



HPC Clusters in the [almost]* Infinite cloud

Brendan Bouffler (@boofla), #scico

WW Research & Technical Computing



Scientific Computing



Science is one of the greatest areas of computation and can benefit from a democratization in cost and global accessibility that the cloud brings.

It's also where we think Amazon can make a huge, really disruptive, impact on the world by participating - which is, at the most basic level, what we are about as a company.



AWS Research & Technical Computing Team



The **Research & Technical Computing** team is a global group of scientists and specialists from Amazon Web Services.

We're responsible for making the sure the cloud continually innovates in ways that benefit the global community of researchers from whom we draw our inspiration.

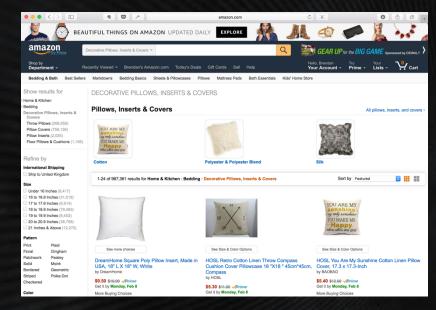
Our aim is to bring the revolutionary benefits of agility and extreme scale to this community so we can all keep making the discoveries that will change the world and impact the lives of everyone on our planet.

We have team members from physics, astronomy, aeronautical engineering, and genomics and all have extensive experience in research and high performance computing. We even have a rocket scientist.



Disrupting science, wherever it's happening.





"... the online book and decorative pillow seller Amazon.com

swooped in and, in 2006, launched its own computer rental system—the future Amazon Web Services. The once-fledgling service has since turned cloud computing into a mainstream phenomenon ..."

Source: Bloomberg Business - April 22, 2015

2006 2016

amazon.com



\$7B retail business 10,000 employees

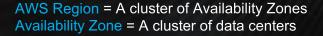
A whole lot of servers

We deploy the equivalent of a top500 supercomputer every day.



Global AWS Regions

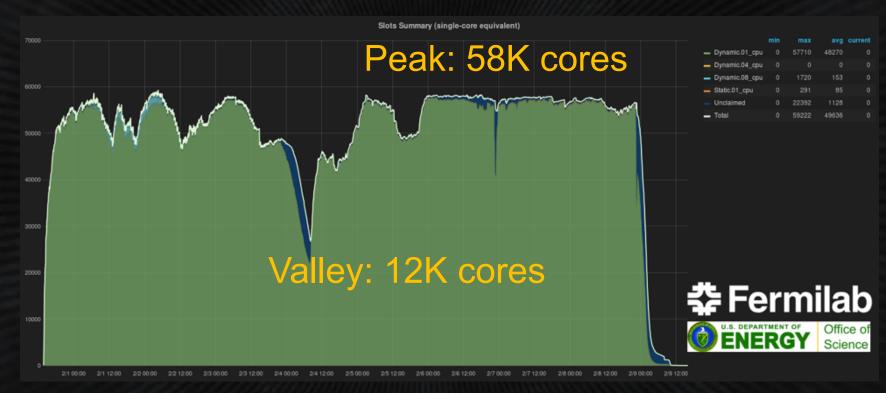




All regions are sovereign, meaning your data never leaves that location unless you cause it to.



Agility is...Paying Only for IT You Use





Science means Collaboration



Collaboration is easier in the cloud





Public Data Sets

1000 Genomes Project and AWS

The 1000 Genomes Project is an international research effort coordinated by a consortium of 75 companies and organizations to establish the most detailed catalogue of human genetic variation. The project has grown

to 200 t can now of more

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AWS is m centralize AWS sen organizat public da or analysi

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Research work with available

TCGA on AWS

The Cancer Genome Atlas (TCGA) is a joint effort of the National Cancer Institute (NCI) and the National Human Genome Research Institute (NHGRI) to accelerate our understanding of the molecular basis of cancer. TCGA-funded researchers across the United States have produced a corpus of raw and processed genomic, transcriptomic, and epigenomic data from thousands of cancer patients.

These data are now freely available on AWS via the National Cancer Institute's Cancer Genomics Cloud pilot to credentialed researchers subject to NIH data sharing policies. As the NIH Trusted Partner for this project, Seven Bridges Genomics is responsible for authorizing access to the data.

The Cancer Genome Atlas is one of the world's largest collections of cancer genome data available. Making the data available on a cloud platform greatly lowers the barrier to entry for researchers that are seeking to work with these data to create better models of disease, and ultimately develop new treatments for cancer. Qualified researchers can use the data on-demand without worrying about download time or storage costs.

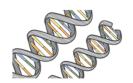
For more information, please visit http://www.cancergenomicscloud.org/. If you have any questions, please email cgc@sbgenomics.com.

Accessing the Data

While the data are hosted within Amazon S3, access is currently only possible through the National Cancer Institute's Cancer Genomics Cloud Pilot. Researchers wishing to access the TCGA controlled data must be registered within that system, and also be listed on an approved TCGA Data Access Request.

