

How Best to Leverage Cloud for (Big) HPC Sites

CUG 2025

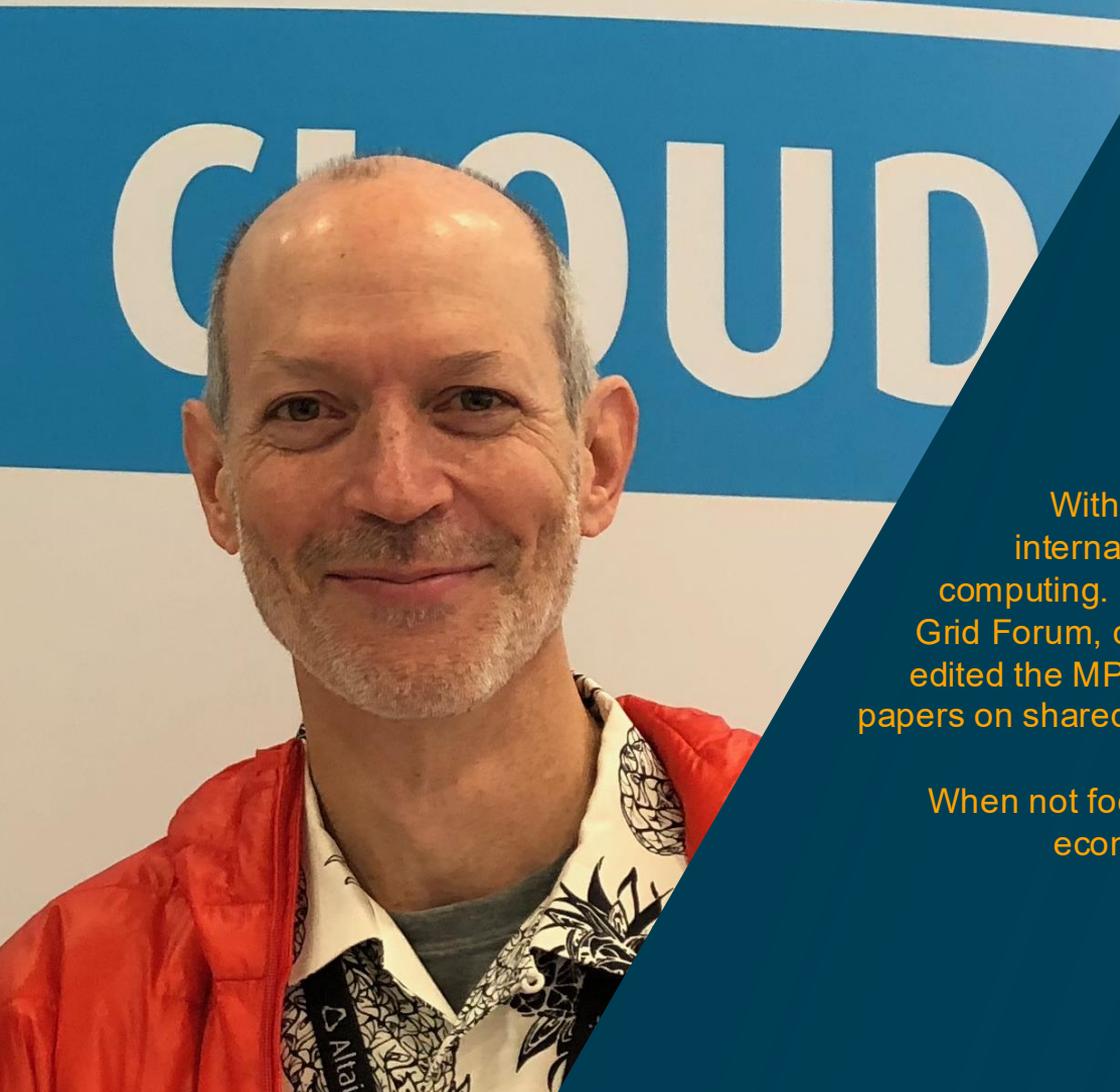
Bill Nitzberg, Chief Scientist
Ian Littlewood, VP, HPCWorks Tools



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WHO IS BILL?

Bill Nitzberg, Chief Scientist, Altair

With over 30 years in computing, Dr. Nitzberg is an internationally recognized expert in high performance computing. Dr. Nitzberg served on the board of the Open Grid Forum, co-architected NASA's Information Power Grid, edited the MPI-2 I/O standard, and has published numerous papers on shared memory, parallel I/O, scheduling, and clouds.

When not focused on HPC, Bill tries to improve his running economy for his long-distance running adventures.

Changing Tomorrow, Together

1985

Founded

16k+

Customers

\$666M

FY2024 Revenue

Altair has been acquired by Siemens, creating the world's most complete AI-powered portfolio of industrial software for simulation, high performance computing, data science, and artificial intelligence as part of the Siemens Xcelerator platform.

