

AWS Whitepaper

Computational Fluid Dynamics on AWS



Computational Fluid Dynamics on AWS: AWS Whitepaper

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Abstract

The scalable nature and variable demand of computational fluid dynamics (CFD) workloads makes them well suited for a cloud computing environment. This whitepaper describes best practices for running CFD workloads on Amazon Web Services (AWS). Use this document to learn more about AWS services, and the related quick start tools that simplify getting started with running CFD cases on AWS.

Introduction

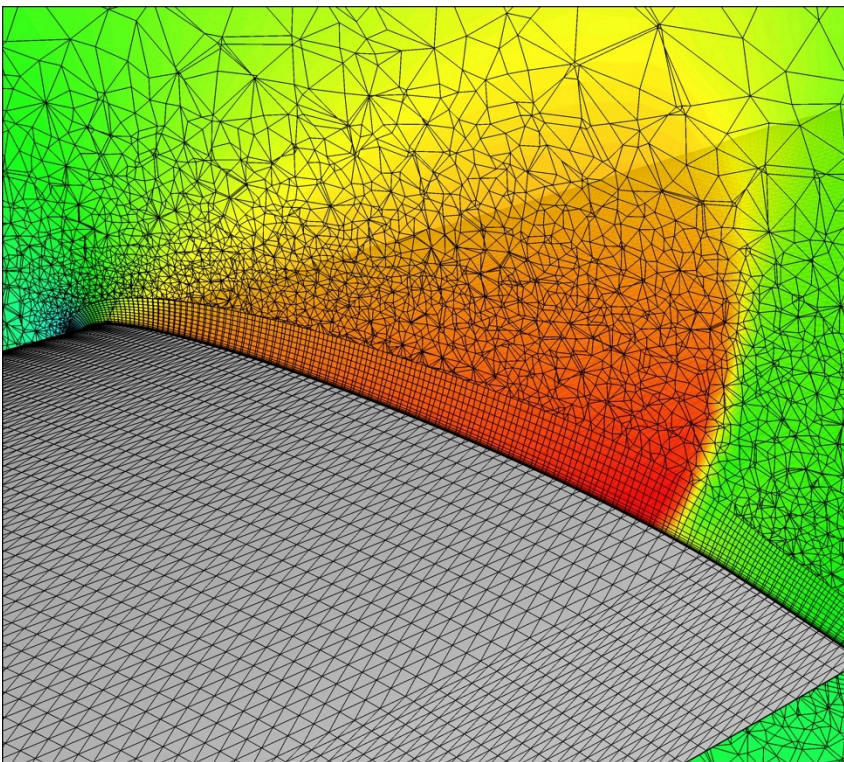
Fluid dynamics is the study of the motion of fluids, usually in the presence of an object. Typical fluid flows of interest to engineers and scientist include flow in pipes, through engines, and around objects, such as buildings, automobiles, and airplanes. Computational fluid dynamics (CFD) is the study of these flows using a numerical approach. CFD involves the solution of conservation equations (mass, momentum, energy, and others) in a finite domain.

Many CFD tools are currently available, including specialized and *in-house* tools. This variety is the result of the broad domain of physical problems solved with CFD. There is not a universal code for all applications, although there are packages that offer great capabilities. Broad CFD capabilities are available in commercial packages, such as ANSYS Fluent, Siemens Simcenter STAR-CCM+, Metacomp Technologies CFD++, and open-source packages, such as OpenFOAM and SU2.

A typical CFD simulation involves the following four steps:

- **Define the geometry** — In some cases, this step is simple, such as modeling flow in a duct. In other cases, this step involves complex components and moving parts, such as modeling a gas turbine engine. For many cases, the geometry creation is extremely time-consuming. The geometry step is graphics intensive and requires a capable graphics workstation, preferably with a Graphics Processing Unit (GPU). Often, the geometry is provided by a designer, but the CFD engineer must “clean” the geometry for input into the flow solver or mesh generation tool. This can be a tedious and time-consuming step and can sometimes require a large amount of system memory (RAM) depending on the complexity of the geometry.

- **Generate the mesh or grid** — Mesh generation is a critical step because computational accuracy is dependent on the size, cell location, and skewness or orthogonality of the cells. In the following figure, a hybrid mesh is shown on a slice through an aircraft wing. Mesh generation can be iterative with the solution, where fixes to the mesh are driven by an understanding of flow features and gradients in the solution. Meshing is frequently an interactive process and its elliptical nature generally requires a substantial amount of memory. Like geometry definition, generating a single mesh can take hours, days, weeks, and sometimes months. Many mesh generation codes are still limited to a single node, so general-purpose [Amazon Elastic Compute Cloud](#) (Amazon EC2) instances, such as the M family, or memory-optimized instances, such as the R family, are often used.



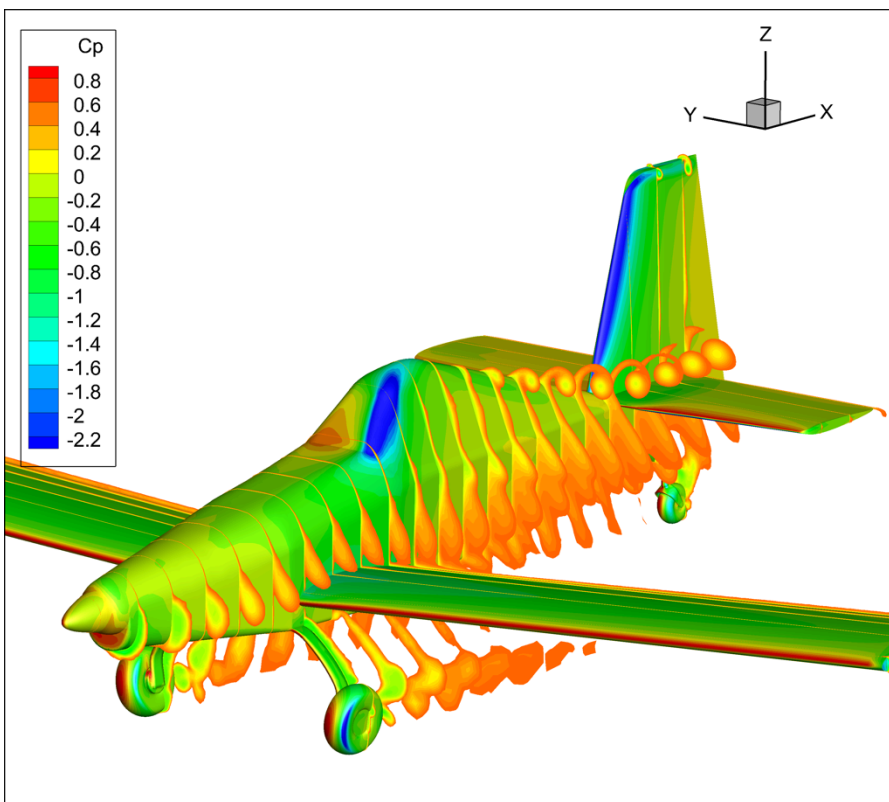
Mesh generation

- **Solve for the solution** — This step is the primary focus of this whitepaper. For some solutions, tens of thousands of cores (processors) run over weeks to achieve a solution. Conversely, some jobs may run in just minutes when scaled out appropriately.

There are choices for model equations depending on the desired solution fidelity. The [Navier-Stokes equations](#) form the basis of the solved equations for most fluid calculations. The addition

of chemical reactions, liquid and gas multi-phase flows, and many other physical properties create increasing complexity. For example, increasing the fidelity of turbulence modeling is achieved with various approximate equation sets such as Reynolds Average Navier-Stokes (RANS), Large Eddy Simulation (LES), Delayed Detached Eddy Simulation (DDES), and Direct Numerical Simulation (DNS). These approaches typically do not change the fundamental computational characteristics or scaling of the simulation.

- **Post process through visualization** — Examples of this step include the creation of images, video, and post processing of flow fields, such as creating total forces and moments. Similar to the geometry and mesh steps, this can be graphics and memory intensive, and graphics processing units (GPUs) are often favored.



Post-processing visualization

Are you Well-Architected?

