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NAVGEM on the Cloud:
Computational Evaluation of Commercial Cloud HPC with a Global Atmospheric Model

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Outline

- Background
  - Computing Resources
  - Cloud Migration
- Test Workload
  - Navy Global Environmental Model
  - Benchmark Specification
- Low resolution forecast performance
- Elastic Fabric Adapter on AWS EC2
- High resolution forecast performance
- Next Steps

Background: Computing Resources

Navy Supercomputing

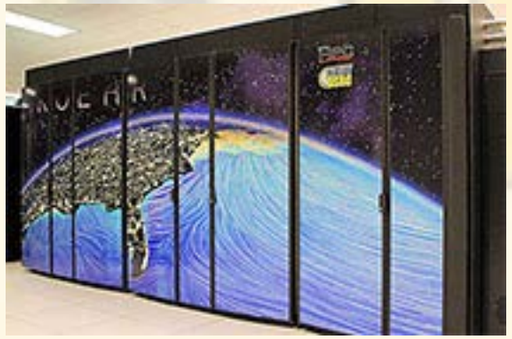
- Navy's arm of DoD HPC Modernization Program
- One of five DoD HPC Centers
- Headquartered with Naval Meteorology and Oceanography Command
- Supports various defense computational areas:
  - Climate/Weather/Ocean Modeling and Simulation
  - Computational Structural Mechanics
  - Computational Electromagnetics and Acoustics
  - Space and Astrophysical Science

Navy DSRC

Stennis Space Center, Mississippi

HPE SGI 8600
3.05 PFLOPS

Gaffney



Koehr

Cray XC40
2 PFLOPS

Conrad

Gordon

Background: Cloud Migration

DoD Priority: Modernization, Cost-Savings, Redundancy

Directive History

- 2012 National Defense Authorization Act
- 2012-2014 Navy Approach to Cloud Computing
- 2015 Acquisition and Use of Cloud Services
- 2017 Navy Cloud First Policy
- 2019 Federal Cloud Computing Strategy – Cloud Smart

Performance Plan for Reduction of Resources Required for Data Servers and Centers:

"Migration… to cloud computing services… that provide a better capability at a lower cost with the same or greater degree of security."

- NDAA FY 2012

Navy's Emphasis

- Transition public facing websites
- Reduce data centers
- Increasing secure capabilities

"… reduce investment in traditional, on –premises… data centers … [including] Special Purpose Processing Nodes…"

- Navy Cloud First Policy

Success with Enterprise Applications

- Public-facing Navy websites
  - Fleet and Family has shifted 100 web-based systems to AWS GovCloud.
  - My Navy Portal team awarded for implementing the first Level 4 data enterprise architecture to the cloud.

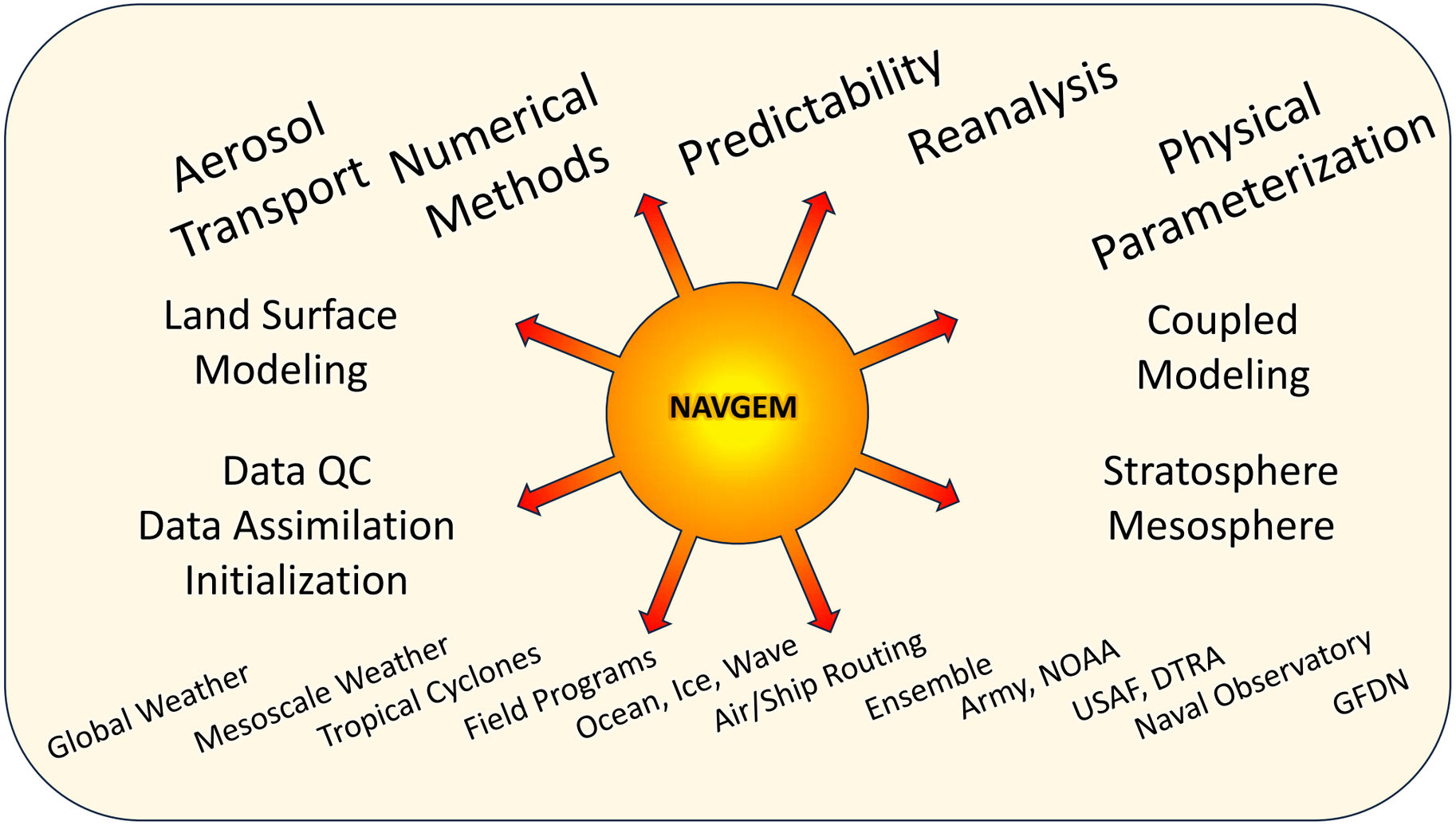
"… agencies must cultivate an organizational mindset of constant improving and learning.

- 2019 Federal Cloud Computing Strategy

Test Workload: Navy Global Environmental Model

NAVGEM

- Global (synoptic) scale weather prediction program written in Fortran/MPI .
- Dynamical core composed of Semi-Lagrangian/Semi-Implicit numerical methods to solve primitive equations on a sphere.
- Ouput products feed in to numerous external programs and organizations.



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Benchmark Specifications

	Navy DSRC - Conrad (Cray XC40)	AWS c4.8xlarge	Azure H16r	Penguin B30 queue	AWS c5n.18xlarge
CPU	- 2.3 GHz Intel Xeon E5-2698 v3 Broadwell - 32 core nodes	- 2.9 GHz Intel Xeon E5-2666 v3 Haswell - 18 core nodes	- 3.2 GHz Intel Xeon E5-2667 v3 - 14 core nodes	- 2.4 GHz Intel Xeon E5-2680 v4 Broadwell - 28 core nodes	- 3.0 GHz Intel Xeon Platinum w/ AVX-512 - 36 core nodes
Network	- Cray Aries / Dragonfly	- 25 Gbps ethernet with SRIOV	- FDR Infiniband	- Intel OmniPath	- AWS EFA

Software Configuration

- Intel Fortran 2018 update 1
- MPI:
  - Intel 2018 update 1
  - EFA: Open MPI 3.1.4
- HDF5 1.8.20

Platform Parameters

- Hyperthreading disabled

- AWS
  - us-west-2 (OR) region
  - Placement Groups
  - CloudFormation

- Azure
  - US Gov Arizona
  - VMSS

- Penguin on Demand
  - PBS resource manager

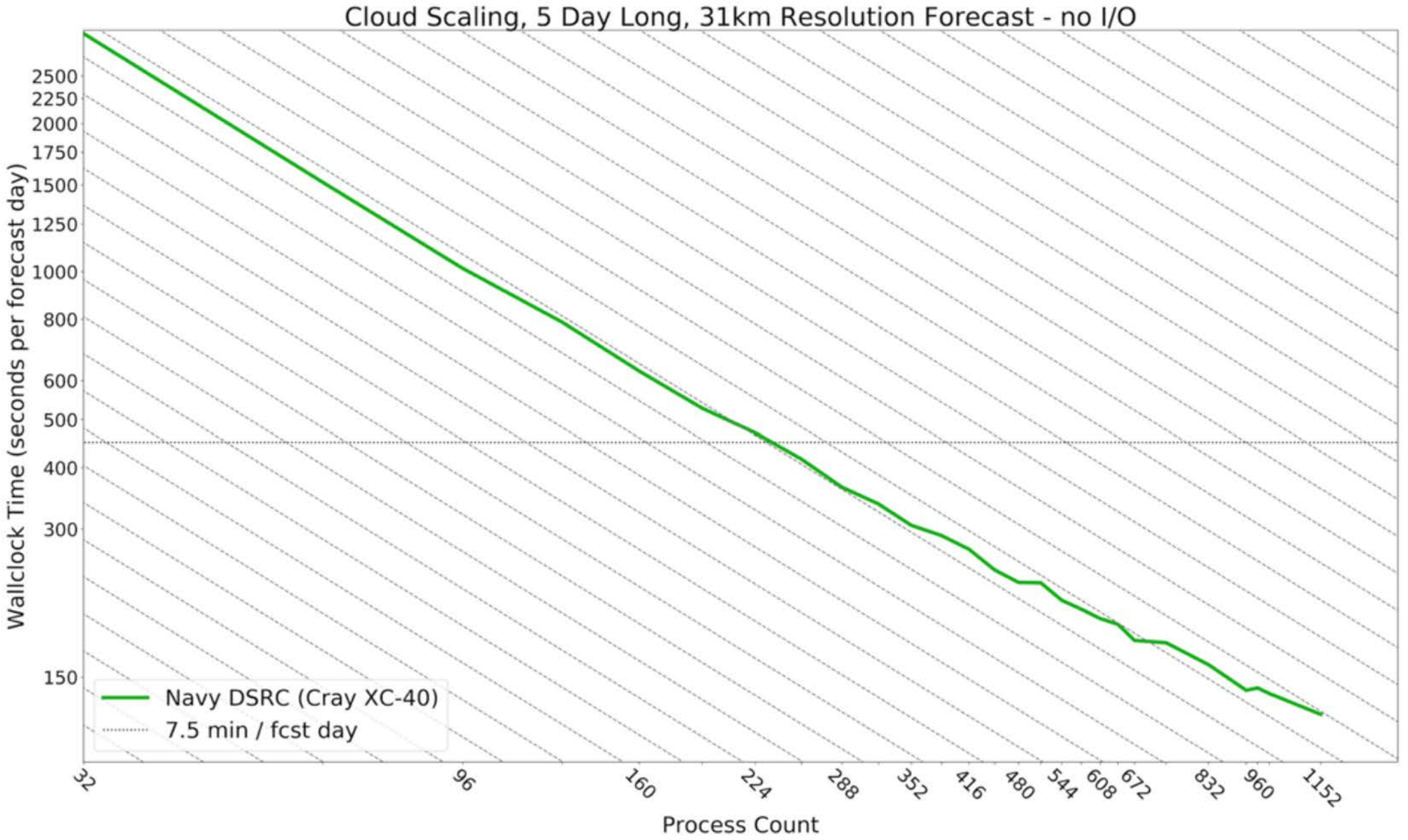
Low Resolution Forecast: Performance - Navy DSRC

