Workflow tradeoffs in the context of cancer phylogeny

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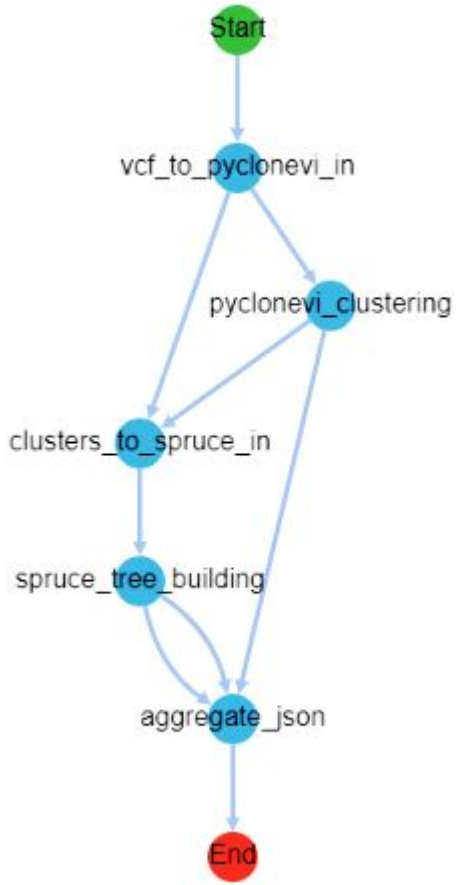
Context

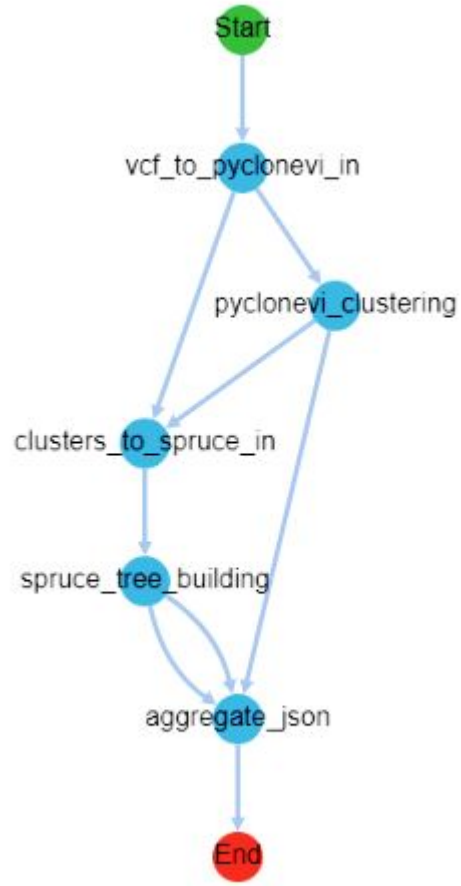
- Cancer phylogenies are graphs that represent the evolutionary relationships and growth of tumors.
- Phylogenetic workflows are pipelines used to build phylogenetic graphs by processing genomic and mutagenic data in a multistep process
- These often use WDL (Workflow Description Language), a bioinformatic framework for executing scientific workflows. The workflow we primarily researched, phyloflow, made heavy usage of WDL.
- Implemented solutions through Parsl, a Python scientific computing framework that enables simplification of workflows, easy parallelization, extension of workflows, and more portability.
- Langchain is a framework that connects LLMs to applications. We have been using it to connect to OpenAI's API.



More on Phyloflow

Workflow steps

- Load a VCF file generated by 'mutect' and its annotated version from VEP (Variant Effect Pipeline).
- Convert the mutations from the VCF file into the required input format for 'pyclone-vi'.
- Execute 'pyclone-vi' to cluster the mutations.
- Adapt the output of the pyclone clustering to be compatible with 'spruce' tree inference.
- Gather the relevant output files and merge them into a JSON file that works with the PhyloDiver visualization tool.