The AWS Well-Architected Framework helps you understand the pros and cons of the decisions you make when building systems in the cloud. The six pillars of the Framework allow you to learn architectural best practices for designing and operating reliable, secure, efficient, cost-effective, and sustainable systems. Using the [AWS Well-Architected Tool](#), available at no charge in the [AWS Management Console](#), you can review your workloads against these best practices by answering a set of questions for each pillar.

For more expert guidance and best practices for your cloud architecture—reference architecture deployments, diagrams, and whitepapers—refer to the [AWS Architecture Center](#).

Why CFD on AWS?

AWS is a great place to run CFD cases. CFD workloads are typically tightly coupled workloads using a Message Passing Interface (MPI) implementation and relying on a large number of cores across many nodes. Many of the AWS instance types, such as the compute family instance types, are designed to include support for this type of workload. AWS has network options that support extreme scalability and short turn-around time as necessary.

CFD workloads typically scale well on the cloud. Most codes rely on domain decomposition to distribute portions of the calculation to the compute nodes. A case can be run highly parallel to receive results in minutes. Additionally, large numbers of cases can run simultaneously as efficiently and cheaply as possible to allow the timely completion of all cases.

The cloud offers a quick way to deploy and turn around CFD workloads at any scale without the need to own your own infrastructure. You can run jobs that once were in the realm of national labs or large industry. In just an hour or two, you can deploy CFD software, upload input files, launch compute nodes, and complete jobs on a large number of cores. When your job completes, results can be visualized and downloaded, and then all resources can be ended – so you only pay for what you use. If preferred, your results can be securely archived on AWS using a storage service, such as [Amazon Simple Storage Service](#) (Amazon S3). Due to cloud scalability, you have the option to run multiple cases simultaneously with a dedicated cluster for each case.

The cloud accommodates the variable demand of CFD. Often, there is a need to run a large number of cases as quickly as possible. Situations can require a sudden burst of tens, hundreds, or thousands of calculations immediately, and then perhaps no runs until the next cycle. The need to run a large number of cases could be for a preliminary design review, or perhaps a sweep of cases for the creation of a solution database. On the cloud, the cost is the same to run many jobs simultaneously, in parallel, as it is to run them serially, so you can get your data more quickly and at no extra cost. The cost savings in engineering time is an often-forgotten part of cost analysis. Running in parallel can be an ideal solution for design optimization.

Cloud computing is a strong choice for other CFD steps. You can easily change the underlying hardware configuration to handle the geometry, meshing, and post-processing. With remote visualization software available to handle the display, you can manage the GPU instance running your post-processing visualization from any screen (laptop, desktop, web browser) as though you were working on a large workstation.

Getting started with AWS

To begin, you must [create an AWS account](#) and an [AWS Identity and Access Management \(IAM\)](#) user. An IAM user is a user within your AWS account. The IAM user allows authentication and authorization to AWS resources. Multiple IAM users can be created if multiple people need access to the same AWS account.

During the first year after account activation, many AWS services are available for free with the [AWS Free Tier](#). The free-tier program provides an opportunity to learn about AWS without incurring significant charges. It provides an offset to charges incurred while training on AWS. However, the compute-heavy nature of CFD means that charges are regularly not covered by the free tier. Training helps limit mistakes resulting in unnecessary charges. You can also set up [AWS billing alarms](#) to alert you of estimated charges.

After creating an AWS account, you are provided with what is referred to as your root user. It is recommended that you do *not* use this root user for anything other than billing. Instead, set up privileged users (through IAM) for day-to-day usage of AWS. IAM users are useful because they help you securely control access to AWS resources within your account. Use IAM to control authentication and authorization for resources. [Create IAM users](#) for everyone, including yourself, and preserve the root user for the required account and service [management tasks](#).

By default, your account is limited on the number of instances that you can launch in a [Region](#), which is a physical location around the world where AWS clusters data centers. These limits are initially set low to prevent unnecessary charges, but you can raise them to preferred values. CFD applications often require a large number of compute instances simultaneously. The ability and advantages of scaling horizontally are highly desirable for high performance computing (HPC) workloads. However, you may need to request an increase to the [Amazon EC2 service limits](#) before deploying a large workload to either one large cluster, or too many smaller clusters at once.

If you want to understand more about the underlying services, a few foundational tutorials can be helpful to get started on AWS:

- [Amazon EC2](#) is the Amazon Web Service you use to create and run compute nodes in the cloud. AWS calls these compute nodes “instances”. This [Launch a Linux Virtual Machine with Amazon Lightsail](#) tutorial will help you successfully launch a Linux compute node on Amazon EC2 within our AWS Free Tier.
- [Amazon S3](#) is a service that enables you to store your data (referred to as *objects*) at massive scale. This [Store and Retrieve a File with Amazon S3](#) tutorial will help you store your files in the

cloud using Amazon S3 by creating an Amazon S3 bucket, uploading a file, retrieving the file, and deleting the file.

- [AWS Command Line Interface](#) (AWS CLI) is a common programmatic tool for automating AWS resources. For example, you can use it to deploy AWS infrastructure or manage data in S3. In this [AWS Command Line Interface](#) tutorial, you learn how to use the AWS CLI to access Amazon S3. You can then easily build your own scripts for moving your files to the cloud and easily retrieving them as needed.
- [AWS Budgets](#) gives you the ability to set custom budgets that alert you when your costs or usage exceed (or are forecasted to exceed) your budgeted amount. In the [Control your AWS costs with the AWS Free Tier and AWS Budgets](#) tutorial, you learn how to control your costs while exploring AWS service offerings using the AWS Free Tier, then using AWS Budgets to set up a cost budget to monitor any costs associated with your usage.

A dedicated [Running CFD on AWS workshop](#) has been created to guide you through the process of running your CFD codes on AWS. This workshop has step-by-step instructions for common codes like Simcenter STAR-CCM+, OpenFOAM, and ANSYS Fluent.

Additionally, the [AWS Well-Architected Framework High Performance Computing \(HPC\) Lens](#) covers common HPC scenarios and identifies key elements to ensure that your workloads are architected according to best practices. It focuses on how to design, deploy, and architect your HPC workloads on the AWS Cloud.

CFD approaches on AWS

Most CFD solvers have locality of data and use sparse matrix solvers. Once properly organized (application dependent), a well-configured job exhibits good strong and weak scaling on simple AWS cluster architectures. “Structured” and “Unstructured” codes are commonly run on AWS. Spectral and pseudo-spectral methods involve [fast Fourier transforms](#) (FFTs), and while less common than traditional CFD algorithms, they also scale well on AWS. Your architectural decisions have tradeoffs, and AWS makes it quick and easy to try different architectures to optimize for cost and performance.

Architectures

There are two primary design patterns to consider when choosing an AWS architecture for CFD applications: the *traditional* cluster and the *cloud native* cluster. Customers choose their preferred architecture based on the use case and the CFD users’ needs. For example, use cases that require frequent involvement and monitoring, such as when you need to start and stop the CFD case several times on the way to convergence, often prefer a traditional style cluster.

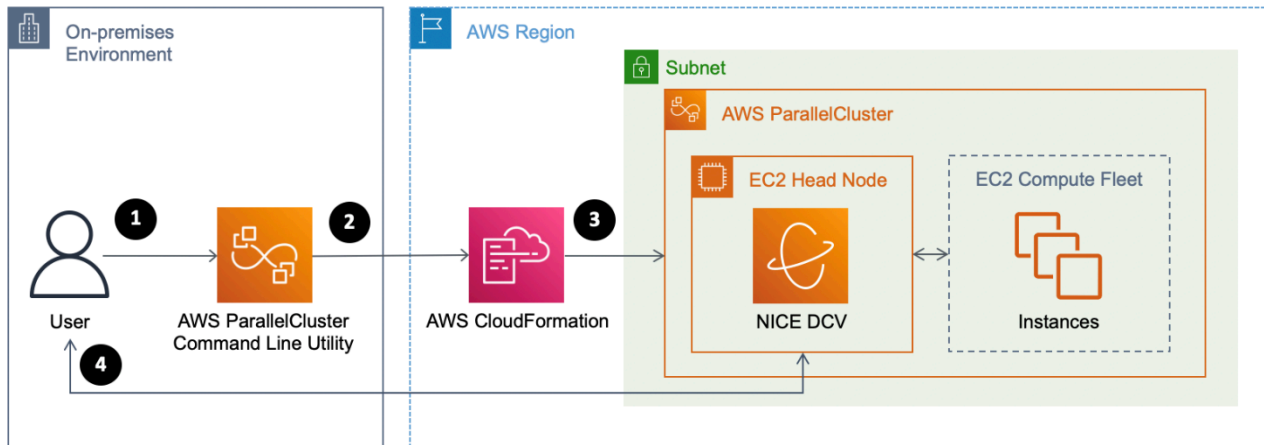
Conversely, cases that are easily automated often prefer a cloud native setup, which enables you to easily submit large numbers of cases simultaneously or automate your run for a complete end-to-end solution. Cloud native is useful when cases require special pre- or post-processing steps which benefit from automation. Whether choosing traditional or cloud native architectures, the cloud offers the advantage of elastic scalability — enabling you to only consume and pay for resources when you need them.