Data Science + Rocket Science™ =



Altair One | Cloud Innovation Gateway



ALTAIR
HYPERWORKS

Design & Simulation Platform

ALTAIR
HPCWORKS

HPC & Cloud Platform

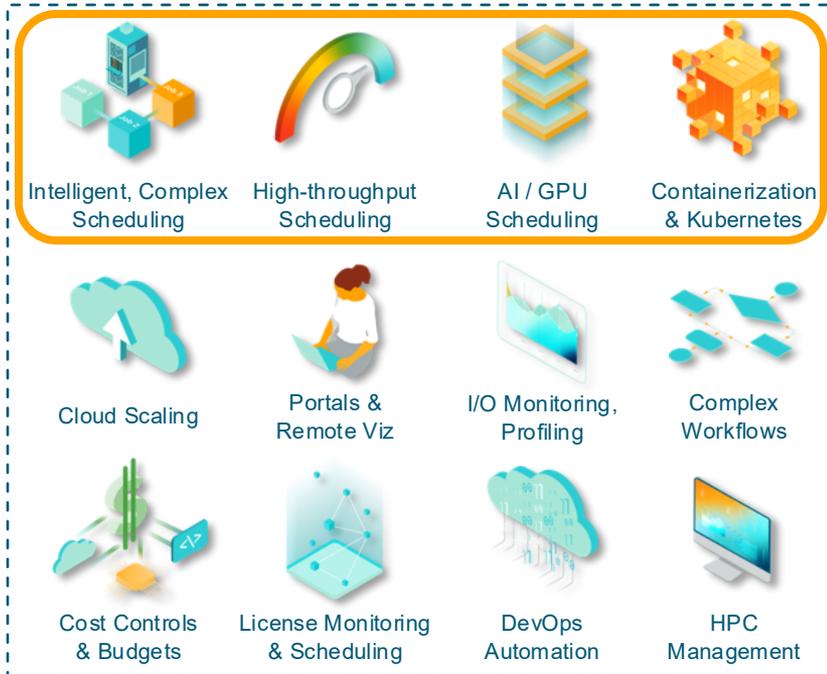
ALTAIR
RAPIDMINER

Data Analytics & AI Platform

Altair HPCWorks Platform

Accelerate and optimize HPC, AI, and Cloud

PBS Pro



Achieving **breakthrough results** requires computing and analyzing more (a lot more), faster (a lot faster), but, it's complex, it's fragile, and it's expensive.

HPCWorks delivers

- Easier access (a lot easier)
- Faster turnaround (a lot faster)
- Rapid Scaling™ for more compute (a lot more)
- Cost controls and visibility (a lot more control)
- Future-proof, open ecosystem (a lot more flexibility)
- Plus... optimize flows, licenses, I/O, energy, GPUs, quantum, emulators, DevOps, Cloud, ... (a lot more efficiency)

Quick Poll...

Which will happen in ≤ 5 years?

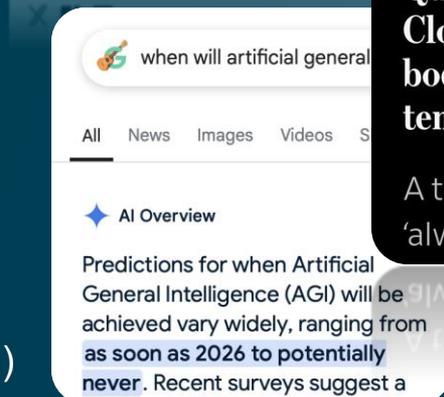
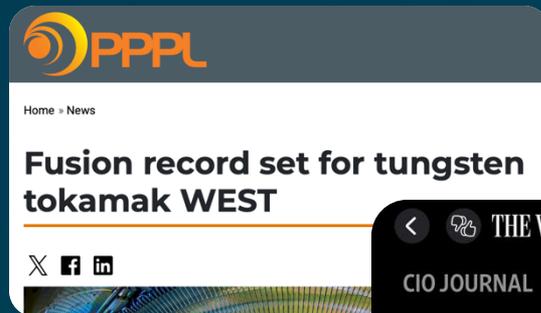
Self-driving cars (for a lot of your car rides)

Fusion energy (for a lot of our energy)

Quantum computing (for a lot of the TOP500)

AGI - Artificial General Intelligence

Cloud “clusters” on TOP500 (for a lot of the TOP500)



WHAT IS CLOUD?

Cloud = Someone Else's Computer (Rented)



$\$664,000 / 50 \text{ years} = \$1.52/\text{hr}$



$\$3099 / 3.5 \text{ years} = \$0.10/\text{hr}$

7-25x
more
\$



$\$280 / 1 \text{ day} = \$11.67 / \text{hr}$



$\$0.55-2.54 / \text{hr}$

WHY CLOUD?

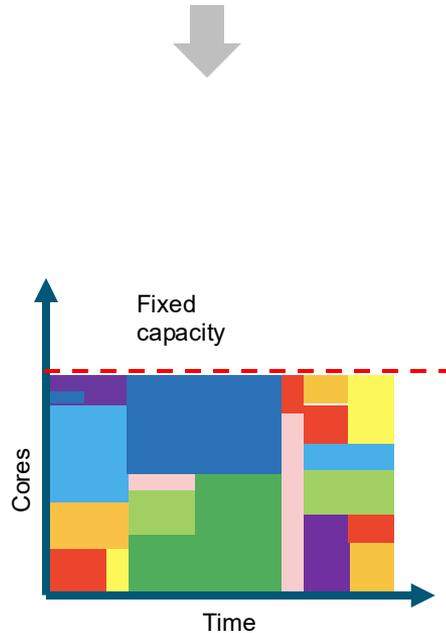
Cloud is a Panacea...

Infinite compute → Infinite Profit

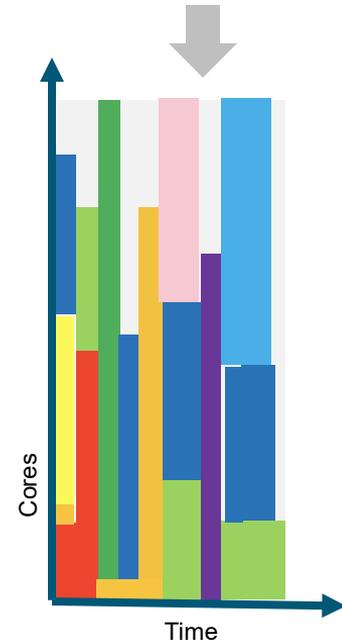


“For every \$1 spent on HPC, businesses see \$463 in incremental revenues and \$44 in incremental profit”

On-premise – constrained



Cloud – infinite compute



Circa 2011...

