Migration and performance of CMAQ & WRF-CMAQ in the public cloud with commercial images

> Arturo Fernandez odyhpc 20th Annual CMAS Conference November 1-5 2021 (virtual)

Outline

- Public cloud environments
- Running HPC apps (CMAQ) in the public cloud
- Integrated product for CMAQ
- Performance evaluation
- Cost analysis
- Final remarks



Public Cloud Environments

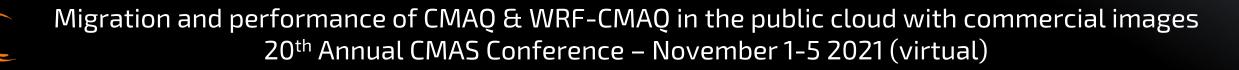
What is the public cloud? \rightarrow Rented IT (a la carte) from Cloud Service Providers (CSPs)

Pros

- Flexibility
- No upfront cost
- Unlimited storage space and other resources
- Availability of new hardware every so often
- What about performance?

Cons:

- New skills (very basic to highly specialized)
- Everything is billed
- Lower performance for HPC workloads?





Running HPC apps (CMAQ) in the public cloud

How do you run HPC apps in the public cloud?

- Choose the right laaS
- Compile and build the app

What is the right laaS?

There is no universal answer as each case is unique. In general, hungrier computational resource apps require more resources \rightarrow Major CSPs

How do you compile and build the app?

- Start from scratch \rightarrow Challenge: The hardware and software must work together
- Use integrated product

Integrated product for CMAQ

Integrated product: CMAQ & WRF-CMAQ

It has precompiled executables optimized for public cloud

infrastructure or Infrastructure as a Service (laaS)

- Currently available from the AWS Marketplace (potential future availability from the Azure Marketplace)
- Dual functionality for single instances and clusters
- It also has postprocessing apps, which can even be used with instances with GPU capabilities



Integrated product for CMAQ

Launch and connect to an instance running CMAQ

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Feedback English (US)

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Integrated product for CMAQ

Launch and connect to a cluster using AWS-Parallelcluster

- Uses slurm as scheduler
- Cluster monitoring tools are also available

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Performance evaluation

Software

- Benchmark: 2016 Southeast U.S.
- Domain size: 100 x 80 x35
- Species tracked: 218
- Input files > 6 GB
- Not very (RAM) memory hungry: Was
- able to run on instances with 8GB

Hardware

Intel Xeon E5-2697 v4 32 cores (dual socket)– 14 nm (2016)

AWS Graviton2 64 cores (single socket) – 7 nm (2019)

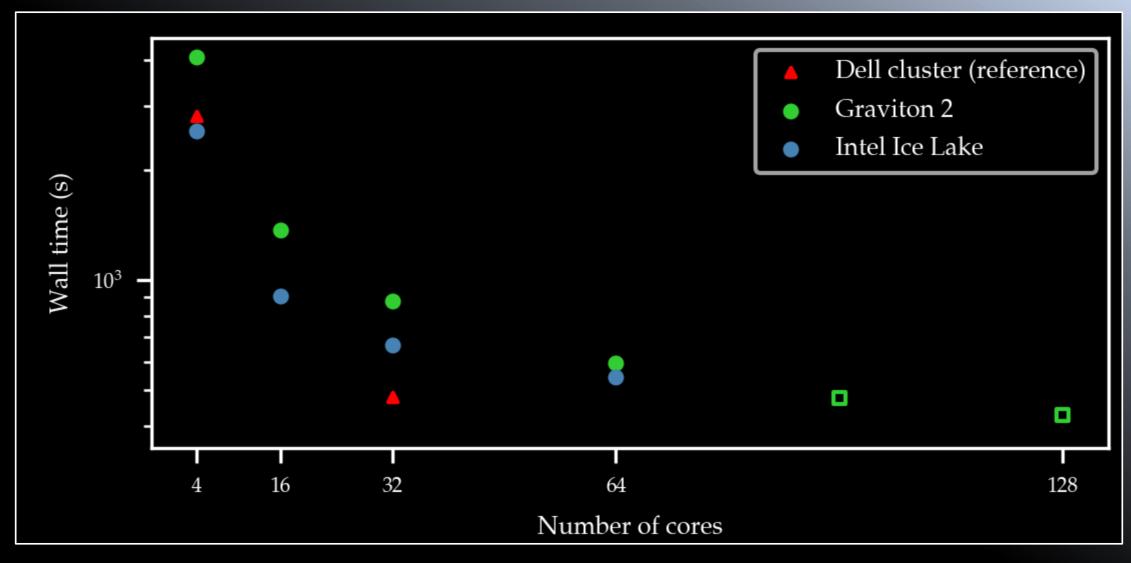


Intel Xeon Platinum 8375C -64 cores (dual socket)– 10 nm (2021)