Platform Specifications:

- 2.3 GHz Intel Xeon E5-2698 v3 Broadwell
- 32 core nodes
- Cray Aries / Dragonfly
- Cray Linux

Results

- Tested on Conrad
- Good scaling
  - minimal variability
  - minor increase in slope.



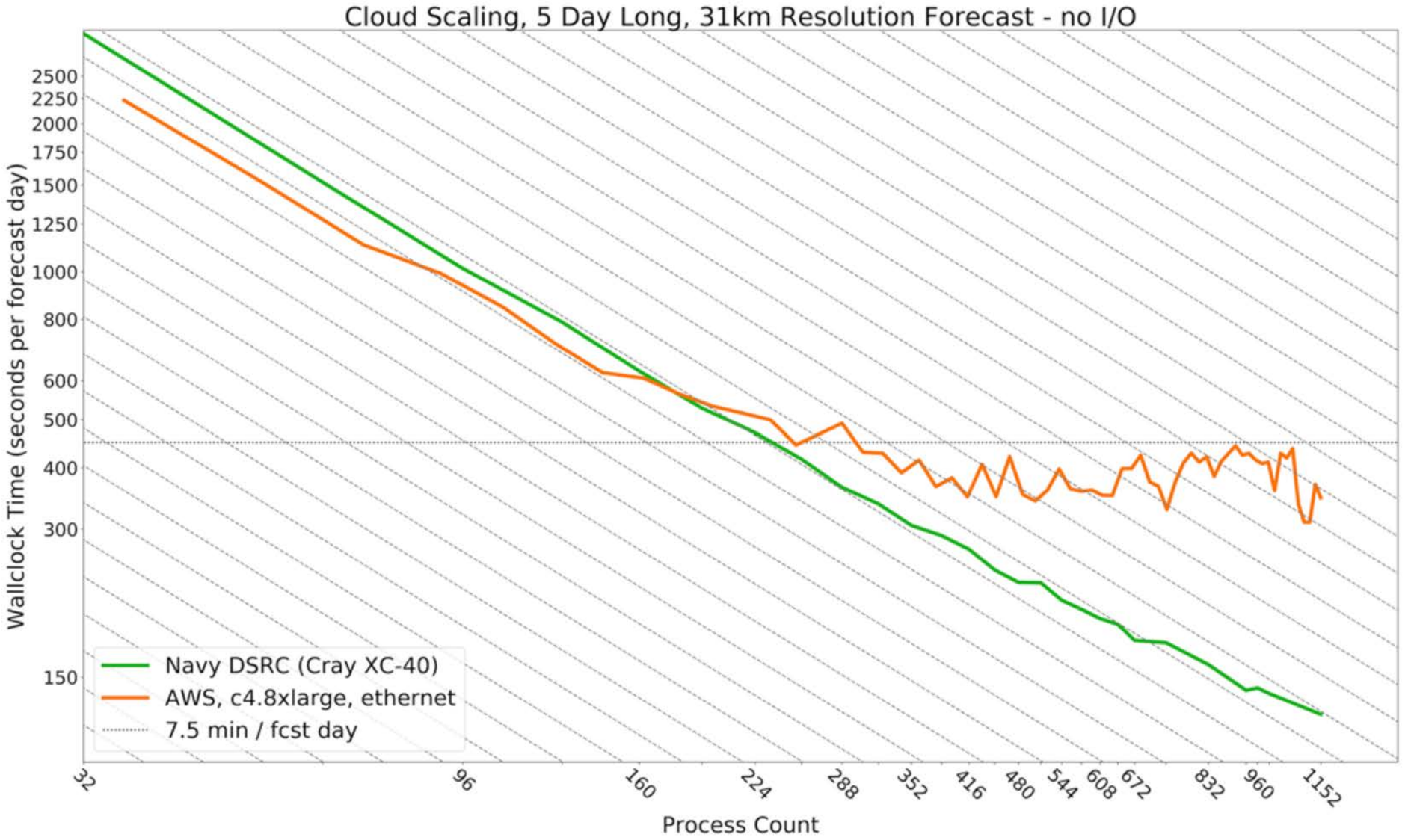
Low Resolution Forecast: Performance - AWS EC2 1

Platform Specifications:

- 2.9 GHz Intel Xeon E5-2666 v3 Haswell
- 18 core nodes
- 25 Gbps ethernet with SRIOV
- Amazon Linux

Results

- AWS's most powerful compute optimized instance at time of testing.
- Adjusted variety of configurations
  - System clocksource
  - Attached storage type
  - Cluster creation tools
  - Processors per node



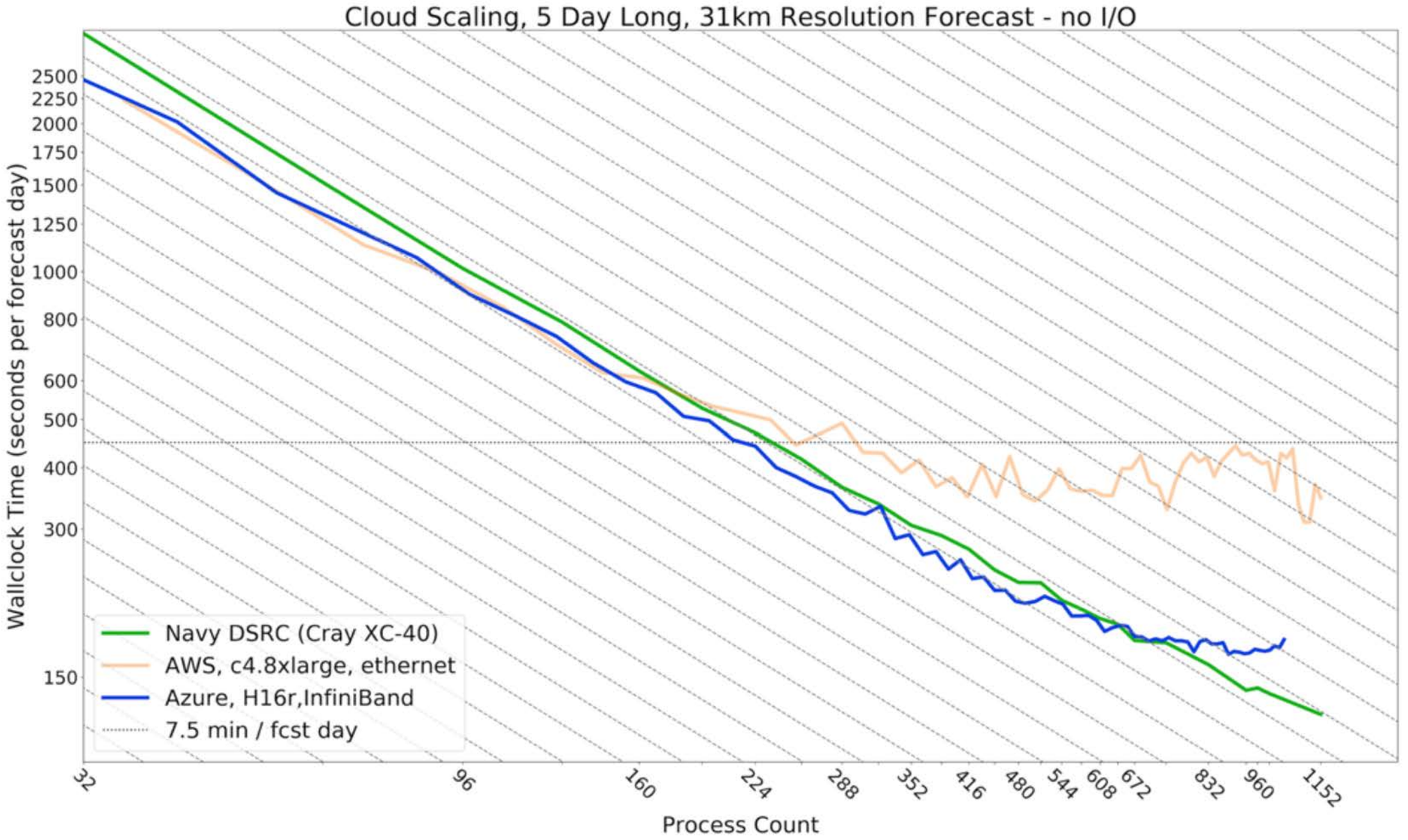
Low Resolution Forecast: Performance - Azure

Platform Specifications:

- 3.2 GHz Intel Xeon E5-2667 v3
- 14 core nodes
- FDR Infiniband
- CentOS Linux

Results

- Infiniband networking likely contributed to improvement.
- Improved performance (plotted) using 14/16 processors per node.
- Eventual flattening of performance.



