The Alliance Cloud Connect Pilot

Potential Use Cases

Digital Research Alliance of Canada | Alliance de recherche numérique du Canada

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Selected Representative Use Cases

Scalable Web Portal for Research Teams

Description & User Experience

A research group has developed a platform for managing access to research data. Access to this data is provided as a service to a specific research community. This access is provided through a web portal that provides the research user with a customized and easy-to-use user interface to find, access, analyze, and/or reuse the interoperable data (aka FAIR). User accounts with authentication are often required to manage access to the portal and sometimes to control access to data that has data sharing restrictions.

The data is typically managed in some sort of repository (database, files on disk, object store, etc.) along with metadata that describes important characteristics of the data. The data can be quite large, so having a scalable repository can be important. Although the most common data access pattern to the data in the repository is through the web portal, it is often required to provide direct access to the data repository through a web-based query API. In this manner, researchers can either use the web portal user interface or use the web query API to access data, depending on their requirements and skill level.

The research group needs to manage the above infrastructure (web portal + repository), including managing software deployment (web portal + repository), devops (web portal + repository), and data curation (repository). These services are persistent services (need to be running all the time) with the ability to scale up resources for specific analysis and query tasks desirable in some cases. A range of uptime and performance monitoring of the services offered is beneficial and can be critical for the research group to monitor these services to ensure responsiveness to the end user.

Example(s)

The iReceptor platform (https://gateway.ireceptor.org) is an example of the above use case. iReceptor uses the Arbutus OpenStack cloud platform to manage and provide its web portal and repository infrastructure and uses the Cedar ARC platform for computation.

The iReceptor platform hosts billions of annotated sequences in the AIRR Data Commons (ADC) and uses a “scale-out” model to scale its repositories. When new data is curated into a repository, if existing repositories are “full”, a new repository instance is added. The iReceptor team manages 14 “production” repository instances of this type (e.g. https://covid19-1.ireceptor.org). These instances are all persistent instances (running all the time) and are currently running on the Arbutus cloud. Each repository instance consists of a set of docker images and these docker images are managed using docker compose on each instance.

The iReceptor Gateway is the web portal that coordinates access to the data in the ADC, and is a web application that runs on a single instance in the Arbutus cloud. The web application is deployed automatically when Git push events happen on a specific Git branch (using Git hooks), with unit and feature tests automatically run and the deployment failing if they do not succeed.

When the iReceptor Gateway performs computationally intensive analysis of data, the data is staged to the Cedar ARC platform and analysis jobs are queued and run using a "community account" on Cedar for all jobs submitted by the iReceptor Gateway. iReceptor uses the Tapis project middleware from the Texas Advanced Computing Centre to stage data and manage jobs on Cedar.

Development instances are used for all components. A set of "staging" repository instances are used as mirrors of specific production repositories to curate data without impacting the production instances (efficient data curation and efficient production searches are not compatible). These instances are used by data curators to load new data sets into the repositories. Development instances are used by development team members to develop both the iReceptor Turnkey repository software stack and the iReceptor Gateway software stack.

Development of the iReceptor Turnkey consists of local development on either the database, data curation, or web API service docker images. Once testing is completed code is pushed to the production branch on github. Docker images are then created and pushed to Docker Hub. Any repository can then be updated (with new Docker images) by performing a docker-compose update on the repository instance, which stops the docker images, pulls new docker images if required, and then restarts the software stack. Repositories are NOT deployed automatically, as automatic deployments on databases are risky.

A set of iReceptor Gateway staging instances are run, with automatic deployment driven by pushes to specific Git branches. Moving software into production typically involves local development on a development gateway instance, merging code into the master branch (which deploys the code to the iReceptor Staging Gateway), and after testing is completed and when a production deployment is approved, a pull request to merge into the production branch is made. Once the pull request is accepted and the merge occurs, the platform is automatically deployed to the iReceptor Production Gateway.

Hybrid Environments

i. Interactive Scalable Computing - Jupyter Notebook

Description & User Experience

Researchers access a web-based preconfigured dashboard portal. The portal will allow the researchers to launch remote desktop applications and sessions for interactive work. The portal will also dynamically leverage cluster resources for parallel applications as needed. Popular research software packages and workflows are pre-packaged and available to launch with a single click. Data transfer is drag and drop, with persistent cloud storage.

