

# **HPC USER FORUM Cloud PANEL**

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**OHPC  
USER FORUM**

# Panel Participants

- **Moderator**

- Sharan Kalwani, KAUST

- **Participants**

- Bill Bryce UNIVA
- Raymond O'Brien NASA
- Shane Canon Lawrence Berkeley National Labs
- Pavan Pant CloudSwitch.com
- Chris Porter Platform Computing
- Jason Stowe CycleComputing.com

# Panel Format

- **3 Questions**

- Provided ahead of time

- **3 minutes (max) per question for each participant response**

- **Follow-up and Audience after each participant has a chance to share**

# Q1. Workflow Pre-qualifications HPC cloud...

➤ ***Please list what qualifies for HPC in the Cloud here.....***

# Q1. Workflow Pre-qualifications HPC cloud...

**There are several general areas that must be addressed to qualify HPC in the cloud they are:**

## **Middleware Software (The HPC Platform)**

- DRM systems, OS Provisioning, User Management, Filesystem Management, Configuration Management, Package/Image Management.
- User Tools, MPI, Parallel Shell
- API to access/Control Cloud
- Hypervisor (VMWare, Xen)

## **Storage**

- Local/Remote, NFS, Hypervisor Storage, Snapshots, NAS Appliances, Storage alignment with Compute nodes.

## **Network**

- Ethernet Gig or 10Gige, Infiniband, Low latency & High Bandwidth, VLAN (Isolation), VPN (bursting).

## Compute Nodes

- Physical Nodes or Virtual, Multi-Core (8,12,16) nodes.  
Sharing vs Dedicated access to nodes.

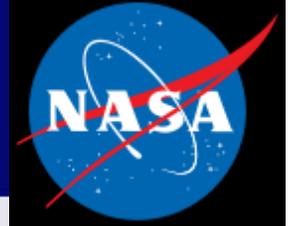
**Any HPC in the Cloud solution has to address all of these areas to be successful.**

**Proper selection of above components provides a 'HPC Platform in a Cloud' and should deliver:**

***Scalability – to 1000+ nodes***

***Reliability – Handle failures of nodes, jobs, etc..***

***Performance – Physical Performance on Virtual Nodes***



## **Workflow Characteristics**

- *Loosely coupled or independent task execution*
- *Able to operate in virtualized environment*
- *Able to operate with heterogeneous set of processors*
- *Ideally, workflow:*
  - *Is tolerant of individual process failures*
  - *Consists of tasks that can be stopped and re-started to allow execution of higher priority work*
  - *Can take advantage of cloud scale up and scale out features*
  - *Can take advantage of a highly scalable object storage capability*

# Q1. Workflow Pre-qualifications HPC cloud...LBNL



- ***High-performance interconnect***
- ***High-performance parallel I/O including concurrently writing to a shared object***
- ***Dedicated access to key resources (CPU, memory bandwidth, interconnect)***
- ***Highly scalable***

## Q1. Workflow Pre-qualifications HPC cloud...

- ***The definition of Cloud includes virtualization to deliver on the on-demand requirement of cloud computing. Therefore, HPC in the cloud requires that the workloads and deployments be able to run in a virtualized environment:***
  - ***This means CPU virtualization (VMWare, XEN, Hyper-V)***
  - ***This often also includes network and storage virtualization***
- ***In addition HPC in the cloud is currently defined by horizontal scale. Most public clouds today have reasonable, bit limited vertical scale.***

## Q1. Workflow Pre-qualifications HPC cloud...

- IaaS providers are not ready for full HPC yet
  - Amazon CCI + GPU instances are moving in the right direction
- Private clouds are the right choice for HPC today
- Private cloud characteristics:
  - Policy-based workload management
  - Flexibility
    - PM &/or VMs
    - Multi OS
  - Accountability
    - Job, user, group, project, OS, instance type

# Q1. Workflow Pre-qualifications HPC cloud...



## HPC in the Cloud Workloads (Type, Data, Hardware, Security, Access)

- Parallel - Only 1-node or non-low-latency sensitive
- Embarrassingly Parallel – Parameter sampling, Monte Carlo
- Data – Doesn't necessarily depend on total size (web 2.0 use PetaBytes), depends upon deltas and bandwidth to transfer
  - Data aware synchronization/placement is a requirement
  - Massive scales are done but still challenging (PB)
- GPUs workloads supported (e.g. Mol. Dyn. workload cost  $\frac{1}{4}$  as much)
- Scheduling w/multi-user support
- Virtualized / Isolated data storage
- Multi-tenant, with virtualized, isolated access/auth
- Programmatic access to Resources (no required phone calls to providers)
- Pay for what you use

