Re-Thinking Experiments

Accelerating Research through Reproducible Experiments at Scale

Vivek Katial

09/12/2019

Slides

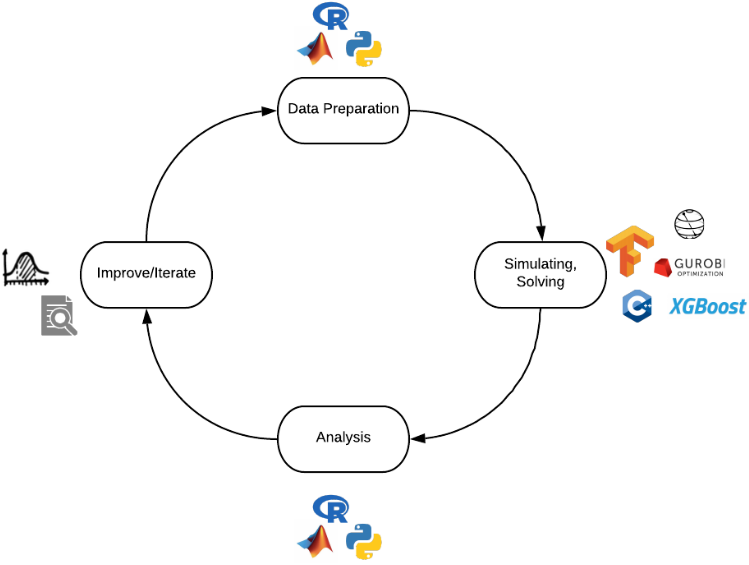
- Check out the slides at https://tinyurl.com/scnb3va

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**

Introducing “EZ-EXPERIMENTr”

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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

```
BootStrap: library
From: ubuntu:16.04

%post
    apt-get -y update
    apt-get -y install fortune lolcat

%environment
    export EXPERIMENT_NAME="example_presentation"

%runscript
    echo "This is an example"

%labels
    Author 'Vivek Katial'
```

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

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experiment:
  name: "three-sat"
  author: "vivek"
  tracking-uri: "http://localhost:5000"
  seed: 1032918
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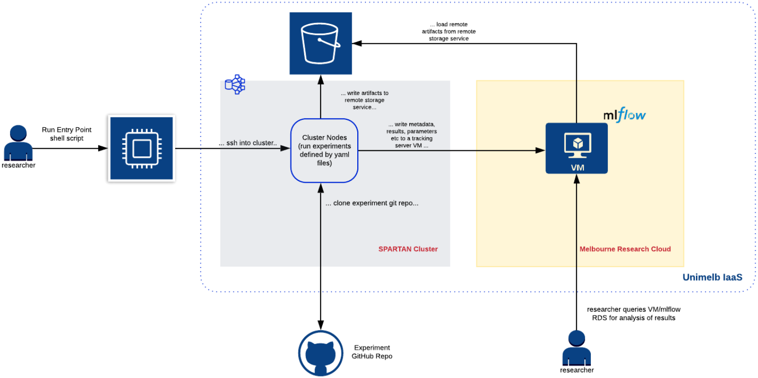
- Example: “https://localhost:5000”

Architecture



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```yaml
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

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

```yaml
experiment:
  name: "three-sat"
  author: "Vivek Katial"
  tracking-uri: "http://<mlflow-server-ip-address>:5000"
  seed: 1032918

initialise:
  source: "src/generate-instances.R"
  params:
    n_qubits: "{{n_qubits}}"
    k: "{{k}}"
    n_sat: "{{n_sat}}"

build_hamiltonians:
  source: "src/run-time-evolution.R"
  params:
    time_T: "{{time_T}}"
    t_step: "{{t_step}}"
    num_energy_levels: "{{num_energy_levels}}"

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

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n_qubits:
  1:20
t_step:
  0.01
  0.1
k:
  1:20
```

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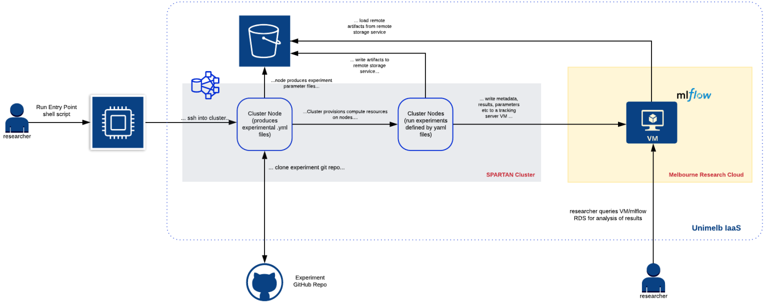
- `singularity run example-image.img PARAMETER_FILE_NAME.yml`

Putting it all together



Thank You!