Argonne NATIONAL LABORATORY

Generic Portals for Science Infrastructure (GPSI)

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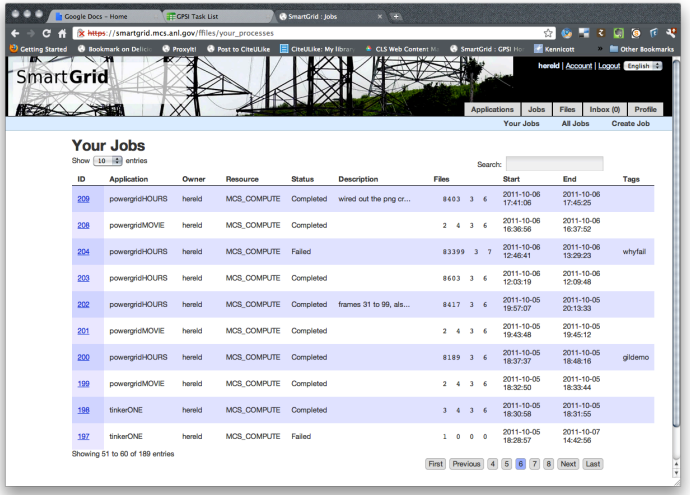
GPSI
Generic Portals for Science Infrastructure

Approach

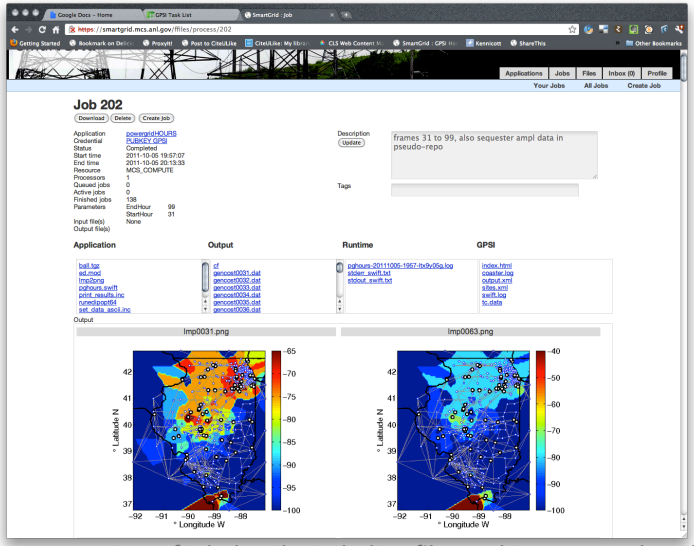
- Simplify execution and data management on compute resources
- Support reproducibility of results through execution and data provenance
- Enable collaboration among researchers working on a science campaign
- Capture details of scientists' idiosyncratic workflows



View of job history

Research Questions

- Effective scheduling of jobs across resources
- Efficient data staging to and from compute resources
- Automated data analysis and feature extraction
- Data filtering for remote analysis



View of job details, including files and images produced

GPSI: Technologies

- Django core (hence Python)
  - Django is widely used in industry, and is the most popular Python web framework
  - Python is widely used in the scientific community
  - Uses a variety of database backends (MySQL, Sqlite)
- Collection of Django apps
  - Apps exist for (nearly) anything one needs
- GPSI is one more Django app
  - Can remain small, focus on only the gateway-related functionality
- Uses Swift for describing workflow and running jobs
- GPSI exposes opportunities for customization by science domains
  - User-driven gateways

