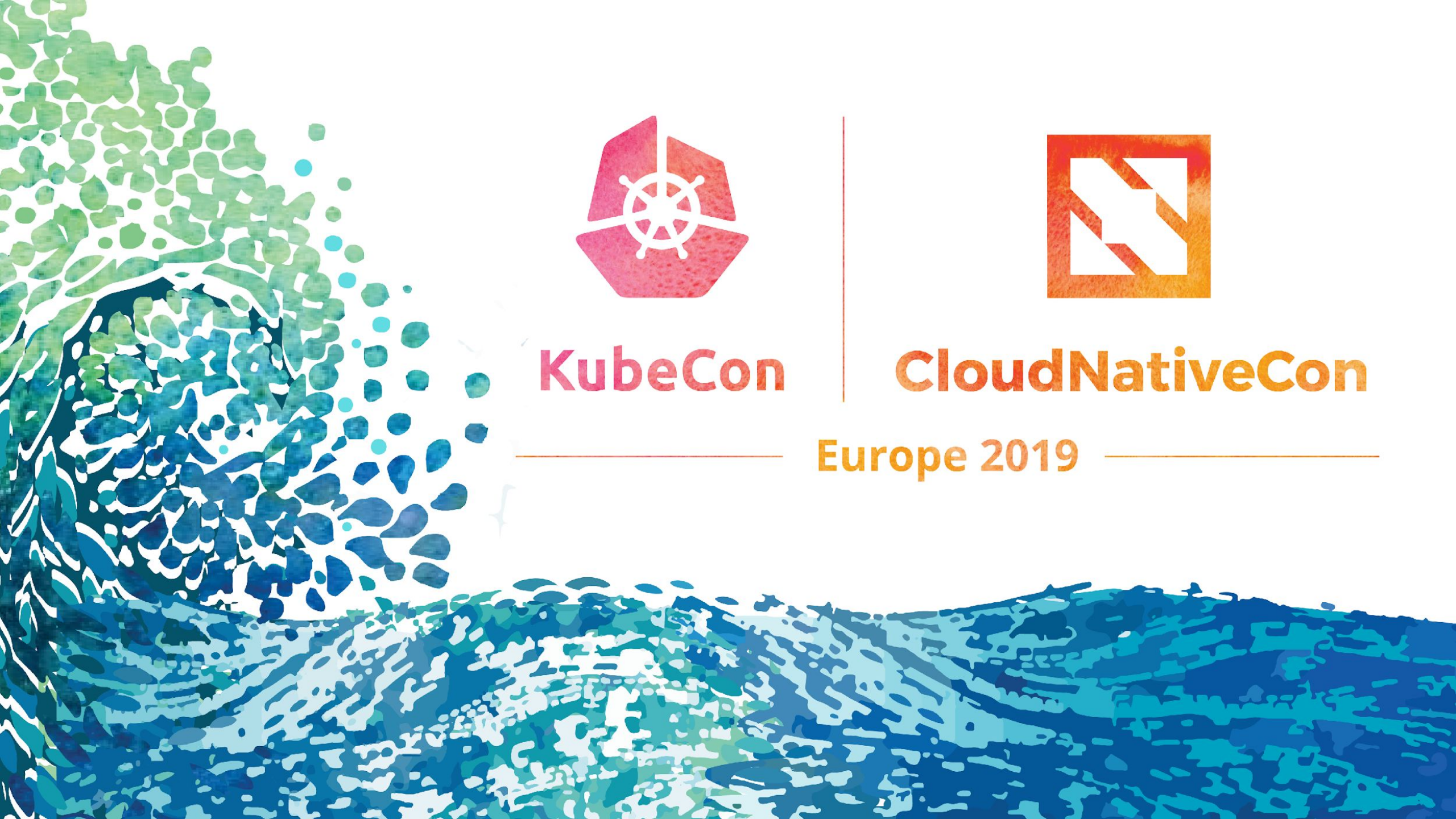

KubeCon
CloudNativeCon
Europe 2019

KubeCon | CloudNativeCon

Europe 2019

Kubernetes the New Research Platform

Bob Killen
University of Michigan

Lindsey Tulloch
Brock University

$ whoami - Lindsey

Lindsey Tulloch

Undergraduate Student at Brock University

Github: @onyiny-ang

Twitter: @9jaLindsey

$ whoami - Bob

Bob Killen

rkillen@umich.edu

Senior Research Cloud Administrator

CNCF Ambassador

Github: @mrbobbytables

Twitter: @mrbobbytables

KubeCon | CloudNativeCon

Europe 2019

Kubernetes the New Research Platform

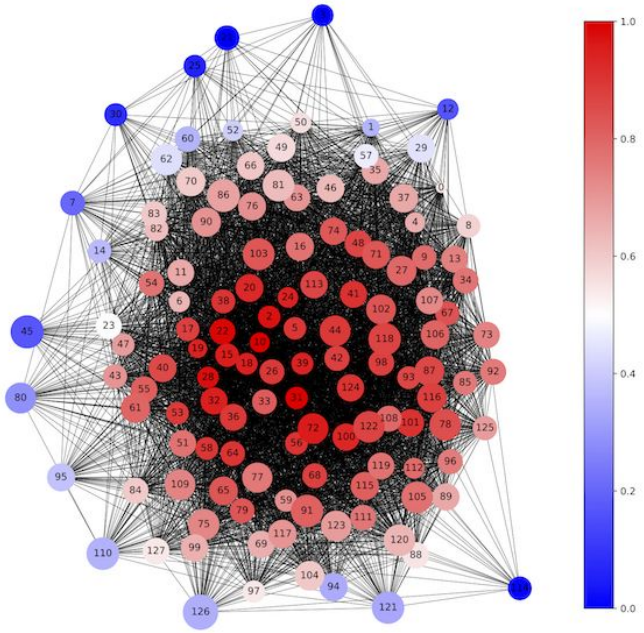
Bob Killen
University of Michigan

Lindsey Tulloch
Brock University

...or a tale of two Research Institutions.

Why?

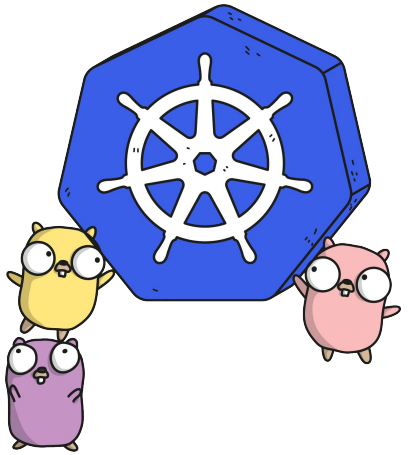
- Increased use of containers...*everywhere*.
- Moving away from strict “job” style workflows.
- Adoption of data-streaming and in-flight processing.
- Greater use of interactive Science Gateways.
- Dependence on other more persistent services.
- Increasing demand for reproducibility.



R. Banerjee et. all - A graph theoretic framework for representation, exploration and analysis on computed states of physical systems

Why Kubernetes?

- Kubernetes has become **the standard** for container orchestration.
- Extremely easy to extend, augment, and integrate with other systems.
- If it works on Kubernetes, it'll work *"anywhere"*.
- No vendor lock-in.
- Very large, active development community.
- Declarative nature aids in improving reproducibility.



- Final Research Project in CS(1 credit)

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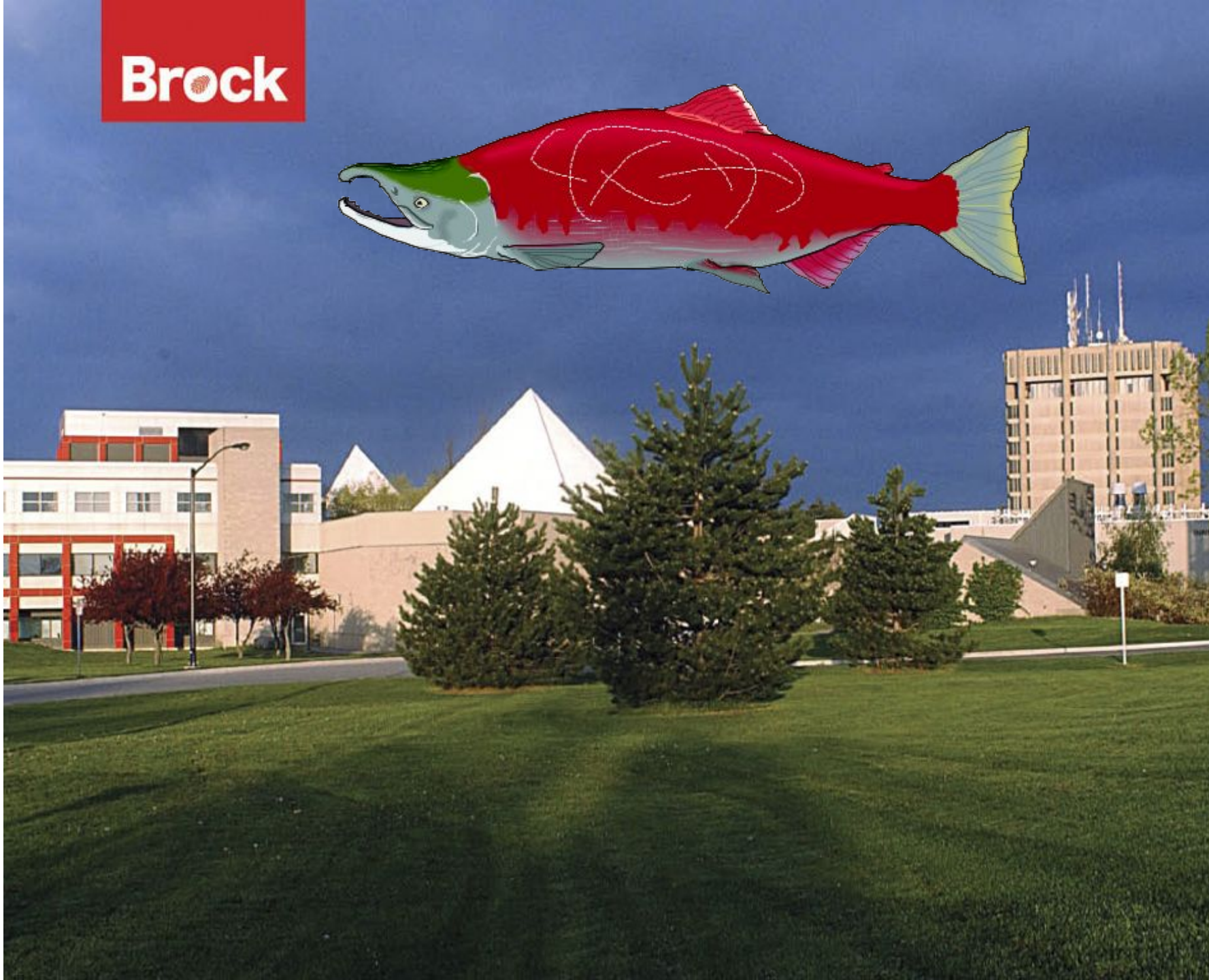
- Bioinformatics