Traditional cluster environments

In the cloud, a traditional cluster is also referred to as a *persistent cluster* due to the persistence of minimal AWS infrastructure required for preserving the cluster environment. Examples of persistent infrastructure include a node running a scheduler and hosting data even after a completed run campaign. The persistent cluster mimics a traditional on-premises cluster or supercomputer experience. Clusters include a login instance with a scheduler that allows multiple users to submit jobs. The compute node fleet can be a fixed size or a dynamic group to increase and decrease the number of compute instances depending on the jobs submitted.

[AWS ParallelCluster](#) is an example of a persistent cluster that simplifies the deployment and management of HPC clusters in the AWS Cloud. It enables you to quickly launch and terminate an HPC compute environment in AWS as needed. AWS ParallelCluster orchestrates the creation of the

required resources (for example, compute nodes and shared filesystems) and provides an automatic scaling mechanism to adjust the size of the cluster to match the submitted workload. You can use AWS ParallelCluster with a variety of batch schedulers, including [Slurm](#) and [AWS Batch](#).



Example AWS ParallelCluster architecture

An AWS ParallelCluster architecture enables the following workflow:

- Creating a desired configuration through a text file
- Launching a cluster through the AWS ParallelCluster Command Line Utility (CLI)
- Orchestrating AWS services automatically through [AWS CloudFormation](#)
- Accessing the cluster through the command line with Secure Shell Protocol (SSH) or graphically with NICE DCV

Cloud native environments

A cloud native cluster is also called an *ephemeral cluster* due to its relatively short lifetime. A cloud native approach to tightly coupled HPC ties each run, or sweep of runs, to its own cluster. For each case, resources are provisioned and launched, data is placed on the instances, jobs run across multiple instances, and case output is retrieved automatically or sent to Amazon S3. Upon job completion, the infrastructure is ended. Clusters designed this way are ephemeral, treat infrastructure as code, and allow for complete version control of infrastructure changes. Login nodes and job schedulers are less critical and often not used at all with an ephemeral cluster. The following are a few frequently used methods to implement such a design:

- **Scripted approach** — A common quick-start approach for CFD users getting started with AWS is to combine a custom [Amazon Machine Image](#) (AMI) with the AWS CLI and a bash script. After

launching an Amazon EC2 instance, software can be added to the instance and an AMI is created to be used as the starting point for all compute nodes. It is typical to set up the [SSH](#) files and the [.bashrc](#) file before creating the custom AMI or “golden image.” Although many CFD solvers do not require a shared file location, one can easily be created with an exported network file system (NFS) volume, or with [Amazon FSx for Lustre](#), an AWS managed Lustre file system.

- **API based** — If preferred, an automated deployment can be developed with one of the [Software Development Kits](#) (SDKs), such as Python, available for programming an end-to-end solution.
- **CloudFormation templates** — [AWS CloudFormation](#) is an AWS Cloud native approach to provisioning AWS resources based on a JSON or YAML template. AWS CloudFormation offers an easily version-controlled cluster provisioning capability.
- **AWS Batch** — [AWS Batch](#) is a cloud-native, container-based approach that enables CFD users to efficiently run hundreds of thousands of batch computing jobs in containers on AWS. AWS Batch dynamically provisions the optimal quantity and type of compute resources (for example, compute or memory-optimized instances) based on the volume and specific resource requirements of the batch jobs submitted.

With AWS Batch, there is no need to install and manage batch computing software or server infrastructure that you use to run your jobs — enabling you to focus on analyzing results and solving problems. AWS Batch plans, schedules, and runs your batch computing workloads across the full range of AWS compute services and features, such as Amazon EC2 and [Spot Instances](#). AWS Batch can also be used as a job scheduler with [AWS ParallelCluster](#).

Software

Installation

CFD software can either be installed into a base AMI, or it can be used from prebuilt AMIs from the AWS Marketplace. If installing into a base AMI, a custom AMI can be created to launch new instances with the software already installed. The [AWS Marketplace](#) offers a listing of software from individual software vendors, which offer software included with AWS services. Finally, you can also add the installation to the cluster deployment scripts and run them at cluster creation.

Licensing

Many commercial CFD solvers are licensed and may require access to a license server, such as [FlexNet Publisher](#). Licensing software in the cloud is much like licensing with any other cluster. If

a license server is necessary, you can configure your networking to use an existing on-premises server, or you can host the license server on the cloud.

If hosting the license server on AWS, burstable general-purpose T instances in small sizes, such as micro, can be used for cost-effective hosting. A Reserved Instance purchase for the license server provides further cost savings.

The FlexNet Publisher license relies on the network interface's MAC address. The easiest way to retrieve the new MAC address for your license is to launch the instance and retrieve the MAC address before the license is issued. You can preserve the MAC address by changing the [ending behavior](#) to prevent deletion of the network interface if the instance is ever terminated. When hosting your own license server, confirm that the security group for the license-server instance allows connectivity on the appropriate ports required by the software package.

If accessing an on-premises license server, create an [AWS Site-to-Site VPN](#) for your Virtual Private Cloud (VPC), or alternatively, if on-premises firewalls allow, you may be able to access the on-premises license server through SSH tunneling.

Cloud-friendly licensing through power-on-demand licensing keys is also growing in popularity and relies on submitting a job with a key provided by the software provider.

Setup

There are multiple strategies for setting up software in clusters. The most widely used examples are below:

Create a custom AMI

This method features the shortest application startup time and avoids potential bottlenecks when accessing a single shared resource. This is the preferred means of distribution for large-scale runs (tens of thousands of MPI ranks) or applications that must load a large number of shared libraries. A drawback is the larger AMI size, which incurs more cost for [Amazon Elastic Block Store](#) (Amazon EBS).

Share an Amazon EBS volume via NFS

This method installs the necessary software into a single Amazon EBS volume, creates an NFS export on a single instance, and mounts the NFS share on all of the compute instances. This approach reduces the Amazon EBS footprint because only one Amazon EBS volume must be

created for the software. This method is useful for large software packages and moderate scale runs (up to thousands of MPI ranks).

To optimize input/output (I/O) performance, different EBS volume types are available offering different performance characteristics. A tradeoff with this method is a small amount of added network traffic and a potential bottleneck with a single instance hosting the NFS share. Ensuring a larger NFS host instance with additional network capabilities mitigates these concerns.

To make this approach repeatable, the exported NFS directory can be decoupled from the root volume, stored on a separate [Amazon EBS volume](#), and created from an [Amazon EBS snapshot](#). This approach is similar to the custom AMI method, but instead it isolates software from the root volume. An additional Amazon EBS volume is created from an Amazon EBS snapshot at instance launch and is mounted as an additional disk to the compute instance. The snapshot used to create the volume contains the software installation. Decoupling the user software from operating system updates that are necessary on the root volume reduces the complexity of maintenance. Furthermore, the user can rely on the latest AMI releases for the compute instances, which provide an up-to-date system without maintaining a custom AMI.

Use a managed shared file system

This approach installs the CFD software into an AWS managed file system service, such as Amazon FSx for Lustre or [Amazon Elastic File System](#) (Amazon EFS), and mounts the shared file system on all of the compute instances. Amazon FSx for Lustre provides a high-performance, parallel file system optimized for HPC workloads. Lustre is optimized for simultaneous access, and its performance can be scaled independently from any single instance size.