*“Infinite capacity –
get results ASAP!”*

*“99.999%
reliability”*

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Rationale for Cloud Computing

“In distributed computing environments, up to
85% of computing capacity sits idle.”

(U.S. Department of Energy, May 18, 2007)

“On average, **70% of IT budget is spent on maintaining
current IT infrastructures** versus adding new capabilities.”

(IDC, December 2006)

“**Energy cost per year can exceed \$105,000**
for a single rack of servers.”

(Gartner, “Technology Trends You Can’t Afford to Ignore”, June 2009)

*“Save \$\$\$
(only pay for
what’s used)”*

*“Shrink you
IT staff”*

*“Cloud has
economy-of-
scale”*

But...

~~“Infinite capacity –
get results ASAP!”~~



Asking for 3 instances i2.4xlarge

- For 12 hours on Nov 6th

 Failed to add capacity - Failed running step create_instances of task CreateInstancesJob. Details: ["An error occurred (InsufficientInstanceCapacity) when calling the RunInstances operation (reached max retries: 4): Insufficient capacity."].

“Infinite capacity? Yes, but for small values of infinity”



Scorecard vs. Circa 2011

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Challenges, cont.

Availability

- Big memory (100's of GB)? Big scale (10,000-way MPI)?



Performance

- Multi-tenant/virtual machines add jitter, killing MPI performance

Reliability – 99.999% means ~5 minutes/year down

- Rebooting 1 node may lose all work for a 1,000-way MPI job



Security – IP protection and Gov't regulations

Data size prohibits movement (non-portability)

- Maybe remote visualization, but physics limits to ~1500mi

~~“Infinite capacity –
get results ASAP!”~~

~~“99.999%
reliability”~~

Data is still a
big issue

~~“Save \$\$\$
(only pay for
what's used)”~~

~~“Shrink you
IT staff”~~

“Cloud has
economy-of-
scale”

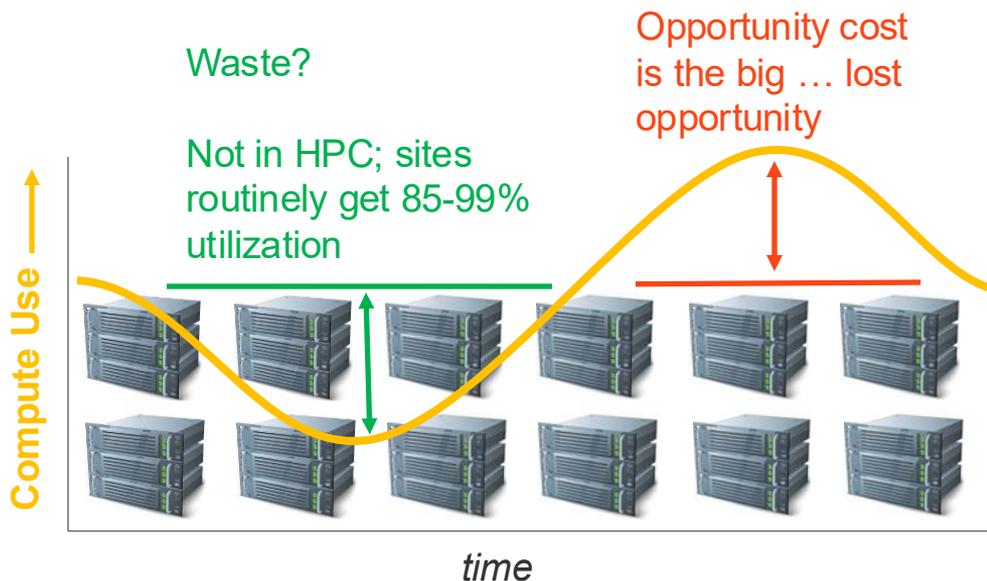
Alas, Cloud for HPC...

- Hard to get resources at scale, e.g., lots of GPUs
- More expensive (and easy to overspend) – 2-10x on-prem costs for traditional HPC sites
 - Oh, and Cloud vendors do not make it easy to control/view costs
- Different and ever changing interface requires a totally new skill set for admins
- Complex to rightsize (benchmark) given the huge set of (ever changing) choices (*)
 - Oh, and different Clouds offer different features at different values
- Prone to vendor lock-in
- Data... yeah...

(*) although, choice is generally good...

SO, WHAT WORKS FOR CLOUD FOR HPC?

