CyberGIS-Compute: Geospatial Middleware for Simplifying Access to High Performance Computing

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AAG Annual Meeting, 2023
March 25th, 2023

Overview of Workshop

- Introduction
- Using the CyberGIS-Compute SDK (Hands-On)
- Making a CyberGIS-Compute Model (Hands-On)
- Wrap-Up/Next Steps
- Q&A

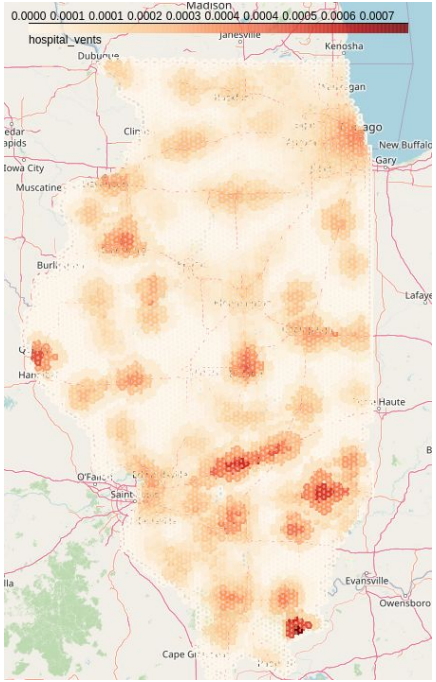
Motivation

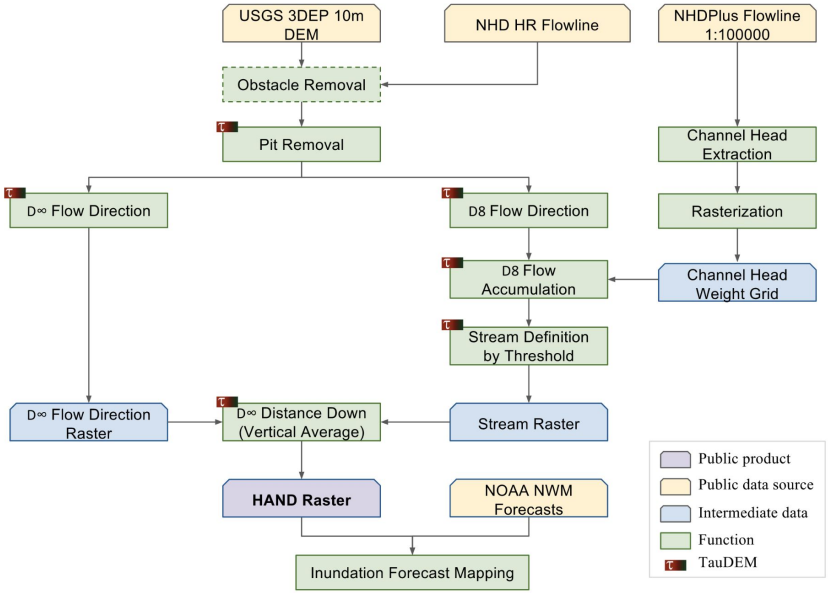
- Geospatial discovery and innovation are increasingly computation and data intensive
- Personal computing environments are limited to resolve such computational intensity
- High-performance computing (HPC) environments are needed to enable computation- and data-intensive geospatial scientific workflows

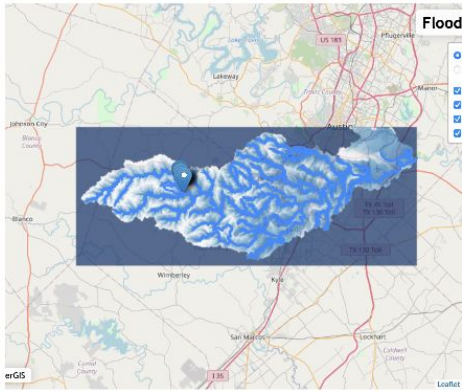
But …

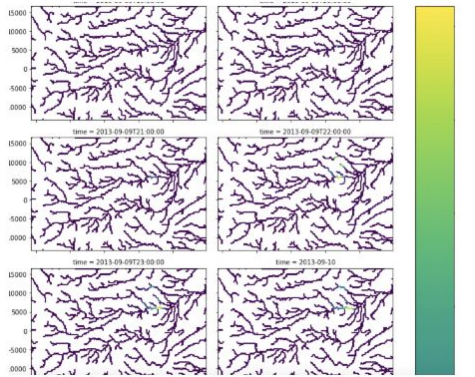
- The learning curve to access and use HPC is very steep!