GPSI: Overall Flow

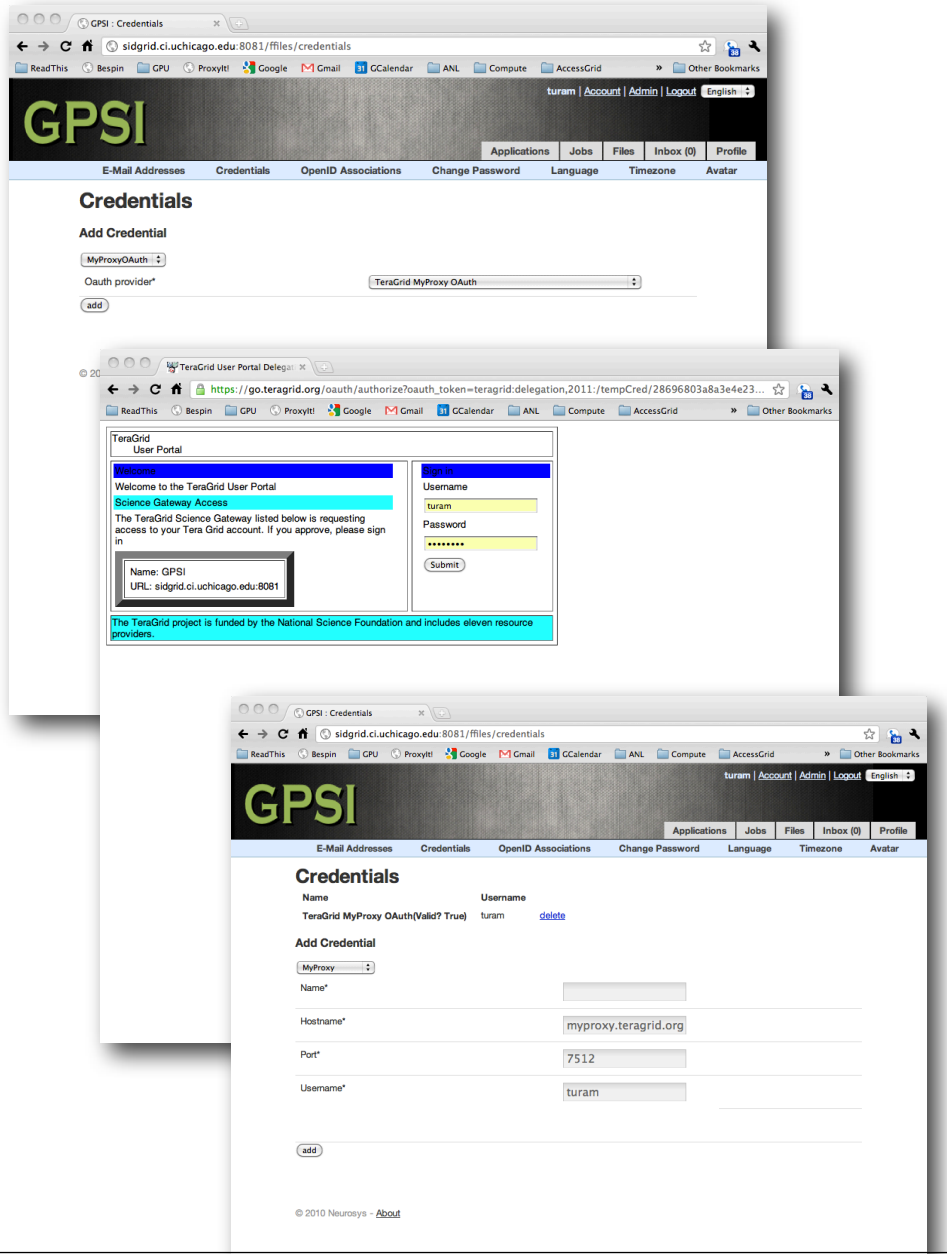
- Introduce data
- Introduce applications
- Schedule jobs
- View/Analyze results
- Reproduce results
- Download
- Share

Compute Resource Setup

- Mechanisms supported by Swift
  - File transfer: gridftp, ssh, http
  - Execution: pbs, gram, sge, ssh, ec2, FutureGrid, ...
- Have run on a variety of resources
  - Ranger, Steele, Blacklight @ ~~TeraGrid~~ XSEDE
  - Compute machines at Argonne, including Fusion cluster
  - PADS at UChicago
  - Third-party resources
- Administratively controlled (for

Credential Management

- Credentials managed by user and associated with particular resources
- Credential types include
  - ssh
  - MyProxy
    - MyProxy server host, port, username and password
    - Credential renewed as needed
  - MyProxy OAuth
    - Avoids collection of MyProxy username and password by gateway
    - Have currently integrated pre-production TeraGrid MyProxy OAuth support

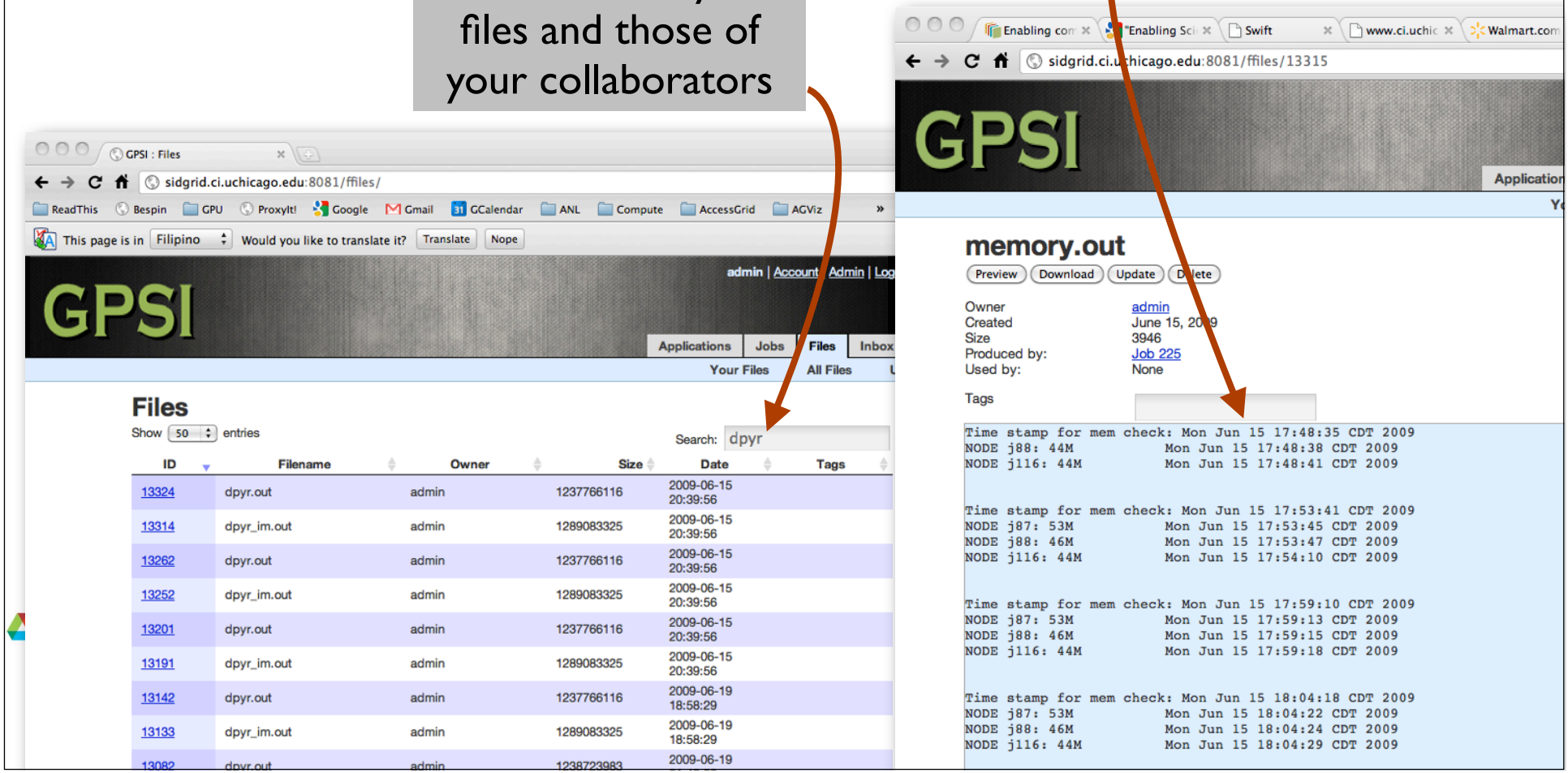


Introduce Data

- Upload relevant files, or ingest on server-side

Search across your files and those of your collaborators

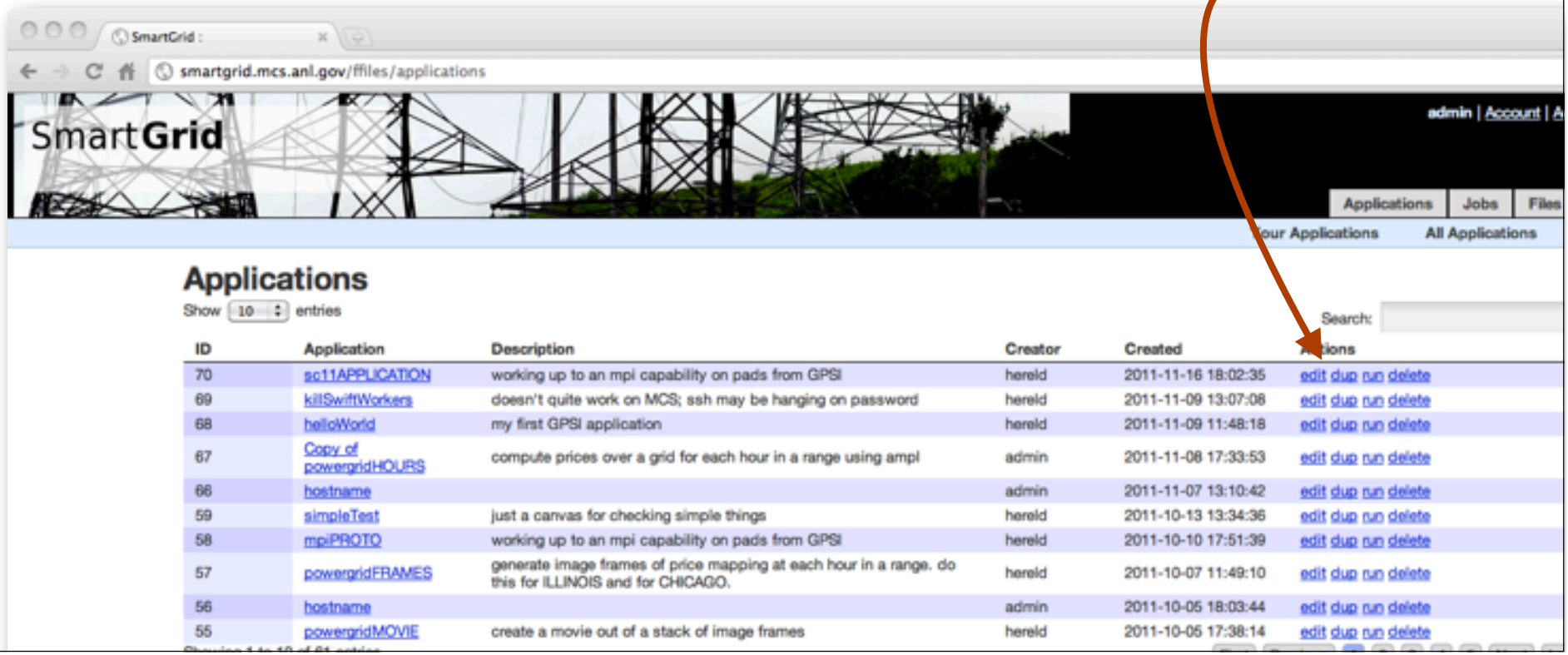
Preview files inline



Introduce Applications

- Upload relevant files
- Application definition relies on required applications residing on compute resource
- Edit Swift script within GPSI

Edit, duplicate, run, delete jobs



Swift

- Language for parallel scripting
- Execution engine with interfaces to various schedulers

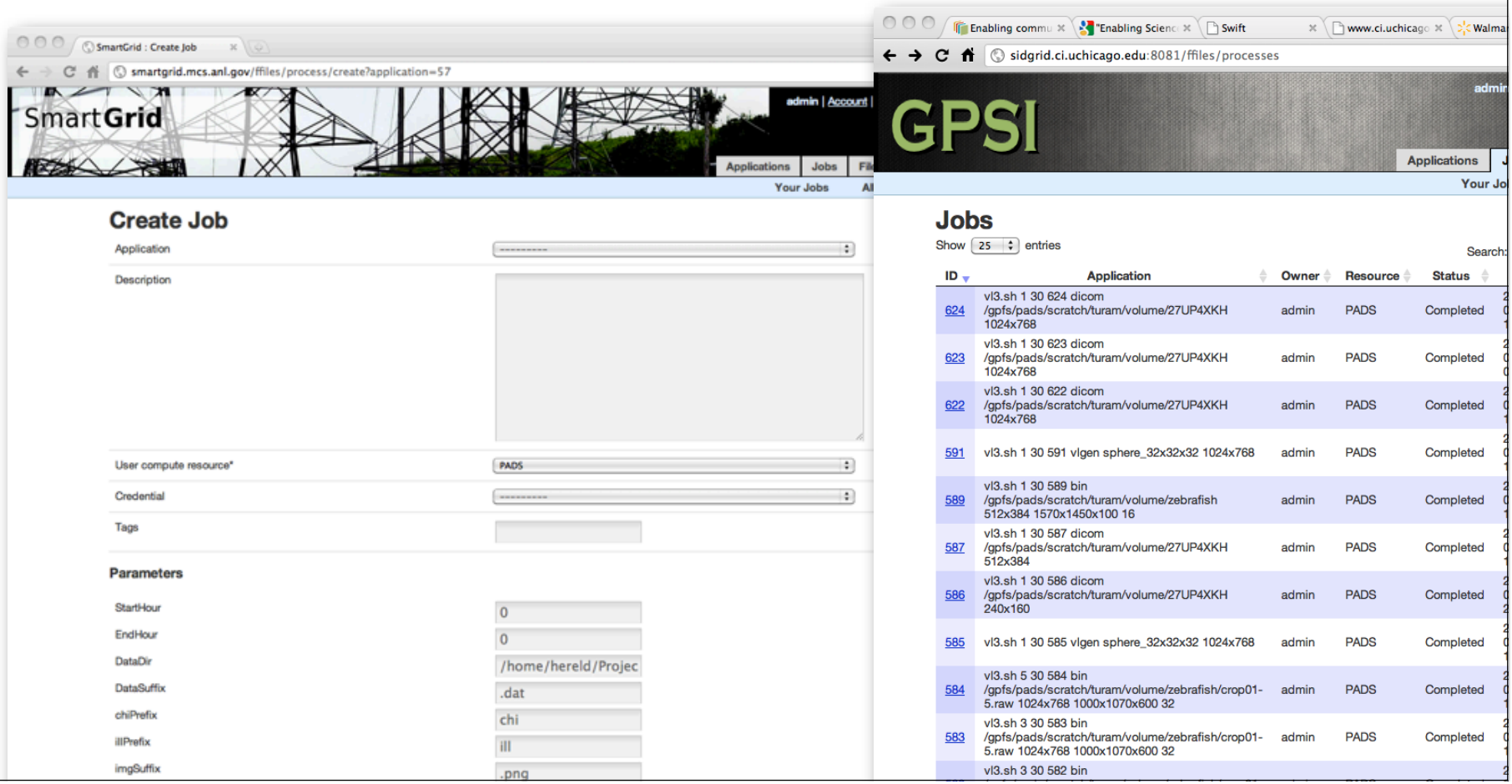
```
# simple script to execute hostname N times
type file;

# Swift app definition; each call will schedule a job
(file t)do_hostname() {
    app {
        hostname stdout=@filename(t);
    }
}
foreach i in [0:50] {
  file outfile <concurrent_mapper;prefix="stdout",suffix=".txt">;
  outfile = do_hostname();
}
```

For info on Swift, see http://www.ci.uchicago.edu/swift

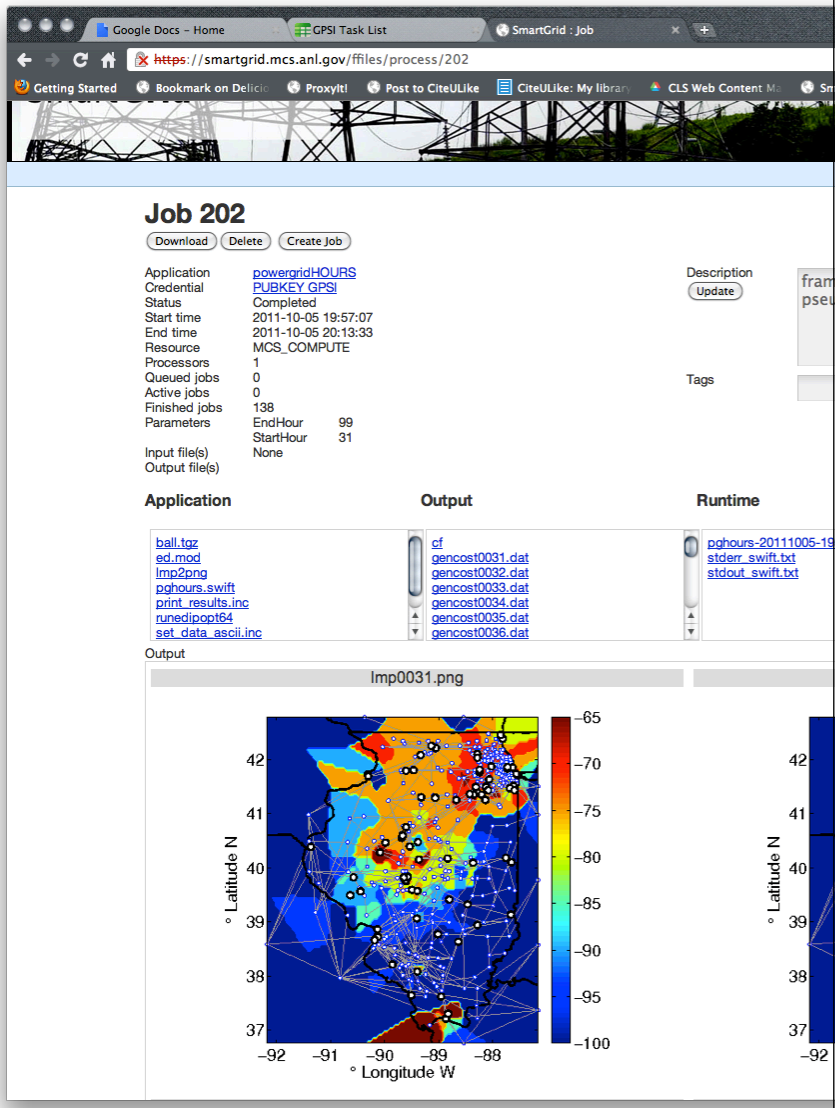
Execute Jobs

- Web form generated by introspecting Swift script, including default values
- Uses server-side proxy certificate for single sign on



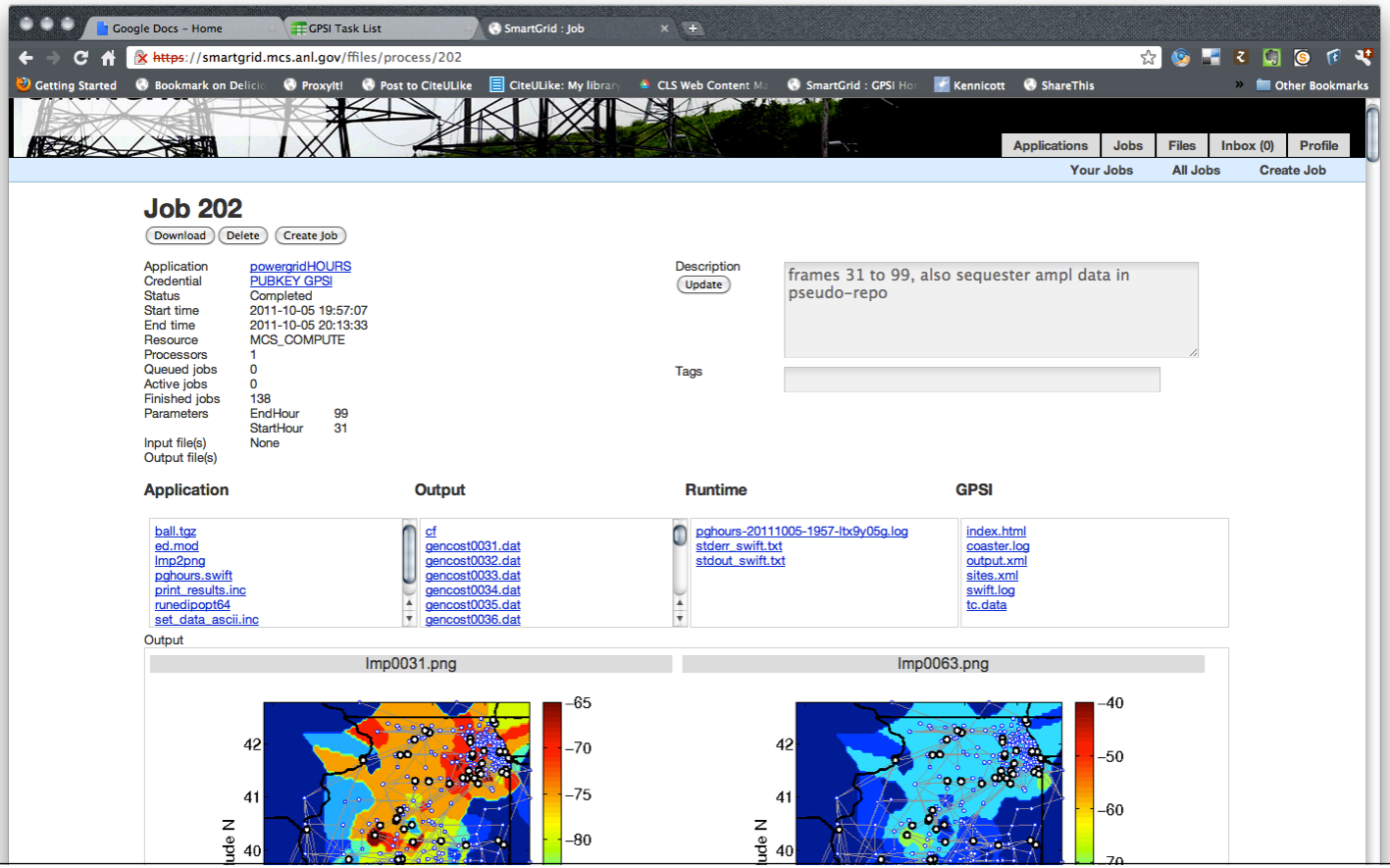
Generate, view, download results: Collaborate

- Well-known data types are presented graphically among job output
- Applications control which job outputs are included and how they're represented
  - XML designation of output files to include
  - XSLT transform of file input to representative HTML
- Users view each other's results, can run each other's apps



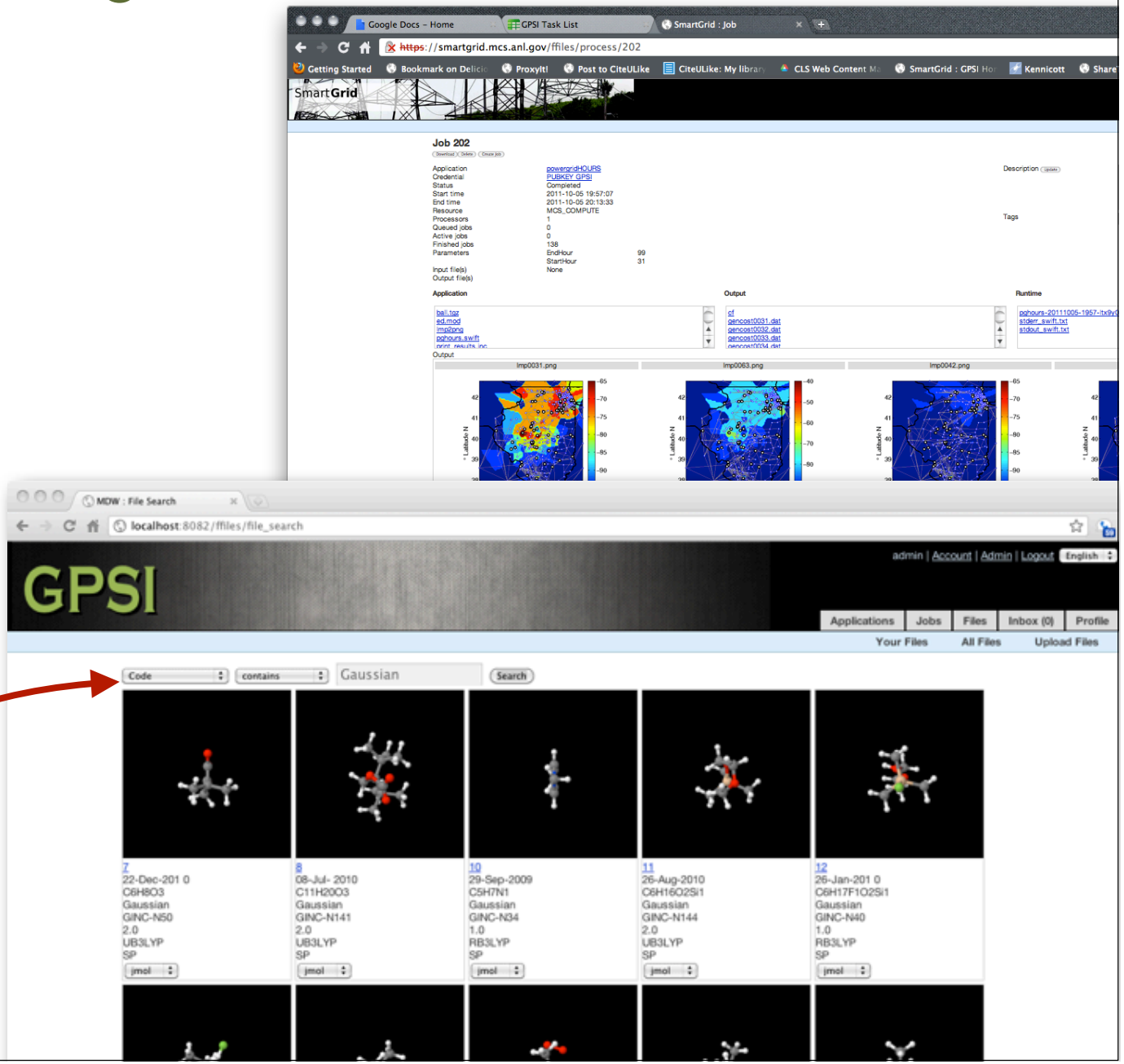
provenance

- Job details captured in one place
  - input, options, compute resource, credential
- Jobs can be rerun from within GPSI, using the original scenario



Where we're using it

- SmartGrid
- Materials
- Phylogenetics



Triple-store for metadata integration and searching

Future Work

- Integrated analysis
- Dynamic provisioning
- SCS integration
- Globus Online integration
- Data cataloging

Acknowledgements

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