
Technology Spotlight

# Smart Orchestration Speeds HPC Workflows in the Cloud

Sponsored by Amazon Web Services

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## HYPERION RESEARCH OPINION

Extrapolated findings from Hyperion Research's most recent worldwide study indicate that HPC sites have rapidly increased the portion of their workloads they perform on third-party clouds. On average, they now send about 20% of all their HPC workloads to third-party clouds, double the 10% average reported in our studies less than two years ago. Cloud services providers (CSPs), and to a lesser extent HPC system vendors offering cloud services, have helped to propel this growth by adding features, functions and partners designed to make their platforms run a broader spectrum of HPC-related workflows cost- and time-effectively.

For years, an important attraction of third-party cloud platforms has been their ability to offer wide selections of hardware, software and storage resources, especially resources that users lack on premises (or lack in sufficient quantity). These selections have expanded more recently to address the growing heterogeneity of HPC workflows, especially with the rise of high performance data analysis (HPDA) and HPC-enabled artificial intelligence (AI). The trend toward increased heterogeneity is nicely described in the U.S. Department of Energy's January 2018 report, *Productive Computational Science in the Era of Extreme Heterogeneity*.

The growing heterogeneity and scale of major CSP offerings has increased the need for mechanisms that help HPC users deploy and manage their workloads in third-party clouds. Automating frequent and repetitive tasks is an important help but does little to manage workflows that might need to pass through a dozen or more stages from start to finish, with each stage requiring a different mix of hardware, software and storage resources. The answer for this complex sequencing of workflows is cloud orchestration. Orchestration aims to give cloud users the ability to program and manage the entire end-to-end sequence a workflow will traverse, no matter how many varied stages that process entails.

This paper discusses the importance of cloud orchestration in the context of expanding HPC cloud usage and workflow heterogeneity. The paper uses Amazon Web Service (AWS), the market-leading HPC cloud service, to illustrate how sophisticated cloud orchestration can happen.

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## HPC CLOUD GROWTH AND THE ROLE OF ORCHESTRATION

### *HPC Cloud Growth*

In Hyperion Research's latest global study of HPC sites that are using clouds, the surveyed users on average said they run 33% of all their HPC work in third-party clouds. Extrapolating from this group of cloud users to the whole HPC community lowers that average to about 20%, which is a significant uptick from the 10% figure in Hyperion Research surveys not long ago. HPC cloud computing is rounding an elbow in the growth curve and is ramping up briskly.

Chief among the reasons driving greater usage is the recognition, at least among major CSPs, that the size and growth rate of the worldwide HPC market make it worth special attention. The market for HPC servers, storage, software and technical support expanded from about $2 billion in 1990 to $27.7 billion in 2018, en route to a Hyperion Research forecast $39.2 billion in 2023. When revenue from public cloud usage is added to the mix this number increases to $45 billion. (See Figure 1.)

### FIGURE 1

### HPC Worldwide Market Forecast ($000)

| Revenues by the Broader HPC Market Areas | | | |
|---|---|---|---|
| | 2018 | 2023 | CAGR 18-23 |
| Server | 13,706,088 | 19,979,016 | 7.8% |
| Storage | 5,547,188 | 7,771,184 | 7.0% |
| Middleware | 1,582,892 | 2,217,801 | 7.0% |
| Applications | 4,627,492 | 6,413,592 | 6.7% |
| Service | 2,229,921 | 2,858,820 | 5.1% |
| Total Revenue | 27,693,580 | 39,240,413 | 7.2% |
| Source: Hyperion 2019 | | | |

HPC cloud (CSP) usage raises forecast to $45 billion

Source: Hyperion Research, 2019

But that's not all, CSPs are also aware that HPC is an important factor for success in the emerging markets for artificial intelligence (AI) and high performance data analysis (HPDA) applications. HPC is nearly indispensable today at the forefront of R&D for automated driving systems, precision medicine, affinity marketing, business intelligence, cyber security, smart cities and the Internet of Things. Today's HPC activity indicates where the mainstream HPDA and AI markets are headed in the future.

