A platform for delivering superior HPC cloud services

A technical overview of Hybrid HPC IaaS for enterprises, cloud providers, and ISVs
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Executive summary

For enterprises, managing on-premises HPC environments is a challenge. Organizations are constrained by data center space, available power, environmental considerations, time and complexity to deploy new infrastructure, and the significant investments required. As the range of HPC workloads has expanded to include Big Data, analytics, and various AI applications, these challenges have become acute.

Not surprisingly, HPC users have long been interested in the potential of cloud computing to address these challenges. However, until recently, cloud providers have struggled to provide the level of performance required, and to deliver it economically. HPC users need secure, state-of-the-art HPC environments that can be managed as easily and seamlessly as standard enterprise cloud computing.

Fortunately, HPE and Intel® led innovations are rapidly making this vision of composable HPC infrastructure as a service (IaaS) a reality. In this paper, we look at the architecture behind the Hybrid HPC IaaS solution from HPE and show how HPC cloud providers, system administrators, and users can leverage a hybrid cloud solution as a platform for high-performance computing. Based on innovative HPC foundation technologies from Intel, the HPC IaaS solution enables enterprises and cloud providers to deliver high-value infrastructure and application services for even the most demanding HPC requirements.

HPC users come in many shapes and sizes. They range from small engineering firms running on-premises CAE applications to large multinationals with multiple data centers.

While the scale of the problem can vary, HPC users face common challenges:

- Rethinking their data center strategies as HPC operations increasingly shift to off-premises or are handled through co-location arrangements
- Becoming more agile in the face of new types of workloads and accelerating change
- Shifting to consumption-based models to avoid large up-front investments

Additionally, as the lines blur between HPC simulation, high-performance data analytics (HPDA) and artificial intelligence (AI), infrastructure requirements for HPC clusters are becoming more complex. Organizations are exploring new analytic techniques including machine learning and deep learning to deliver better predictive outcomes for a variety of applications including robo-advisors, personalized medicine, and predictive system maintenance. Some of these applications require the use of specialized hardware and solutions with the latest generations of GPUs and accelerators as an example.

As the simulation-intensive HPC applications used in automotive, aerospace, and life sciences are here to stay, HPC centers need to find ways to support these additional applications within constrained IT budgets. Faced with these challenges, HPC users are exploring a variety of consumption-based models for HPC hardware and software to reduce risk, contain costs, and help free up capital to where it can be deployed most productively.

New opportunities for Hybrid HPC Deployments

Fortunately, while managing HPC environments has become more challenging, traditional barriers to running HPC using cloud delivery models and technologies have become easier. Improvements in network bandwidth and latency, remote visualization, data replication solutions, and container technologies are making it more cost-effective to run HPC applications in a cloud environment.

While large public clouds are an option for some organizations, other users may have unique requirements sometimes better served by specialized providers with domain expertise. HPC users want the environments to be tailored to their unique workloads without worrying about the complexity of managing high-performance bare-metal clusters and on-demand provisioning. They need an environment that supports a variety of applications as well as multiple deployment models including on-premises, off-premises, and public cloud. A variety of HPC-as-a-service models ranging from simple IaaS to platform as a service (PaaS) to complete software-as-a-service (SaaS) solutions are required to address user’s individual needs.
To address these challenges, HPE has developed a Hybrid HPC IaaS solution and reference architecture purpose-built to deliver high-performance bare-metal clusters with a cloud experience to IT administrators and end users. The solution is based on a variety of innovative technologies from Intel.

A high-level view of this solution is shown in Figure 1. Today, the solution is deployed using HPE Insight Cluster Management Utility (CMU) along with various open-source components. As the solution evolves, it will leverage additional OpenStack® and Kubernetes components to provide cloud operators with greater flexibility.

The HPC IaaS solution can:

- Auto-provision state-of-the-art infrastructure for modern HPC workloads on demand
- Present a variety of service entry points including application-level (SaaS), platform-level (PaaS), and infrastructure-level (IaaS) offerings
- Improve partitioning, multitenancy, and security of HPC clusters
- Support a variable cost-consumption-based model attractive to HPC users

The following Hybrid HPC users, partners, and providers can benefit from this solution:

- Cloud-service providers offering hosted infrastructure or application services
- Systems Integrators delivering HPC-managed services
- Private or public enterprises employing a shared services model to deliver private cloud to groups within their organizations
- HPC, analytics, or AI software ISVs delivering SaaS models either themselves or in partnership with one or more cloud providers

HPE HPC IaaS puts service provider partners and customers firmly in control of their environment. Cloud providers and administrators can choose multiple entry points, relying on HPE for infrastructure only, taking advantage of various aspects of the IaaS solution to deliver self-service IaaS, PaaS, or SaaS environments. Hybrid HPC partners can use the solution to deliver their own software solutions or work with HPE partners to deliver full-stack SaaS solutions including third-party ISV application services.

