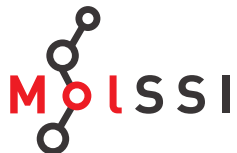


Distributed, high-throughput quantum chemistry with QCArchive and Parsl

Benjamin Pritchard

Molecular Sciences Software Institute
Virginia Tech

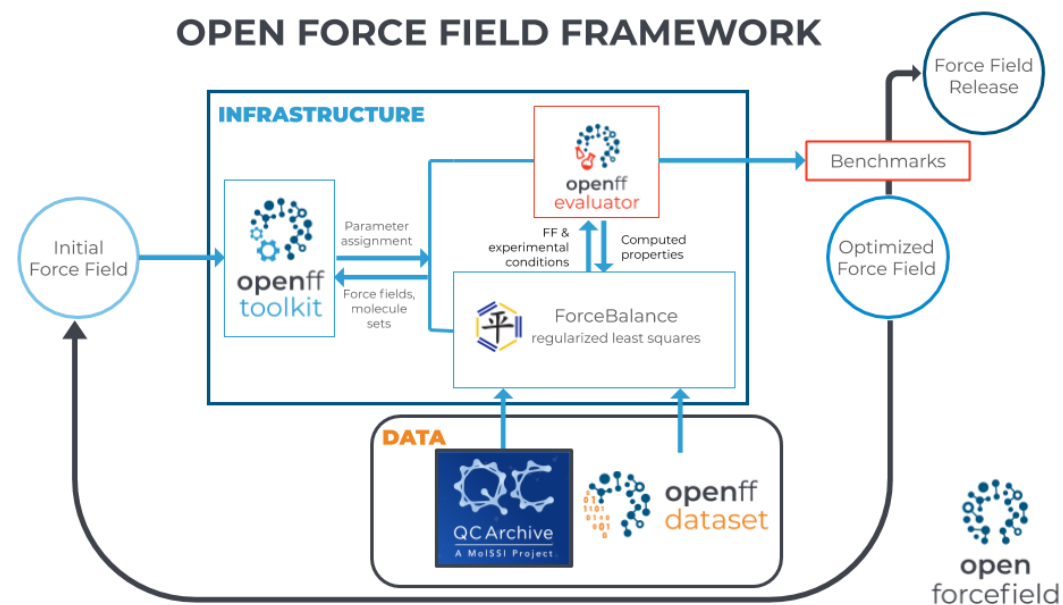


Data generation is important

Many areas require high-quality simulations

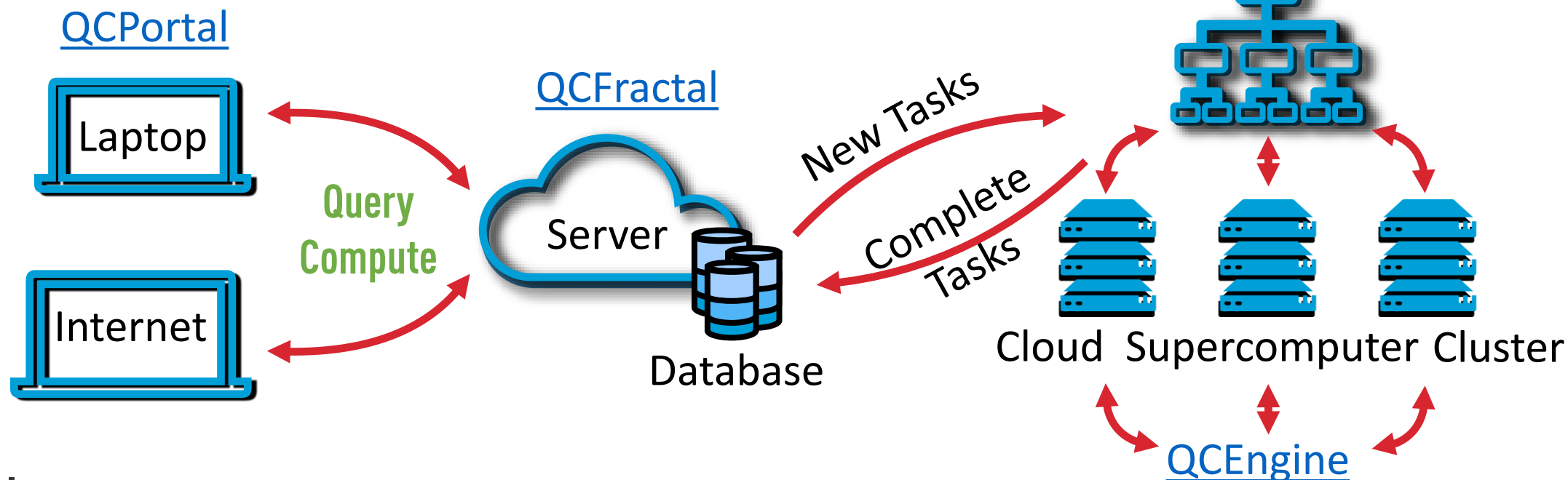
- Artificial Intelligence/Machine Learning
- New classical force fields
- New semi-empirical models
- Reaction networks/pathways
- Old-fashioned data analysis

