

Increasing performance with AMD

Amazon EC2 Hpc7a instances benchmarking





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1. Introduction

Do IT Now deployed an HPC cluster in the cloud, using AMD-based HPC-optimized instances on AWS, installed Altair applications on the infrastructure, and conducted benchmarks with reference models for each application. Do IT Now also compared results in terms of performance and costs for each application and instance combination.

During this analysis, Do IT Now also explored possible optimization patterns and parameters to tune the applications, the instances, and the overall HPC architecture in the cloud.

1.1 Objective

The objective of this project is to provide the results of the benchmarks conducted in the cloud environment, showing the baseline performance results and any additional optimizations that the Do IT Now team applied to the infrastructure, the software, and its parameters.

As an additional objective, Do IT Now will present and describe the various design steps, any issue and how it was solved, and the lessons learned during the project execution.

1.2 About the cloud instances

The selected cloud instances are based on AMD EPYC[™] processors of two different generations, all within the same AWS HPC instance family:

- Amazon EC2 Hpc6a instances, featuring two 3rd Gen AMD EPYC[™] 7003 series 48-core processors with up to 3.6 GHz all-core turbo frequency and 100 Gb/s networking (<u>https://aws.amazon.com/ec2/instance-types/hpc6a/</u>)
- Amazon EC2 Hpc7a instances, featuring two 4th Gen AMD EPYC[™] 9004 series 96-core processors with up to 3.7 GHz all-core turbo frequency, DDR5 RAM, and 300 Gb/s networking. Hpc7a instances also offer 24-, 48-, or 96-core 4th Gen AMD EPYC[™] processors. (<u>https://aws.amazon.com/ec2/instance-types/hpc7a/</u>)

In case of Hpc7a, AWS is offering smaller instance sizes that make it easier for customers to pick a smaller number of CPU cores to activate while keeping all other resources constant based on their workload requirements. In fact, the smaller sizes (with 96, 48, and 24 cores) increase the memory per core and memory bandwidth per core. This can have a serious impact on solver performance and becomes tangible in the case of commercial software that's licensed on a per-core basis. Additionally, the best core topology configuration is automatically selected by AWS, maximizing performance and eliminating the need for complicated core pinning configurations at run time.

We ran the benchmarks on Hpc6a and all Hpc7a sizes.



1.2.1 Amazon EC2 hpc6a.48xlarge

Full specifications:

- CPU: AMD EPYC[™] 7R13 Processor @ 3.6 GHz
- Cores: 48 x 2 sockets, 1 thread per core, 96 total physical cores
- RAM: 384 GiB
- Network: 1 x Elastic Fabric Adapter network interface, 100 Gb/s bandwidth

1.2.2 Amazon EC2 hpc7a.96xlarge

Full specifications:

- CPU: AMD EPYC[™] 9R14 Processor @ 3.7 GHz
- Cores: 96 x 2 sockets, 1 thread per core, 192 total physical cores
- RAM: 768 GiB
- Network: 2 x Elastic Fabric Adapter network interface, 300 Gb/s bandwidth

1.2.3 Amazon EC2 hpc7a.48xlarge

Full specifications:

- CPU: AMD EPYC[™] 9R14 Processor @ 3.7 GHz
- Cores: 48 x 2 sockets, 1 thread per core, 96 total physical cores
- RAM: 768 GiB
- Network: 2 x Elastic Fabric Adapter network interface, 300 Gb/s bandwidth

1.2.4 Amazon EC2 hpc7a.24xlarge

Full specifications:

- CPU: AMD EPYC[™] 9R14 Processor @ 3.7 GHz
- Cores: 24 x 2 sockets, 1 thread per core, 48 total physical cores
- RAM: 768 GiB
- Network: 2 x Elastic Fabric Adapter network interface, 300 Gb/s bandwidth

1.2.5 Amazon EC2 hpc7a.12xlarge

Full specifications:

- CPU: AMD EPYC[™] 9R14 Processor @ 3.7 GHz
- Cores: 12 x 2 sockets, 1 thread per core, 24 total physical cores
- RAM: 768 GiB
- Network: 2 x Elastic Fabric Adapter network interface, 300 Gb/s bandwidth



1.3 About the software

The software used for the benchmarks are part of the Altair CAE product line:

• Altair[®] Radioss[®], a leading analysis solution to evaluate and optimize product performance for highly nonlinear problems under dynamic loadings. Used worldwide across all industry sectors, it improves the crashworthiness, safety, and manufacturability of complex designs.