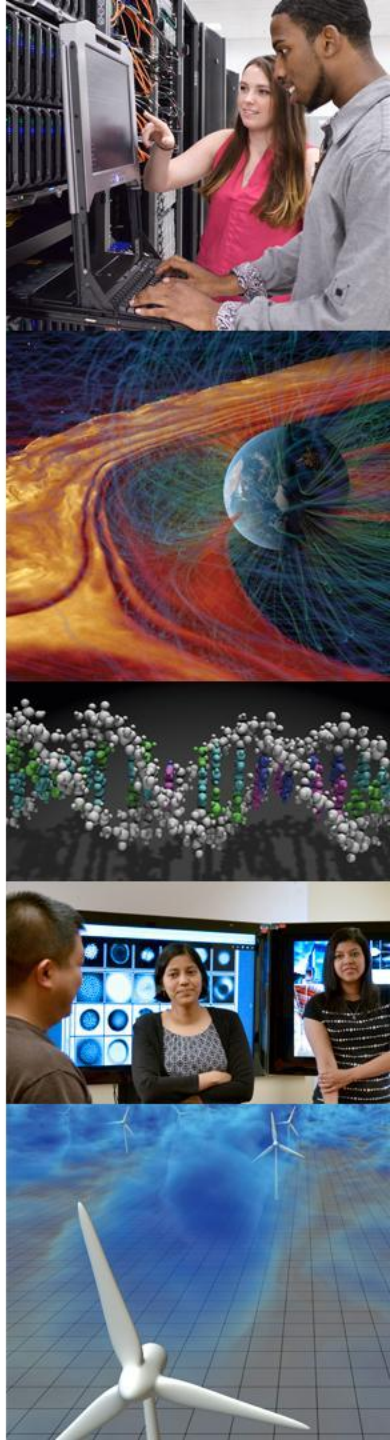
WDL to Parsl Workflow Translation

Why translate the Phyloflow workflow?

- To compare the ease of use of Parsl against WDL on a scientific workflow.
- To test how easy it is to extend a workflow with the parallelizable capabilities of Parsl.
- To make it easier to integrate AI tools developed for Python.

{wdl}

Parsl



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WDL to Parsl Workflow Translation

Workflow Translation Process

Understanding Phyloflow workflow

- Tasks and dependencies.

Running the workflow locally

- Setting up running environments.

Translating the workflow to Parsl

- WDL tasks into Parsl Apps.
- Bash scripts into python functions.
- Filesystem Management.
- Containerization.

Documenting the Process:

- https://github.com/grimloc-aduque/Phyloflow-Parsl-Implementation

CONDA

docker

@python_app

@bash_app

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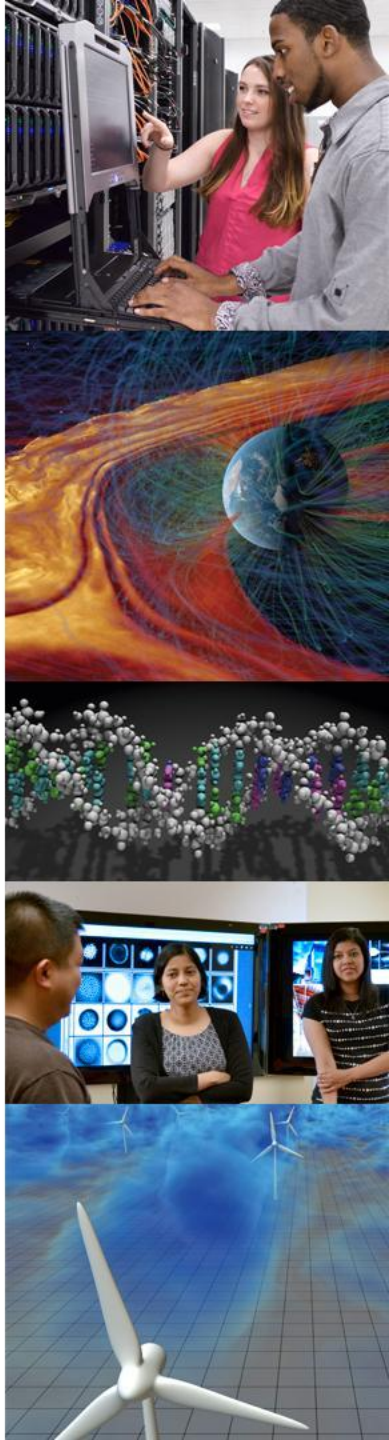
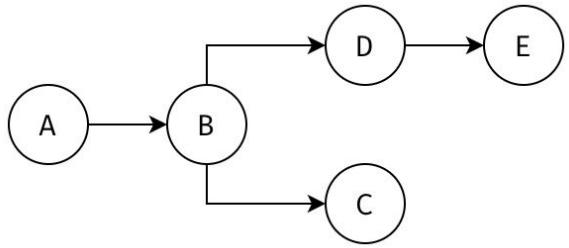


WDL to Parsl Workflow Translation

Developer Experience with Parsl

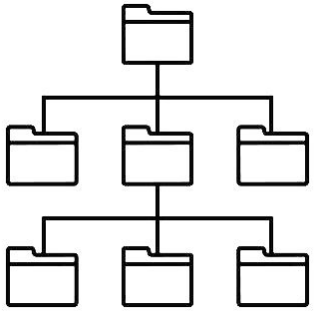
Parsl Advantages

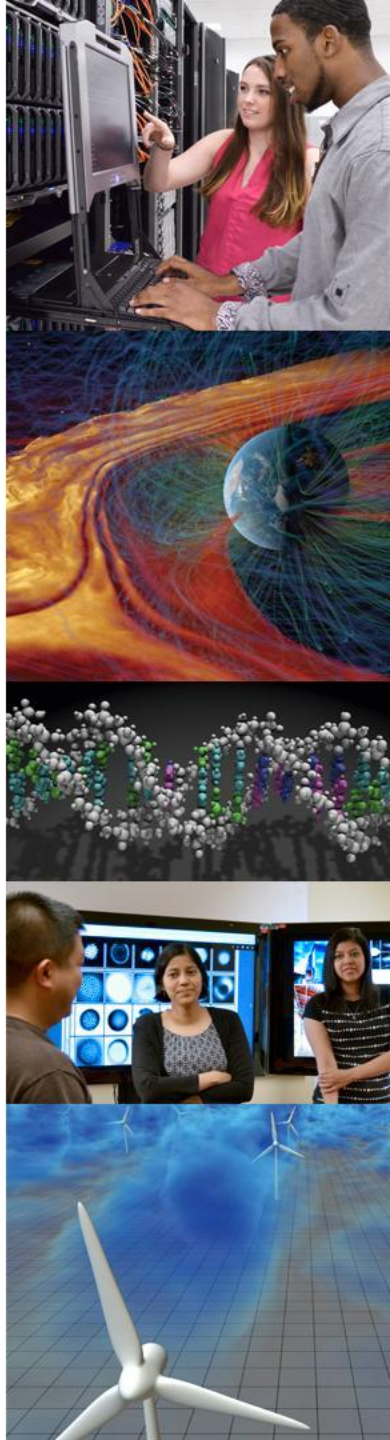
- Finer control over the file dependencies.
- Easy to extend with native python functionality.
- Straightforward parallelization.



Parsl Disadvantages

- Requires more experience with the filesystem.
- Harder to run tasks with conflicting environment dependencies.
- Retrieving inputs and outputs by indexing an array is confusing and error prone.





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Workflow Integration with AI

Integration of AI in phylogenetic workflows

Explore ways to use Langchain along with OpenAI LLM's

Workflow translation

- Generate Parsl code from existing WDL workflows.

Workflow generation

- Generate Parsl code with NLP.
- Zero-shot and One-shot prompting.
- RepoReader for document indexing.

Workflow usage

- Execute workflow tasks using NLP.
- OpenAI function calling.

LangChain

OpenAI

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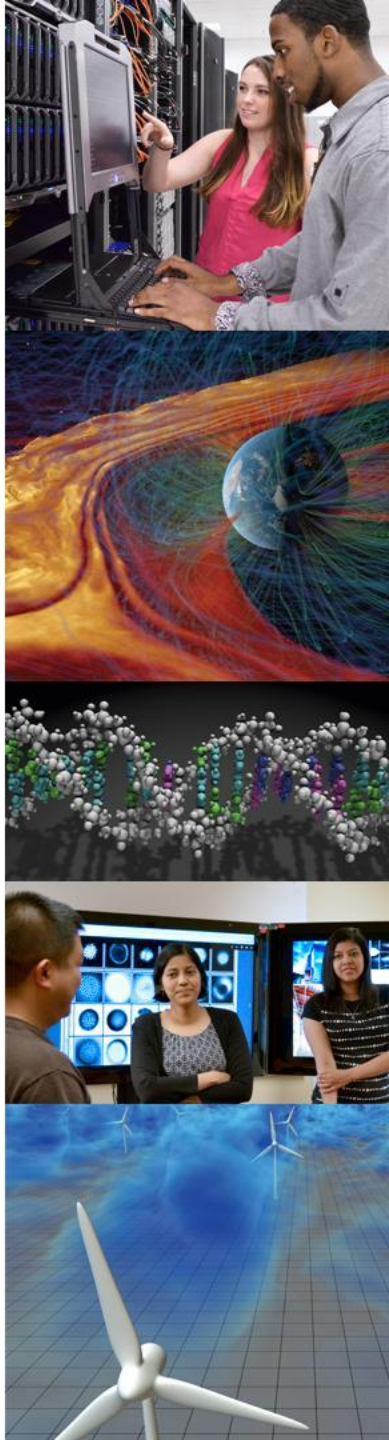

Workflow Integration with AI

Next Steps

- Concatenate function call requests to compose multiple tasks.
- Explore ways to use Langchain along with function calling.
- Implement the Variant Effect Predictor as a node of the workflow.

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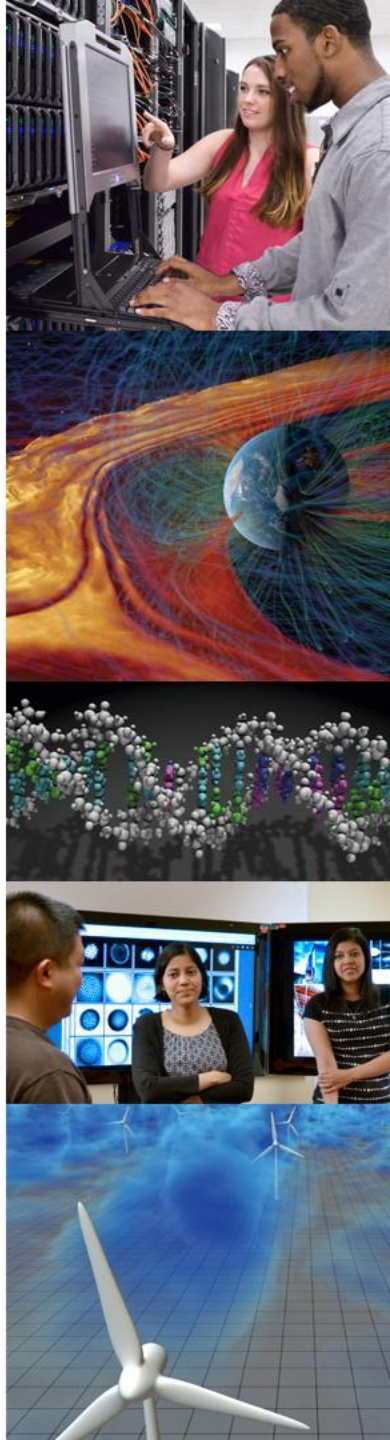

References

- Phyloflow: https://github.com/ncsa/phyloflow
- Parsl: https://parsl.readthedocs.io/en/stable/
- Langchain: https://python.langchain.com/docs/
- OpenAI API: https://platform.openai.com/docs/api-reference
- Function calling: https://openai.com/blog/function-calling-and-other-api-updates