Re-Thinking Experiments

Accelerating Research through Reproducible Experiments at Scale

Vivek Katial

09/12/2019

Slides

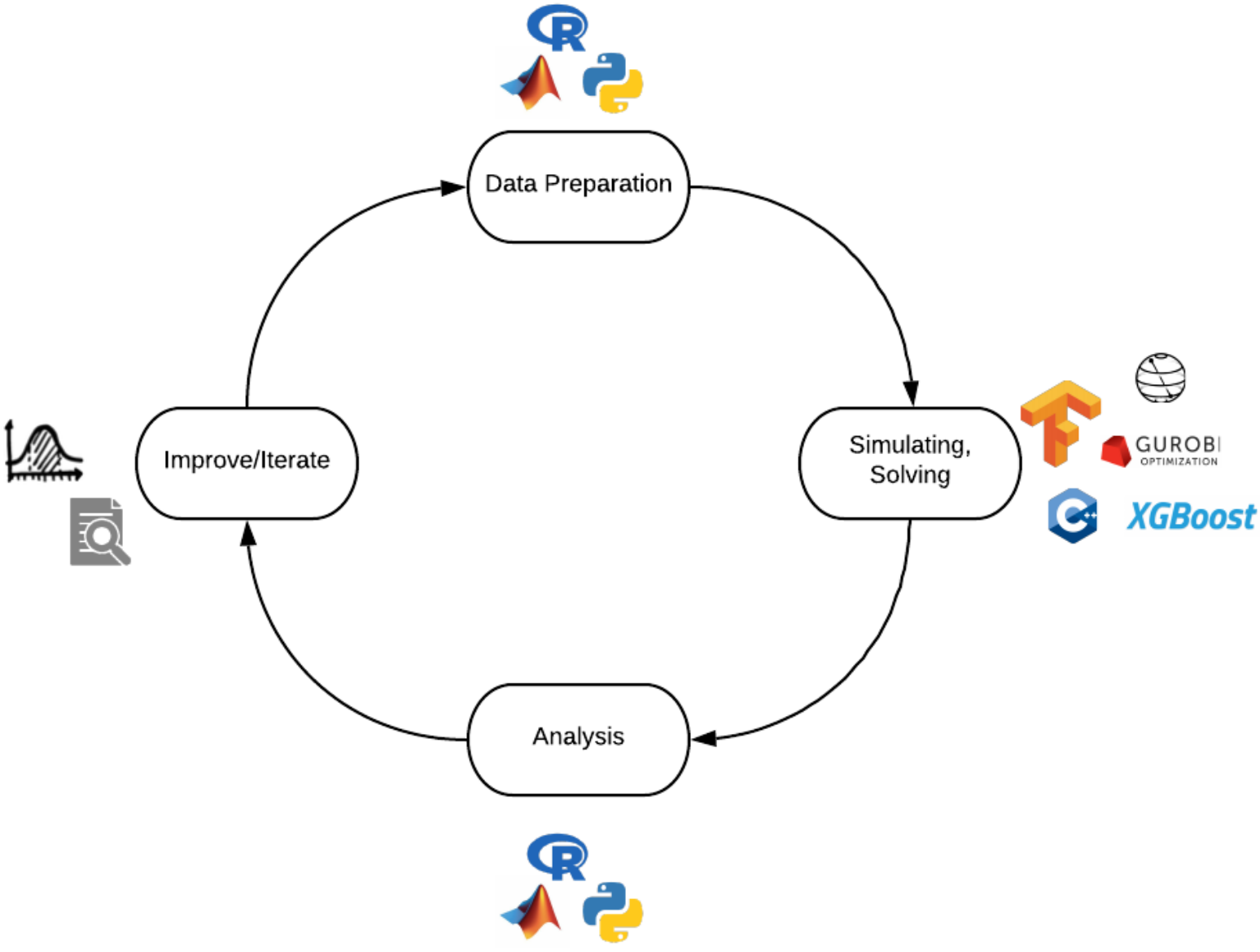
- Check out the slides at https://tinyurl.com/scnb3va

About Me

- Vivek Katial (vkatial@student.unimelb.edu.au)
  - PhD Candidate (Optimisation on Quantum Computers)
  - Data Scientist (3 years)

Motivation

Running Experiments and Developing ideas is Complex



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- Other issue is that this all needs to **scale**

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  - *mlflow* to track parameters, metrics at scale

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  - Similar to AWS, Microsoft Azure, GCP

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- Singularity is a container-technology designed for use in HPC environments.