Figure 1 – Altair refined version derived from originally developed NCAC FE Taurus model (image/courtesy of Altair)

 Altair[®] AcuSolve[®], a leading general-purpose Computational Fluid Dynamics (CFD) solver that is capable of solving the most demanding industrial and scientific applications. Robust and scalable solver technology empowers users by providing unparalleled accuracy.



Figure 2 – Altair® AcuSolve® example output (image/courtesy of Altair)





1.4 About the models

1.4.1 Altair[®] Radioss[®]

The model used for this software is the publicly available "Taurus 10 million finite elements" model, recovered from the OpenRadioss™ public repository. It is well suited to benchmarking HPC performance in HPC clusters with many CPUs. This benchmark has a refined mesh with 10 million finite elements.



Figure 3 – Altair refined version derived from originally developed NCAC FE Taurus model (image/courtesy of Altair)

The model has three different settings, based on the simulation time:

- Full simulation, 120 milliseconds.
- Shorter simulation, 10 milliseconds: best suited for fast performance and scalability testing on many nodes/CPUs.
- Very short simulation, 2 milliseconds: useful to test the HPC cluster functions.

For our benchmarks we use the "Shorter" simulation test case, with 10 milliseconds of simulation time.

1.4.2 Altair® AcuSolve®

The model used for AcuSolve has been sent to us directly from Altair, as they considered it a good example of a simulation that will demonstrate high scalability in an HPC environment.



Figure 4 – "Impinging Nozzle" model (image/courtesy of Altair)



The "Impinging Nozzle" is a fairly substantial model (7.8 million nodes and 7.7 million elements) that simulates a steady water flow through a nozzle using a Navier–Stokes-based solver, and a Spalart–Allmaras turbulence model.

The simulation for this benchmark has been limited to 200 time-steps.

2. Architecture design

The architecture is based on an AWS ParallelCluster standard deployment.



Figure 5 – AWS architecture diagram

A HeadNode is installed, providing centralized user authentication, job scheduling services, and autoscaling integration for two job queues. Each job queue is associated with a specific instance type in a separated Availability Zone.

An Amazon FSx for Lustre deployment provides the shared filesystem that will contain the applications, the user input, and output data while also acting as a high-performance scratch filesystem for compute jobs.

All systems are using RedHat Enterprise Linux 8.8.

On HPC instances, EFA networking (<u>https://aws.amazon.com/hpc/efa/</u>) is enabled.

An external License Server provides the software with the networked licenses that are required to run the simulations.



3. Installation

3.1 AWS ParallelCluster

The deployment of the architecture was performed using AWS ParallelCluster and choosing the appropriate dimensions and base AMI for the instances and instance specifications. The compute instance timeout was set to 10 minutes to avoid incurring costs while the instances are not actively used for compute jobs.

3.1.1 Scheduler

The Slurm scheduler was also deployed using AWS ParallelCluster, which helped configuring the proper partitions (aka job queues) with the association of a specific instance type to each partition. All auto-scaling operations are directly controlled by Slurm, which takes care of deploying compute instances based on each job's resource requests.

3.1.2 Storage

FSx for Lustre storage was also deployed via AWS ParallelCluster, to ensure that the HeadNode and each compute instance can access the same data with the highest possible performance. We considered the possibility of using EBS with NFS for the users' home directories, but we deemed it unnecessary as this is not a production-ready environment, and we wanted to contain overall costs by cutting what we considered to be non-essential features.

