# SimplifyHPC: A Framework to Simplify HPC Codes Deployment

## NASA SBIR Phase I

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**Advanced Modeling & Simulation (AMS) Seminar Series**
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*Established 2009; Headquarters: San Diego, CA*

# EP Analytics

- As performance analysis, code modernization, and optimization experts, we utilize specialized tools and methodologies to develop performance characterizations of HPC applications and systems
  - Specialized tools to analyze production applications running on cloud resources and production HPC systems
  - Methodologies determine computations within applications that are affected by (or are sensitive to) the limitations of the systems/hardware
- Expertise in analyzing HPC workloads from DoE, NNSA, NSF, NASA, & DoD



**Laura Carrington, PhD**
Co-Founder, CEO

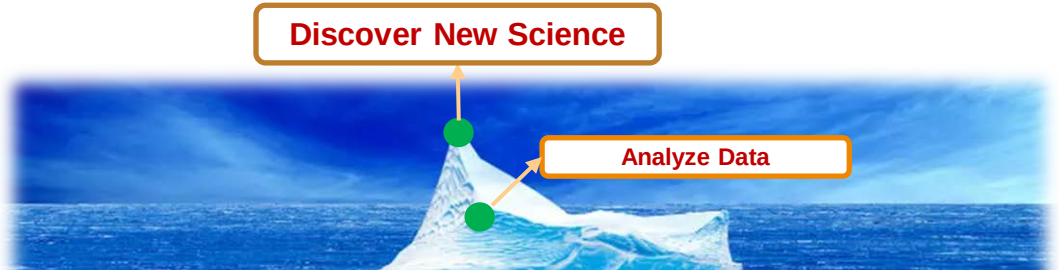


**Ananta Tiwari, PhD**
Principal Investigator



**Sarom Leang, PhD**
Senior Computational Scientist

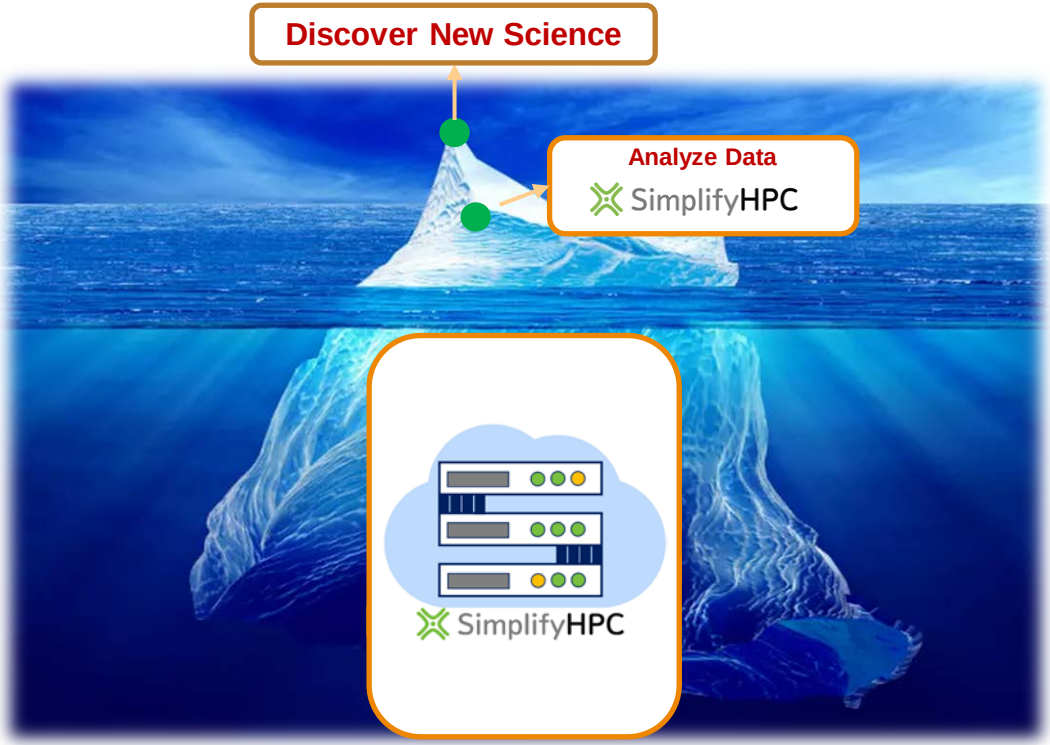
# HPC Codes are Complex



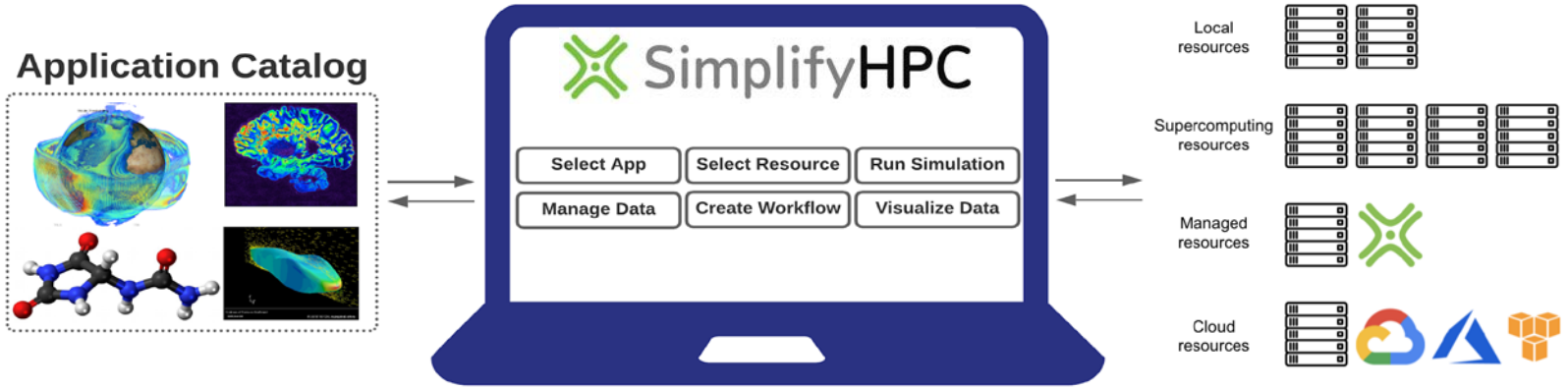
# HPC Codes are Complex



# HPC Codes are Complex



# SimplifyHPC Overview



# Key Components of SimplifyHPC

- Data manager: keeps track of all the calculations and simulation data
  - A centralized methodology that helps avoid data loss, which can lead to duplicated calculations
  - Fosters **reproducibility**
  - Allows for easy **sharing** of scientific results

- Visualization manager: provides domain- and application-specific visualization capabilities
  - Plug-and-Play integration of third-party visualization tools
  - Supports **in-situ** (or remote) visualizations to reduce data movement costs

- Performance manager: monitors and analyzes the performance of codes
  - Ensures optimal turnaround times for simulations
  - Allows for cost-performance tradeoff studies