FSx for Lustre works natively with Amazon S3 and can be automatically populated with data residing in S3, which enables users to have a Lustre file system running only while compute jobs are active and easily discard it afterwards.

Amazon EFS provides a simple, scalable, fully managed elastic NFS file system that can be used as a location for home directories. However, EFS is not recommended for other aspects of a CFD cluster, such as hosting simulation data or compiling a solver, due to performance considerations.

Maintenance

New feature releases and patches to existing software are a frequent need in the CFD application workflow. All distribution strategies can be fully automated. When using the AMI or Amazon EBS snapshot strategy, the software update cycle can be isolated from the application runs. Once a

new AMI or snapshot has been created and tested, the cluster is reconfigured to pick up the latest version. Software updates cycles in the strategies using file sharing via NFS or FSx for Lustre must be coordinated with application runs because a live system is being altered.

In general, automating CFD application installation with scripting tools is recommended and is usually referred to as a Continuous Integration/Continuous Deployment (CI/CD) pipeline on AWS. The automation process reduces the manual processes required to build and deploy new software and security patches to HPC systems. This is useful if you want to use the latest features in software packages with fast update cycles. You can read more about CI/CD pipelines in the [AWS Continuous Delivery documentation](#).

Cluster lifecycle

AWS offers a variety of unique ways to design architectures that deploy HPC workloads. Your choice of deployment method for a particular workload depends on a number of factors, including your desired user experience, degree of automation, experience with AWS, preferred scripting languages, size and number of cases, and the lifecycle of your data. The [High Performance Computing Lens](#) whitepaper covers additional best practices for architectures beyond what is discussed in this paper.

While the architecture for a cluster is typically unique and tailored for the workload, all HPC clusters benefit from lifecycle planning and management of the cluster and the data produced — allowing for optimized performance, reliability, and cost.

It is not unusual for an on-premises cluster to run for many years, perhaps without significant operating system (OS) update or modification, until the hardware is obsolete thus rendering it useless. In contrast, AWS regularly releases new services and updates to improve performance and lower costs. The easiest way to take advantage of new AWS capabilities, such as new instances, is by maintaining the cluster as a script or template. AWS refers to this as “Infrastructure as Code” because it allows for the creation of clusters quickly, provides repeatable automation, and maintains reliable version control.

Examples of “cluster as code” are the [AWS ParallelCluster configuration file](#), deployment scripts, or [CloudFormation templates](#). These text-based configurations are easy to modify for a new capability or workload.

A view of the cluster lifecycle includes infrastructure as code that starts before the cluster is deployed with the maintenance of the deployment scripts. Elements of a cluster maintained as code include:

- Base AMI to build your cluster
- Automated software installation scripts
- Configuration files, such as scheduler configs, MPI configurations, and .bashrc
- Text description of the infrastructure, such as a CloudFormation template, or an AWS ParallelCluster configuration file
- Script to initiate cluster deployment and subsequent software installation

While the nature of a cluster changes depending on the type of workload, the most cost-effective clusters are those that are deployed only when they are actively being used.

The cluster lifecycle can have a significant impact on costs. For example, it is common with many traditional on-premises clusters to maintain a large storage volume. This is not necessary in the cloud because data can be easily moved to S3 where it is reliably and cheaply stored. Maintaining a cluster as code allows you to place a cluster under version control and repeatedly deploy replicas if needed.

Each cluster maintained as code can be instantiated multiple times if multiple clusters are required for testing, onboarding new users, or running a large number of cases in parallel. If set up correctly, you avoid idle infrastructure when jobs are not running.

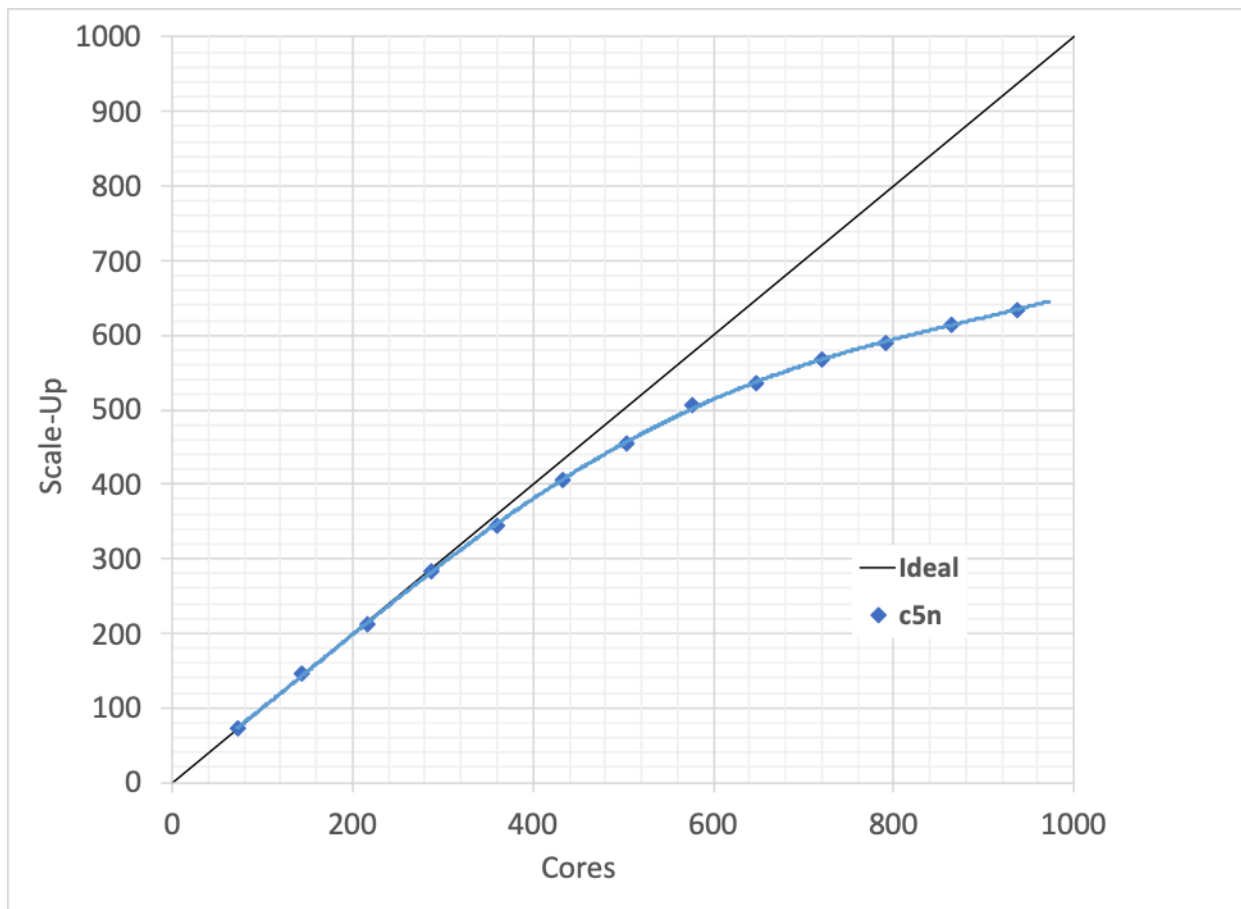
CFD case scalability

CFD cases that cross multiple nodes raise the question, “How will my application scale on AWS?” CFD solvers depend heavily on the solver algorithm’s ability to scale compute tasks efficiently in parallel across multiple compute resources. Parallel performance is often evaluated by determining an application’s scale-up. Scale-up is a function of the number of processors used and is defined as the time it takes to complete a run on one processor, divided by the time it takes to complete the same run on the number of processors used for the parallel run.

$$ScaleUp(N) = \frac{Time\ to\ Run\ on\ 1\ Compute\ Node}{Time\ to\ Run\ on\ N\ Compute\ Nodes}$$

Scale-up equation

Scaling is considered to be excellent when the scale-up is close to or equal to the number of processors on which the application is run. An example of scale up as a function of core count is shown in the following figure.



