Reproducible Quantum Chemistry in JupyterLab

Chris Harris (Kitware)

@openchem

O'REILLY

jupytercon

Overview

- Scientific Use Case
- Why Jupyter?
- Approach
- Demo
- Architecture
  - Backend
  - Frontend
- Deployment
- Future

Project and Team

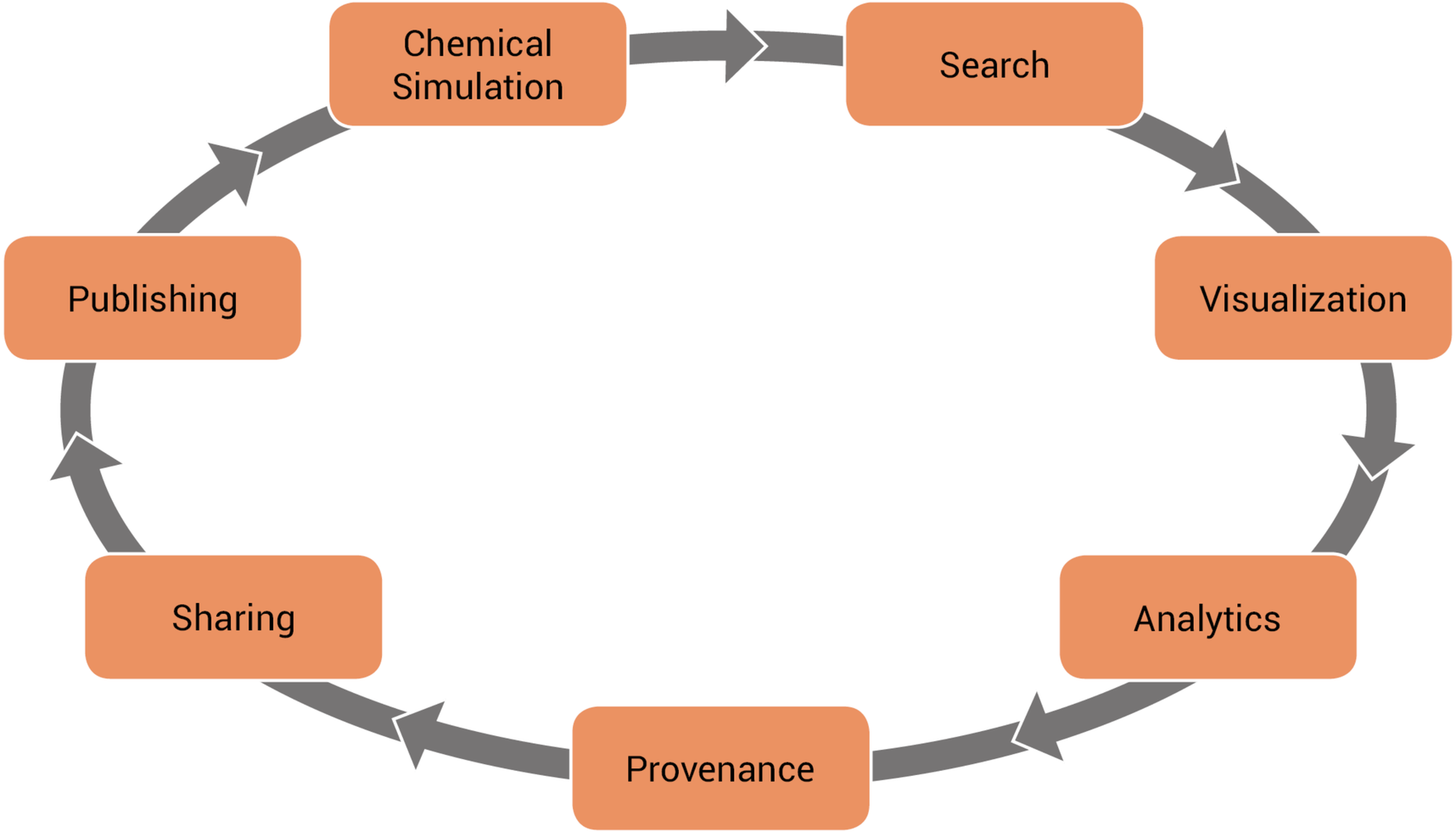
- Department of Energy SBIR Phase II (Office of Science contract DE-SC0017193)
- Marcus D. Hanwell (Kitware)
  - Background in physics, experimental data, nanomaterials, visualization
- Chris Harris (Kitware)
  - Computer science, AI, HPC
- Bert de Jong (Berkeley Lab)
  - Developer of NWChem computational chemistry code, machine learning, quantum computing
- Johannes Hachmann (SUNY Buffalo)
  - Expertise in chemistry, machine learning, chemical library generation