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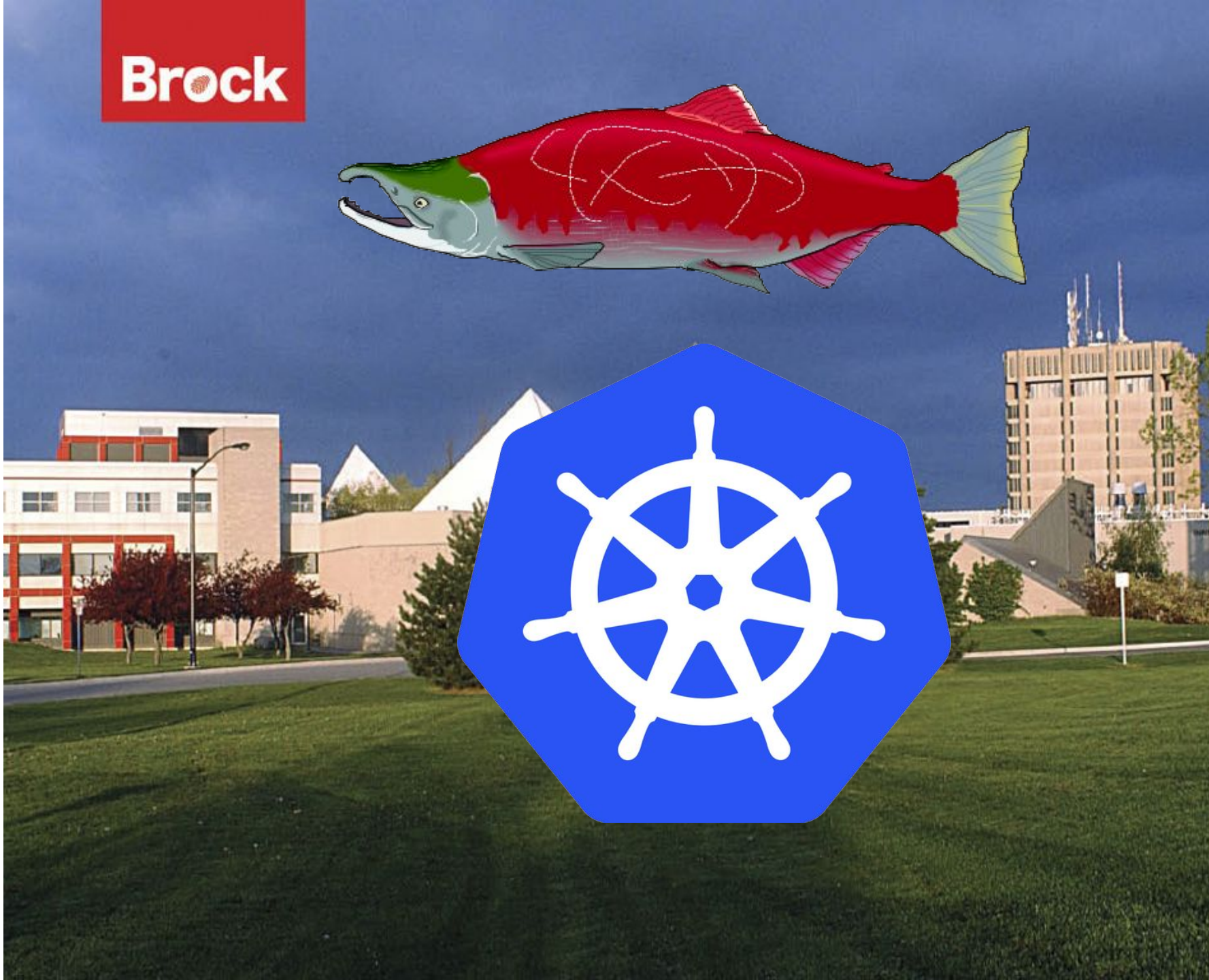
- Bioinformatics
- Kubernetes



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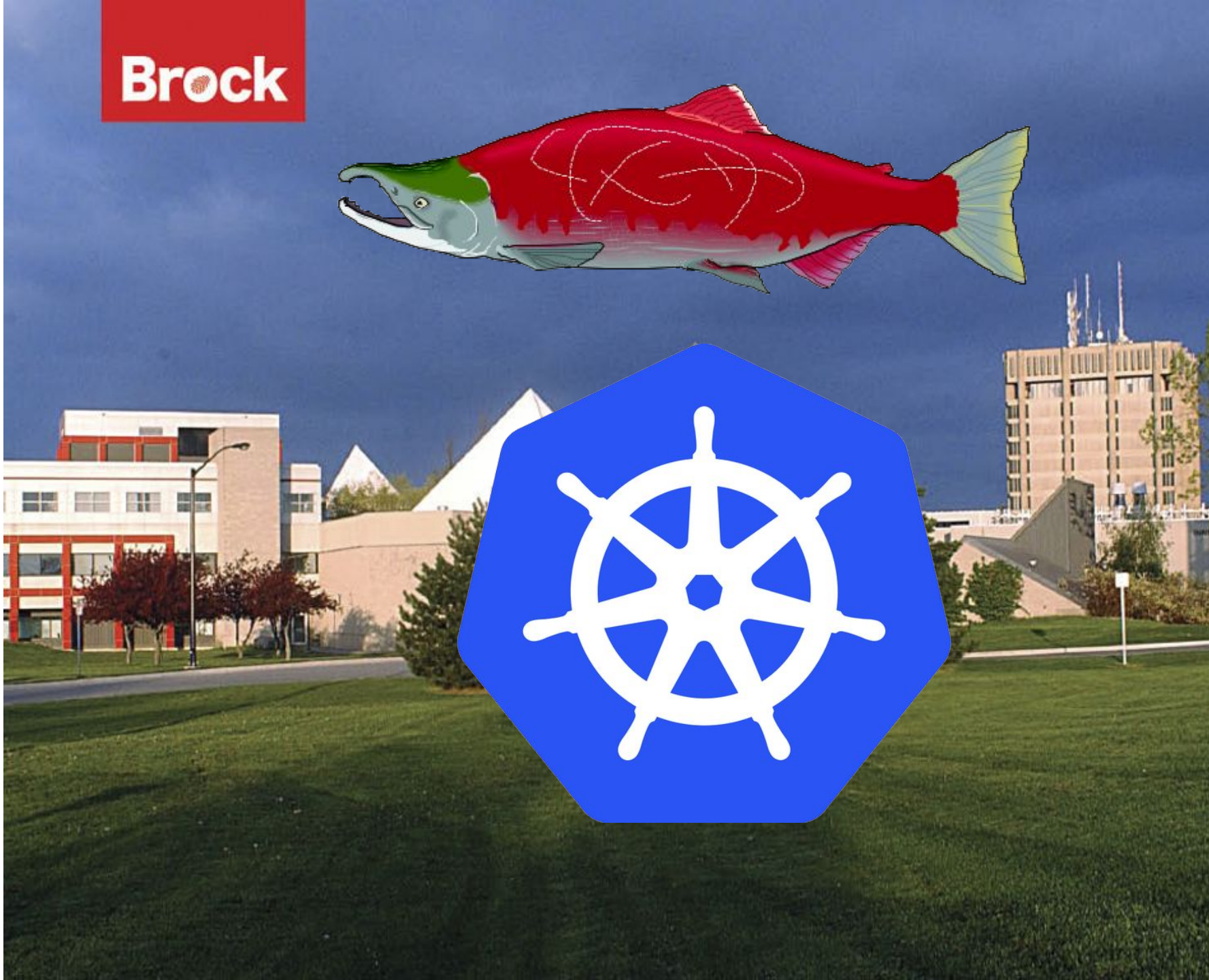
- Kubernetes
- Bioinformatics on Kubernetes!