Figure 1. High-level view of HPE Hybrid HPC Cloud solution
These various approaches and business models in Figure 2 illustrate how Hybrid HPC providers can leverage the HPE HPC IaaS solution.

**HPC IaaS solution**

The HPC IaaS solution is a multitenant composable infrastructure that helps enterprises and cloud infrastructure providers deliver Hybrid HPC services more effectively. It enables system administrators to easily deploy ready-to-use, dedicated bare-metal clusters using a flexible REST API, a command-line interface (CLI), or a cloud management platform like the Micro Focus® Hybrid Cloud Management suite. It also provides flexibility, allowing customers to easily scale their HPC services based on business requirements, paying only for the infrastructure and application services they consume.

The IaaS solution is targeted for both cloud users and cloud providers. HPC customers can leverage the IaaS solution as the technology foundation of their own cloud service to deliver high-value application-level services tailored to specific industries or vertical markets. By leveraging a proven HPC IaaS framework, cloud providers can also get to market faster, reduce development costs, and reduce business risk.

**Based on Intel’s HPC foundation**

The HPC IaaS platform leverages a variety of innovative foundational technologies from Intel. Built for the continuing convergence of HPC and AI, and supported by a broad software ecosystem, the Intel-based HPC platforms offered by HPE provide balanced HPC system performance, lower latency, greater capacity, and improved efficiency.

Intel’s innovative HPC foundation, based on the Intel® Xeon® Scalable processors, includes critical platform innovations in memory, storage, and acceleration technologies to address the complex spectrum of diverse HPC workload requirements. Given the criticality of HPC fabric in scale-out deployments, Intel Omni-Path Architecture (OPA) provides low-latency interconnect for scalable performance of multi-node environments.

**Architectural overview**

An architectural overview of the HPC IaaS 1.0 solution in its present form is shown in Figure 3. End users typically interact with the environment using a cloud provider’s web-based interface or a third-party cloud marketplace platform (CMP). The web interface or CMP, in turn, leverages the IaaS REST API to deploy and manage clustered environments tailored to each customer’s requirements.

Cloud deployments can be structured to present large or sophisticated users with a Python-based CLI allowing them to script the deployment and teardown of frequently required application environments to reduce friction in the cluster provisioning process.
The HPC IaaS management environment (pictured in the lower right portion of Figure 3) provides command and control functions for the overall HPC data center environment.

The HPC IaaS solution presents a RESTful interface on a user-selectable port and accepts calls from multiple internal or external clients along with in-house utilities that cloud operators might develop for their convenience. The REST API can be exposed to a web-based management interface or marketplace, or optionally, it can be exposed outside the firewall to authorized clients with appropriate credentials.

The HPC IaaS management environment uses OpenStack Mistral to manage the process of provisioning tenant clusters. For example, a create cluster request made via the REST API would trigger an associated workflow in Mistral to perform the steps involved in deploying the tenant cluster.

Mistral provides several benefits for Hybrid HPC cloud deployments. It is an open, reliable workflow engine that can schedule, manage, and automate a virtually unlimited number of tasks with automated error handling to reduce administrative workload. Also, the Mistral Workflow Language is easy to use and supports familiar YAML constructs, and service providers can build on HPE supplied workflow templates to deliver new functionality easily. The IaaS environment is designed so that system administrators can use proven DevOps approaches to manage workflows and supporting task definitions using Git to track changes and essentially manage infrastructure as code.

The private tenant cluster is pictured attached to the green network diagram in Figure 3. Behind the scenes, Mistral interfaces with multiple components and APIs to provision hardware and configure various services appropriately. Depending on Mistral workflow, these interfaces include:

- HPE Insight Cluster Management Utility (CMU) API
- HPE Integrated Lights Out Management (iLO) API
- Intel Omni-Path (OPA) Subnet Manager API
- Ethernet switches (VLAN) API
- NFS Server APIs

Mistral uses Ansible Playbooks (Ansible YAML scripting language) to configure components of the delivered cluster including Intel OPA or InfiniBand fabrics, compute servers, and their various components, login servers, and storage resources.