# Key Components of SimplifyHPC

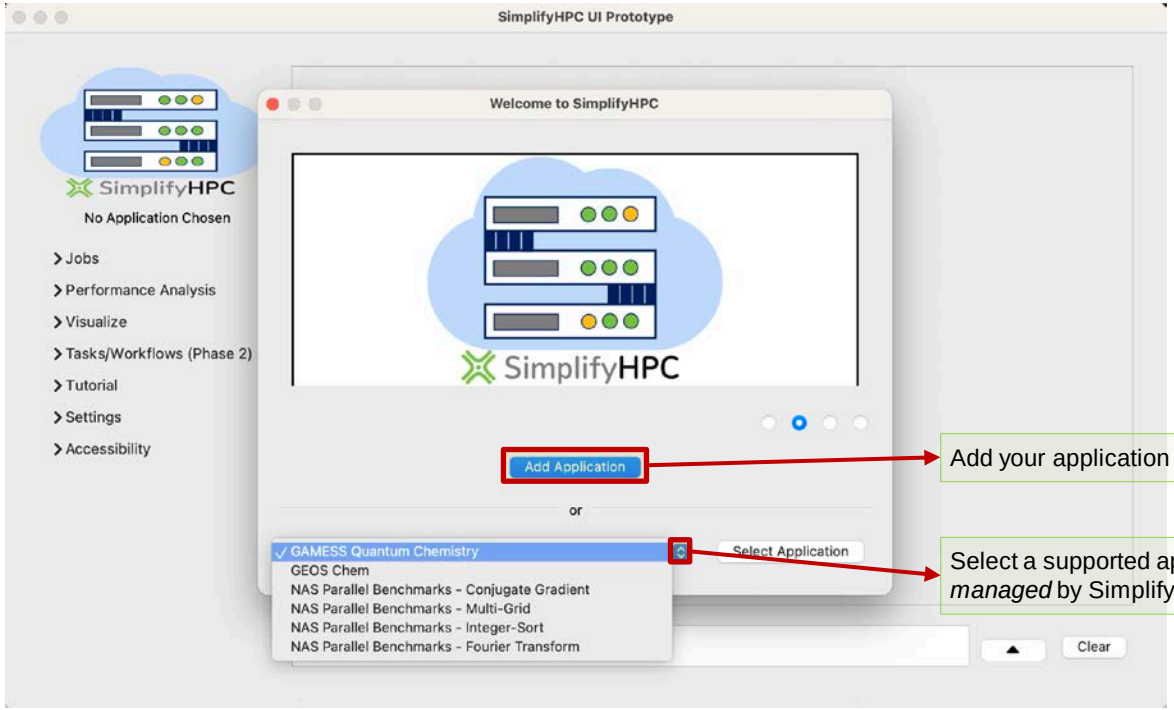
- Resource manager: manages the computational resources and stages simulations
  - Can farm out calculations to the cloud resources with a click of a button
    - NASA's interest in cloud HPC is well-documented
  - Add your own resources
    - Supported resources: remote Linux-based clusters with SLURM/PBS queues, private cloud resources and local Desktop/Laptop

- Software-as-a-service (SaaS): provides access to cloud resources managed by EP Analytics
  - Infrastructure-as-Code (IaC)
  - Customized machine images (or AMI) in Phase I; containers in Phase II
  - Pay-per-use

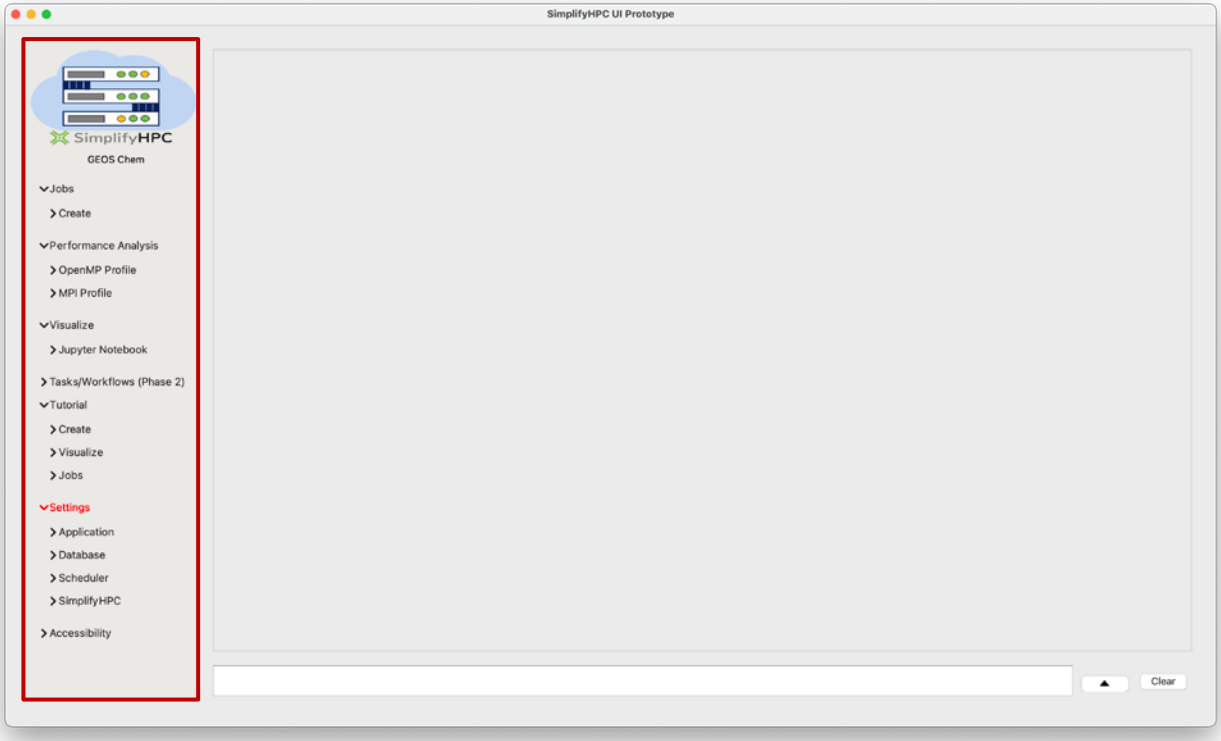
# Key Components of SimplifyHPC

- Application portfolio: HPC codes managed by EP Analytics
  - GEOS-Chem: atmospheric chemistry code
    - SimplifyHPC is a tool that has the potential to **radically transform** the GEOS-Chem community. SimplifyHPC gives users an intuitive graphical interface that can be used to **configure and run GEOS-Chem and visualize** the results. It **facilitates reproducibility** and **builds performance analysis right into the GUI**, making it almost trivial to identify poorly performing code. – *Mr. Robert Yantosca, Senior Software Engineer, GEOS-Chem Support Team*
    - Dr. Daniel Jacob, GEOS-Chem Model Scientist, has expressed interest in making SimplifyHPC "accessible to the GEOS-Chem community by being incorporated into the standard model as an option for 'out-of-the-box' simulations and advertised as such on the GEOS-Chem website"
  - GAMESS: computational chemistry code with more than 100K users worldwide
  - In initial discussions with the application teams for FUN3D, OVERFLOW and CART3D
  - Let us know if you are interested in adding your application to our portfolio!