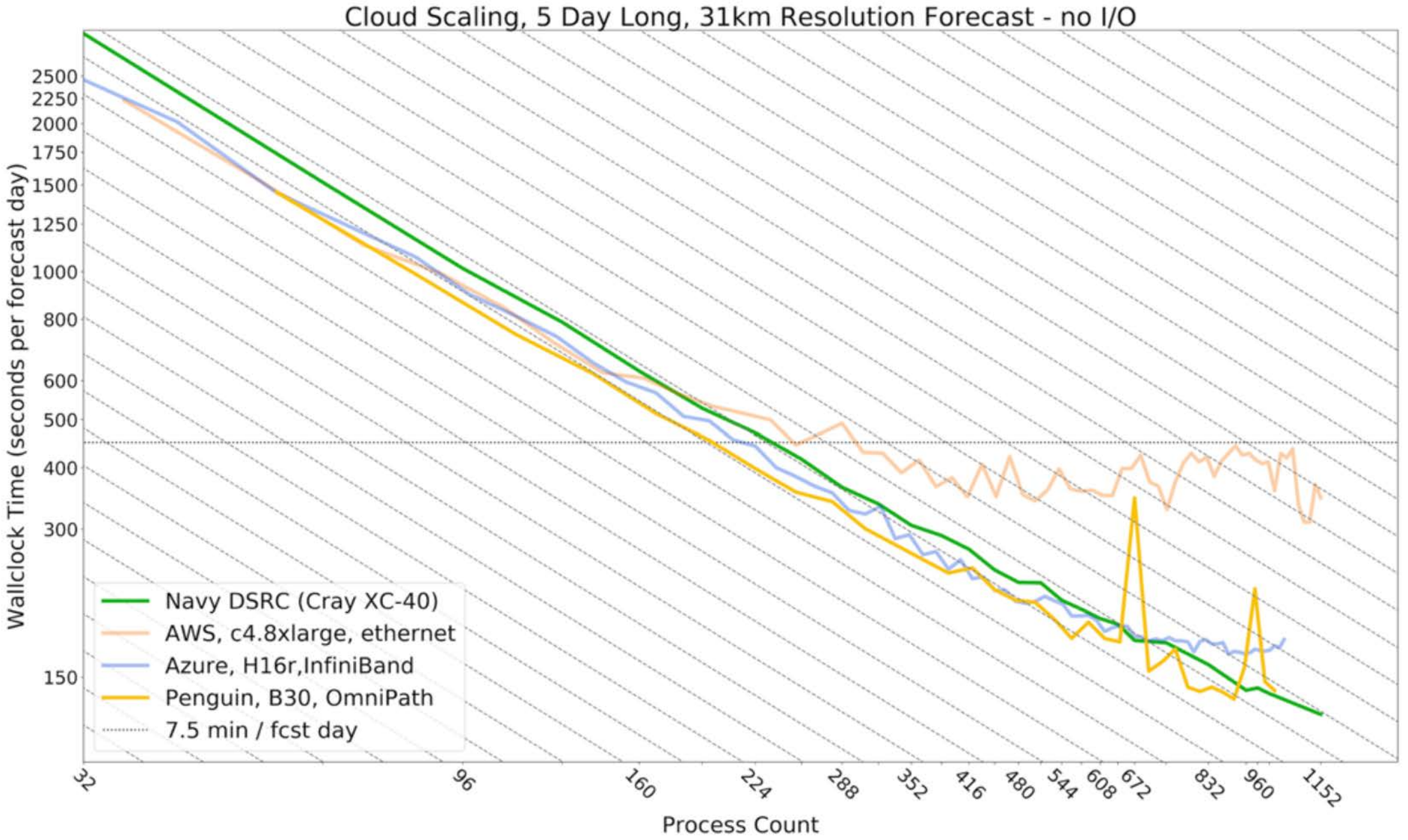
Low Resolution Forecast: Performance - Penguin

Platform Specifications:

- 2.4 GHz Intel Xeon E5-2680 v4 Broadwell
- 28 core nodes
- Intel OmniPath

Results

- Improved scaling expected considering Penguin's "traditional" system design.
- Required use of batch scheduler and waiting for system resources at larger cluster sizes.
- Variability and unexplained spikes at higher core counts.



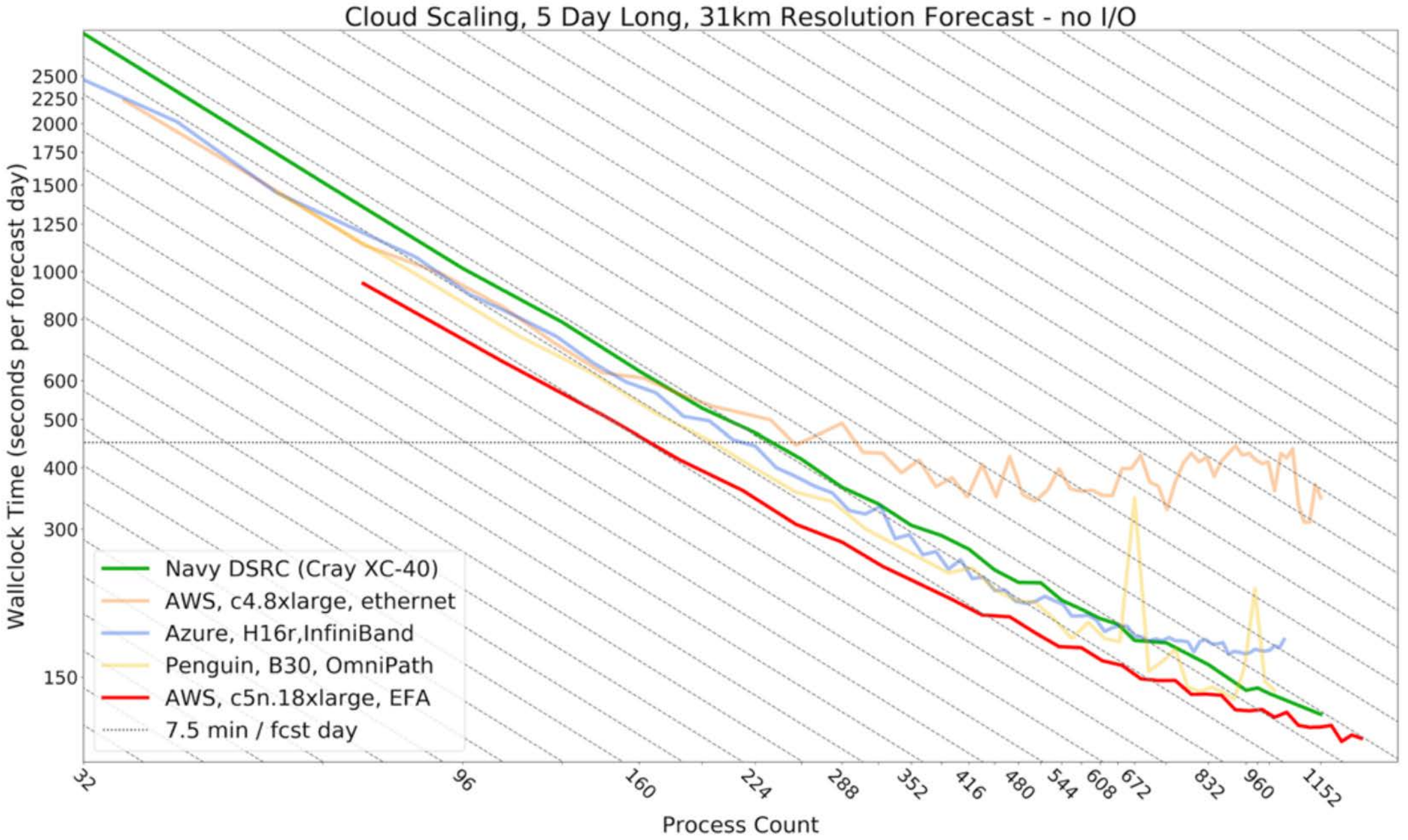
Low Resolution Forecast: Performance - AWS EC2 EFA

Platform Specifications:

- 3.0 GHz Intel Xeon Platinum w/ AVX-512
- 36 core nodes
- AWS Elastic Fabric Adapter
- Amazon Linux 2

Results

- Smooth scaling up to ~450 cores.
- Slight variability beyond – “stair step” performance beyond.
- Required use of Open MPI; Intel MPI now supported but not yet tested successfully with NAVGEM.



