearly with the size of the cluster. Low-end clusters may not satisfy productivity requirements. For a given problem size, the optimal number of nodes in the cluster typically

falls in the middle of the performance/price spectrum. The choices within this narrow range should be evaluated closely (using ROI analysis) to determine optimal cluster size.

As an example, loading around 150K cells per core seems like a reasonable compromise in calculating the cluster size. Using this guideline, the size of the cluster is computed as follows:

Number of cores required to run a single ANSYS Fluent simulation = Size of the problem (in million cells) / Recommended loading of each core

Number of nodes required for each job = Number of cores required to run ANSYS Fluent / Maximum Number of cores in a Node

The number of nodes is rounded up to the nearest integer value.

Total Number of nodes required = Number of nodes required for each job * Average number of simultaneous jobs in the system

An illustration:

Recommended loading per core =	150,000 cells
Average size of ANSYS Fluent simulation:	4 million cells
Maximum number of cores in a node:	16
Average number of simultaneous jobs in the system:	7
Number of cores required to run a single ANSYS Fluent simulation =	$4,000,000 / 150,000 = 27$ cores
Number of nodes required for each job =	$27 / 16 = 1.68 = 2$ (rounded)
Total Number of nodes required =	$2 * 7 = 14$

Number of PureFlex chassis:	1
Number of 25U Racks:	1
High-speed network:	Infiniband
Leaf switch:	1
Spine switch:	none

ANSYS Fluent is a very highly scalable application. Depending on the ANSYS Fluent model size, a large number of compute cores can be used to realize productivity gains with high levels of efficiency. For example, in the tests conducted on cluster of 14 PureFlex System nodes using truck_14m, an ANSYS Fluent standard benchmark model, a near linear speed-up of 13.75 was observed. This translates into a simulation which takes over two days to complete on a workstation can be done in about 4 hours.

ANSYS Mechanical

The solvers used in ANSYS are both computationally intensive and also use a large amount of memory. Sparse solver in ANSYS is the default solver for virtually all analyses. The memory requirements vary significantly depending on whether input matrices are symmetric (most matrices created in ANSYS Mechanical are symmetric) or non-symmetric. Symmetric matrices require approximately 10 GB of memory for 1 million degrees of freedom (DOF). In the case of non-symmetric matrices, the memory consumption could be approximately 15 to 20 GB. Also, ANSYS Mechanical solvers do not tend to scale to much larger than 96 cores. If there is sufficient memory on the system where solver is running, then the problem can be solved in-core. Otherwise, the problem is solved in out-of-core mode because the

intermediate results need to be written to the disk and read back throughout the solution phase. In a single compute node, the maximum memory to operate at the rated speed of 1600 MHz is 256 GB. If the problem is too large to solve in-core then there are two options.

1. The solver can run on a cluster of nodes, there by increasing the available physical memory so that problem can be solved in-core.
2. If the problem is solved out-of-core, a robust local storage system is recommended. We recommend an array of 8 fast 15K RPM SSA 300 GB drives with RAID0 on each of the compute nodes where the ANSYS Mechanical solvers are run.

Significant productivity gains can be realized using multiple cores to solve ANSYS Mechanical simulations. For example, in the tests conducted on a cluster of 6 nodes using V14cg-1, an ANSYS Mechanical standard benchmark model, a speed-up of 5 was observed. This translates into a simulation which takes over two days to complete on a workstation can be done overnight in about 10 hours.

Sample Configurations

In order to simplify the equipment procurement, several representative cluster sizes for ANSYS Fluent and ANSYS Mechanical are defined and entered into the IBM procurement system. Each of these configurations includes all the components required for a successful implementation of a specific ANSYS application or mix of applications. IBM technical sales representatives and business partners are encouraged to start with one of these that closely satisfy the customer's requirements. Adjustments such as adding/deleting nodes, adding memory, etc. to these configurations can be made if the customer requirements dictate deviation from these configurations. The following configurations are recommended to implement the ANSYS application suite. Please see the [Configurator](#) Guide in the Resources Chapter.

Application	Configuration			
	Small	Medium	Large	Mixed
ANSYS Fluent	6 nodes	10 nodes	14 nodes	
ANSYS Mechanical		8 nodes	16 nodes	
ANSYS Fluent and ANSYS Mechanical				16 nodes (Fluent) 6 nodes (Mechanical)

The details of each of these configurations are described in the following tables/figures.