3.2 Altair software and licensing services

Altair licensing software was installed on a separate machine, outside of the HPC architecture. The license server is also on AWS, has a fixed public IP, and strict security access rules to be reachable only by the machines within the HPC infrastructure.

All Altair CAE software was installed directly on the FSx for Lustre filesystem, to be accessible from all the compute instances with a consistent filesystem path.

3.3 User Data Repository

User data was also stored in the FSx for Lustre filesystem, organized in "models" and "runs" for each solver.

4. Benchmark execution

The different job directories were carefully prepared with all the required data to run the simulations in different configurations. Simulation results were produced within each job's directory.

4.1 Baselining

To provide a baseline for performance and scalability, we ran each simulation on a single instance for each of the instance types covered in this study.



4.2 MPI tuning

The two instance types have processors from different generations with a different number of cores and a different network configuration. This required fine-tuning the MPI libraries to best suit the characteristics of each instance type.

The MPI library used for both instance types was Intel[®] MPI, version 2021 Update 9. In fact, the same library at the same version was included in the Altair software and in the AWS ParallelCluster system image, with the latter also providing an external libfabric (version 1.17) customized by AWS for better EFA support.

The MPI configurations were the same for all software used in our benchmarks.

4.2.1 Amazon EC2 Hpc6a MPI settings

The following environment variables were set at each job's run time:

- 1. export FI_EFA_FORK_SAFE=1
- 2. export I_MPI_OFI_LIBRARY_INTERNAL=0
- 3. export I_MPI_FABRICS=shm:ofi
- 4. export I_MPI_OFI_PROVIDER=efa
- 5. export I_MPI_DEBUG=5

This is the baseline configuration that we used for all tests to:

- provide reliable process spawn on EFA network (FI_EFA_FORK_SAFE)
- make use of the AWS-provided libfabric (I_MPI_OFI_LIBRARY_INTERNAL)
- select the correct fabrics for optimal performance within the nodes and for node-to-node communications (I_MPI_FABRICS)
- select the required fabric provider for AWS Elastic Fabric Adapter (I_MPI_OFI_PROVIDER)
- enable debug mode with enough details to analyze the fabric configuration in detail (I_MPI_DEBUG)

4.2.2 Amazon EC2 Hpc7a MPI settings

The following environment variables were set at each job's run time:

- 1. export FI_EFA_FORK_SAFE=1
- 2. export I_MPI_OFI_LIBRARY_INTERNAL=0
- 3. export I_MPI_FABRICS=shm:ofi
- 4. export I_MPI_OFI_PROVIDER=efa
- 5. export I_MPI_DEBUG=5
- 6. export FI_EFA_SHM_AV_SIZE=256
- 7. export I_MPI_MULTIRAIL=1

The key difference from Hpc6a are the last two environment variables:

- FI_EFA_SHM_AV_SIZE is required with ParallelCluster versions older than 3.7.0 because of the increased number of processors that Hpc7a has on a single node. Without the proper setting, the simulations were crashing at MPI process spawn.
- I_MPI_MULTIRAIL is required to fully take advantage of the two EFA interfaces on the Hpc7a nodes and increase the overall network bandwidth available to the MPI processes of the simulations.



4.3 Scalability

To test scalability, the same simulations were run on different node configurations: Starting from the baseline, the number of cores was increased to 2 times and 4 times the original amount. However, since Hpc6a instances have half the cores per node than Hpc7a, we went up to 8 times with the former to have a proper core-per-core comparison with the latter. This brought our maximum core number per simulation to 768.

4.4 Performance results

Note: We are missing some data points for low-core sizes of Hpc7a instances, as we could not run the full scale of benchmarks due to limitations to the maximum number of instances and licensed cores in our environment.