Strong scaling demonstrated for a 14M cell external aerodynamics use case

The example case in preceding figure is a 14 million cell external aerodynamics calculation using a cell-centered unstructured solver. The mesh is composed largely of hexahedra. The black line shows the ideal or perfect scalability. The blue diamond-based curve shows the actual scale-up for this case as a function of increasing processor count. Excellent scaling is seen to almost 1000 cores for this small-sized case. This example was run on Amazon EC2 c5n.18xlarge instances, with Elastic Fabric Adapter (EFA), and using a fully loaded compute node.

Fourteen million cells is a relatively small CFD case by today's standards. A small case was purposely chosen for the discussion on scalability because small cases are more difficult to scale. The idea that small cases are harder than large cases to scale may seem counter intuitive, but smaller cases have less total compute to spread over a large number of cores. An understanding of strong scaling vs. weak scaling offers more insight.

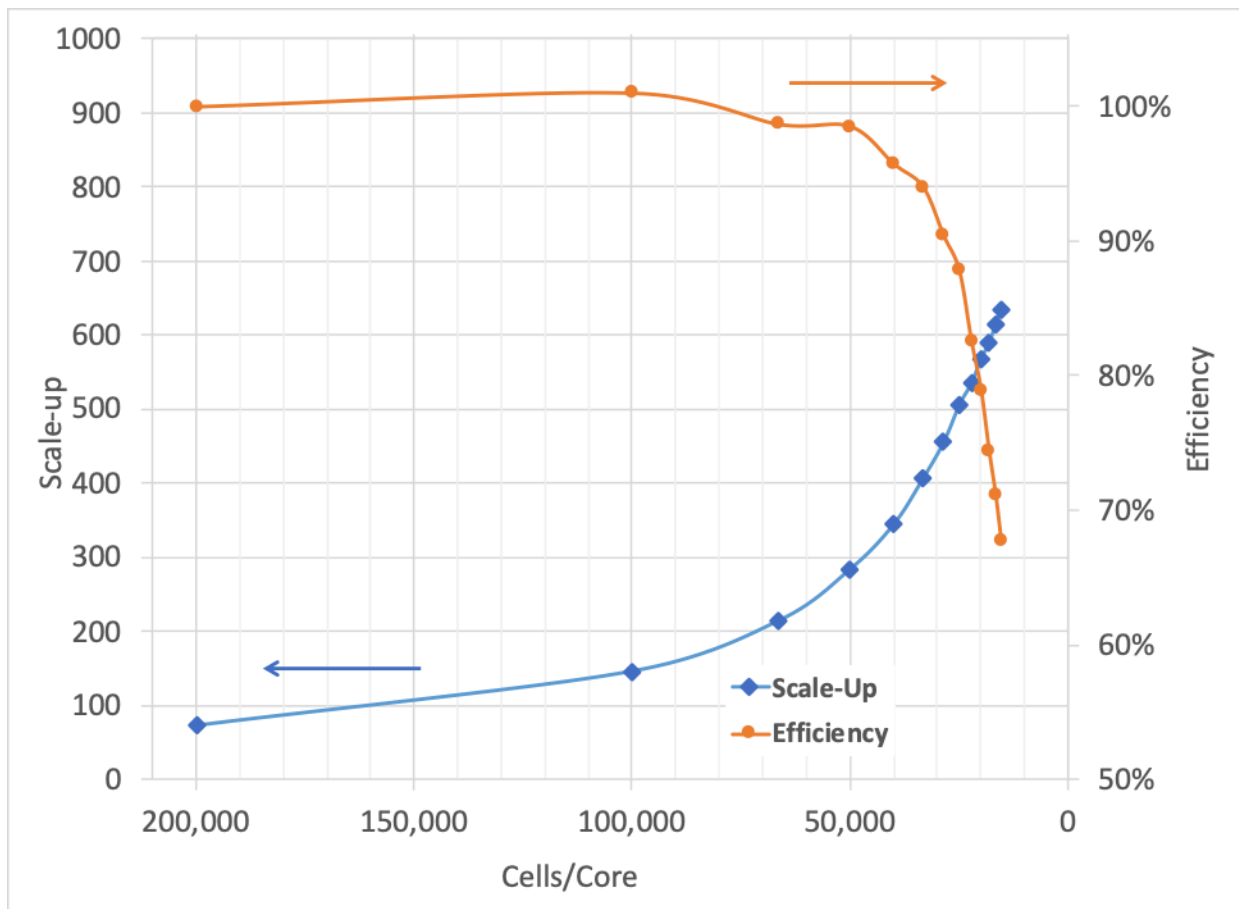
Strong scaling vs. weak scaling

Case scalability can be characterized two ways: strong scaling or weak scaling. Weak does not mean inadequate — it is a technical term facilitating the description of the type of scaling.

Strong scaling, as demonstrated in the following figure, is a traditional view of scaling, where a problem size is fixed and spread over an increasing number of processors. As more processors are added to the calculation, good strong scaling means that the time to complete the calculation decreases proportionally with increasing processor count.

In comparison, weak scaling does not fix the problem size used in the evaluation, but purposely increases the problem size as the number of processors also increases. The ratio of the problem size to the number of processors on which the case is run is constant. For a CFD calculation, problem size most often refers to the number of cells or nodes in the mesh for a similar configuration.

An application demonstrates good weak scaling when the time to complete the calculation remains constant as the ratio of compute effort to the number of processors is held constant. Weak scaling offers insight into how an application behaves with varying case size. Well-written CFD solvers offer excellent weak scaling capability allowing for more cores to be used when running bigger applications. The scalability of CFD cases can then be determined by looking at a normalized plot of scale-up based on the number of mesh cells per core (cells/core). An example plot is shown in the following figure.



Scale-up and efficiency as a function of cells per processor

Running efficiency

Efficiency is defined as the scale-up divided by the number of processors used in the calculation. Scale-up and efficiency as a function of cells/core is shown in the preceding figure. In this figure, the cells per core are on the horizontal axis. The blue diamond-based line shows scale-up as a function of mesh cells per processor. The vertical axis for scale-up is on the left-hand side of the graph as indicated by the lower blue arrow. The orange circle-based line shows efficiency as a function of mesh cells per core. The vertical axis for efficiency is shown on the right side of the graph and is indicated by the upper orange arrow.