Small-scale hardware resources are available free of charge (both in community cloud, and commercial cloud), while larger resource requests will be queued, or alternatively will be run on commercial cloud resources, with researchers' acknowledgment and commitment to pay-per-use. Alliance acts as an intermediary between the users and commercial cloud vendors, and will charge the researchers on a monthly or quarterly basis. The platform will have proper budgeting and cost control (etc. instant stop if over budget) measures.

Example(s)

Science workflow cloud management portal. Computer Science grad student leveraging commercial cloud via a GUI-based middleware portal that manages images, launching, scaling and budget controls, allowing the student to have on-demand, immediate access to customized compute resources at scale. The stack could consist of e.g. Ronin for cloud management, with persistent head node running Jupyter notebook for prototyping and for running PostgreSQL database instance. Larger simulations would be submitted to the local SLURM scheduler, to be executed in an auto scaling cluster managed by Ronin.

2i2c/Syzygy: Jupyter Notebooks enable interactive computing by allowing users to meld code, equations, visualizations and exposition in the familiar environment of their browsers. Syzygy of UBC/PIMS has built and operates the largest network of JupyterHubs in the world, delivering notebooks-as-as-service to more than 21,000 people at 18 higher education institutions. It is currently being used by thousands of people every day. Increasingly, data is at the heart of research and teaching. Proficiency in manipulating data, visualizing results, and integrating techniques such as machine learning have become core skills across disciplines, both in academia and beyond. In the Alliance Cloud Connection pilot, the Syzygy platform could be established as a national service, leveraging both community and commercial clouds.

ii. Hybrid Custom Workflow Kubernetes / Container Environment

Description & User Experience

The researcher logs into a web portal providing a community cloud-based, highly customized scientific grid-type computing platform and workflow. Traditionally the sophisticated platform has been running on a community cloud, but an updated version now allows easy extension of compute capacity to the public cloud. Within the allotted credits (available via a separate public cloud management portal), the platform will allow the user to launch compute instances in the public cloud, in particular for burst type time sensitive compute needs. Compute instance and research software setup, and data migration for the public cloud are handled automatically by the platform.

The Alliance acts as an intermediary between the users and commercial cloud vendor(s), and will charge the researchers (or their representative organizations, e.g. CANFAR) on a monthly or quarterly basis. The platform will have proper budgeting and cost control (etc. instant stop if over budget) measures.

Example(s)

Canadian Advanced Network For Astronomical Research's (CANFAR) Science Portal provides a science platform for the analysis and distribution of observational astronomical data.. The platform allows Canadian and international astrophysicists to store, share, and calibrate and analyze very large observational datasets. The platform utilizes customized containers and Kubernetes to provide virtual machines, running primarily on the Alliance community cloud. The Cloud Connect pilot will add seamless public cloud burst capability to the platform. CANFAR would be responsible for allocating the credits and absorbing the potential costs of running its user's jobs on public cloud. CANFAR would be primarily responsible for guardrailing this usage and managing it within the budget they have for this purpose.

iii. On-Prem HPC Cluster with Automatic or User-Initiated/Manual bursting to Public Cloud

Description & User Experience

A user with a resource allocation (a project designated as a research priority) that has significantly underutilized that resource allocation to date submits a job to an on-prem HPC run by an HPC provider (e.g. The Alliance). The on-prem HPC is over-subscribed, with many jobs in the queue (many of them without resource allocations), meaning the job from the user with the resource allocation will wait in the queue a significantly long time. This results in a poor experience for the user and a negative experience around the Alliance HPC Service and its resource allocation process.

Automatic Bursting: In order to better satisfy the research needs of the user with the resource allocation, the scheduler chooses to burst the job into the public cloud. The end user does not necessarily know that this occurred, with the end result being that their job ran more quickly than it would have without the public cloud bursting and the end user being more satisfied with the Alliance HPC service than they would have been without the cloud bursting.

The cost of the public cloud bursting is absorbed by the Alliance as part of its HPC service, the end user does not see a cost. The Alliance has budgeted for both on-prem HPC as well as for public cloud bursting as part of its strategy to meet the HPC needs of the Canadian research community. A cloud bursting budget is provided to both provide added capacity as well as to more effectively meet the needs of the bursty workloads of those users that have resource allocations.