4.4.1 Altair® Radioss®

The execution time of each Radioss job was taken from the output files, using the reported time from the "engine" solver itself. This is because the "starter" process runs at the beginning of the job on a single node, preparing the input files for each single "engine" process that will run the simulation. The time for the "starter" process to prepare the input files increases linearly with the number of cores the simulation will run. In the end, we chose not to include "starter" timings in the benchmark elapsed time to provide a more precise, apples-to-apples comparison between different runs.



Altair[®] Radioss[®] Performance (lower is better)

Figure 6 – Performance chart for Altair $^{\ensuremath{\mathbb{R}}}$ Radioss $^{\ensuremath{\mathbb{R}}}$ on Hpc6a and Hpc7a



hpc6a.48xlarge	96 cores	192 cores	384 cores	768 cores
Job Elapsed Time (seconds)	9282	4895	2903	1759
Scalability (using 96 cores as the reference)	100%	94.8%	79.9%	66.0%

Figure 7 – Scalability for Altair® Radioss® on hpc6a.48xlarge

hpc7a.96xlarge	96 cores	192 cores	384 cores	768 cores
Job Elapsed Time (seconds)	5914	4310	2577	1690
Scalability (using 96 cores as the reference)	100%	68.6%	57.4%	43.7%

Figure 8 – Scalability for Altair® Radioss® on hpc7a.96xlarge

On Hpc6a, Altair[®] Radioss[®] has very good scalability (66%) when increasing the number of cores from 96 to 768.

On Hpc7a, the picture is a bit different, depending on the actual size of the instance.

The default size, hpc7a.96xlarge, is a bit less efficient with a scalability of 43.7% when increasing the number of cores from 96 to 768.

Considering just the 192 cores data point, using multiple hpc7a.12xlarge nodes gives a shorter job elapsed time than using just one hpc7a.96xlarge instance (2812 seconds vs 4310 seconds).

We can see a similar pattern at the 384 cores data point, where using the hpc7a.24xlarge size can reduced the elapsed time to 1921 seconds compared to 2577 seconds obtained with hpc7a.96xlarge instances.

In general, we can see that the test case performed better on lower-core Hpc7a instances. This means that having more memory per core and more memory bandwidth per process is enhancing the simulation performance, potentially overcoming a memory bottleneck by leveraging EFA networking features.

Summing it up:

- Hpc7a has a definite performance advantage vs. Hpc6a in all situations.
- While Hpc6a scalability is more efficient vs. the base instance shape of Hpc7a, the latter clearly overcomes the former in all iso-core situations by making use of Hpc7a lower-core sizes.
- If your software license is based on the total number of cores, Hpc7a low-core shapes could provide a significant opportunity to enhance performance with the same overall core usage.





4.4.2 Altair® AcuSolve®

The execution time taken into consideration for AcuSolve was the overall elapsed time, in seconds, between the start and the end of the whole computation. Like Radioss, AcuSolve has a preparation phase to subdivide the simulation data for each solver process. However, since AcuSolve automatically uses a different approach than Radioss for distributed computations, the duration of this preparation phase is negligible in the context of the overall duration of the simulation (0.1% to 0.5%).



Figure 9 – Performance chart for Altair® AcuSolve® on Hpc6a and Hpc7a

hpc6a.48xlarge	96 cores	192 cores	384 cores	768 cores
Job Elapsed Time (seconds)	32938	15894	7978	3692
Scalability (using 96 cores as the reference)	100%	103.7%	103.3%	111.6%

Figure 10 - Scalability for Altair® AcuSolve® on hpc6a.48xlarge

hpc7a.96xlarge	96 cores	192 cores	384 cores	768 cores
Job Elapsed Time (seconds)	12342	11925	6109	2902
Scalability (using 96 cores as the reference)	100%	51.7%	50.5%	53.2%

Figure 11 – Scalability for Altair® AcuSolve® on hpc7a.96xlarge

hpc7a.48xlarge	96 cores	192 cores	384 cores	768 cores
Job Elapsed Time (seconds)	12376	6367	3240	1863
Scalability (using 96 cores as the reference)	100%	97,1%	95.5%	83.0%

Figure 12 – Scalability for Altair® AcuSolve® on hpc7a.48xlarge



On Hpc6a, Altair[®] AcuSolve[®] has excellent scalability (111%) with the test case when increasing the number of cores from 96 to 768.