## Q2. Best HPC in the Cloud example?.....

- **In your experience, which is the most successful HPC in the cloud implementation and what was different about it?**
- **Your citation here....**

## A2. Best HPC in the cloud usage/implementation

- **Amazon EC2 is the best HPC cloud.**
  - EC2 has many limitations but...
  - VPC (Virtual Private Cloud),
  - CCI (Cluster Compute Instances)
  - Dedicated access to hypervisors
  - Multiple instance 'sizes'
  - 'De-facto' standard API
  - Clearly the most popular and used HPC cloud

## A2. Best HPC in the cloud usage/implementation

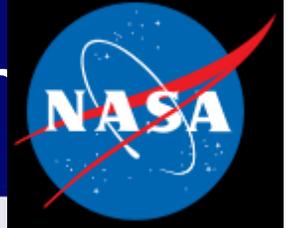
- Examples:
  - NASA JPL
  - Pathwork Diagnostics
  - Cycle Computing
  - Abaqus in EC2 (Univa)



- **NASA Wide Field IR Survey Explorer Project**

- 4 IR cameras have imaged entire sky *each*
- Needed: resolution enhancement, deconvolution
- Project 1: 2000 distant galaxies
  - Increase resolution with processing = 100 CPU hrs *each*.
- Project 2: Some sky areas require huge RAM-based processing.
  - - Set up an 80 GB RAM instance
  - - Finished first phase on Nebula in two days.
  - - WISE scientist: "I am amazed"

## A2. Best HPC in the cloud usage/implementer



- **Quotes from Dominic Benford, WISE project scientist:**

“After having access to Nebula for only a few days, I find that I am already able to accomplish more data-intensive calculations than I can do on any of the local servers we have here, and with no difficulties at all!

“The system is easy to access and use, and offers a capability that I absolutely need occasionally but for which I could never justify the expense if it were for my needs alone.

## A2. Best HPC in the cloud usage/implementer



- **Additional quote from Dominic Benford, WISE project scientist:**

“With the recent addition of a large-RAM instance, I am now able to conduct calculations that could not be done on our project's large server farm. Nebula has provided me with a tool for science data analysis that far surpasses anything that I could envision in a single-user context. NASA Cloud computing may be the way forward for our data-intensive projects in the future, since only a NASA system could provide the necessary reliability and proprietary controls on our data “

## A2. Best HPC in the cloud usage/implementer



- **Cloud is well suited for NASA projects:**

- With HPC workloads possessing the characteristics described earlier
- Constrained by availability of compute resources
- That cannot justify the cost of dedicated infrastructure for key processing which is only required occasionally or for a limited duration

- **Another example:**

- See NASA presentation titled: Proposed Use of the NASA Ames Cloud Computing Platform for Numerical Weather Prediction and the Distribution of High Resolution Satellite Imagery
- By Ashutosh S. Limaye, Andrew L. Molthan, and Jayanthi Srikishen
- 2010 AGU Fall Meeting, San Francisco, CA
- Session IN21D-08: "Research Clouds: Virtualization of Infrastructure, Tools, and Services I"

Available from the NASA Aeronautics and Space Database

## A2. Best HPC in the cloud usage/implementation



- **In your experience, which is the most successful HPC in the cloud implementation and what was different about it?**
- **What do we mean by successful?**
  - Best known?
  - Most profitable?
  - **Most useful to the user/customer!**

# A2. Is an HPC Center Cloud-like enough?



## HPC Centers ?

- **Resource pooling.**
- **Broad network access.**
- **Measured Service.**
- **Rapid elasticity.**
  - Usage can grow/shrink; pay-as-you-go.
- **On-demand self-service.**
  - Users cannot demand (or pay for) more service than their allocation allows
  - Jobs often wait for hours or days in queues



## A2. Best HPC in the cloud usage/implementation

- **Automated provisioning (PXE boot of nodes, ROCKS configuration)**
- **Data set sizes reasonable for transport across Internet / WAN (both initial set, and results)**
- **Latency between the DC and the Cloud was not a significant factor – interactive performance, reach-back was not in-line with processing**
- **Provided an outlet for overtaxed internal resources**