For more information on gaining accessing to these data, visit: http://www.cancergenomicscloud.org/controlled-access-data or http://docs.cancergenomicscloud.org/.

Tools and Tutorials



Project Updates

(XXX) XXX XXXX

If you are interested in using the TCGA data or learning more about this project, please fill out the form below.

Last Name*	
Email Address*	
Job Role *	
Select	٠
Telephone*	

NASA NEX

NASA NEX is a collaboration and analytical platform that combines state-of-the-art supercomputing, Earth system modeling, workflow management and NASA remote-sensing data. Through NEX, users can explore

and analyz projects ar

Landsat on AWS

Three NAS simulations data set, p
Terra and /
record fron land.

Landsat 8 data is available for anyone to use via Amazon S3. All Landsat 8 scenes from 2015 are available along with a selection of cloud-free scenes from 2013 and 2014. All new Landsat 8 scenes are made available each day, often within hours of production.

Accessing AWS is makin

AWS Com

Amazon E

The Landsat program is a joint effort of the U.S. Geological Survey and NASA. First launched in 1972,

Simple HT the Landsat series of satellites has produced the

longest continuous record of Earth's land surface as seen fr

Amazon E launch
 perform
The data is he

Available system

Available satellite archivi

charge

the U.S

invento

AWS h

Amazo

Sentinel-2 on AWS

Sentinel-2 data is available for anyone to use via Amazon \$

About the data

Data structure

Browse through data

Accessing the Data

Accessing the Data Featured uses

Sentinel-2 data is available for anyone via Arnazon S3, either over Internet or within AWS. All Sentinel-2 scenes are made available, often within hours of production.

Earth observation data provided by the Sentinel-2 satellites are revolutionizing the market of space applications. Free, full and open access to data with very short revisit times, high spatial resolution, and good spectral resolution can benefit several sectors - agriculture, environmental and land-change monitoring, natural disaster response, insurance and others.

The Sentinel-2 mission is a land monitoring constellation of two satellites (Sentinel-2A was launched on 23 June 2015 and Sentinel-28 will fellow in the second half of 2016) that provide high resolution optical imagery and provide continuity for the current SPOT and Landsat missions. The mission will provide a global coverage of the Earth's land surface every 10 days with one satellite (and 5 days with 2 satellites), making the data of great use in one-poing studies.

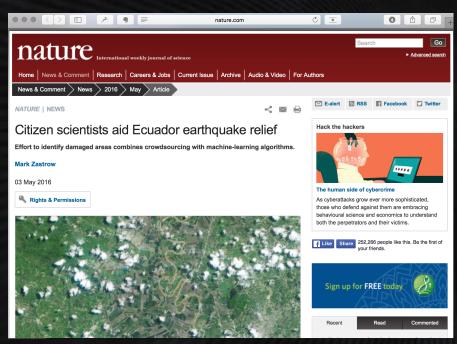
Sentinel-2 delivers high-resolution optical images for land monitoring, emergency response and security



Saving People

ESA, Planet Labs, Copernicus data from ESA's Sentinels & Zooniverse's network of citizen scientists

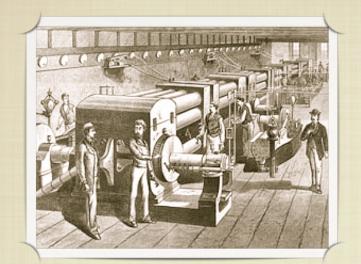
The first live public test for an effort dubbed the Planetary Response Network (PRN)



"Within 2 hours of the Ecuador test project going live with a first set of 1,300 images, each photo had been checked at least 20 times. "It was one of the fastest responses I've seen," says Brooke Simmons, an astronomer at the University of California, San Diego, who leads the image processing. Steven Reece, who heads the Oxford team's machine-learning effort, says that results — a "heat map" of damage with possible road blockages — were ready in another two hours."



http://www.nature.com/news/citizen-scientists-aid-ecuador-earthquake-relief-1.19861



