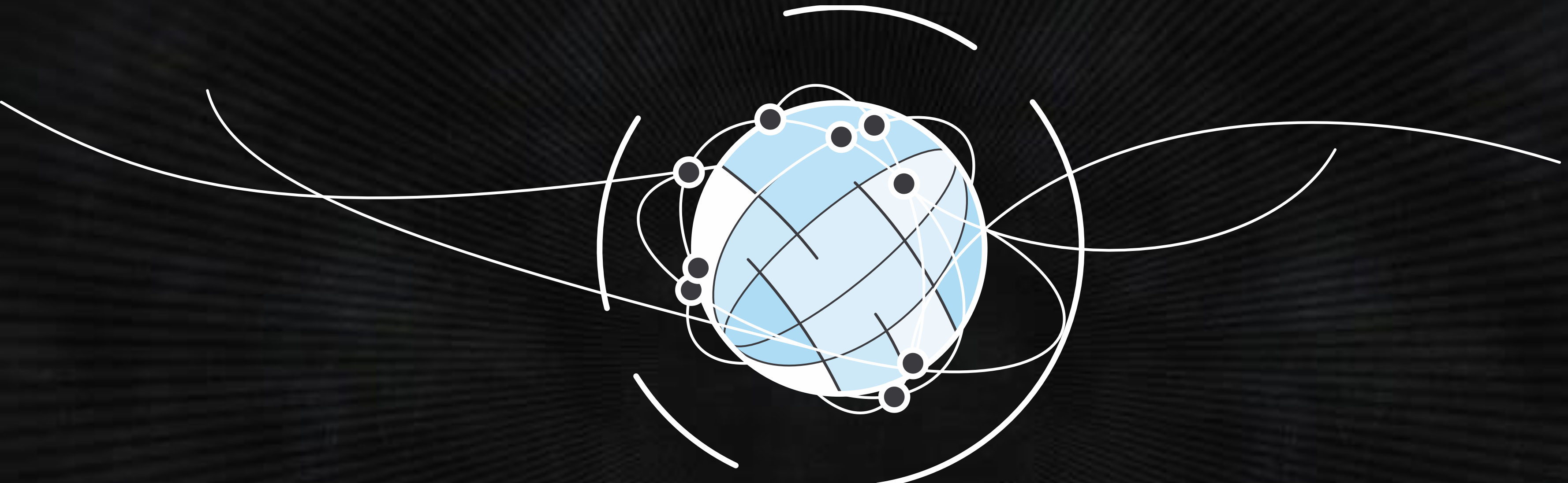
Scaling Tightly Coupled Algorithms on AWS



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aws

Research Computing @ AWS

AWS Worldwide Research & Technical Computing

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Unlimited infrastructure

Low cost with flexible pricing

Efficient clusters

Why AWS for HPC?

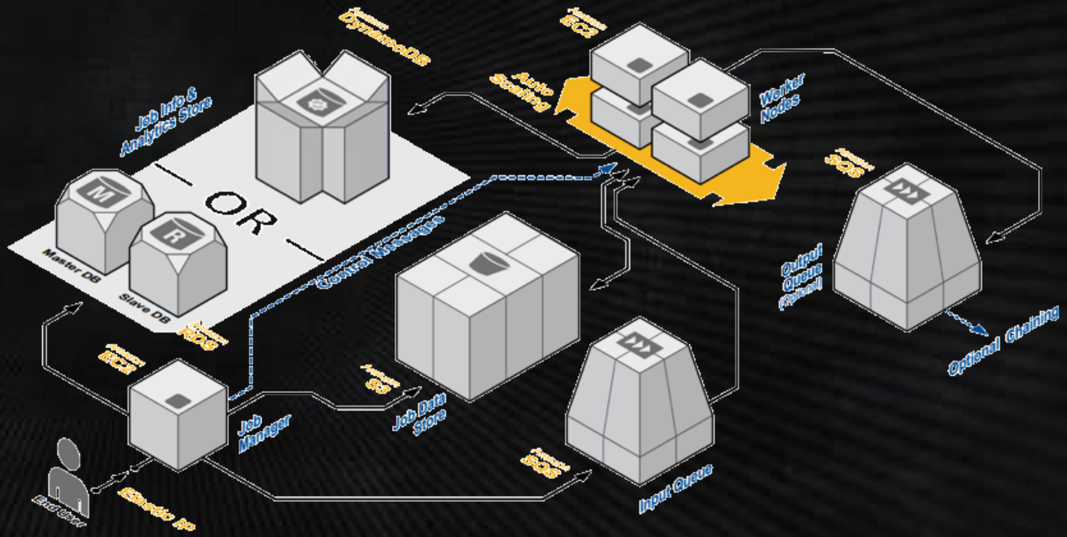
Faster time to results

Increased collaboration

Concurrent clusters on-demand

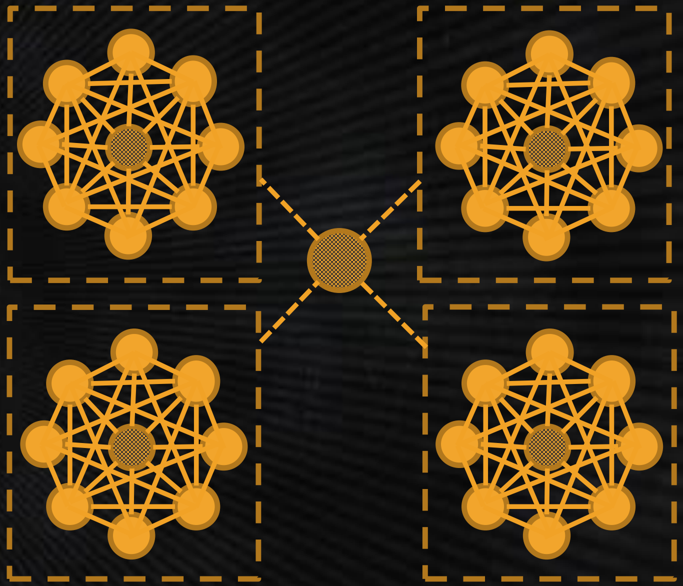
Great Features for HPC Workloads

- Experimentation without Fear!
- Start and stop instances!
- Spot Pricing
- Continuous Updates
  - Compute
  - Network
  - Storage
  - Services



Cloud Improves Workload Throughput

- Run many Jobs in Parallel
  - Eliminate HPC resource contention
  - Eliminate queue wait
  - Use it when you need it
- Right-size clusters and resources
  - Optimize each workload for performance
  - Pay for only what you use

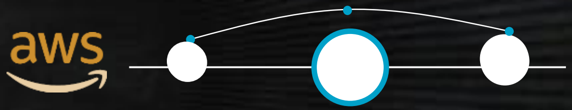


Cost advantages

On Premises
Capital Expense Model

- High upfront capital cost
- High cost of ongoing support

Amazon Web Services
Pay As You Go Model



- Use only what you need
- Multiple pricing models

Popular HPC workloads on AWS

Genomics Processing

Modeling and Simulation

Government and Educational Research

Monte Carlo Simulations

Transcoding and Encoding

Computational Chemistry

… and many more

Defining HPC – example use cases

Clustered (Tightly coupled)

Data Light

Minimal requirements for high performance storage

Data Heavy

Benefits from access to high performance storage

Clustered / Data Light:
- Fluid dynamics
- Weather forecasting
- Materials simulations
- Crash simulations