Example Container

Check it out at: https://sylabs.io/singularity/

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YAML

- A recursive acronym for: *YAML Ain't Markup Language*

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experiment:
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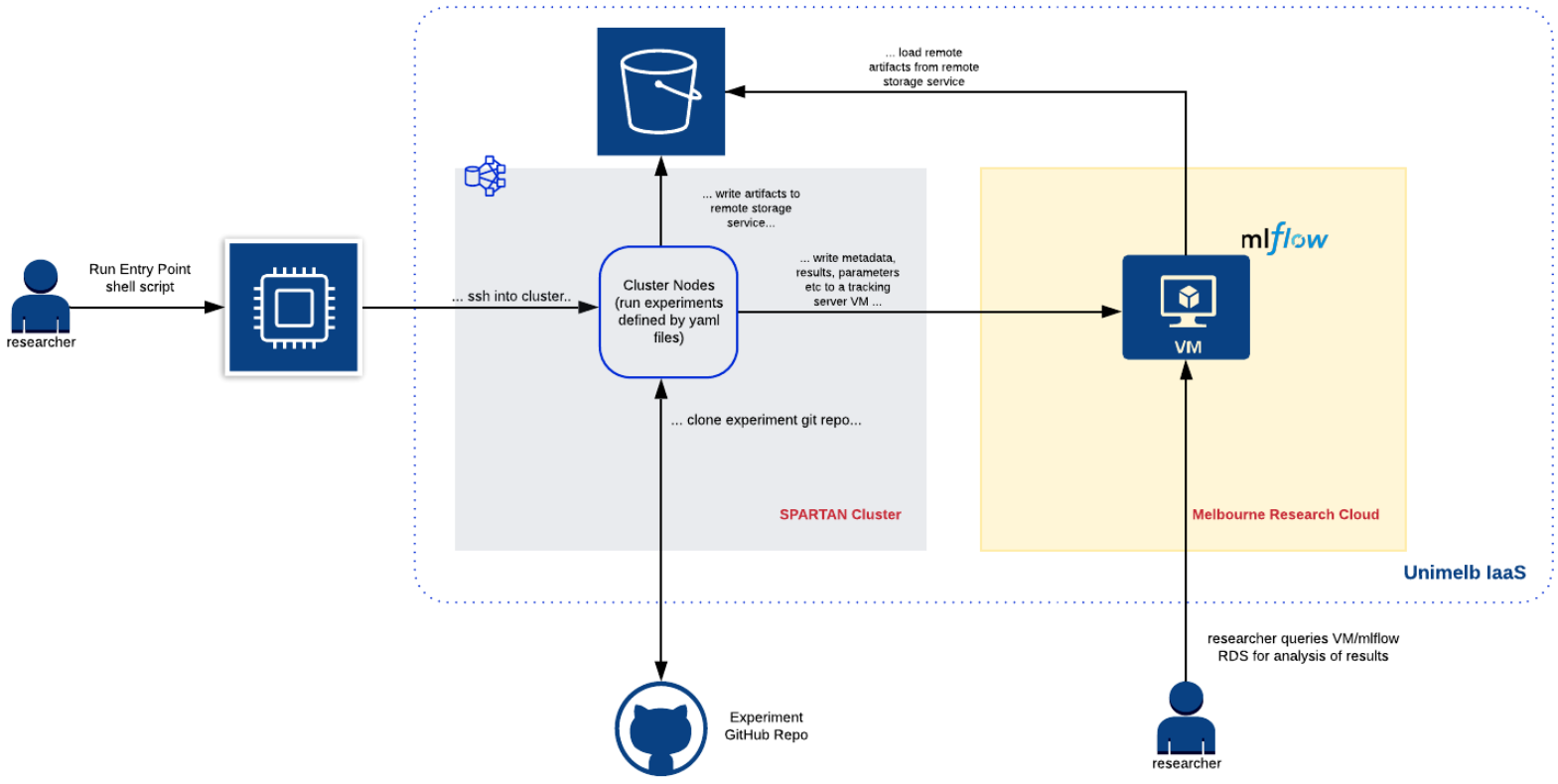
- Easily integrates with workflow
- Example: “https://localhost:5000”

Architecture



Concepts

Experiments and Runs

- The tool is organized around the concept of *experiments* and *runs*.
- An experiment can be considered the wider project.
  - Each experiment is defined by a **GitHub** repository
- A run is an execution of one-configuration of that experiment.
  A run consists of:
  - Code Version
  - Parameters
  - Metrics
  - Artifacts

Define an Experiment

- Each experiment is defined by a text file
- The text file specifies:
  - One configuration of the experiment
  - Parameters
  - Path to scripts
- Easy to understand

```
experiment:
  repository: "aqc-three-sat-sim" # GitHub Repostiry
  github_url: "https://github.com/vivekkatial/aqc-three-sat-sim"
  cluster_uri: "/data/cephfs/punim1074/"
  cluster_scratch_dir: "/scratch/punim1074/"
  cluster_provider: "unimelb_SPARTAN"
  singularity_image_uri: "ubuntu@115.146.94.33:aqc-three-sat-sim/portable-image.img"
```

An example of a run

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initialise:
  source: "src/generate-instances.R"
  params:
    n_qubits: "5"
    k: "4"
    n_sat: "3"

build_hamiltonians:
  source: "src/run-time-evolution.R"
  params:
    time_T: "100"
    t_step: "0.1"
    num_energy_levels: "4"

results:
  source: "src/produce-plots"
```