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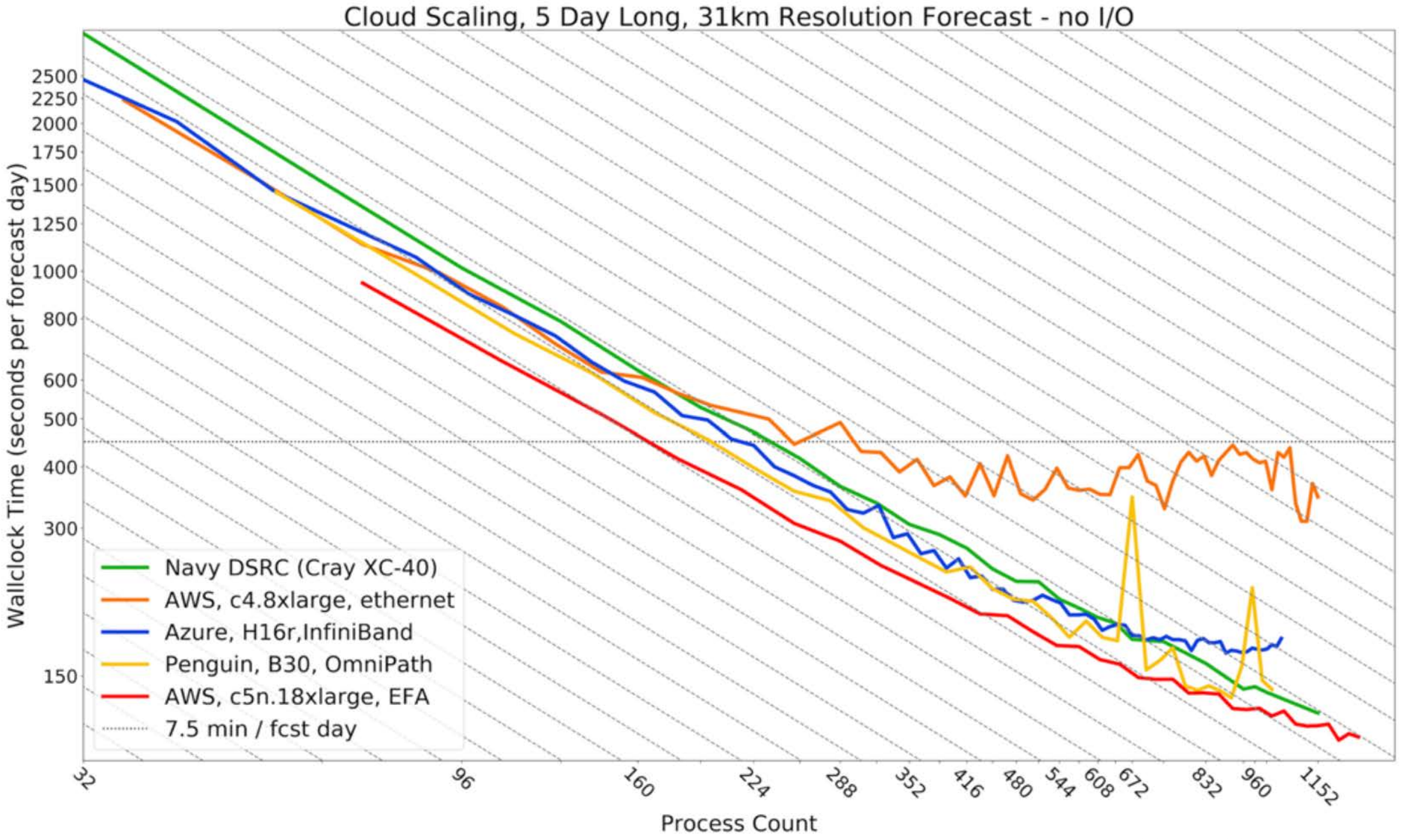
Low Resolution Forecast: Performance - Comparison

Performance Improvements: c5n with EFA on AWS EC2

- At the highest core counts:
  - 13% faster than Penguin
  - 39% faster than Azure
  - 192% faster than previous AWS
  - 6% faster than Navy DSRC

- Min size estimated to meet 7.5 min:
  - 6% faster than Penguin
  - 16% faster than Azure
  - 74% faster than previous AWS
  - 29% faster than Navy DSRC

- Min size cost estimate:
  - Penguin: $12.95
  - Azure: $21.31
  - Previous AWS: $18.65
  - C5n with EFA: $13.76



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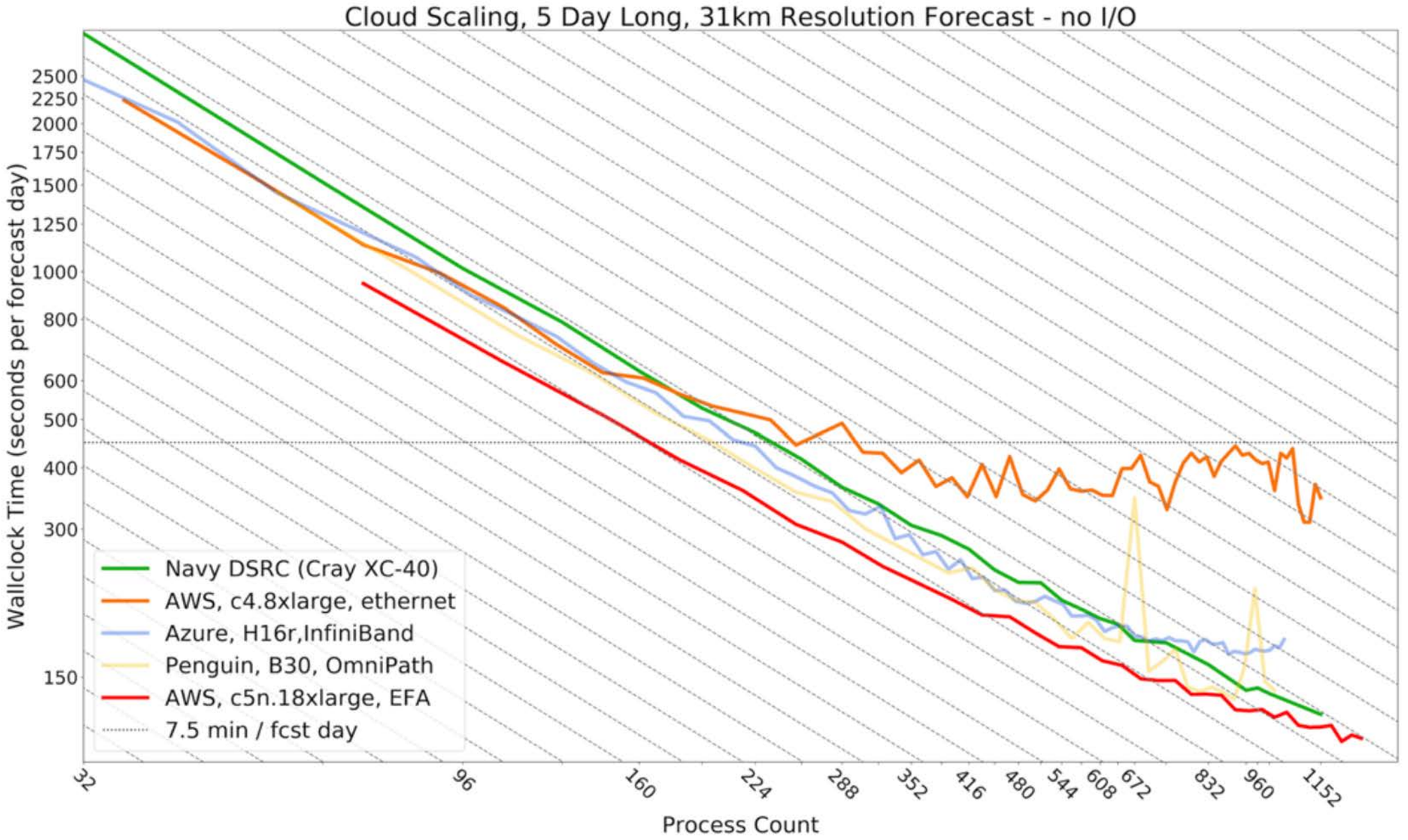
Elastic Fabric Adapter on AWS EC2

Elastic Fabric Adapter

- Updated networking capability launched April 2019
- Hardware:
  - 3rd gen Nitro chip
- Software:
  - Scalable Reliable Datagram
- EFA provider has been upstreamed to most recent libfabric release
- Currently available on 4 large instance types.
- Supports Open MPI and Intel MPI.



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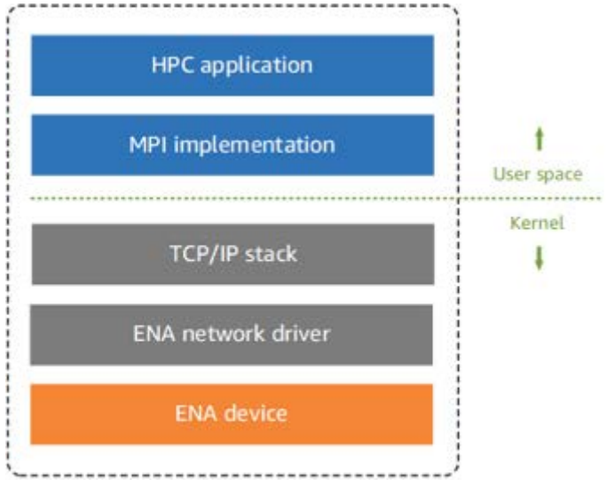
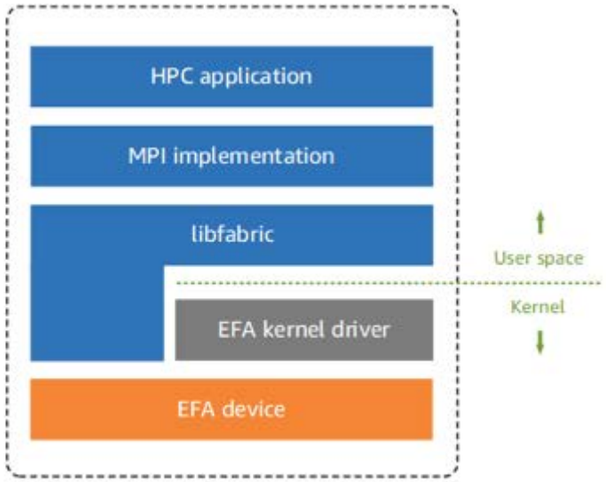
Elastic Fabric Adapter on AWS EC2

Elastic Fabric Adapter

- Updated networking capability launched April 2019.
- Hardware:
  - 3rd gen Nitro chip
- Software:
  - Scalable Reliable Datagram
- EFA added as network fabric provider supported by libfabric library.
- Currently available on 4 large instance types.
- Supports Open MPI and Intel MPI.