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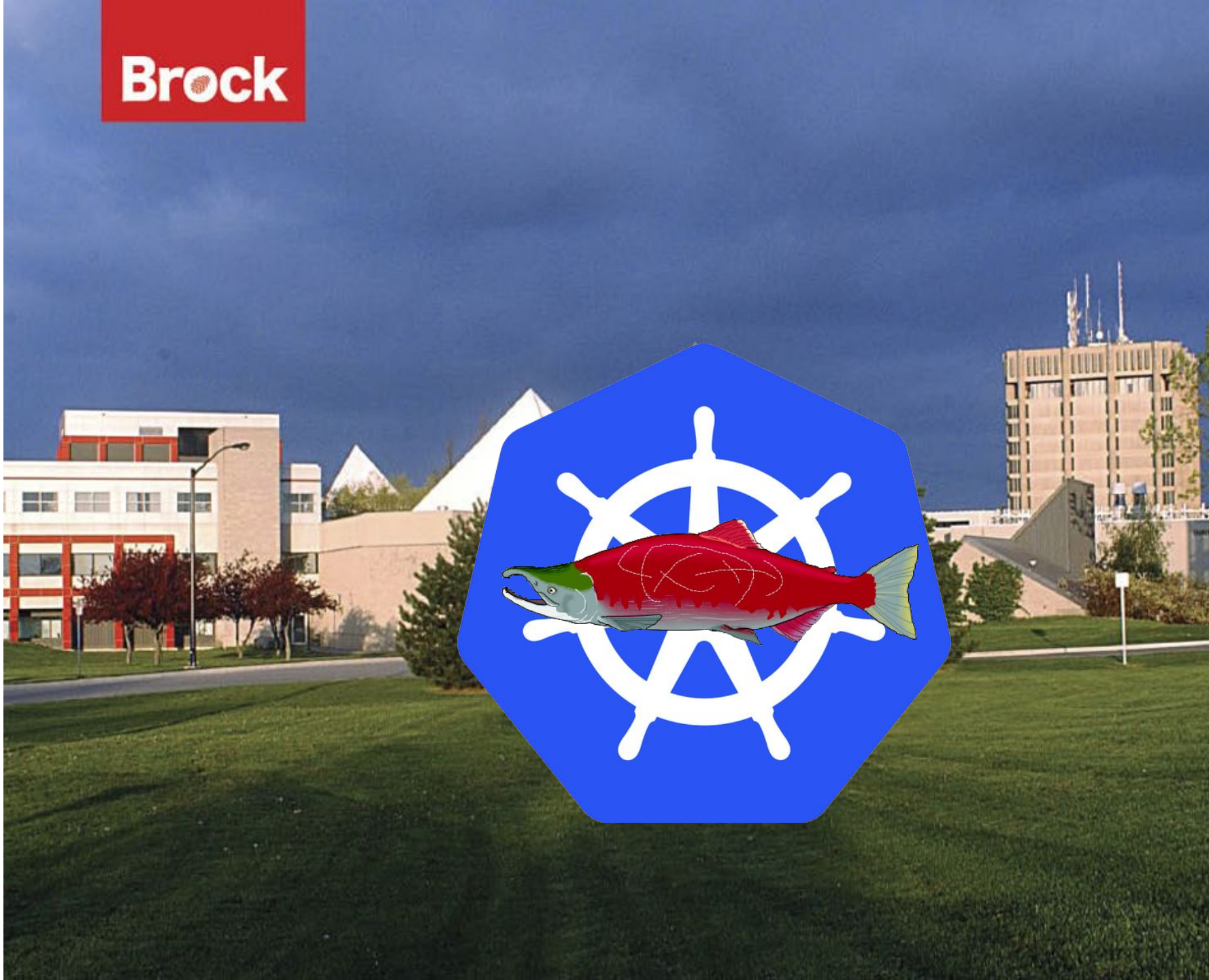

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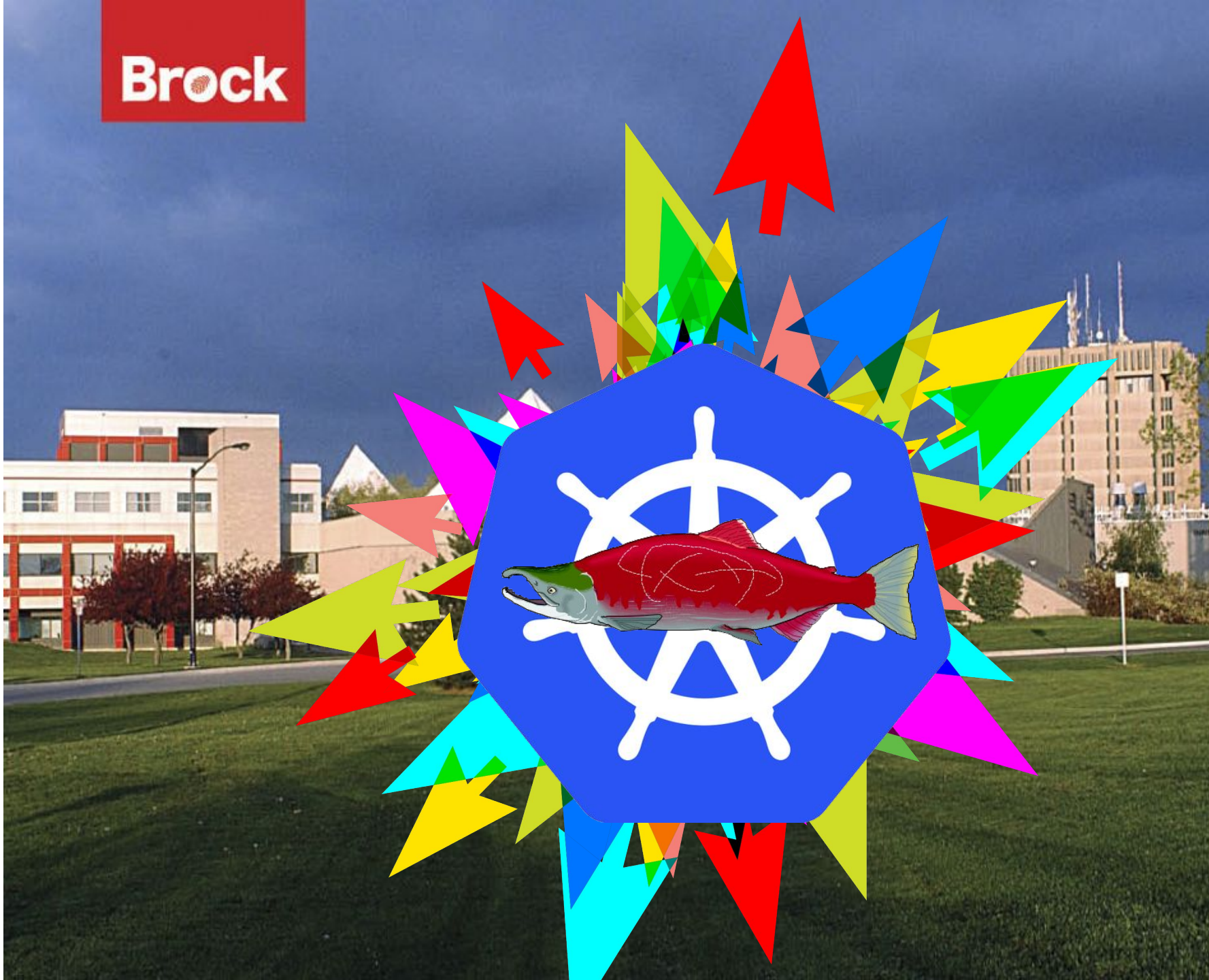
- Kubernetes
- Bioinformatics on Kubernetes!
- on Compute Canada?



Compute Canada

Regional and Government Partners

compute canada | calcul canada

ACENET accelerate discovery

Atlantic Canada Opportunities Agency | Agence de promotion économique du Canada atlantique