Examples









Spatial Accessibility Calculation

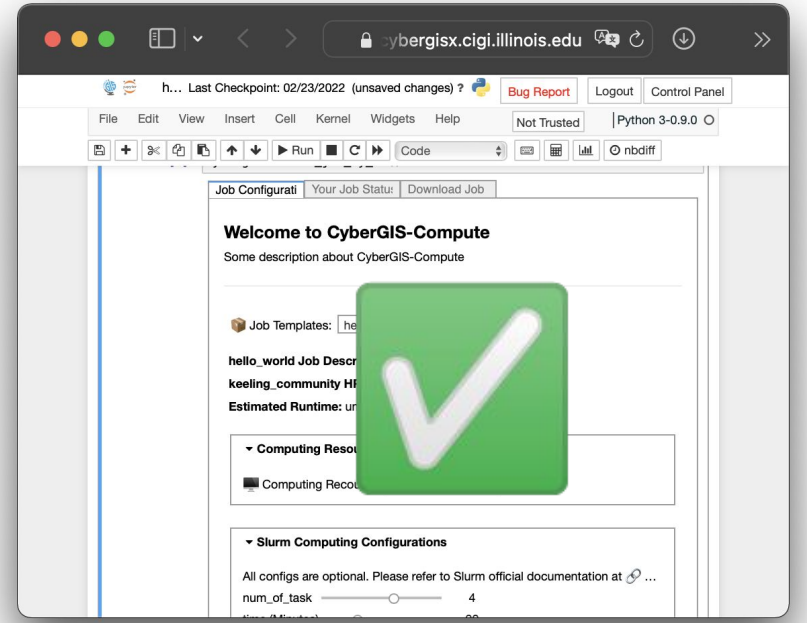
Estimate Height Above Nearest Drainage

WRFHydro Model

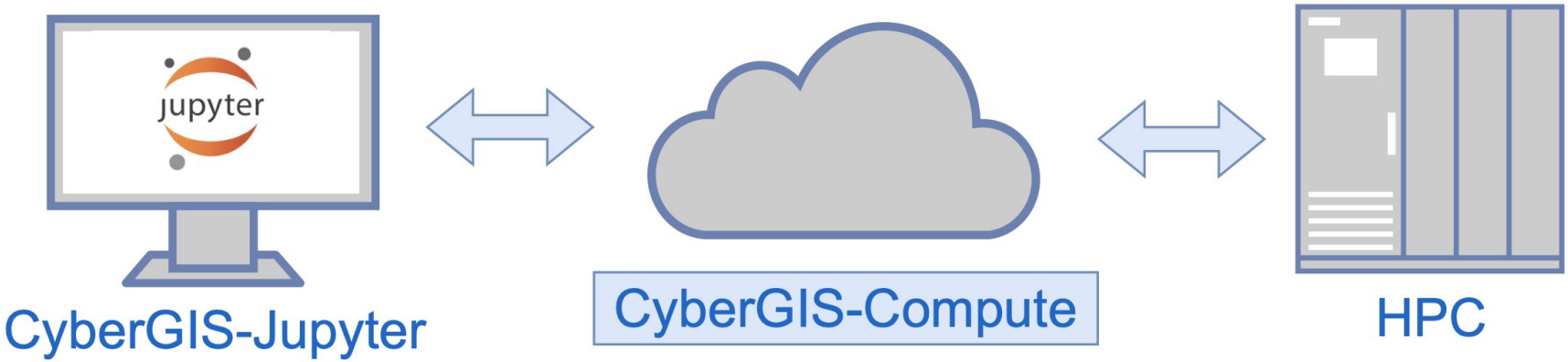
What is CyberGIS-Compute?

- Simplify access to HPC
- Bridge the gap between interactive computing environments (e.g. CyberGIS-Jupyter) and HPC
- Enable computation- and data-intensive geospatial workflows