Traditional HPC software stack in EC2



HPC software stack in EC2 with EFA

TCP	InfiniBand	SRD
Stream	Messages	Messages
In-order	In-order	Out-of-order
Single path	Single(ish) path	ECMP spraying with load balancing
High limit on retransmit timeout (>50ms)	Static user-configured timeout (log scale)	Dynamically estimated timeout (usec resolution)
Loss-based congestion control	Semi-static rate limiting (limited set of supported rates)	Dynamic rate limiting
Inefficient software stack	Transport offload with scaling limitations	Scalable transport offload (same number of QPs regardless of cluster size)

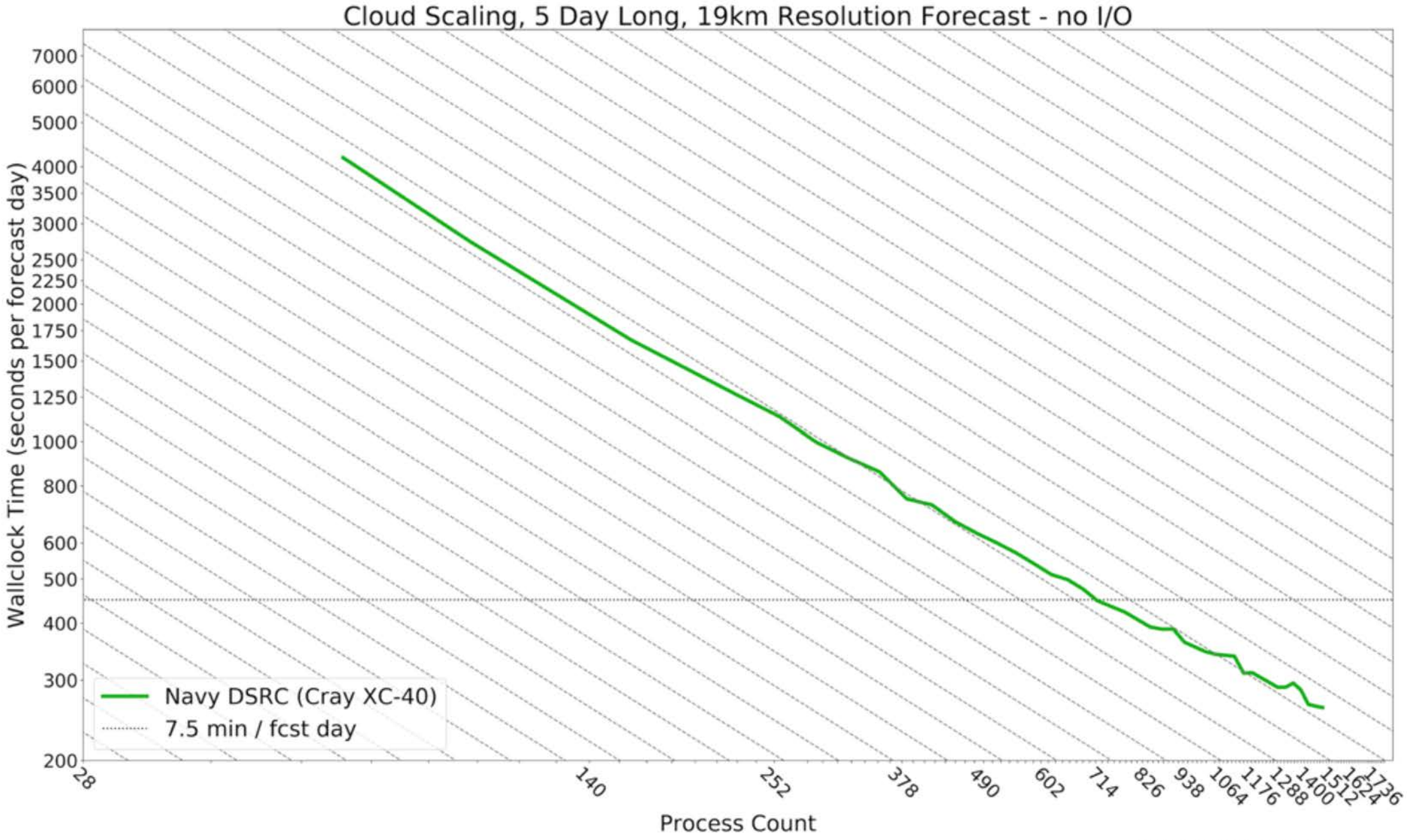
High Resolution Forecast: Performance - Navy DSRC

Platform Specifications:

- 2.3 GHz Intel Xeon E5-2698 v3 Broadwell
- 32 core nodes
- Cray Aries / Dragonfly
- Cray Linux

Results

- Good scaling maintained on Navy resources.
- Larger cluster sizes required to meet 7.5 min/day standard.



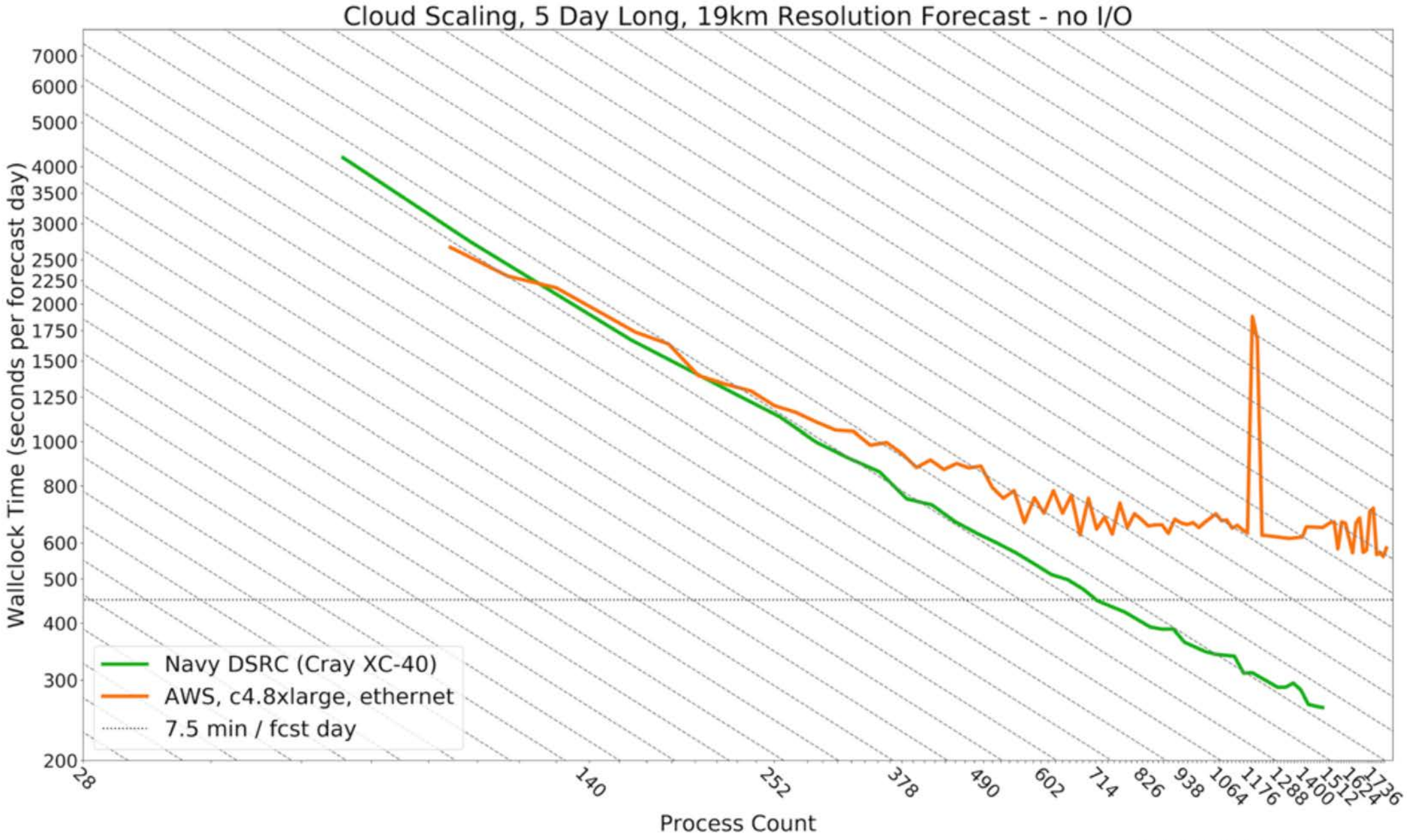
High Resolution Forecast: Performance - AWS EC2 1

Platform Specifications:

- 2.9 GHz Intel Xeon E5-2666 v3 Haswell
- 18 core nodes
- 25 Gbps ethernet with SRIOV
- Amazon Linux

Results

- Variability and performance flattening delayed.
- Cannot meet 7.5 min/day goal.



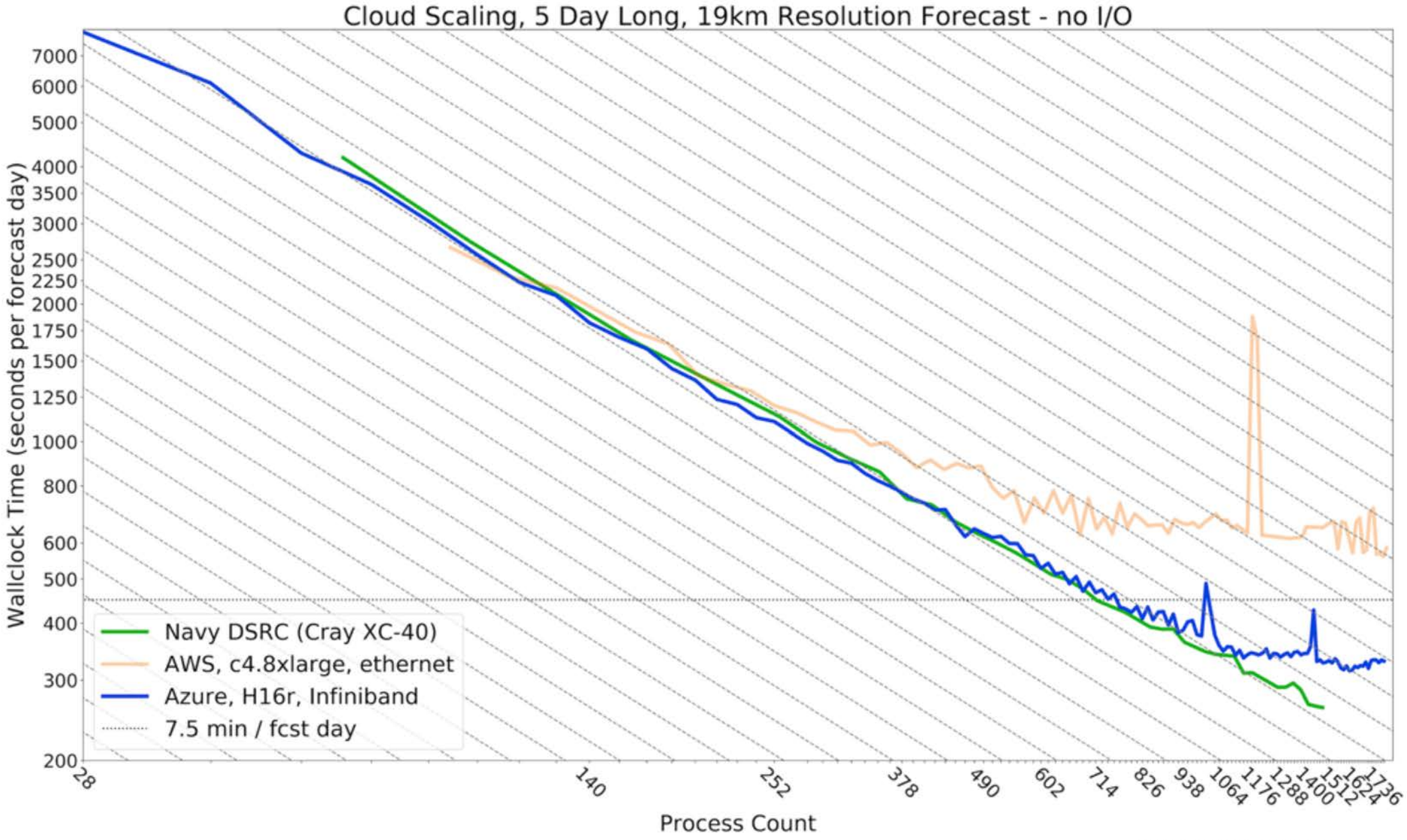
High Resolution Forecast: Performance - Azure

