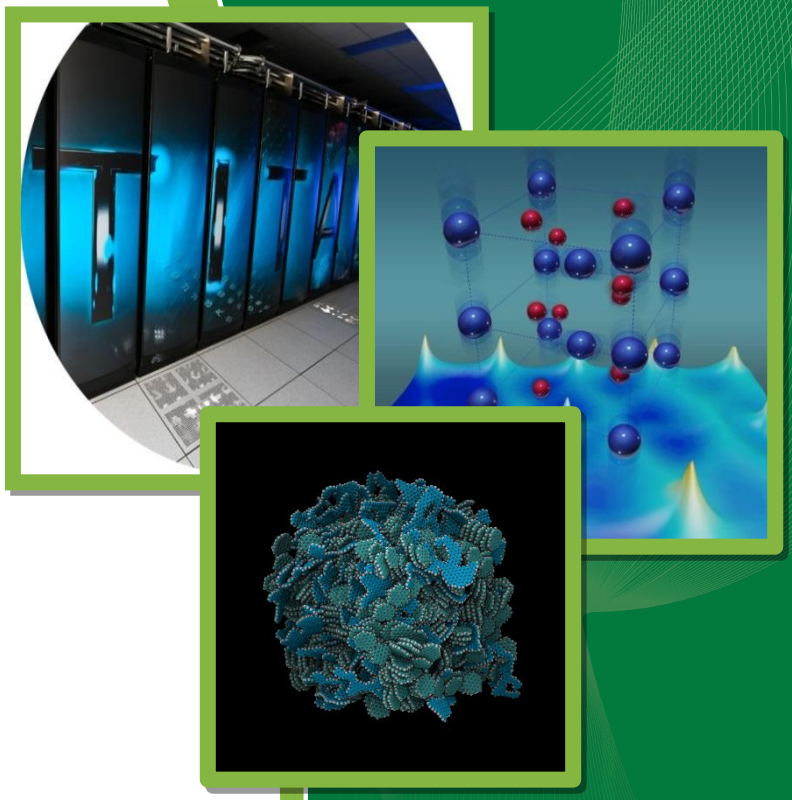
The New Energy Science and Technology Software Center



Jay Jay Billings, ORNL & OSTI
with contributions from the rest of the DOE Code Team

20170221
@jayjaybillings

ORNL is managed by UT-Battelle
for the US Department of Energy

OAK RIDGE National Laboratory

Don’t worry: We’re not making you stop using GitHub! (or any other repo service)

Office of Scientific and Technical Information

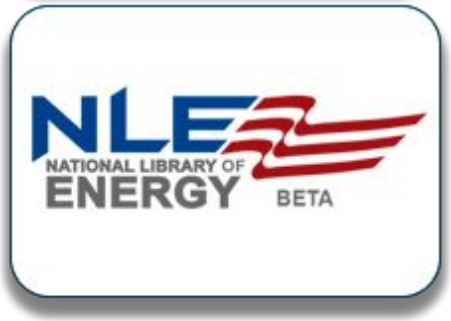
“OSTI”

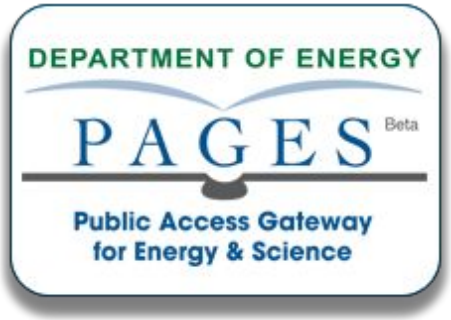
What is OSTI?

"...the Department of Energy (DOE) office that collects, preserves, and disseminates DOE-sponsored research and development (R&D) results that are the outcomes of R&D projects or other funded activities at DOE labs and facilities nationwide and grantees at universities and other institutions."