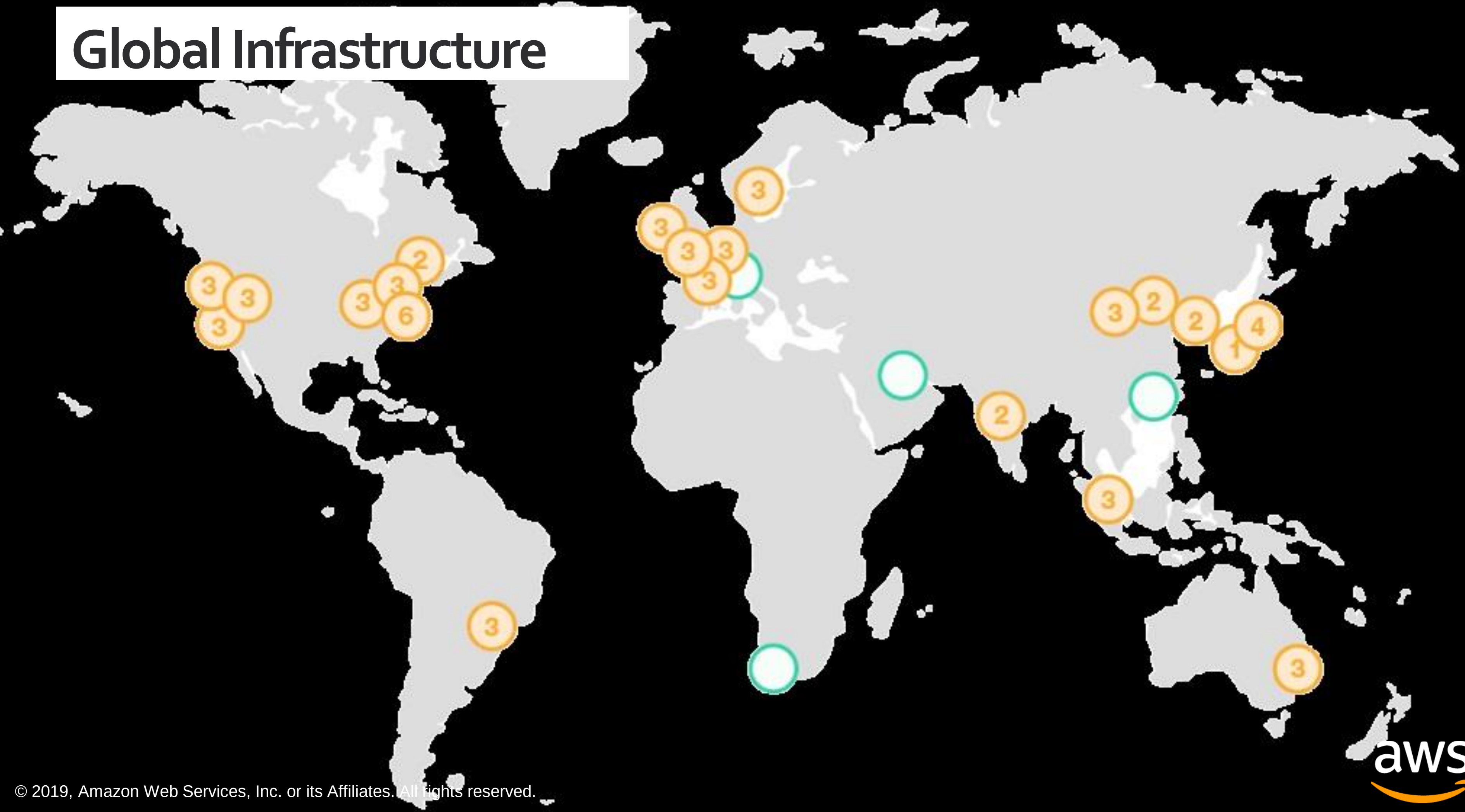
Clustered / Data Heavy:
- Seismic processing
- Metagenomics
- Astrophysics
- Deep learning

Distributed / Data Light:
- Risk modeling
- Molecular modeling
- Contextual search
- Logistics simulations

Distributed / Data Heavy:
- Animation and VFX
- Semiconductor verification
- Image processing/GIS
- Genomics

Distributed / Grid (Loosely coupled)

Global Infrastructure



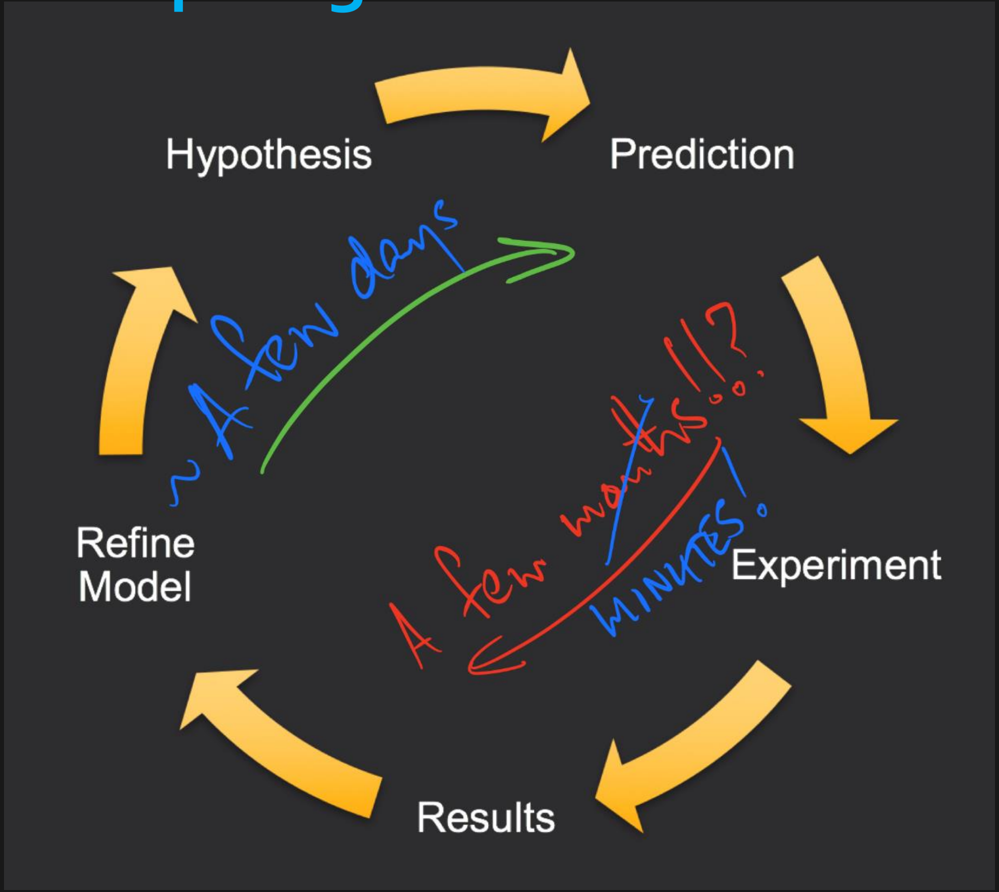
Important enablers for HPC on the cloud

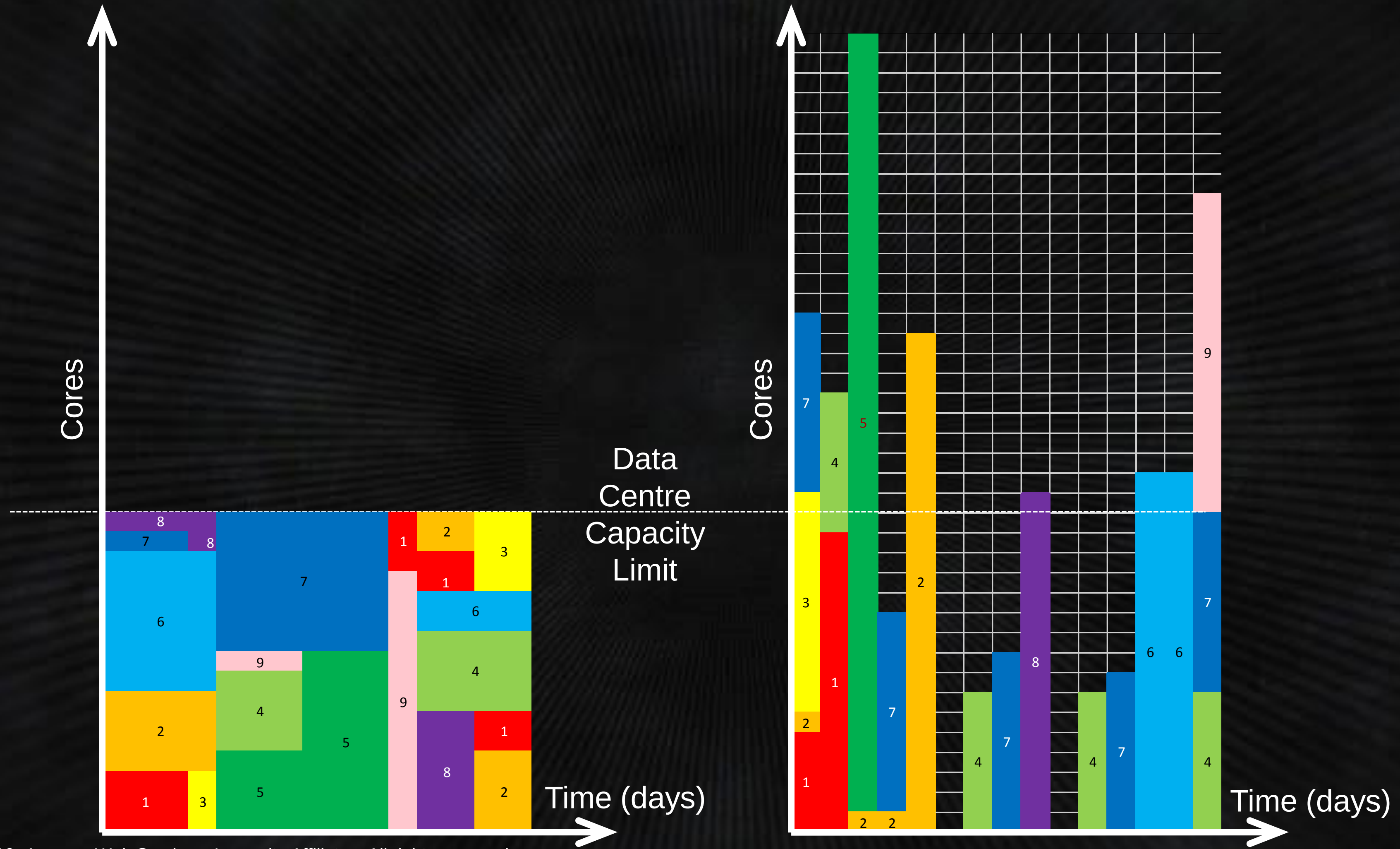
- Compute performance – CPUs, GPUs, FPGAs
- Memory performance – high RAM requirements in many applications
- Network performance – throughput, latency, and consistency
- Storage performance – including shared filesystems
- Automation and cluster/job management
- Remote graphics for interactive applications
- ISV support – including license management