40% of HPC cloud users believe that all their HPC jobs could be run in the cloud, pointing to substantial headroom for cloud growth. The ultimate limiter of this growth may be data locality, the inefficiency of moving large data volumes to third-party clouds when the data is already in the same locale as the applications and computing resources.

With the combined HPC, HPDA and AI market opportunity in mind, leading CSPs have been adding features, functions and partners designed to make their platforms run a broader spectrum of HPC related workloads cost- and time-effectively.

Elasticity, heterogeneous hardware and software, along with extensibility (providing headroom for future growth), are key attractions of cloud computing for HPC users. Together, these resources enable users to create custom-fit computing environments, and to alter these environments for each stage of workflows that may need to pass through a dozen or more stages, each with its own set of hardware, software and processing requirements. Each HPC workload is provided with an appropriate set of resources and run on bare metal or in virtual machines in the form of lightweight containers.

### *The Role of Orchestration*

The goal is not just to complete demanding workflows, but to do so in the quickest, most-efficient way possible, i.e., by compressing the workflows.

Automating frequently used processes and templating configurations for reuse compresses solution times for workflows but doesn't go far enough. Users also need the ability to program and manage the entire end-to-end sequence a workflow will traverse, no matter how many varied stages that requires. This ability is orchestration.

Major CSPs provide orchestration tools that allow users to program the sequence of resources and automated (and other) processes that will be applied to an HPC workflow en route to its completion. CSPs' cloud orchestration platforms all have the ability to provision and deploy servers, software, storage and processes, including previously automated tasks. Beyond that, they can vary considerably from each other, especially in their ease of programming and use, security and compliance, and especially the speed and sophistication with which they process workflows. These differences can result in very dissimilar workflow completion times, along with varying user involvement and costs.

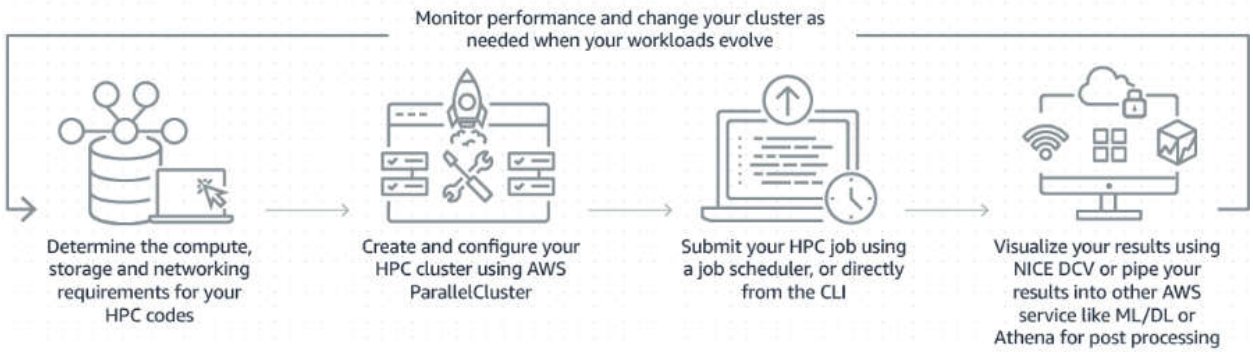
Hyperion Research's most recent study shows that AWS remains the preferred CSP for surveyed HPC user organizations worldwide, with a strong lead over the others. AWS reports that its orchestration tools have played an important, growing role in this success.

## HPC CLOUD ORCHESTRATION AND CLUSTER MANAGEMENT ON AWS

Moving High Performance Computing (HPC) workloads to the cloud can provide a custom-fit compute, storage, and networking environment to meet the unique requirements of every stage of a workflow. The ability to leverage the resource heterogeneity and extreme scalability of the cloud depends to a large extent on the cloud orchestration and management capabilities that come with it. Figure 2 illustrates the approachable process for getting started with HPC on AWS.

## FIGURE 2

### Running HPC Workloads on AWS




Source: Amazon Web Services, 2019

For those users whose data sets are not already resident in the cloud, all workflows begin with data migration. AWS provides AWS DataSync to automate the movement of data between on-premises storage and Amazon S3 or Amazon Elastic File System (Amazon EFS). DataSync is designed to automatically handle running instances, encryption, managing scripts, network optimization, and data integrity validation.