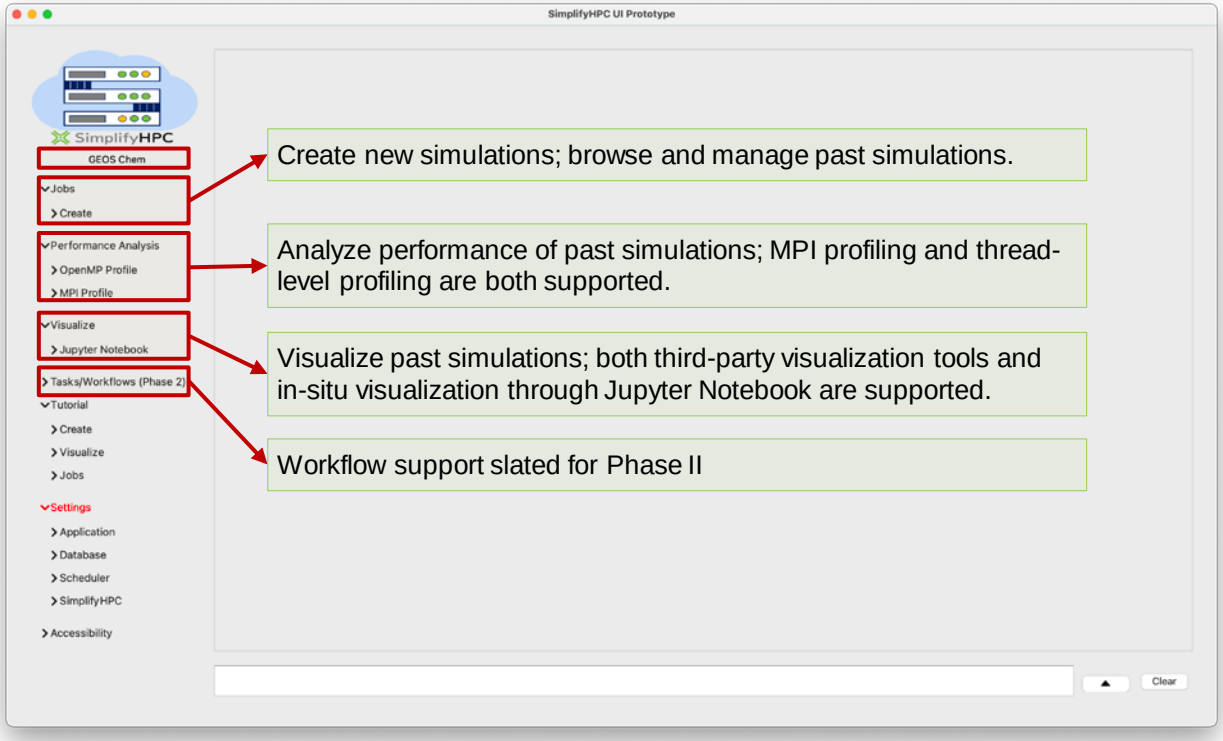
# The Front-door



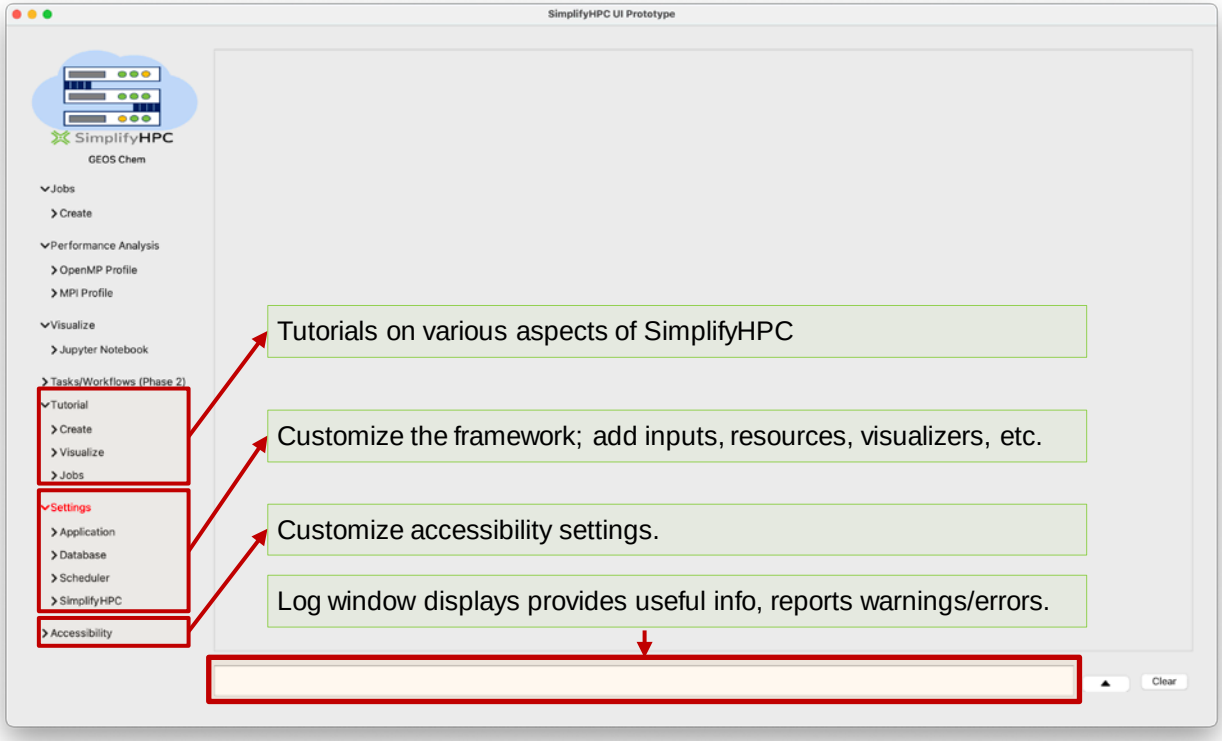
# Accordion-style navigation



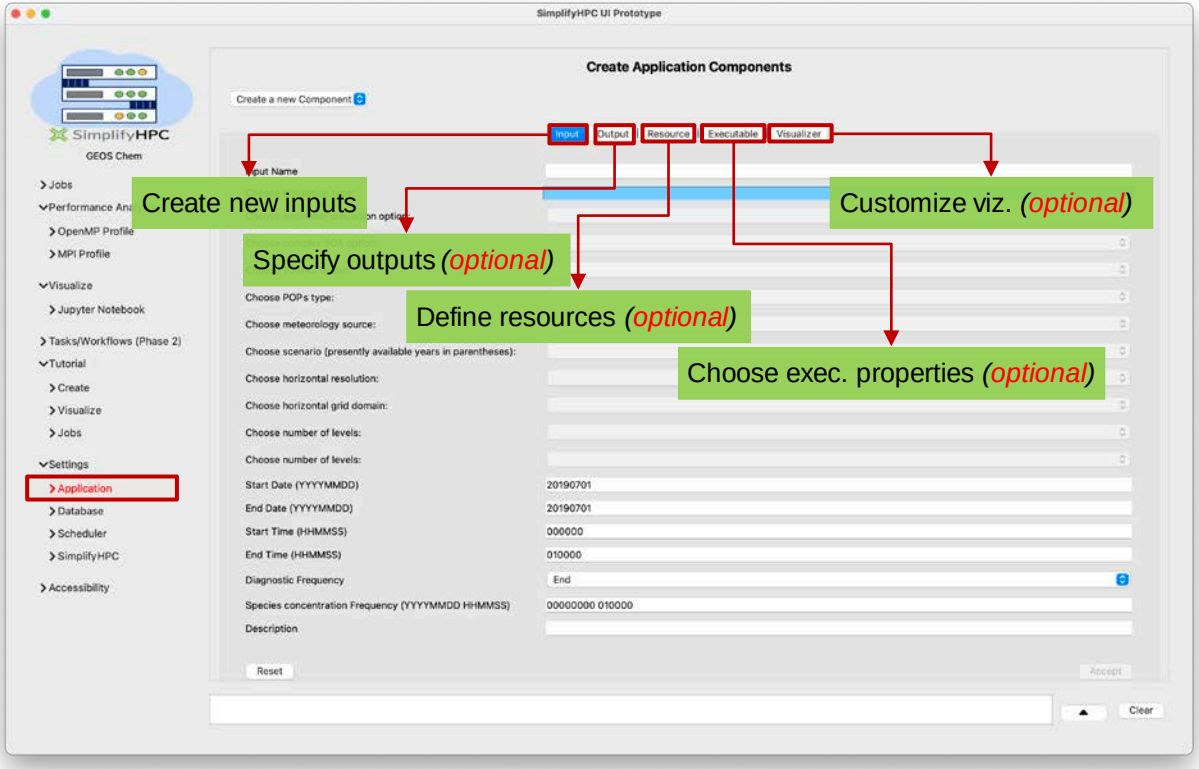