...and SCALE

The Scientific Computing Method

Credit: Aristotle



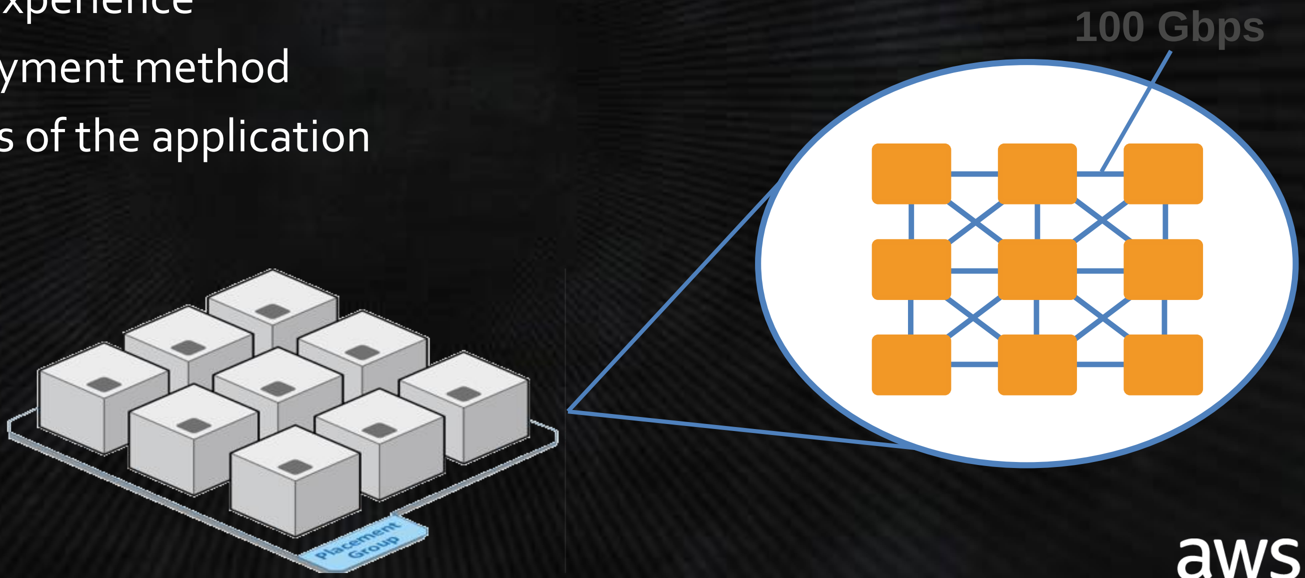

Cores
Time (days)
Data
Centre
Capacity
Limit
Cores
Time (days)

Deploy multiple HPC clusters

Running at the same time, and tuned for each workload

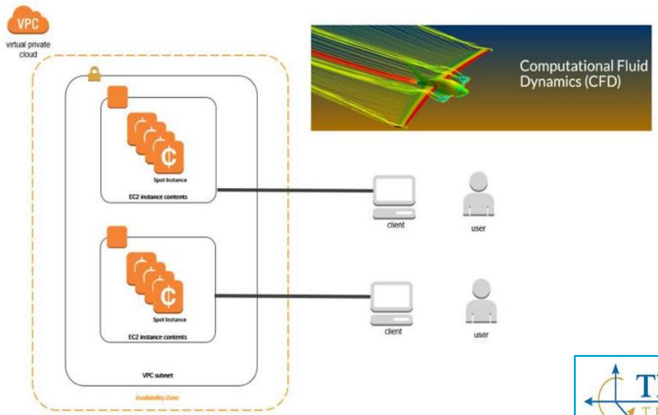
Which architecture Do I choose?

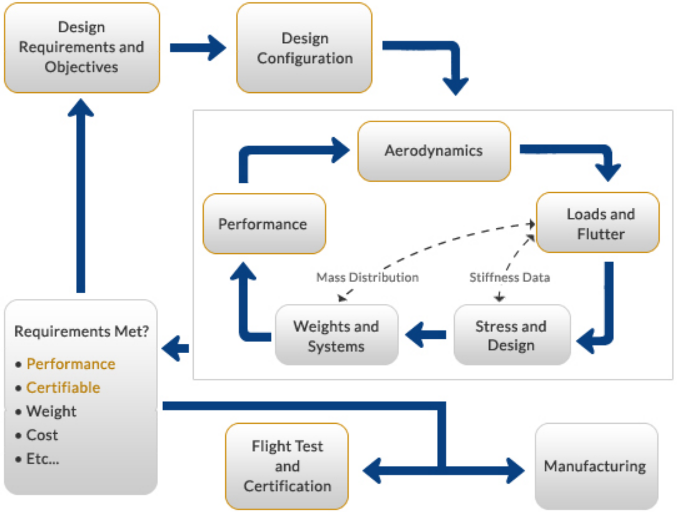
- One size does not fit all
- Architectures are an opportunity for optimization
- The chosen architecture depends on:
  - The desired user experience
  - The desired deployment method
  - The characteristics of the application



Example in aerospace

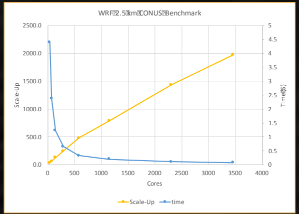
- Running parallel CFD studies using Siemens STAR-CCM+
  - Goal: shorten the time between Design Requirements and Configuration, and Flight Testing
- 1000+ cores per CFD study, multiple studies required for each workflow iteration
- Job-level optimizations:
  - Enhanced Networking, Placement Groups
  - Amazon Linux, Hyper-threading disabled
- Workflow optimizations:
  - Spot instances, multiple clusters
  - Multiple parallel studies for faster throughput





Performance considerations

For tightly-coupled cluster workloads



Test using real-world examples

- Use large cases for testing: do not benchmark scalability using only small examples

Domain decomposition

- Choose number of cells per core for either pre-core efficiency or for faster results

Processor states

- Use P-states to reduce processor variability

MPI libraries

- Test with Intel MPI and OpenMPI 4.0, and make use of available tunings

Network

- Use a placement group
- Enable enhanced networking

Hyper-threading and affinity

- Test with Hyper-threading (HT) on and off – usually off is best, but not always
- Use CPU affinity to pin threads to CPU cores when HT is off

Amdahl’s Scaling

What is Amdahl's Law?

$$Speedup = \frac{1}{(1-p)+\frac{p}{n}}$$

p – fraction of code that can be run in parallel
n – system resource improvement (number of processors)

Ideal: $\lim_{n \to \infty} speedup = \frac{1}{1-p}$

Or: $\lim_{p \to 1} speedup = n$

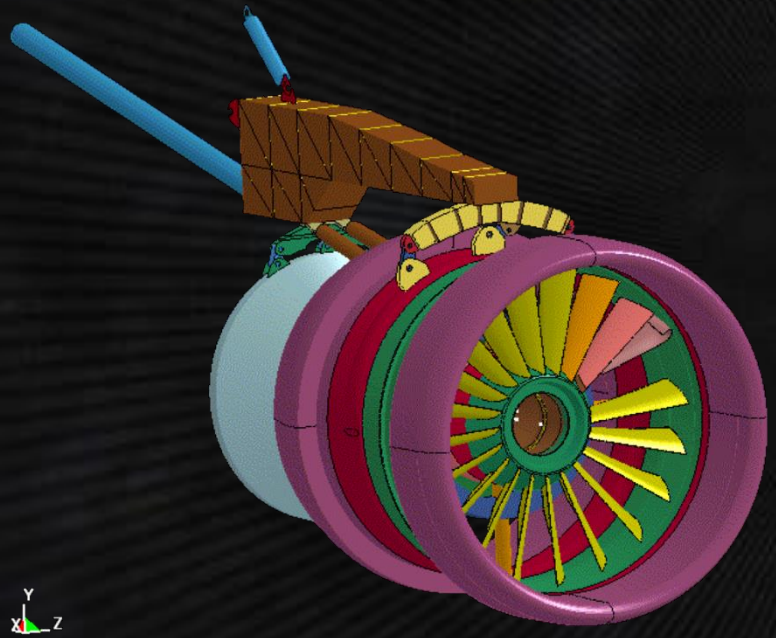
How is it used?