Calcul Québec

Québec

Compute • Calcul Ontario

WESTGRID

British Columbia

Government of Saskatchewan

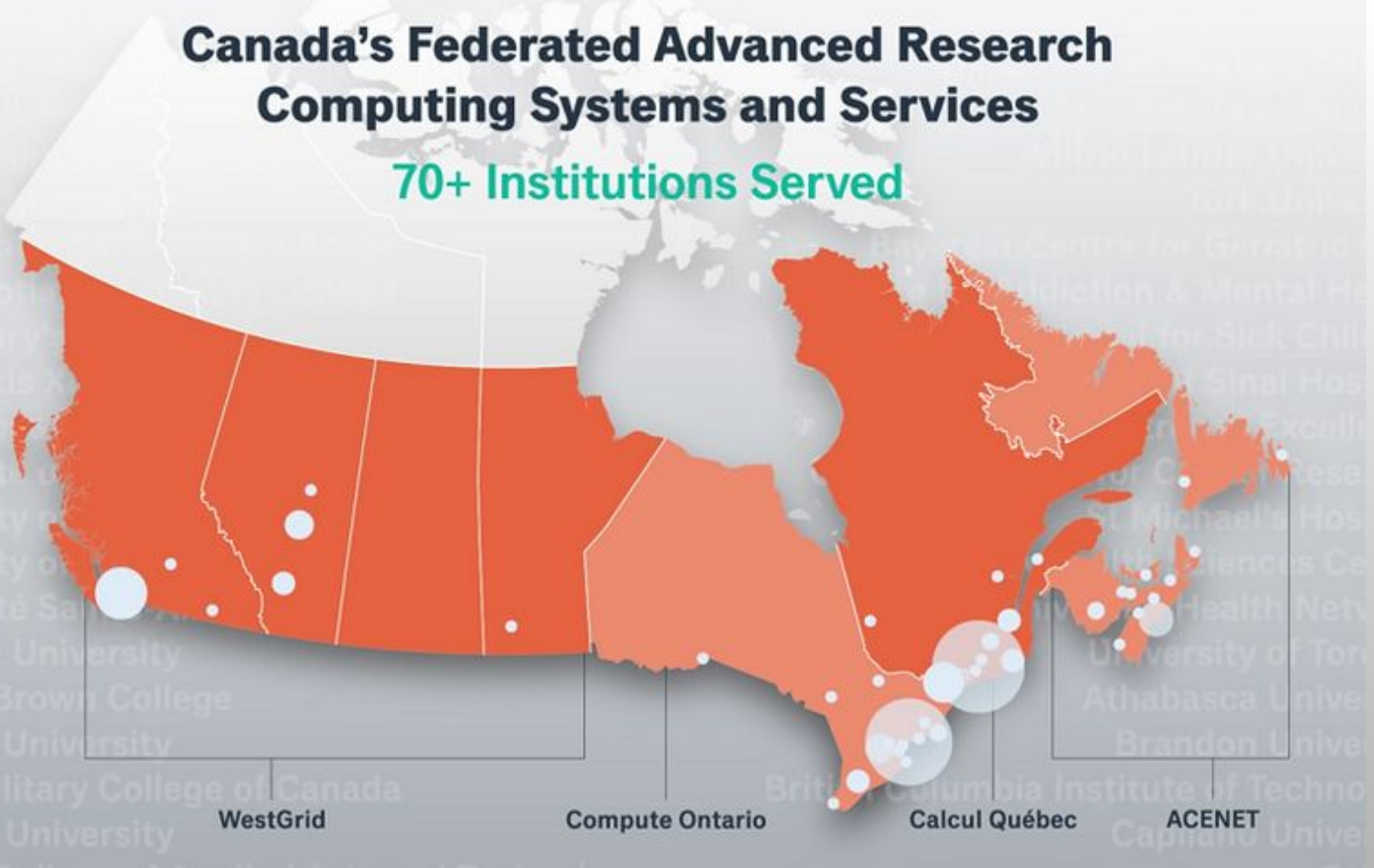
Ontario

Manitoba

Alberta Government

Canada's Federated Advanced Research Computing Systems and Services

70+ Institutions Served



Compute Canada

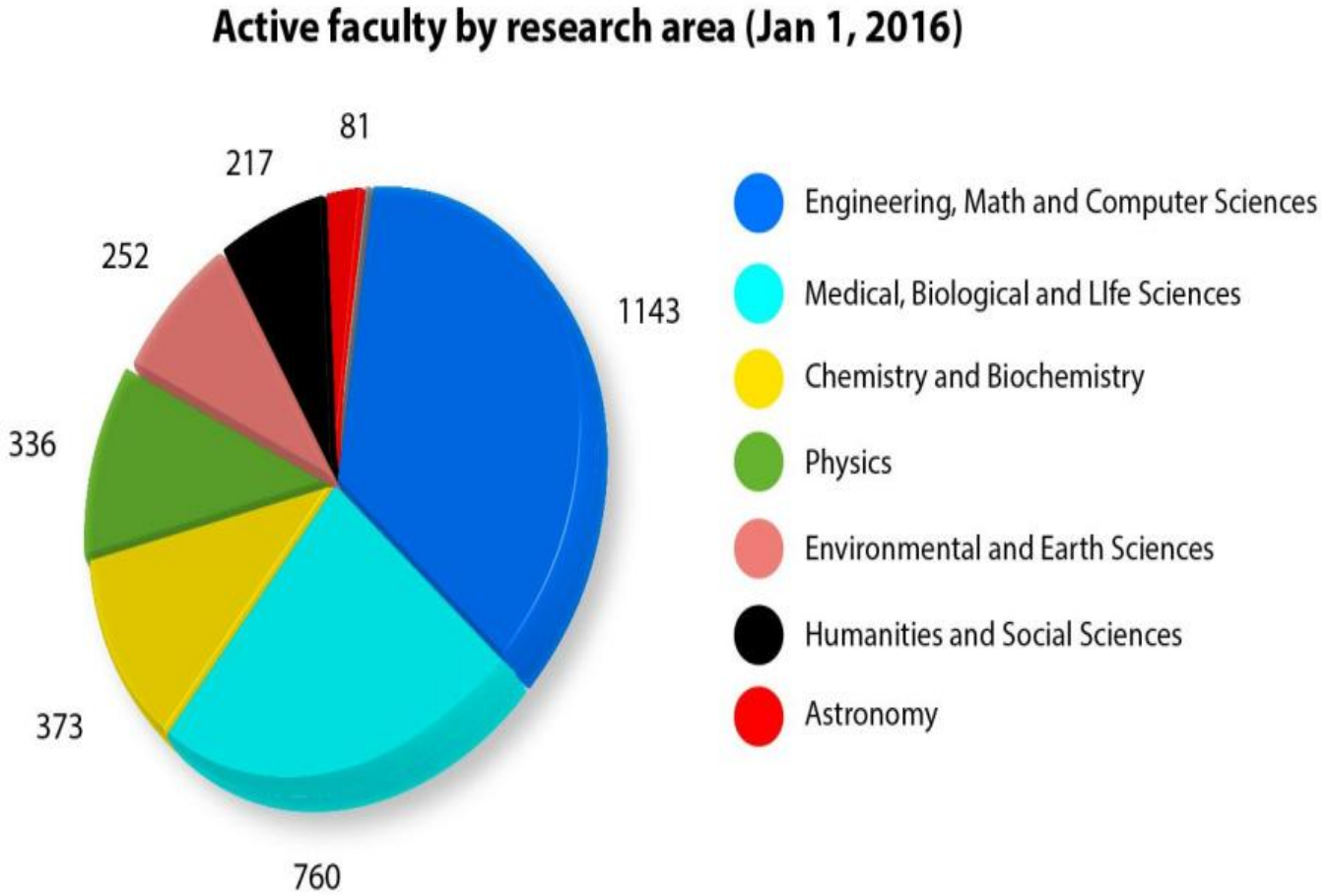
- Not-for-profit corporation

- Membership includes most of Canada's major research universities

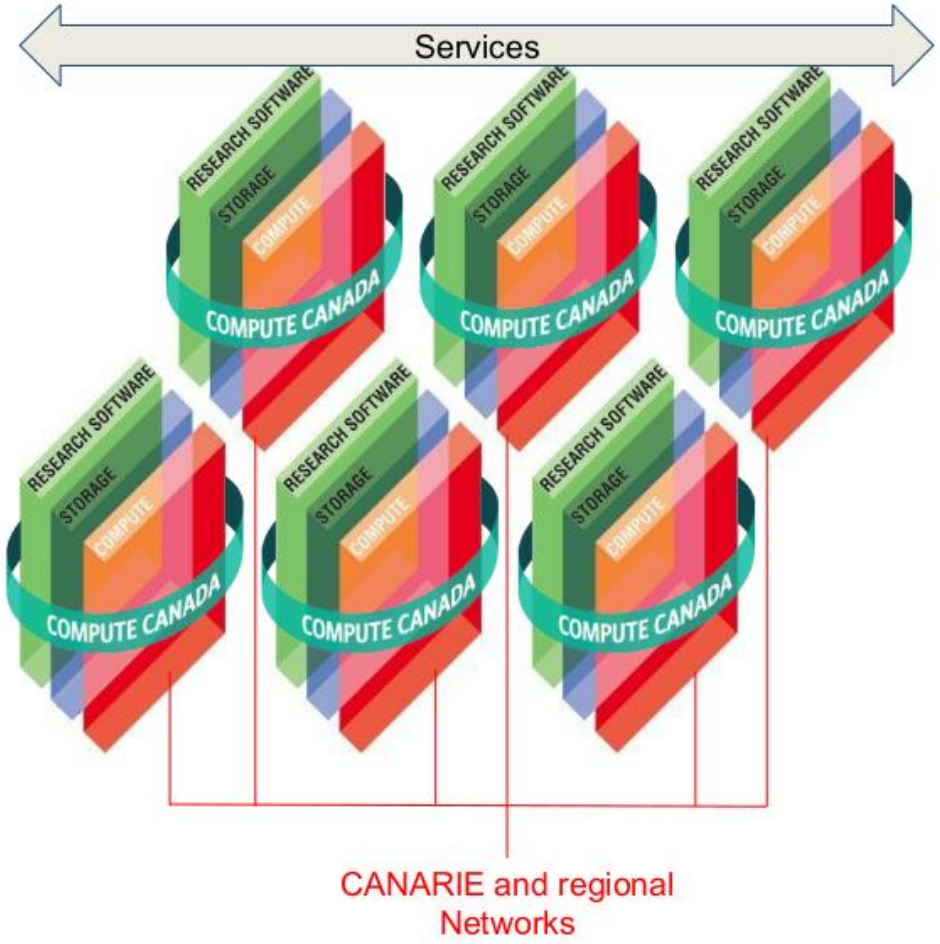
- All Canadian faculty members have access to Compute Canada systems and can sponsor others:
  - students
  - postdocs
  - external collaborators

- No fee for Canadian university faculty

- Reduced fee for federal laboratories and not-for-profit orgs



Compute Canada



- Compute and storage resources, data centres
- Team of ~200 experts in utilization of advanced research computing
- 100s of research software packages
- Cloud compute and storage (openstack, owncloud)

- 5-10 Data Centres
- 300,000 cores
- 12 Pflops, 50+ PB

Compute Canada

Researchers drive innovation

- The CC user base is broadening, bringing a broader set of needs.

- Tremendous interest in services enabling Research Data Management (RDM)

Back to Salmon

KubeCon CloudNativeCon Europe 2019

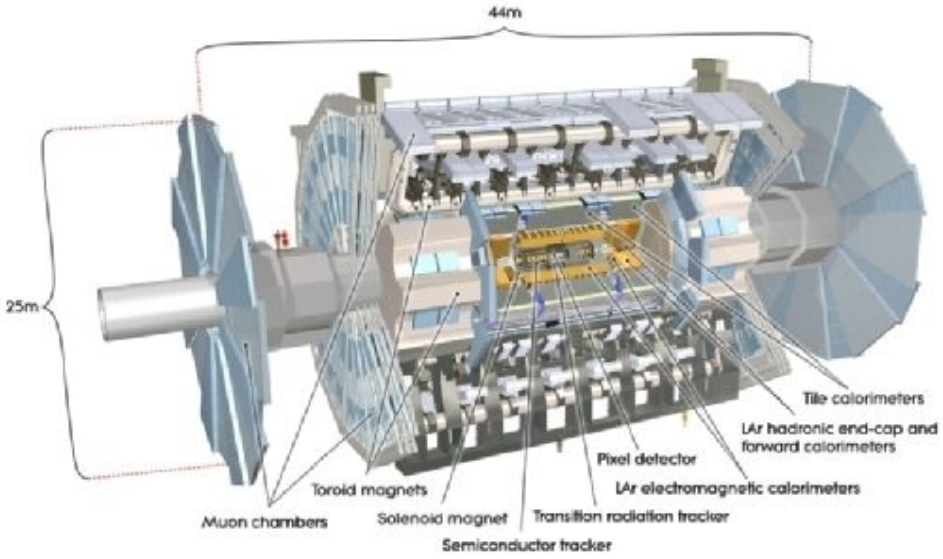
Researchers drive innovation

- No restrictions on researchers ≠ admin privileges
- ~200 experts ≠ ~200 Kubernetes experts
- ≠ 1 Kubernetes expert. . .
- How is this going to work?????