Manual Bursting: Researchers run traditional HPC workloads on a traditional on-prem HPC cluster leveraging a scheduler (e.g. SLURM). When an immediate priority compute need arises, the user chooses a scheduler queue for bursting to the public cloud. The system verifies that the user has credits and sufficient budget for the public cloud compute task, and upon verification will automatically configure and execute the job in the public cloud. After the job finishes, the system will shutdown the public cloud instances, and present the output data and results in the originating file system.

The allotted credits can be managed via a separate public cloud management portal, provided by the Alliance. Compute instance and research software setup, and data migration for the public cloud are handled automatically by the platform. Alliance acts as an intermediary between the users and commercial cloud vendor(s), and will charge the researchers on a monthly or quarterly basis. The platform will have proper budgeting and cost control (etc. instant stop if over budget) measures.

Example(s)

Automatic Bursting: The Alliance runs traditional HPC workloads on a traditional on-prem HPC cluster leveraging a scheduler (e.g. SLURM). These on-prem resources have a fixed scale and do not deal well with bursty workloads. The Alliance strategically allocates budget to public cloud to enhance its on-prem HPC capabilities. The Alliance bursts workloads to the public cloud of its choosing (the user doesn't choose what bursts to cloud, the Alliance does). The cost of bursting to the public cloud is absorbed by the Alliance as part of its HPC service to the research community in Canada.

In this manner, the Alliance can choose which jobs are burst to the public cloud based on criteria of its choosing, such as:

- Jobs are suitable for execution in the cloud, for example jobs that need to move lots of data to run will not be burst into the cloud.

- Jobs that will benefit from certain cloud capabilities such as large memory nodes and specific hardware capabilities (special purpose GPUs, FPGAs etc) will be burst into the cloud.
- Jobs that have resource allocations (a project that has been identified as a scientific priority) that are under utilized but waiting a long time in the queue (bursty workloads) will be burst into the cloud.

This job bursting is transparent (for the most part) to the end user. The end user gets a better experience. The end user doesn't need to worry about costs. The Alliance is better able to provide fit-for-purpose resources to its users. The Alliance is able to manage how much public cloud is used. No user accounts and cost management is required on the cloud platform.

Manual Bursting: This is a subset of the above use case, where one option for the user is to submit a job to a "cloud burst" queue, and if they have a public cloud account and money in the account to cover the cost of their job, the job is burst into the public cloud. This essentially adds another criteria to the bullet list above:

- Jobs that are submitted to a "public cloud" queue from users who have sufficient funds/credits in the Alliance cloud service to cover the costs of running that job.

HPC in the cloud examples using **Magic Castle:**

- On-demand virtual HPC cluster via MC-Hub service
    - Two modes of operation
        1. Single cloud project shared by all users of the hub.
           Single hub, single cloud, single project
           https://mc.computecanada.dev/
        2. Users register their cloud credentials associated with a specific cloud project they own.
           Single hub, multiple cloud, multiple projects
           https://dev.mc.computecanada.dev/
    - Both modes of operation are currently limited to OpenStack because MC-Hub only implements OpenStack quota fetching.
    - JetStream2 uses Magic Castle as its solution virtual Slurm cluster in CACAO
        - https://docs.jetstream-cloud.org/ui/cacao/deployment_magic_castle/
- Research Compute
    - SD4Health private cluster platform for research on sensitive data
        - provider: Calcul Quebec Juno OpenStack Cloud
    - Arbutus HPC cloud cluster
        - provider: WestDRI Arbutus OpenStack Cloud
        - permanent instances:
            - 15 x 56 cores, 240GB RAM
            - 1 x 4 cores, 22GB RAM, 1 V100 8GB VGPU
    - autoscaling instances:
        - 12 x 32 cores, 120GB RAM
        - 10 x 4 cores, 22GB RAM, 1 V100 8GB VGPU
- EESSI CI/CD platform for software deployment on CVMFS

    - provider: AWS
    - autoscaling instances:
        - 8 x AWS Graviton2 16 cores, 32GB RAM (c6g.4xlarge)
        - 4 x AWS Graviton3 16 cores, 32GB RAM (c7g.4xlarge)
        - 8 x Intel Haswell 16 cores, 30 GB RAM (c4.4xlarge)
        - 4 x Intel Skylake 16 cores, 32 GB RAM (c5.4xlarge)
        - 4 x AMD Zen2 16 cores, 32 GB RAM (c5a.4xlarge)
        - 4 x AMD Zen3 16 cores, 32 GB RAM (c6a.4xlarge)
- Machine Learning for Combinatorial Optimization Competition at NeurIPS 2021
    - provider: WestDRI Arbutus OpenStack Cloud
    - References:
        - https://www.ecole.ai/2021/ml4co-competition/