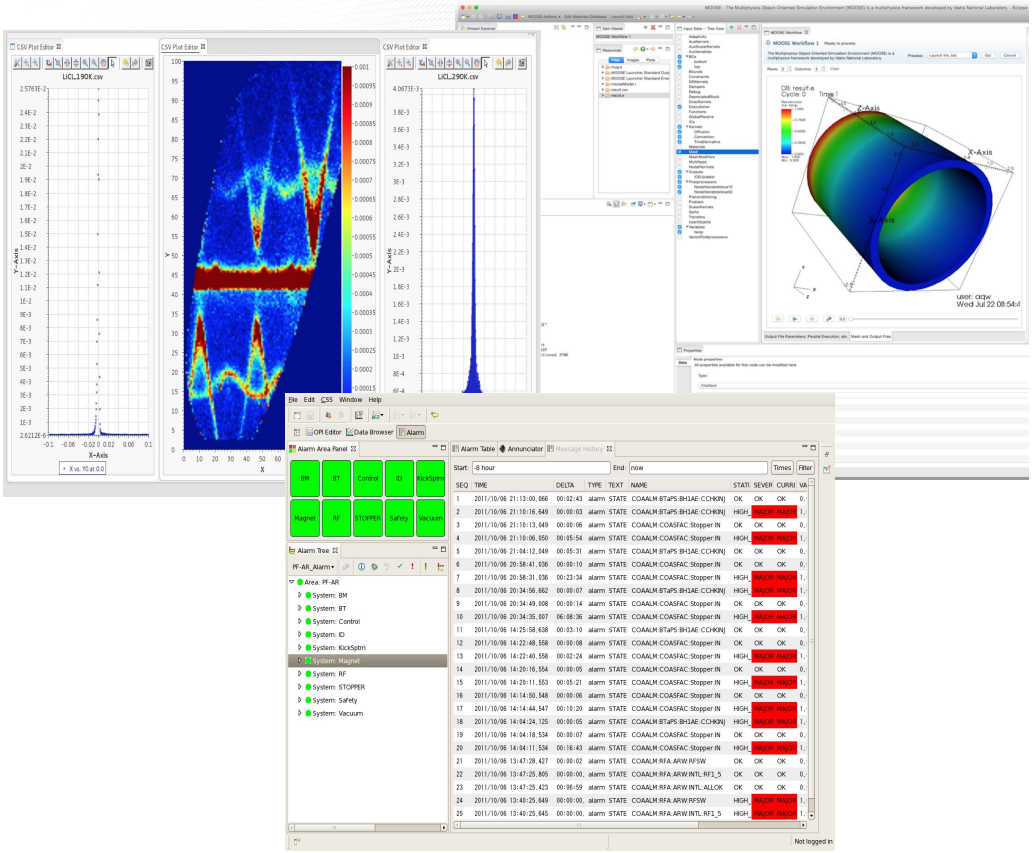
OSTI HQ in Oak Ridge, TN

OSTI Products





Tracking DOE Scientific Software



\+ System Software, etc.

Think Scientific Software - not business software

What is the ESTSC?

The Energy Science and Technology Software Center (ESTSC)...

- is the DOE's centralized software management facility
- licenses and distributes scientific and technical software
- was moved to OSTI in 1991
- originally started at ANL in 1960 by Margaret Butler
- has >3517 packages

Energy Science & Technology
Software Center

What is the ESTSC?

Two Big Problems

1. Not a modern product; has a poor user experience.

   Literally still uses CDs. →

   This is the <u>entire</u> product. →

2. Misses most modern DOE software.

   ⟶ What is a *"release?"*

ESTSC misses many “in development” projects

We expect there are between 5x-10x more codes in the wild than those already available in the ESTSC.

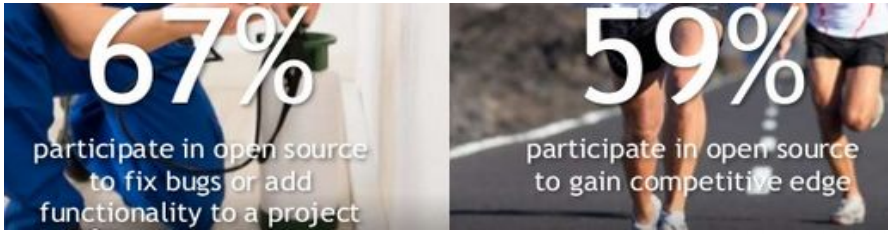
There are more than 900,000 mentions of “Department of Energy” on GitHub alone.