ATLAS Collaboration

compute canada | calcul canada

University of Victoria

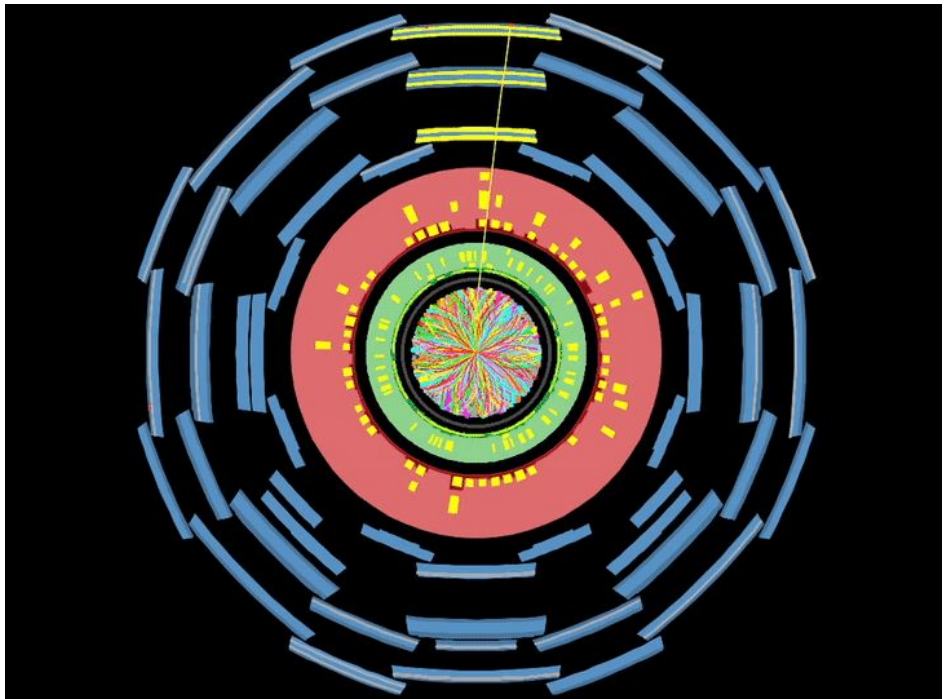


CERN

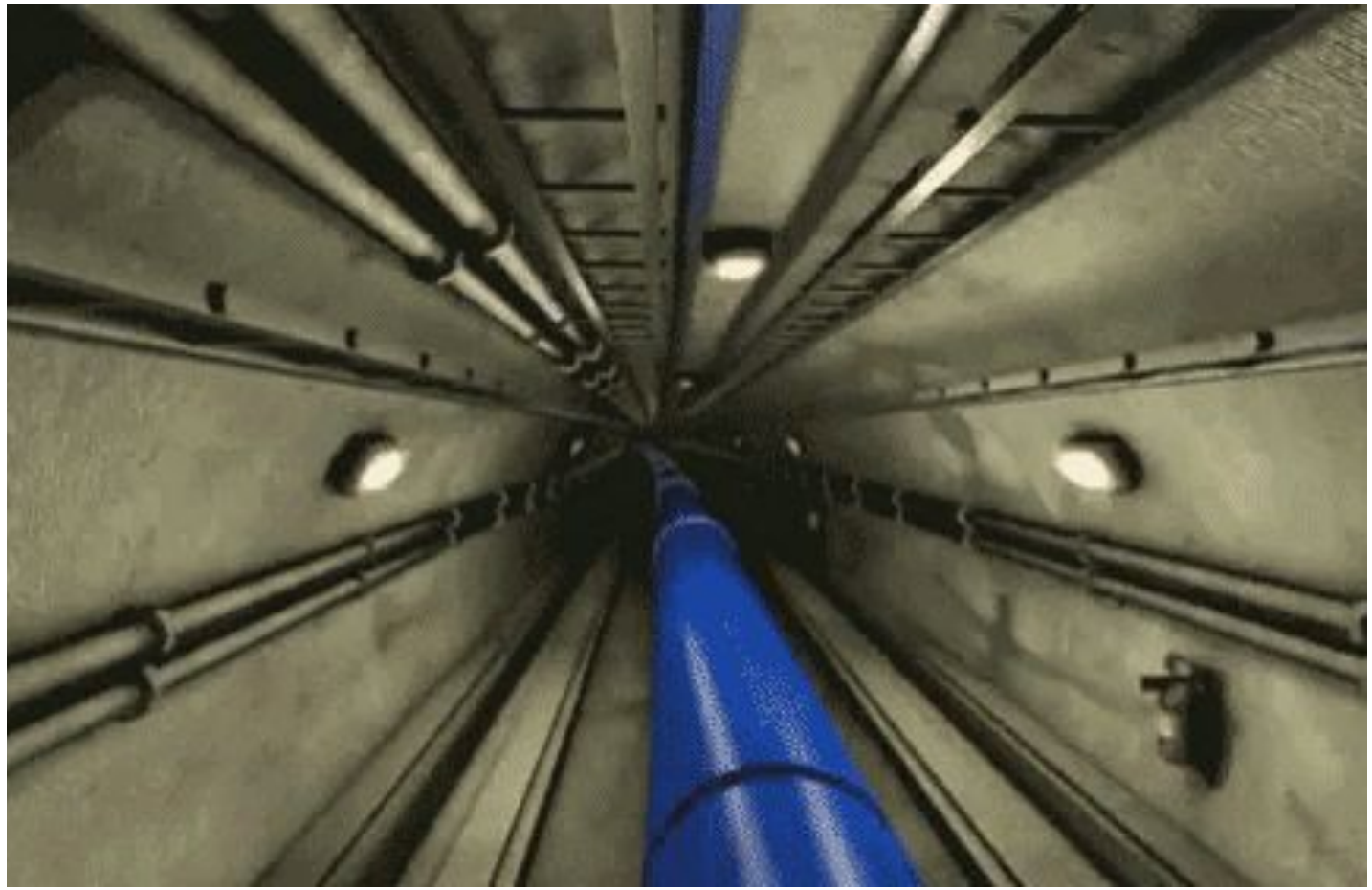
ATLAS Collaboration

What is ATLAS?

- located on the Large Hadron Collider ring
- detects and records the products of proton collisions in the LHC
- The LHC and the ATLAS detector together form the most powerful microscope ever built
- allow scientists to explore:
    - **space and time**
    - **fundamental laws of nature**



ATLAS Collaboration



NBD

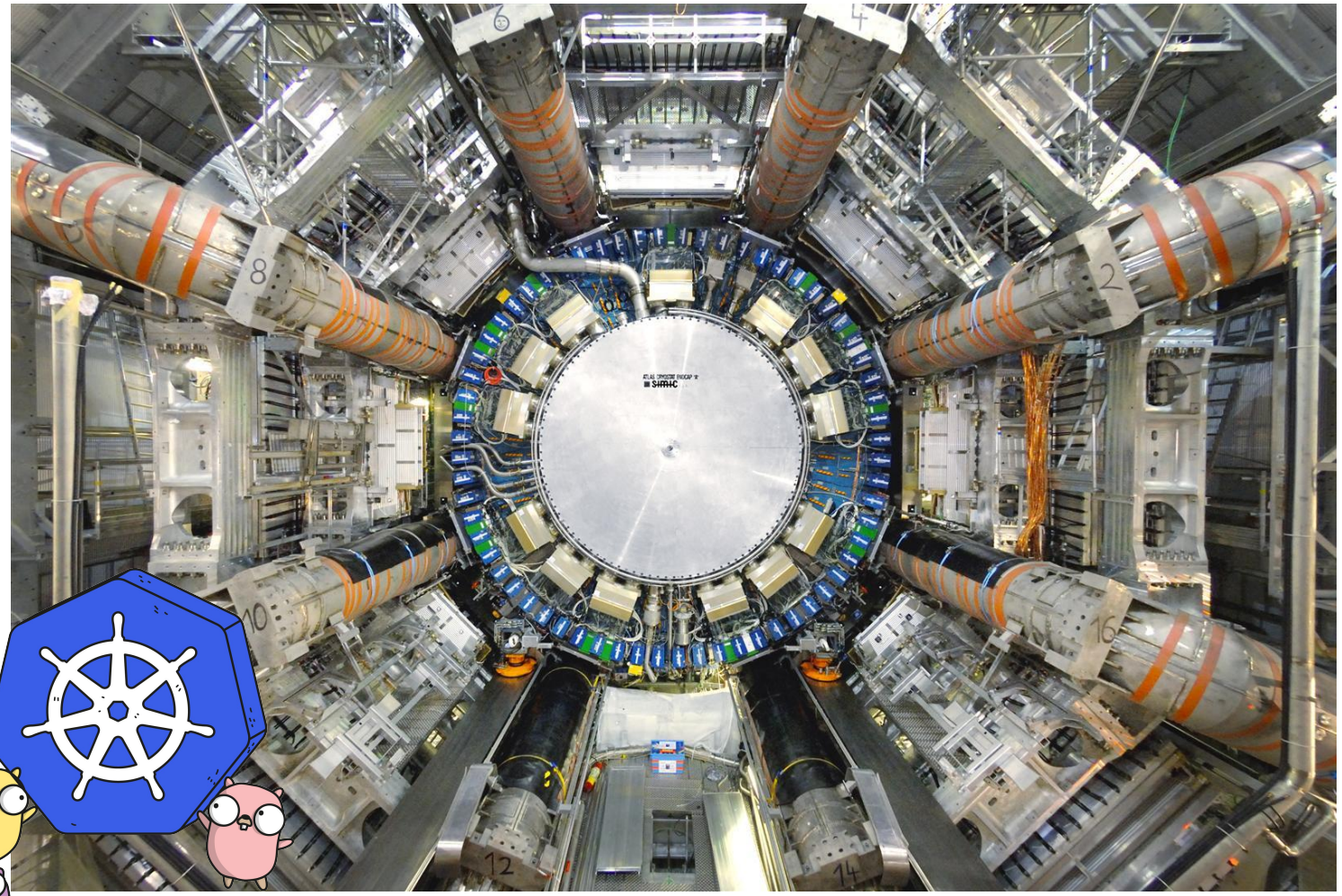
ATLAS Collaboration

- ATLAS produces several peta-bytes of data/year
- Tier 2 computing centers perform final analyses (Canadian Universities like UVic)

  UVic-ATLAS group:

