HPC Current Use and Practice: Industry

Cloud Use-Cases, Architectures, and Security

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Motivations for Cloud in HPC

Scalability and Agility

Secure Global Collaboration

Big Data Convergence with HPC
Scale Matters: for Big Compute and Big Data
Scientists: Evidence of New, Unknown Particle?

By Jim Algar, Tech Times | January 12, 9:52 AM

An unexpected "bump" in the data coming out of collision experiments with the Large Hadron Collider in Switzerland has scientists wondering if they've witnessed evidence of previously-unknown subatomic particles.

The collision, which cannot be explained by the Standard Model of physics, may have been evidence of a previously undiscovered particle, or maybe even two particles, researchers say.
Constructing Models, Running Simulations, Viewing Results

This is Big Compute
High Throughput Computing at Scale
Innovation in Energy Management

Observe. Model. SIMULATE YOUR NETWORK

About Us
Providing a virtual world environment uniquely tailored for power distribution management. Roames’ asset network models facilitate comprehensive vegetation management, infrastructure condition evaluation and enhanced performance monitoring - reducing costs and resources.

Services
- 3D Virtual World
- Vegetation Management
- Conductor Clearance
- Asset Condition Assessment

News
- 15 Oct: Fugro Awarded National Grid Framework Contract in the UK
- 8 Jul: Fugro Roames Aids Network Providers in Meeting AER Requirements
- 2 Jul: Award Winning Roames Service Gains Momentum in UK
Big Data meets Big Compute

- Aircraft equipped with cameras, laser sensors
- Repeated overflights of power networks
- Captured data is used to render detailed 3D models of the power lines, and the environment
- Analytics and simulations are run to generate actionable reports
- Goal: directing post-disaster repair and prioritizing ongoing maintenance

“Fugro Roames has enabled Ergon Energy to reduce the cost of vegetation management from AU$100 million to AU$60 million per year.”

- Josh Passenger, Technical Architect, Fugro Roames
Primary Goal: Improve Throughput

- Run many jobs in parallel for large-scale parameter studies
- Reduce or eliminate HPC resource contention and queue wait times
- Right-size clusters and computing resources for each workload
- Optimize resources for each application, without procuring new hardware
What Does This Mean for Industry?

Go Wide: Expand the Simulation Domain
Run larger numbers of parallel, clustered HPC jobs
The High Cost of Queues for On-Premise HPC

Conflicting goals

- HPC users seek fastest possible time-to-results and have varying needs for scale
- IT support team seeks highest possible utilization of a fixed-size cluster

Result:

- The job queue becomes the capacity buffer
- Job completion times are hard to predict
- Users are frustrated and run fewer jobs
- Innovation is throttled by IT resources
HGST applications for engineering:
- Molecular dynamics, CAD, CFD, EDA
- Collaboration tools for engineering
- Big data for manufacturing yield analysis

Running drive-head simulations at scale:
Millions of parallel parameter sweeps, running months of simulations in just hours.

Over 85,000 Intel cores running at peak, using EC2 Spot instances
Mapping HPC Use-Cases: Examples

Clustering vs. Distributed/Grid

Data Light
- Minimal requirements for high performance storage
- Fluid dynamics
- Weather forecasting
- Materials simulations
- Crash simulations

Data Heavy
- Benefits from access to high performance storage
- Seismic processing
- Metagenomics
- Astrophysics
- Deep learning

Risk simulations
- Molecular modeling
- Contextual search
- Logistics simulations

Animation and VFX
- Semiconductor verification
- Image processing/GIS
- Genomics

Clustered (Tightly Coupled)

Distributed/Grid (Loosely Coupled)
Cloud Performance Testing: CFD on AWS
ANSYS Fluent

- AWS c4.8xlarge
- 140M cells
- F1 car CFD benchmark

http://www.ansys-blog.com/simulation-on-the-cloud/
Fluid dynamics on AWS
Metacomp CFD++

Fluid Dynamics and other tightly-coupled simulations can scale effectively on AWS

“Metacomp Technologies is very familiar with AWS HPC architecture and is well able to support CFD++ on it with confidence”

Dr. Sukumar Chakravarthy, President and Founder, Metacomp
16M cell, polyhedral, external aero case, STAR-CCM+

Running on threads, c4.8xlarge instances

Demonstrates excellent scalability for typical CFD models

Shape of this curve depends on domain decomposition (cells per thread)

Larger CFD cases can scale higher

Ideal Scaling
Hybrid HPC is a Common Pattern

Corporate Data Centers

On-Premise HPC Resources

Integration

Cloud Resources
Sample Hybrid HPC Workflow with Auto Scaling
AWS Direct Connect and VPC

Use AWS Direct Connect to establish a private virtual interface from your on-premise network directly to your Amazon VPC.