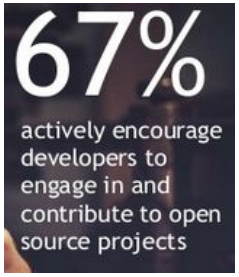
That’s roughly 1000-10000 codes.

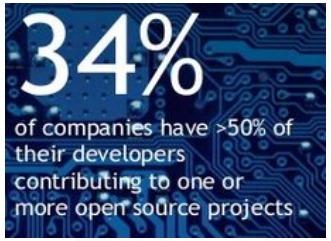
What's important for a "modern" ESTSC?

Modern Software is Open Source

According to the 2016 Future of Open Source Survey...
(1313 Companies Participating)







https://www.blackducksoftware.com/2016-future-of-open-source

Modern Software is Collaboratively Developed

Either through open *social coding* sites like...

- **GitHub**
- **BitBucket**
- **Sourceforge.net**

Or through "Software Foundations" like...

- **The Eclipse Foundation**
- **The Apache Software Foundation**
- **The Linux Foundation**

Modern Software is a Social Activity

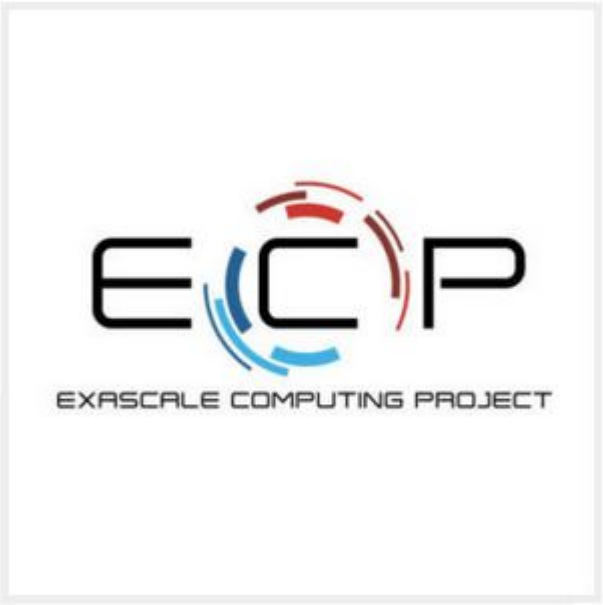
c.f. - “Hackathons”

AT&T Hackathon

ORNL Hackathon

True for Science?

ORNL receives Exascale Computing Project awards to develop next-gen applications



All 22 ECP projects are multi-institution projects that depend on open source in one way or another.

Exascale Computing Project (ECP) Awards $39.8 million for Application Development

What would a “modern” ESTSC look like?

