

Cloud-first data science at the Turing

Martin O'Reilly Principal Research Software Engineer The Alan Turing Institute

@martinoreilly | @turinginst

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The Alan Turing Institute is the national centre for data science, headquartered at the British Library.



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 Cloud-first data science at the Turing



Research engineering group

A permanent team of research software engineers and data scientists who work with researchers to increase the impact of their work.



https://www.turing.ac.uk/research-engineering/

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Challenges

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Challenge 1: How much compute can we afford?

Tier 1 national cluster



Tier 2 regional clusters





Tier 3 institutional clusters



Turing Cray and Intel clusters



Partner university institutional clusters

Institutional cloud compute



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Challenge 2: The cloud learning curve

Model A: Workstation++

- Runs a handful of big VMs
- Gets more personal compute resource than can fit under a desk
- Manages VMs and workload manually

Model B: High throughput "cluster"

- Generally running large or urgent jobs
- Generally existing cluster users
- Need to deploy lots of workers

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Challenges to self-sufficiency

- Unfamiliar compute / data abstractions
- Deploying cloud resources on demand
- Can't simply "lift and shift" existing code
- Usage / cost management





Outcomes

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Azure core-years if spent on one compute type

| CPU node type | On demand cores | Reserved cores (3yr reservation) | • • |
|--|--------------------------------------|--|---|
| Low memory HTC (2 GB / core) | 2,667 | 7,280 | 11,356 |
| Low memory HTC (4 GB / core) | 2,351 | 6,003 | 11,284 |
| Medium memory HTC (8 GB / core) | 1,697 | 4,513 | 8,477 |
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| Medium memory HPC (7 GB /core) | 678 | 2,325 | 4,537 |
| High memory HPC (14 GB / core) | 908 | 1,735 | 3,388 |
| | On domand | Reserved GPUs | Low priority |
| GPU node type | GPUs | (3yr reservation) | • • |
| GPU node type Kepler K80 HTC | | (3yr reservation) | batch GPUs |
| | GPUs | (3yr reservation) 282 | batch GPUs 627 |
| Kepler K80 HTC | GPUs 125 | (3yr reservation) 282 257 | batch GPUs 627 570 |
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On-premise cluster comparisons

National (Tier 1):

ARCHER: 118,080 cores with 0.75 or 1.5 GB / core*

Regional (Tier 2):

- CIRRUS: 10,080 cores with 4 GB / core
- JADE: 176 Pascal P100 GPUs
- Emerald: 372 Fermi M2090 GPUs [retired]

Institutional (Tier 3):

- UCL Grace: 10,944 cores with 5.3 GB / core
- QMUL Apocrita HTC: 2,280 cores with 2 or 10 GB / core**
- QMUL Apocrita HPC: 1,808 cores with 1.3 or 8 GB / core***
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Figures ignore storage costs and are based on Azure Linux VM pricing for East US region as at 11/04/2018 with 1 USD = 0.74 GBP. HTC = RDMA interconnect.

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Storage costs as data size grows

| | | Download £ / year (for N annual downloads of full dataset) | | | | |
|--------------|------------------|--|---------------|----------------|-----------------|--|
| Dataset size | Storage £ / year | 1 | 10 | 100 | 1000 | |
| 1 GB | £0.19 | £0.00 | £0.00 | £0.00 | £0.00 | |
| 10 GB | £1.87 | £0.03 | £0.27 | £2.71 | £27.08 | |
| 100 GB | £18.72 | £0.51 | £5.15 | £51.46 | £514.58 | |
| 1 TB | £191.69 | £5.52 | £55.20 | £551.96 | £5,519.58 | |
| 10 TB | £1,916.93 | £55.44 | £554.40 | £5,543.96 | £55,439.58 | |
| 100 TB | £19,169.28 | £493.23 | £4,932.27 | £49,322.67 | £493,226.67 | |
| 1 PB | £196,293.43 | £3,489.45 | £34,894.51 | £348,945.07 | £3,489,450.67 | |
| 10 PB | £1,962,934.27 | £33,373.87 | £333,738.67 | £3,337,386.67 | £33,373,866.67 | |
| 100 PB | £19,629,342.72 | £332,218.03 | £3,322,180.27 | £33,221,802.67 | £332,218,026.67 | |

1,000,000 = £737,000



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Outcome 2: The cloud learning curve

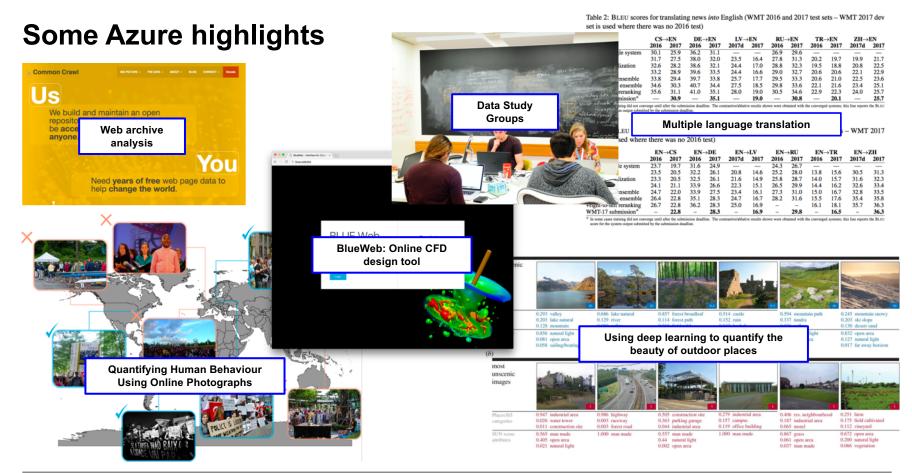
Current support

- Training sessions
- "Azure club" support sessions
- Support from research engineering
- Some orchestration scripts
- Azure tooling such as Batch Shipyard

Current adoption

- Better than last year but a way to go
- A few big "high throughput" users
- Most use "workstation++" model
- Most deploy via portal
- Most don't use low priority
- Even cluster users struggle









Future

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Future

More compute for our \$\$\$

- More use of low priority compute
- Compute directly on data stored outside of Azure
- Both require use of more sophisticated workflows, so need an easier learning curve
- More proactive monitoring of spending

Making the learning curve easier

- Make the Azure compute / data abstractions more transparent
- Provide easy to use workflows for a range of "standard" Turing use cases



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