## A2. Best HPC in the cloud usage/implementation

- **Our most successful HPC cloud deployment was a 1000 core compute node with ROCKS and Sun Grid Engine for use in the Pharma industry. It was a good deployment because:**
  - It provided on-demand scaled compute deployment
  - The application was designed for horizontal scale
  - Had reasonable network and storage bandwidth requirements

## A2. Best HPC in the cloud usage/implementation

- **Pfizer**

- IAAS provider: Amazon EC2
- Technical ingredients:
  - Amazon VPC
  - Serial, memory-bound workload
  - Application: RosettaDock
  - Embarrassingly parallel
  - Small data
- <http://biopharmadirectory.com/news/?p=159>

# Q2. Best HPC in the Cloud example?.....

CycleCloud has started 2000+ clusters since 2007, for **Pfizer, Schrodinger, Varian, Inc., Fortune 500 Insurance/ Finance, Genomic Health**, many, many others & read about numerous others' work.

My favorite is our CycleCloud cluster announced on 4/5/11:

**Single click creates 10000-core cluster in Cloud, for Genentech, in minutes, for \$1060/hour (Cycle + IaaS)**

## NETWORKWORLD

This story appeared on Network World at <http://www.networkworld.com/news/2011/040611-linux-supercomputer.html>

### 10,000-core Linux supercomputer built in Amazon cloud

Cycle Computing builds cloud-based supercomputing cluster to boost scientific research.

By [Jon Brodtkin](#), Network World  
April 06, 2011 03:15 PM ET

## The Register®

*Being the hand that feeds IT*



Original URL: [http://www.theregister.co.uk/2011/04/06/cycle\\_computing\\_hpc\\_cloud/](http://www.theregister.co.uk/2011/04/06/cycle_computing_hpc_cloud/)

Cycle Computing fires up 10,000-core HPC cloud on EC2

Only \$1,060 per hour, management included

By [Timothy Prickett Morgan](#)

Posted in Cloud, 6th April 2011 16:05 GMT

## A2. Best HPC in the cloud usage/implementation

- Full cluster environment with Shared File system (TBs), and Scheduler
- Secured data transfer and at-rest using AES 128-/256-bit
- Researcher demand: 80000 compute hours for protein binding simulations
- Run-time: 8 hours on 1250 servers, 10000 cores
- Up-front costs: \$0, no software to buy, pay for what you use
- Operating Cost: \$1060/hr ~\$.106/hr, Total cost: \$8500
- User Effort: Single click, no programming / IT admin (unless you want to)

# A2. Best HPC in the cloud usage/implementation

Scientists were able to focus on the science, get immediate results

Great for Peak/Parameter Sweep/Monte Carlo workloads

In General:

- <http://blog.cyclecomputing.com> 2000-core, 80GPU, 4000-core, 10000-core
- Support Any Scheduler (GridEngine, Torque, Condor, as well as licensed)

- Using CycleCloud:

Sign up for an account,  
Configure cluster (Filesystem, etc.)  
Launch cluster  
Log in 5-20 minutes later



## Q3. What HPC in the cloud is not?....

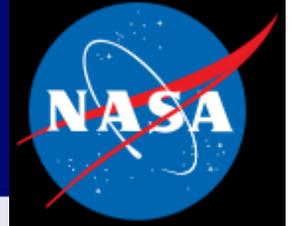
➤ *Examples of HPC in the cloud gone awry.....*

## A3. What HPC in the cloud is not? ....

### ➤ **Not:**

- **A Solution for moving your data in and out of cloud**
- **Applicable to all applications**
  - **Sometimes things don't scale the same way**
- **A solution to license management**
  - **Some commercial applications have 'expensive' license schemes.**
- **Cheaper than your own cluster!**
  - **It is more expensive per hour than internal**
  - **Assuming you need to use the cluster all the time**
- **Guaranteed Secure**
  - **Unless you get the dedicated, storage, network and compute!**
  - **Or you are running on a Cloud with Intel 'Trusted Compute'**

