Adaptive Tool Selection in a Scalable Genomics Pipeline

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My Project

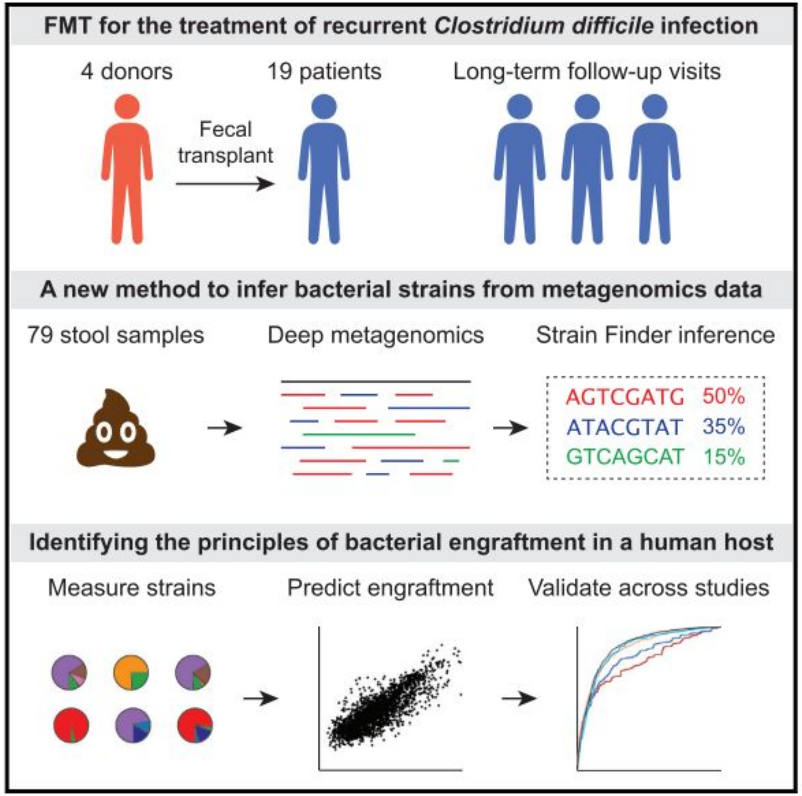
Created FMT viral detection pipeline as part of my undergraduate research