$$Efficiency(N) = \frac{ScaleUp}{N} * 100$$

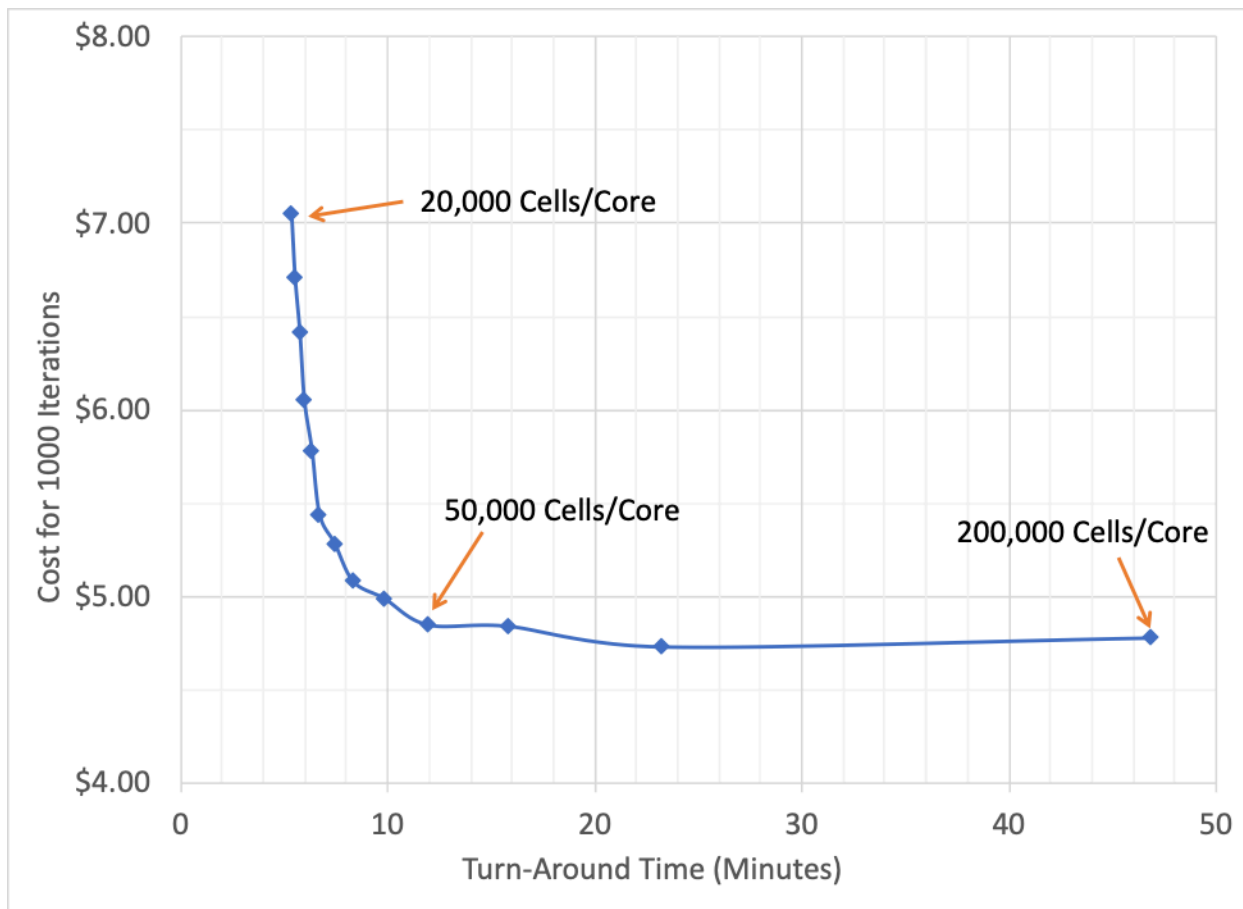
Running efficiency and scale-up equation

For similar case types, running with similar solver settings, a plot like the one in this figure can help you choose the desired efficiency and number of cores running for a given case.

Efficiency remains at about 100% between approximately 200,000 mesh cells per core and 100,000 mesh cells per core. Efficiency starts to fall off at about 50,000 mesh cells per core. An efficiency of at least 80% is maintained until 20,000 mesh cells per core, for this case. Decreasing mesh cells per core leads to decreased efficiency because the total computational effort per core is reduced. The inefficiencies that show up at higher core counts come from a variety of sources and are caused by “serial” work. Serial work is the work that cannot be effectively parallelized. Serial work comes from solver inefficiencies, I/O inefficiencies, unequal domain decomposition, additional physical modeling such as radiative effects, additional user-defined functions, and eventually, from the network as core count continues to increase.

Turn-around time and cost

Plots of scale-up and efficiency offer an understanding about how a case or application scales. However, what matters most HPC users is case turn-around time and cost. A plot of turn-around time versus CPU cost for this case is shown in the following figure. As the number of cores increases, the inefficiency also increases, which leads to increased costs.



Cost for per run based on on-demand pricing for the c5n.18xlarge instance as a function of turn-around time

In the preceding figure, the turn-around time is shown on the horizontal axis. The cost is shown on the vertical axis. The price is based on the “on-demand” price of a c5n.18xlarge for 1000 iterations, and only includes the computational costs. Small costs are also incurred for data storage. Minimum cost was obtained at approximately 50,000 cells per core or more. As the efficiency is 100% over a range of core counts, the price is the same regardless of the number of cores. Many users choose a cell count per core to achieve the lowest possible cost.

As core count goes up, inefficiencies start to show up, but turn-around time continues to drop. When a fast turn-around is needed, users may choose a large number of cores to accelerate the time to solution. For this case, a turn-around time of about five minutes can be obtained by running on about 20,000 cells per core. When considering total cost, the inclusion of license costs may make the fastest run the cheapest run.

Optimizing HPC components

The AWS Cloud provides a broad range of scalable, flexible infrastructure services that you select to match your workloads and tasks. This gives you the ability to choose the most appropriate mix of resources for your specific applications. Cloud computing makes it easy to experiment with infrastructure components and architecture design. The HPC solution components listed below are a great starting point to set up and manage your HPC cluster. Always test various solution configurations to find the best performance at the lowest cost.

Compute

The optimal compute solution for a particular HPC architecture depends on the workload deployment method, degree of automation, usage patterns, and configuration. Different compute solutions may be chosen for each step of a process. Selecting the appropriate compute solution for an architecture can lead to higher performance efficiency and lower cost.

There are multiple compute options available on AWS, and at a high level, they are separated into three categories: instances, containers, and functions. Amazon EC2 instances, or servers, are resizable compute capacity in the cloud. Containers provide operating system virtualization for applications that share an underlying operating system installed on a server. Functions are a serverless computing model that allows you to run code without thinking about provisioning and managing the underlying servers. For CFD workloads, EC2 instances are the primary compute choice.

Amazon EC2 lets you choose from a variety of compute instance types that can be configured to suit your needs. Instances come in different families and sizes to offer a wide variety of capabilities. Some instance families target specific workloads, for example, compute-, memory-, or GPU-intensive workloads, while others are general purpose. Both the targeted-workload and general-purpose instance families are useful for CFD applications based on the step in the CFD process.

When considering CFD steps, different instance types can be targeted for pre-processing, solving, and post-processing. In pre-processing, the geometry step can benefit from an instance with a GPU, while the mesh generation stage may require a higher memory-to-core ratio, such as general-purpose or memory-optimized instances. When solving CFD cases, evaluate your case size and cluster size.

If the case is spread across multiple instances, the memory requirements are low per core, and compute-optimized instances are recommended as the most cost-effective and performant choice.

If a single-instance calculation is desired, it may require more memory per core and benefit from a general-purpose, or memory-optimized instance.

Optimal performance is typically obtained with compute-optimized instances (Intel, AMD, or Graviton), and when using multiple instances with cells per core below 100,000, instances with higher network throughput and packet rate performance are preferred. Refer to the [Instance Type Matrix](#) for instance details.

AWS enables simultaneous multithreading (SMT), or hyper-threading technology for Intel processors, commonly referred to as “hyperthreading” by default for supported processors. Hyperthreading improves performance for some systems by allowing multiple threads to be run simultaneously on a single core. Most CFD applications do not benefit from hyperthreading, and therefore, disabling it tends to be the preferred environment. Hyperthreading is easily disabled in Amazon EC2. Unless an application has been tested with hyperthreading enabled, it is recommended that hyperthreading be disabled and that processes are launched and pinned to individual cores.

There are many compute options available to optimize your compute environment. Cloud deployment allows for experimentation on every level from operating system to instance type to bare-metal deployments. Time spent experimenting with cloud-based clusters is vital to achieving the desired performance.

Network

Most CFD workloads exceed the capacity of a single compute node and require a cluster-based solution. A crucial factor in achieving application performance with a multi-node cluster is optimizing the performance of the network connecting the compute nodes.

Launching instances within a cluster placement group provides consistent, low latency within a cluster. Instances launched within a cluster placement group are also launched to the same Availability Zone.

To further improve the network performance between EC2 instances, you can use an Elastic Fabric Adapter (EFA) on select [instance types](#). EFA is designed for tightly coupled HPC workloads by providing an operating system (OS)-bypass capability and hardware-designed reliability to take advantage of the EC2 network. It works well with CFD solvers. OS-bypass is an access model that allows an application to bypass the operating system’s TCP/IP stack and communicate directly with the network device. This provides lower and more consistent latency and higher throughput than

the TCP transport traditionally used. When using EFA, your normal IP traffic remains routable and can communicate with other network resources.

CFD applications use EFA through a message passing interface (MPI) implementation using the [Libfabric](#) API. EFA usage can be confirmed with the MPI runtime debugging output. Each MPI implementation has environment variables or command-line flags for verbose debugging output or explicitly setting the fabric provider. These options vary by MPI implementation, and access to these options vary by CFD application. Refer to [Getting Started with EFA and MPI documentation](#) for additional details.

