A Serverless Tool for Platform Agnostic Computational Experiment Management

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Keyword 1 | Keyword 2 | Keyword 3 | ...

- Computational sciences are becoming more and more common and necessary.
- Standards are emerging to aid in the reproducibility and shareability of tools and data
  - Boutiques
  - BIDS
  - BIDS apps
- Virtualization tools make analysis software increasingly portable
  - Docker
  - Singularity
- Platforms enable running workflows at scale on a variety of computational resources
  - CBRAIN
  - LONI
  - Nipype
- Execution provenance is becoming increasingly focal and we are recognizing its importance
  - NIDM (neuroscience prov)
  - ReCAP (infrastructure stats/prov)
  - Reprozip (file i/o prov)
- Tools have varying use-cases and barriers for adoption
  - CBRAIN/LONI are designed for production-level pipelines
  - Nipype is complex for tool consumption or simple workflow construction
  - NIDM is very rich and requires deep integration with the tool
  - ReCAP monitors machine resources in virtual machine-based clouds
  - Reprozip has limited compatibility when run around containers, depending on infrastructure
- Clowdr accessibly leverages these approaches where possible and builds-up pipelines with increased deployability, provenance, and shareability
  - Accessible deployment environment closer to development
  - Makes tool consumption very easy
  - Records rich cpu and memory provenance everywhere
  - Records reprozip provenance whenever possible
  - Enables apps/containers that leverage NIDM, Nipype, Reprozip, etc., internally to do their thing, and only adds further richness to provenance records
  - Provides accessible web interface to browse, download, and share executions

Methods

- Data awareness with BIDS
- Cluster and cloud interface with SLURM and Amazon APIs (and extensible)
- Containerization with Singularity or Docker
- Parameter sweeping with boutiques/clowdr
- Tool encapsulation with Boutiques
- Provenance capture using reprozip*, memprofile, cputiming
- Data sharing and publication with Flask
- Figure 1: workflow diagrams (done)

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GK did things, SB provided help and advice, TG provided help and advice and co-supervised, AE co-supervised.

The authors declare no conflicts of interest in this work.

- Supplement repos?
  - Dockerfile
  - Boutiques descriptor
  - Invocations
  - Clowdr command
  - Dataset

Results.

- Figure 2: instructions infographic (i.e. steps to use clowdr)
- Figure 3: we ran, find provenance "here" (i.e. clowdr share)
  - running ndmg on hcp data (compute canada)
  - 1-voxel analysis (compute canada cloud?)
  - Bids example (amazon)
- example provenance analysis (i.e. instance size optimization)
  - Mem usage comparisons (do)
  - CPU usage comparisons (do)

Discussion.

- other uses of provenance information
  - Reprozip trace comparisons (cite)
  - Extrapolate for informed decision making on cloud resource selection (cite)

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