Platform Specifications:

- 3.2 GHz Intel Xeon E5-2667 v3
- 14 core nodes
- FDR Infiniband
- CentOS Linux

Results

- Similar improvement in variability and performance over AWS compared to low resolution forecast.
- Slight performance improvement over Navy DSRC in low resolution forecast has disappeared.



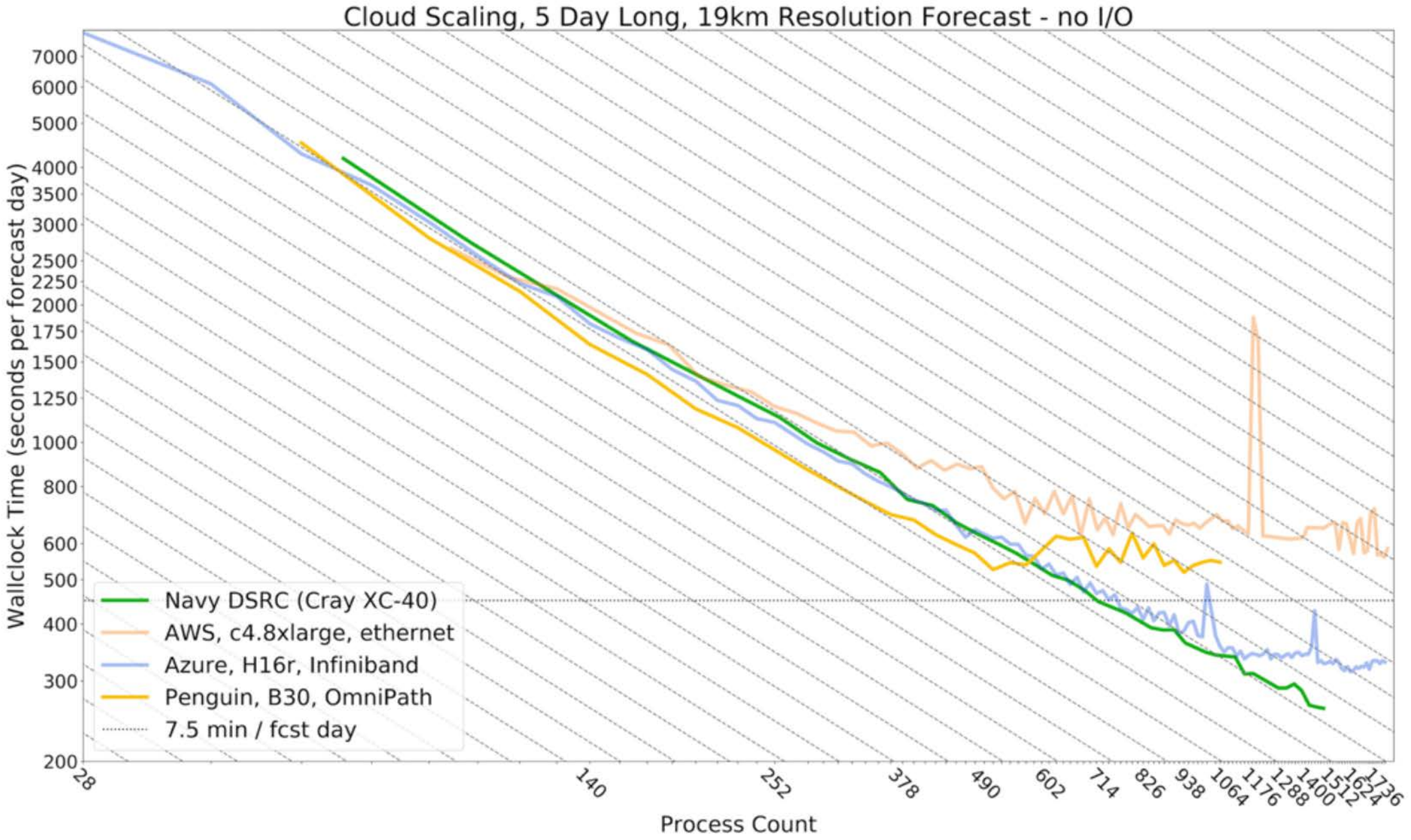
High Resolution Forecast: Performance - Penguin

Platform Specifications:

- 2.4 GHz Intel Xeon E5-2680 v4 Broadwell
- 28 core nodes
- Intel OmniPath

Results

- Good scaling and slight improvement over Navy DSRC until ~500 cores.
- Unable to obtain larger cluster runs to due to system limitations and excessive job queue wait times.



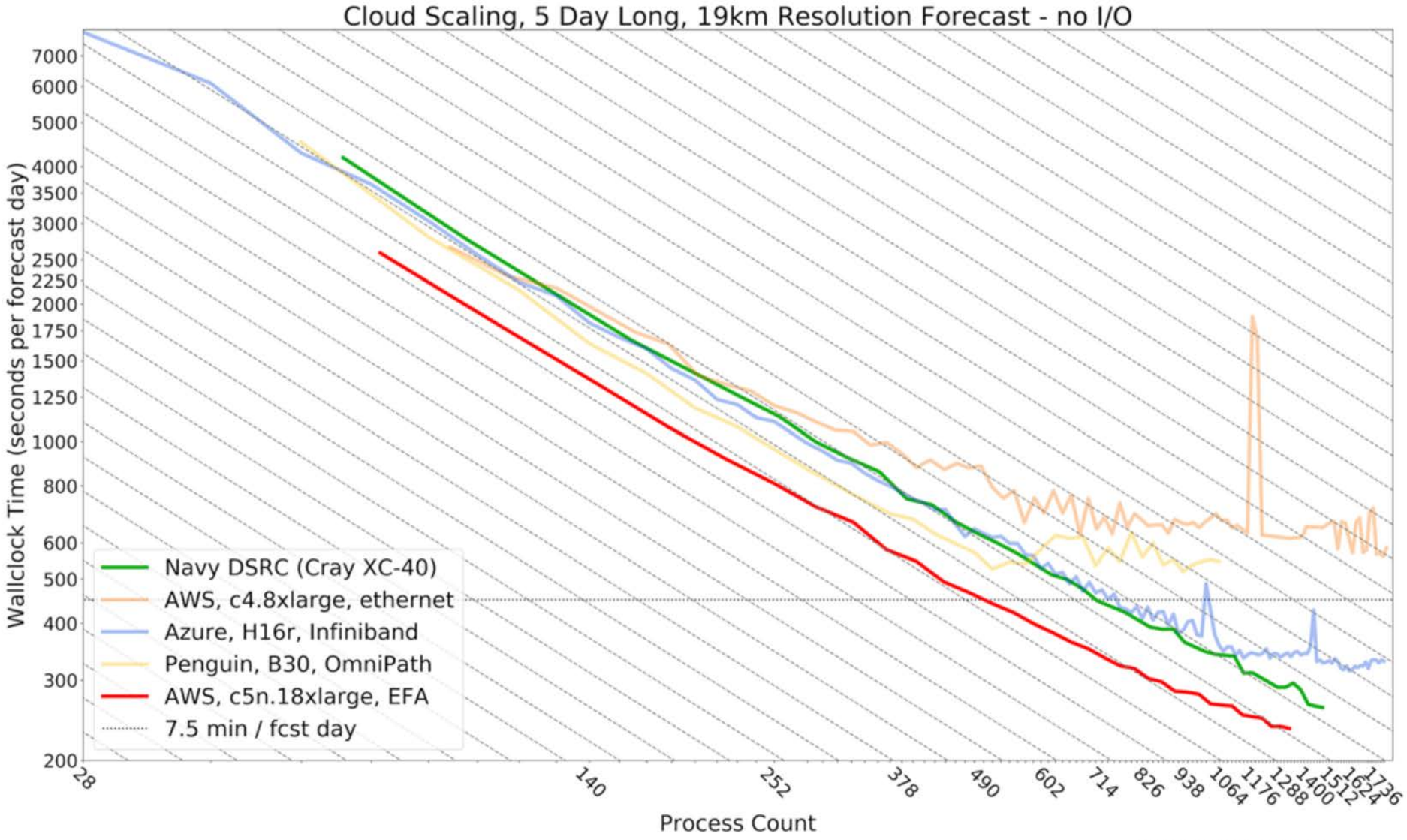
High Resolution Forecast: Performance - AWS EC2 EFA

Platform Specifications:

- 3.0 GHz Intel Xeon Platinum w/ AVX-512
- 36 core nodes
- AWS Elastic Fabric Adapter
- Amazon Linux 2

Results

- Similar performance improvement over all platforms as exhibited in low resolution forecast.



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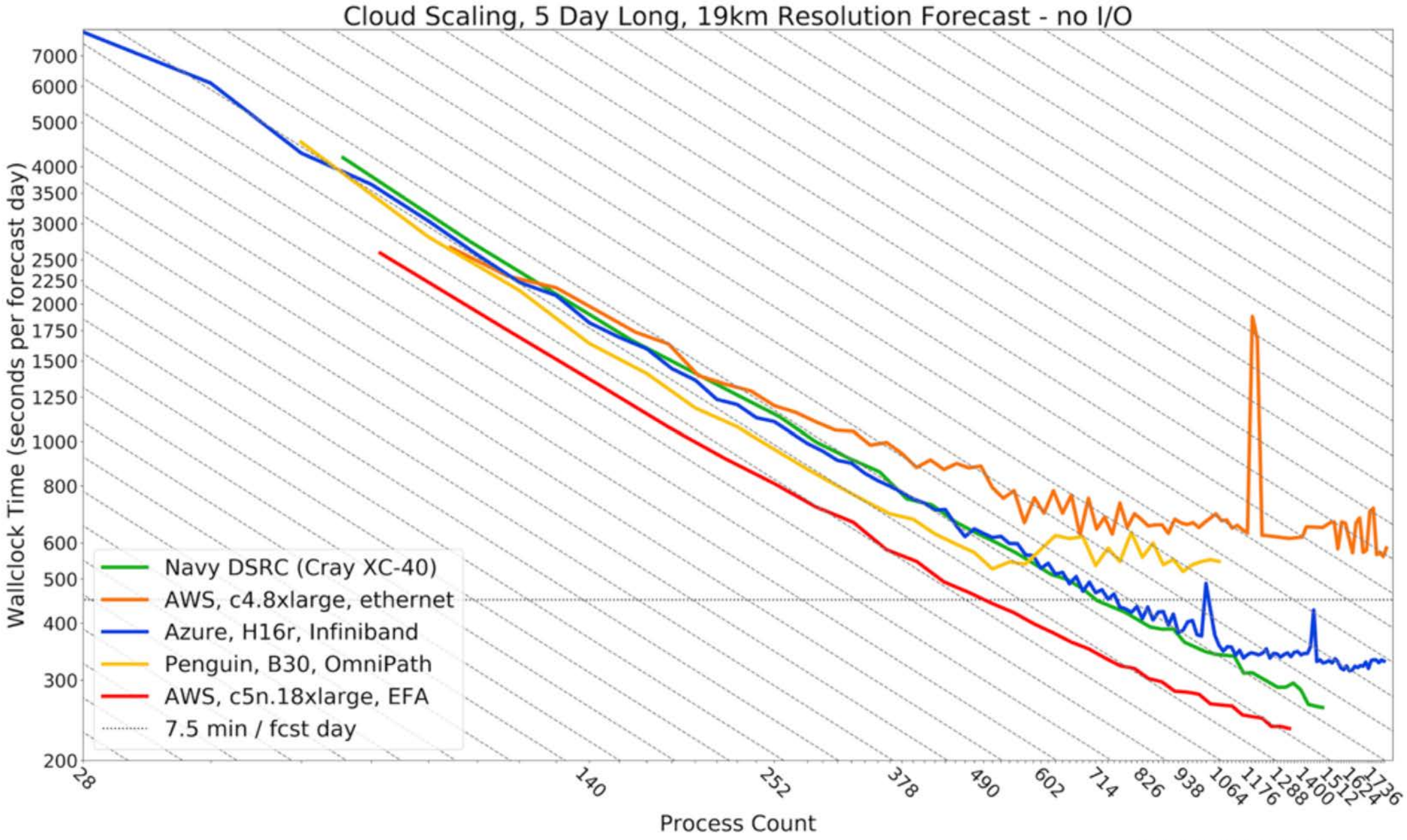
High Resolution Forecast: Performance - Comparison

Performance Improvements: C5n with EFA on AWS EC2

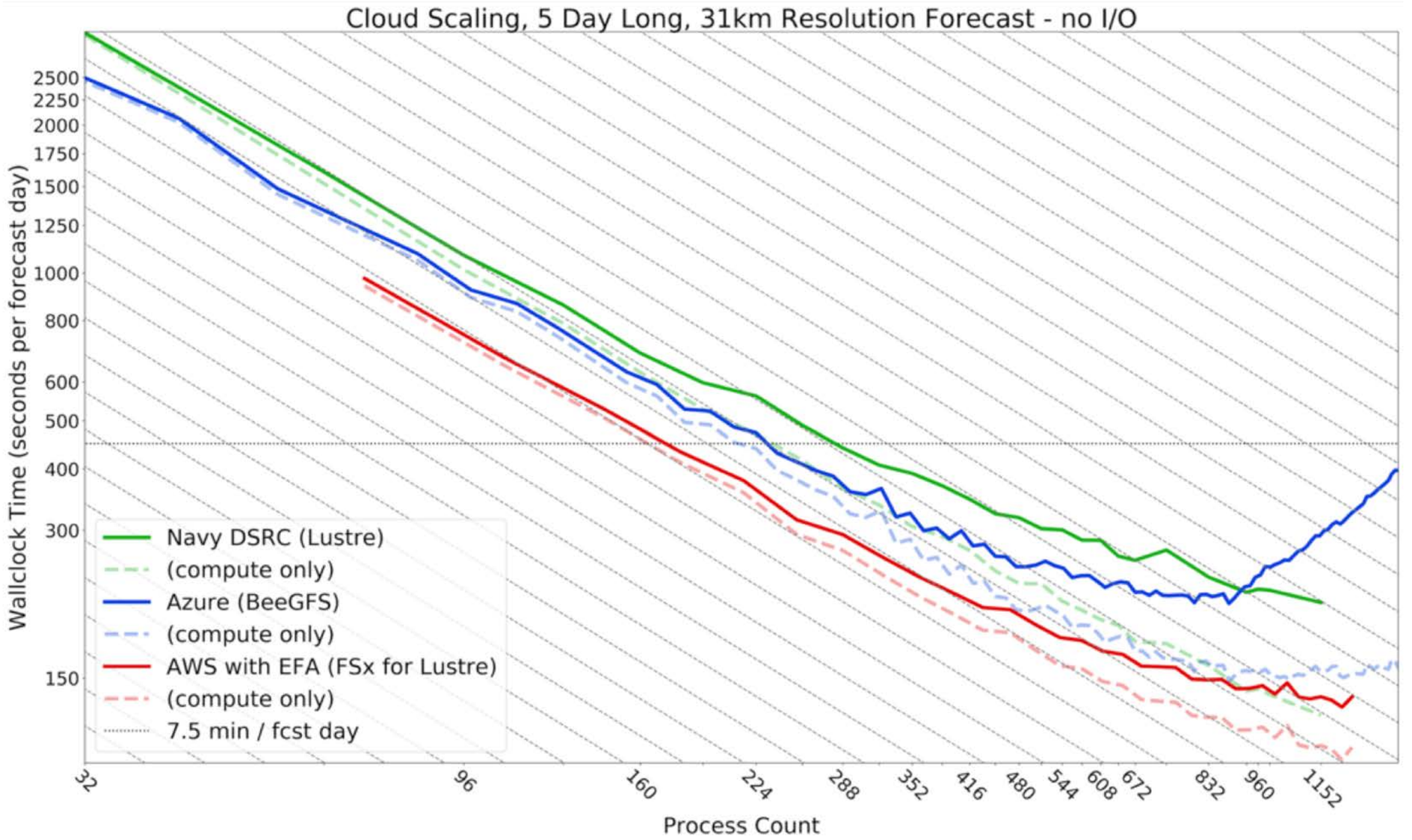
- At the highest core counts:
  - 107% faster than Penguin
  - 43% faster than Azure
  - 160% faster than previous AWS
  - 25% faster than Navy DSRC
- Min size estimated to meet 7.5 min:
  - 33% faster than Azure
  - 23% faster than Navy DSRC
- Min size forecast cost estimate:
  - Azure: $82.97
  - C5n with EFA: $44.02



Low Resolution Forecast with I/O - Comparison

Incorporating I/O: T425 31 km (low) resolution

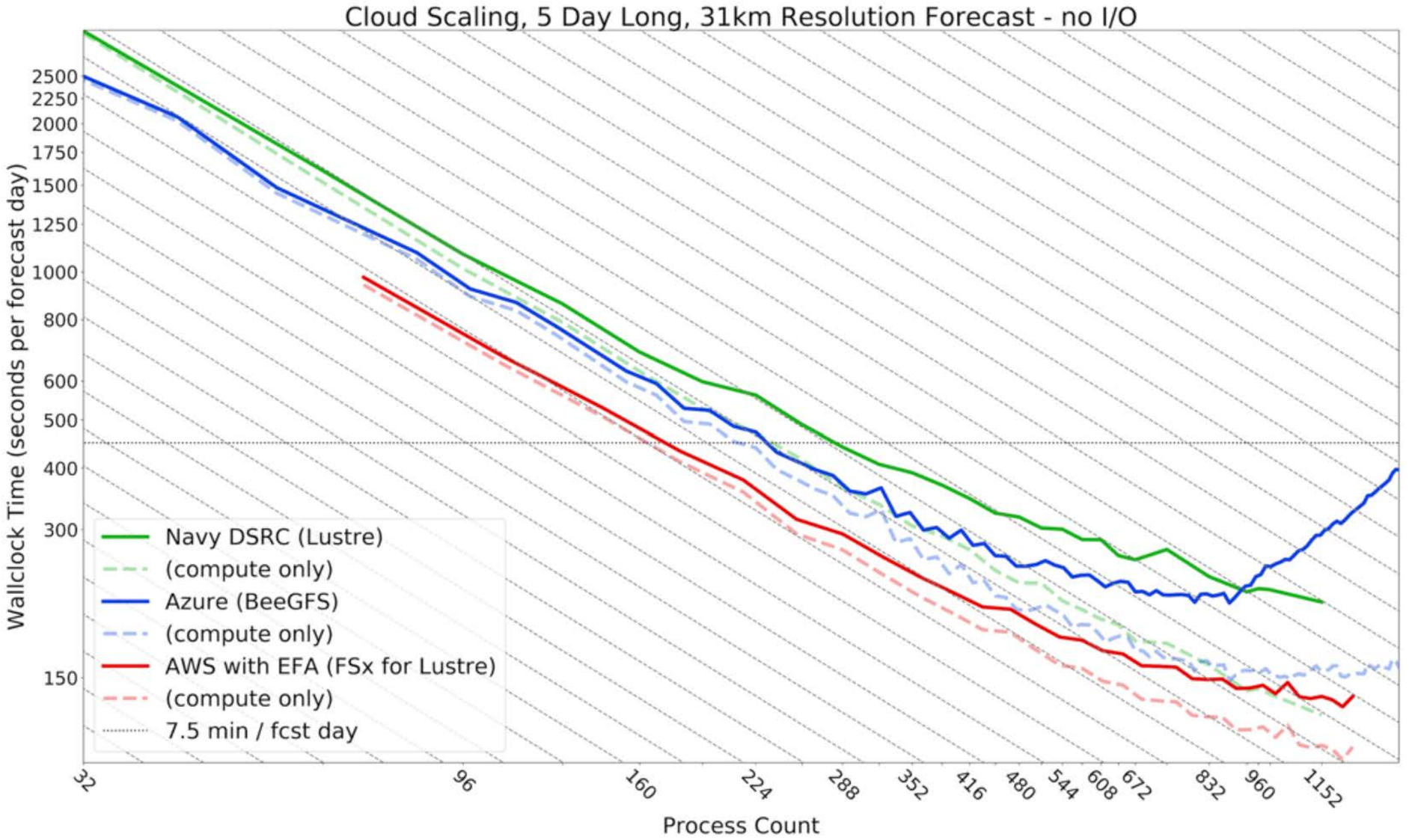
- NAVGEM can output checkpoint data files at specified intervals:
  - ~1.2 GB in size
  - One every sim hour for the first 10 sim hours
  - One every 3 sim hours for the remainder
- All vendors tested offered parallel file systems, we tested on AWS and Azure