Storage

AWS provides many storage options for CFD, including object storage with [Amazon S3](#), block storage with [Amazon EBS](#), temporary block-level storage with [Amazon EC2 instance store](#), and file storage with [Amazon FSx for Lustre](#). You can utilize all these storage types for certain aspects of your CFD workload.

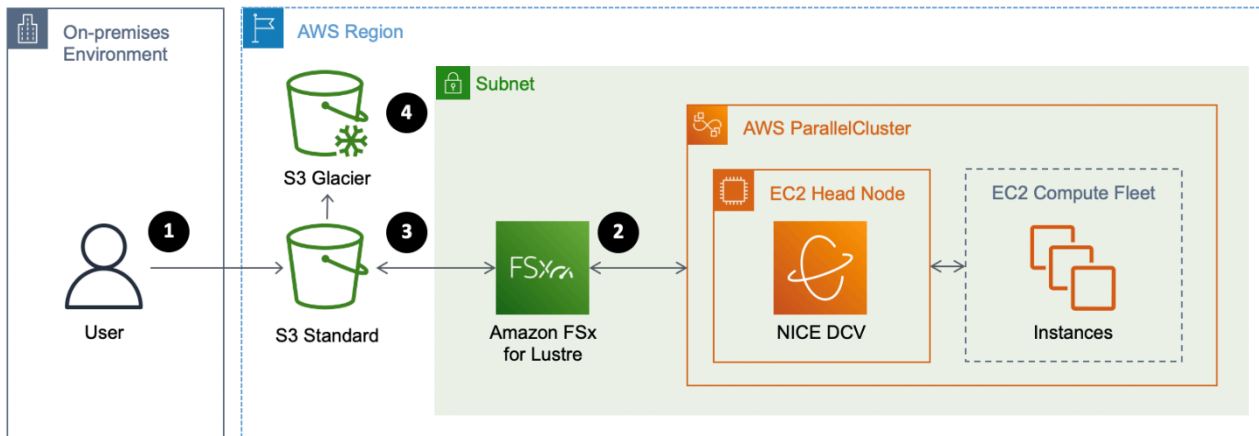
A vital part of working with CFD solvers on AWS is the management of case data, which includes files such as CAD, meshes, input files, and output figures. In general, all CFD users want to maintain availability of the data when it is in use and to archive a subset of the data if it's needed at some point in the future.

An efficient data lifecycle uses a combination of storage types and tiers to minimize costs. Data is described as hot, warm, and cold, depending on the immediate need of the data.

- **Hot data** is data that you need immediately, such as a case or sweep of cases about to be deployed.
- **Warm data** is your data, which is not needed at the moment, but it may be used sometime in the near future; perhaps within the next six months.
- **Cold data** is data that may not ever be used again, but it is stored for archival purposes.

Your data lifecycle can occur only within AWS, or it can be combined with an on-premises workflow. For example, you may move case data, such as a case file, from your local computing facilities, to Amazon S3, and then to an EC2 cluster. Completed runs can traverse the same path in reverse back to your on-premises environment or to Amazon S3 where they can remain in the S3 Standard or S3 Infrequent Access storage class, or transitioned to [Amazon S3 Glacier](#) through a [lifecycle rule](#) for archiving. Amazon S3 Glacier and S3 Glacier Deep Archive are S3 storage tiers that

offer deep discounts on storage for archival data. The following figure is an example data lifecycle for CFD.



Data lifecycle

1. Transferring input data to AWS
2. Running your simulation with input (hot) data
3. Storing your output (warm) data
4. Archiving inactive (cold) data

Transferring input data

Input data, such as a CAD file, may start on-premises and be transferred to AWS. Input data is often transferred to Amazon S3 and stored until you are ready to run your simulation. S3 offers highly scalable, reliable, durable, and secure storage. An S3 workflow decouples storage from your compute cluster and provides a cost-effective approach. Alternatively, you can transfer your input data to an existing file system at runtime. This approach is generally slower and less cost effective when compared to S3 because it requires more expensive resources, such as compute instances or managed file systems, to be running for the duration of the transfer.

For the data transfer, you can choose a manual, scripted, or managed approach. Manual and scripted approaches can use the AWS CLI for transferring data to S3, which helps optimize the data transfer to S3 by running parallel uploads. A managed approach can use a service, such as [AWS DataSync](#), to move input data to AWS. AWS DataSync makes it simple and fast to move large amounts of data online between on-premises storage and Amazon S3.

Running your CFD simulation

Input data for your CFD simulation is considered “hot” data when you are ready to run your simulation. This data is often accessed in a shared file system or placed on the head node if the CFD application does not require a shared drive.

If your CFD workload requires a high-performance file system, Amazon FSx for Lustre is highly recommended. FSx for Lustre works natively with Amazon S3, making it easy for you to access the input data that is already stored in S3. When linked to an S3 bucket, an FSx for Lustre file system transparently presents S3 objects as files and allows you to write results back to S3.

During the simulation, you can periodically checkpoint and write intermediate results to your S3 data repository. FSx for Lustre automatically transfers Portable Operating System Interface (POSIX) metadata for files, directories, and symbolic links (symlinks) when importing and exporting data to and from the linked data repository on S3. This allows you to maintain access controls and restart your workload at any time using the latest data stored in S3.

When your workload is done, you can write final results from your file system to your S3 data repository and delete your file system.

Storing output data

Output data from your simulation is considered “warm” data after the simulation finishes. For a cost-effective workflow, transfer the output data off of your cluster and terminate the more expensive compute and storage resources. If you stored your data in an Amazon EBS volume, transfer your output data to S3 with the AWS CLI. If you used FSx for Lustre, create a [data repository task](#) to manage the transfer of output data and metadata to S3 or export your files with [HSM commands](#). You can also periodically push the output data to S3 with a data repository task.

Archiving inactive data

After your output data is stored in S3 and is considered cold or inactive, transition it to a more cost-effective storage class, such as [Amazon S3 Glacier and S3 Glacier Deep Archive](#). These storage classes allow you to archive older data more affordably than with the S3 Standard storage class. Objects in S3 Glacier and S3 Glacier Deep Archive are not available for real-time access and must be [restored](#) if needed. Restoring objects incurs a cost, and to keep costs low yet suitable for varying needs, S3 Glacier and S3 Glacier Deep Archive provide multiple retrieval options.

Storage summary

Use the following table to select the best storage solution for your workload:

Table 1 — Storage services and their uses

Service	Description	Use
Amazon EBS	Block storage	Block storage or export as a Network File System (NFS) share
Amazon FSx for Lustre	Managed Lustre	Fast parallel high-performance file system optimized for HPC workloads
Amazon S3	Object storage	Store case files, input, and output data
Amazon S3 Glacier	Archival storage	Long-term storage of archival data
Amazon EFS	Managed NFS	Network File System (NFS) to share files across multiple instances. Occasionally used for home directories. Not generally recommended for CFD cases.

Visualization

A graphical interface is useful throughout the CFD solution process, from building meshes, debugging flow-solution errors, and visualizing the flow field. Many CFD solvers include visualization packages as part of their installation. As an example, [ParaView](#) is packaged with [OpenFOAM](#). In addition to visualization tools within the CFD suites, there are third-party visualization tools, which can be more powerful, adaptable, and general.

Post processing in AWS can reduce manual extractions, lower time to results, and decrease data transfer costs. Visualization is often performed remotely with either an application that supports client-server mode or with remote visualization of the server desktop. Client-server mode works well on AWS and can be implemented in the same way as other remote desktop set-ups. When using client-server mode for an application, it is important to connect to the server using the public IP address and not the private [IP address](#), unless you have private network connectivity configured, such as a Site-to-Site VPN.

AWS offers [NICE DCV](#) for local display of remote desktops. NICE DCV is easy to implement and is free to use with EC2. There are a variety of ways to add NICE DCV to your HPC cluster. The simplest approach is to launch AWS ParallelCluster. If you are using AWS ParallelCluster, you can [enable NICE DCV](#) on the head node when launching the cluster with a short addition in the configuration file. A graphics-intensive instance can be easily launched running a Linux or Windows NICE DCV AMI to have NICE DCV pre-installed. Refer to [Getting Started with NICE DCV on Amazon EC2](#) for more information.