With the IaaS 1.0 API, cluster nodes are provisioned on bare-metal servers using HPE Insight CMU. Future API versions will also support Ironic, the OpenStack bare-metal provisioning facility and HPE Performance Cluster Manager, the cluster management tool for HPE Apollo, SGI, and ProLiant DL systems. A Git repository, implemented within the IaaS management plane is used to store the Ansible Playbooks that perform various configuration tasks.
This architecture has several benefits for Hybrid HPC computing:

- **Cloud deployments** can easily offer multiple application images and tailor workflows behind the scenes to offer a variety of application environments.

- **Hybrid HPC providers** can precisely control the customer experience. For example, a provider offering a packaged SaaS solution might expose simple interface with hardware options preselected and details about infrastructure from application user.

- **A standard cloud provider** delivering a more traditional IaaS service might ask a variety of questions enabling the infrastructure to be tailored based on a customer’s preferences.

Regardless of the approach taken, the architecture has the benefit that it is open and standards-based, and therefore easily extensible and customizable by cloud operators.

### Industry-leading HPC infrastructure

The HPC IaaS environment is a software infrastructure for deploying customized tenant clusters tailored to the client and application requirements. Service providers can use any HPE server in their environment supported by HPE Insight CMU, Docker Enterprise Edition (Docker EE), and OpenStack.

**HPE servers** incorporate Intel HPC foundation components ensuring a balanced, high-performance, and scalable HPC environment. Among the key technologies, the components are:

- **Intel Xeon Scalable processors** offer up to 28 cores and highly enhanced per core performance, significant increases in memory with up to six memory channels and I/O bandwidth expanding up to 48 PCIe lanes. These innovations combined with HPC advances like Intel Advanced Vector Extensions (Intel AVX-512) deliver up to 1.73X HPC performance compared to prior generations. When using the latest Intel-optimized AI libraries, these processors offer up to 127X improvement in training throughput over previous generation processors.

- **With the Intel Xeon Phi™ processor**, HPC system gains ultra-wide vector capabilities in highly parallel computing with up to 72 powerful and efficient cores.

The following HPE Apollo servers are recommended for use in the HPC IaaS solution. Servers can be mixed and matched depending on performance, density, and storage requirements.

- **HPE Apollo 2000 series servers** are dense, rack-optimized systems powered by the latest Intel Xeon Scalable processors. HPE Apollo servers are purpose-built for high-performance computing and Big Data analytics workloads. HPE Apollo 2000 series servers are versatile HPC systems providing up to four servers in a 2U chassis with single or dual CPUs up to 22 cores per CPU, 512 GB per node, up to 24 SSD/HDD drives per node, and a variety of add-on options including Intel Xeon Phi 5110P or NVIDIA® Tesla GPUs.

- **HPE Apollo 4000 series servers** are available in two storage dense configurations. There is a 2U model (HPE Apollo 4200 Gen9 Server) and a larger 4U model (HPE Apollo 4510 Gen10 System) supporting up to 68 LFF large form factor 3.5" drives. The HPE Apollo 4200 LFF system is ideal for smaller object storage implementations and the HPE Apollo 4200 SFF system (small form factor supporting 2.5" drive technology) being ideal for Hadoop or NoSQL datastores.

- **HPE Apollo 6000 system** is a dense, rack-optimized platform powered by the latest Intel Xeon Scalable processors. The HPE Apollo 6000 is a highly integrated solution supporting up to 24 dual Intel Xeon Scalable processor nodes, hot-plug redundant power supplies with common cooling, and a high-speed 100 Gb/s interconnect with integrated switches in a compact 12U chassis.

- **HPE Apollo 6500 servers** are also available for sites requiring even greater scalability and density with the GPU-optimized HPE Apollo 6500 system supporting up to eight GPUs per server, NVIDIA NVLink® for fast GPU-to-GPU communication, Intel Xeon Scalable processors support, and choice of high-speed/low latency fabric. These node types are appropriate for GPU-intensive applications found in CAE, life sciences, and deep learning applications.