New Name and Branding

DOE(Code){}

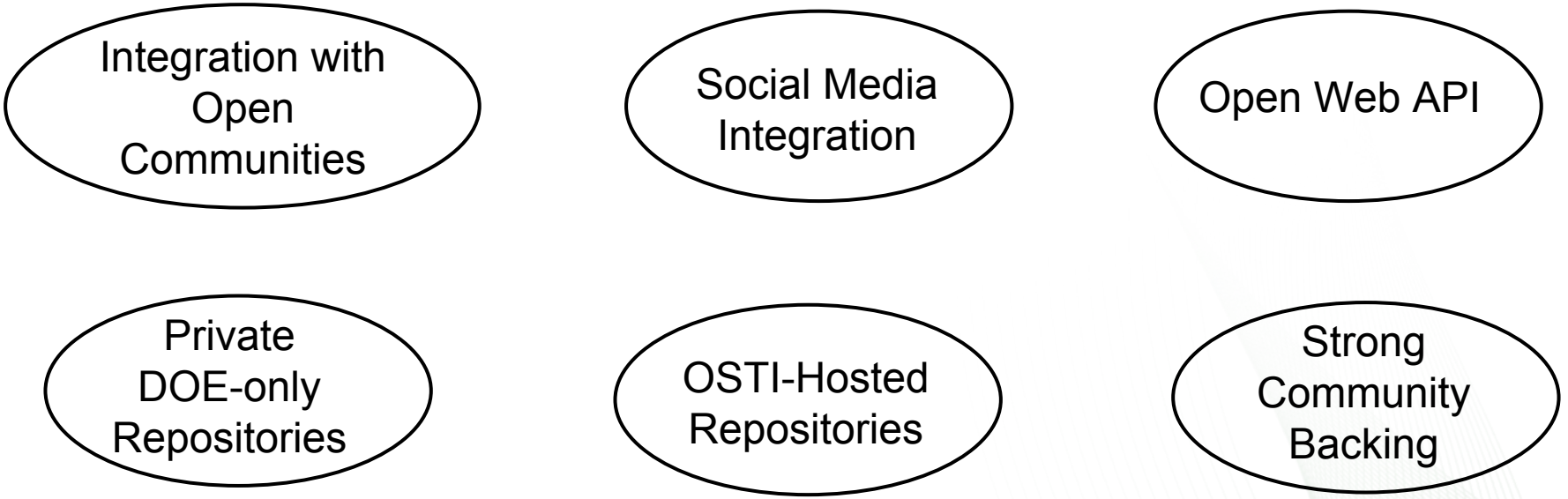
The DOE depends on code, which these ***super nerdy*** "Constructor" logos acknowledge and celebrate.

DOE
(Code){}

A “Modern” Software Experience

DOECode will...

- **Focus on enabling social coding**
- **Integrate researchers, data, etc. *with* the Software**
- **Be open source and developed by the whole DOE community**
  - **OSTI, ORNL, etc.**



Strong Community Backing

We have engaged the DOE Research Community through Requirements Teams

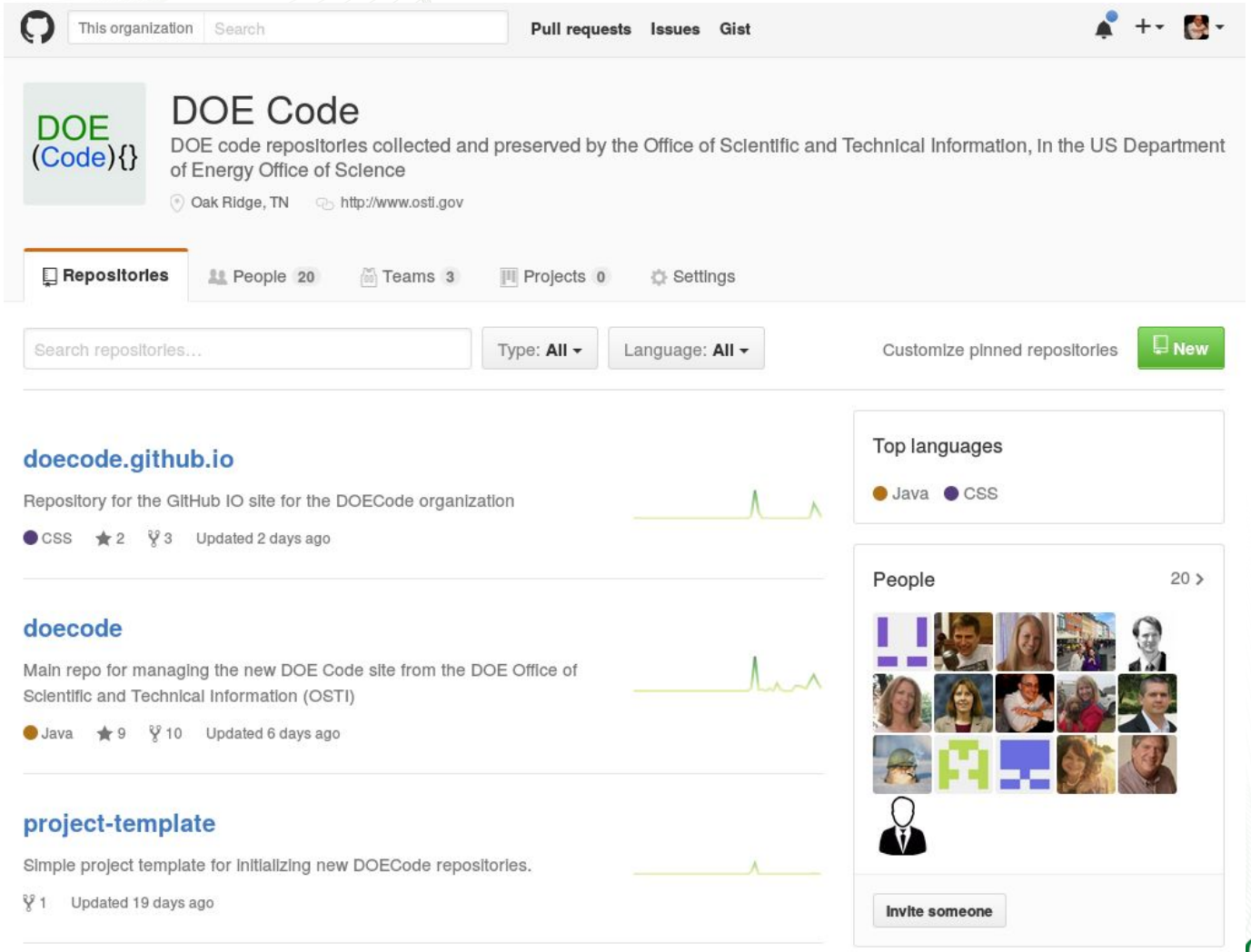
- "Core Requirements"
- OSTI – Technical
- OSTI – Policy
- DOE – GC
- Labs – Software
- Labs – HPC
- Labs – Data
- DOE ASCR