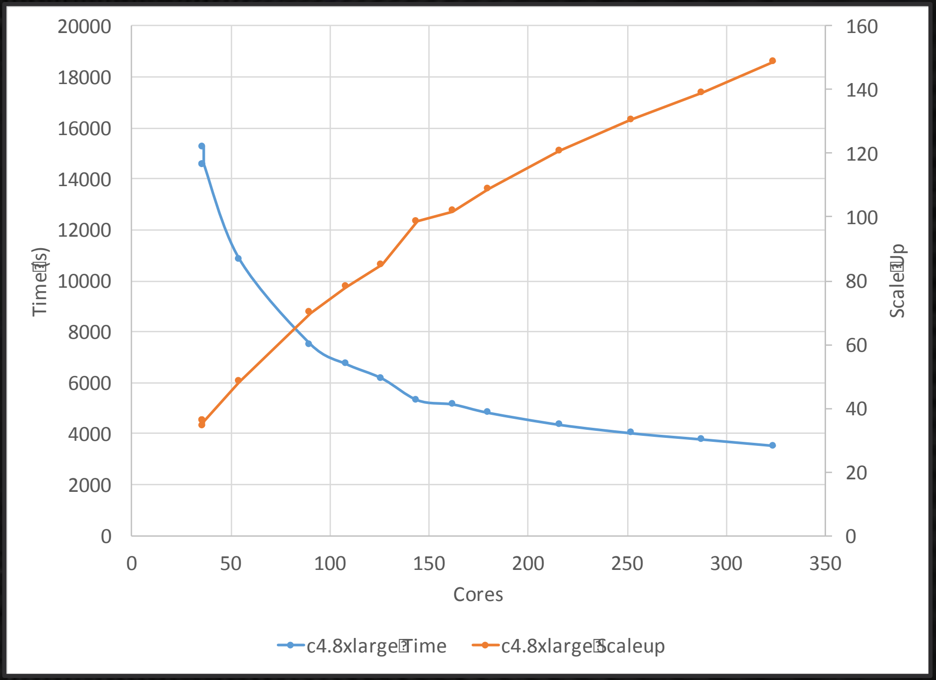
- Amdahl's Law assumes a fixed problem size.
- Example: a CFD calculation with a fixed number of cells – eg. 40M
- As the number of processors increases, the number of CFD mesh cells per compute core decreases.   At some point communication between nodes and cores becomes a bottleneck. This is the driver for low-latency networks.
- Note: The lower the latency the fewer CFD mesh cells per compute node are necessary for good scaling.   Lower latency usually means better speedup when considering Amdahl's law.

Coding Goals

- The following have been routine in code architectures since the first vector computers:
- Choose algorithms where *p* is maximized
-
- Reprogram codes
- Look for ways to avoid/reduce dependencies
- Consider tradeoffs between recalculating and storing
- Monitor code execution to find bottlenecks

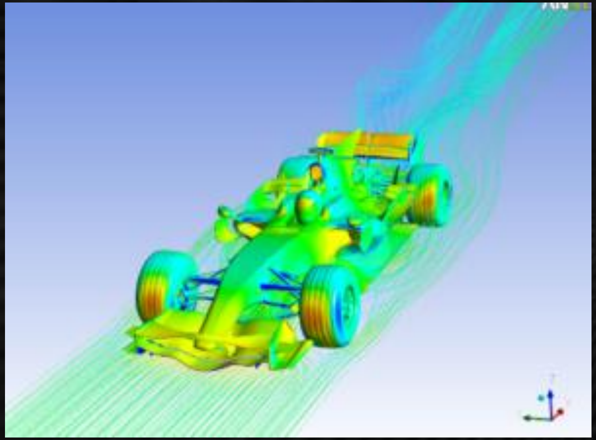
Structural simulation

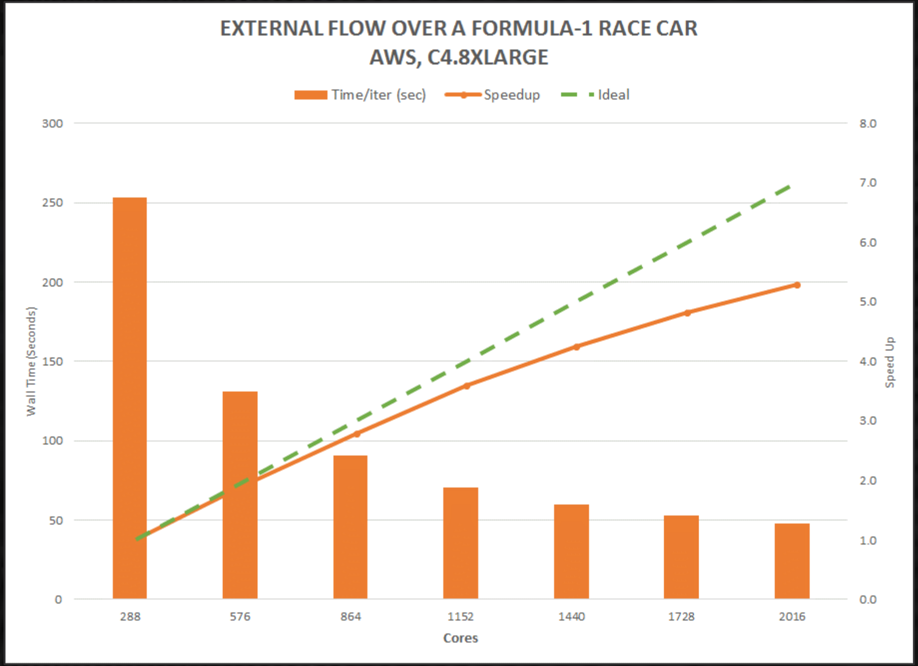




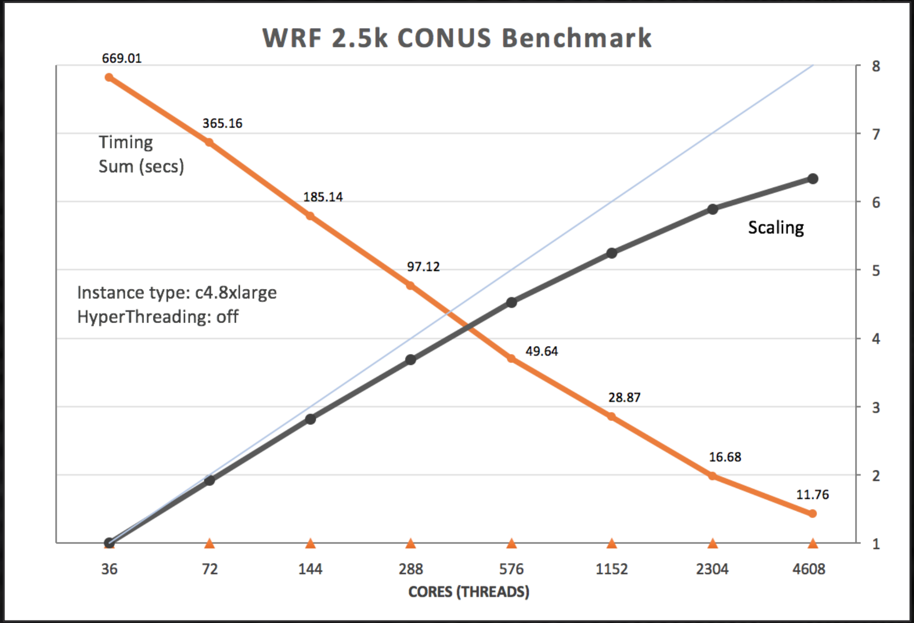
Fluid dynamics – Ansys Fluent

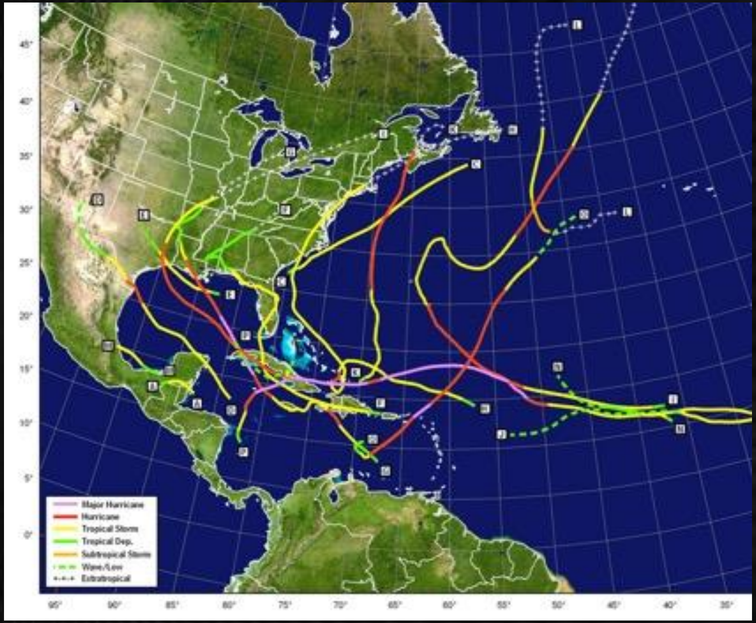
- C4.8xlarge instance type
- 140M cell model
- F1 car CFD benchmark





