Web APIs for the Big Science Enterprise

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Our computing & data apparatus is getting bigger.

Increasingly Big Science relies on the machinery of software.

prototypes \(\rightarrow\) reliable infrastructure

GO is getting some serious traction

http://en.wikipedia.org/wiki/Big_Science

How to maintain / sustain?

How can we make reliable plans together?
Evolution of LHC computing

In chronological order:
1. Copy as much data as feasible to analysis centers worldwide, with hierarchical distribution.
2. Relax the hierarchy and rely on caching.
3. Use “federated data stores” to fetch portions of relevant data sets from remote storage (anywhere), just before they’re needed.

Increasing faith in global science networks. Enterprise.

<table>
<thead>
<tr>
<th></th>
<th>Netflix</th>
<th>LHC Computing</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bandwidth per client</td>
<td>1.5Mbit/sec</td>
<td>1MByte/sec</td>
</tr>
<tr>
<td>Clients</td>
<td>1M*</td>
<td>100k cores</td>
</tr>
<tr>
<td>Serving</td>
<td>1.5Tbits</td>
<td>0.8Tbits</td>
</tr>
<tr>
<td>Total Data Distributed</td>
<td>12TB</td>
<td>20PB</td>
</tr>
<tr>
<td>Annual Budget</td>
<td>&gt;$4B</td>
<td>&lt;$ .04B</td>
</tr>
</tbody>
</table>

Similar Problems: Not all files are equally accessed

Bill and Ted’s Excellent (European) Adventure
Science Facilities are Now Coupled by Science Networks

- Networks and software are part of the apparatus.
- Recent beam time on free-electron laser (LCLS) at SLAC to take ‘snapshots’ of catalytic reaction in Photosystem II (Nick Sauter et al.).
- Data transported to a nearby HPC resource (NERSC) for real-time computational analysis.
- This one experiment *tripled* NERSC’s network utilization.

**X-ray emission spectroscopy** (Chemistry at the catalytic site)

- charge density/spin state
- ligand environment

One Experiment == 150 TB, growing

All NERSC Traffic

PS II Study
Big Science: Beamline in a Browser

- Establish HPC conduit to NERSC capabilities for ALS users to analyze data in real time
- Develop new visualization tools for displaying multi-dimensional datasets
- Introduce reverse modeling tools for understanding plastic deformation at the mesoscale and guiding experiments

Q→ Craig Tull (BESCGWG)
Big Science: Global Telescope Choreography

Very Large Telescopes (4x8.2m)
Cerro Paranal, **Chile**

Gran Telescopio Canarias (10.4m)
La Palma, **Canary Islands**

South African Large Telescope (9.2m)
Sutherland, **South Africa**

Keck Telescopes (2x10m)
Mauna Kea, **Hawaii**

Hobby-Eberly Telescope (9.2m)
McDonald Observatory, **Texas**

Gemini Telescopes (8.1m)
Hawaii and **Chile**

Dark Energy Camera

Web App + API

New Supernova Candidates from **Images**

Requests and Responses for **Spectrograph** Data

Q → Rollin Thomas (LBL)
Let’s Talk About Data culture:

Are you a HEP or a BES?

@CERN
Let’s talk about a data plan for the next 10 years

Unleash the data team on this problem.

Initiating globally distributed data analysis in 3,2,1.

Let me tell you about our middleware software stack...

@ the Beamline
I need the data tomorrow. Deadline is next week.

Minions? There are 3 people on my team.

How can I trust any computer that’s not right in front of me?

Let me tell you about Netflix, Big Data when I want it.
Topics for Globus World

- RESTful Web APIs for Science
- NEWT a web API for HPC
- Examples running at NERSC now
- What’s Wrong with APIs
REST: A software architecture (for the web) that we can actually use. Roy did that.

“app enabler”

Everyone “knows” how to make a RESTful API.

HATEOAS

Maybe a little too cool.

There are now 32 bazillion of them

hypermedia

Which one is the best?

Why were they all written by data providers?

Why do I have to learn yours?

Why didn’t you do yours the “right” way?
REST APIs have brought science resources into a new era of accessibility. This magnifies value of those resources and enables new science.

Of critical importance going forward into Big Data

Must understand enterprise level value propositions

190 REST APIs for Science

RESTful Interface Circa 1955

http://www.w3.org/community/hpcweb/

W3C Community and Business Groups: HPCWEB
NEWT: An API for HPC Stuff

- Authenticate using NERSC credentials
- Check machine status
- Upload and download files
- Work with Big Data remotely
- Submit a compute job
- Monitor a job, check your workflow
- Get user account information
- Store app data (not scientific data)
- Issue UNIX commands

Q: Do this all in your browser?
A: Yes with a science gateway!
Map resources to URI that use web friendly formats (HTML, JSON, etc.) that deliver or accept information about the state of a resource.

What’s a resource? It’s whatever you want it to be.