Scientific Use Case

- Using quantum mechanics to characterize chemical systems
- Has seen vast improvements in both veracity and volume of data
- Lack of transparent and reproducible workflow
  - Ad-hoc data management
  - Complexity associated with codes
  - The intricacies of HPC

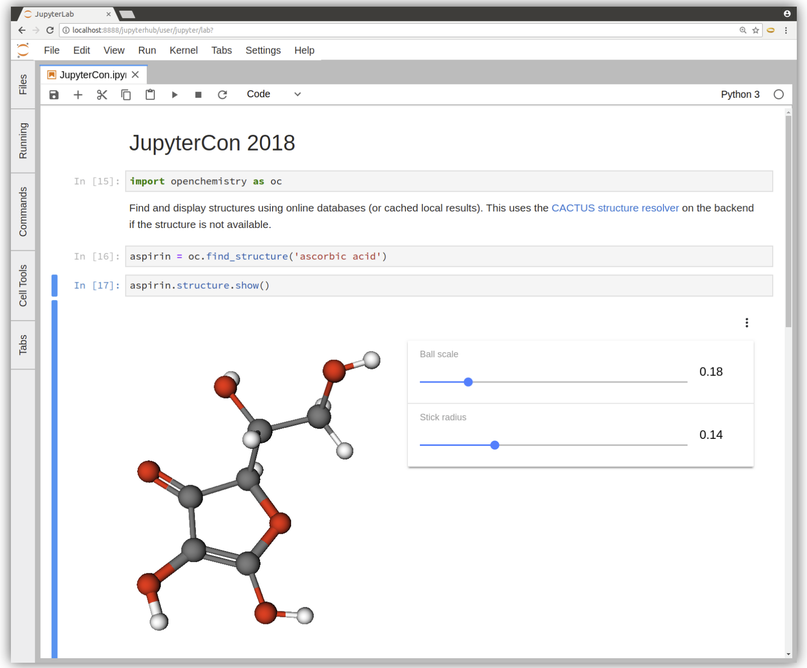
$$\left[\frac{-\hbar^2}{2\mu}\nabla^2 + V(\mathbf{r})\right]\Psi(\mathbf{r}) = E\Psi(\mathbf{r})$$

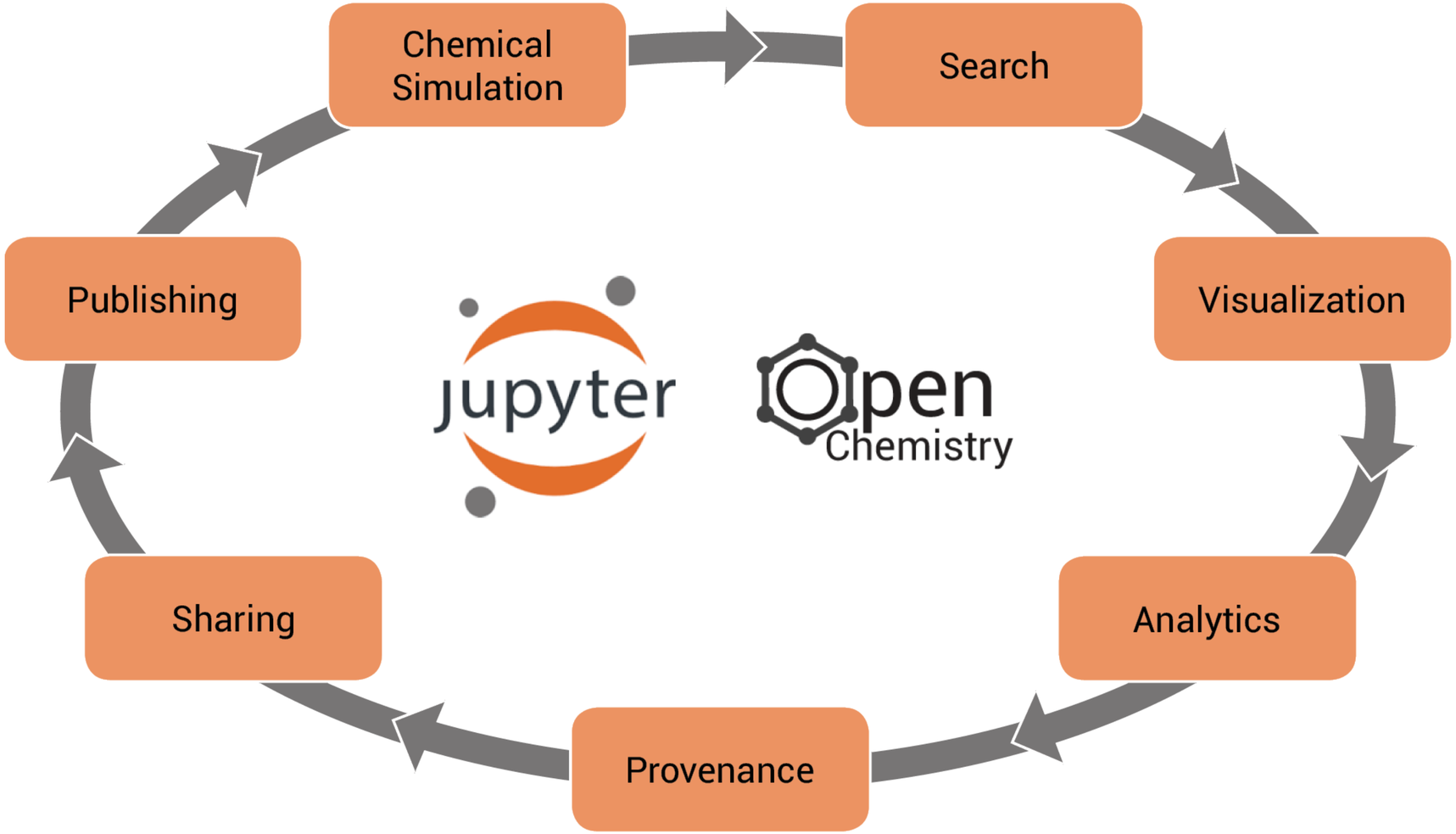
- Lack of integration with environments for visualization and analysis
- Need a platform to enable **end-to-end workflows** from simulation setup, simulation submission, right through to analytics and visualization of the result