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2. “Amazing Inference Performance with Intel Xeon Scalable processors,” Intel, 2018
The HPC IaaS solution also leverages high-speed networking and storage technology from Intel including:

- **Intel Omni-Path Architecture (OPA) switches** and ePCI adapters are ideal for large-scale HPC applications or neural network training requirements delivering 100 Gb node-to-node connectivity, low latency, and the ability to scale to very large numbers of nodes. The use of Intel OPA fabrics provides HPC cloud operators a distinct advantage over competitors that typically use slower 10GbE or FDR InfiniBand interconnects.

- **Intel Optane™ SSD** is a new technology in the data center that is extremely responsive under any load and delivers the low latency, high performance, and high endurance demanded by HPC clusters. Intel 3D NAND SSDs provide greater storage performance with higher density and reliability than hard disk drives. Both SSD technologies deliver the high performance and reliability that users expect making them excellent choices for cloud operators.

**OpenStack and Kubernetes—an open, extensible approach**

In its present form, the HPC IaaS solution leverages OpenStack Mistral and Docker EE. As the HPC IaaS solution evolves, it will expose additional open source projects such as OpenStack, Kubernetes, and Singularity.

Using the current HPC IaaS solution based on HPE Insight CMU, Hybrid HPC cloud deployments can provision clusters running Docker EE containerized application services to deliver both PaaS and SaaS services to customers. In this section, we focus on the IaaS control plane and how it will evolve to use Kubernetes internally and deliver more OpenStack functionality for Hybrid HPC applications.

The beauty of accessing infrastructure services through a backward compatible REST API is that as new functionality is introduced, existing application integrations will continue to work allowing service providers to embrace new technologies at their own pace. The REST API decouples the customer interface from underlying implementation details.

By relying on open-source software, Hybrid HPC users benefit from the latest open-source innovations. They can easily extend or modify their environment as needs change and they avoid becoming locked into a single provider. With over 150 companies supporting the OpenStack community and projected market growth of 28.3% CAGR through 2022,³ OpenStack is an open, flexible framework that delivers rich functionality.

OpenStack supports not only virtualized machine deployments with Nova but bare-metal deployments using OpenStack Ironic and containerized deployments with OpenStack Magnum. HPE has gained significant expertise with OpenStack, contributing to multiple projects including Neutron, Ironic, TripleO (OpenStack On OpenStack), and Cinder.

Recently, HPE made its iLO drivers available (delivering integrated lights-out functionality) for OpenStack Ironic to improve the management of bare-metal HPE nodes. This driver replaces the default IPMI driver used for bare-metal host provisioning. The HPE iLO driver supports features like RAID configuration, secure/trusted boot, and other capabilities essential for cloud providers like the ability to reset server ROM settings to known baseline values and securely erase disks before physical servers are re-allocated to different tenants.

**New service delivery options for HPC providers**

While the existing HPC IaaS solution supports the deployment of nodes running Docker EE, future releases will more tightly integrate Kubernetes and container technologies. Management functions will be implemented as containerized services running on a customer’s preferred Kubernetes environment as shown in Figure 4.

The use of Kubernetes, production-proven at Google™, helps ensure that management services are both scalable and reliable. Kubernetes also allows customers and service providers to benefit from the increasing variety of containerized application services built for Kubernetes.

³ “Global $5.6 Bn OpenStack Service Market 2018–2022 by Component, Organization Size, Vertical and Region” Research and Markets, 2018
Using Kubernetes as a single environment for management services provides clear benefits to enterprises and cloud operators:

- New services can be deployed at any time without the need to add infrastructure.
- Updates are simplified and involve simply pulling Docker images from appropriate registries.
- Kubernetes ensures that services are scalable and resilient using concepts like Deployments and ReplicaSets to deliver auto-scale functionality so that services scale based on demand.
- Service providers can configure Kubernetes Ingresses, selectively exposing various web interfaces and APIs outside the Kubernetes environment and even outside the service provider’s firewall, the IaaS REST API end point being just one example.
- Functionality like health checks and rolling updates of Kubernetes Deployments help providers ensure reliability and perform software maintenance and updates with zero service downtime, automatically falling back to known good configurations in the event of a problem.

While Kubernetes will be used in future IaaS releases to support internal management functions, some cloud operators will also want to deploy Kubernetes on tenant clusters used by their customers. Kubernetes can be used as a platform for delivering containerized HPC applications, or some cloud providers might elect to expose Kubernetes to their customers, delivering a PaaS offering similar to Google GKE, Microsoft® AKS, or Amazon EKS.