User Interface

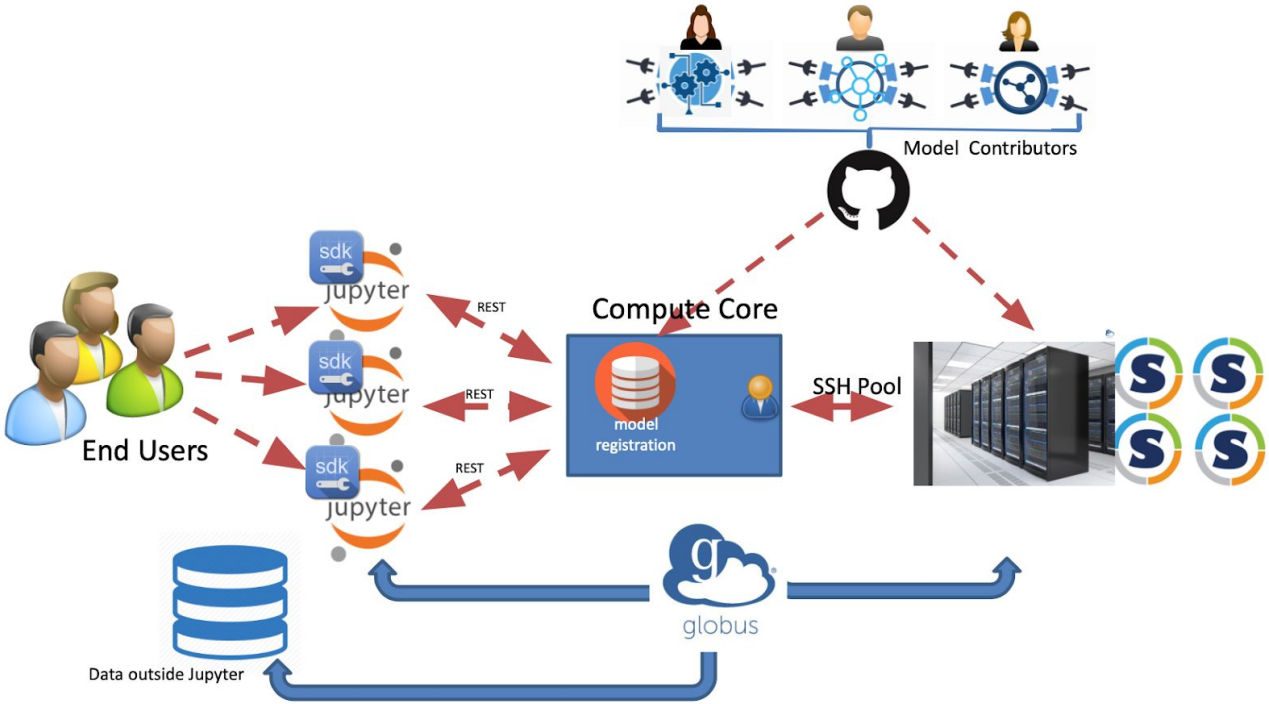


Bridging Ease of Use with Powerful Computing



- Padmanabhan, A., Vandewalle, R.. C., Xiao, Z., Baig, F., Michels, A., Li, Z., and Wang, S. (2021) “CyberGIS-Compute for enabling computationally intensive geospatial research”. In: *Proceedings of the 3rd ACM SIGSPATIAL International Workshop on Geospatial Data Access and Processing APIs,* https://doi.org/10.1145/3486189.3490017.
- Yin, D., Liu, Y., Hu, H., Terstriep, J., Hong, X., Padmanabhan, A., and Wang, S. (2018) “CyberGIS-Jupyter for Reproducible and Scalable Geospatial Analytics”. *Concurrency and Computation: Practice and Experience*. https://doi.org/10.1002/cpe.5040

Geospatial Middleware



A **scalable middleware framework** for enabling high-performance and data-intensive geospatial research and education

Key Components

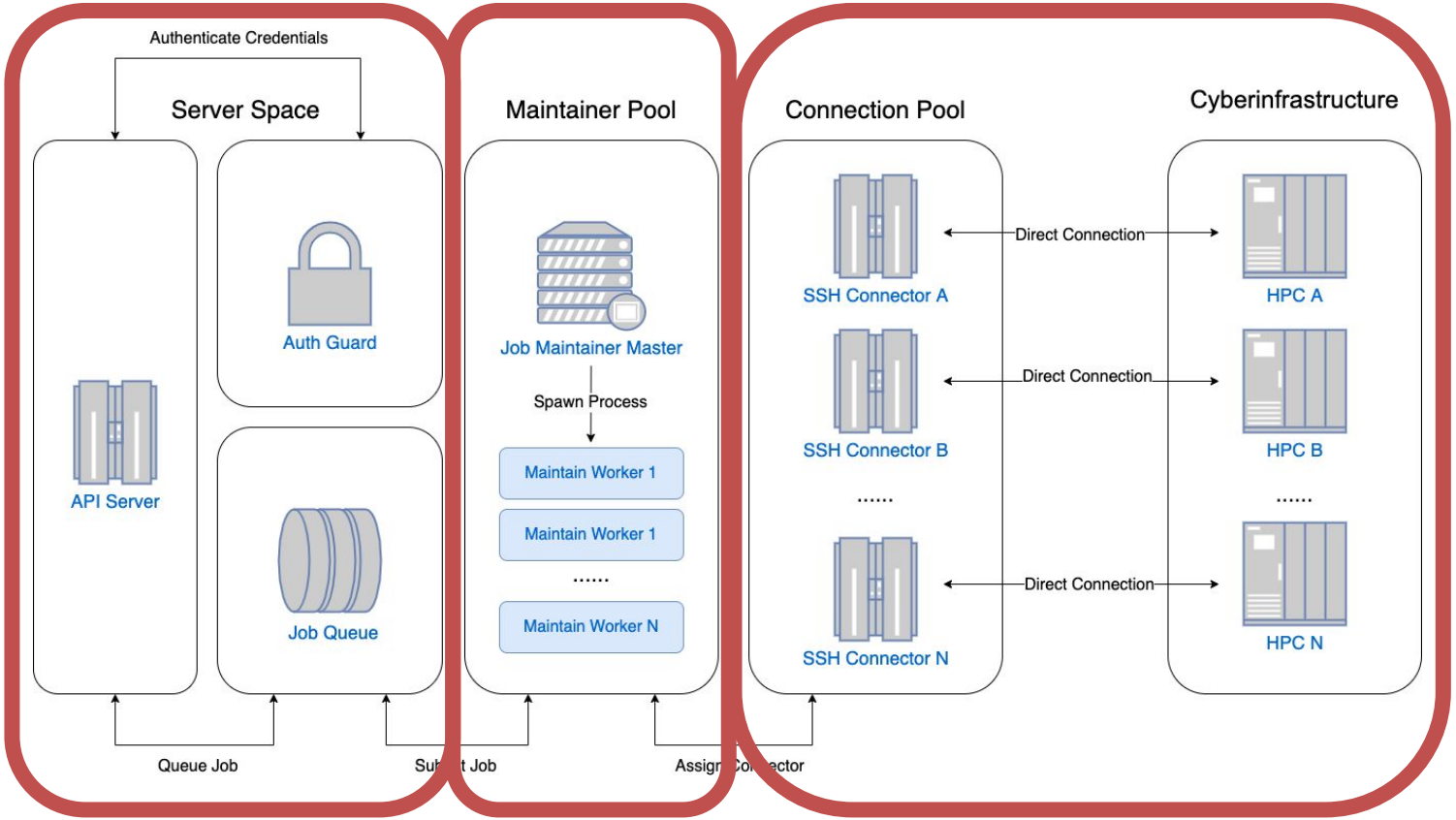
- **Core**: middleware server that automates job submission to HPC
- **SDK**: interactive client for Jupyter Notebook with code-less UI support
- **Contribution**: developer API that enables workflow contribution with little to no modification of existing code