## A3. What HPC in the cloud is not? ....

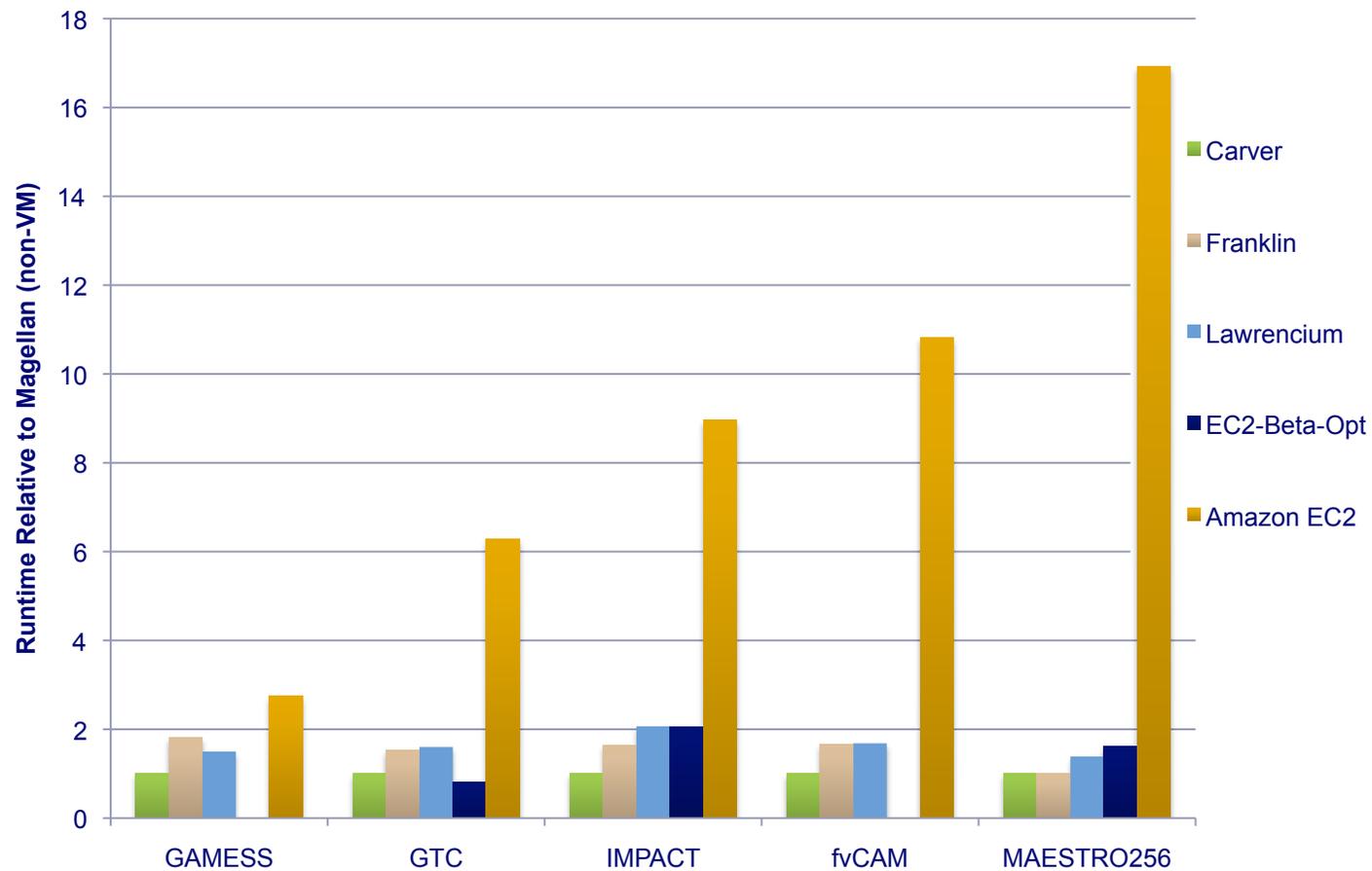


- A substitute for the highly optimized HEC systems NASA operates to address most large-scale CFD and similar workloads
- Yet readily accepted within NASA as a substitute for project-specific infrastructure due to:
  - Historical reliance on, and comfort with, “owned infrastructure,” despite the inherent constraints
  - A business model for NASA cloud services that is still under development
  - User concerns about the effectiveness of cloud security
  - Current lack of a solution engineering group to assist projects with cloud adoption