IBM Configurations to implement ANSYS Fluent			
	Small	Medium	Large
Compute Server	6	10	14
Management Node	1	1	1
Visualization Node*		1	1
Network	10GbE; GbE	FDR IB, 10GbE, GbE	FDR IB, 10GbE, GbE
Total number of compute Cores	96	160	224
Total Memory (GB)	192	320	448
		1	1
File System (Optional)	DS3524	DS3524	DS3524
Packaging - PureFlex Chassis	1	1	1
25U Rack	1	1	1
Software	LSF and PAC	LSF and PAC	LSF and PAC
	Platform HPC	Platform HPC	Platform HPC
Example Usage Scenarios			
Largest Single Job (million cells)	15+ million cells using all 96	25+ million cells using all 160 cores	35+ million cells using all 224 cores
Approx. Number of simultaneous jobs; each job size = 5 million cells	3	5	7
Approx Number of simultaneous jobs; each job size = 2.5 million cells	6	10	14

* Visualization Node can serve as a back-up to Management Node

Table 2: IBM Application Ready Configurations to implement ANSYS Fluent

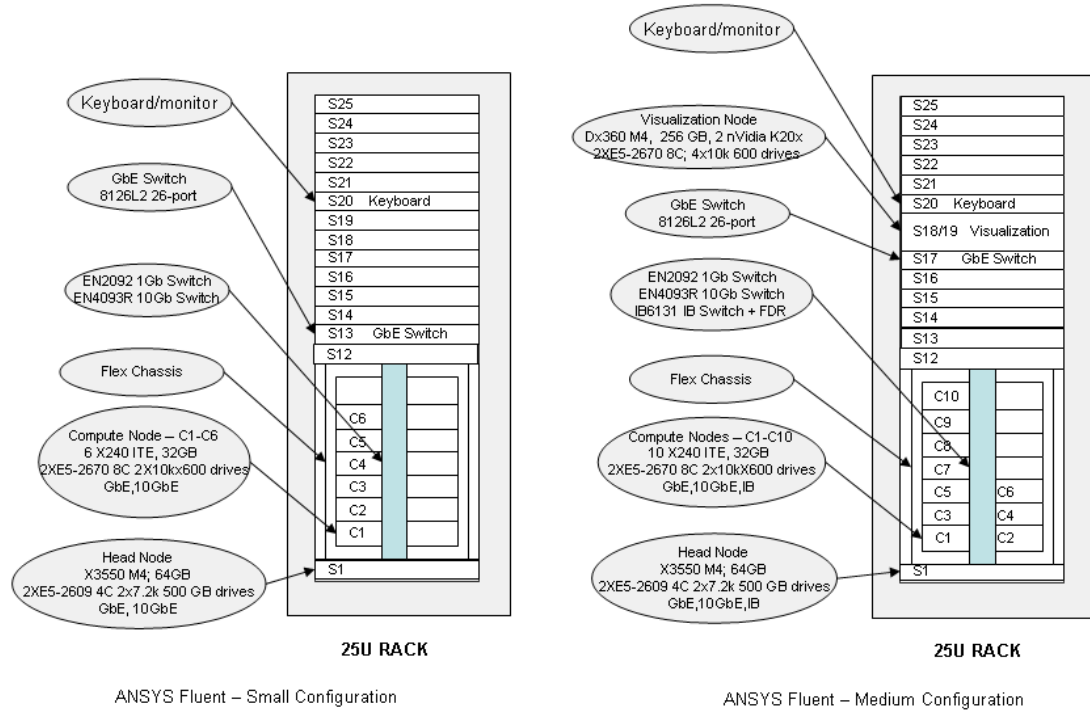


Figure 10A: Deployment diagram for ANSYS Fluent - Small and Medium configurations