Cloud computing for Specialized HPC Workloads

Description & User Experience

The researcher logs into the public cloud provider's HPC-as-a-service portal for the purpose of running HPC simulations for specialized scenarios where on-prem resources are not sufficient or available. The Alliance research cloud support team has configured the HPCaaS to accommodate the specific use case and research software and hardware stack. The cloud usage credits and budgeting are managed via a separate third party central cloud management system, providing both Alliance staff and the researchers visibility and control over the financials.

Example(s)

Specific use cases could include:

- For improved speed or additional functionality, the researcher needs access to state-of-the-art GPU technology that is not available/provided on-prem.
- Researcher needs access to very large memory and/or high core number servers that are not available on-prem.
- The public cloud provider offers a unique research software stack, visualization tools, or workflow offering. Leveraging public cloud will enable quick time-to-solution and provide overall positive total-cost-of-operations compared to time and cost of building the service offering in-house.
- Researcher has a time-sensitive workload, need for very fast turn-around time, and has the funds to run the workload in the public cloud.

Advanced Technology R&D Access

Description & User Experience

A researcher is interested in testing advanced computing technology (e.g. quantum computing or simulation, RISC architecture, advanced custom AI chips, etc.) that could potentially be applicable for their research. The advanced technology is still in R&D phase and acquiring the infrastructure in-house would be prohibitively expensive. The researcher consults Alliance research computing support that will then direct the researcher to an advanced technology access platform provided by a public cloud provider. The researcher will be supported by Alliance subject matter experts and public cloud provider's specialist teams. The testing phase cloud costs will be covered by the Alliance via public cloud vendor credits.

Example(s)

The quantum computing market is still in a very strong research & development and growth phase until the foreseeable future with multiple, different, and very expensive competing technologies and systems in development. Public cloud-based quantum computing platforms will allow researchers to access and test a variety of quantum computing platforms and technologies.

The Alliance Cloud Connect pilot would not commit to or endorse any particular quantum technology. The Vendor CFP would cast a wide net for interested participants who would provide discounted or complimentary access to their quantum technology in the cloud. Alliance would act as an intermediary and handle the negotiations with the CSVs, usage costs, budgeting and allocation of usage credits.

The roster of advance technology platforms would be offered in the Researcher CFP to interested researchers.

Potential Involved Technologies and Vendors

Multiple commercial cloud providers, each with their own quantum technology stack offering.

There are several different categories of quantum computing devices, and then different technologies inside those categories. Within those technologies there are then different vendors who offer various devices operating at different size-scales, fidelities, error rates, and coherence times. Within this plethora of options, it will be very important to consider what the priority use cases of the research community in Canada is for quantum devices, and what options are already available to the community via other initiatives. The following section will detail cloud quantum computing options available from several different vendors, which cross the different quantum computing categories and technologies.

Quantum Annealing

Quantum annealing is a class of quantum computing more limited than the more popular gate-based quantum computing, but has shown to be a more readily applicable technology in select use cases. The strength of quantum annealing is in optimization, for example finding a global minimum of a function that may contain many local minima. The famous travelling salesman problem fits into this category. However, the same does not apply to all quantum algorithms, for example, Shor's algorithm cannot be done on a quantum annealing device. Quantum annealing is not plagued by many of the issues facing gate-based quantum computing as it is faster (making decoherence less of an issue) and does not suffer from the same error challenges. Recent advances include:

Bioinformatics: https://www.nature.com/articles/s41598-021-88321-5
Materials Science:
https://journals.aps.org/prxquantum/abstract/10.1103/PRXQuantum.1.020320
Pharmaceuticals: https://www.nature.com/articles/d43747-023-00021-3

Dwave - Superconducting Qubits
A Canadian company, DWave is the main North American vendor for quantum annealing devices, and their system is available in the cloud. Furthermore, they were the vendor included in the quantum initiative funded by ISED as part of the Alliance MYFP. That program was launched by QAI this past fall and has provided training and access to the DWave Leap system, their quantum annealing cloud system, which includes the infrastructure for hybrid classical-quantum computing. Through it, DWave claims to be able to support optimization models with up to 1 million variables and 100,000 constraints.