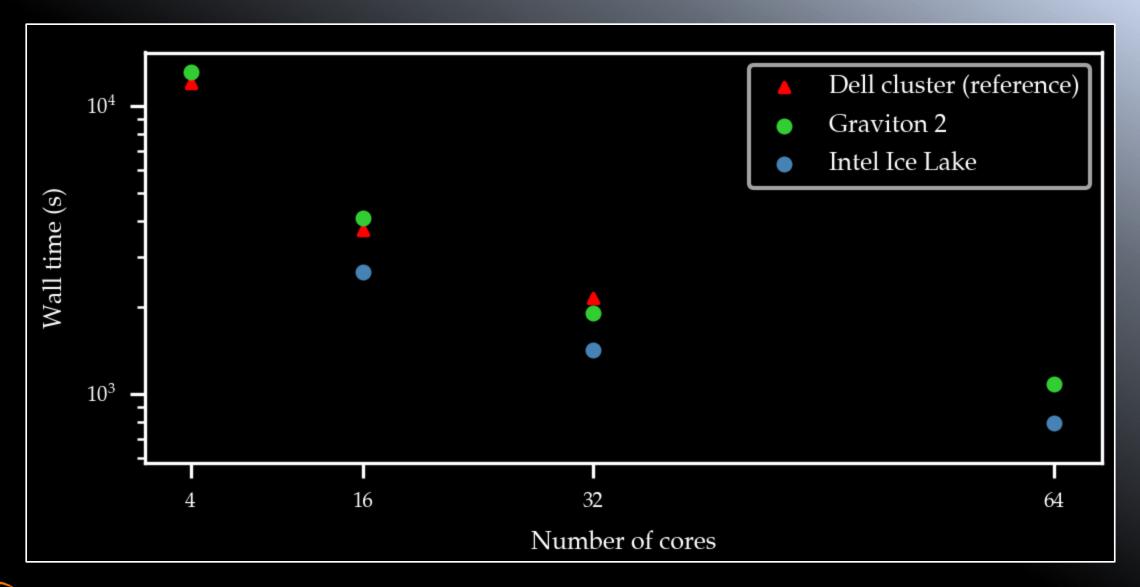




Performance evaluation – CMAQ measurements



Performance evaluation – WRF-CMAQ measurements



Cost analysis

Performance evaluation is relatively straightforward but cost analysis is more complex. A full analysis requires a total cost of ownership (TCO), which is unique for each organization. As a minimum, it must include:

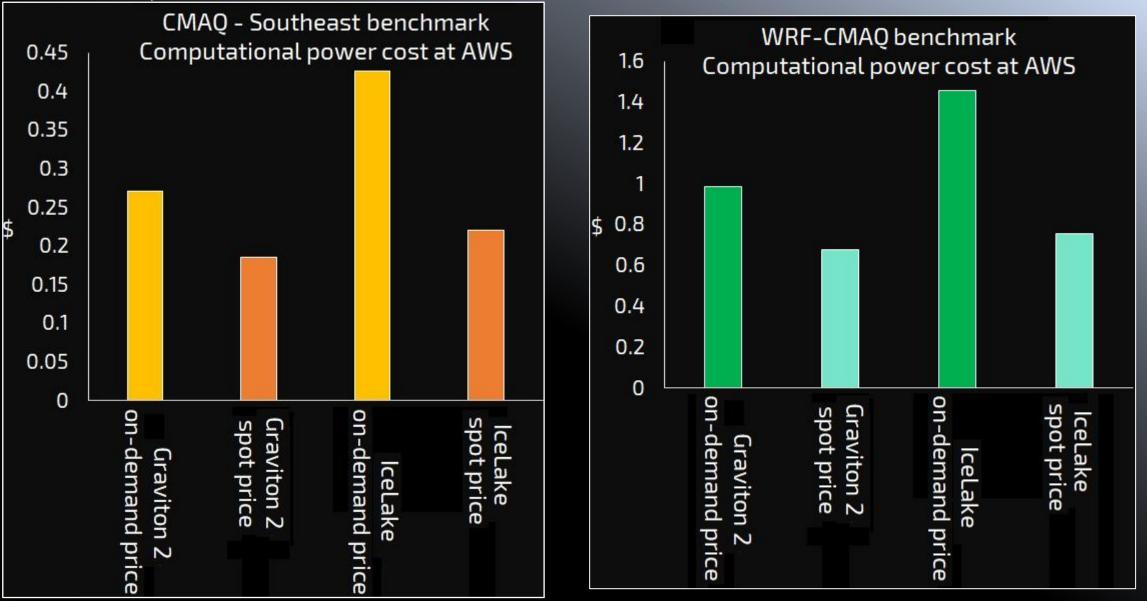
- Computational power account for most of the cost but not all of it
- Storage
- Outbound traffic (can also add up for HPC apps)
- Commercial AMI fees must also be considered Many categories have several tiers and conditions

Preliminary cost analysis

- It focuses on computational power plus AMI fees
- It categorizes cost associated with computational power into 2:
 - **On-demand prices (maximum cost)**
 - Spot prices (maximum savings)



Cost analysis – cost estimates



Conclusions

The main conclusions from the study are the following:

- CMAQ & WRF- CMAQ are available as an integrated image from the AWS Marketplace
- Performance is good and they can be run with many cores using clusters of several instances
- Two choices: Intel IceLake vs. Graviton2 (performance vs. cost)
- Matching the CMAQ case with the right hardware is important to maximize performance and keep expenses low

Questions?