# Accordion-style navigation



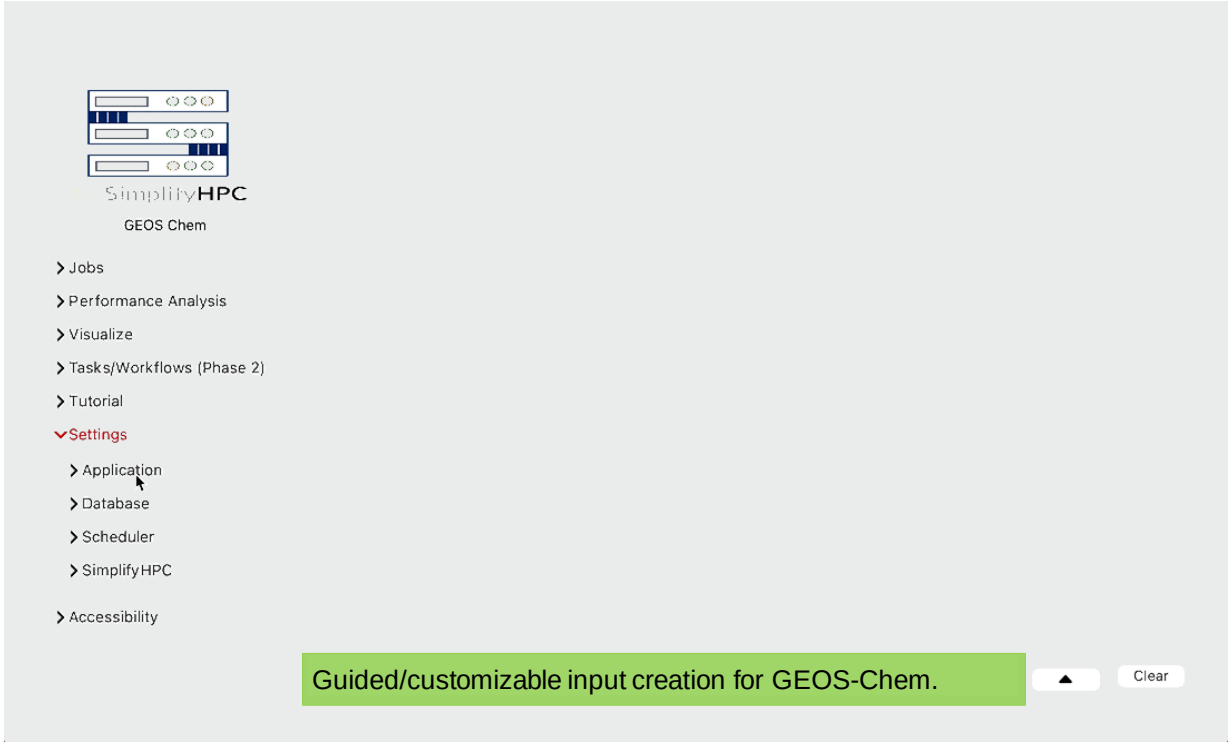
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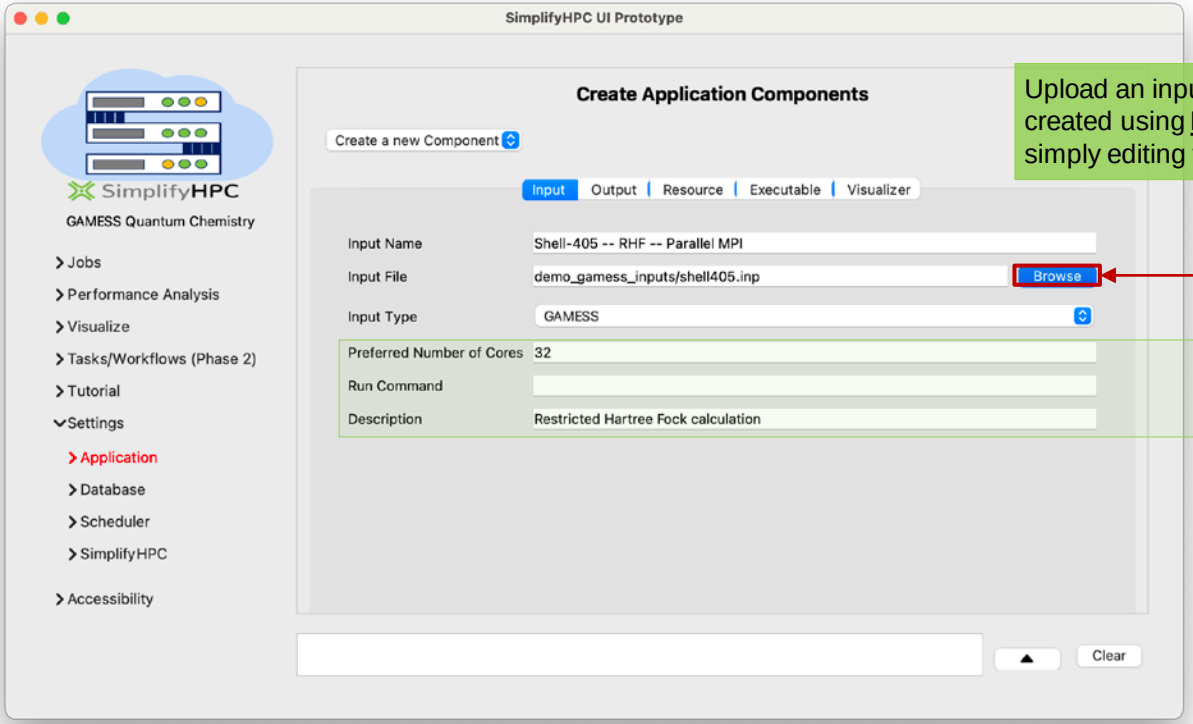
# Application Customization