<table>
<thead>
<tr>
<th>VERB</th>
<th>RESOURCE</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>POST</td>
<td>/queue/R</td>
<td>Submits POST data to queue on R; returns job id</td>
</tr>
<tr>
<td>GET</td>
<td>/file/R/path/</td>
<td>Returns directory listing for /path/ on R</td>
</tr>
<tr>
<td>GET</td>
<td>/account/user/U</td>
<td>Returns user account info for U</td>
</tr>
<tr>
<td>DEL</td>
<td>/store/DB/DOC</td>
<td>Deletes object DOC in DB</td>
</tr>
</tbody>
</table>

See Roy Fielding’s Thesis
Client: Web Application
HTML 5/AJAX

http request

Authentication
MyProxy CA

lots of state.... session, cred, user information

http request

JSON data

NEWT

System Resources (via Globus)
- Files
- Batch Jobs
- Shell Commands
- Status

Persistent Store (NoSQL DB)
- MongoDB

Accounting Information
- NIM
The web augments the command line when you need it, web when you don’t use HTML+APIs to make science gateways (web apps).
Data Headaches Circa 2013

Overheard between Dr. Computing & Dr. Science
“I can’t collaborate with you because my data is too big for you kiddo. You could get pieces, but your connection is so weak that you’d never be able to really work with the data. Best if we just say no.”
“I can’t show you my data analysis workflow because the moving parts are too big. There’s no small parts you can interact with.”
“I’d write an API but I am not sure what people want. Could be a huge waste for my team, and a little embarrassing, if nobody came knocking.”
“How can I provide data access in graduated ways? I want to provide more data to teams who prove they are doing world-class stuff with my world-class data, not waste time on tourists.”

Our progress is measured by the extent to which these go away.
Data Headaches Circa 2013

Overheard between Dr. Science vs. Dr. Computing:

“I can’t collaborate with you on that Big Data proposal because I am a simple spectroscopist. You’d probably ask me to learn a bunch a CS rigamarole before I could even ‘ls’ your data. Phooey.”

“I know I could demonstrate something very cool if I had access to that data set, even a little slice. How can I persuade Dr. Computing of this without asking for the whole thing? I don’t even know which part to ask for? How can I stay away from the parts I don’t need?”

“I can’t collaborate with you because your API doesn’t do what I want. Asking you to change it would probably be imposing. You wrote the API so you must know”

Our progress is measured by the extent to which these go away.
NEWT Futures
NEWT 1.0:
- NERSC Web Toolkit REST API that covers things people do at HPC centers
- Batch and interactive oriented execution
- HTTP based file/data movement

NEWT 2.0:
- Refactoring around flatter URLs
- Batch, interactive, and pipeline oriented execution
- High Throughput Computing (HTC)
- New approaches for wildcarding
- Data analysis provenance through tagging
- Extensibility: requests to extend/modify API through POSTS
- Take discussion to W3C
A Design Target for NEWT: Enable Materials Genomics

computational survey drivers

- ICSD
  - enumerated structures (e.g., MOFs)
  - structure predictor
  - experimental data
  - PV, defects, x-ray data …

simulation engines

- VASP, Zeo++, BerkeleyGW, PARATEC, QEspresso

(A)

Hands-off Expertise Automation (A)
High Throughput Computing (A)
Big Data Materials Ontologies (B)
Probabilistic Data Management (B)
Anomaly Detection (C)
Consistency / V&V (C)
Query Language / Web Gateway (D)

(B)

operational In 2012

(C)

Community Web Gateway

(D)

functional
electronic materials

phosphors & scintillator

carbon storage

critical materials...

materials genome

(!)
Big Data Enterprise means acknowledging true costs

Big Data is not free (as in beer)

My Big Data costs $1.75 per download

Real infrastructure,
Real costs
Real money

Awesome. I’ve got $3.50. Make mine a double. I’ll take a small schema too. To go.

I’d buy four if you charged $1.25.

Nights and weekends are easier for my team.

Sold.
Data Discovery

Whatcha looking for? Whatcha got?

I need it in another format. No problem?

What does this data even look like? Give me just a little bit and I’ll get back to you.

“Insight before a terabyte”

People who liked data XYZ also like YZXV.

Data is the easiest product in the universe to test-drive. Why aren’t we doing that?
Reflections on NEWT 1.0, thoughts on 2.0

A web API tailored for HPC purposes

Very Accessible

Took 2 people 7 years to write, we needed a REST

Toolkit approach (ugh)

small data

Popular w/ NERSC users
(always a good sign)

“stiff”

no HTC

limited vocabulary

We can rebuild him better. We have the technology.

(remember that one time when scientists invented the world wide web?)
The **Tyranny** of the API

How many APIs do you want to learn?

Written in a one-sided way

Speculation by publisher as to user

No way to vote on what you like, suggest improvements

My team wants that data/resource our way.

Sometimes need to mask multiple APIs under a single unified view

All those errors

Why are so many APIs written by the data publisher? I could do better.
Imagine that the API spec was a google doc someplace. What if you let some people comment/suggest changes or alternatives? What if you let people you trust make actual changes to the spec? What if every version of the spec and every transaction against every version was logged? What if you could copy one spec to another? Imagine you had fine grained controls. What if you could do all this through a RESTful interface?

Quack? .....presto!...... Ok. Quack.

Thanks!