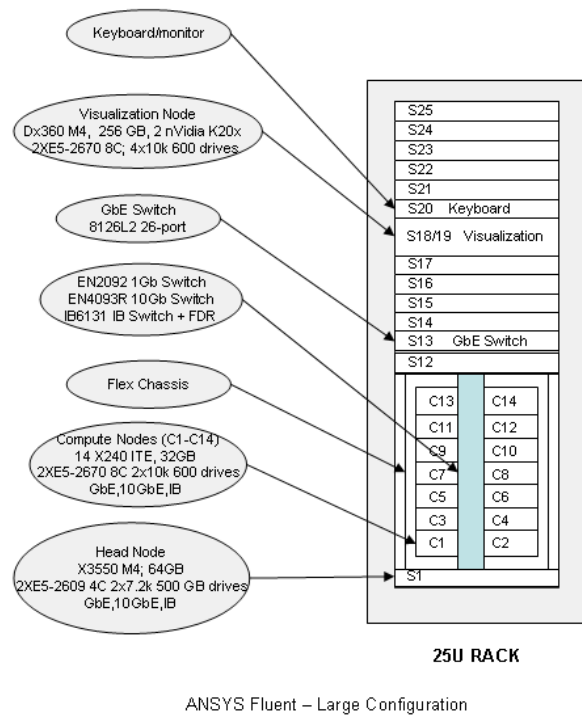


Figure 10B: Deployment diagram for ANSYS Fluent - Large configuration

IBM Configurations to implement ANSYS Mechanical		
	Medium	Large
Compute Server	8	16
Management Node	1	1
Visualization Node*	1	1
Network	10GbE; GbE;	FDR IB, 10GbE, GbE
Total number of compute Cores	128	224
Total Memory (GB)	512	1024
File System (Optional)	DS3524	DS3524
Packaging - 25U Rack	1	1
Software	LSF and PAC	LSF and PAC
	Platform HPC	Platform HPC
Example Usage Scenarios		
Approx. Number of simultaneous jobs; each job size = 5 to 10 Million DOF	3	8
Approx Number of simultaneous jobs; each job size = 2 to 5 million DOFs	8	16

* Visualization Node can serve as a back-up to Management Node

Table 3: IBM Application Ready Configurations to implement ANSYS Mechanical

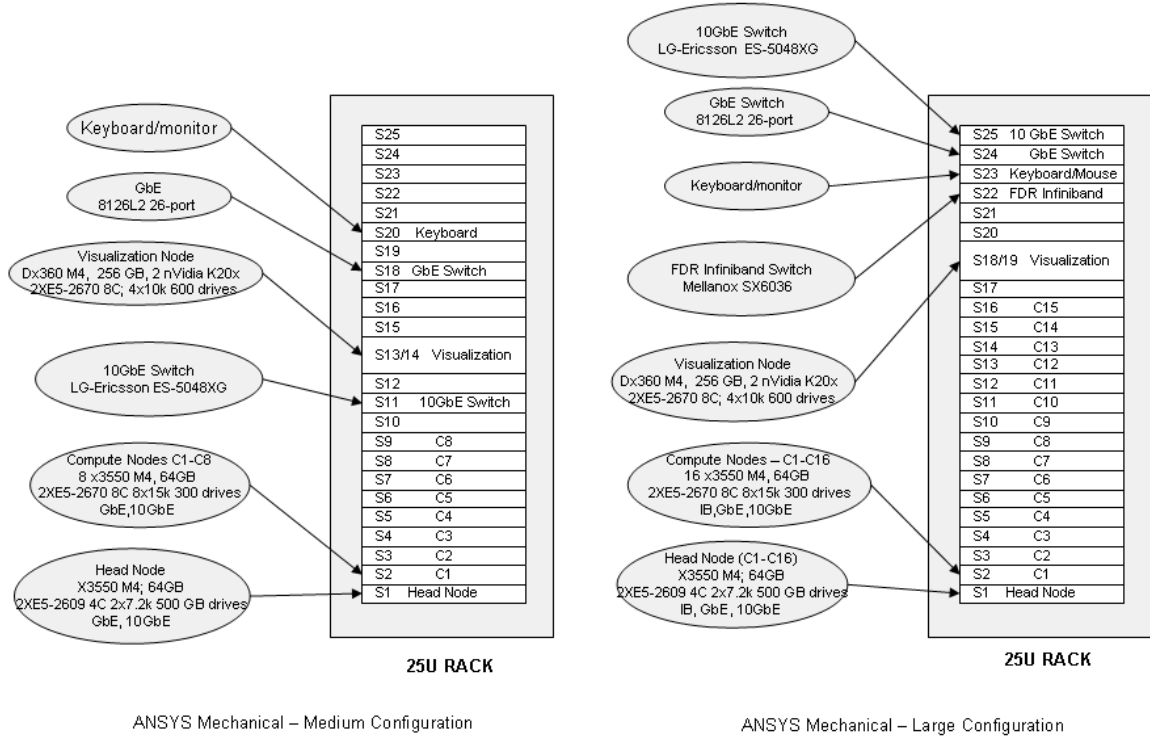


Figure 10C: Deployment diagram for ANSYS Mechanical - Medium and Large configurations

IBM Configurations to implement ANSYS Fluent and ANSYS Mechanical			
	Applies to both	Fluent	Mechanical
Compute Server		14	6
Management Node	1		
Visualization Node*	1		
Total Compute Coress		224	96
Total memory (GB)		512	384
Network	10GbE, GbE, FDR IB		
File System	DS3524		
Packaging			
Pure Flex Chassis	1		
25U Rack	1		
	1		
Software	LSF and PAC		
	Platform HPC		