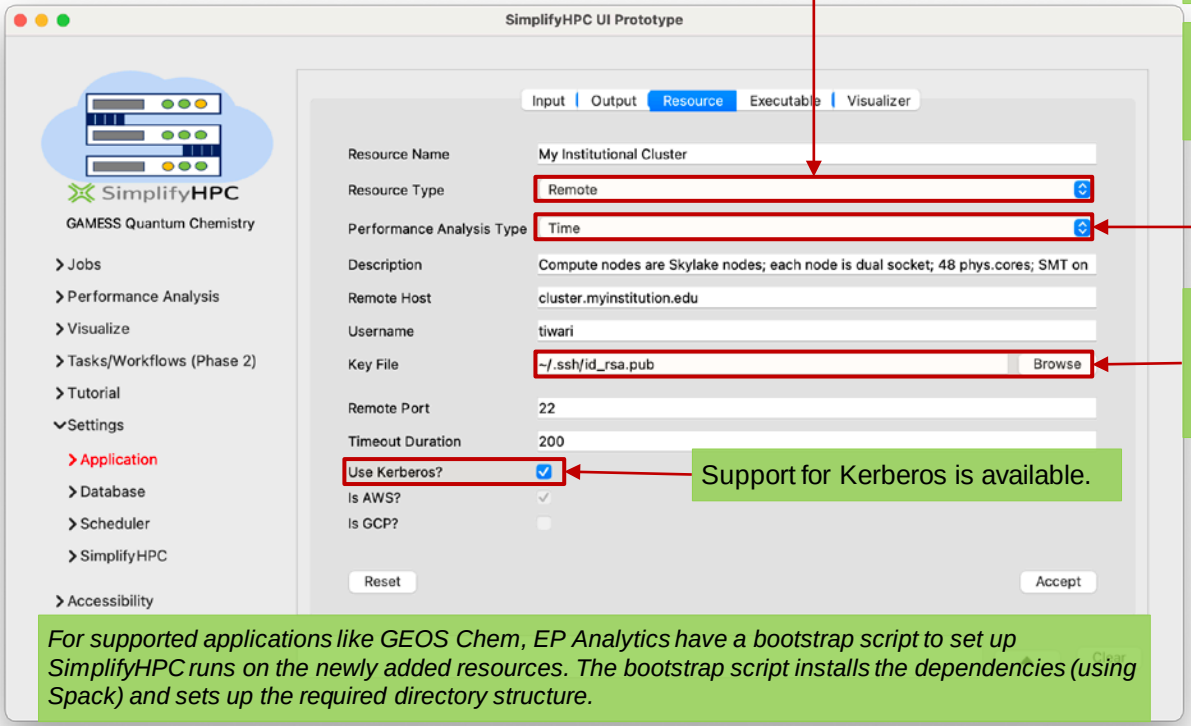
# Creating an Input – GEOS-Chem



# Creating an Input – GAMESS



# Adding a new resource




Options: Remote, Private Cloud

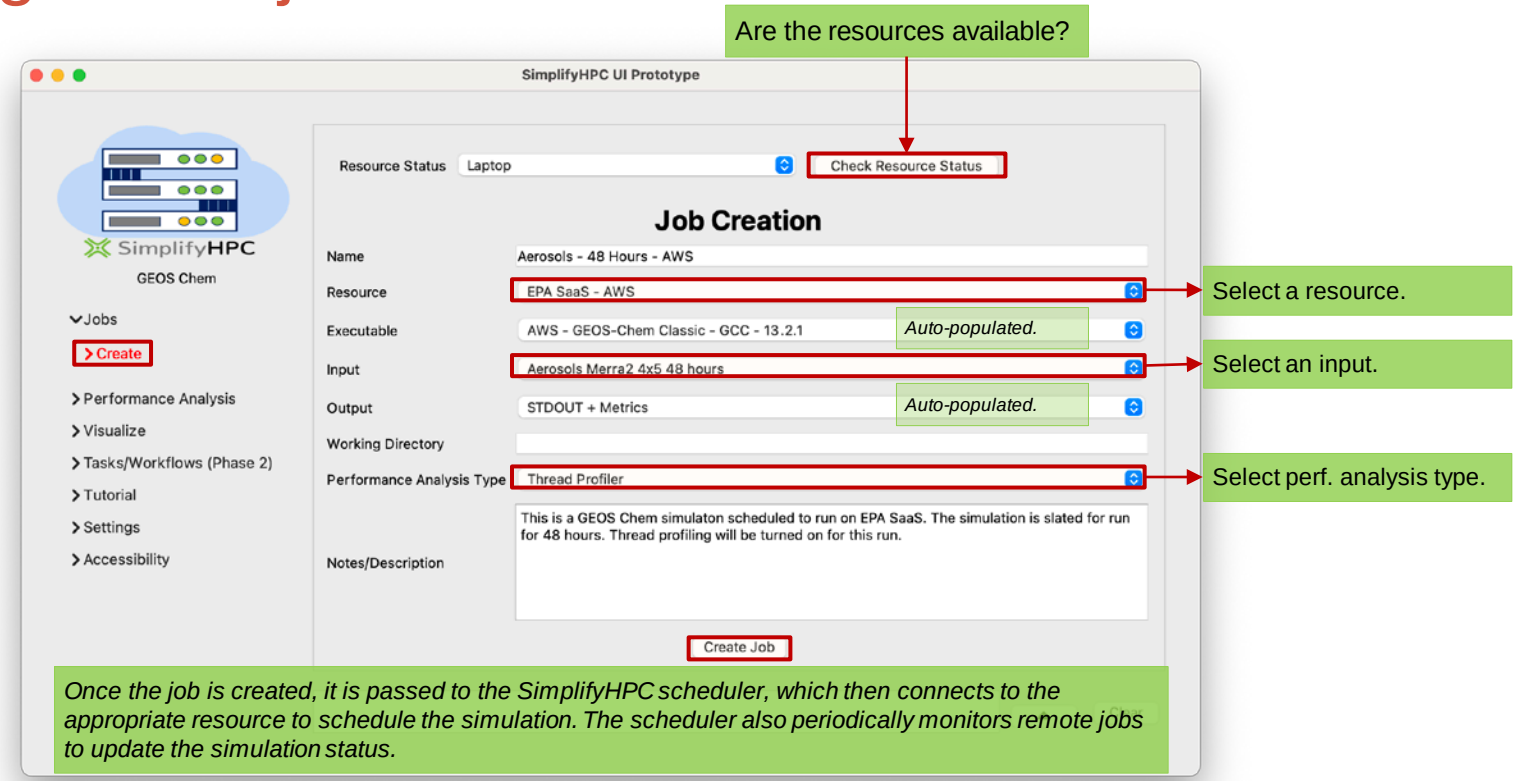
Options: Execution time, MPI Profiling and Thread Profiling

For private cloud resources, this will be the key provided by your admin.