As developers increasingly embrace containers and microservice delivery models, Kubernetes is emerging as a popular solution. While traditional HPC applications may not support Kubernetes natively, HPC applications are distributed in Docker containers, which run on Kubernetes clusters. Also, high-performance frameworks used in machine learning and deep learning (e.g., TensorFlow, Caffe) are leveraging containers both for model training and for the scalable deployment of the predictive models themselves.

Figure 5 illustrates how OpenStack Magnum can be used to deliver customer-ready Kubernetes clusters on virtual machines or bare metal. This technology has been demonstrated by HPE running on the IaaS HPC solution.
The flexibility to deploy traditional HPC environments, as well as Kubernetes on tenant clusters, is important for HPC service providers who need to ensure that their environment is future-proof and easily extensible to new application workloads and changing customer requirements.

**Bare-metal advantage**

While virtualization has been widely embraced in the enterprise, it has proven to be less popular with HPC users where performance is a primary concern.

HPC applications often demand 100% of cluster resources for sustained periods, and any software with the potential to cause additional latency for high-speed interconnects, specialized GPUs, and fast disk subsystems are a liability to HPC systems. For HPC applications, there is simply no substitute for dedicated bare-metal hardware and fast local storage.

Other concerns about virtual machines include latency issues, noisy-neighbor problems, and concerns about infrastructure being over-subscribed leading to unpredictable performance.

Similarly, for customers in finance, healthcare, and government concerned about security, dedicated bare-metal hardware can be a major selling feature. Tenants want to know if their applications, network traffic, and data are secure and physically isolated from other users. HPC users are technically savvy, and while they may introduce virtualization into their environments, they typically want to do so on their terms. They want control over details like the selection of the hypervisor and various OS and hypervisor level configuration settings. The HPC IaaS solution provides this flexibility.

HPE HPC IaaS environment provides operators and end customers—the best of all worlds:

- **Flexibility and ease of management**—With a simple, automated provisioning and management API that makes bare-metal clusters as easy to deploy as virtual environments
- **Unrivaled performance**—With dedicated hardware, dedicated switched network ports, and fast local storage
- **Security and peace of mind**—Knowing that applications and data are secure, isolated from other tenants and when clusters are deprovisioned, all traces of customer data are wiped away
HPC-ready storage and data management

Just as OpenStack provides flexible provisioning of compute resources including bare metal, virtualized, and containerized environments, it also provides rich capabilities for storage. Depending on the HPC applications, storage requirements can vary widely, and OpenStack gives providers the flexibility to deliver a variety of storage services easily and cost-effectively.

Before delving into some of the HPC-specific storage capabilities provided by the HPC IaaS solution, it's useful to review the standard storage services available in OpenStack available to cloud deployments:

Cinder is a block storage service that virtualizes the management of block storage devices. With Cinder, storage resources can be consumed without applications needing to know where the storage is located or the type of storage device used.

Swift is a highly available, distributed, eventually consistent object store suited to inexpensive storage of large volumes of data. Swift is used for storing Glance images (VM images) and snapshots, and can be used by applications as a general-purpose object store.

Manila is an OpenStack project that provides a shared file system services. While Cinder provides block-level services only, Manila provides coordinated access to a shared file system.

Ceph is another open-source storage service that service providers can use. Ceph is unique in providing object, block, and POSIX file storage in a single unified system. It is also easy to manage, making it a good foundation for a variety of storage services.

Ceph can be configured to provide:

- Block storage capabilities for Cinder supporting Ironic and virtualized Nova compute instances
- Object storage for Swift

The HPC IaaS solution can present Ceph storage to underpin Cinder and Swift storage in cases where performance is not the overriding requirement. Among Ceph's features are:

- Amazon S3 and Swift compliant APIs
- Flexible striping options
- Support for snapshots and incremental backups
- Dynamic rebalancing
- File system compatibility with NFS, SMB/CIFS
- Support for Hadoop (replacing HDFS)

While service providers may not choose to expose all this functionality to their customers immediately, the variety of storage services offered by OpenStack and Ceph provide flexibility and the opportunity to deliver additional application or infrastructure services in the future as business needs evolve.