Hybrid = Best Use Case for HPC Cloud

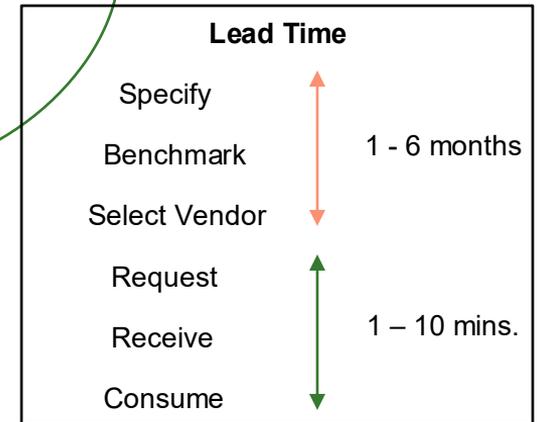
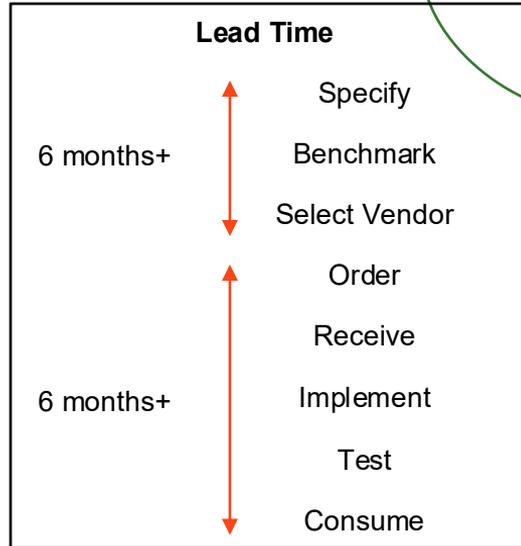


Opportunities

- Meet project deadlines
- Quickly scale for dynamic workloads
- Test new / rarely-used tech, e.g., GPUs/Quantum
- Offload “cloud-friendly” workloads
- Cover for (planned) outages, e.g., chiller
- Disaster recovery (with right contracts)

(* when opportunity \gg extra costs)

Note 1: Quickly Scale (On-prem vs. Cloud)

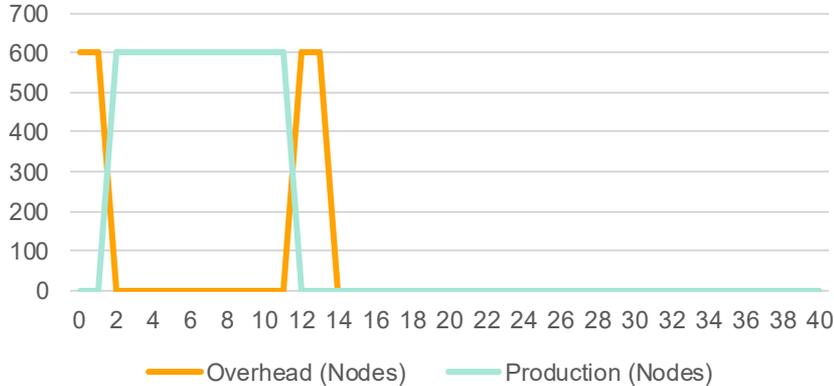


Note 2: Quickly Scale

The devil is in the details... too quickly can be inefficient...

Aggressive Scaling

(100 Node minutes of compute)



Delivery Focus

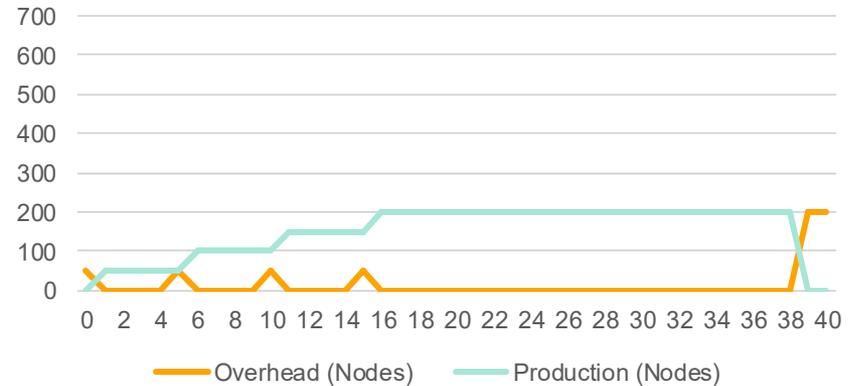
Total Cost: \$5,939

Overhead: \$1,697

Efficiency: 60%

Rapid Scaling™ with HPCWorks

(100 Node minutes of compute)



SLA Focus

Total Cost: \$4,737

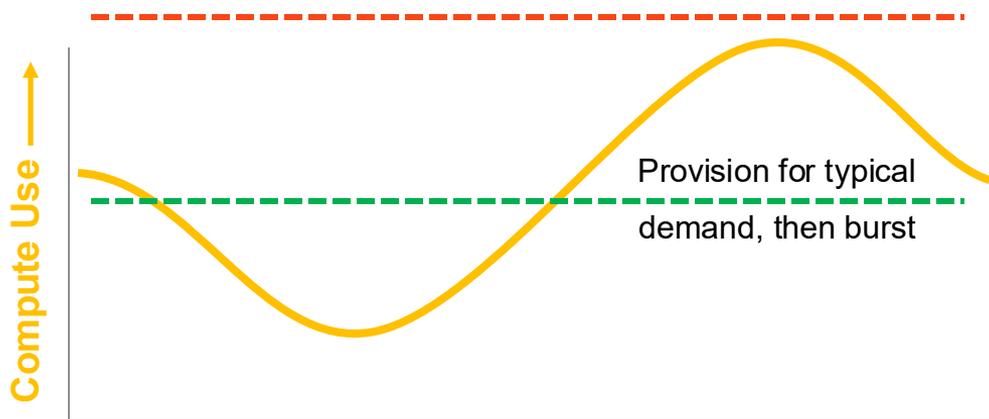
Overhead: \$424

Efficiency: 90%

Saving: 20%

Note: In this illustrative example overhead relates to nodes during provisioning or de-provisioning which are unproductive but being paid for.