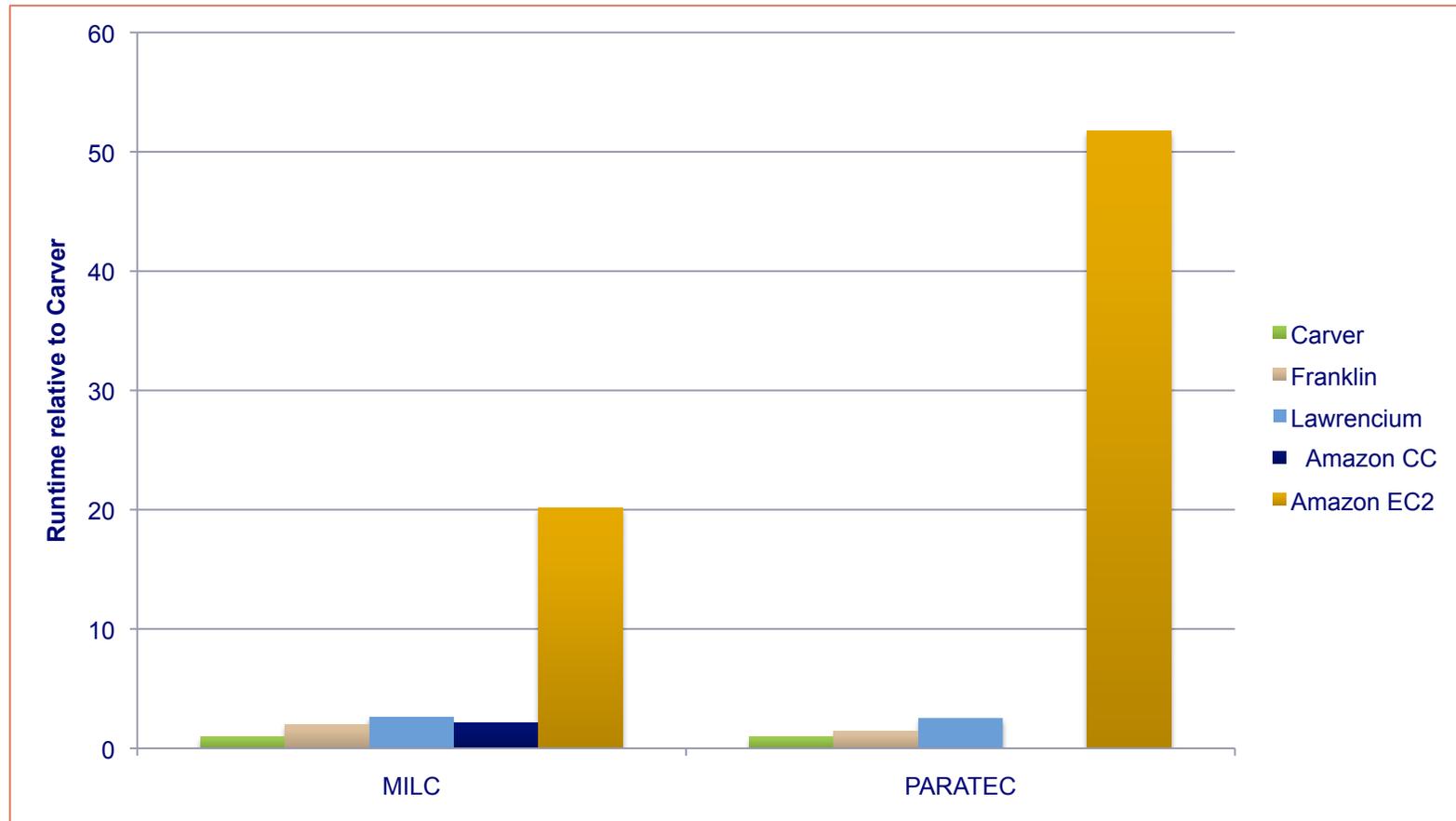
## A3. What HPC in the cloud is not? ....