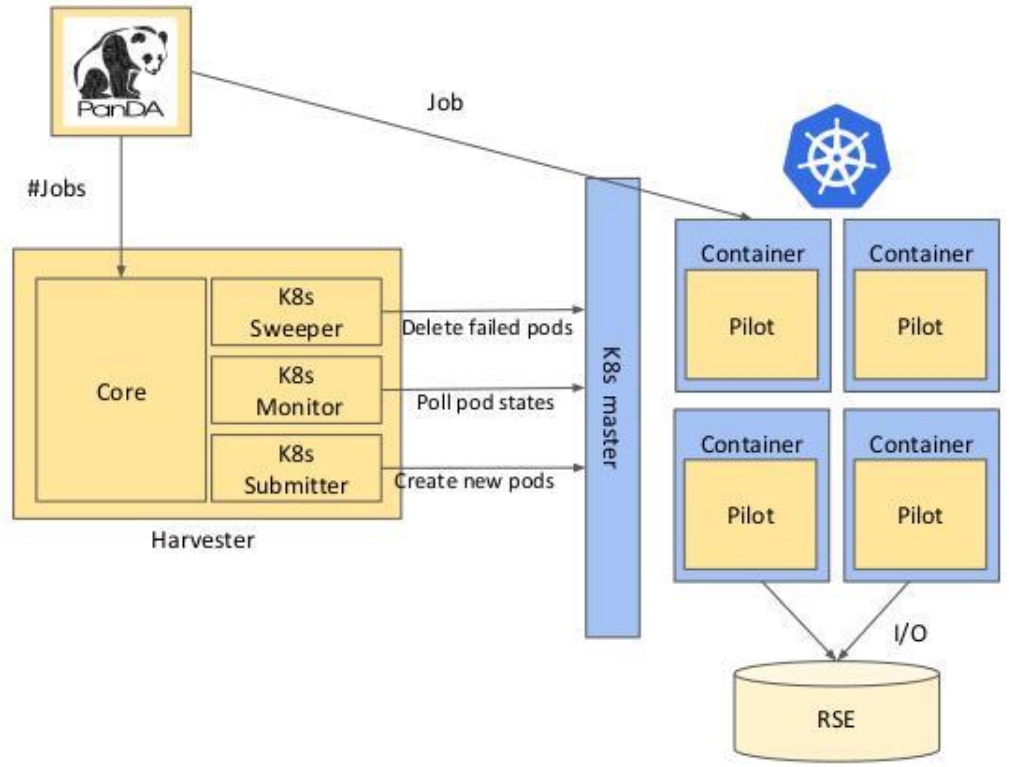
  - 25 scientists (students, research associates, technicians, computer experts, engineers and physics professors)

ATLAS + Kubernetes



Where does Kubernetes fit in?

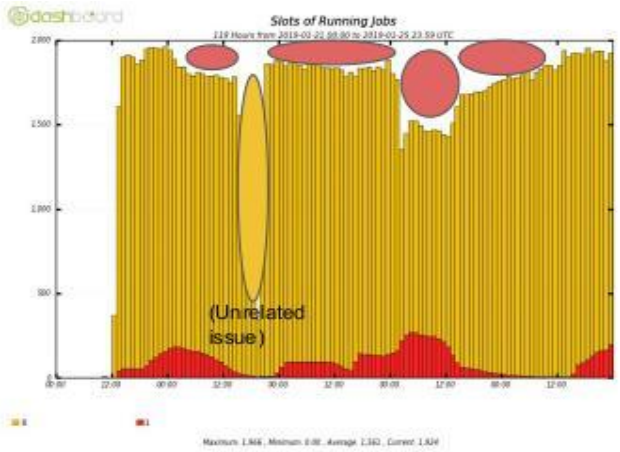
Compute Canada and CERN



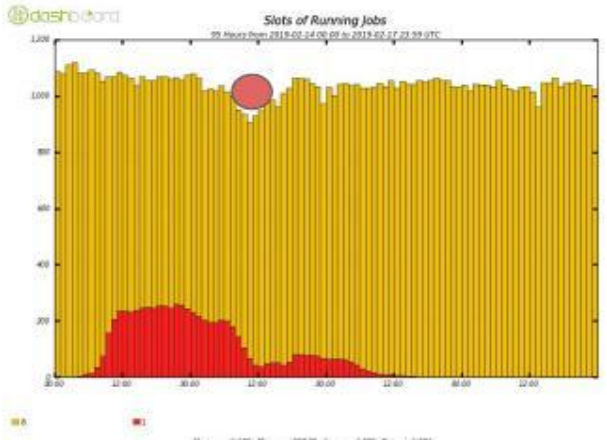
- Use Kubernetes as a batch system
- Based on SLC6 containers and CVMFS-csi driver
- Proxy passed through K8s secret
- Still room for evolution, eg. allow arbitrary container/options execution, maybe split I/O in 1-core container, improve usage of infrastructure
- Tested at scale for some weeks thanks to CERN IT & Ricardo Rocha

FaHiu Lin, Mandy Yang

Compute Canada and CERN



With default K8s Scheduler (round robin load balance)



With policy tuning to pack nodes

- Create your own cluster with certain number of nodes (=VMs)
- Kubernetes orchestrates pods (=containers) on top
- Need custom scheduling
- Need to improve/automate node management with infrastructure people
  - Lost half the nodes during the exercise

FaHiu Lin

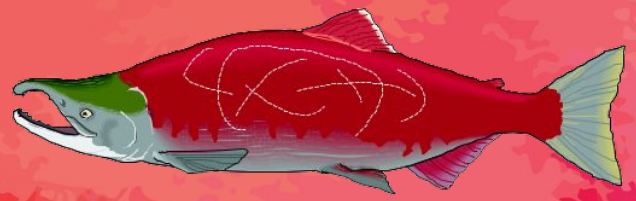
Thanks to Danika MacDonell

Salmon on Kubernetes

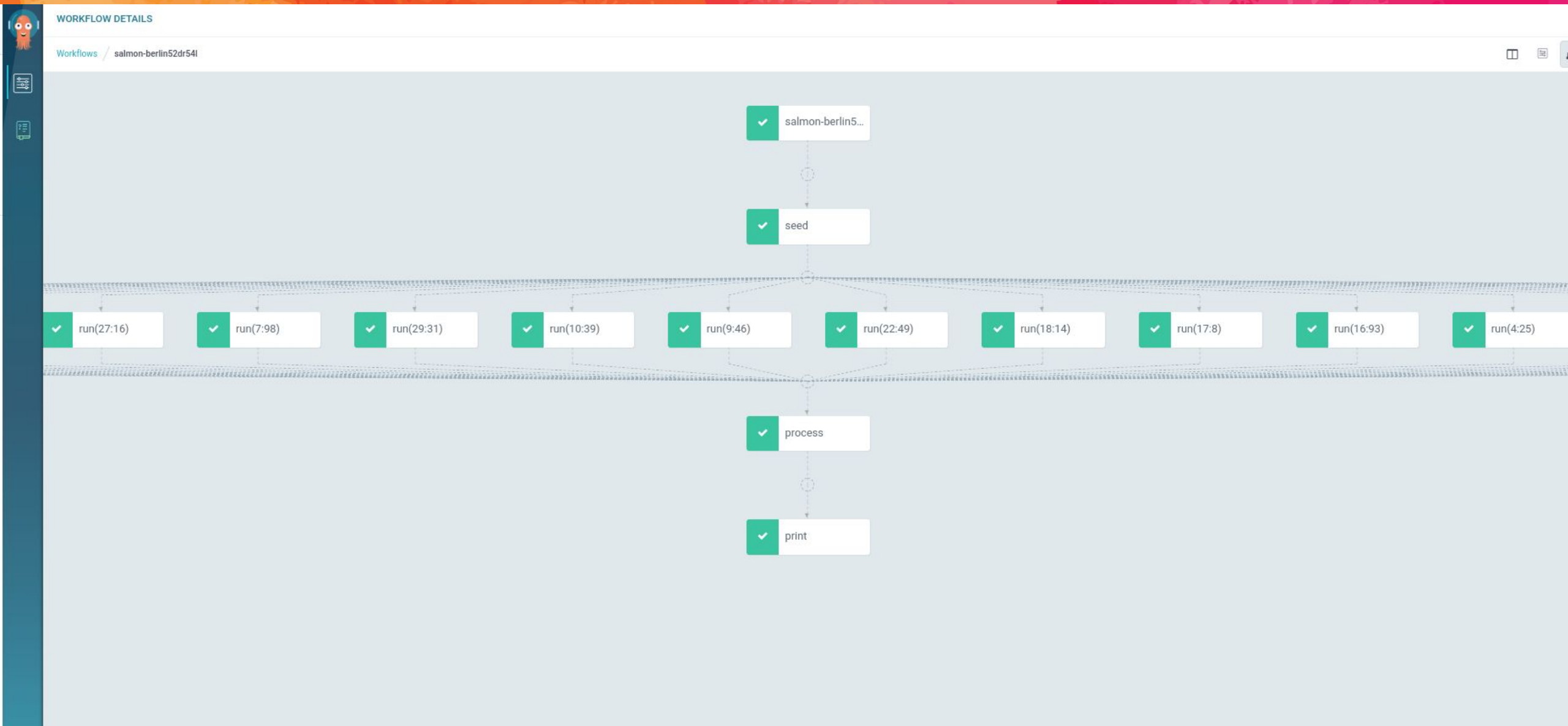
KubeCon CloudNativeCon Europe 2019

- Arbutus Cloud Project Access
  - Openstack
  - Maximum Resource Allocation
    - 5 Instances, 16 VCPUs, 36GB RAM, 5 Volumes, 70GB Volume Storage
    - 5 Floating IPs, 6 Security Groups
- Deploy Kubernetes with Kubespray, Terraform and Ansible
- Containerize the Salmon Algorithm
- Create Argo workflow

Salmon runs



KubeCon CloudNativeCon Europe 2019



Salmon Results

KubeCon CloudNativeCon Europe 2019

```
The length of the best path is 7549.29
It occurred first in generation 67
This program took 27.14 seconds to complete.
The best path is 30 21 0 48 31 44 18 40 7 8 9 42 32 50 10 51 12 13 46 25 26 27 11 24 3 5 14 4 23 47 36 37 39 38 35 34 33 43 45 15 28 49 19 22 29 1 6 41 20 16 2 17
The average of best paths found in 30 runs was: 7832.7970000000005
The seeds used were: [10, 94, 81, 88, 25, 92, 84, 98, 1, 46, 39, 15, 34, 57, 5, 77, 93, 8, 14, 30, 37, 97, 49, 69, 73, 9, 28, 16, 91, 31]
```

run(7:98)

Future of Kubernetes at CC

- Interest from some staff
- CERN seems to be driving Kubernetes innovation
- Other researchers?
  - Learning curve is steep and time is precious (installing Kubernetes on bare metal just to run your workflow is probably not worth it)
  - Lack of expertise with essential tools (yaml, docker, github)

University of Michigan

- 19 school and colleges
- 45,000 students
- 8,000 faculty
- Largest Public Research Institution within the U.S.
- 1.48 billion in annual research expenditures.