Private connectivity from private data center to an Amazon VPC

http://aws.amazon.com/directconnect/
1. VPN or DirectConnect
2. GPU instances for pre- and post-processing
3. Proxy server for secure remote access
4. Source code or library repository
5. Continuous Integration server
6. Simple Queueing Service for job submission
7. Application-specific compute nodes, automatically scaling
8. Simulation models, results, job logs pushed to S3 durable storage
9. Other management nodes, for example used in monitoring
10. Block storage for compute clusters, for example to create NFS mounts
Secure, Petabyte Scale Data Transport

Ruggedized case
“8.5G Impact”

E-ink shipping label

50TB & 80TB
10G network

Rain & dust resistant

Tamper-resistant case & electronics

All data encrypted end-to-end
Secure Graphics and Collaboration

Cloud can be used for pre-and post processing as well as HPC

- Use GPUs in the cloud for remote rendering and remote desktops

Cloud is more secure for collaboration

- Encrypt the data in flight and at rest
- Manage your own keys and credentials
- Deliver pixels to your collaborators, not the actual data
Thin Client Remote Collaboration

*Calgary Scientific PureWeb™*
Enabling Global Collaboration

Bring the users to the data, don’t send the data to the users
GE on AWS

GE’s Global Business Integration Technologies Laboratory wanted to advance traditional manufacturing and create a dynamic network of people and machines that would allow collaboration, rapid prototyping, and product development for complex systems. GE had to adhere to U.S. International Traffic in Arms Regulations (ITAR) regulations and other compliance requirements. By using AWS GovCloud (US), GE developed a revolutionary manufacturing platform, Crowd-driven Ecosystem for Evolutionary Design (CEED), which connects people, materials, models, simulation, and equipment in an ITAR-compliant, secure, and distributed global environment.

Smart manufacturing Crowd-driven Ecosystem for Evolutionary Design (CEED)

Design  Share  Simulate  Schedule
Thermal  Mechanical  Electrical  Manufacturing

People, materials, models, simulation, equipment, all connected in one distributed global environment.
Security

SECURITY & COMPLIANCE

- Identity Management
- Access Control
- Key Management & Storage
- Monitoring & Logs
- Configuration Compliance
- Web application firewall
- Assessment and reporting
- Resource & Usage Auditing
Security, Monitoring, Governance

Infrastructure Security

• **Network firewalls** are built into Amazon VPC

• **Web Application Firewall** lets you create private networks, and control access to your instances and applications

• **Encryption in transit** with TLS across all services

• **Connectivity options** that enable private, or dedicated, connections from your office or on-premises environment
Security, Monitoring, Governance

Inventory and Configuration

- **Amazon Inspector** automatically assesses applications for vulnerabilities or deviations from best practices, including impacted networks, OS, and attached storage.

- **Deployment tools** help manage the creation and decommissioning of resources according to organization standards.

- **AWS Config** helps identify AWS resources and then track and manage changes to those resources over time.

- **AWS CloudFormation** to create standard, preconfigured, secure environments.
Data Encryption

- **Flexible key management** options including AWS Key Management Service
- Choose whether to have AWS manage the encryption keys, or keep complete control over your keys
- **Dedicated, hardware-based cryptographic key storage** is available using AWS CloudHSM
- AWS APIs allow you to integrate encryption and data protection with any of the services you develop or deploy in an AWS environment
Identity and Access Control

- **Identity and Access Management** lets you define individual user accounts with permissions across AWS resources.

- **AWS Multi-Factor Authentication** for privileged accounts, including options for hardware-based authenticators.

- **AWS Directory Service** allows you to integrate and federate with corporate directories to reduce administrative overhead.

- **Native identity and access management integration** across many AWS services, plus API integration with any of your own applications or services.
Monitoring & Logging

• **AWS CloudTrail** provides deep visibility into API calls, including who, what, who, and from where calls were made.

• Includes log aggregation options, streamlining investigations and compliance reporting.

• **Amazon CloudWatch** to alert on specific events, or if thresholds are exceeded.

• **AWS monitoring tools** give you the visibility you need to spot issues before they impact the business.
Logs → Metrics → Alerts → Actions

API calls from most services

Monitoring data from AWS services

CloudWatch / CloudWatch Logs / CloudWatch Events

CloudWatch alarms

Custom metrics

AWS Lambda

Amazon SNS

HTTP/S notification

Email notification

SMS notifications

Mobile push notifications

HTTP

Amazon EC2 OS logs

AWS Config

AWS CloudTrail

Amazon VPC Flow Logs

AWS Lambda

Amazon SNS

splunk

Alert Logic

sumo logic

AWS CloudTrail

Amazon EC2 OS logs

AWS Config

AWS CloudTrail

Amazon VPC Flow Logs

AWS Lambda

Amazon SNS

splunk

Alert Logic

sumo logic
Resources

aws.amazon.com/hpc
aws.amazon.com/big-data/
aws.amazon.com/security

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