Chemical Simulation
Search
Visualization
Analytics
Provenance
Sharing
Publishing

Why Jupyter?

- Supports interactive analysis while preserving the analytic steps
  - Preserves much of the provenance
- Familiar environment and language
  - Many are already familiar with the environment
  - Python is the language of scientific computing
- Simple extension mechanism
  - Particularly with JupyterLab
  - Allows for complex domain specific visualization
- Vibrant ecosystem and community




Chemical Simulation
Search
Visualization
Analytics
Provenance
Sharing
Publishing
jupyter
Open Chemistry

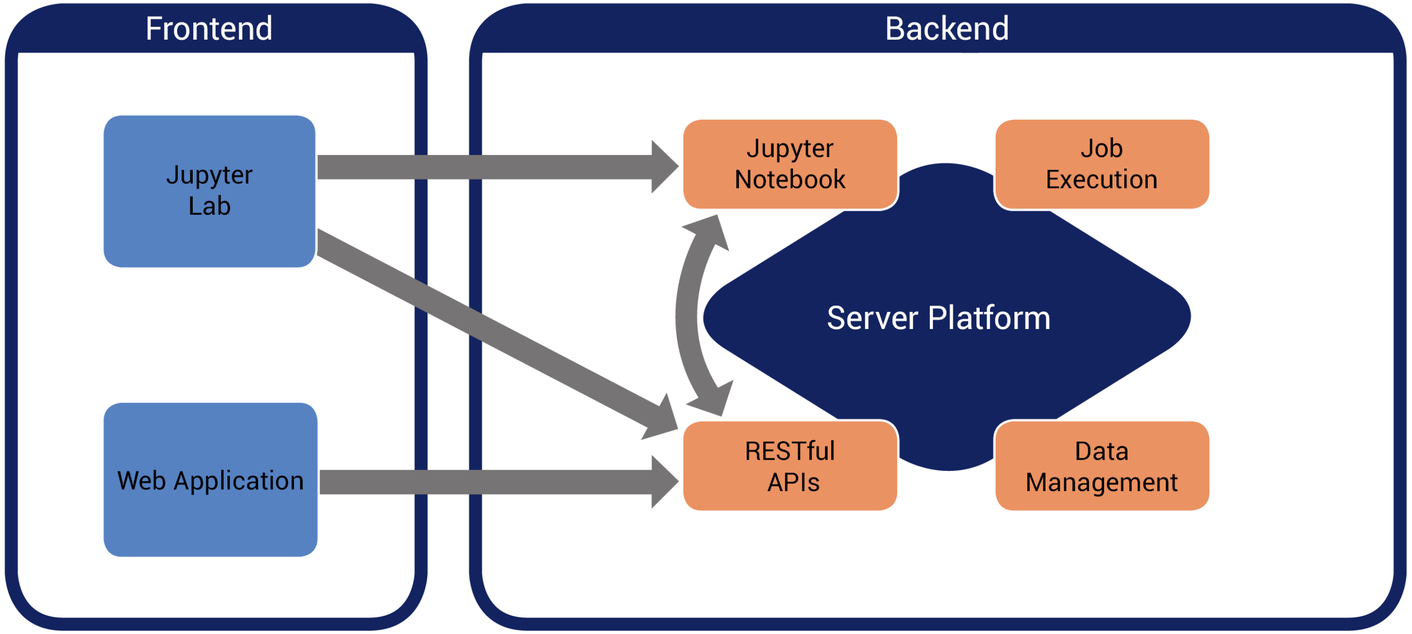
Approach

- Data is the core of the platform
  - Start with simple but powerful data model and data server
- RESTful APIs everywhere
  - Allows access anywhere
    - Notebooks, web apps, command line, desktop applications, etc
- Jupyter notebooks for interactive analysis
  - Provide a simple high-level domain specific Python API for use within the notebooks
- Web application
  - Authentication, access control and user management
  - Launching/managing notebooks
  - Enable users to interact with data without having to launch notebooks