Cloud Cost Control



Manage and automate ... everything

- Automated rules for use
- Auto-detect & shutdown idle
- Use spot, etc.
- Right-size instances
- Cost controls, quotas, et. al.
- Use WLM, e.g., PBS Pro

Percentages based on sample TCO reduction calculation based on AWS deployment example

OK, all Cloud (lift-and-shift) makes sense too sometimes, e.g., to balance CAPEX-OPEX

Getting Hybrid Cloud Right

Business-policy driven and flexible – what, why, when, where – including:

- SLAs: budget, deadlines, backlog
- Preferences: on-prem first, energy costs, ...
- Filters: projects, accounts, groups, queues, priorities, software, licenses, job class, OS, node types
- Custom categories: cloud eligible, security level, database req, parallel env, ...
- Fully admin controlled, but with ability for users to request exact specs, esp. for benchmarking

Open

- All Clouds, workload, WLMs, ...

Automated

- Ideally, users not required to change behavior
- Scale up and scale down
- Right-size infrastructure
- Also: DevOps, deployment, tracking, ...

Bulletproof accountability and full visibility

- Cost: estimation, real-time use, quotas, limits, reporting
- End-to-end logging, for fast troubleshooting and to keep CSPs honest

EXAMPLES

Altair Cloud: Subaru

Efficient Crash Simulation

Tier 1 Automotive Manufacturer

- Oracle Cloud Infrastructure (OCI)
- Apps requiring Infiniband:
OCI bare metal instances
- 16 Instances/Job, circa 300 max.
- Bursting from a single cloud native
PBS Pro cluster

Results

- **Better time-to-market**
- **Bare-metal speed**



Altair HPCWorks

Powering Drug Discovery



Johnson & Johnson – Janssen Pharmaceuticals

- Drug discovery – COVID 19 vaccine
- Capacity @ scale (3x bigger)
- HPC in Cloud, ~20 clusters, all different
- Multi-tenant environment
- ~1.500 users; moving to 10K cores

Results

- **Scale (fast) to match demand**
- **On-demand science**



The solution including Altair Grid Engine and NavOps enabled us to scale in the cloud and grow our HPC infrastructure to support critical science and research, including COVID-19 vaccine development.

Martin Dellwo, Manager, Advanced Computing, Janssen R&D



Altair HPCWorks

Energy efficient powertrains

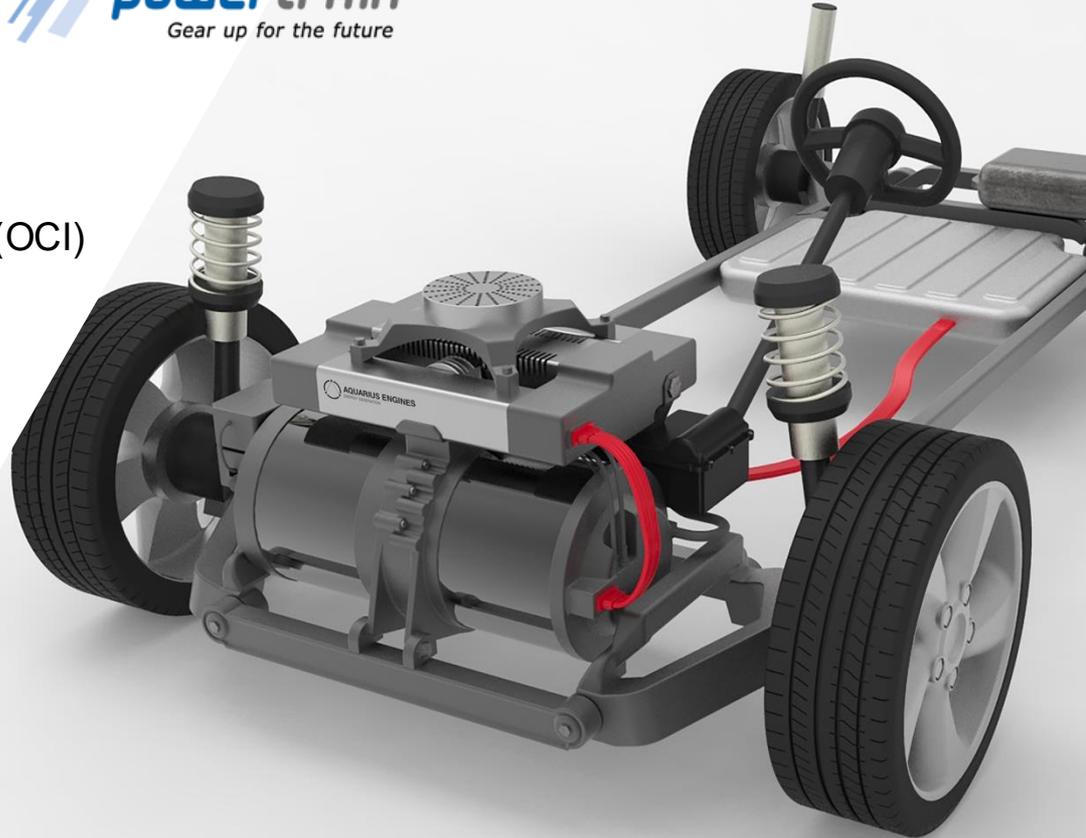


Punch Powertrain

- Multi-cloud: Oracle Cloud Infrastructure (OCI) and Google Cloud Platform (GCP)
- Apps requiring Infiniband: OCI bare metal instances
- GCP for other apps
- Bursting from a single *PBS Pro* on-prem cluster into both clouds

Results

- **Route work for best ROI**
- 25 **On-prem & multi-cloud**



Altair HPCWorks

Harnessing the power of wind, sun and water

GE Wind Energy

- AWS Spot Instances in multiple AZs within the local region
- Round robin on AZs to harvest spot instances; spot pricing support
- Mix of Windows and Linux
- Batches of 5K job arrays
500+ burst nodes