Use Parsl make my original pipeline more efficient and scalable

Apply adaptive tool selection with Academy

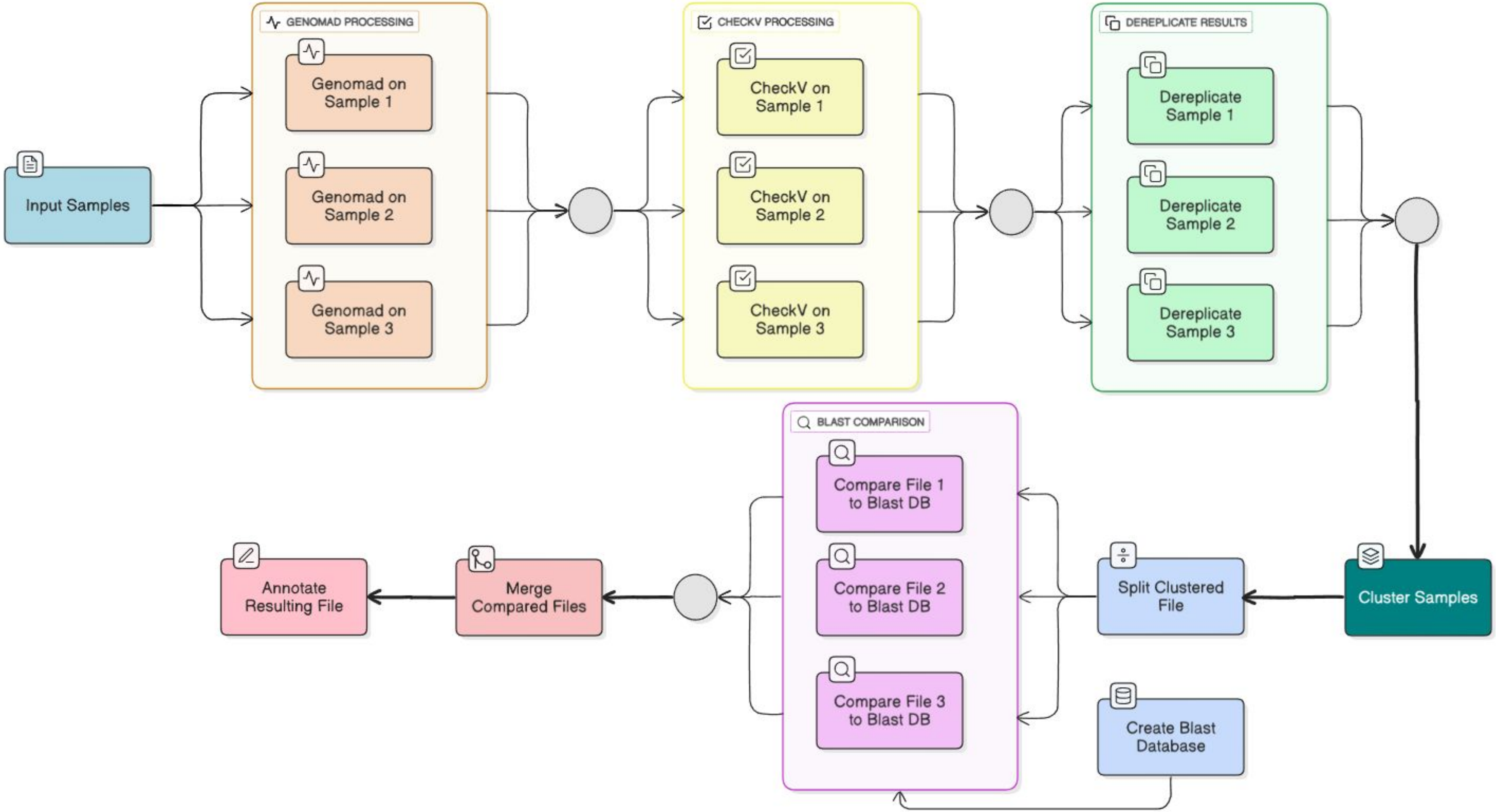
FMT Viral Detection

- FMT for C. diff
- Tracking viruses
- From donor to patient, and over time
- Metagenomic approach
- Assembled contigs → annotated viruses



