



Mountain



Rocky Linux



Apptainer



Warewulf



Fuzzball



Ascender

Fuzzball for portable, reproducible workflows

David Godlove - Lead Technical Product Writer

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CIQ supported tools



CIQ supported tools



Rocky Linux



CIQ supported tools



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Ascender



CIQ supported tools



Mountain



CIQ supported tools

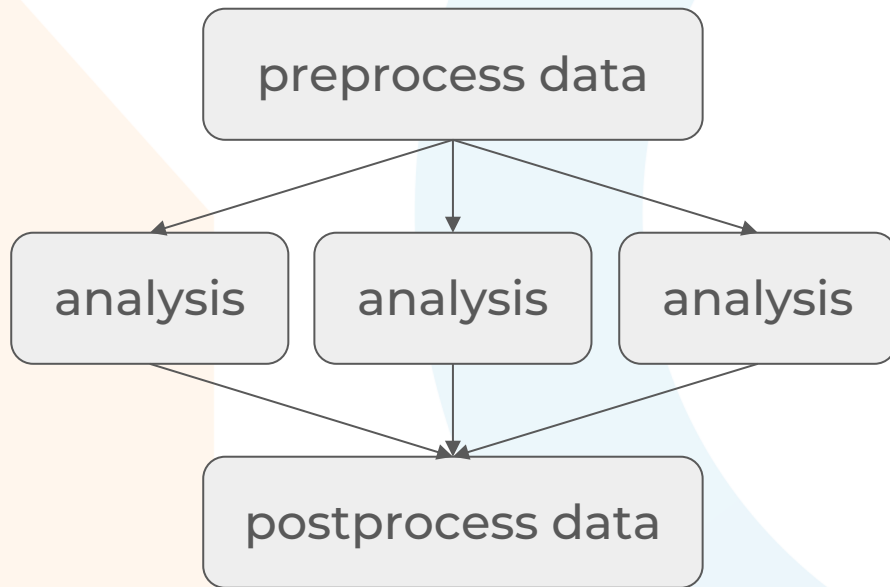
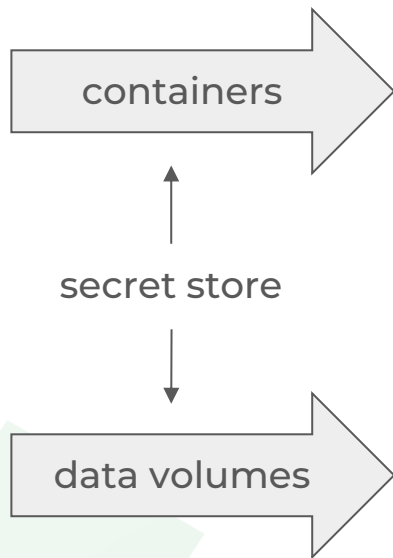


CIQ supported tools

Fuzzball



Fuzzball workflows



MPI



GPUs



fabrics



Fuzzball is a Modern and Container-Based Solution

- container orchestration for *jobs*
- jobs run in a lightweight container runtime (called *Substrate*) with virtually no overhead
- approach blends the best aspects of *cloud*, *enterprise*, and *HPC* providing a solution for all 3



Fuzzball is API driven with a clean web GUI and CLI

The screenshot displays the Fuzzball Workflow Editor interface. On the left, a sidebar contains navigation options: 'SA' (selected), 'Workflows', 'Workflow Editor', and 'ACCOUNT CONFIGURATION' (with sub-items: 'Resource Definitions', 'Secrets', 'Users', and 'Volumes'). The main workspace shows a workflow diagram with the following steps: 'create-dirs' (top), 'retrieve-query-sequence' (left), 'retrieve-database-sequences' (right), 'make-blast-database' (center, highlighted in green), and 'run-blast' (bottom). These steps are connected by dashed lines indicating a sequential flow. On the right, a panel titled 'Edit make-blast-database' is open, showing configuration options for the 'make-blast-database' step. The panel has tabs for 'Job', 'Environment' (selected), and 'Resources'. Under the 'Environment' tab, the following settings are visible: 'Image' (URI: 'docker://ncbi/blast:2.12.0'), 'Secret' (a dropdown menu), 'Mounted Volumes' (a table with columns 'VOLUME' and 'ABSOLUTE PATH' showing 'blast-volume' mapped to '/data'), 'Environment Variables' (a dropdown menu), and 'CWD' (set to '/data/fasta'). At the bottom of the panel are 'Delete' and 'Close' buttons. The top right of the interface shows a user profile for 'dgodlove@ciq.co'.

Workflow Editor

Workflow Diagram:

```
graph TD; create-dirs[create-dirs] --> retrieve-query-sequence[retrieve-query-sequence]; create-dirs --> retrieve-database-sequences[retrieve-database-sequences]; retrieve-query-sequence --> make-blast-database[make-blast-database]; retrieve-database-sequences --> make-blast-database; make-blast-database --> run-blast[run-blast];
```

Edit make-blast-database

Environment Tab:

- Image:** URI: `docker://ncbi/blast:2.12.0`
- Secret:** Select a secret
- Mounted Volumes:**

VOLUME	ABSOLUTE PATH
blast-volume	/data

[Add Mounted Volume](#)
- Environment Variables:** [Add Environment Variable](#)
- CWD:** `/data/fasta`