CyberGIS-Compute Core

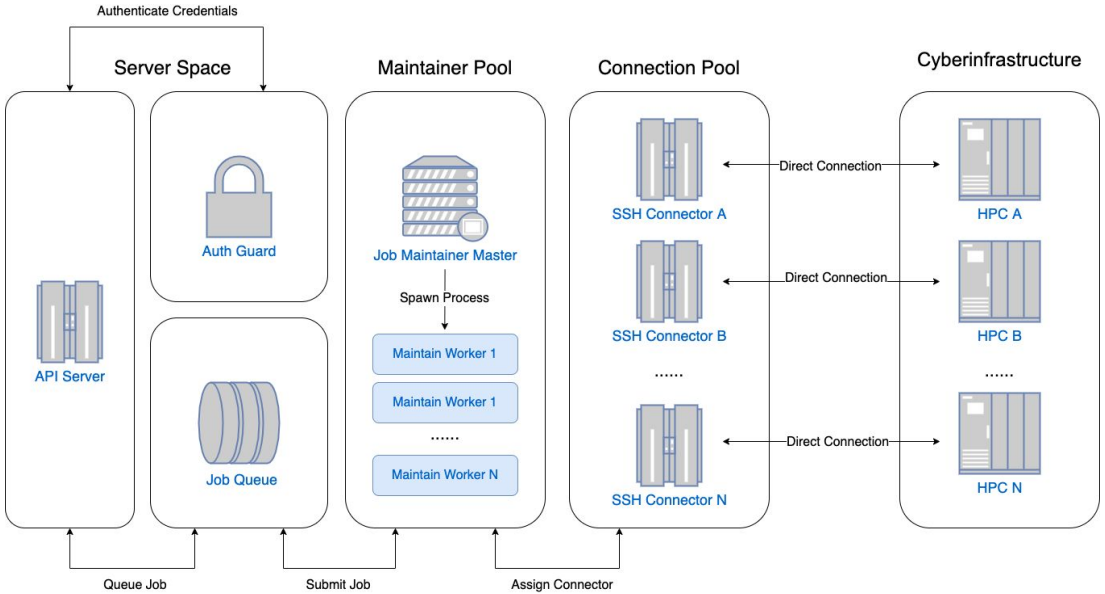
CyberGIS-Compute SDK

Contribution

Architecture



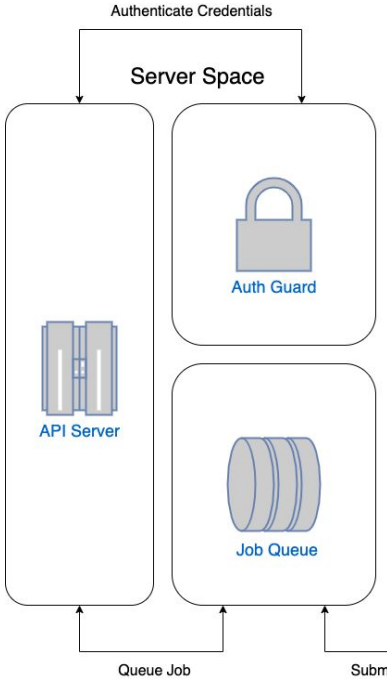
Middleware Server



- 🎯 Manages job submission to HPC
- Three layers
  - API Server Space
  - Maintainer Pool
  - Connection Pool