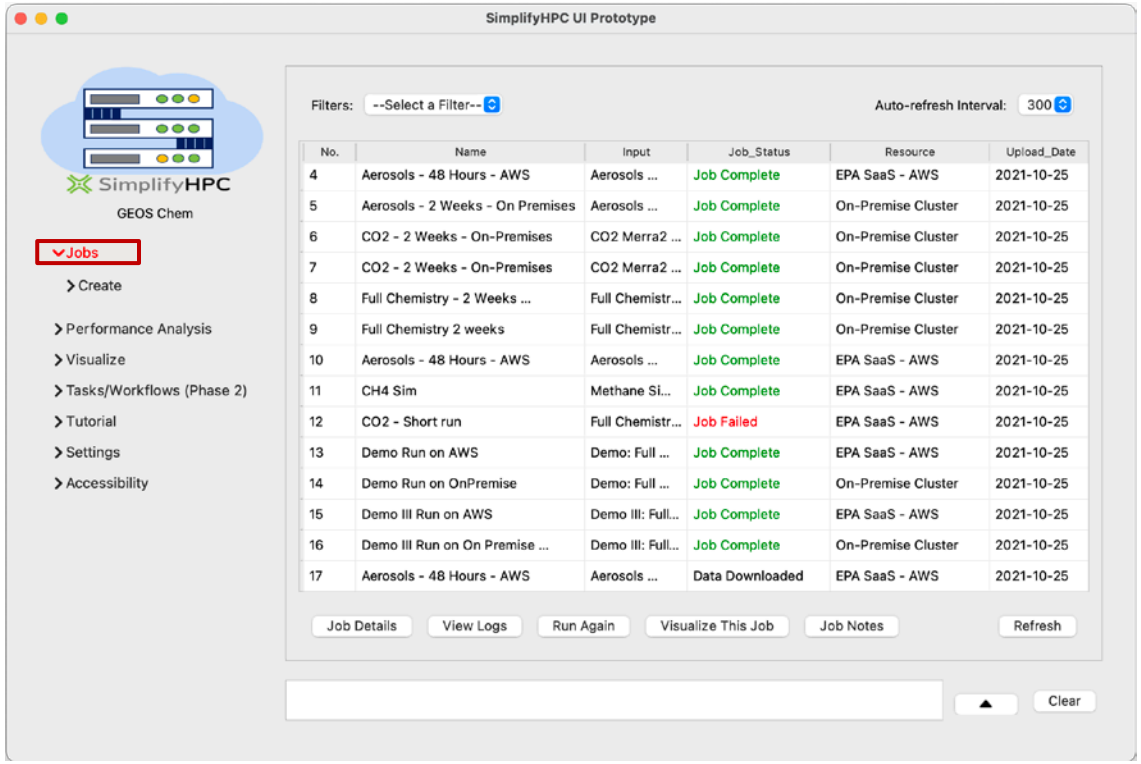
Support for Kerberos is available.

*For supported applications like GEOS Chem, EP Analytics have a bootstrap script to set up SimplifyHPC runs on the newly added resources. The bootstrap script installs the dependencies (using Spack) and sets up the required directory structure.*