- ***Business/Web solutions repurposed as HPC***
  - ***Virtualized and shared with other users (unpredictable/variable performance)***
  - ***Commodity network***
  - ***Spread across a data center (or multiple data centers)***
  - ***No simple IO solution***

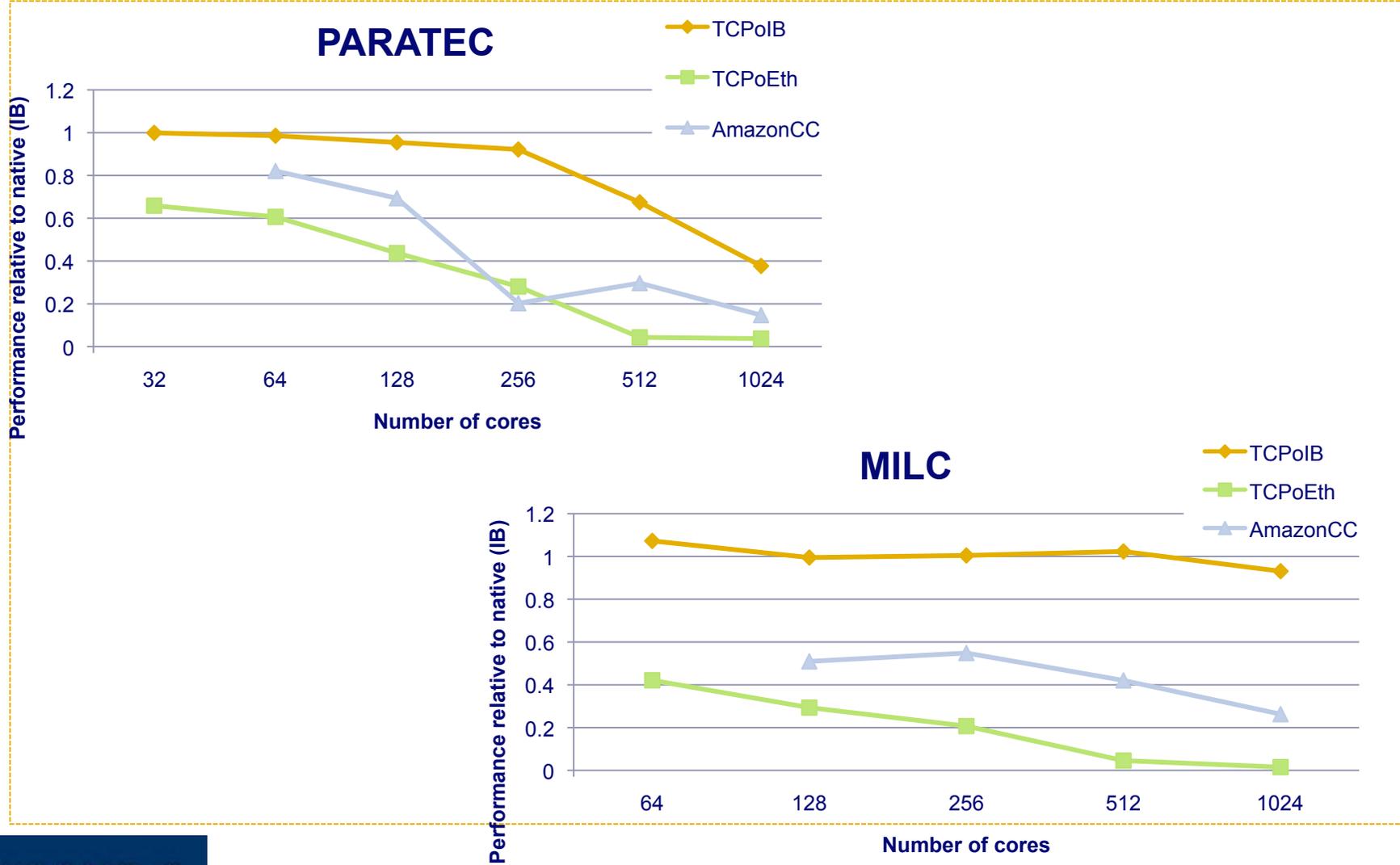
# A3. What HPC in the cloud is not? ....