Gate-Based Quantum Computing
Gate-based quantum computing is the more well-known of the two paradigms, and relies on the execution of quantum circuits made up of a series of quantum-gates. One can think of the gates being like steps or operations in the calculation. Some well known quantum gate examples include Hadamard, CNOT, and different axis rotations. The long sought holy grail of quantum computing has been a fault-tolerant, scalable, universal quantum computer. Universal means that the system can run any quantum algorithm. This is guaranteed for computers that can run any combination of quantum gates (up to the limit where the state decoheres of course). At this point, all universal quantum computers are gate-based, but not all gate-based systems are universal. Fault-tolerant means that errors incurred during the execution of the circuit can be corrected, enabling confidence that the results can be clearly distinguished from the system noise. Scalable indicates that the number of qubits can be increased orders of magnitude while maintaining the required connectivity, maintaining a reasonable coherence length (this is what limits how big a quantum circuit can be), and not exponentially increasing the system noise.

Xanadu - Squeezed-state Photonic Qubits (their technology isn't the most ready at this point, their strength at this point is their software, which is excellent, but they are a vendor to watch. They are available on Amazon Braket).

Photonic - Universal Photonic Qubits, to be made available on Azure soon.

PASQAL - Neutral Atoms

IONQ - Trapped-Ions

MonarQ - Superconducting Qubits

IBM - Superconducting Qubits

Training

Description & User Experience

A researcher is interested in learning how to use Linux-based HPC clusters for scientific computing and signs up for a hands-on training course or workshop conducted by Alliance affiliate organization. At the start of the course, each participant will get unique temporary login credentials for accessing a custom-built on-demand HPC cluster. The researcher can access the HPC cluster from their local workstation using commonly available free or built-in tools. Once logged in to the cluster, the researcher will have access to a fully functional HPC computing environment, leveraging the standard command-line-interface (CLI) and job scheduler for operating in the environment. The end-user does not need to be aware of the details of the cloud backend infrastructure, or whether the computing is done on-prem or in public cloud.

A lecturer requires on-demand access to configurable and scalable HPC cluster for teaching and training purposes. The course sizes can range from a dozen to even hundreds of students. Since the on-prem HPC cluster and community cloud services are heavily utilized with potentially long wait times, leveraging on-demand public clouds for teaching how is a viable option since launching a traditional HPC cluster in the public cloud for limited-time training needs allows for immediate access to needed compute resources. The HPC cluster in the cloud service is configured so that it closely resembles the on-prem HPC cluster. Alliance training services will support the lecturer in setting up and configuring the cluster, and Alliance-provided credits will cover any potential public cloud costs.

Example(s)

Customized on-demand HPC Linux cluster environments for teaching and training:

- Alliance's regional partners' training (community cloud, Arbutus or Beluga)
    - Calcul Québec's entire 2023-2024 training program and spring school use Magic Castle as their hands-on exercise platform
    - WestDRI's 2023-2024 training program uses Magic Castle as their hands-on exercise platform (over 20 courses).
    - University of Alberta uses it for its semestrial bootcamp (spring, fall, and winter).

    - ACENET uses Magic Castle for its summer school, regular workshops, as a support training tool for external organizations’ workshops (i.e.: Institute for Comparative Genomics).
    - Compute Ontario …
- Calcul Québec offering virtual cluster for graduate courses in AI and HPC
    - UL GLO-7030: Apprentissage par réseaux de neurones profonds
    - UQAC 8INF919: Apprentissage automatique pour les données massives
    - Concordia PSYC 458: Behavioural Neuroscience Advanced Issues
    - UQAM INF5171: Programmation concurrente et parallèle
    - McGill BIOC 600:Advanced Strategies in Genetics and Genomics
- Magic Castle as a platform for teaching Magic Castle at SC23
    - Tutorial taught using cloud credits from AWS
- U Sherbrooke’s International Summer School on Computational Quantum Materials 2022 used Magic Castle for various training needs during the school, including: batch computing with MPI, Jupyter notebook, and virtual desktops. (community cloud, Beluga)