* Visualization Node can serve as a back-up to Management Node

Table 4: IBM Application Ready Configurations to implement mixed ANSYS Fluent and ANSYS Mechanical

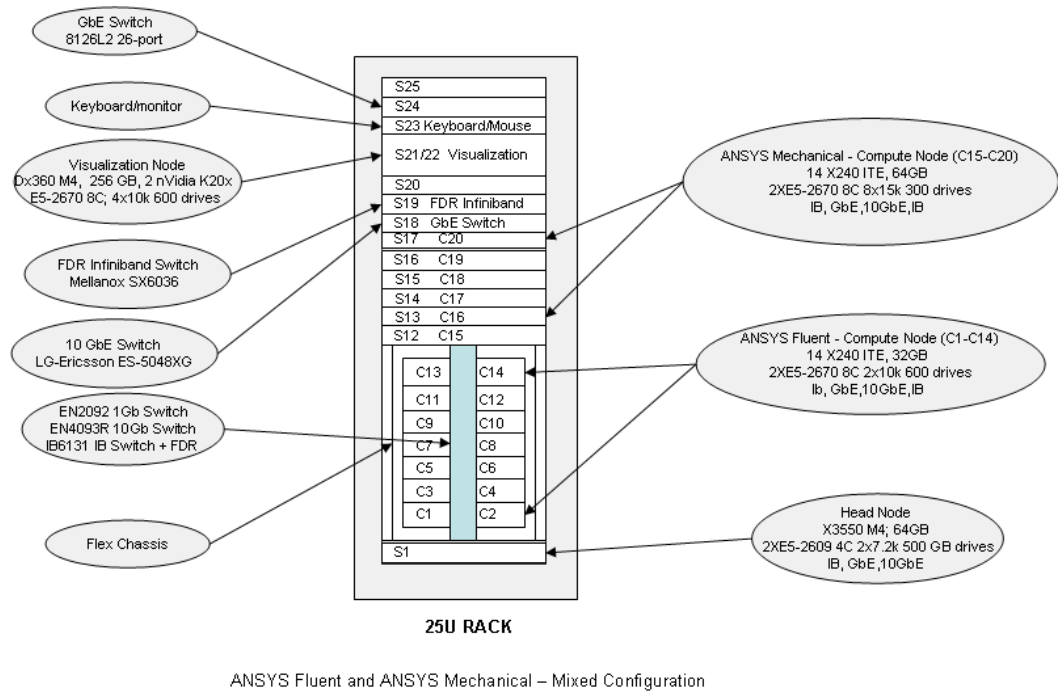


Figure 10D: Deployment diagram for ANSYS Mechanical and ANSYS Fluent Mixed Configuration

Resources

References

- IBM Application Ready Solutions for Technical Computing
<http://www.ibm.com/support/techdocs/atmastr.nsf/WebIndex/WP102288>
- IBM System x: <http://www.ibm.com/systems/x/?lnk=mpSY-sysx-usen>
- IBM PureSystems: <http://www.ibm.com/ibm/puresystems/us/en/?ad=messagedetect-6>
- IBM Platform Computing: [ibm.com/platformcomputing](http://www.ibm.com/platformcomputing)

Installation Scripts

Installation scripts and guide for System x are available to help install and bring up the system and are found at the link below. It is named fix pack: TechSolInst1.0

<http://www-933.ibm.com/support/fixcentral/swg/selectFix?product=ibm%2FOther+software%2FPlatform+HPC+for+System+x&fixids=TechSolInst1.0&source=dbluesearch&function=fixId&parent=Platform%20Computing>

Configurator Guide

Here are the steps to access the templates:

Access the configurator at the following link:

<https://www-01.ibm.com/products/hardware/configurator/americas/bhui/asit/index.html>

- 1) From the x-config starter screen, select the "Express" button (with Cluster Support ON).



- 2) On the next screen, select "No-options solutions" from the "Solution" drop-down box.
- 3) Then select "IBM Application Ready Solutions" from the "Type" drop-down box.
- 4) Then select the applicable Application Ready Solution from the "Template" drop-down box.

The following are the pre-configured template names to select from:

IBM Application Ready Solution CAE fluid dynamics small
IBM Application Ready Solution CAE fluid dynamics medium
IBM Application Ready Solution CAE fluid dynamics large
IBM Application Ready Solution CAE mechanical medium
IBM Application Ready Solution CAE mechanical large
IBM Application Ready Solution CAE fluid dynamics/mechanical mixed large

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