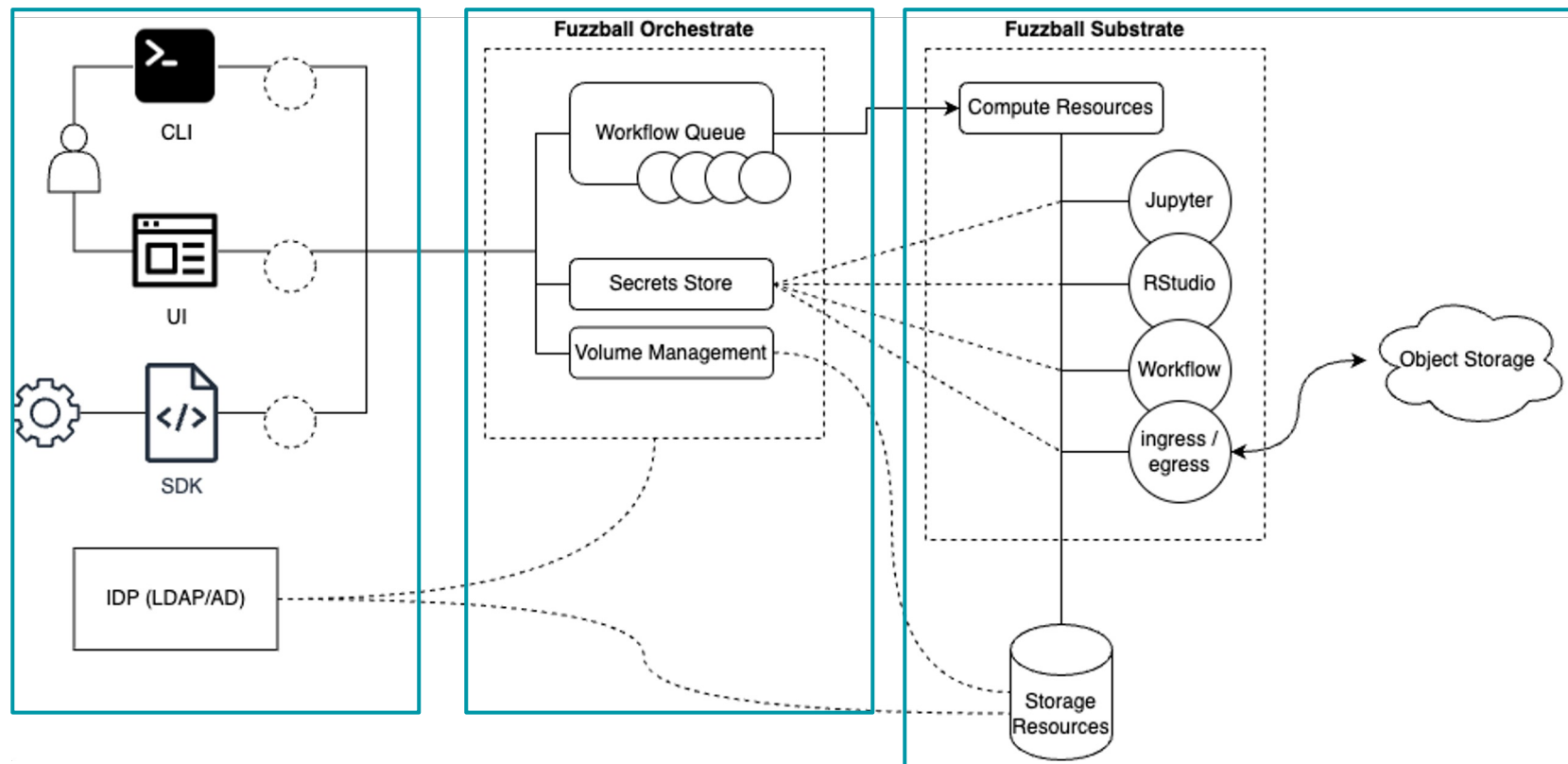
Absolute path of the working directory used by the job

[Delete](#) [Close](#)

Fuzzball Allows Each User to Focus on their Specialty

- no need to open a terminal and `ssh` into a login node
- can forget about using `scp`, `rsync`, etc to move data
- permissions and file ownership no longer an issue
- can simply use containers instead of worrying about installing software
- also eliminates administrative tasks like user management and software installation

Fuzzball Architecture



Fuzzball: Proven Use Cases

GenAI / Tech

- *Meta's Llama 2/3 (LLM), Stable Diffusion (image gen), GPT-like models (LLMs)*
- *Training/inference with major AI frameworks*
 - PyTorch
 - Tensorflow
 - JAX-based models
 - Hyperparameter tuning with W&B
- *Interactive Jupyter notebooks*
- *Salmon and similar Python-based bioscience tools*
- *Specialized Use Cases*
 - GasNET/Chapel language support
 - Exascale Computing Project apps
 - Remote GPU profiling via NVIDIA tools
 - Satellite signal processing submitted via Fuzzball SDK
 - VNCs into programming language debuggers/interfaces like R

Industry Examples

- *Life Sciences / Pharma*
 - GROMACS (drug discovery)
 - LAMMPS (drug discovery, NL nuclear apps)
 - STAR genomic alignment (genomics)
- *Simulation / Manufacturing*
 - MATLAB
 - Ansys tools
 - Altair OpenRadioss (FEM, structural simulation, etc.)
 - WRF (weather simulation for public power utilities)
 - OpenFOAM w/ Paraview visualization (CFD, aerodynamics, fluid flow)
 - QMCPACK (quantum dynamics)
 - Quantum ESPRESSO (quantum dynamics)
 - Arkouda - Exploratory Data Analysis



THANK YOU



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