ARC-TS

- Advanced Research Computing and Technology Services.
- Streamline the Research Experience.
- Manage **all** computational Research Needs.
- Provide infrastructure and architecture consultation services.

ARC-TS

- Primary Shared HPC Cluster - 27,000 cores.
- Secondary restricted data HPC Cluster.
- Additional clusters with ARM, POWER architectures.
- Data Science (HADOOP + Spark)
- On-prem virtualization services
- Cloud Services.

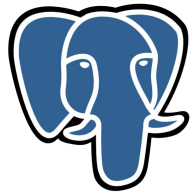
ARC-TS Needs

- Original adoption of Kubernetes spurred by internal needs to easily host and manage internal services.
  - High availability
    - Hosting artifacts and patch mirrors
    - Source repositories
    - Build Systems
  - Minimal overhead
  - Logging & Metrics

Research Needs


No. Really.
Research Needs

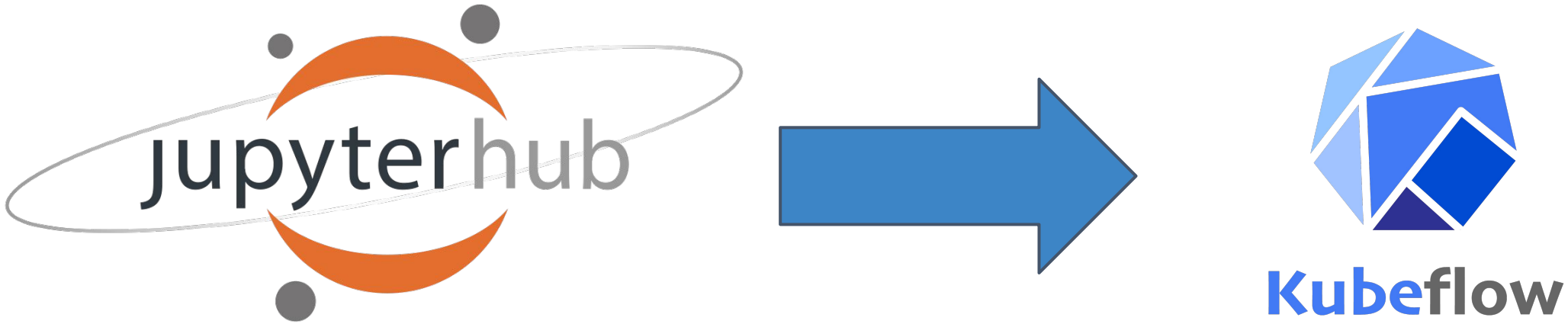
A few services..



PostgreSQL

Airflow

#1 Requested Service.

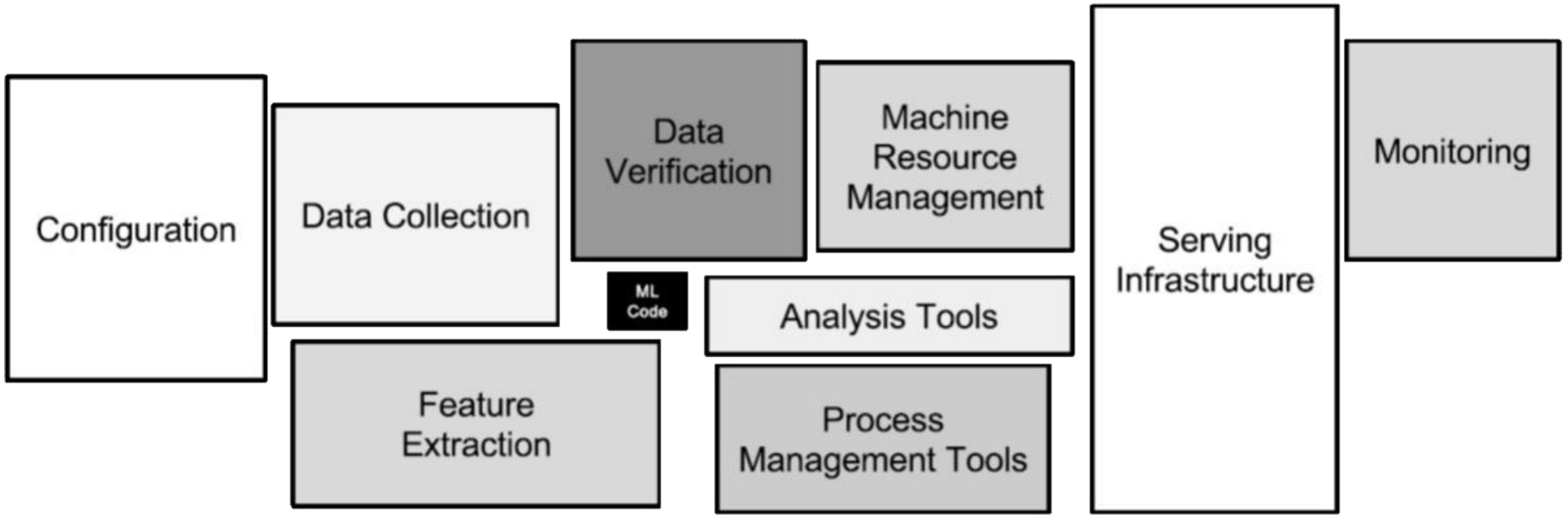


Demand shifting from JupyterHub to Kubeflow.

Why Kubeflow?

- Chainer Training
- Hyperparameter Tuning (Katib)
- Istio Integration (for TF Serving)
- Jupyter Notebooks
- ModelDB
- ksonnet
- MPI Training
- MXNet Training
- Pipelines
- PyTorch Training
- Seldon Serving
- NVIDIA TensorRT Inference Server
- TensorFlow Serving
- TensorFlow Batch Predict
- TensorFlow Training (TFJob)
- PyTorch Serving

The New Research Workflow



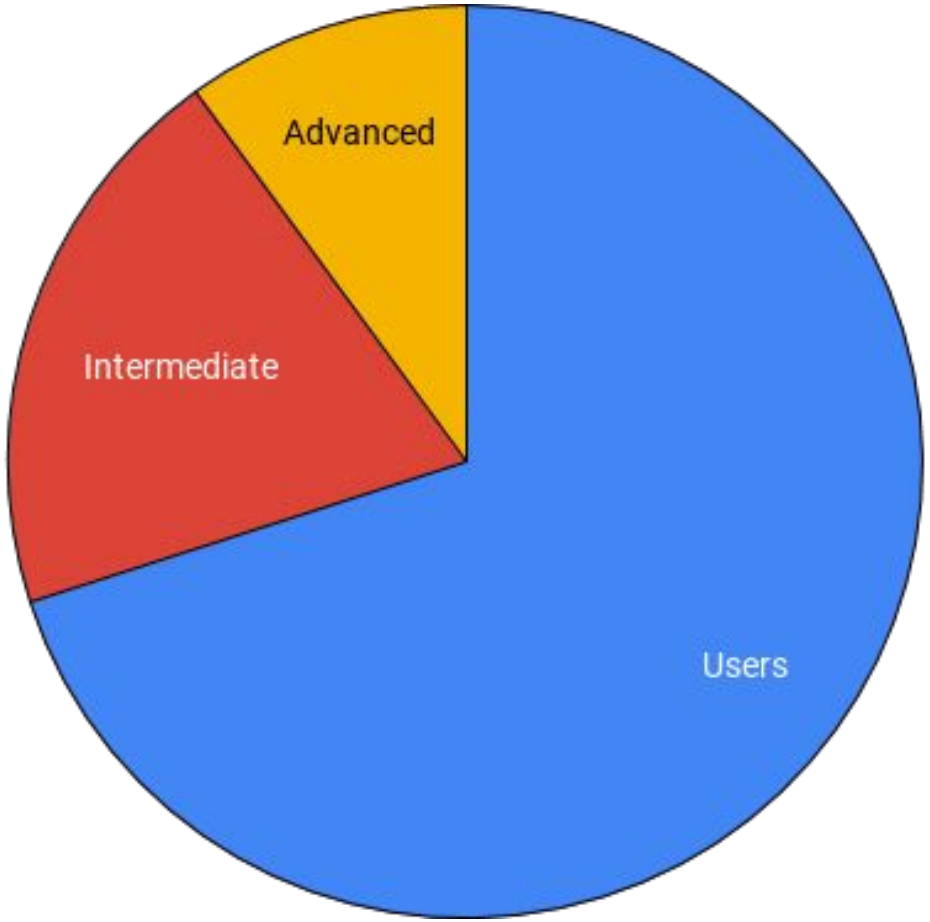
Sculley et al. - Hidden Technical Debt in Machine Learning Systems

Challenges

- Difficult to integrate with classic multi-user posix infrastructure.
    - Translating API level identity to posix identity.
- Installation on-prem/bare-metal is still challenging.
- No “native” concept of job queue or wall time.
    - Up to higher level components to extend and add that functionality.
- Scheduler generally not as expressive as common HPC workload managers such as Slurm or Torque/MOAB.

Current User Distribution

- **General Users - 70% -** Want a consumable endpoint.
- **Intermediate users - 20% -** Want to be able to update their own deployment (Git) and consume results.
- **Advanced users - 10% -** Want direct Kubernetes Access.



Future @ UofM

- Move to Bare Metal.
- Improve integration with institutional infrastructure.
- Investigate Hybrid HPC & Kubernetes.
  - Sylabs SLURM Operator
  - IBM LSF Operator
- Improved Kubernetes Native HPC
  - Kube-batch
  - Volcano

Sylabs.io

IBM Spectrum LSF

Future @ UofM

Outreach and training for both Faculty and Students.