Demo

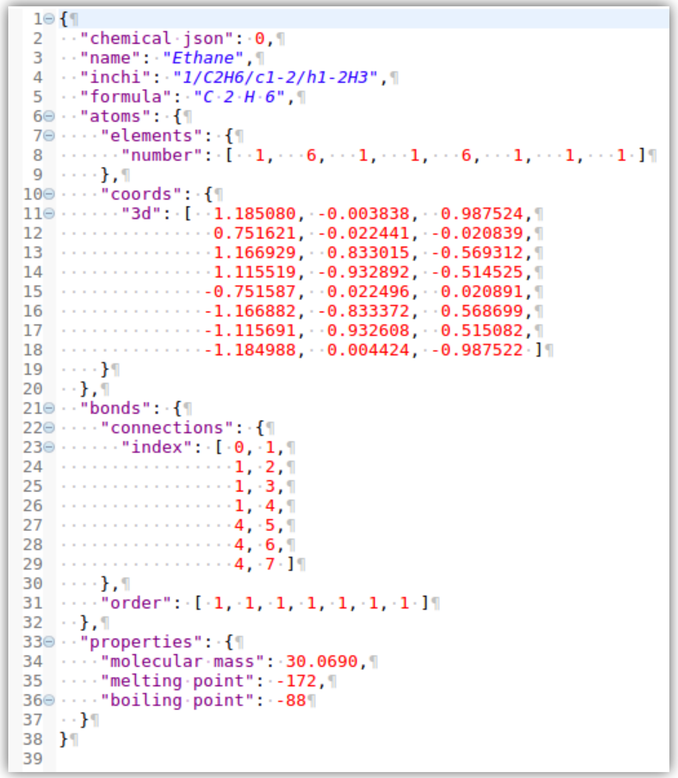
Architecture

- Backend
  - Data Management
  - Job Execution
  - Notebook management
- Frontend
  - Web components
  - JupyterLab Extensions
  - Web application



Data Management

- Computational chemistry codes produce a wide variety of output
  - Often non-standard, even non-structured
  - Need to convert to single format
- Chemical JSON (CJSON)
  - Simple JSON format for representing chemical information
  - Efficient binary representation
  - MolSSI standard being developed
- Support export in multiple standard formats
  - Facilitate integration



```
{
  "chemical json": 0,
  "name": "Ethane",
  "inchi": "1/C2H6/c1-2/h1-2H3",
  "formula": "C 2 H 6",
  "atoms": {
    "elements": {
      "number": [ 1, 6, 1, 1, 6, 1, 1, 1 ]
    },
    "coords": {
      "3d": [ 1.185080, -0.003838, 0.987524,
              0.751621, -0.022441, -0.020839,
              1.166929, 0.833015, -0.569312,
              1.115519, -0.932892, -0.514525,
             -0.751587, 0.022496, 0.020891,
             -1.166882, -0.833372, 0.568699,
             -1.115691, 0.932608, 0.515082,
             -1.184988, 0.004424, -0.987522 ]
    }
  },
  "bonds": {
    "connections": {
      "index": [ 0, 1,
                 1, 2,
                 1, 3,
                 1, 4,
                 4, 5,
                 4, 6,
                 4, 7 ]
    },
    "order": [ 1, 1, 1, 1, 1, 1, 1 ]
  },
  "properties": {
    "molecular mass": 30.0690,
    "melting point": -172,
    "boiling point": -88
  }
}
```

Data Management

- Girder
  - Web-based data management platform
    - Enable quick and easy construction of web applications:
      - Data organization and dissemination
      - User management & authentication
      - Authorization management
  - Extended via the development of plugins
    - Expose new data models and RESTful endpoints