The default size of Hpc7a, hpc7a.96xlarge, shows a very good performance compared to Hpc6a nodes. The elapsed time goes from 32,938 seconds to 12,342 seconds for 96 cores. When using more nodes, the scalability is around 50% but stable: adding more nodes will decrease the elapsed time in proportion to the number of nodes added.

The test case performed better on lower-core Hpc7a instances. With hpc7a.48xlarge nodes, scalability is much better (83.0% for 768 cores). Using instances with a lower core count is usually better and will slightly decrease the job elapsed time.

Summing it up:

- Overall performance heavily favors Hpc7a with a performance uplift of ~3X compared to Hpc6a.
- The best performance is obtained with lower core count sizes of Hpc7a, with hpc7a.12xlarge providing the most efficient solution.
- In case your software license is based on the total number of cores, Hpc7a low-core shapes could provide a significant opportunity to enhance performance with the same overall core usage.

4.5 Job price results

To calculate each job price and compare it properly, the following formula was used:

JobPrice = (JobInstanceNum * HourlyInstancePrice * JobExecutionTimeInSecs / 3600)

Please note that we took storage out of the equation, since all instances are using the same FSx for Lustre filesystem for their storage needs. The hourly rates for each instance type have been retrieved from the publicly available listings on November 6th, 2023.





4.5.1 Altair[®] Radioss[®]

The following charts plot the comparative job price against the core count for each job of Radioss:



Figure 13 – Cost per job chart for Altair[®] Radioss[®] on Hpc6a and Hpc7a

Considering the 384 cores data point and including performance numbers:



Figure 14 – Cost per job and performance chart for Altair® Radioss® @ 384 cores on various instance types/sizes

While the cheapest option is the Hpc6a with 96 cores, Hpc7a provides a superior reduction in time-tosolution while increasing the job cost by a small amount (less than \$0.001 per simulation second).



4.5.2 Altair® AcuSolve®

The following charts plot the comparative job price against the core count for each job of AcuSolve:



Figure 15 – Cost per job chart for Altair® AcuSolve® on Hpc6a and Hpc7a

The situation is much different than the one we saw on the Altair Radioss chart: Most of the job prices are in the same range, with an exception made for the ones where the scalability efficiency was approaching the limit.







It's clear that hpc7a.48xlarge provides excellent performance while being aligned in terms of cost, while the cheapest option is provided by hpc7a.96xlarge with almost double the elapsed time-to-solution.



5. Conclusions

In terms of pure performance, Hpc7a instances always have the edge against the still excellent Hpc6a. The higher cores-per-instance count and the more than double bandwidth for the high-speed interconnect are powerful tools that both multi-thread and multi-process solvers can use to achieve greater performance.

In terms of price, it's important to note that the per-price job scales less than performance, meaning that adding a host to the computation to get better performance will not actually increase the price of the job by that instance's hourly price, but for a fraction. This fraction will follow the scalability curve.

This can be achieved thanks to the scalability properties of the Altair solvers, the advanced architecture of AMD processors, and the AWS optimizations of the HPC-series instances and EFA network interfaces.

The price comparison favors the older generation of the AWS HPC instances for Altair[®] Radioss[®], while the opposite is true for Altair[®] AcuSolve[®]. In both cases, prices are not that far from each other even though performance on the Hpc7a is clearly better.

Additionally, the different sizes of Hpc7a instances help in achieving even faster performance and can provide more cost-efficient options.

5.1 Credits and special thanks

Many thanks go to AMD and AWS, for sponsoring this study.

A special thanks to Altair, for providing the licenses for the solvers.