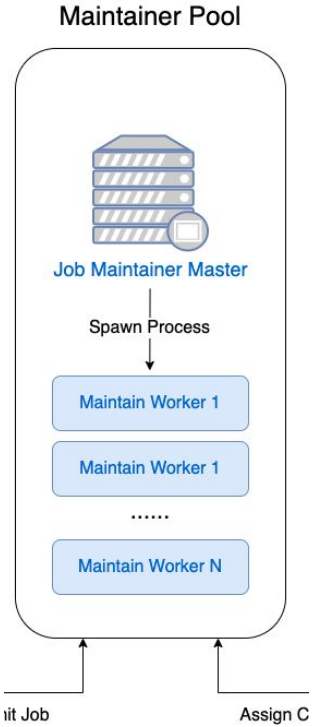
Padmanabhan, A., Xiao, Z., Vandewalle, R, C., Michels, A., and Wang, S. (2021) ”Enabling computationally intensive geospatial research on CyberGIS-Jupyter with CyberGISCompute”. In: *Proceedings of the Gateways 2021 Conference*, October 19 – 21, 2021, DOI: 10.5281/zenodo.5570056

API Server



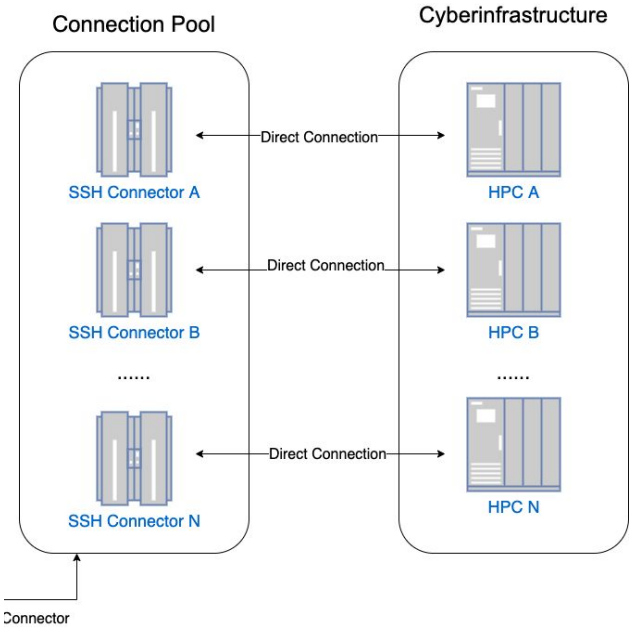
- Provides a **user-facing RESTful web interface** (API Server) for authentication and interaction with internal components of CyberGIS-Compute
- Pushes computation jobs into an internal job queue that the Maintainer Pool consumes

Maintainer Pool



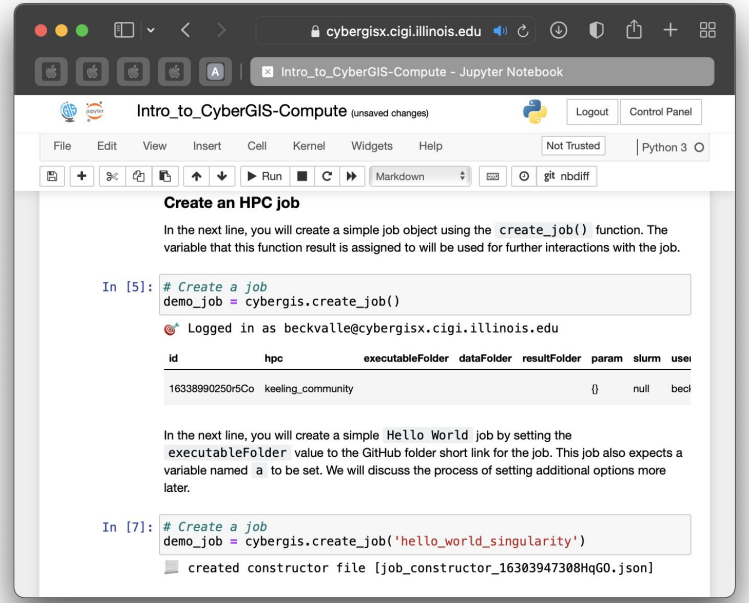
- Maintainer Pool has a multithreaded life cycle that spawns and oversees worker processes called **Maintainer Workers** that contain **logic** on submitting, stopping, resuming, and ending a task executing on a remote HPC resource
- A Maintainer Worker can use a **Connector** to interact with remote HPC via SSH

Connectors



- A Connector is a **long-living SSH connection** between the CyberGIS-compute core and HPC
- To reduce the connection rate, connectors are shared between Maintainer Workers and a **Mutex** is implemented to avoid race conditions in executing commands

SDK: Client Package



- A **Python-based Jupyter Notebook client** that integrates CyberGIS-Compute Core functionalities into CyberGIS-Jupyter
- Provides **seamless** interaction with HPC
- Provides **code-less** interactive UI

https://cybergis.github.io/cybergis-compute-python-sdk/index.html

Hands-On Part 1: Using the SDK

Please open this link:
https://github.com/cybergis/AAG2023-ComputeTutorial

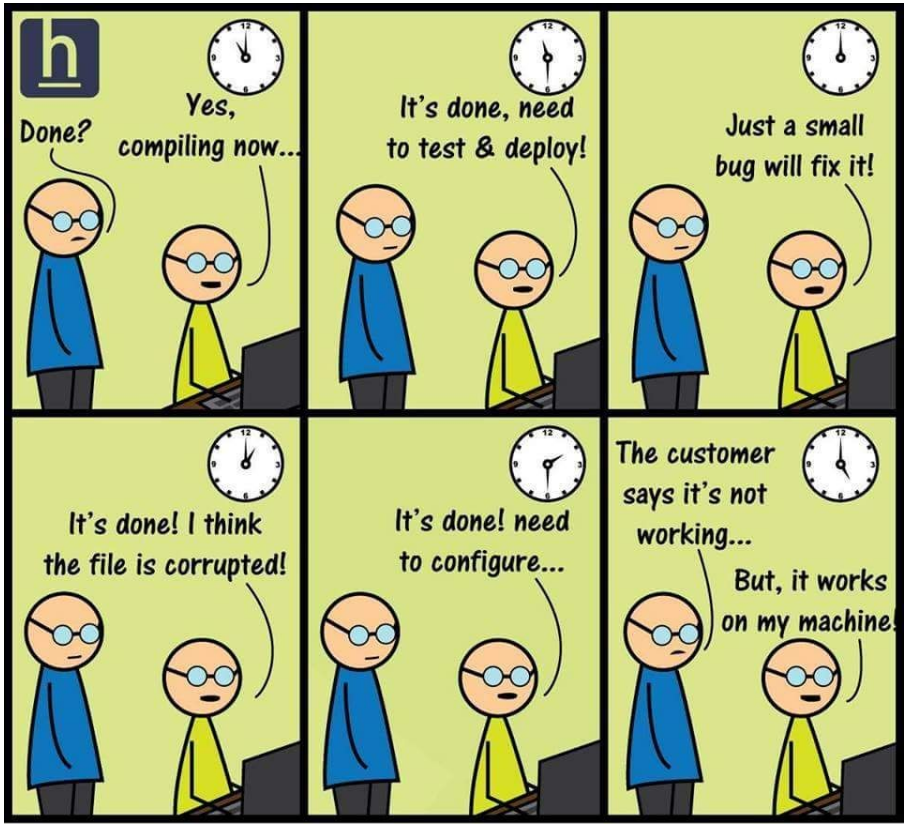
Navigate to CyberGISX (create an account if you don't have one)

Open the repo on CyberGISX

Seamless Access to HPC

Containerization: Run code in familiar environments

Transparently interfaces with batch systems (e.g. Slurm): Manage Slurm on behalf of developers



Why We use Containers

CyberGIS-Compute Contribute

CyberGIS-Compute Contribute allows users to **submit workflow code hosted on GitHub repositories** to be executed on HPC resources

Submissions are verified through a checking process

Provides configurations, system environment, and developer API

Git commit version lock for security

Contribution Process

github.com

```python
import json
import os

print('running main...\n')

print('./job.json\n')
job = json.load(open('./job.json',))

print('SLURM_NODEID\n')
print(os.environ['SLURM_NODEID'])

print('SLURM_PROCID\n')
print(os.environ['SLURM_PROCID'])

print('job_id')
print(os.environ['job_id'])
```

manifest.json

ready for HPC

Hands-On Part 2: Creating a Model

Please open this link:
https://github.com/cybergis/AAG2023-ComputeTutorial

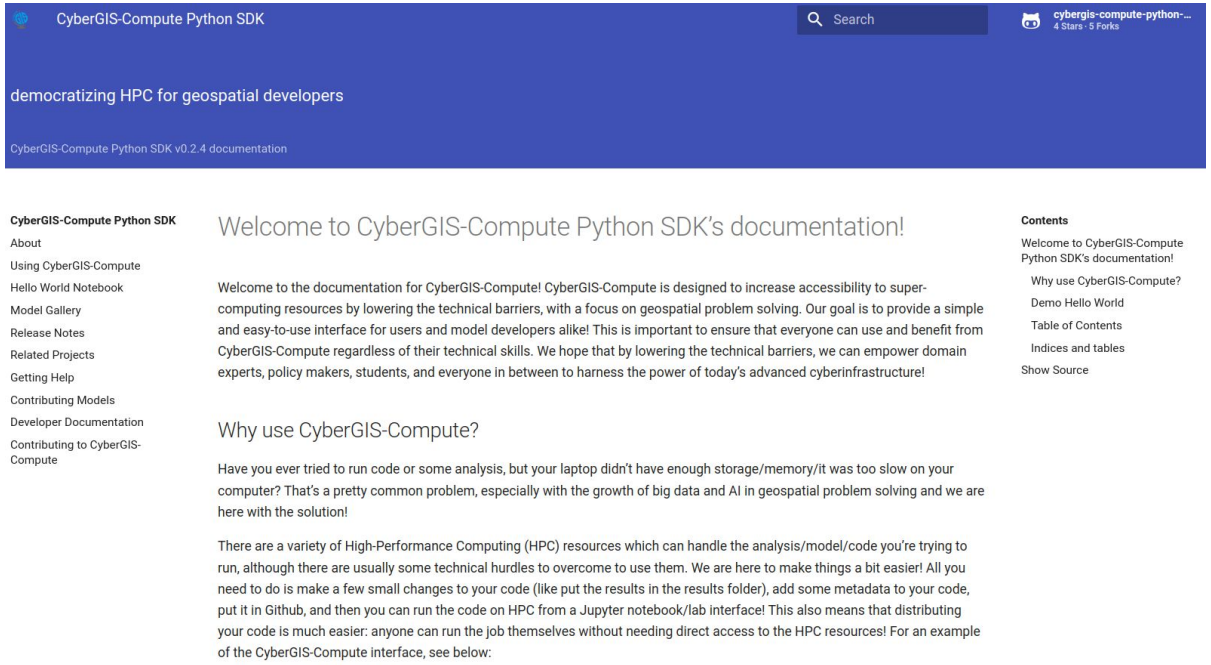
Go to the “cybergis-compute-examples” repo and follow the directions on the README.md

Next Steps for Contributing a Model

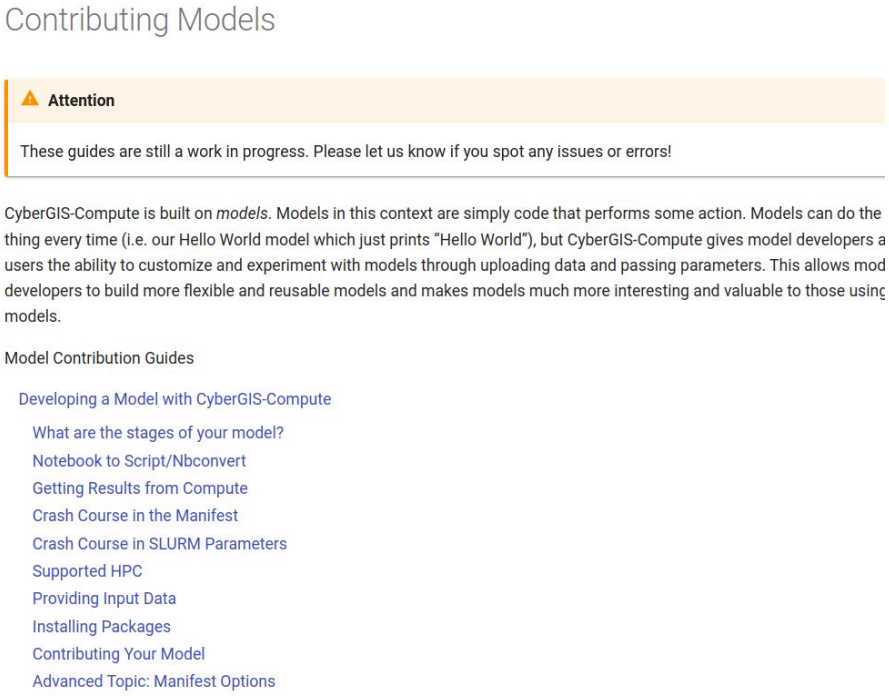
- Work with someone at the CyberGIS-Center (or other organization hosting a Core server) to have your model added.
- Test and debug your model just to make sure everything works.
- You're done and everyone else can now easily run your model on HPC!

Documentation

As you develop models, be sure to check out the CyberGIS-Compute documentation!



Contributing Models Docs



Contributing Models

Attention

These guides are still a work in progress. Please let us know if you spot any issues or errors!

CyberGIS-Compute is built on *models*. Models in this context are simply code that performs some action. Models can do the thing every time (i.e. our Hello World model which just prints "Hello World"), but CyberGIS-Compute gives model developers a users the ability to customize and experiment with models through uploading data and passing parameters. This allows mod developers to build more flexible and reusable models and makes models much more interesting and valuable to those using models.