Pearl Street Power Station



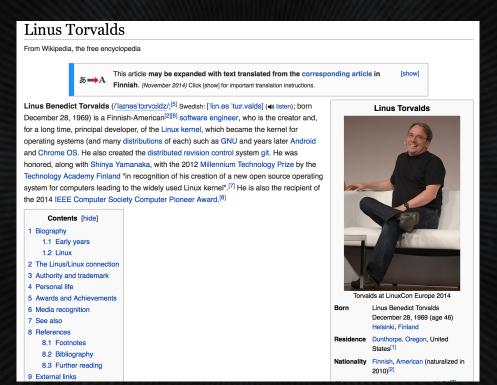


Cray Supercomputer





< Please insert revolution >







Cray Supercomputer





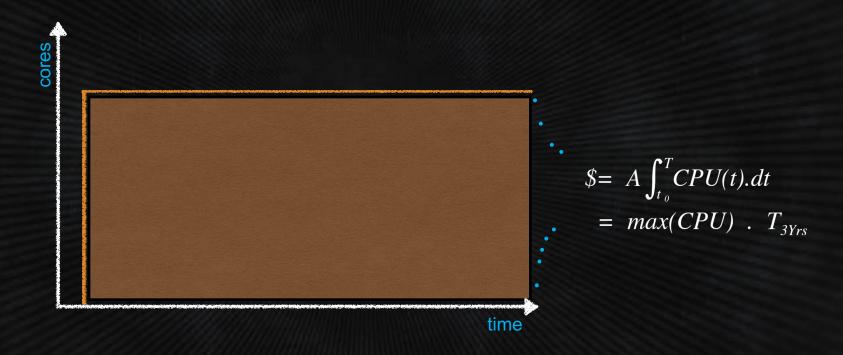


Beowulf Cluster



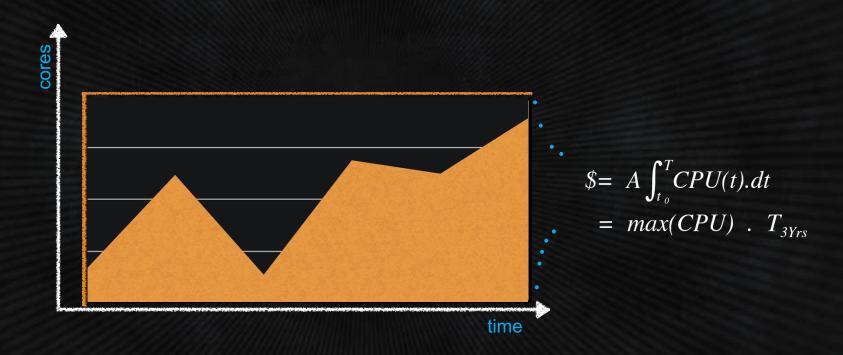


The spherical model of owning a supercomputer



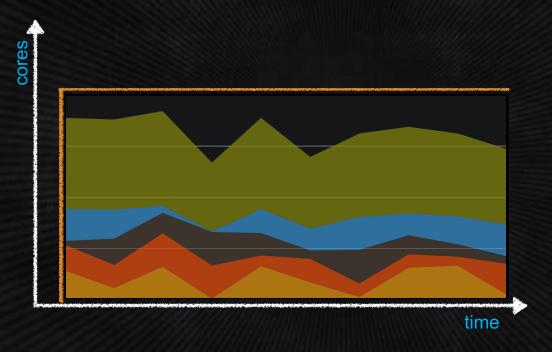


Empirical data





Meeeeelions of uncorrelated workloads

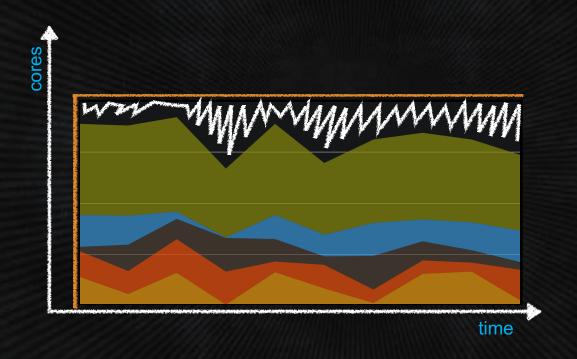


Collective action

When everyone comes together in the cloud to share the resource, and only pays for what they use, the efficiency is huge.



Spot Market



Spot Market

Our ultimate space filler.

Spot Instances allow you to name your own price for spare AWS EC2 computing capacity.

Great for workloads that aren't time sensitive, and especially popular in research (hint: it's really cheap).



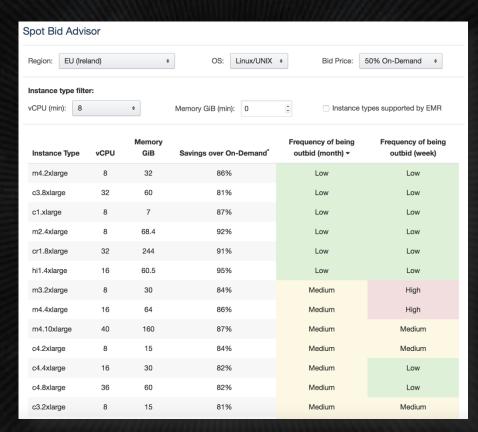
Spot Market Behavior

Spot Bid Advisor

The Spot Bid Advisor analyzes Spot price history to help you determine a bid price that suits your needs.

You should weigh your application's tolerance for interruption and your cost saving goals when selecting a Spot instance and bid price.

The lower your frequency of being outbid, the longer your Spot instances are likely to run without interruption.



Bid Price & Savings

Your bid price affects your ranking when it comes to acquiring resources in the SPOT market, and is the maximum price you will pay.

But frequently you'll pay a lot less.



Spot Market Behavior

```
bash-3.2$ python get_spot_duration.py \
--region us-east-1 \
--product-description 'Linux/UNIX' \
--bids c3.large:0.05,c3.xlarge:0.105,c3.2xlarge:0.21,c3.4xlarge:0.42,c3.8xlarge:0.84
```

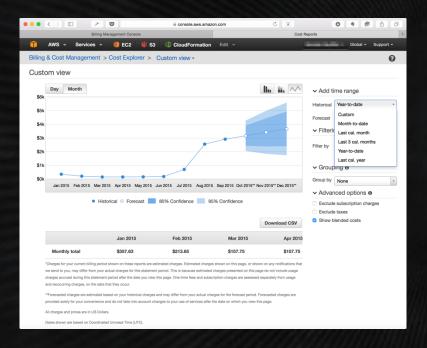
```
Duration
                                Availability Zone
                Instance Type
168.0
       c3.8xlarge
                        us-east-la
168.0
       c3.8xlarge
                        us-east-1d
168.0
       c3.8xlarge
                        us-east-le
168.0
       c3.4xlarge
                        us-east-1b
168.0
       c3.4xlarge
                        us-east-1d
168.0
       c3.4xlarge
                        us-east-le
168.0
       c3.xlarge
                        us-east-1d
168.0
       c3.xlarge
                        us-east-le
168.0
       c3.large
                        us-east-1b
       c3.large
168.0
                        us-east-1d
168.0
       c3.large
                        us-east-le
168.0
       c3.2xlarge
                        us-east-1b
168.0
       c3.2xlarge
                        us-east-le
117.7
       c3.large
                        us-east-la
36.1
       c3.2xlarge
                        us-east-1d
34.5
       c3.4xlarge
                        us-east-la
23.0
       c3.xlarge
                        us-east-1b
21.9
       c3.2xlarge
                        us-east-la
17.3
       c3.8xlarge
                        us-east-1b
0.1
       c3.xlarge
                        us-east-la
```

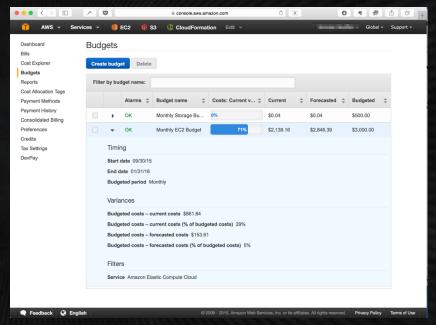
Spot Bid Advisor

As usual with AWS, anything you can do with the web console, you can do with an API or command line.



Cost Control & Budgeting







Galaxies in the Cloud

CHILES will produce the first HI deep field, to be carried out with the VLA in B array and covering a redshift range from z=0 to z=0.45. The field is centered at the COSMOS field. It will produce neutral hydrogen images of at least 300 galaxies spread over the entire redshift range.

The team at ICRAR in Australia have been able to implement the entire processing pipeline in the cloud for around \$2,000 per month by exploiting the SPOT market, which means the \$1.75M they otherwise needed to spend on an HPC cluster can be spent on way cooler things that impact their research ... like astronomers.





Computing efforts

Single Machine

Big desktop: 48 Gb RAM

Good for testing Would take ~vear to finish

Conventional Cluster (pleiades) 5 nodes each node has 2x Intel Xeon X5650

2.66GHz CPUs (6 cores / 12 HTs) with 64-192 GB of RAM

Enough computing power, however disk access limitations



Super computer (MAGNUS) Cray XC40 - 24 cores per node

PHISCC 2015, 16-18 March, New Jersey





Breakthrough discoveries in the Cloud

The CHILES project astronomers have detected radio emissions from hydrogen in a galaxy more than 5 billion light years away, shattering the previous record by almost twice. This has important implications for our understanding of how galaxies have evolved over time.

The team at ICRAR in Western Australia estimates that the amount of compute capacity required to shift and crunch this data would have made this work infeasible.

By using AWS, they were able to quickly and cheaply build their new pipelines, and then scale them as massive amounts of data arrived from their instruments.



Embargoed Press Release

Under embargo until:

June 1st: 8pm EST (New York), Midnight GMT (London) June 2nd: 2am CEST (Amsterdam), 8am AWST (Perth), 10am AEDT (Melbourne & Sydney)

Astronomers smash cosmic records to see hydrogen in distant galaxy

An international team of scientists has pushed the limits of radio astronomy to detect a faint signal emitted by hydrogen gas in a galaxy more than five billion light years away—almost double the previous record.

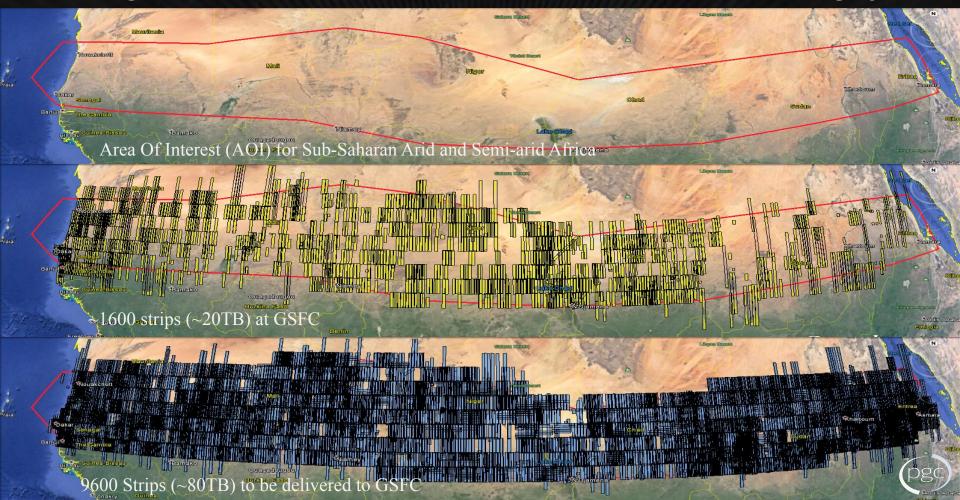
Using the Very Large Array of the National Radio Astronomy Observatory in the US, the team observed radio emission from hydrogen in a distant galaxy and found that it would have contained billions of young, massive stars surrounded by clouds of hydrogen gas.

As the most abundant element in the Universe and the raw fuel for creating stars, hydrogen is used by

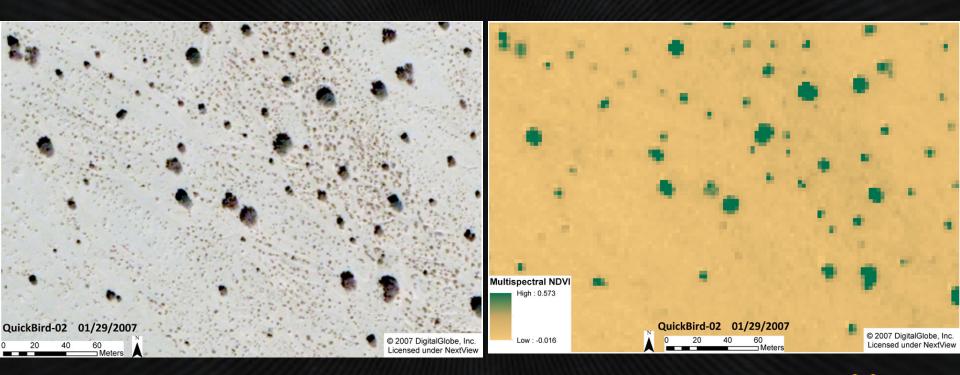




Existing Sub-Saharan Arid and Semi-arid Sub-meter Commercial Imagery

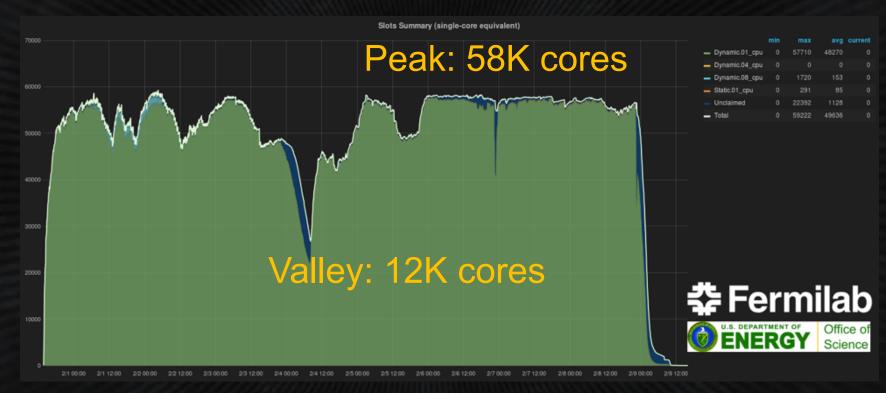


Panchromatic & Multi-Spectral Mapping at the 40cm - 50cm Scale



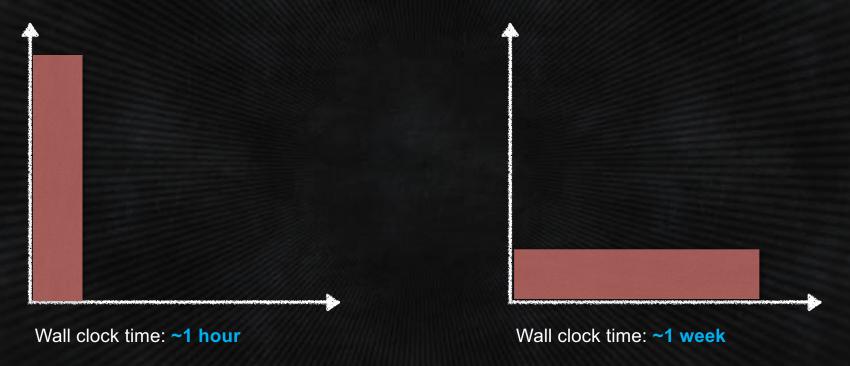


Agility is...Paying Only for IT You Use





Time travel for job queues



Cost: the same



Choices



When you only pay for what you use ...

 If you're only able to use your compute, say, 30% of the time, you only pay for that time.

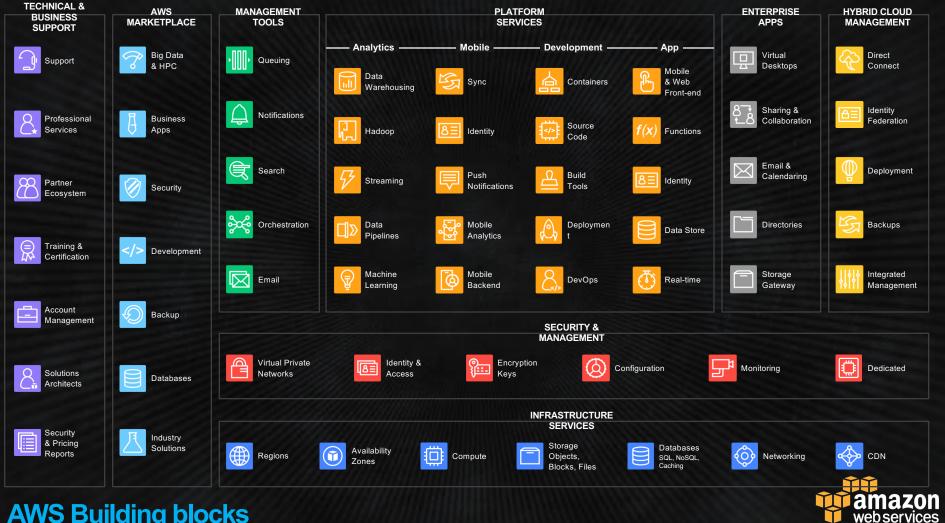


... you have options.

 Do 3x the science, or consume 3x the data.

- Go faster
 Use 3x the cores to run your jobs at 3x the speed.
- Pocket the savings
 - Buy chocolate
 - Buy a spectrometer
 - · Hire a scientist.





Finding what you're not looking for

(Widefield ouTlier Finder)



'WTF is that?' How we're trawling the Universe for the unknown

By Eamonn Bermingham 9TH OCTOBER 2015





The Australian Square Kilometre Array Pathfinder. Credit: Alex Cherney

WTF's cloud-based backend is hosted on Amazon Web Services servers, where the researchers are able to access software for data reduction, calibration and viewing right from their desktop. The team is currently issuing a challenge using data peppered with "EMU (Easter) Eggs" – objects that might pose a challenge to data mining algorithms.

This way they hope to train the system to recognise things that systematically depart from known categories of astronomical objects, to help better prepare for unanticipated discoveries that would otherwise remain hidden.





There's a couple dozen EC2 compute instance types alone, each of which is optimized for different things.

One size does not fit

Memory Optimized

R3

R3 instances are optimized for memory-intensive applications and have the lowest cost per GiB of RAM among Amazon EC2 instance types.

Features:

- · High Frequency Intel Xeon E5-2670 v2 (Ivy Bridge) Processors
- · Lowest price point per GiB of RAM
- SSD Storage
- · Support for Enhanced Networking

Model	vCPU	Mem (GiB)	SSD Storage (GB)
r3.large	2	15.25	1 x 32
r3.xlarge	4	30.5	1 x 80
r3.2xlarge	8	61	1 x 160
r3.4xlarge	16	122	1 x 320
r3.8xlarge	32	244	2 x 320

Use Cases

We recommend memory-optimized instances for high performance databases, distributed memory caches, in-memory analytics, genome assembly and analysis, larger deployments of SAP, Microsoft SharePoint, and other enterprise applications.

GPU

G2

This family includes G2 instances intended for graphics and general purpose GPU compute applications.

Features:

- · High Frequency Intel Xeon E5-2670 (Sandy Bridge) Processors · High-performance NVIDIA GPU with 1,536 CUDA cores and
- 4GB of video memory On-board hardware video encoder designed to support up to
- eight real-time HD video streams (720p at 30fps) or up to four real-time FHD video streams (1080p at 30 fps).
- · Support for low-latency frame capture and encoding for either the full operating system or select render targets, enabling highquality interactive streaming experiences.

SSD Storage (GB) g2.2xlarge 1 x 60

Game streaming, video encoding, 3D application streaming, and other server-side graphics workloads.

http://aws.amazon.com/ec2/instance-types/

C4 instances are the latest generation of Compute-optimized instances, featuring the highest performing processors and the lowest price/compute performance in EC2.	Model	vCPU	Mem (GiB)	Storage	Dedicated EBS Throughput (Mbps)
Features:	c4.large	2	3.75	EBS-	500
 High frequency Intel Xeon E5-2666 v3 (Haswell) processors optimized specifically for EC2 	c4.large	2	3.75	Only	300
EBS-optimized by default and at no additional cost	c4.xlarge	4	7.5	EBS- Only	750
Ability to control processor C-state and P-state configuration on the c4.8xlarge instance type	c4.2xlarge	8	15	EBS- Only	1,000
Support for Enhanced Networking and Clustering	c4.4xlarge	16	30	EBS- Only	2,000
	c4.8xlarge	36	60	EBS-	4,000

High Frequency Intel Xeon E5-2680 v2 (Ivy Bridge) Processors	Model	vCPU	Mem (GiB)	SSD Storage (GB)
Support for Enhanced Networking	c3.large	2	3.75	2 x 16
Support for clustering	c3.xlarge	4	7.5	2 x 40
SSD-backed instance storage	c3.2xlarge	8	15	2 x 80
	c3.4xlarge	16	30	2 x 160
	c3.8xlarge	32	60	2 x 320

This family includes the M3 instance types and provides a balance of compute, memory, and network resources, and it is a good choice for many applications.	Model	vCPU	Mem (GiB)	SSD Storage (GB)
Features:	m3.medium	1	3.75	1 x 4
High Frequency Intel Xeon E5-2670 v2 (Ivy Bridge) Processors*	m3.large	2	7.5	1 x 32
SSD-based instance storage for fast I/O performance	m3.xlarge	4	15	2 x 40
Balance of compute, memory, and network resources	m3.2xlarge	8	30	2 x 80
	Use Cases			

Small and mid-size databases, data processing tasks that require additional memory, caching fleets, and for running backend servers for SAP, Microsoft SharePoint, and other enterprise applications.



C4

Intel Xeon E5-2666 v3, custom built for AWS.

Intel Haswell, 16 FLOPS/tick

2.9 GHz, turbo to 3.5 GHz

Feature	Specification
Processor Number	E5-2666 v3
Intel® Smart Cache	25 MiB
Instruction Set	64-bit
Instruction Set Extensions	AVX 2.0
Lithography	22 nm
Processor Base Frequency	2.9 GHz
Max All Core Turbo Frequency	3.2 GHz
Max Turbo Frequency	3.5 GHz (available on c4.2xLarge)
Intel® Turbo Boost Technology	2.0
Intel® vPro Technology	Yes
Intel® Hyper-Threading Technology	Yes
Intel® Virtualization Technology (VT-x)	Yes
Intel® Virtualization Technology for Directed I/O (VT-d)	Yes
Intel® VT-x with Extended Page Tables (EPT)	Yes
Intel® 64	Yes

AWS Official Blog

New Compute-Optimized EC2 Instances

by Jeff Barr | on 13 NOV 2014 | in Amazon EC2 | Permalink

Our customers continue to increase the sophistication and intensity of the compute-bound workloads that they run on the Cloud.

Applications such as top-end website hosting, online gaming, simulation, risk analysis, and rendering are voracious consumers of CPU cycles and can almost always benefit from the parallelism offered by today's multicore processors.

The New C4 Instance Type

Today we are pre-announcing the latest generation of compute-optimized Amazon Elastic Compute Cloud (EC2) instances. The new C4 instances are based on the Intel Xeon E5-2666 v3 (code name Haswell) processor. This custom processor, designed specifically for EC2, runs at a base speed of 2.9 GHz, and can achieve clock speeds as high as 3.5 GHz with Turbo boost. These instances are designed to deliver the highest level of processor performance on EC2. If you've got the workload, we've got the instance!

Here's the lineup (these specs are preliminary and could change a bit before launch time):

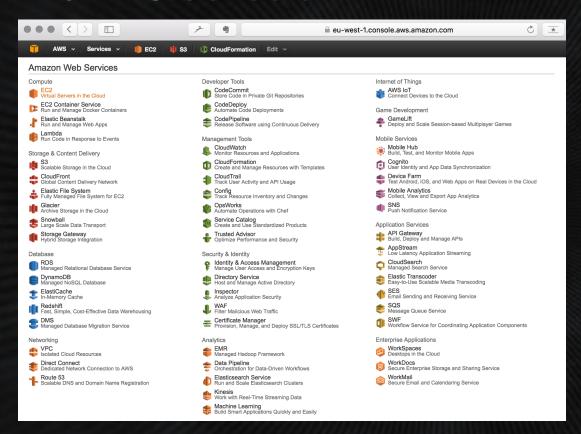
Instance Name	vCPU Count	RAM	Network Performance
c4.large	2	3.75 GiB	Moderate
c4.xlarge	4	7.5 GiB	Moderate
c4.2xlarge	8	15 GiB	High
c4.4xlarge	16	30 GiB	High
c4.8xlarge	36	60 GiB	10 Gbps

These instances are a great match for the SSD-Backed Elastic Block Storage that we introduced earlier this year. EBS Optimization is enabled by default for all C4 instance sizes, and is available to you at no extra charge. C4 instances also allow you to achieve significantly higher packet per second (PPS) performance, lower network litter, and lower network latency using Enhanced Networking.