AWS also offers managed desktop and application streaming services, such as [Amazon WorkSpaces](#) or [Amazon AppStream 2.0](#). Amazon WorkSpaces is a Desktop-as-a-Service solution providing Linux or Windows desktops while Amazon AppStream 2.0 is a non-persistent application and desktop streaming service for Windows environments.

In general, visualizing CFD results on AWS reduces the need to download large data back to on-premises storage, and it helps reduce cost and increase productivity.

Costs

AWS offers a pay-as-you-go approach for pricing for cloud services. You pay only for the individual services you need, for as long as you use them, without long-term contracts or complex licensing. Some services and tools incur no charge, such as [AWS ParallelCluster](#), [AWS Batch](#), and [AWS CloudFormation](#); however, the underlying AWS components used to run cases incur charges.

AWS charges arise primarily from the compute resources required for the CFD solution. Storage and data transfer also incur charges. Depending on your implementation, you may use additional services in your architecture, such as [AWS Lambda](#), [Amazon Simple Notification Service](#) (Amazon SNS), or [Amazon CloudWatch](#), but cost accumulated by usage of these services is rarely significant when compared to the compute costs for CFD.

It is common to stand up a cluster for only the time period in which it is needed. In a simple scenario, costs are associated with EC2 instances and Amazon EBS volumes. Costs incurred after shut down of the cluster include any snapshots taken of Amazon EBS volumes and any data stored on Amazon S3.

While data transfer into Amazon EC2 from the internet is free, data transfer out of AWS can incur modest charges. Many users choose to leave their data in S3 and only move the smaller post-processed data out of AWS. Data can also be transitioned to Amazon S3 Glacier for archival storage to reduce long-term storage costs.

When AWS ParallelCluster is maintained for an extended period of time, the login node and Amazon EBS volumes continue to incur costs. The compute nodes scale up and down as needed, which minimizes costs to only reflect the times when the cluster is being used.

When developing an architecture, you must monitor your workload (automatically through monitoring solutions or manually through the console) and ensure that your resources scale up and down as expected. Occasionally, hung jobs or other factors can prevent your resources from scaling properly. Logging on to the compute node and checking processes with a tool, such as [top](#) or [htop](#), can help debug issues.

AWS provides four different ways to [pay for EC2 instances](#):

- On-Demand Instances
- Reserved Instances
- Savings Plans

- **Spot Instances**

Amazon EC2 instance costs can be minimized by using Spot Instances, Savings Plans, and Reserved Instances.

- **On-Demand Instances** — With On-Demand Instances, you pay for compute capacity by the hour or the second, depending on which you run. No long-term commitments or upfront payments are needed. You can increase or decrease your compute capacity depending on the demands of your application and only pay the specified per-hour rates for the instance you use.

On-Demand Instances are the highest cost model for computing and require no upfront commitment. Cost saving is gained because costs are only incurred while the instances are in a running state. For a dynamic workload, the savings can be large. Savings occur because you can select the newest processor types, which may speed up the computations significantly.

- **Reserved Instances** — Reserved Instances (RIs) provide you with a significant discount (up to 75%) compared to On-Demand Instance pricing. For customers that have steady state or predictable usage and can commit to using EC2 over a 1- or 3-year term, Reserved Instances provide significant savings compared to using On-Demand Instances.
- **Savings Plans** — Savings Plans are a flexible pricing model that provides savings of up to 72% on your AWS compute usage. This pricing model offers lower prices on Amazon EC2 instances usage, regardless of instance family, size, OS, tenancy or AWS Region, and also applies to [AWS Fargate](#) usage.

Savings Plans offer significant savings over On-Demand Instances, just like EC2 Reserved Instances, in exchange for a commitment to use a specific amount of compute power (measured in \$/hour) for a one- or three-year period. You can sign up for Savings Plans for a one- or three-year term and easily manage your plans by taking advantage of recommendations, performance reporting, and budget alerts in the [AWS Cost Explorer](#).

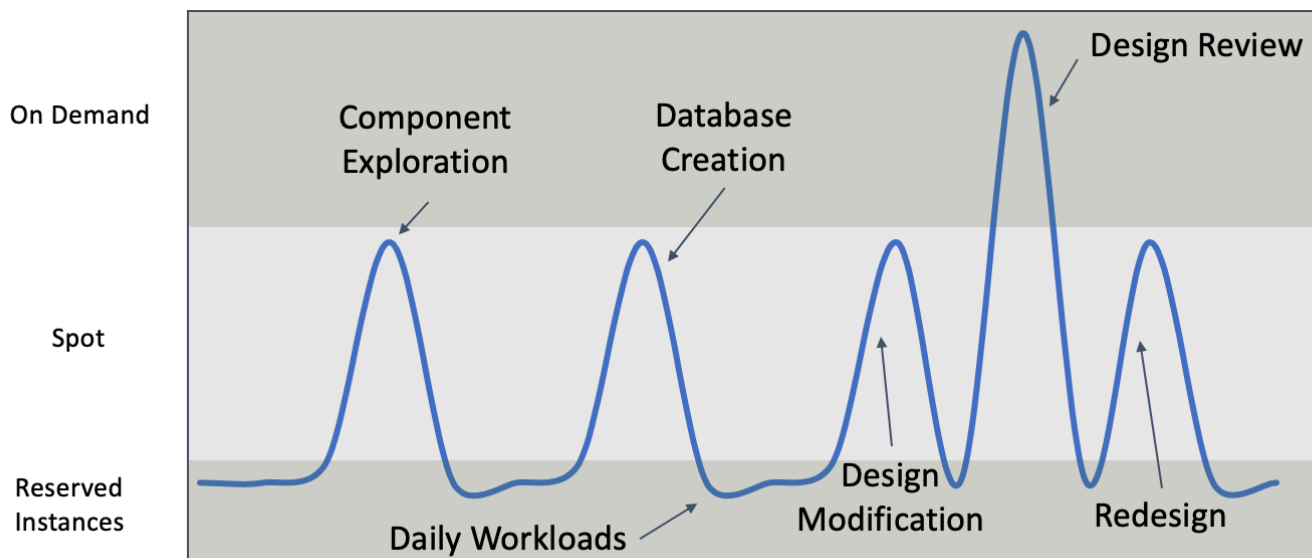
- **Spot Instances** — Amazon EC2 Spot Instances let you take advantage of unused EC2 capacity at up to a 90% discount compared to On-Demand prices. However, Spot Instances can be interrupted when EC2 needs to reclaim the capacity. Spot Instances are frequently the most cost-effective resource for flexible or fault-tolerant workloads and can also be used for CFD cases. Spot availability varies by spot pool (for example, Region, Availability Zone, and instance type). Consider your deployment strategy and interruption impact when determining the most cost-effective resources for your case.

When a Spot Instance is interrupted, your case is interrupted. The interruption impact to your case depends on how your CFD application handles the interruption, and you can minimize this impact by checkpointing your simulation if supported. In addition, you can minimize the risk of Spot Instance interruption by working with the Spot Advisor, being flexible on instance type and Availability Zone, and using advanced features, such as the capacity-optimized allocation strategy in EC2 Fleet, to launch your Spot Instances. Overall, the need to occasionally restart a workload can be offset by the cost savings of Spot Instances.

- **Combined approach** — You can easily combine Spot Instances with On-Demand and RIs to further optimize workload cost with performance. For example, in the following figure, you could use Reserved Instances for your daily workloads, Spot Instances for component exploration, and On-Demand Instances for design review.

Cost Optimization

Computational Fluid Dynamics



EC2 cost optimization for CFD cases

Conclusion

This whitepaper describes best practices for using AWS for computational fluid dynamics (CFD). The paper presents the advantages of using AWS for CFD workloads, covers the getting started process, discusses AWS approaches for CFD, and addresses the options for optimizing the HPC components for CFD workloads. Following the best practices presented in this paper allows you to architect and optimize your environment for CFD workloads.

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Further reading

For additional information, refer to:

- [CFD Workshop](#)
- [CFD on AWS](#)
- [HPC on AWS](#)
- [AWS Well-Architected Framework](#)
- [Introduction to HPC on AWS](#)

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AWS Glossary

For the latest AWS terminology, see the [AWS glossary](#) in the *AWS Glossary Reference*.