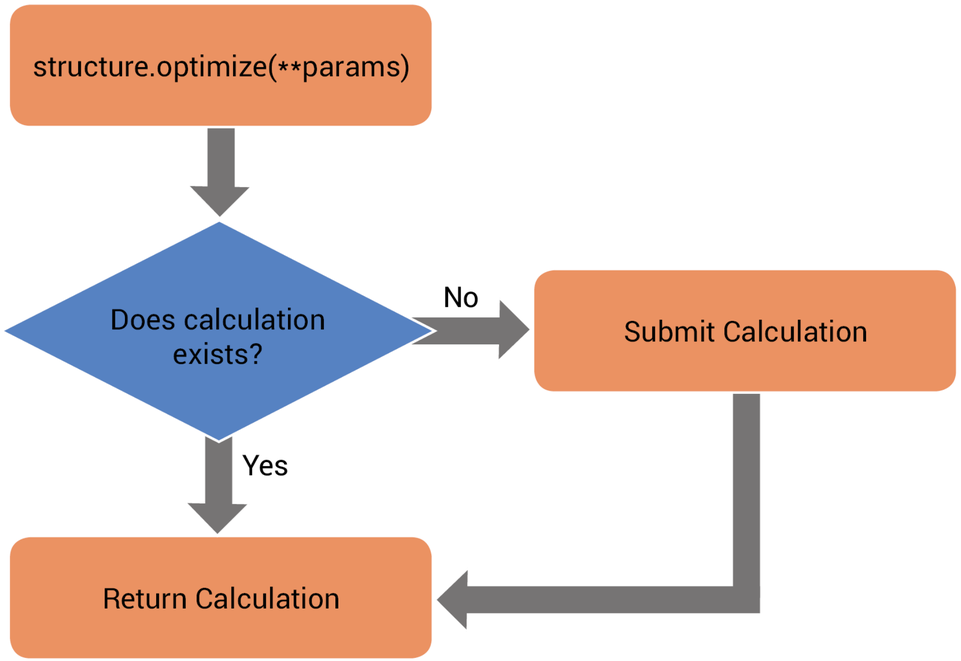
Job Execution

- What's involved in submitting a job to run on HPC resource?
  - Input generation
    - Code specific and often pretty esoteric
  - Moving the required data onto the resource
  - Generate submission script
    - Scheduler specific
  - Submit and monitor job
    - Scheduler specific
  - Post-processing or ingestion of result

Focus on knowledge discovery, not job execution...

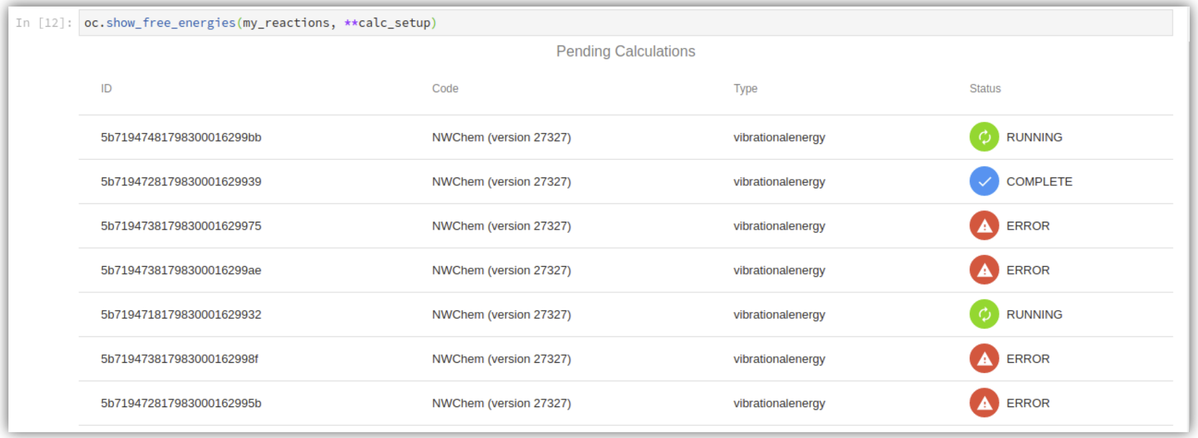
Job Execution

- Shield the end-user from the complexities
- Job execution is implicit with sane defaults
  - A result of requesting a given data set that doesn't exist
  - Concentrate on the data and analysis



Job Execution

- Provide a scheduler abstraction
  - SGE, PBS and Slurm (+NEWT)
- Template input decks
- Distributed task queue to support long running operations
  - Job submission and monitoring
  - Support "offline" execution of jobs



```
In [12]: oc.show_free_energies(my_reactions, **calc_setup)
```