BeeGFS parallel file systems

For many HPC applications, the performance of NFS filers, object stores, or Cinder volumes is not sufficient. Parallel HPC workloads including CFD and crash simulations write very large files to intermediate scratch space. Cluster nodes need to be able to read and write to the file system in parallel, and massive disk I/O bandwidth (typically tens of GB/s) is required between cluster hosts and the underlying file system.

The HPC IaaS solution supports the deployment of a high-performance BeeGFS parallel file system across bare-metal cluster nodes, using local Intel SSDs or other drive technology for maximum performance. BeeGFS leverages the high-performance Intel OPA fabric between cluster nodes to deliver massive levels of bandwidth and I/O for the most demanding applications.

The IaaS REST API makes it easy to deploy cluster nodes with a scalable BeeGFS file system preinstalled. HPC applications can use the parallel file system for demanding storage requirements and leverage other types of storage including NFS for less performance-critical applications as shown in Figure 6.
A RESTful API for automated deployment

The HPC IaaS platform exposes a comprehensive RESTful API and CLI to enable self-service provisioning and management of various types of high-performance clusters.

Service providers can call the API from their in-house developed portal or leverage integrations with Micro Focus Cloud Service Automation (CSA) or other cloud management platforms to provide a customer-friendly marketplace. The benefit of exposing a REST API is that service-providers can control how customers, developers, and ISVs interact with their service and present a simple interface that hides the underlying complexity from users of their service.

For developers experienced with RESTful APIs, the IaaS software API is easy to use. Developers will use standard HTTP operations including GET, POST, and DELETE using their preferred programming or scripting language to provision and manage tenant clusters through their lifecycle.

The REST API exposes multiple API end points as shown in Figure 7. The various end points accept JSON-format commands and can be queried in flexible ways, returning JSON formatted responses that are easily parsed.
By calling the various API end points with appropriate HTTP operations, a variety of tasks can be automated. Some examples are:

- Creating or removing customer-ready clusters
- Adding or removing cluster nodes or associated storage
- Adding and mounting storage volumes after customer creation
- Manipulating utility nodes such as login servers or visualization servers
- Querying clusters belonging to a specific customer
- Retrieving information about available node types

A simple example showing API usage is provided in Figure 8. A customer, using a web interface or program written to the API, can easily create a bare-metal cluster tailored to their application requirements, in this case, ANSYS Fluent.

```json
{
  "clusterName": "myansyscluster",
  "description": "My ANSYS Fluent Cluster",
  "domain": "customer",
  "computeNodes": [
    {
      "count": 4,
      "type": "8/coreXeon.e5-2680-v3@1.80GHz/32.0GiB/3x11GiB",
      "glanceImage": "fc7364b1-28f3-0d01-3b4a-6c10cf3e1294",
      "image": "<restapi-url>:8080/v1/images/fc7364b1-28f3-0d01-3b4a-6c10cf3e1294"
    }
  ]
}
```

![Figure 8. Example of provisioning a tenant cluster using the HPC IaaS REST API](image)

The client application will POST a JSON message to the appropriate end point to create a new cluster, in this case, `http://<restapi-url>:8080/v1/clusters`.

Included in the JSON message are details like:

- The name and description of the cluster
- Details about the cluster environment including the number of nodes, the type of hardware, and the disk image (CMU or Glance) to be associated with each host
- Details about utility nodes (i.e. login nodes) including the type of node, their role, and if appropriate SSH credentials that can be used to log in once provisioned
- The JSON can also stipulate storage to be mounted by each node including details like the name of the volume, the amount of storage, and the type of storage (i.e. NFS)

When the JSON message is posted to the API end point, the end point will respond with a cluster-id and a task-id associated with the create cluster operation.

Behind the scenes, the API will execute a Mistral workflow comprised of several discrete tasks associated with cluster creation. Developers can call the `/v1/task` end point to monitor progress by providing the task-id returned by the cluster create operation.
The API provides multiple benefits to cloud providers:

- Developers see a straightforward, well-defined interface that hides implementation details. This means that service providers can evolve their back-end environments without breaking client functionality.
- Service providers can easily provide their own custom images depending on the types of application services they want to provide to their customers.
- To the extent that end customers use the APIs to self-provision and self-manage resources, processes are automated, reducing errors and improving efficiency since the operator’s technical staff doesn’t need to be involved with every customer request.

The back end of the API interfaces with the OpenStack Mistral Executor, which in turn executes workflows that manage the provisioning process using components like the HPE Insight Cluster Management Utility (CMU), OpenStack Ironic (in future releases), and Ansible Playbooks.

**Realizing an HPC App Store**

The HPC IaaS solution exposes HPC clusters as a set of services to internal or external customers. In addition to providing infrastructure services, customers, service providers, and ISVs can also use the IaaS platform to deliver their own branded App Store. To help realize this vision, cloud operators can leverage innovations from HPE and various partners solutions described in the following.

**The end-user experience: Low-touch, self-service access to HPC applications**

Often, end users don’t want to be bothered with infrastructure. For example, an engineer running a CAE application probably prefers to use a familiar application interface to build, run, monitor, and visualize their simulations. They don’t necessarily care about underlying details like hardware, MPI versions, and storage as long as they have adequate capacity to do their work. The same is true in other disciplines as well including life sciences, seismic analysis, and high-performance data analytics.

**Using containers to deliver HPC application services**

Containers are a useful tool for helping service providers deliver ready-to-use application services. HPC applications frequently have environmental dependencies on things like math libraries, run-time interpreters, MPI libraries, and more. Containers allow application software to be packaged along with prerequisite components into an image that can run reliably across any physical machine with a container run time.

While there are multiple container platforms and formats, for HPC users, Docker and Singularity are popular choices. Enterprises may choose to use the commercially support version of Docker, Docker Enterprise Edition (Docker EE).

Figure 9 shows how the HPC IaaS environment can be used with Docker EE to deliver simplified access to container-based application services. Users interact with a portal that presents an application catalog and they select their preferred application (i.e., ANSYS) along with any ordering options that the service provider exposes to the customer. After a few minutes, when provisioning is complete, the user is presented with a URL and login credentials that they can access a secure, private application environment that is ready to use.

![Figure 9. Delivering an HPC App Store using the Hybrid Cloud IaaS Solution](image-url)
To realize this vision of an HPC App Store, automated steps take place behind the scenes. While the details are a little more complicated, the high-level flow is as follows:

1. Once a user has selected their preferred application environment using the App Store or cloud management platform, the client calls the HPC IaaS REST API posting a JSON message. The JSON includes details like the type of hardware required, cluster name, description, number of nodes, disk images, storage requirements, and such.

2. The HPC IaaS API triggers a Mistral workflow appropriate to the application environment that the customer has requested as shown in Figure 8. The Mistral workflow might use either HPE Insight CMU or OpenStack facilities to provision the cluster depending on the underlying technology the service provider elects to use and the REST API version.

3. Once the tenant cluster is provisioned, the Mistral workflow makes sure that Docker EE or a similar container run time is installed on each cluster host if it is not already present. In other cases, the workflow might use OpenStack Magnum (as shown in Figure 5) or other Kubernetes installers to automatically install a Kubernetes environment across the tenant cluster.

4. With the physical cluster and container run times deployed, the application environment can be automatically installed. For simple requirements, service providers can obtain and run Docker containers directly from an appropriate container registry (using Docker pull and Docker run respectively) to start containerized applications on a cluster host. For more complicated multihost application deployments, Kubernetes provides more flexibility. The installation scripts can use kubectl, the Kubernetes administrative facility, to install the containerized application across cluster hosts based on specifications in a YAML template, providing detailed preferences related to application containers, versions, storage, and networking.

Unlike some Kubernetes microservices applications where containers are minimalist by design, in the case of HPC applications, containers are used for portability and ease of deployment. Each cluster host will typically run a small number of large application containers or even a single container.

The HPC IaaS solution provides cloud operators with flexibility. While the example mentioned previously describes how Docker and Kubernetes can be used to support turnkey application services, cloud providers can devise their own solutions for application deployment including simply installing applications on bare-metal hosts using tools like Ansible, Chef, or Puppet or packaging them in virtual machines.

For service providers wishing to implement an App Store and deliver SaaS solutions, UberCloud provides prebuilt, containerized HPC applications for the HPC IaaS solution.

**UberCloud container solutions**

UberCloud provides a variety of packaged CAE application containers and includes the ability to meter and manage ISV license costs relieving service providers or large IT organizations of this burden. UberCloud also provides facilities that allow containerized applications to run MPI efficiently across hosts and share resources like GPUs to deliver bare-metal performance on a containerized infrastructure.

While not all UberCloud application containers are certified for use with the HPC IaaS solution presently, the increasing variety of available applications provides cloud providers with flexible deployment options.

- ANSYS Mechanical, CFX, Fluent, and such
- NUMECA FINE™/Marine
- Dassault Abaqus and CST
- Siemens STAR-CCM+
- CFD Support OpenFOAM
- DYNAMORE LS-DYNA & LS-OPT
- Univa Grid Engine
- NICE Desktop Cloud Visualization (DCV)

Deploying application environments in containers is becoming a standard practice and many open-source projects and ISVs already provide Docker images and templates to simplify application deployment on Kubernetes. UberCloud provides a commercially supported application environment ready for production supercomputing workloads.
Rich opportunities for Hybrid HPC Solutions

HPE HPC IaaS puts service provider partners and customers firmly in control of their environment. Cloud deployments can choose multiple entry points, relying on HPE for infrastructure only, taking advantage of various aspects of the IaaS solution to deliver self-service IaaS, PaaS, or SaaS environments. HPE partners can use the solution to deliver their own software solutions or work with HPE partners to deliver full-stack SaaS solutions including third-party ISV application services.

Getting started

The HPC IaaS solution is a powerful and flexible architecture for building self-service HPC environments. It is suitable for traditional HPC as well as compute and data-intensive applications including Big Data, analytics, machine learning, and deep learning.

Existing HPC users may have on-premises HPE infrastructure, application environments, and cluster management software such as HPE Insight CMU. For these customers, HPE consultants can help chart an evolutionary path to a Hybrid Cloud environment that preserves existing investments in software and management approaches while gradually introducing capabilities like self-service, cloud-bursting, and access to hybrid environments. These customers will typically use the following technologies and services as part of their Hybrid HPC environment:

• HPE Apollo systems
• HPE Insight Cluster Management Utility
• HPE Hybrid HPC IaaS solution
• Services from HPE Pointnext

Enterprises or service providers pursuing a management strategy based on OpenStack can also take advantage of the HPC IaaS solution leveraging OpenStack behind the scenes to present internal or external users with self-service access to infrastructure via the same easy to use REST API. For these environments, customers might consider the following products and services:

• HPE Apollo systems
• SUSE OpenStack Cloud 8 (or other OpenStack distributions with HPE iLO support)
• HPE Hybrid HPC IaaS solution
• Services from HPE Pointnext

There are a variety of potential deployment scenarios depending on a customer’s existing HPC environment. HPE Pointnext or HPE partners can provide guidance and technical assistance to help organizations take advantage of the HPC IaaS solution, embrace Hybrid Cloud computing, and optionally take advantage of containers for workload deployment using Docker EE or Singularity. Other solutions worth mentioning are:

• Bright OpenStack and Bright Cluster Manager from Bright Computing—Bright OpenStack is a complete solution for deploying and managing OpenStack software on bare-metal clusters. Bright Cluster Manager simplifies software deployment for HPC clusters.
• Navops Command and Navops Launch from Univa—Navops Command brings advanced scheduling capabilities to Kubernetes and enables traditional HPC workloads to run on Kubernetes without modification. Navops Launch (formerly UniCloud) can be used for automating the deployment of HPE clusters based on policy controls or enabling on-premises or cloud-based clusters to burst to a variety of public or private providers based on workload demand.
HPE advantage

HPC customers and partners face a variety of challenges managing on-premises environments including space, cost, complexity, and security concerns related to data. For some organizations, an on-premises environment will make the most sense. For others, running some applications partially or entirely in the cloud can be an attractive option because it allows them to outsource non-core requirements, shift to a variable cost model, and free up capital to where it can be employed more productively. By offering a mixed/hybrid approach to HPC, HPE addresses both scenarios.

The shift to the cloud represents an opportunity for both service providers, and IT organizations to re-think how they deploy HPC infrastructure and evolve from fixed-cost models to usage-based models. Cloud providers can provide a spectrum of services from IaaS to PaaS to full-service application offerings (SaaS) delivered by professionals with application domain expertise.

By leveraging HPE’s customizable IaaS framework, enterprises and service providers can

- Reduce risk by leveraging proven infrastructure components
- Reduce development costs
- Accelerate time to market for new application services

Using the HPC IaaS solution based on the latest Intel HPC foundation technologies, organizations can quickly deploy a proven, self-service, composable infrastructure solution, helping customers move to a more flexible, variable cost model for HPC and related application services at their own pace.

Learn more at