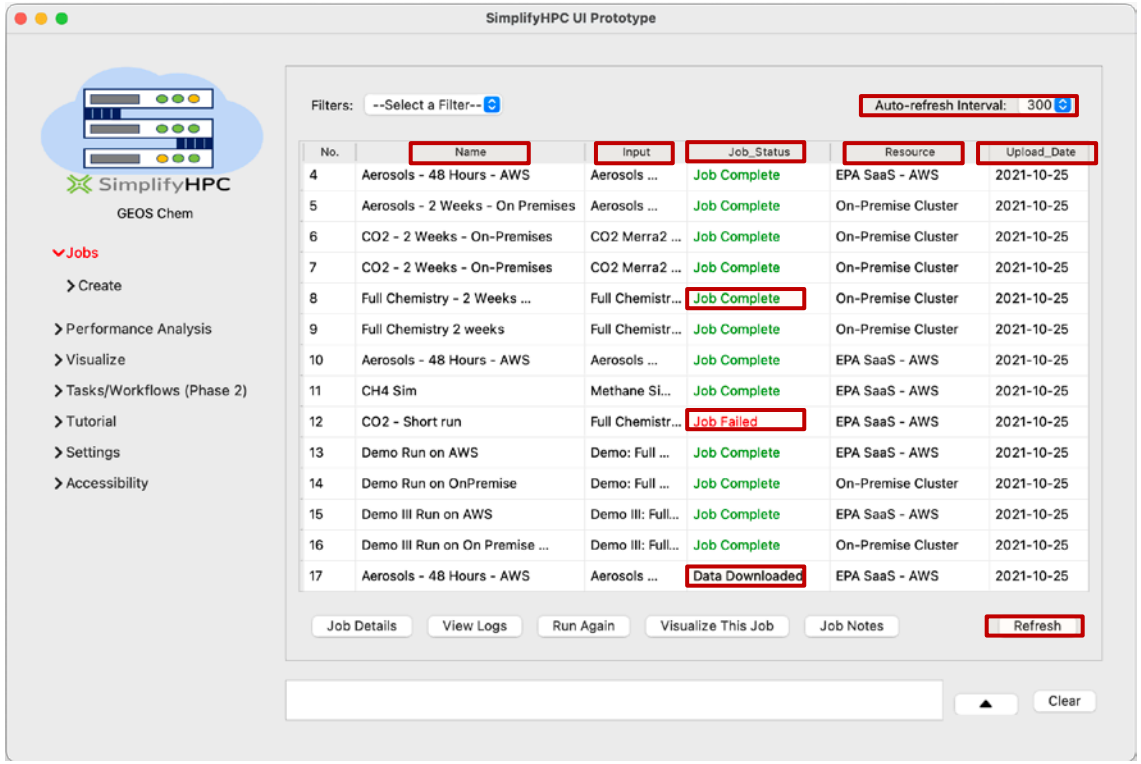
# Submitting a new job



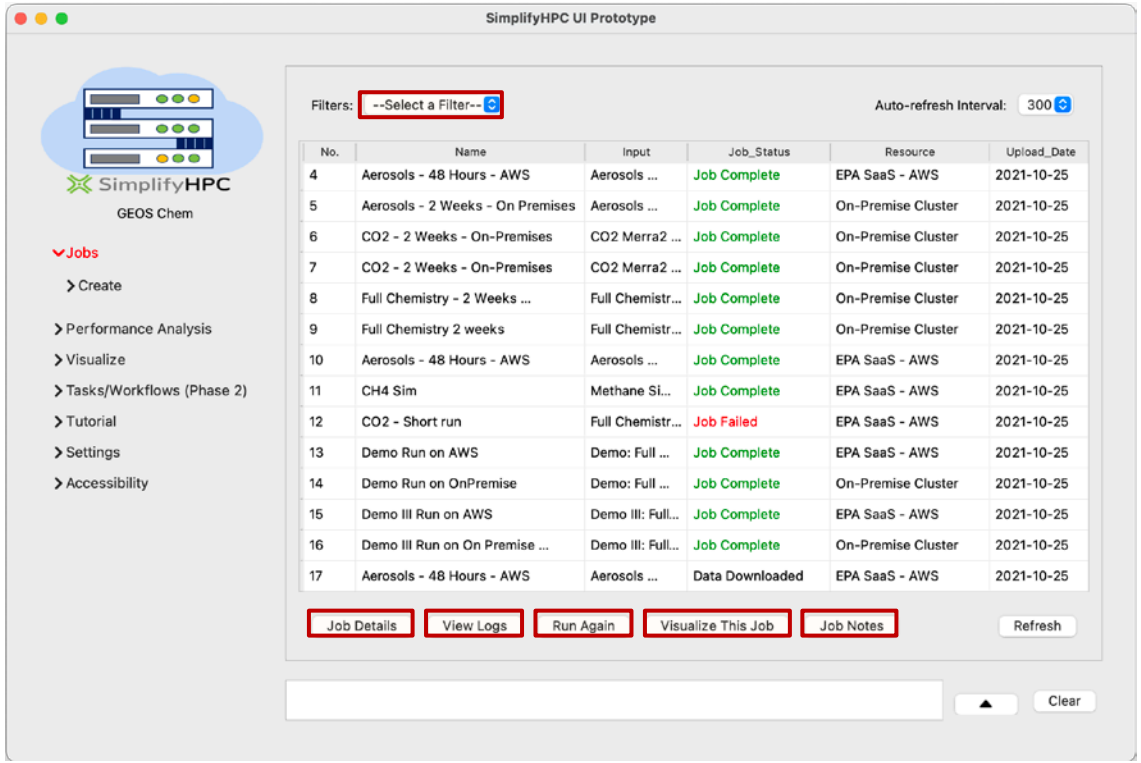
# The Job Dashboard



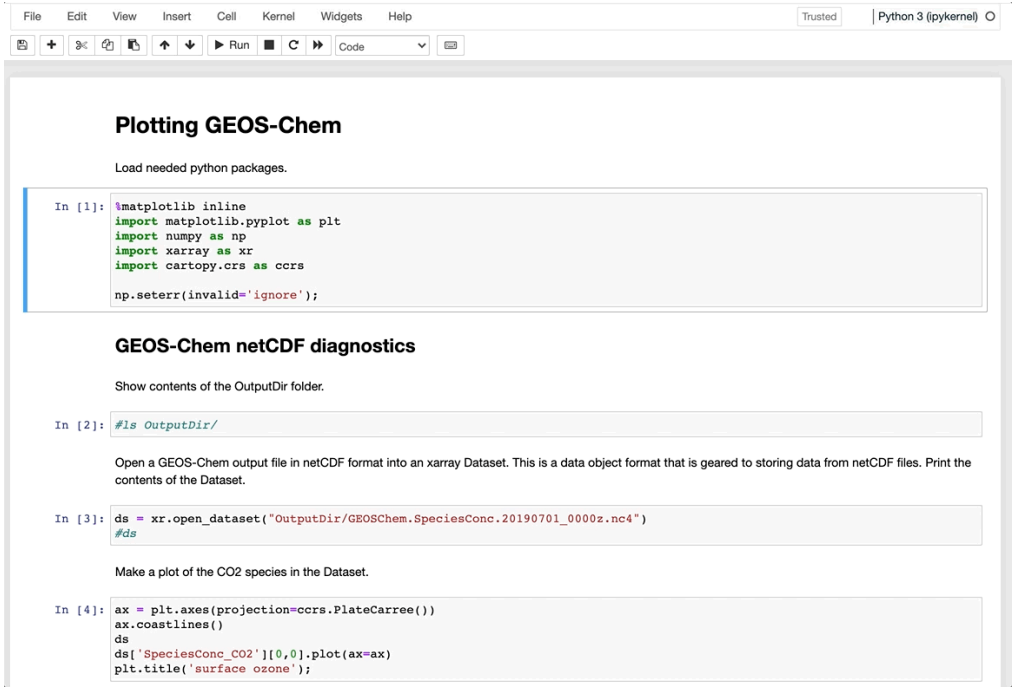
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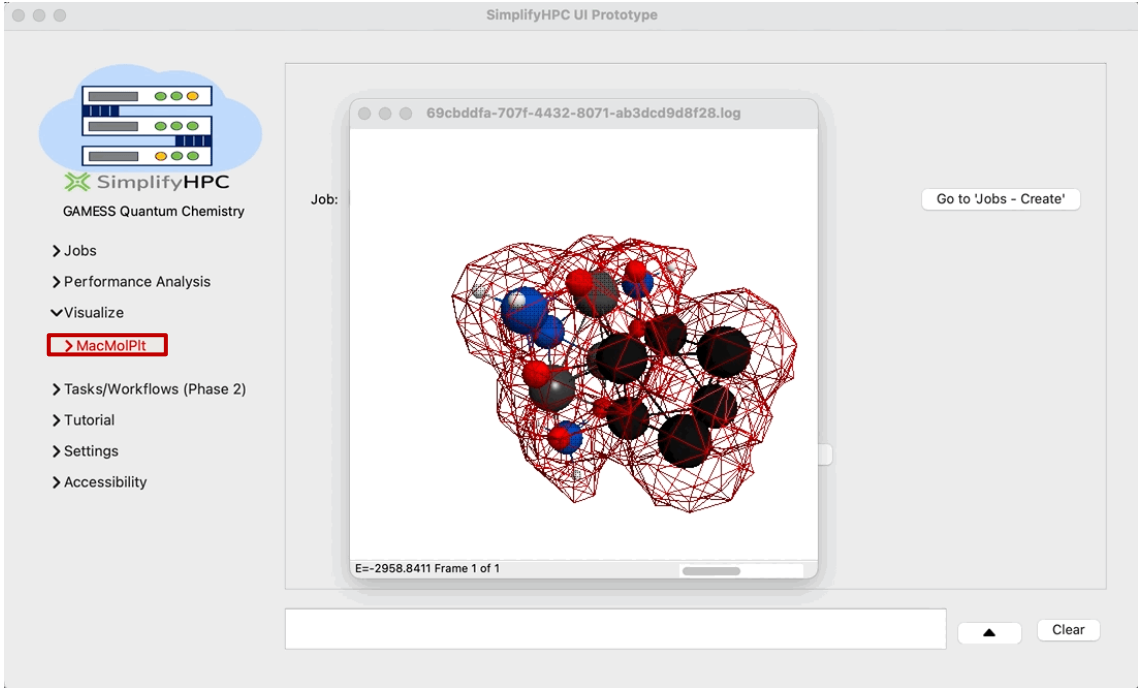


# Visualize a job – interactive and in-situ

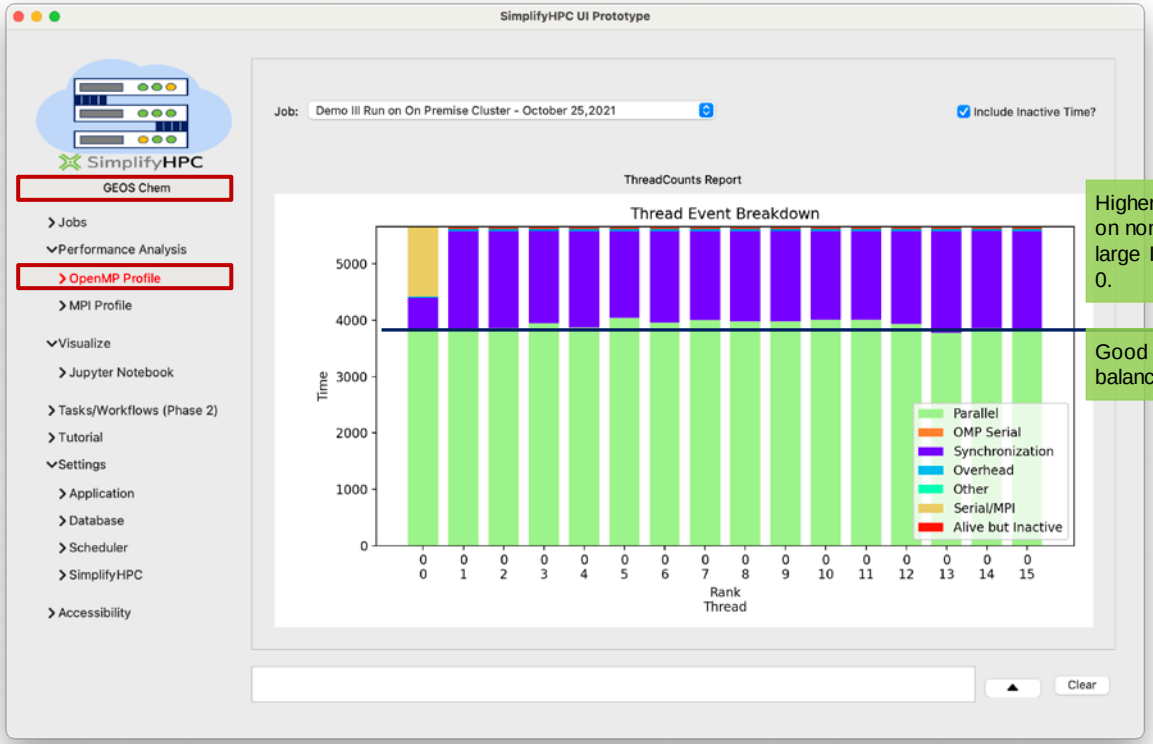



Large data-files do not leave the cloud resources.