Model Contribution Guides

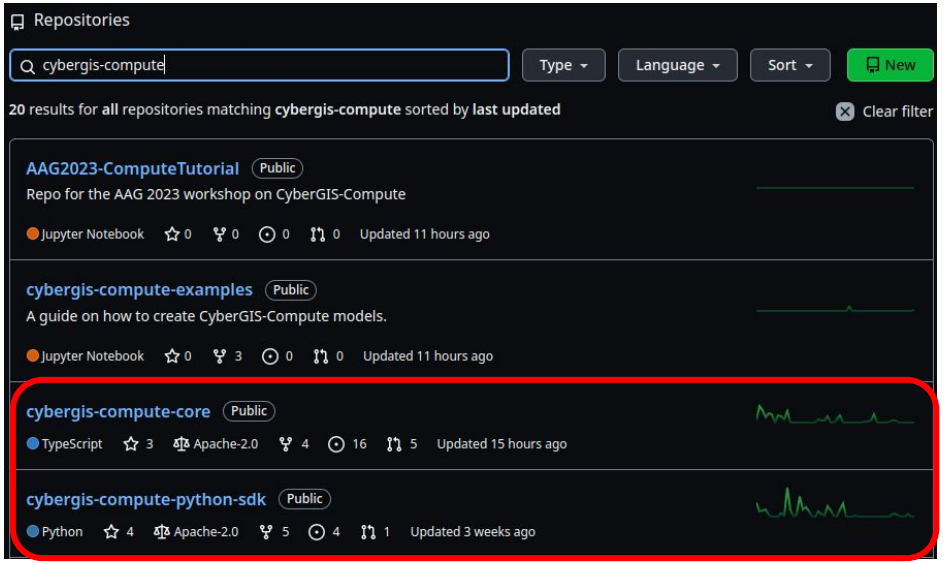
- Developing a Model with CyberGIS-Compute
  - What are the stages of your model?
  - Notebook to Script/Nbconvert
  - Getting Results from Compute
  - Crash Course in the Manifest
  - Crash Course in SLURM Parameters
  - Supported HPC
  - Providing Input Data
  - Installing Packages
  - Contributing Your Model
  - Advanced Topic: Manifest Options

We have documentation on our site to guide you through creating a model!

It also details advanced options and answers FAQs!

Developers Welcome!

Both the Core and SDK are open-sourced and available on Github for anyone interested in contributing to the codebase!



Works in Progress

- **Eliminating containers**. You just use CyberGIS-Jupyter kernels!
- **Simplified UI.** A simplified UI for model users to avoid overwhelming them.

We hope to have these changes rolled out over the next year.

CyberGIS-Compute Team

- Mit Kotak
- Alexander Michels
- Anand Padmanabhan
- John Speaks
- Shaowen Wang
- Zimo Xiao
- Taylor Ziegler

Links

Project Development doc:

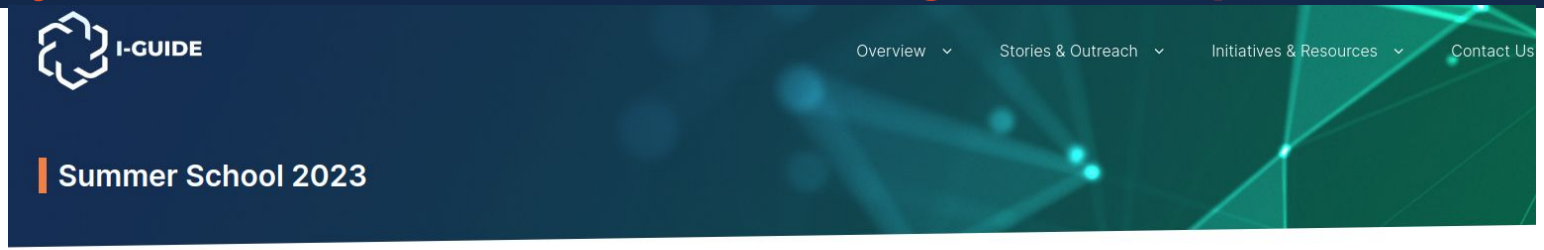
http://github.com/cybergis/cybergis-compute-core

SDK doc:

http://github.com/cybergis/cybergis-compute-python-sdk

Hello World doc:

http://github.com/cybergis/cybergis-compute-hello-world



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Convergence Science in Action

UCAR campus in Boulder, Colorado
August 7-11, 2023

The Institute for Geospatial Understanding through an Integrated Discovery Environment, I-GUIDE, will lead a week-long Summer School in August 2023 on ***Convergence Science in Action.*** Certain complex and compelling societal problems require a convergent research approach, when knowledge, tools, and modes of thinking from multiple disciplines are strategically integrated and merged. About 25 graduate students and early career scholars will collaborate with project members of I-GUIDE to develop novel solutions to complex problems that rely on computation- or data-intensive geospatial data science. The participants will experience the collaborative and professional interactions that are key to comprehensively working on convergence science problems, including geoethics, geo-enabling reproducible and open science, geovisualization, and geoAI and spatial data science via cloud and high-performance computing.

This year our application areas will include topics such as climate change, biodiversity, water security, sustainable development, and implications of these as studied via social science data.

The Summer School will be hosted on the UCAR campus in Boulder, Colorado, from Monday August 7 to Friday, August 11, 2023. If you are a graduate student or early-career scholar new to geospatial data science and want to learn more about integrating this into your research, or are already working with data-intensive geospatial science approaches, this Summer School will offer new and exciting opportunities for your professional development, and will help you develop interdisciplinary skills and build new connections with others in related fields.

Learn more:

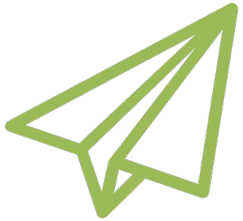
https://iguide.illinois.edu/summer-school-2023/

Acknowledgments

- **National Science Foundation**
  - 2118329
  - XSEDE
- Virtual ROGER

Thanks !

Comments / Questions?



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