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6. Appendix

6.1 Example submission command for Slurm

sbatch -N<nodeNum> -n<coreNum> --exclusive --mem=0 <jobscript>

6.2 Job scripts

6.2.1 Radioss

```
#!/bin/bash
RADIOSS_DIR="/shared/apps/altair/2023/altair/scripts/"
RADIOSS_INP="TAURUS_A05_FFB50_0000.rad"
NDOMAINS=0
ulimit -s unlimited
cd ${SLURM_SUBMIT_DIR}
NCPUS=${SLURM_NTASKS}
if [ $NDOMAINS -lt 1 ]; then
    NDOMAINS=${NCPUS}
    NTHREADS=1
else
    [ $((NCPUS % NDOMAINS)) -ne 0 ] && exit 1
    NTHREADS=$((NCPUS / NDOMAINS))
fi
NHOSTS=${SLURM_NNODES}
[ $((NDOMAINS % NHOSTS)) -ne 0 ] && exit 1
NDOMAINS_PER_NODE=$((NDOMAINS / NHOSTS))
NODEFILE=nodefile.txt
scontrol show hostnames "$SLURM_JOB_NODELIST" > ./slurm_hosts.${SLURM_JOBID}
for host in $(cat slurm_hosts.${SLURM_JOBID}); do
    printf $host'\n%.0s' {1..${SLURM_NTASKS}} >> ./${NODEFILE}.${SLURM_JOBID}
done
```



6.2.2 AcuSolve

#!/bin/bash

source /shared/apps/altair/2023/altair/hwcfdsolvers/acusolve/linux64/script/acusim.sh ulimit -s unlimited cd \${SLURM_SUBMIT_DIR} export ALTAIR_LICENSE_PATH="6200@10.0.0.1" # Acusolve recognizes the platform automatically and takes care of MPI settings, even between Hpc6a and Hpc7a #export FI_EFA_FORK_SAFE=1 #export I_MPI_OFI_LIBRARY_INTERNAL=0 #export I_MPI_OFI_LIBRARY_INTERNAL=0 #export I_MPI_OFI_PROVIDER=efa #export I_MPI_OFI_PROVIDER=efa #export FI_EFA_SHM_AV_SIZE=256 #export I_MPI_MULTIRAIL=1 acuRun -slurm | tee acuRun.\${SLURM_JOBID}.out



6.3 ParallelCluster configuration files

6.3.1 Amazon EC2 Hpc6a in eu-north-1

Region: eu-north-1
Image:
Os: rhel8
HeadNode:
InstanceType: t3.medium
Networking:
SubnetId: subnet-Offfffffffffffff
Ssh:
KeyName: amd-benchmark
Scheduling:
Scheduler: slurm
SlurmQueues:
- Name: hpc6a
ComputeResources:
- Name: hpc6a48xlarge
Instances:
- InstanceType: hpc6a.48xlarge
MinCount: 0
MaxCount: 10
Efa:
Enabled: true
Networking:

Enabled: true
Networking:
PlacementGroup:
Enabled: true
SubnetIds:
- subnet-0222222222222222
CustomActions:
OnNodeStart:
Script: s3://amd-benchmarking/create-users.sh
SharedStorage:
- MountDir: /shared
Name: AmdBenchmarkingSharedLustre
StorageType: FsxLustre
FsxLustreSettings:
StorageCapacity: 1200
DeploymentType: PERSISTENT_2
PerUnitStorageThroughput: 125
Tags:
- Key: Project
Value: AMD



6.3.2 Amazon EC2 Hpc7a in eu-west-1

Region: eu-west-1
Image:
Os: rhel8
HeadNode:
InstanceType: t3.medium
Networking:
SubnetId: subnet-0eeeeeeeeeeeeeeee
Ssh:
KeyName: amd-benchmark-2
Scheduling:
Scheduler: slurm
SlurmQueues:
- Name: hpc7a
ComputeResources:
- Name: hpc7a96xlarge
Instances:
- InstanceType: hpc7a.96xlarge
MinCount: 0
MaxCount: 10
Efa: