Research Computing in a time of disruption: Trends, highlights and new ways of innovating

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WW Research & Technical Computing

*Does not apply to mathematicians with specialties in Cantorian set theory who should immediately ask for a copy of my very long disclaimer.
“… 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
Disrupting science, wherever it’s happening.
The Research & Technical Computing team is a global group of scientists and specialists from Amazon Web Services.

We're responsible for making 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.
Science means Collaboration and EU is centre
European Centrality
Brendan Bouffler ("boof")
London

Brendan Bouffler has 20 years of experience in the global IT industry dealing with very large systems in high performance environments. He has been responsible for designing and building hundreds of HPC systems for commercial enterprises as well as research and defense sectors all around the world and has quite a number of his efforts listed in the top500, including some that have placed in the top 5.

Brendan previously lead the HPC Organization for Dell in Asia and joined Amazon in 2014 to help accelerate the adoption of cloud computing in the scientific community globally. He holds a degree in Physics and an interest in testing several of its laws as they apply to bicycles. This has frequently resulted in hospitalization 🚑.
HPC since the dawn of … Beowulf

Thanks: Jeff Layton
When your only tool is a hammer ...
Linus Torvalds

From Wikipedia, the free encyclopedia

Linus Benedict Torvalds ([ˈlɪnəs ˈtɔːr.vɑlðs] (listen) [ˈlinus ˈtɔːr välz]; born December 25, 1969) is a Finnish-American software engineer, who is the creator and, for a long time, principal developer of the Linux kernel, which became the kernel for operating systems (and many distributions of each) such as GNU and years later Android and Chrome OS. He also created the distributed revision control system git. He was honored, along with Shinya Yamanaka, with the 2012 Millennium Technology Prize by the Technology Academy of Finland in recognition of his creation of a new open source operating system for computers leading to the widely used Linux kernel. He is also the recipient of the 2014 IEEE Computer Society Computer Pioneer Award.

Contents

1 Biography
  1.1 Early years
  1.2 Linux
2 The Linux/Linux connection
3 Authority and trademark
4 Personal life
5 Awards and achievements
6 Media recognition
7 See also
8 References
   8.1 Footnotes
   8.2 Bibliography
   8.3 Further reading
9 External links
Beowulf Cluster
HPC since the dawn of … Beowulf

Thanks: Jeff Layton
Polishing the cannonball ...

Thanks: Infiniband Industry
Working at Amazon is very different

1. Customer Obsession
2. Ownership
3. Invent and Simplify
4. Are Right, A Lot
5. Learn and Be Curious
6. Hire and Develop the Best
7. Insist on the Highest Standards
8. Think Big
9. Bias for Action
10. Frugality
11. Earn Trust
12. Dive Deep
13. Have Backbone; Disagree and Commit
14. Deliver Results

Leadership Principles

Our Leadership Principles aren’t just a pretty inspirational wall hanging. These Principles work hard, just like we do. Amazonians use them every day. Whether they’re discussing ideas for new products, deciding on the best solution for a customer’s problem, or interviewing candidates. It’s just one of the things that makes Amazon popular.

Customer Obsession

Leaders start with the customer and work backwards. They work vigorously to earn and keep customer trust.

Although leaders pay attention to competitors, they obsess over customers.

Ownership

Leaders are owners. They think long term and don’t sacrifice long-term value for short-term results. They act on behalf of the entire company, beyond just their own team. They never say “that’s not my job”.

Invent and Simplify

Leaders expect and require innovation and invention from their teams and always find ways to simplify. They are externally aware, look for new ideas from everywhere, and are not limited by “not invented here”. As we do new things, we accept that we may be misunderstood for long periods of time.

https://www.amazon.jobs/en/principles
Direction

Customer Obsession
Everything we do starts with a customer and we work backwards from there.
We work vigorously to earn and keep customer trust.
Disrupt

Bias For Action
Speed of decision making does matter, and despite what you think, most decisions are reversible, so we value “why the hell not?” more than “let’s wait and see”.

Frugality
Constraints breed resourcefulness, self-sufficiency and invention. There are no points for growing headcount.

Think Big
Thinking small is a self-fulfilling prophecy. Think differently and look around corners for ways to serve customers.
Failure is a data point

Lowering the cost of failure leads to greater experimentation and thus innovation.
Failing Fast

... is just the scientific method sped up a little.
Failing cheaply

Low cost of failure

More experimentation
### AWS Building blocks

**AWS Marketplace**
- Big Data & HPC
- Business Apps
- Security
- Development
- Backup
- Databases
- Industry Solutions

**Management Tools**
- Queuing
- Notifications
- Search
- Orchestration
- Email

**Platform Services**
- Analytics
  - Data Warehousing
  - Hadoop
  - Streaming Pipelines
  - Machine Learning
- Mobile
  - Sync
  - Identity
  - Push Notifications
  - Mobile Analytics
  - Mobile Backend
- Development
  - Containers
  - Source Code
  - Build Tools
  - Deployment
- App
  - Mobile & Web Front-end
  - Functions
  - Mobile & Web Front-end

**Enterprise Apps**
- Virtual Desktops
- Sharing & Collaboration
- Email & Calendaring
- Direct
- Identity Federation
- Deployment
- Backups
- Integrated Management

**Hybrid Cloud Management**
- Backups
- Deployment
- Integrated Management

**Security & Management**
- Virtual Private Networks
- Identity & Access
- Encryption Keys
- Configuration
- Monitoring
- Dedicated

**Infrastructure Services**
- Regions
- Availability Zones
- Compute
- Storage
- Networking
- CDN
Global AWS Regions

AWS Region = A cluster of Availability Zones
Availability Zone = A cluster of data centers

All regions are sovereign, meaning your data never leaves that location unless you cause it to.
Meeeeeelions 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.
Time travel for job queues

Wall clock time: ~1 hour

Wall clock time: ~1 week

Cost: the same
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).
Agility is…Paying Only for IT You Use

Peak: 58K cores

Valley: 12K cores
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.
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.
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.

1 Go Large
• Do 3x the science, or consume 3x the data.

2 Go faster
• Use 3x the cores to run your jobs at 3x the speed.

3 Pocket the savings
• Buy chocolate
• Buy a spectrometer
• Hire a scientist.
AWS Lambda is a compute service where you can upload your code into the cloud and the service can run the code on your behalf using AWS infrastructure.

After you upload your code and create what we call a Lambda function, AWS Lambda takes care of provisioning and managing the servers that you use to run the code.

1 Million free lambda requests per month in the free tier.
Changing the way the world computes

Spin up a cluster?

Process images and mash up against geo data?

Notify a subscriber list?

No Servers to Manage
AWS Lambda automatically runs your code without requiring you to provision or manage servers. Just write the code and upload it to Lambda.

Continuous Scaling
AWS Lambda automatically scales your application by running code in response to each trigger. Your code runs in parallel and processes each trigger individually, scaling precisely with the size of the workload.

Subsecond Metering
With AWS Lambda, you are charged for every 100ms your code executes and the number of times your code is triggered. You don’t pay anything when your code isn’t running.
Changing the way the science scales

Scale:

- From laptop to server
- From server to cluster
- From CPU to GPU

... in minutes.
Primordial Soup
Collaboration is easier in the cloud

More time spent computing the data than moving the data.
Public Datasets

Invent & Simplify
Be the best platform we can be and remove the undifferentiated heavy lifting so others can be the best that they can be.
Lesson – Jed’s Laws of Open Data

I. Put the data somewhere
II. Document it
III. Make sure it’s there tomorrow
Big Open Data

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 complete reference of human genetic variation. The project has sequenced over 200 genomes and made the data available to more than 1,000 researchers.

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 new and processed genomic, transcriptomic, and epigenetic data from thousands of cancer patients.

Access

AWS is a trusted partner of TCGA and has organized public data sets at Amazon S3. At any time, you can access TCGA data by simply using the Amazon S3 service.

Accessing the Data

While the data is hosted within Amazon S3, access is currently only possible through the National Cancer Institute’s Cancer Genomics Cloud (CGC). Researchers wanting to access the TCGA controlled data must be registered within this system and also be listed on an approved TCGA Data Access Request.

Tools and Tutorials

For more information on viewing the data, visit the TCGA website at http://tcga.cancer.gov/ and http://tcga.cancer.gov/tutorials/.

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 analyze projects at NASA and access data.

Landsat on AWS

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

Access

AWS account

Simple Key

AWS Code

Amazon S3

Landsat by date

Access the data

A new scene is available via AWS Cloud

Sentinel-2 on AWS

Sentinel-2 data is available for anyone to use via Amazon S3. Each scene is made available within hours of production.

Landsat data may be used freely for non-commercial purposes.

Disclaimer

NASA does not accept or retain any responsibility for the content or accuracy of data generated by Third Party Participants using Landsat data.

Amazon Web Services

Amazon Web Services is a platform for building, deploying, and scaling applications.

Sentinel-2 data is available for anyone to use via Amazon S3.
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.”
A top500 supercomputer ... 2013-style

Ready in ~100 seconds

For ~ $100/hr
Self-service Science … 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.

http://boofla.io/u/alcesFlight
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.
Flight enables collaboration

Access the graphical console of your control node simultaneously with your collaborators

- Run visual apps that use the elastic cluster to drive visual results and you can work together with the visual console in real-time

Shared & secure cloud workspaces

- Control access and focus on data analysis
- Make more discoveries faster
  - Save lives
  - Change the world

Collaborative IGV (Integrative Genomics Viewer) workspace for variant analysis
M4.16xL

Intel Xeon 2686 v4, custom built for AWS.

Intel Broadwell, 16 FLOPS/tick

2.2 GHz, turbo to 3.60 GHz

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Expanding the M4 Instance Type – New M4.16xlarge

by Jeff Barr on 27 SEP 2016 in Amazon EC2, Launch | Promote | ☰ Comments

EC2's M4 Instances offer a balance of compute, memory, and networking resources and are a good choice for many different types of applications.

We launched the M4 instances last year (read The New M4 Instance Type to learn more) and gave you a choice of five sizes, from large up to 10xlarge. Today we are expanding the range with the introduction of a new m4.16xlarge with 64 vCPUs and 256 GB of RAM. Here’s the complete set of specs:

<table>
<thead>
<tr>
<th>Instance Name</th>
<th>vCPU Count</th>
<th>RAM</th>
<th>Instance Storage</th>
<th>Network Performance</th>
<th>EBS-Optimized</th>
</tr>
</thead>
<tbody>
<tr>
<td>m4.large</td>
<td>2</td>
<td>8 GB</td>
<td>EBS Only</td>
<td>Moderate</td>
<td>480 Mbps</td>
</tr>
<tr>
<td>m4.xlarge</td>
<td>4</td>
<td>16 GB</td>
<td>EBS Only</td>
<td>High</td>
<td>750 Mbps</td>
</tr>
<tr>
<td>m4.2xlarge</td>
<td>8</td>
<td>32 GB</td>
<td>EBS Only</td>
<td>High</td>
<td>1,090 Mbps</td>
</tr>
<tr>
<td>m4.4xlarge</td>
<td>16</td>
<td>64 GB</td>
<td>EBS Only</td>
<td>High</td>
<td>2,030 Mbps</td>
</tr>
<tr>
<td>m4.10xlarge</td>
<td>40</td>
<td>120 GB</td>
<td>EBS Only</td>
<td>10 Gbps</td>
<td>4,000 Mbps</td>
</tr>
<tr>
<td>m4.16xlarge</td>
<td>64</td>
<td>256 GB</td>
<td>EBS Only</td>
<td>20 Gbps</td>
<td>10,000 Mbps</td>
</tr>
</tbody>
</table>

The new instances are based on Intel Xeon E5-2680 v4 (Broadwell) processors that are optimized specifically for EC2. When used with Elastic Network Adapter (ENA) inside of a placement group, the instances can deliver up to 20 Gbps of low-latency network bandwidth.

To learn more about the ENA, read my post, Elastic Network Adapter – High Performance Network Interface for Amazon EC2.
P2

Intel Xeon E5-2686v4 CPU 2.7 GHz, custom built for AWS (Intel Broadwell, 16 FLOPS/tick)

8 x K80 = 16 x GK210 GPU dies per P2.16xL

Tesla K80 DELIVERS 5-10X BOOST IN KEY APPLICATION PERFORMANCE

<table>
<thead>
<tr>
<th>GPU</th>
<th>NVIDIA Tesla K80</th>
<th>NVIDIA Tesla K20</th>
<th>CPU</th>
</tr>
</thead>
<tbody>
<tr>
<td>Performance Boost</td>
<td>14.3x</td>
<td>7.1x</td>
<td>2.5x</td>
</tr>
</tbody>
</table>

TNELSA K80 DELIVERS 5-10X BOOST IN KEY APPLICATION PERFORMANCE

Now P2 Instance Type

This new instance type incorporates up to 8 NVIDIA Tesla K80 accelerators, each running a pair of NVIDIA GK210 GPUs. Each GPU provides 12 GB of memory (accessible via 240 GB/second of memory bandwidth), and 2,496 parallel processing cores. They also include ECC memory protection, allowing them to fix single-bit errors and to detect double-bit errors. The combination of ECC memory protection and double-precision floating point operations makes these instances a great fit for all of the workloads that I mentioned above.

Here are the instance specs:

<table>
<thead>
<tr>
<th>Instance Name</th>
<th>GPU Count</th>
<th>vCPU Count</th>
<th>Memory</th>
<th>Parallel Processing Cores</th>
<th>GPU Memory</th>
<th>Network Performance</th>
</tr>
</thead>
<tbody>
<tr>
<td>p2.xlarge</td>
<td>1</td>
<td>4</td>
<td>81 GB</td>
<td>2,496</td>
<td>12 GB</td>
<td>High</td>
</tr>
<tr>
<td>p2.2xlarge</td>
<td>2</td>
<td>32</td>
<td>488 GB</td>
<td>19,968</td>
<td>96 GB</td>
<td>10 Gigabit</td>
</tr>
<tr>
<td>p2.16xlarge</td>
<td>16</td>
<td>64</td>
<td>732 GB</td>
<td>30,036</td>
<td>192 GB</td>
<td>20 Gigabit</td>
</tr>
</tbody>
</table>
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.
We Feel Emotion Explorer

- Twitter ‘decahose’ (thanks to GNIP)
- AWS Kinesis
- Natural language processing / sentiment analysis.

Used by the Blackdog Institute in Australia for research into depression and it's causes.

http://wefeel.csiro.au
The Zooniverse is heavily reliant on Amazon Web Services (AWS), particularly Elastic Compute Cloud (EC2) virtual private servers and Simple Storage Service (S3) data storage. AWS is the most cost-effective solution for the dynamic needs of Zooniverse’s infrastructure …


... cost is a factor – running a central API means that when the Zooniverse is quiet and there aren’t many people about we can scale back the number of servers we’re running (automagically on Amazon Web Services) to a minimal level.
Thank You
Python Serverless Micro-framework

In just 45 seconds, we can create a new project, inspected its code file (app.py), deployed it to a public API endpoint, and using curl, made a successful HTTP GET request to the endpoint. Because our goal is to minimize the time it takes to get started, we hope you'll enjoy the simple and fast experience offered by the new microframework.

https://youtu.be/BkB5-8IFYek