# A3. What HPC in the cloud is not? ....



# A3. What HPC in the cloud is not? ....



## A3. What HPC in the cloud is not? ....

- *Deploying applications into the Cloud from an environment where the compute, storage, and networking is highly tuned.*
- *Vertical scale applications – i.e. E15K*
- *Specialized/dedicated hardware*

## A3. What HPC in the cloud is not? ....

- ***Applications that require highly tuned Storage back-end (i.e. Tuned SAN)***
  - ***The public clouds today have poor SLA/QOS attributes. This leads to varying performance of the storage and networking infrastructure based on multi-tenant loading.***
  - ***Any applications that are sensitive to this will bottleneck, or potentially fail – and at least they will have unpredictable run-times***
- ***HPC that requires specialized H/W – this is impacted by both virtualization, and cloud vendor hardware selection.***
- ***For virtualization, the issues is if (and how well) the virt. Platform can deliver the functionality. For the vendor selection – the clouds are designing for majority use cases (and may not be focused on HPC)***

# A3. What HPC in the cloud is not? ....

- **A good choice for fine grained parallel jobs**
  - Network latency
- **A good choice for jobs with large data (in/out)**
  - Data charges + time for transfer
- **A good choice for long running parallel jobs**
  - Reliability still in question

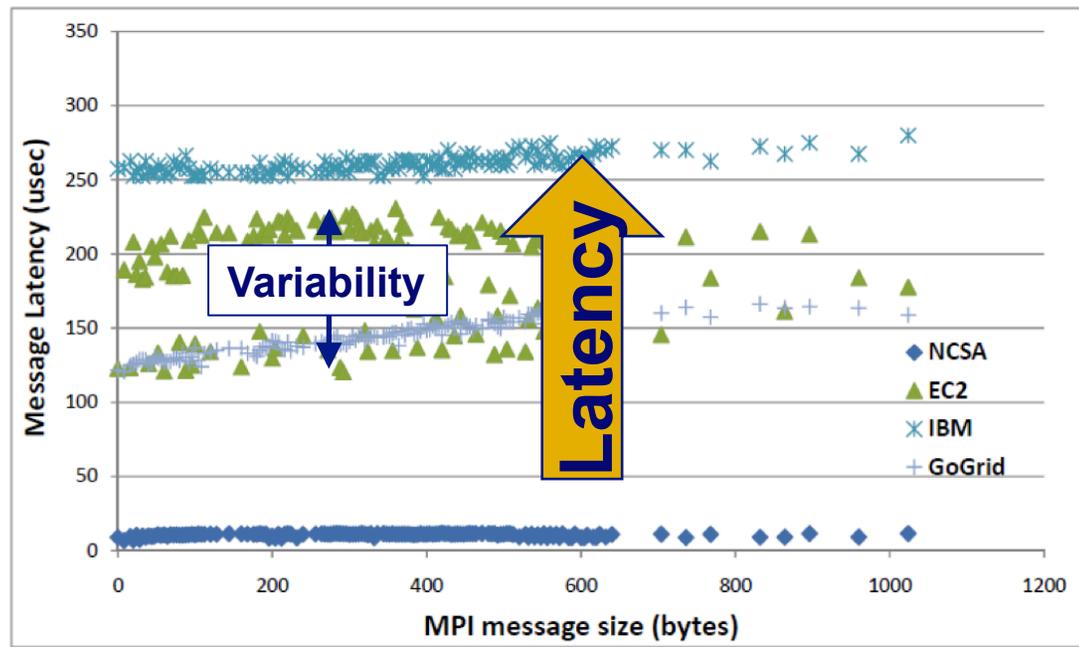


Chart: Q. He, S. Zhou, B. Kobler, dc Duffy, and T. mcglynn,  
"Case study for running HPC applications in public clouds", in Proc. HPDC, 2010

## Q3. What HPC in the cloud is not?....

### ➤ HPC in the Cloud is

- Massive Scale, On-Demand, Cost transparency, with no upfront expense, Performance conscious, Data conscious, & “No phone calls required”

### Is not:

- Current “Cloud-bursting” methodologies in various schedulers, and various tools
  - Automatically shifting tasks to cloud resources
  - Ignores the data, provisioning a VPN causes far more downloading of data, latency, etc.
  - Bad for your bill, bad for performance (upside?)

## A3. What HPC in the cloud is not? ....

- Non-instantaneous capacity
  - Counter to Cloud agility, no phone should be needed
  - Low-latency, extremely big I/O
- Various “automated”-VPN software layers for servers
  - These hurt performance, are proprietary, encourage security laziness (dangerous), use open source tools
- Shared environments that don't use low-level virtualization or dedicated server/strict auth systems to quarantine data.
- Systems that require Web API programming and don't do managed data placement

# General Audience Q&A and wrap up

➤ *Open floor....*