Results

- **Fast, cost-effective scaling**



Altair HPCWorks (Beta/PoC)

NCAR

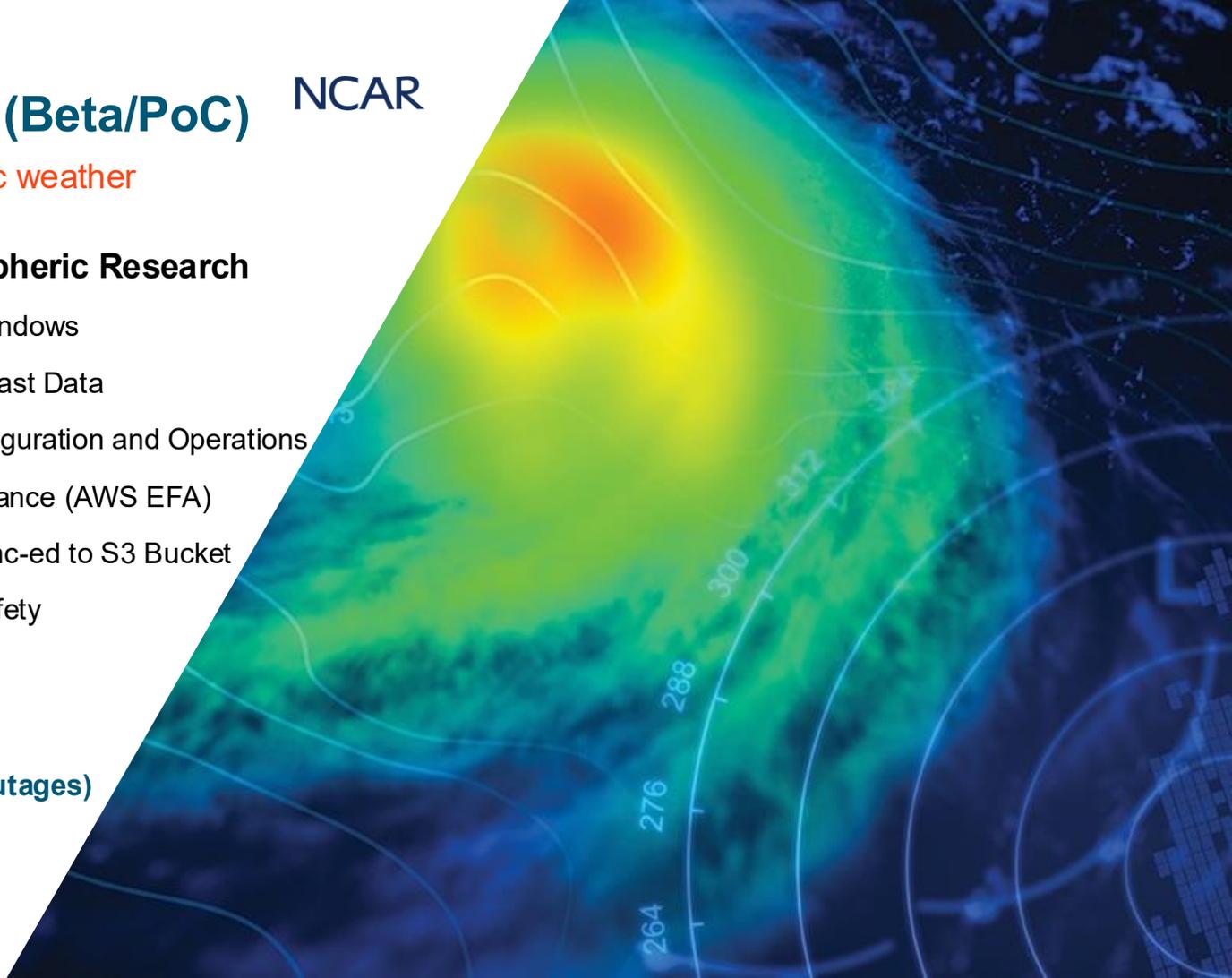
AMPS: Predicting Antarctic weather

National Center for Atmospheric Research

- Coverage for Maintenance Windows
- Provide Mission Critical Forecast Data
- Automated Deployment, Configuration and Operations
- Scale 100s of IB Enabled Instance (AWS EFA)
- Automation of Lustre FSX Sync-ed to S3 Bucket
- Supporting Antarctic Team Safety