- **New discoveries will require new data**
- Quantum chemistry is one source



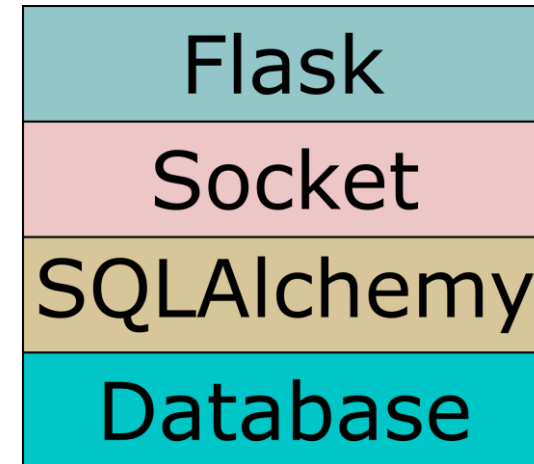
QCArchive

- Started in 2019 by Daniel Smith
- High-throughput quantum chemistry
- Laptop to multi-physical site orchestration
- Can run many different QM programs
- Share & collaborate via structured data
- Self-hosted
- Modular, with reusable components (QCElemental, QCEngine)



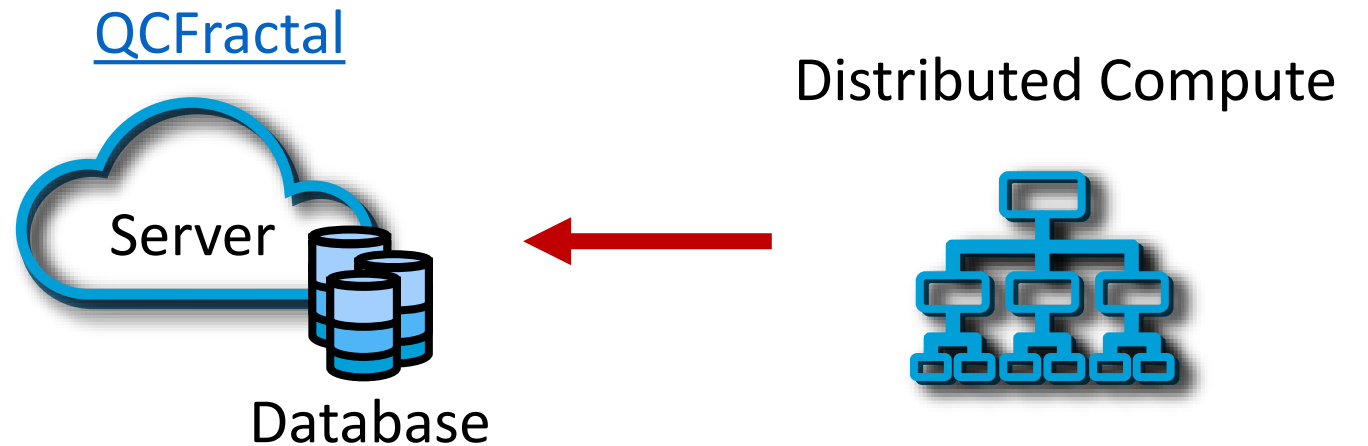
Server Software stack

- Postgres database + SQLAlchemy
- Alembic – database migrations
- Flask – web API
- Requests – Client HTTP access
- Pydantic – validation (lots of it)
- Extensive use of type hints
- Pytest + Github actions
- Docker/Docker compose – coming!



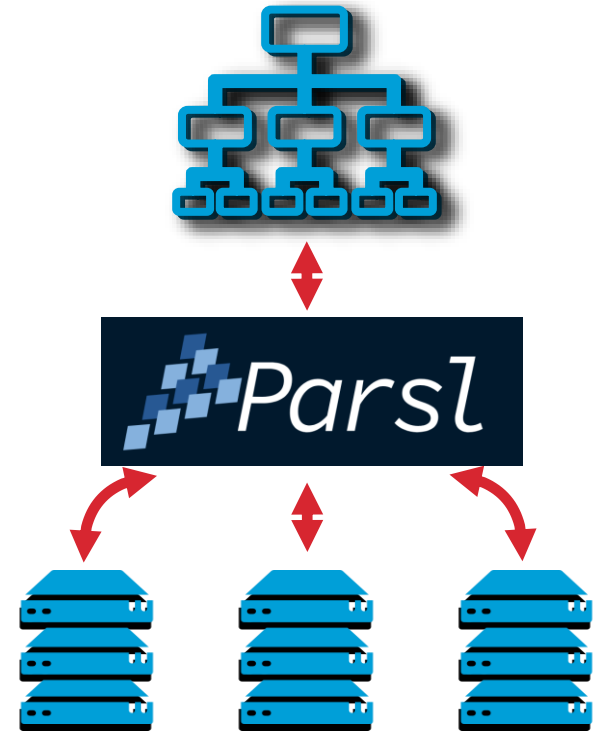
Task Distribution

- QCArchive works with a pull-based model
- Advantages:
 - Easy to scale
 - Bypasses authentication issues



Task Computation

- Compute worker then needs to do something with the task
- **Can submit tasks to HPC via Parsl!**
- Manager process runs on head node, connecting to server
- This process uses Parsl to submit/manage tasks with Slurm



MolSSI QCArchive Server

- MolSSI has its own server
- Current stats:
 - **109M** computations
 - **3.7TB** of data
- Starting to outgrow our server



Advanced Research Computing



Future

- Major work is on-going in a separate branch
 - Expected release: November
- Stable for new instances
- MolSSI-hosted service for other users?
- Looking to expand/polish capabilities related to Parsl
 - Possible hosting with the main server?

Thank you!

Interested in QCArchive? Questions?

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