Tightly-coupled HPC – weather





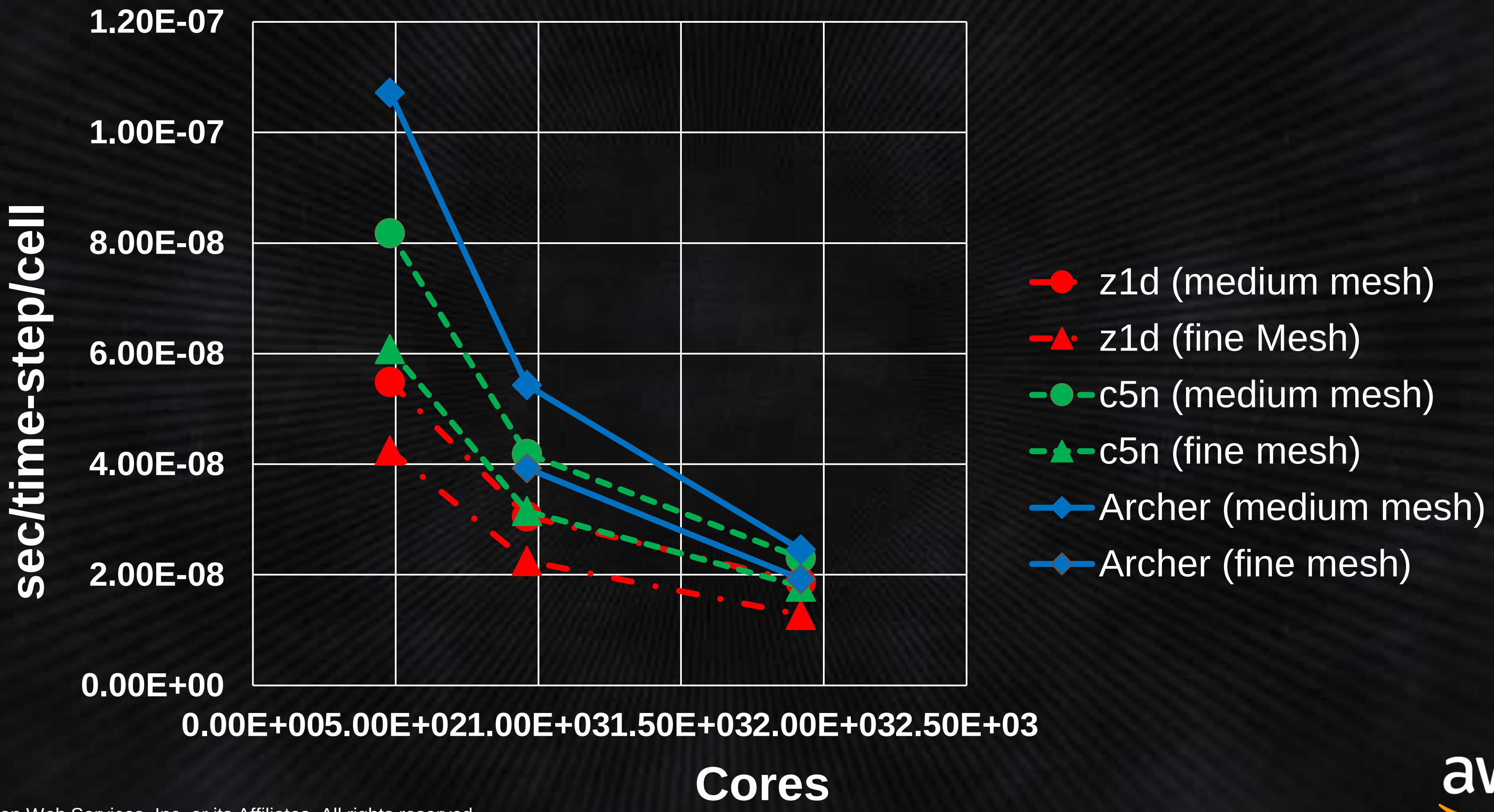
Resources used in this study

- Archer: Cray XC30 supercomputer
  - two 2.7 GHz, 12-core Intel E5-2697 v2 (Ivy Bridge)
- AWS:
  - z1d: 4.0 GHZ Intel®Xeon®Scalable Processors; 24 core per instance; 16GB Ram per core; 25 Gigabit network bandwidth
  - c5n: 3.0/3.5 GHZ Intel®Xeon®Scalable Processors; 36 core per instance; 5.3 GB Ram per core; 100 Gigabit network bandwidth; New Elastic Fabric Adaptor (EFA) for fast networking

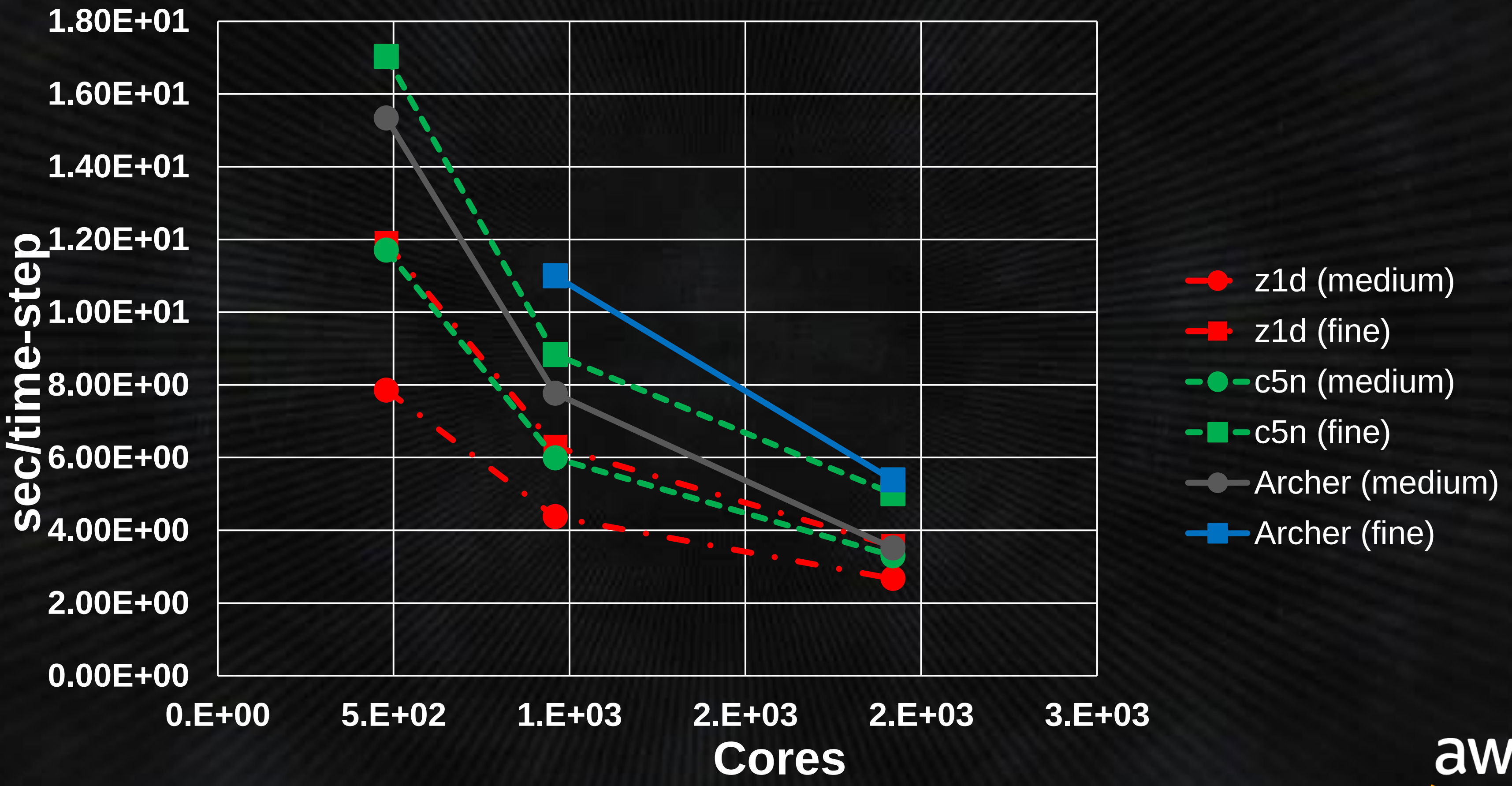
Methodology

- OpenFOAM v1806 in Double Precision (pimpleFoam)
- Scotch decomposition for solving, hierarchical (i.e constant x/y/z loading) for meshing
- SST-DDES Turbulence Model
- ANSA generated 143/280M cell unstructured mesh
- Time Step=5e-^{4}s with 5 inner iterations
- Preconditioned Conjugant Gradient Linear Solver