Results

- **Reliable forecasting (thru outages)**

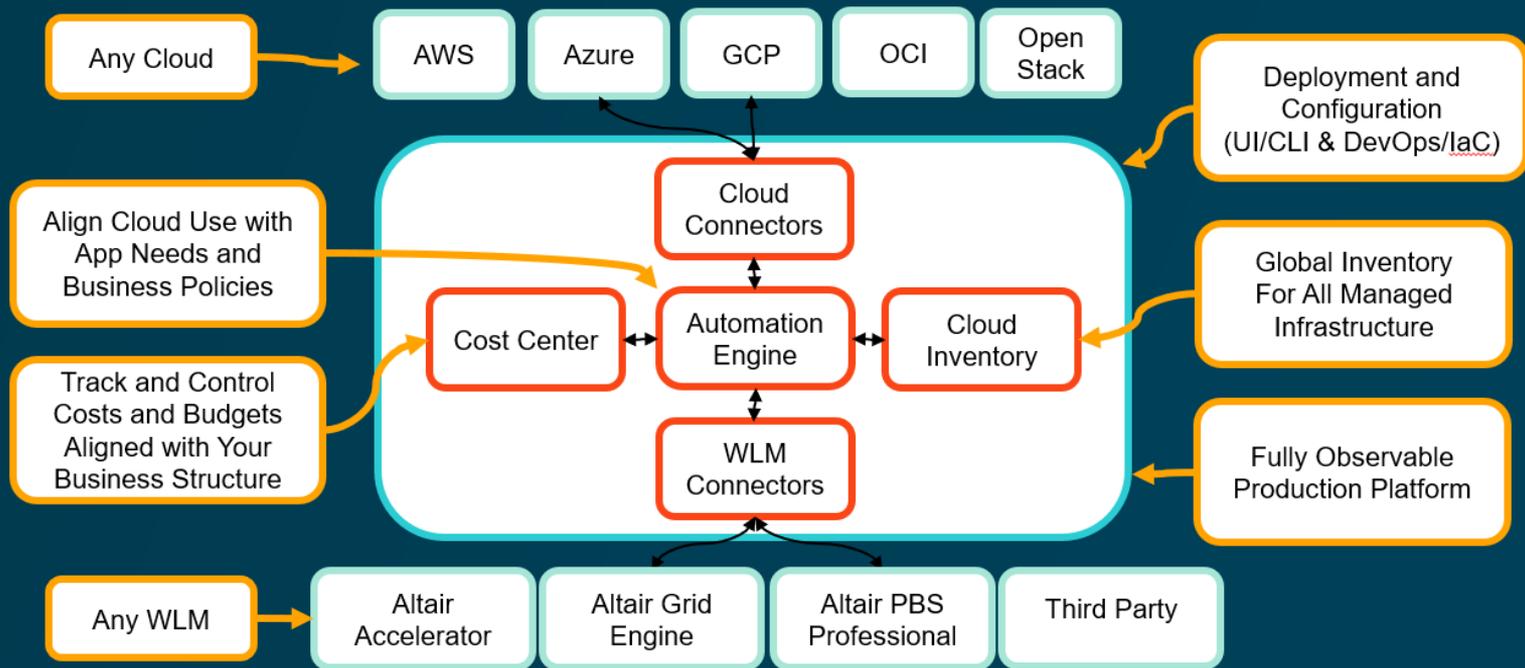


ALTAIR NAVOPS®

ENTERPRISE CLOUD SCALING FOR HPC

Altair NavOps

Any Workload, Any Cloud, Any Scale, Anywhere



Altair NavOps

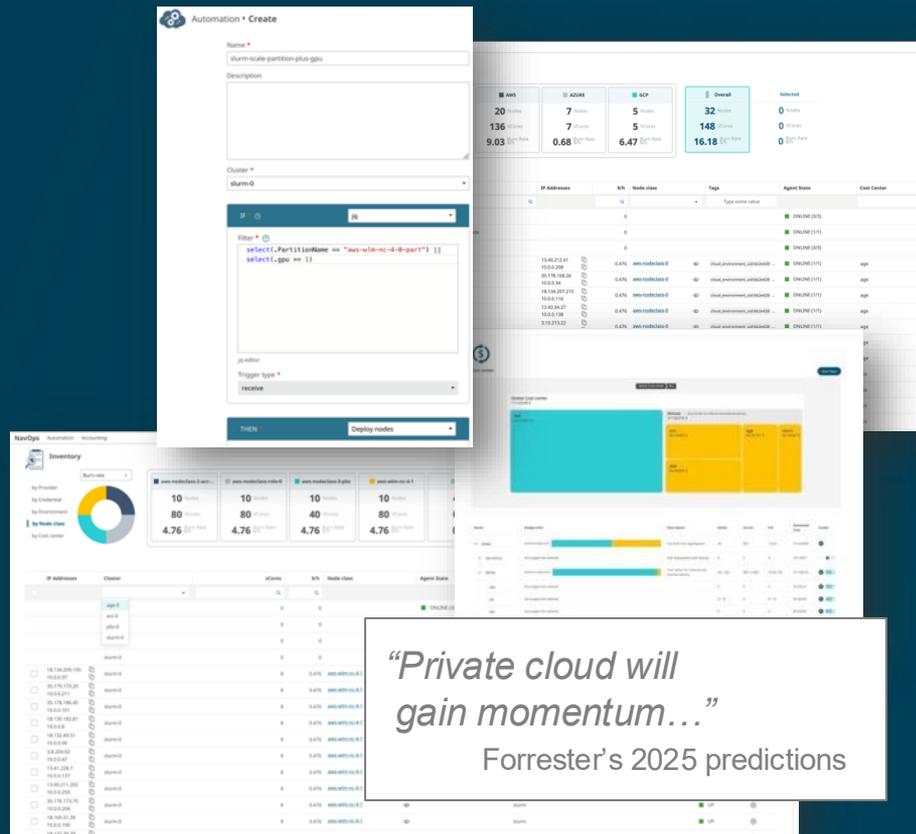
Hybrid Multi-cloud scaling & bursting

- All uses – hybrid, Cloud native, lift-and-shift
- All workloads – AI & HPC (PBS Pro, AGE, Accel., Slurm, K8s, ...)
- All clouds -- no lock-in, exploit arbitrage, inc. specific capabilities, e.g., spot
- All scales –naïve user to global enterprises

Enterprise-level DevOps/IaC platform

- Automation Engine with Rapid Scaling™ delivers business needs fast and efficiently
- API-first (w/great GUI), budgets, limits, cluster deployment, full observability

Centralized cost controls and dashboarding



“Private cloud will gain momentum...”