# Visualize a job – third-party tools



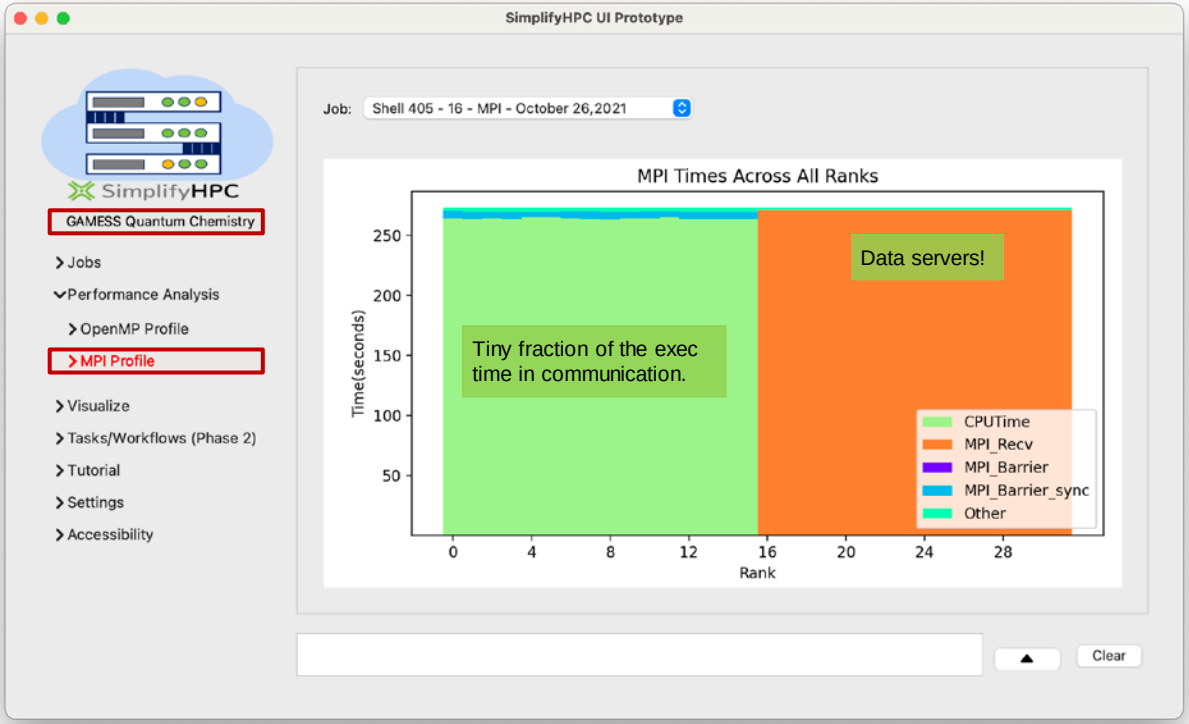
# In-depth performance analysis – thread-level profile



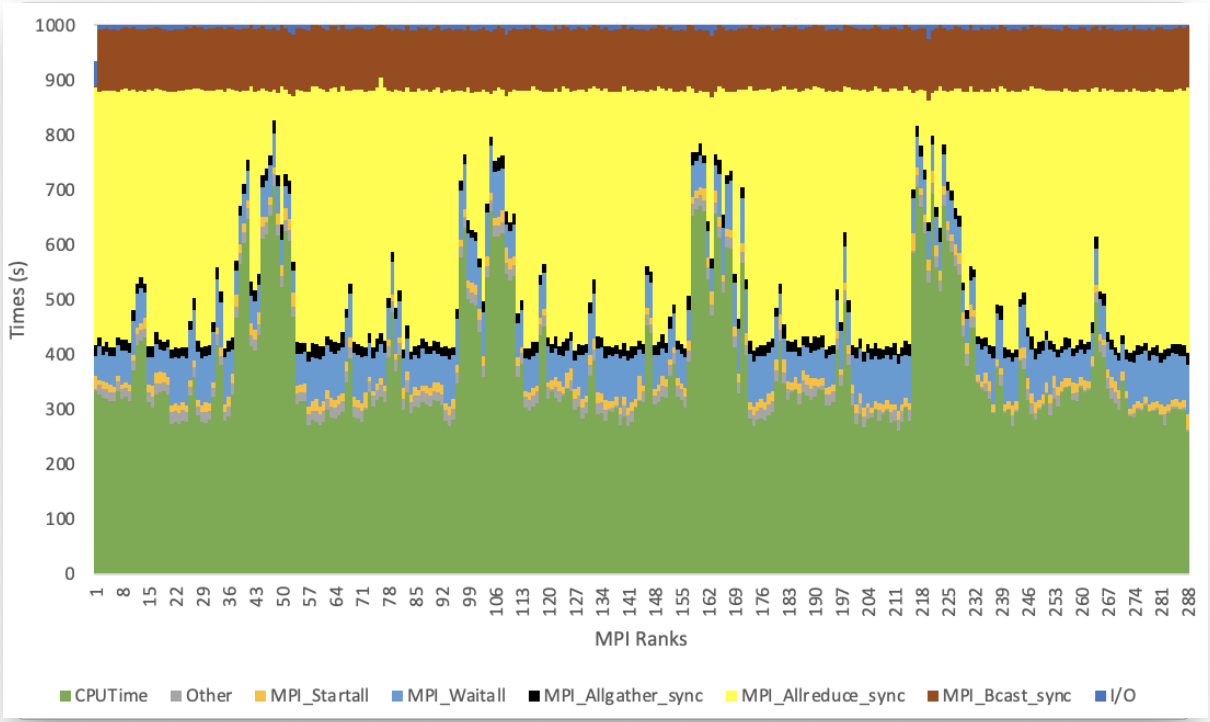

Higher synchronization times on non-zero threads due to large I/O activities on thread 0.

Good thread-level load balancing

# In-depth performance analysis – rank-level profile



# In-depth performance analysis – rank-level profile



# Phase II

- Full-featured SimplifyHPC framework
  - Build on the prototypes developed in Phase I
- Extend SaaS to include all major cloud service providers (CSPs)
  - Allow for easy mobility across the CSPs based on cost-performance tradeoffs
- Develop container based methodology to handle multi-platform deployment of HPC codes
- Extend performance analysis features to include fine-grained analysis of MPI and OpenMP hotspots
- Develop workflow manager
- Extend the application portfolio and customer base
  - *Contact us if you would like us to integrate your application within the SimplifyHPC framework in Phase II*

# QUESTIONS / THANK YOU

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