Low Resolution Forecast with I/O - Comparison

Incorporating I/O: C5n with EFA on AWS EC2

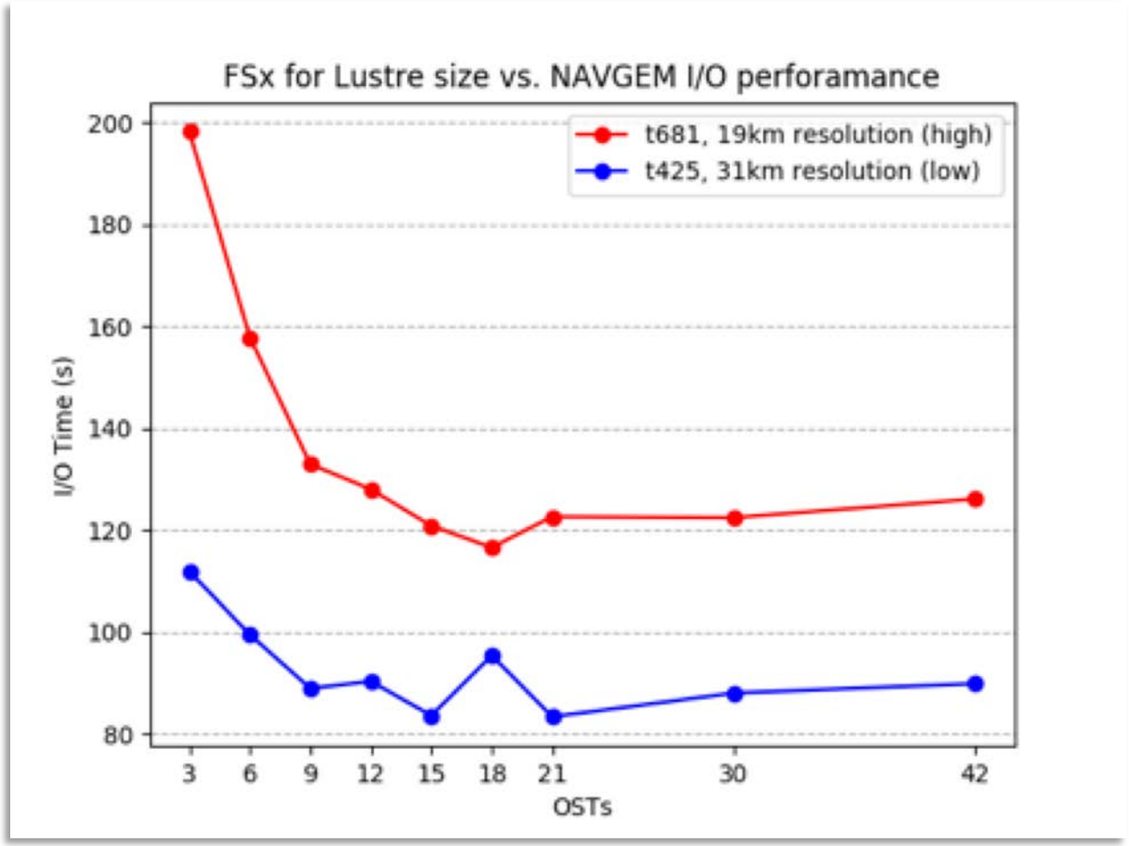
- At the highest core counts:
  - 35% faster than Azure
  - 36% faster than Navy DSRC
- Min size estimated to meet 7.5 min:
  - 18% faster than Azure
  - 33% faster than Navy DSRC
- On AWS, additional cost is minor (<$1) for small scratch parallel file systems provisioned only for length of model run



Low Resolution Forecast with I/O - Comparison

Incorporating I/O: C5n with EFA on AWS EC2

- Cloud allows for “custom” parallel file systems
- FSx for Lustre on AWS: throughput is a function of size provisioned (i.e. larger file system = more Lustre OSTs = higher data throughput)
- Exclusive use offers chance to tune configurations to particular model data



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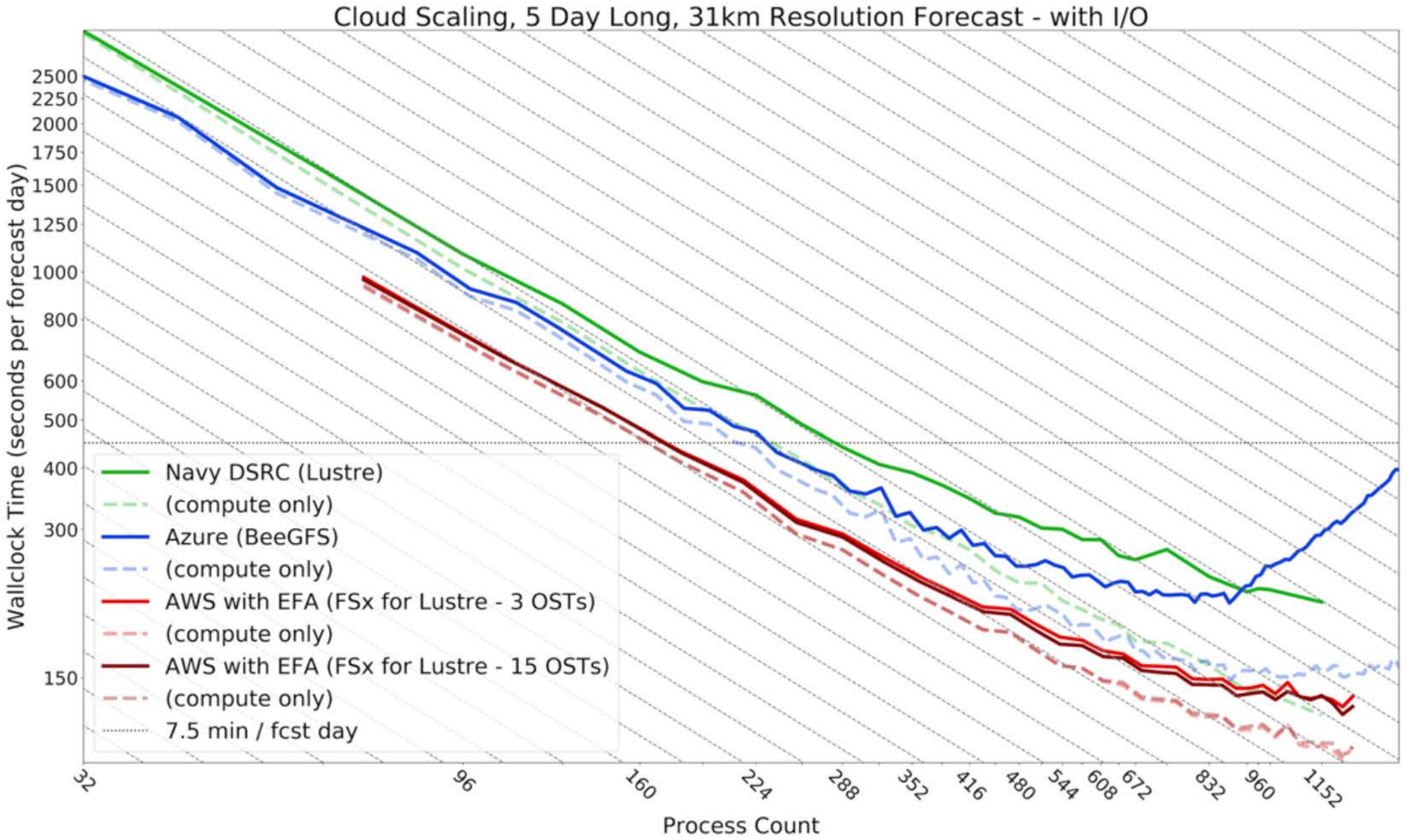
Low Resolution Forecast with I/O - Comparison

Incorporating I/O: C5n with EFA on AWS EC2

- Utility of optimizing file system size is questionable.
- Minor improvement:
  - At higher core counts, larger file system only an average of 10 sec faster for a 5-day forecast
- Cost difference can add up:
  - 3 OSTs: + $0.70/hr
  - 15 OSTs: + $3.49/hr



Next Steps

Future Areas of Research

- Test full NAVGEM ensemble
- Test next-generation forecast programs – NEPTUNE
- Incorporate on-going updates to cloud systems to further reduce costs and optimize performance.

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Questions

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