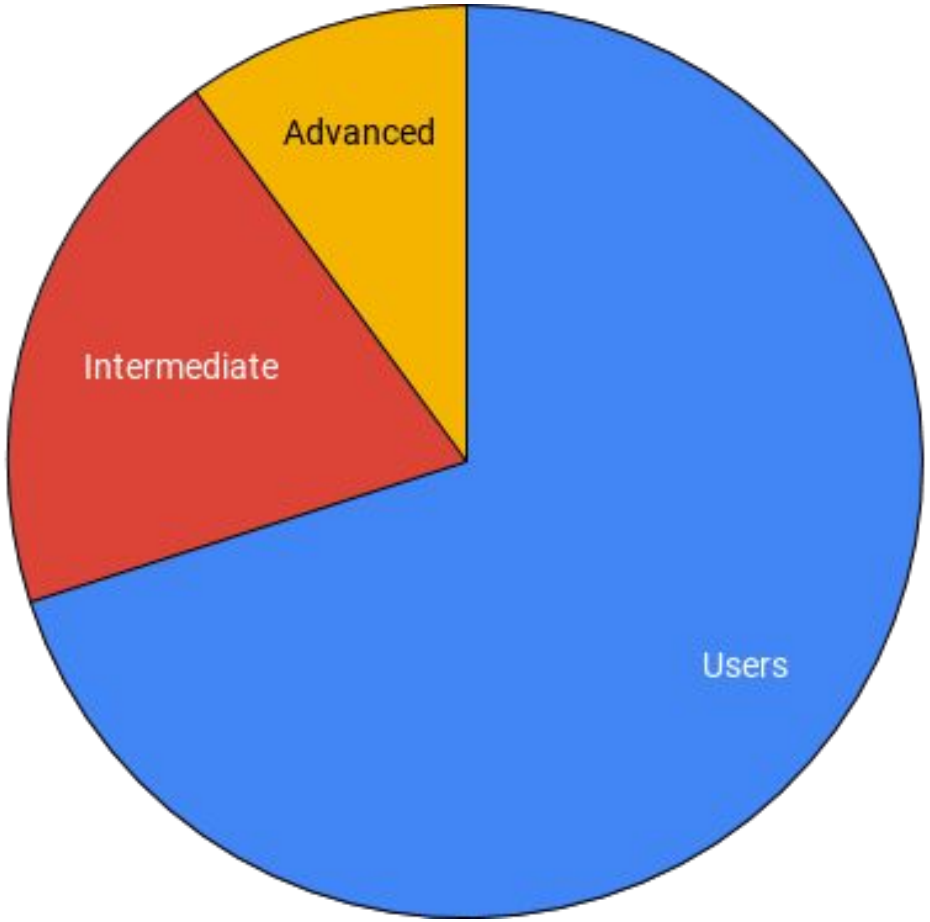
Expected User Distribution

Demand for direct access growing with continued education.

General Users - 70% ↘ 30%

Intermediate - 20% ↗ 40%

Advanced - 10% ↗ 30%



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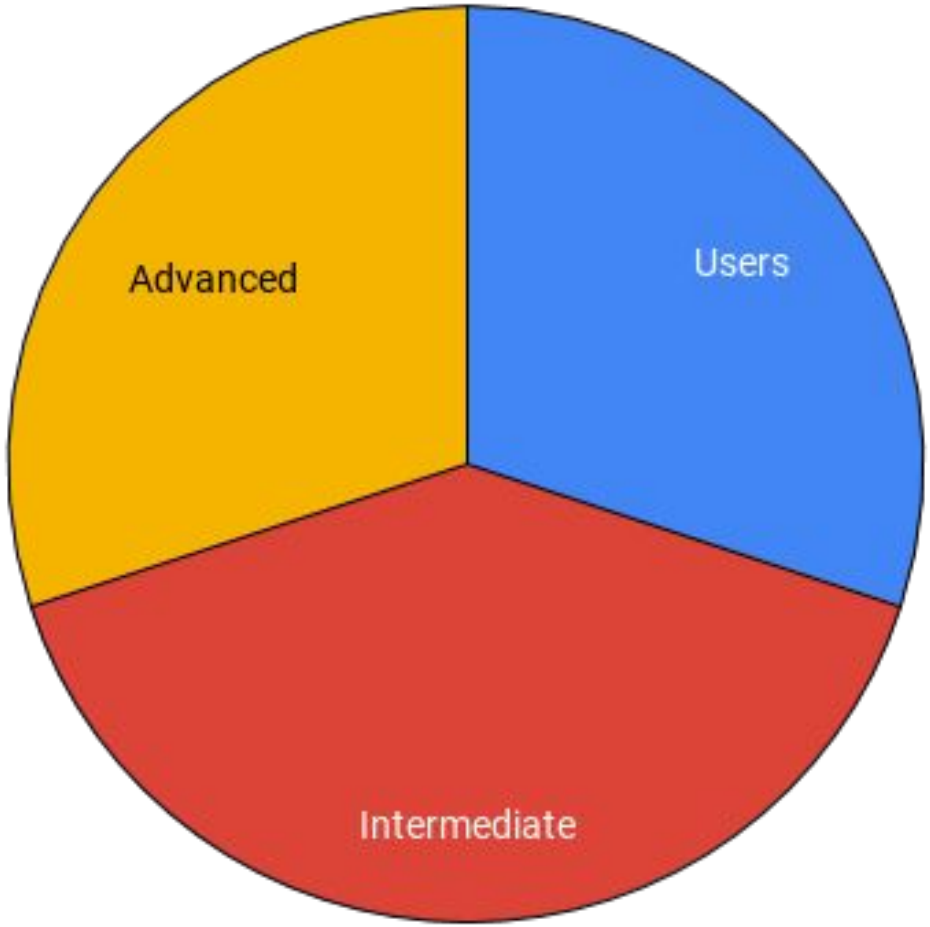
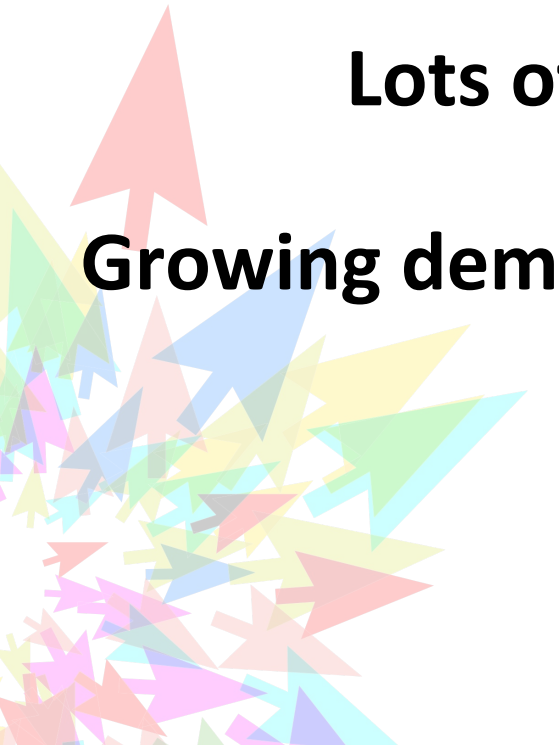


Recap:

Kubernetes is great.

Lots of applications to facilitate research workflows.

Growing demand for research that would benefit from Kubernetes.



Suggestions for increasing Kubernetes Adoption

Providers

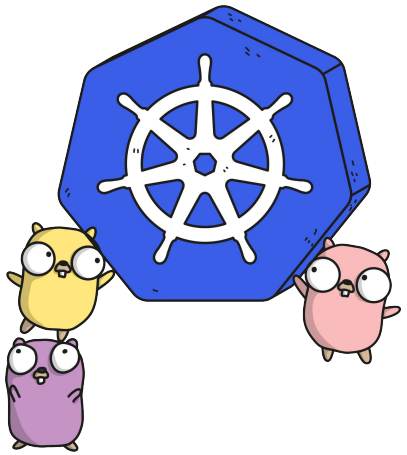
- Offer Kubernetes for people to consume
- Get involved with the Kube community
- Learn as much as you can
- Provide outreach to researchers and anyone that might need to be ramped up

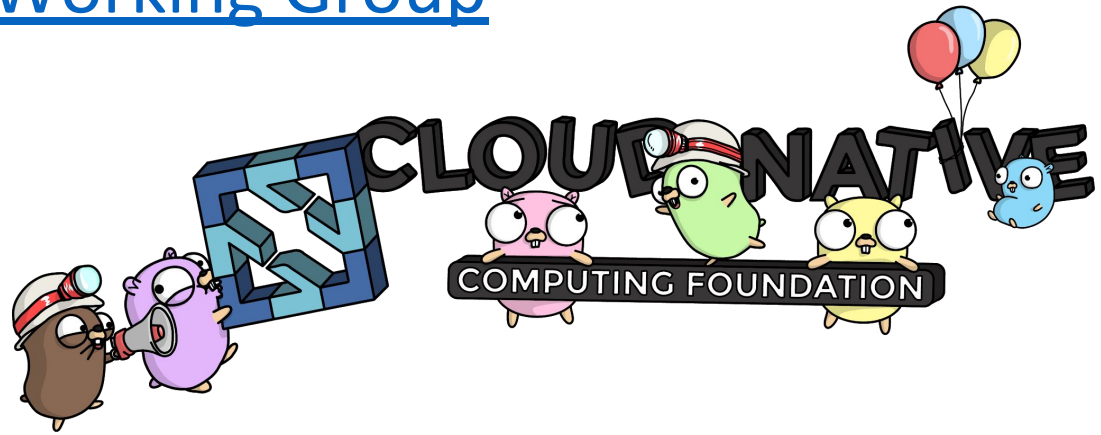
Researchers

- Engage with research institutions
- Get involved with the Kube community
- Learn as much as you can
- Provide outreach to researchers and anyone that might need to be ramped up

Useful Links

- CNCF Academic Mailing List
- CNCF Academic Slack (#academia)
- Batch Jobs Channel (#kubernetes-batch-jobs)
- Kubernetes Big Data User Group
- Kubernetes Machine Learning Working Group





Credits and Thanks

- ATLAS images were sourced from the CERN document server: https://cds.cern.ch/
- VISPA website: https://www.uvic.ca/science/physics/vispa/research/projects/atlas/
- Compute Canada usage information: https://www.computecanada.ca