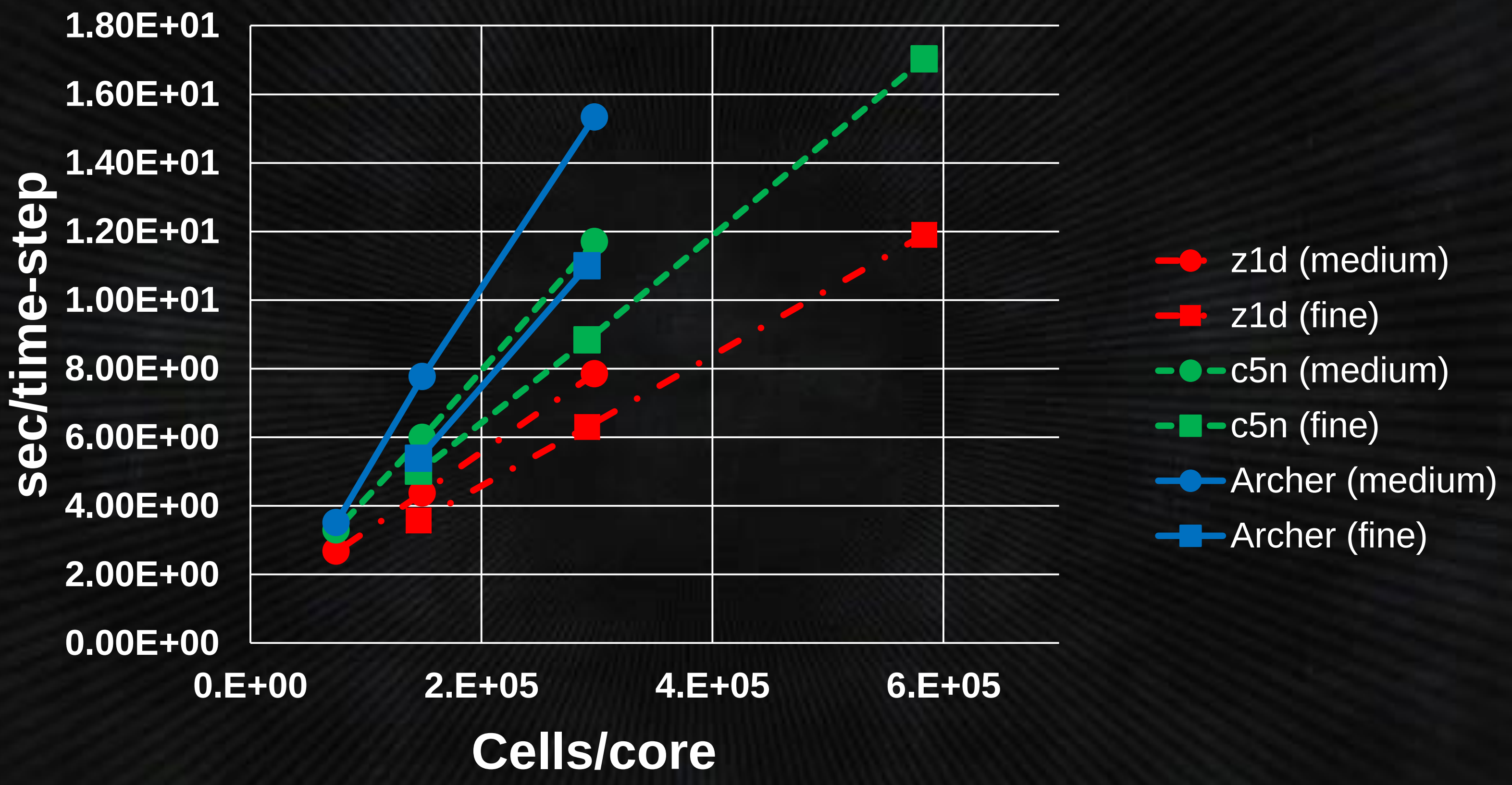
Amdahl Scaling: openFoam (pimpleFoam)



Amdahl Scaling, Alternate View



Amdahl Scaling, 2nd Alternate View



Scaling

Gustafson-Barsis Scaling (aka Gustafson's Law)

What is Gustafson's Law?

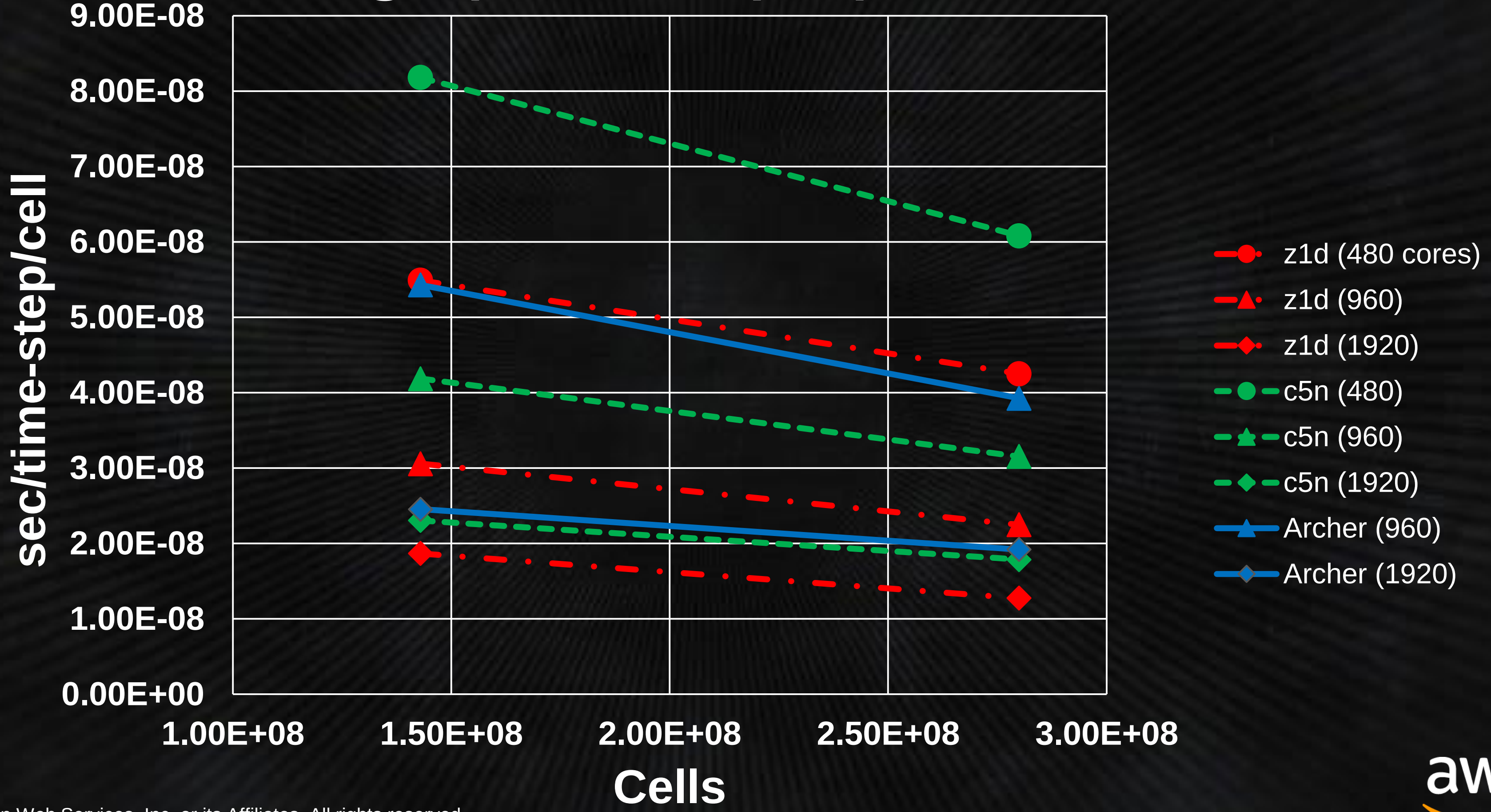
$$Speedup = (1 - p) + \frac{p}{n}$$

Gustafson's Law assumes a workload will increase in size linearly with the number of processors. (scalable workload)