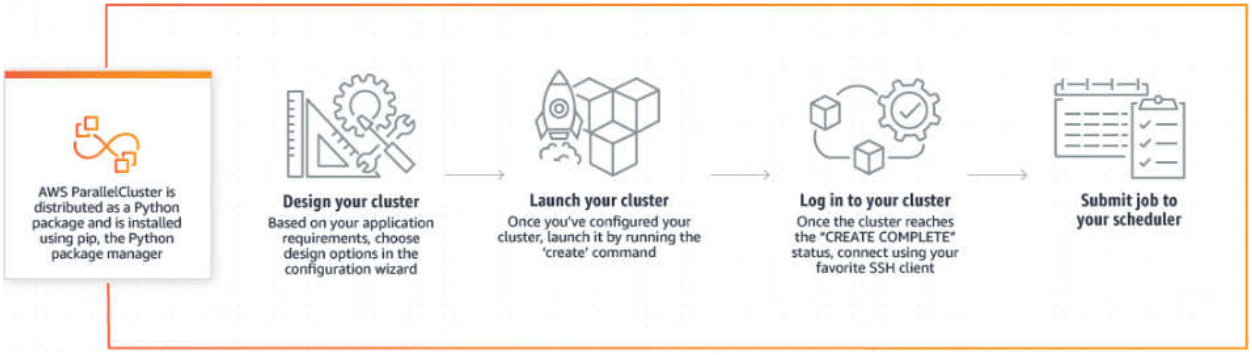
For most AWS HPC users, AWS ParallelCluster is the first step in setting up and managing an elastic HPC cluster. AWS ParallelCluster, built on the open source CfnCluster project, is an AWS-supported Open Source cluster management tool to deploy and manage HPC clusters in the AWS cloud. AWS ParallelCluster aims to provision resources in a safe, repeatable manner, allowing users to build and rebuild their infrastructure, without having to perform manual actions or write custom scripts.

AWS CloudFormation is the core service used by AWS ParallelCluster. AWS CloudFormation provides a common language for users to describe and provision all the infrastructure resources in their cloud environment. CloudFormation allows users to employ a simple text file to model and provision the resources needed for their applications in an automated and secure manner. All resources required by the cluster are defined within the AWS ParallelCluster AWS CloudFormation template.

Here is a quick overview of how AWS ParallelCluster works (Figure 3).

## FIGURE 3

### How AWS ParallelCluster Works




Source: Amazon Web Services, 2019

All HPC clusters depend upon their scheduler as a key portion of their workflow. AWS ParallelCluster supports a number of typical on-premises schedulers including Slurm, SGE, and Torque, as well as AWS's own scheduler, AWS Batch.

**AWS Batch.** AWS Batch is the AWS-managed job scheduler that dynamically provisions the optimal quantity and type of compute resources (for example, CPU or memory-optimized instances). It provisions resources based on the volume and the requirements of the batch jobs that are submitted. With AWS Batch, AWS says there is no need to install and manage batch computing software or server clusters to run jobs. For HPC clusters that are based on AWS Batch, AWS ParallelCluster relies on the elastic scaling capabilities provided by AWS Batch.

**Amazon EC2 Auto Scaling.** When deployed with schedulers other than AWS Batch (e.g., SGE or Slurm), AWS ParallelCluster implements the scaling capabilities using the Amazon EC2 Auto Scaling. Amazon EC2 Auto Scaling helps maintain application availability by automatically adding or removing EC2 instances according to conditions that the user defines. Scaling up is achieved by evaluating the current number of instances required by the pending jobs in the queue. If the total number of busy nodes and requested nodes is greater than the current desired value in the auto scaling group, more nodes are added. Another process evaluates the idle time of the node. An instance is terminated if that node has no jobs for a period of time longer than a defined value and there are no pending jobs in the cluster.

**Amazon CloudWatch** collects and tracks metrics, monitors log files, sets alarms, and automatically reacts to changes in the user's AWS resources.

**AWS Identity and Access Management (IAM).** AWS ParallelCluster uses IAM to ensure that the user who creates the cluster has the appropriate level of permissions.

Beyond infrastructure orchestration and security/access management, AWS offers options for cost and budget management.