Forrester’s 2025 predictions

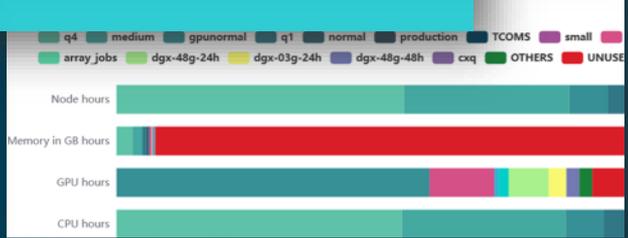
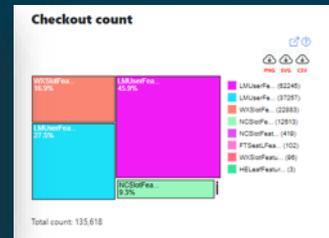
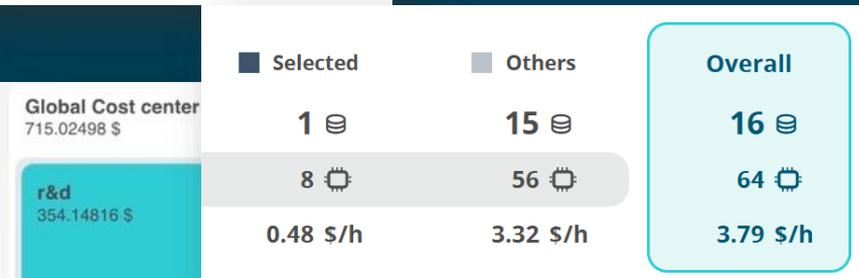
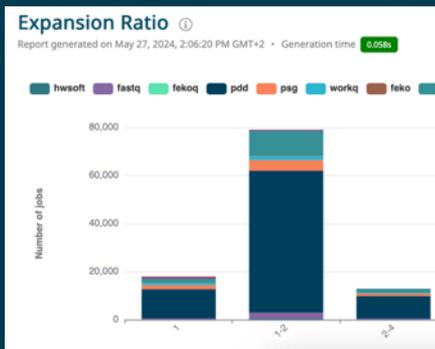
Altair InsightPro™

Manage to business priorities: 360° visibility

- Projects, costs, budgets, quotas
- Rightsize infrastructure, eliminate waste
- Chargeback, tune, troubleshoot

Analytics for HPC Infrastructure and Use

- Turnkey → custom expansion → open APIs
- Data for “everything”: workload, hardware, software licenses, performance, faults, \$/costs, energy, carbon, ...



Altair NavOps: Example

Scaling for SLURM

The screenshot shows the Altair NavOps 'Inventory' page for a SLURM cluster. It features a 'Burn rate' donut chart and a summary table. The summary table shows 4 nodes, 0 vCores, and 0 Burn Rate. Below this is a table with columns for IP Address, Cluster, vCores, S/h, Node class, Cost Center, and Node State. One node is listed as 'slurm-0' with a state of 'UP'.

IP Address	Cluster	vCores	S/h	Node class	Cost Center	Node State	Actions
	slurm-0	0	0			UP	

The screenshot shows an AWS WLM terminal window displaying SLURM node details. It includes a table of nodes with columns for JOBID, PARTITION, NAME, USER, STATE, TIME, TIME_LIMIT, NODES, and NODELIST(REASON). Below this is a table of node details with columns for NODELIST, NODES, PARTITION, STATE, CPU, S/CPU, MEMORY, TMP_DISK, WEIGHT, AVAIL, REASON, and more. The terminal also shows a clock and system information for London.

```
Every 2.0s: squeue -l; echo; who -m "Busy SLURM Nodes: "; scontrol show nodes | grep ALLOCATED | ... | fp-10-0-0-165: Mon Nov 11 19:04:08 2024
```

```
Mon Nov 11 19:04:08 2024
```

JOBID	PARTITION	NAME	USER	STATE	TIME	TIME_LIMIT	NODES	NODELIST(REASON)
2800	aws-slurm	job_ah	centos	PENDING	0:00	10:00	2	{PartitionConfig}
2804	aws-slurm	job_ah	centos	PENDING	0:00	10:00	2	{PartitionConfig}
2805	aws-slurm	job_ah	centos	PENDING	0:00	10:00	2	{PartitionConfig}
2802	aws-slurm	job_ah	centos	PENDING	0:00	10:00	2	{PartitionConfig}
2801	aws-slurm	job_ah	centos	PENDING	0:00	10:00	2	{PartitionConfig}
2809	aws-slurm	job_ah	centos	PENDING	0:00	10:00	2	{PartitionConfig}

```
Busy SLURM Nodes: 0  
Idle SLURM Nodes: 1
```

```
Mon Nov 11 19:04:08 2024
```

NODELIST	NODES	PARTITION	STATE	CPU	S/CPU	MEMORY	TMP_DISK	WEIGHT	AVAIL	REASON
fp-10-0-0-165	1	aws-slurm	idle	8	1:4:2	12000	0	1	on-prem	none
fp-10-0-0-165	1	aws-slurm	idle	8	1:4:2	12000	0	1	on-prem	none

```
UID
```

UID	HOSTNAME	NODE CLASS	UID
249000cf-363c-4248-0749-03010207f6fe	aws-slurm-03010207f6fe	up	
ec444799-5d79-4475-baac-bc78c4a4a993	aws-baac-bc78c4a4a993	up	
237c40e7-9911-40a0-0a6f-288228408370	aws-0a6f-288228408370	up	
f4679495-f4ef-4425-936a-ac876ca17651	aws-936a-ac876ca17651	up	

Showing page 1 of 1, 25 Items per page

Get the **right resources**
to the **right person** (agent)
at the **right cost**
and at the **right moment.**

Powered by Altair® HPCWorks® and Altair® RapidMiner®