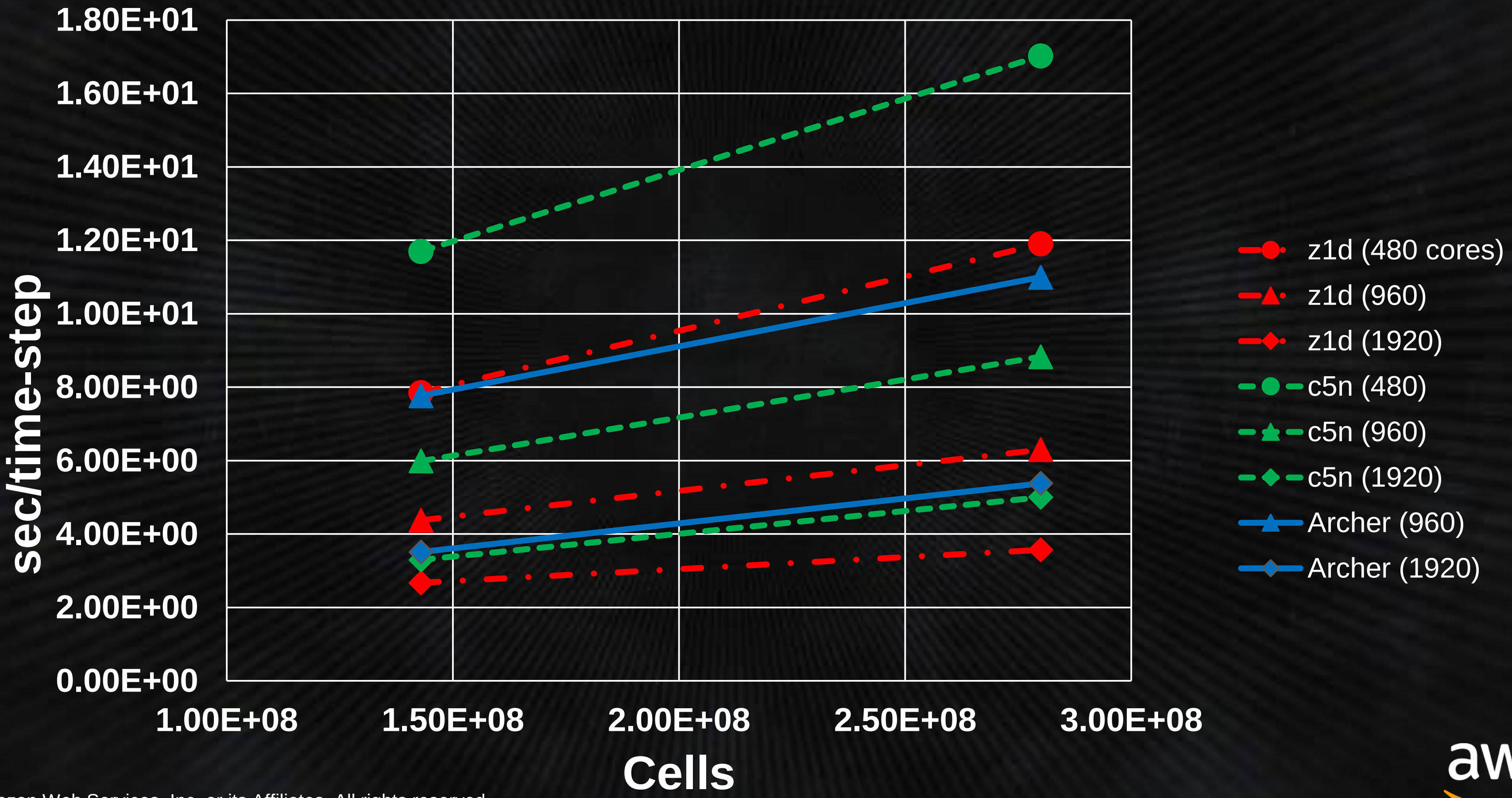
For example, scaling is measured at constant CFD mesh cells per core

Ideal: $\lim_{n \to \infty} speedup = 1 - p$

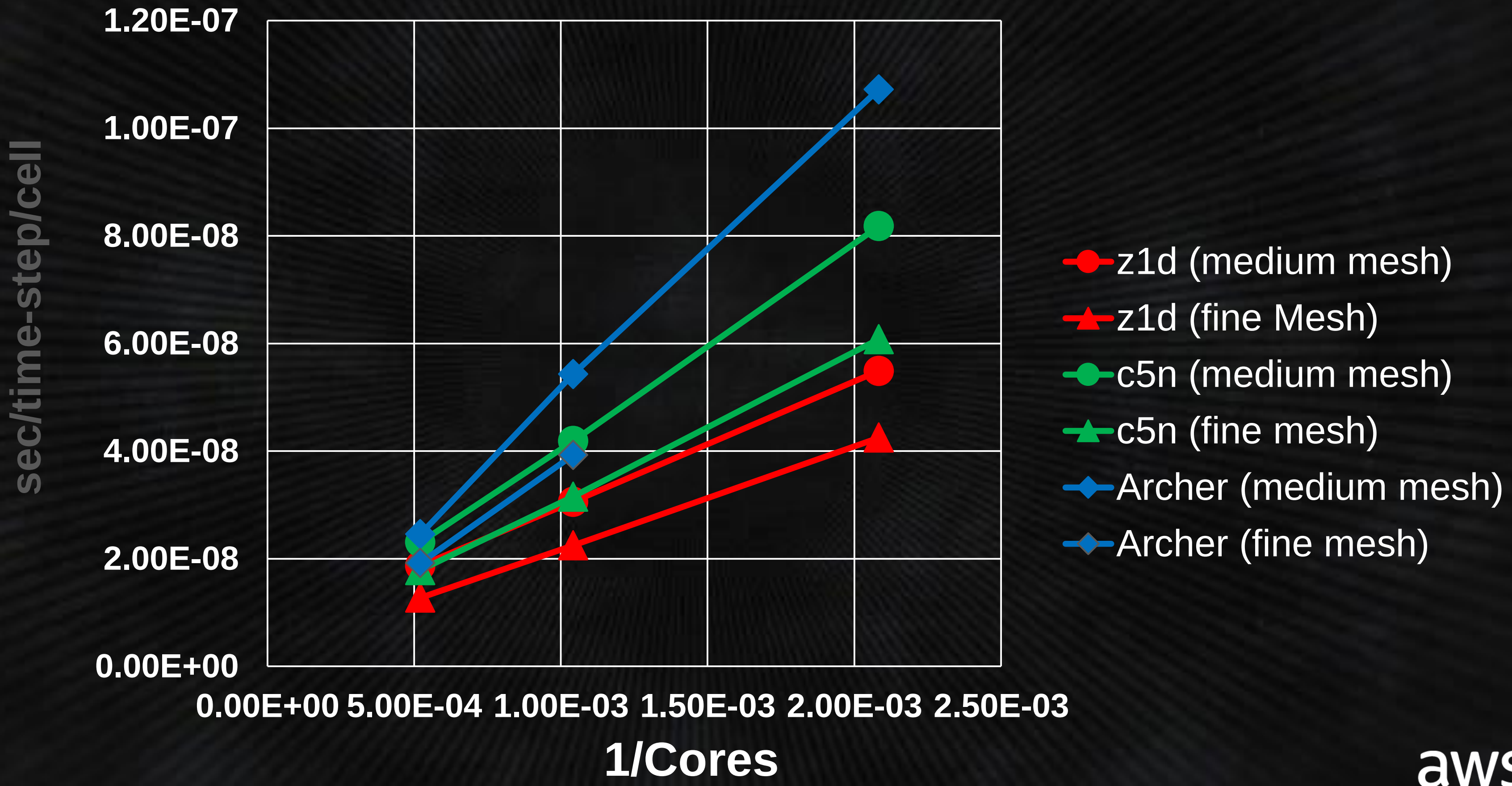
Gustafson Scaling: openFoam (pimpleFoam)