**Trusted Advisor.** With Trusted Advisor, users can provision resources following best practices to improve system performance and reliability, increase security, and look for opportunities to save money.

**AWS Cost Explorer** gives users additional ability to analyze costs and usage. Using a set of default reports, HPC users or admins can get started with identifying the underlying cost drivers and usage trends. Cost Explorer enables the user to filter and group data according to resource tags and map resources and workloads to the appropriate cost center within the organization.

## AMAZON SUCCESS STORIES

### *Western Digital*

In late 2018, AWS and Western Digital evaluated the impact of running the customer's electro-magnetic simulations on a massive HPC cluster built on AWS using Amazon EC2 Spot Instance. As part of this pioneering collaborative work, Western Digital ran 2.3 million simulation jobs on an Amazon EC2 Spot Instances-based cluster of a little over one million vCPUs, taking only 8 hours to complete the job. Western Digital reports that doing the same work on a cluster of 16,000 on-premises CPUs at a time would have taken about 20 days. This project also showcased the scaling and orchestration capabilities of AWS. AWS CloudFormation template was used to start the Univa Grid Engine job scheduler and launch the cluster. The cluster grew to one million vCPUs in only 1 hour and 32 minutes. When there were no more undispatched tasks available, Grid Engine began to shut the instances down, reaching the zero-instance point in about an hour.

### *OpenEye Scientific*

OpenEye, a provider of computational drug discovery software, counts pharmaceutical giants Pfizer and Merck among its customers. OpenEye built Orion, its software-as-a-service (SaaS) computer-aided drug-design platform, on AWS. Using Orion, chemists at pharmaceutical firms can create, share, model, calculate, visualize, analyze, and organize chemical collections of different sizes and complexities. Orion uses AWS to give companies highly scalable, maintenance-free access to up to hundreds of thousands of processors. Orion runs on Amazon EC2 instances and takes advantage of Auto Scaling to automatically monitor compute capacity and adjust it as needed. OpenEye also uses Amazon EC2 Spot Instances—spare compute capacity available at a discount compared to on-demand prices. Additionally, Orion relies on AWS Identity and Access Management (IAM) to control access to AWS services, and AWS CloudFormation templates to provision resources. OpenEye reports that now, instead of spending time setting up and managing an HPC infrastructure, customers can implement complete research data centers in weeks instead of months. OpenEye customers have deployed 100,000 cores in a few days, instead of the six months it would typically take with on-premises infrastructure.

## FUTURE OUTLOOK

Hyperion Research forecasts that the global market for running HPC workloads in third-party clouds will reach about $6 billion in 2023, representing about 13% of our projected $45 billion in overall spending on HPC in that year. CSPs have been turning more attention to the global HPC market, because this market has become a sizable opportunity and because HPC is at the forefront of R&D for economically important, emerging HPDA-AI use cases.

Leading CSPs will continue to enhance their capabilities in order to address more existing and emerging HPC workflows time- and cost-effectively. Addressing this increasingly heterogeneous mix of workflows will require CSPs to make increasingly heterogeneous hardware, software and storage resources

available, but that's not all. CSPs also need to offer mechanisms that help HPC users to deploy and manage their workloads in third-party clouds. Automating frequent and repetitive tasks will not be enough. CSPs also need to provide sophisticated orchestration that makes it easier for cloud users to program and manage the entire end-to-end sequence a workflow will traverse, no matter how many varied the stages that process entails. Hyperion Research believes that Amazon Web Services is a leader in cloud orchestration for HPC workflows and is well positioned to benefit from and help drive the growth Hyperion Research forecasts for HPC cloud use.

## About Hyperion Research, LLC

Hyperion Research provides data driven research, analysis and recommendations for technologies, applications, and markets in high performance computing and emerging technology areas to help organizations worldwide make effective decisions and seize growth opportunities. Research includes market sizing and forecasting, share tracking, segmentation, technology and related trend analysis, and both user & vendor analysis for multiuser technical server technology used for HPC and HPDA (high performance data analysis). We provide thought leadership and practical guidance for users, vendors and other members of the HPC community by focusing on key market and technology trends across government, industry, commerce, and academia.

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