Pending Calculations

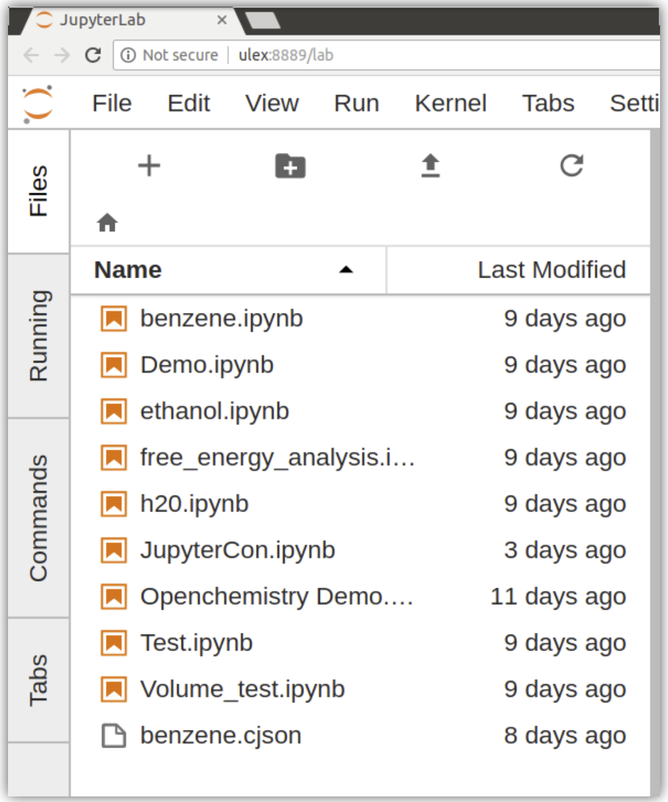
ID	Code	Type	Status
5b71947481798300016299bb	NWChem (version 27327)	vibrationalenergy	RUNNING
5b719472817983000162939	NWChem (version 27327)	vibrationalenergy	COMPLETE
5b719473817983000162975	NWChem (version 27327)	vibrationalenergy	ERROR
5b719473817983000162999ae	NWChem (version 27327)	vibrationalenergy	ERROR
5b719471817983000162932	NWChem (version 27327)	vibrationalenergy	RUNNING
5b719473817983000162998f	NWChem (version 27327)	vibrationalenergy	ERROR
5b719472817983000162995b	NWChem (version 27327)	vibrationalenergy	ERROR

Notebook Management

- JupyterHub to enable multi-user environment
  - DockerSpawner
    - Users do not need to have account on server
    - Simple deployment of complex Jupyter configurations
  - JupyterHub Girder authenticator
    - Allows cross-site authentication
  - Jupyter servers are launched with a simple redirect

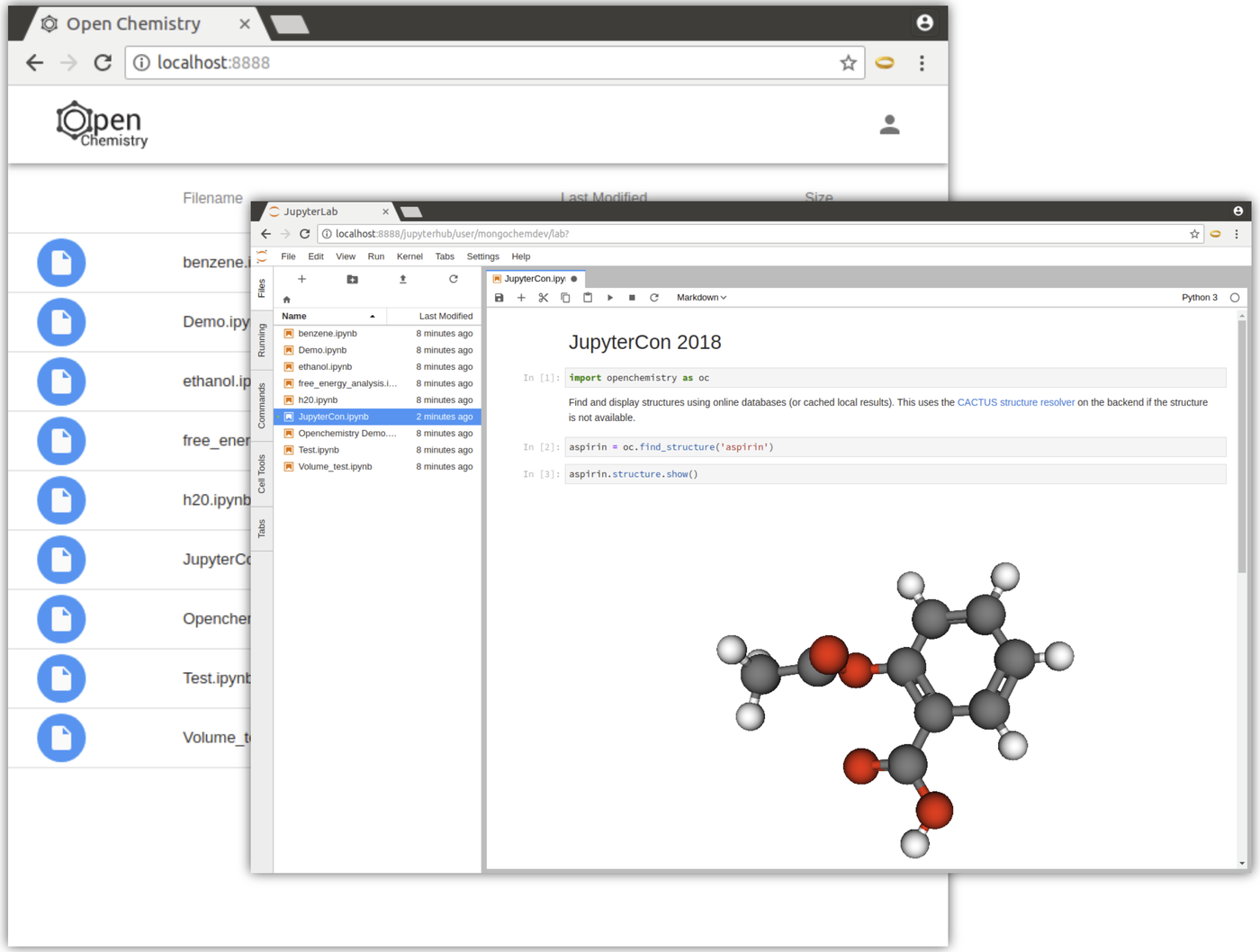
Notebooks as data

- The notebooks encode the workflow
  - Are as valuable as the calculation output
- Store in the data management system along with the output
  - Make them searchable
  - Make them available to others
  - Version
- Girder Contents Manager
  - Implements Jupyter Contents API
  - Notebooks can be stored in Girder



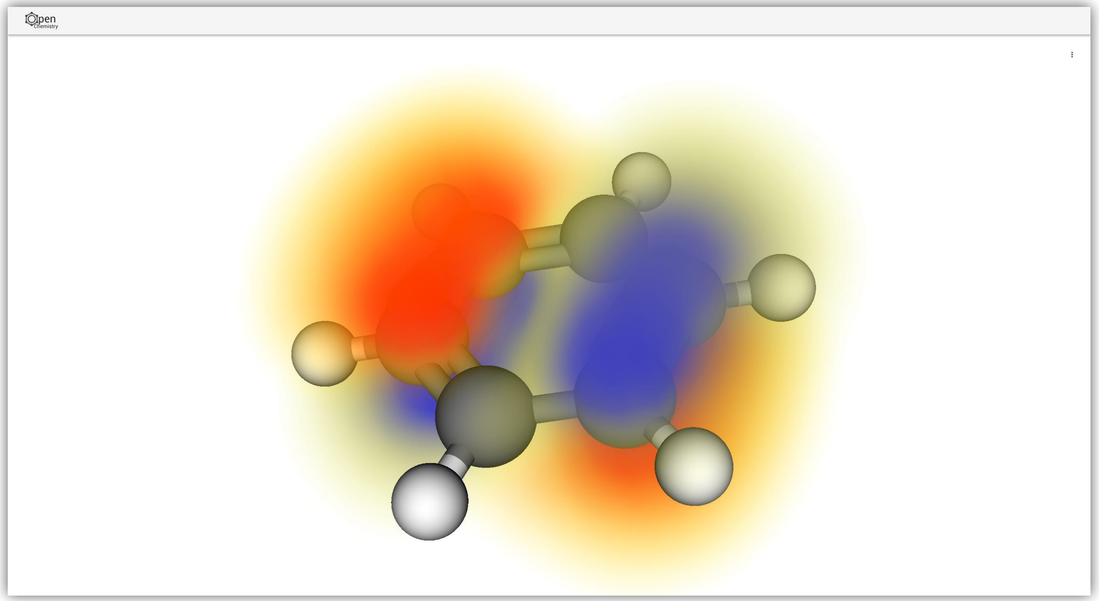
Frontend

- Users have two interaction modes
  - Web application
  - JupyterLab



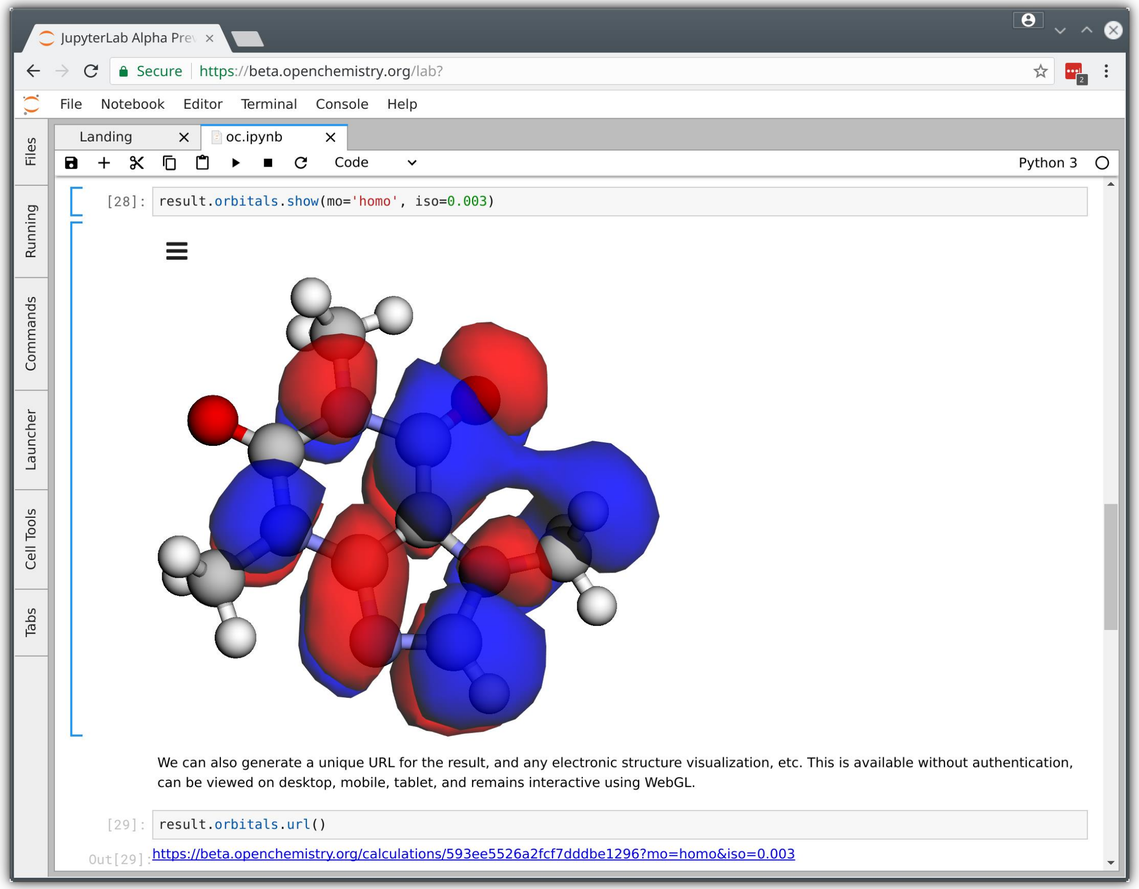
Web components

- Allows the creation of new custom, reusable, encapsulated HTML tags
- stenciljs web component compiler
- Low level visualization components
  - Shared between JupyterLab extensions and web application
  - VTK.js for volume rendering
  - 3DMol.js for 3D chemical structures



JupyterLab Extensions

- MIME renderer extensions
  - React/Redux components
  - Fetch data direct from data server
- Components are "thin" by design
- How to store "interactive" provenance?
- Adopted TypeScript

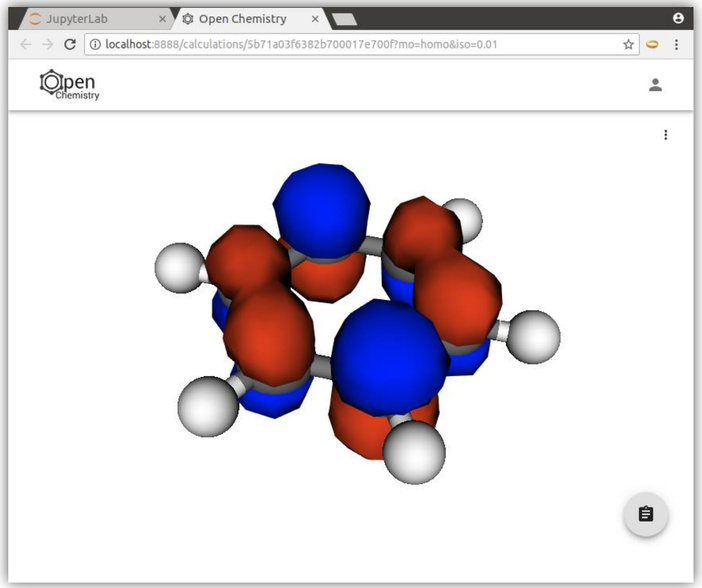


Deployment

- docker-compose
- Ansible for runtime configuration
- AWS
  - Running jobs on small cloud cluster
- National Energy Research Scientific Computing Center (NERSC)
  - Uses NERSC login credentials
  - Jobs run on Cori

Future Work

- Extend collaboration features
  - Fork notebooks
  - Real time editing of notebooks
- Integrate more computational chemistry and materials codes
  - Psi4, NWChemEx, Orca
- Add machine learning capabilities
  - Bulk downloads for training datasets
- Semantic web
  - Enriching data and make it more discoverable



Thank you!

- Please come visit!
  - https://openchemistry.org/
  - https://github.com/openchemistry/