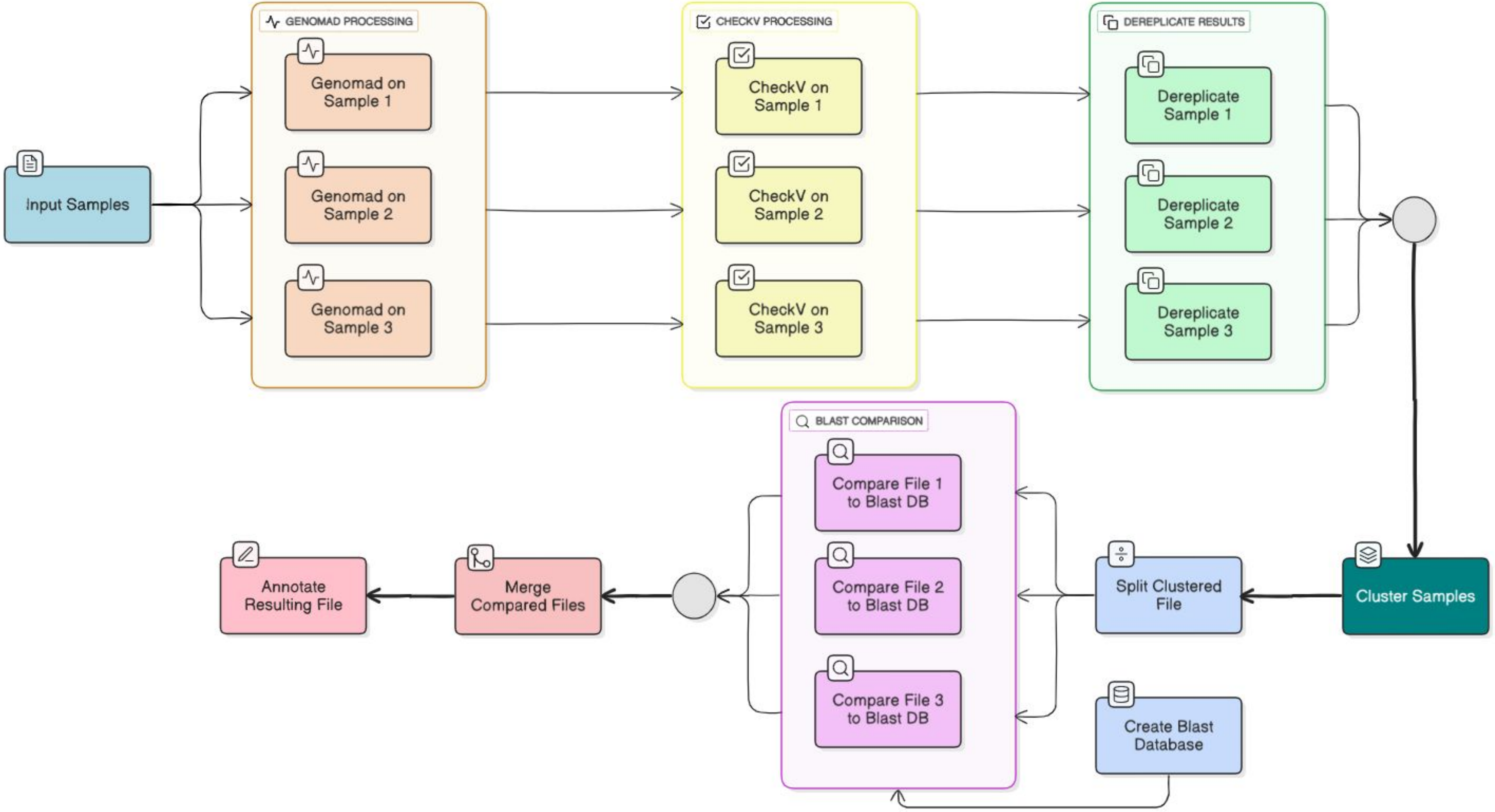
From: Smillie et al., *Cell Host Microbe* 2018;23(2):229–240.
DOI: 10.1016/j.chom.2018.01.003.

Funded by the U.S. National Science Foundation, Grant #2127548



Parsl

- Apps run concurrently
- Parsl creates a dynamic graph of tasks and their dependencies
- Tasks executed when their dependencies are met
- “Natural parallel programming!”



Input Samples

GENOMAD PROCESSING

Genomad on Sample 1

Genomad on Sample 2

Genomad on Sample 3

CHECKV PROCESSING

CheckV on Sample 1

CheckV on Sample 2

CheckV on Sample 3

DEREPLICATE RESULTS

Dereplicate Sample 1

Dereplicate Sample 2

Dereplicate Sample 3

Cluster Samples

Split Clustered File

Create Blast Database

BLAST COMPARISON

Compare File 1 to Blast DB

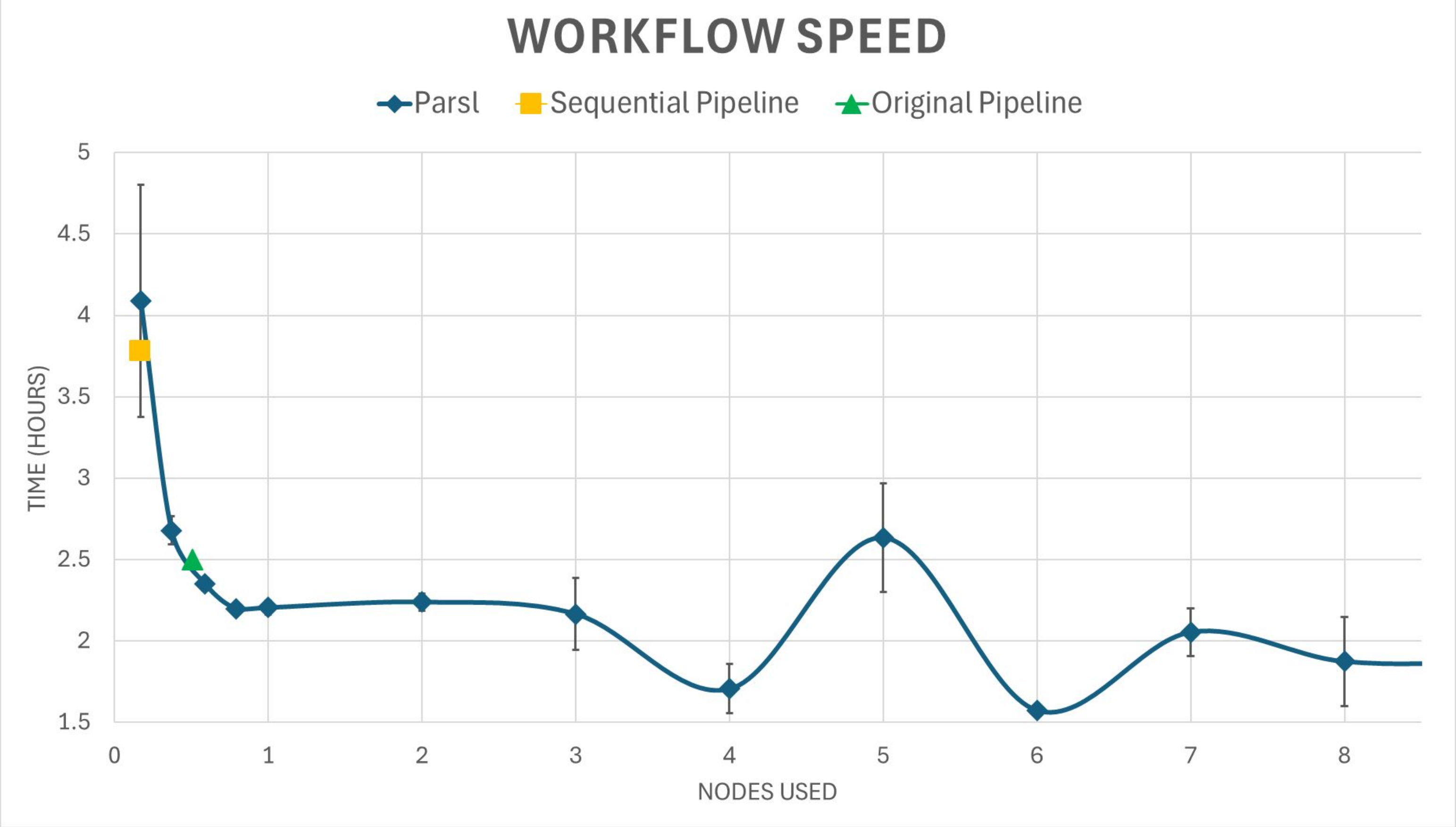
Compare File 2 to Blast DB

Compare File 3 to Blast DB

Merge Compared Files

Annotate Resulting File

Scaling the Workflow



Academy

- Modular middleware for building autonomous agents
- Manage inter-agent communication
- “Deploy agents across distributed, federated, and heterogeneous resources”

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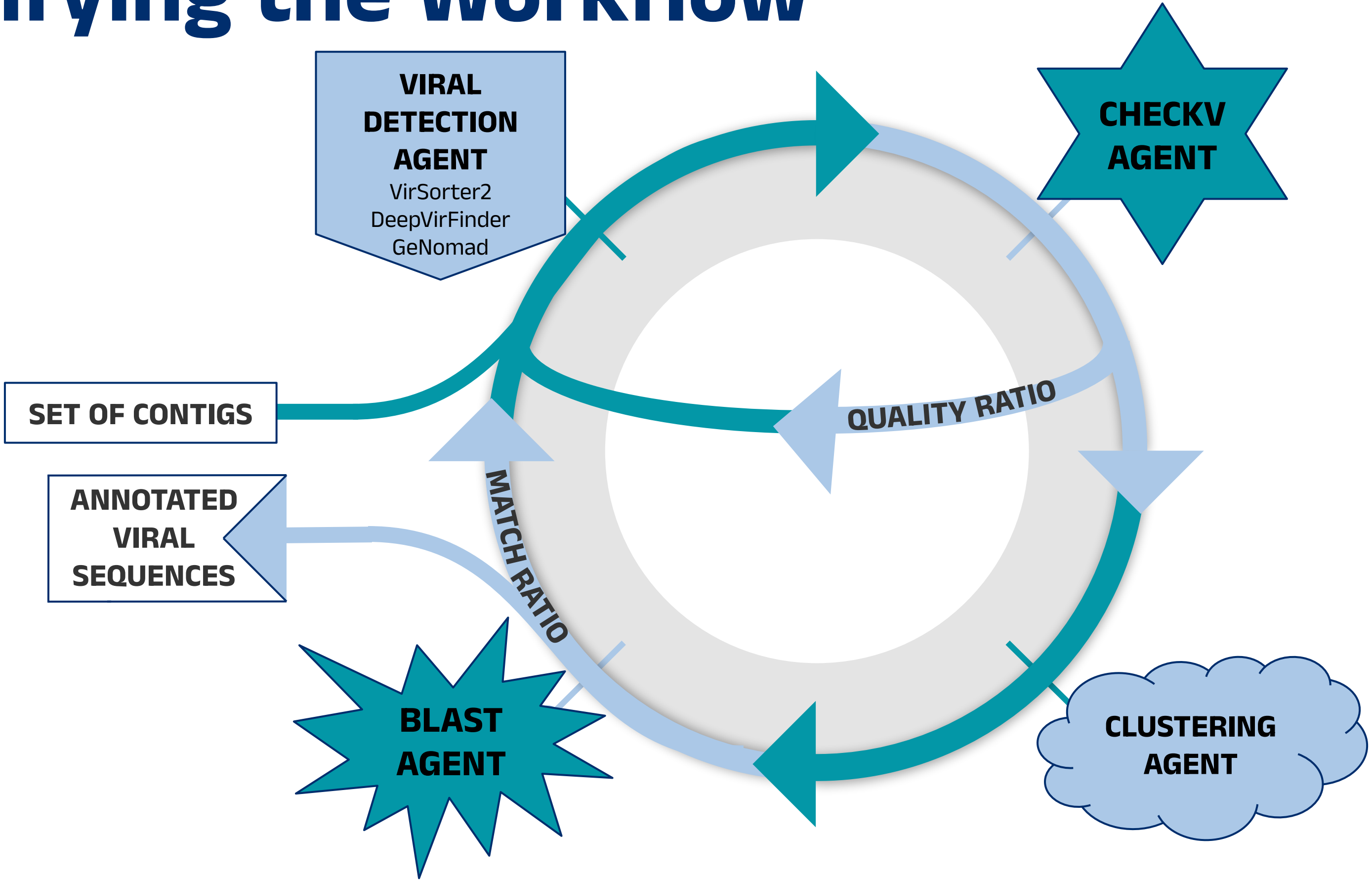
Agentifying the Workflow



VIRAL DETECTION AGENT
VirSorter2
DeepVirFinder
GeNomad

CHECKV AGENT

SET OF CONTIGS

QUALITY RATIO

ANNOTATED VIRAL SEQUENCES

MATCH RATIO

BLAST AGENT

CLUSTERING AGENT

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Skills Learned and Takeaways

1. Understanding of HPC and resource management
2. Understanding of workflow management (Parsl, Academy, etc)
3. Learned about autonomous agents and how to agentify a workflow
4. Data collection and documentation
5. Creativity in a workflow

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Future of the Project

Submitting poster to the ACM Student Research Competition at SC25

Expanding to other datasets to understand and explore tool selection process

Exploring possibilities of agents (annotation, clustering, etc.)

Acknowledgments

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Check out my code!

https://github.com/globus-labs/academy-fmt-viral-workflow