http://docs.aws.amazon.com/AWSEC2/latest/UserGuide/c4-instances.html



The AWS Console





The AWS API

Almost anything you can do in the GUI, you can do on the command line or via our API

```
# use power user policy
resp = iam.get_policy({policy_arn: "arn:aws:iam::aws:policy/PowerUserAccess"})
policy_arn = resp.policy.arn
# create an output CSV document
output = File.open("users.csv", 'a+')
output.puts(%w{ UserName Password AwsAccessKeyId, AwsSecretAccessKey}.to_csv)
users.each do luserl
    # create user
    iam.create_user({user_name: user[:name]})
   # attach policy
    iam.attach_user_policy({
        user_name: user[:name].
        policy_arn: policy_arn
    # create login
    iam.create_loain_profile({
       user_name: user[:name].to_s,
       password: user[:pw].to_s,
        password_reset_required: false,
    # create access keys
   resp = iam.create_access_key({user_name: user[:name]})
   user[:access_key_id] = resp.access_key.access_key_id
   user[:secret_access_key] = resp.access_key.secret_access_key
    output.puts(
            user[:name],
            user[:pw],
           user[:access_key_id],
           user[:secret_access_kev]
        1.to_csv
    puts "--\n"
                             #{MY_URL}\n"
    puts "Portal:
    puts "Username:
                             #{user[:name]}\n"
                            #{user[:pw]}\n"
    puts "Password:
   puts "Access Key ID:
                             #{user[:access_key_id]}\n"
    puts "Secret Access Key: #{user[:secret_access_key]}\n"
end
```

http://boto.readthedocs.org/en/latest/

Java
Python
Ruby
PHP
Shell
...
... and in most popular languages.





Cray Supercomputer







Beowulf Cluster





A top500 supercomputer ... 2013-style





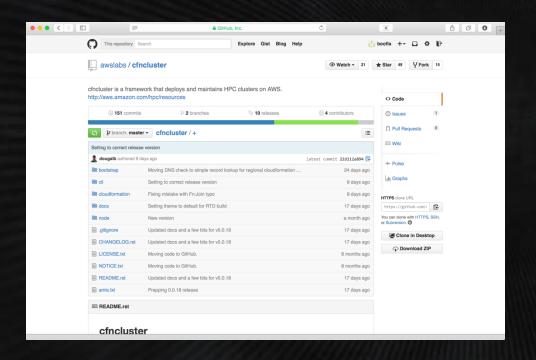
Ready in ~100 seconds

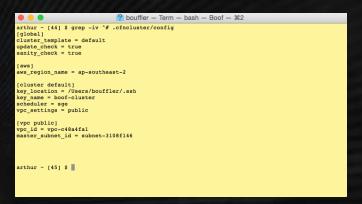
For ~ \$100/hr



cfnCluster - provision an HPC cluster in minutes

cfncluster is a sample code framework that deploys and maintains clusters on AWS. It is reasonably agnostic to what the cluster is for and can easily be extended to support different frameworks. The CLI is stateless, everything is done using CloudFormation or resources within AWS.







https://github.com/awslabs/cfncluster





Self-service Supercomputing ... 2016

Introducing Alces Flight - self-scaling HPC clusters instantly ready to compute, billed by the hour and using the AWS Spot market by default to achieve supercomputing for ~1c per core per hour.

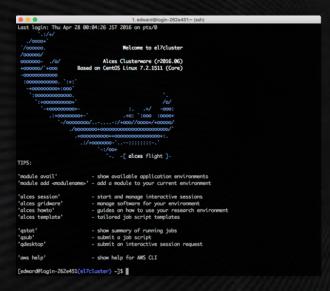


- 750+ popular scientific applications
 - Pre-installed & ready to run.
 - Multiple versions, complete with libraries and various compiler optimizations, ready to run
- Available via the AWS Marketplace (the cloud's "App Store") and launched within minutes.
- Deployable anywhere on Earth ... immediately.

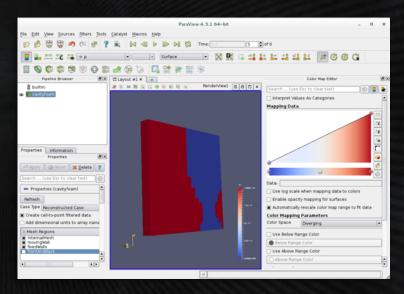


Flight is very accessible

All the traditional command-line tools will be familiar, but you can also create an Alces "session" and immediately launch a desktop view of your cluster to run graphical apps.



Command Line (ssh)



Graphical Console



Filesystems in the marketplace, too

There are cluster filesystem options, too—for when you need extreme I/O scaling.

- BeeGFS is a scalable parallel cluster filesystem developed with a strong focus on performance and designed easy installation and management developed by the Fraunhofer Institute.
- Intel Lustre® Cloud Edition is a scalable, parallel file system purpose-built for HPC and with a long history in the field supporting a range of workloads.
- There's more to come the AWS Marketplace is growing all the time and new offerings are added frequently. Watch this space.









Thank You