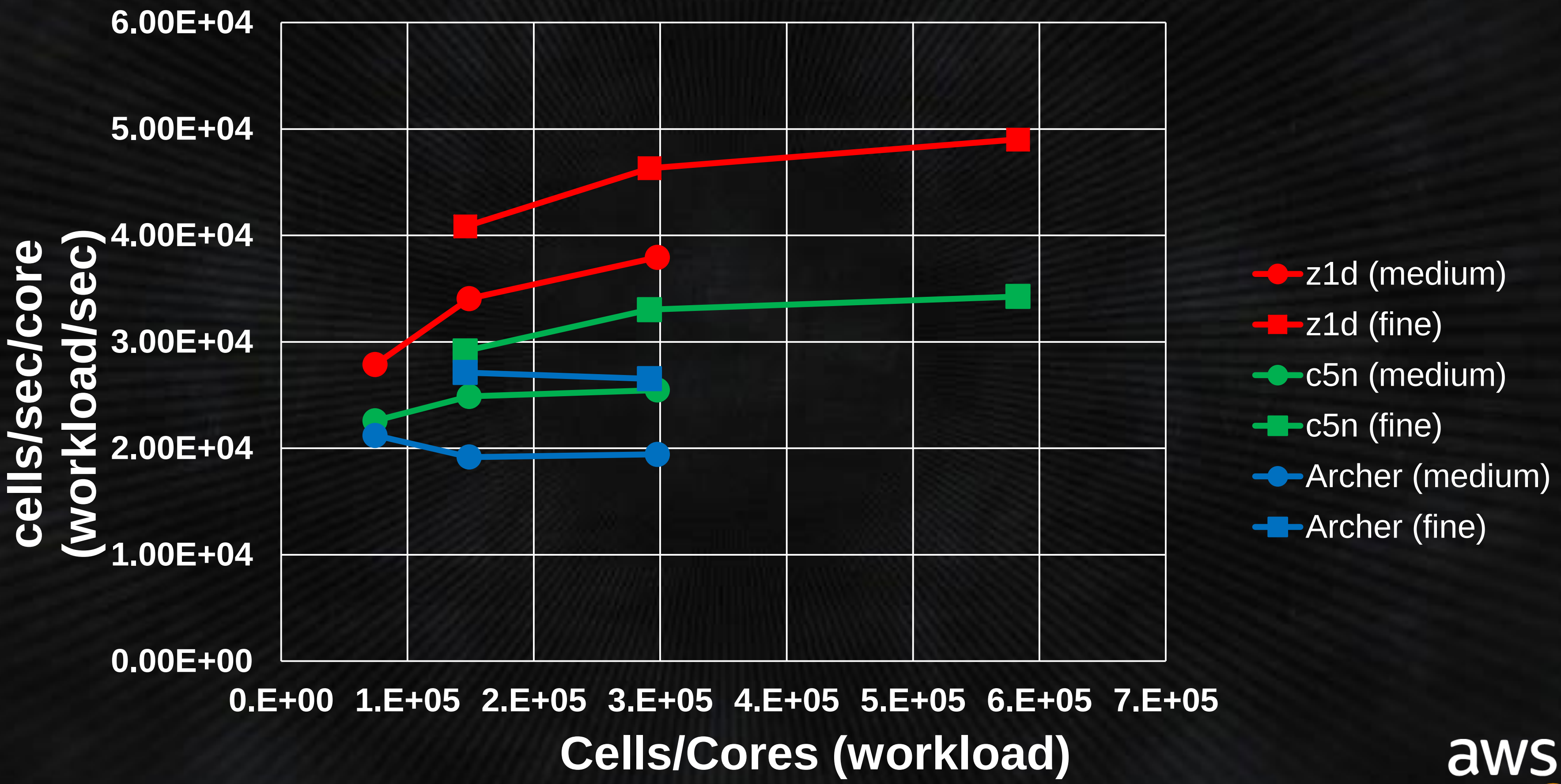
Gustafson Scaling: Alternate View



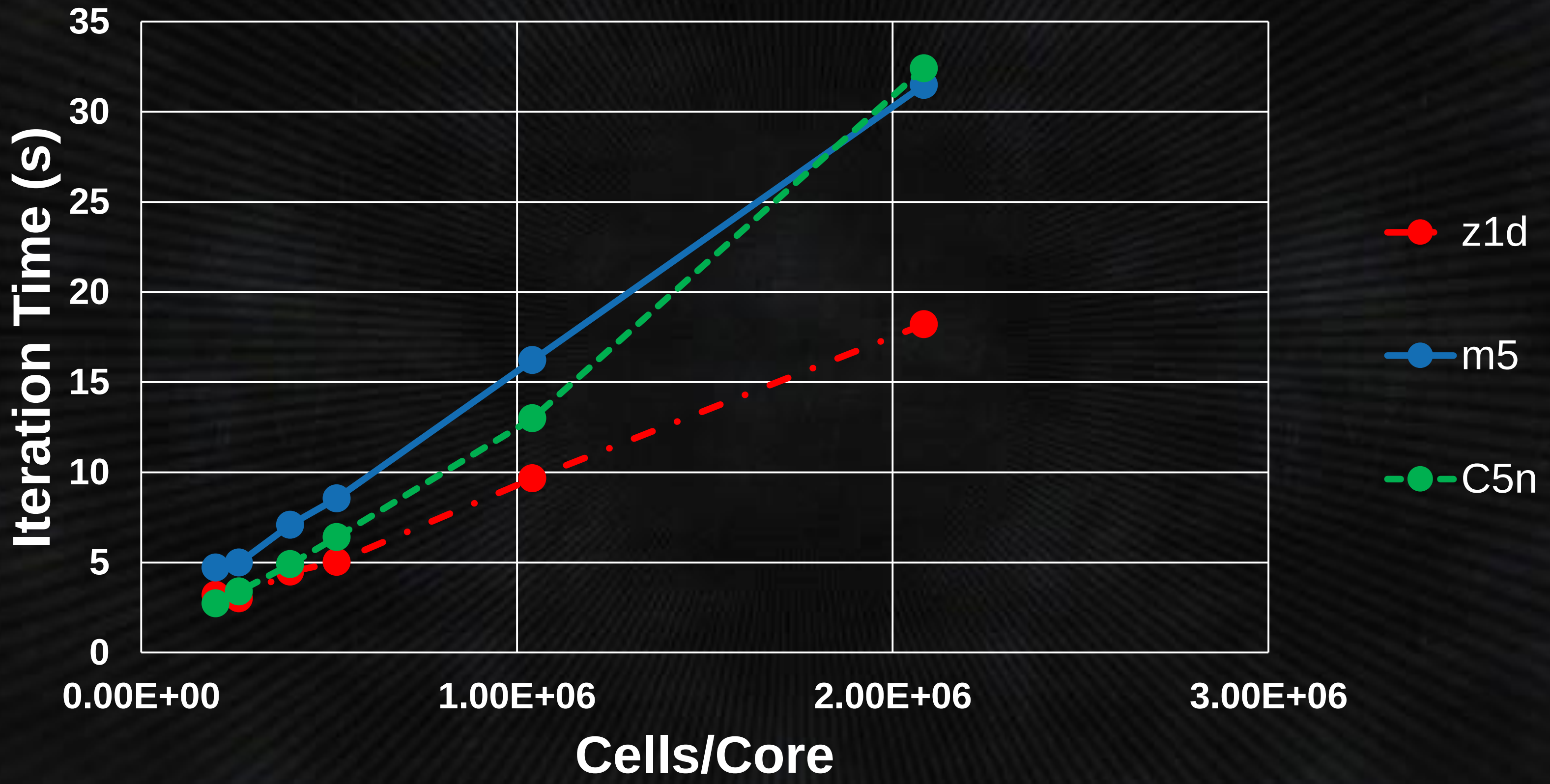
Gustafson: Speedup ∝ p/n



Gustafson: workload



400 Cell scaling



Obvious Question:

Why not include 400M cell case with others?

Answer:
They were done by two different people and two different workloads and, therefore, do not follow a consistent process

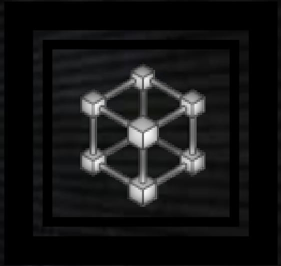
Latency

- Amdahl and Gustafson scaling both measure latency.   Latency includes:
  - Non parallel code
  - Memory latency
  - Cache latency
  - Network latency
  - Storage latency

Comments

- At high cell/core, or low core count, memory or cache more likely to slow processing (possibly see this in Archer)
- At low cell/core, or high core count, network latency more likely to slow processing (see in AWS-z1d and AWS-c5n)
- Total execution scaling based on processor workload (cells/core) is linear in all cases
- Slope of processor workload (cells/core) seems to follow network latency – faster network → steeper slope = better scaling
- Faster network does not mean faster execution time
- Coarser mesh has better scaling than finer mesh in all cases, but AWS-c5n has largest difference (best guess: PCG routines)

Discussion?



Acknowledgement

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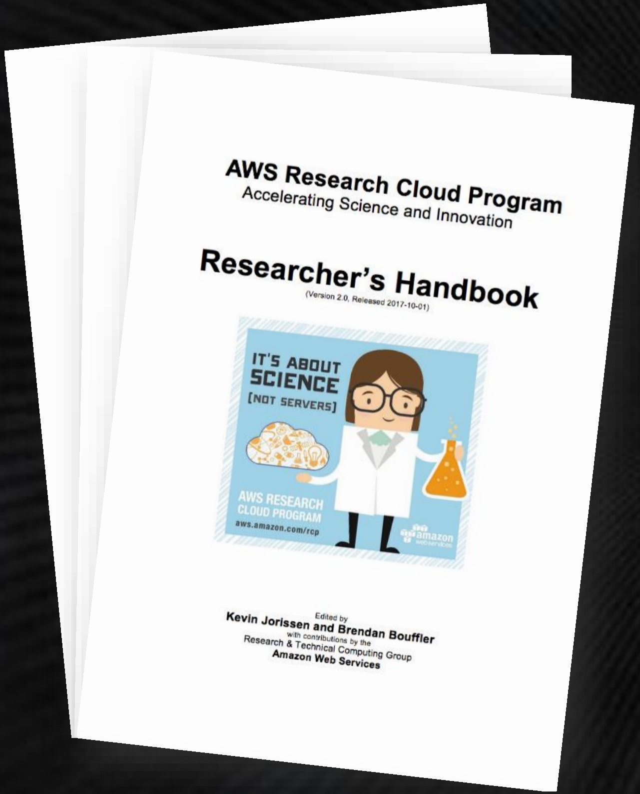
AWS Researcher's Handbook

The 200-page "missing manual" for science in the cloud.



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