- Students
- Post Graduates
- Labs – Ops
- Labs – STI Managers
- Exascale Computing Program
- DOE Other Offices
- University Partners

Teams are roughly 4-5 people (sometimes more) and a set of interviews.

Strong Community Backing - We're on GitHub!

https://github.com/doecode



Strong Community Backing - Events

We're hitting the road!

Accepted Conference Events

- ICSTI TACC Workshop
- Supercomputing 2016
- SIAM CSE 2017 Spring Conference in Atlanta

Currently submitting to several more!

Leveraging - not replacing! - existing services

A profile on DOECode will combine info plus...

Your repo location from, e.g. -

Your papers from, e.g. -

SciTech Connect

Your data from, e.g. -

DOE Data Explorer

(Among others!)

Integrations we're thinking about

What if your code already has a DOI, i.e. - from Zenodo?

What about code.gov, the OMB's Open Source pilot?

Some cool requests thus far

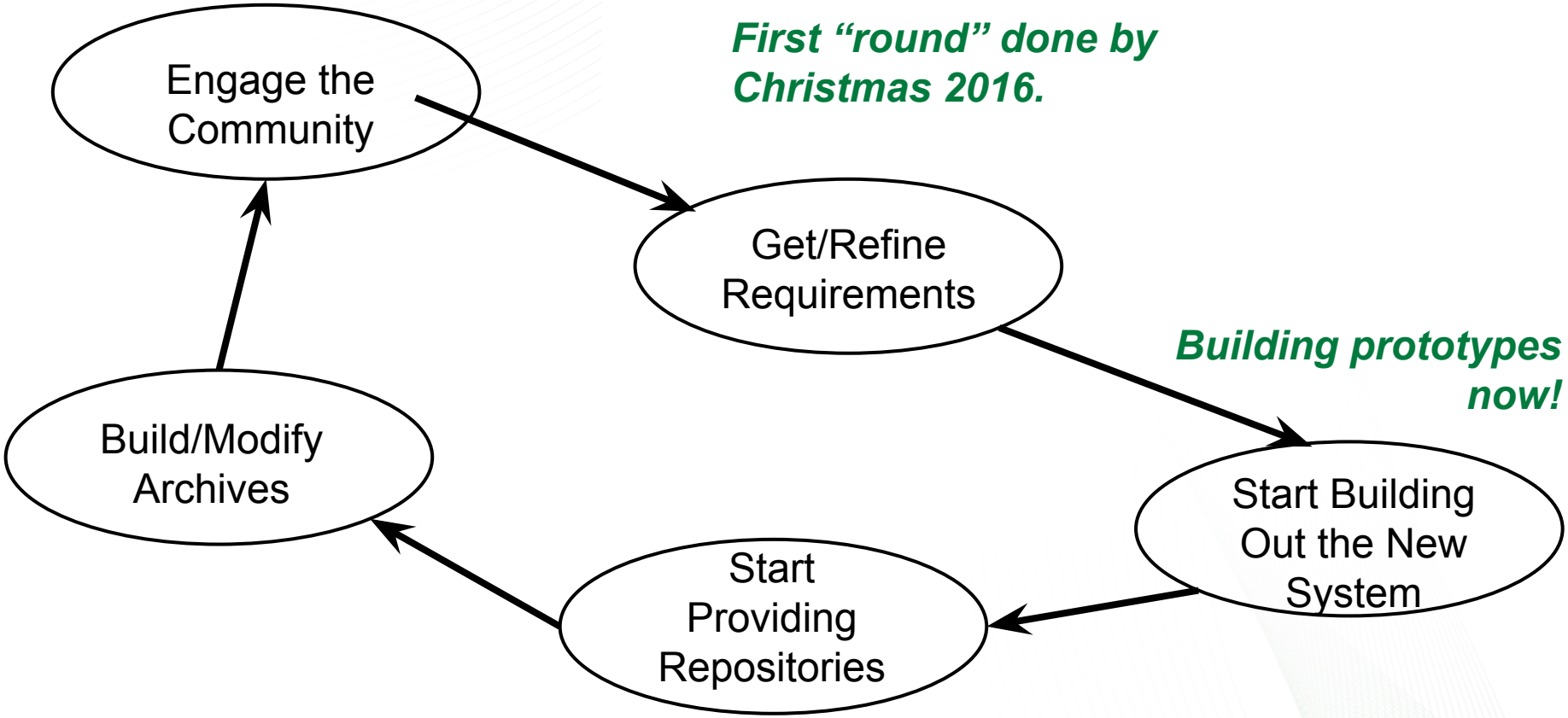
- Automated metadata ingest
- DOIs for software!
- Code Scanning - Performance, Quality, Security
- Automatic provisioning of containers on clouds
- Metrics and Analytics Dashboard
- Social Media Features for Authors and Users
- Portfolios and Lists
- “Success story” blog posts
- Long-Term Download Support for old versions

Path Forward

Iteratively developing this product with community support!

2yr development plan with many iterations!

First "round" done by Christmas 2016.



Current Technical and Policy Questions

Example Technical Questions

- Should we use web frameworks?
- Security concerns?
- UI Wireframes to drive design

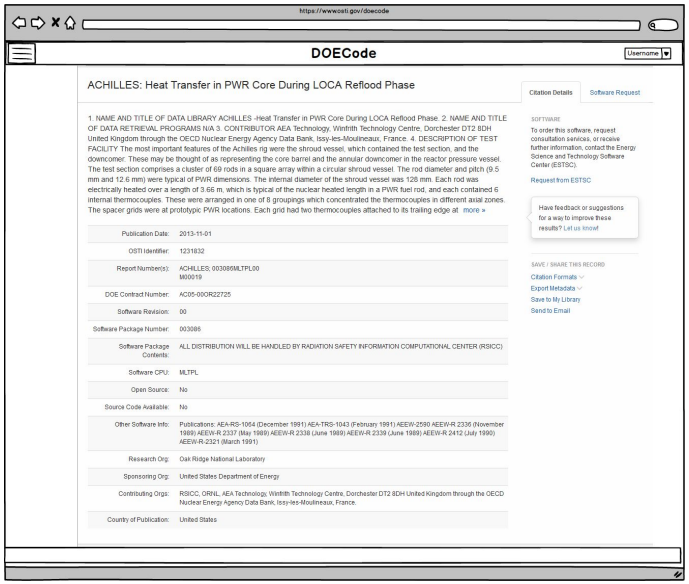
Example Policy Questions

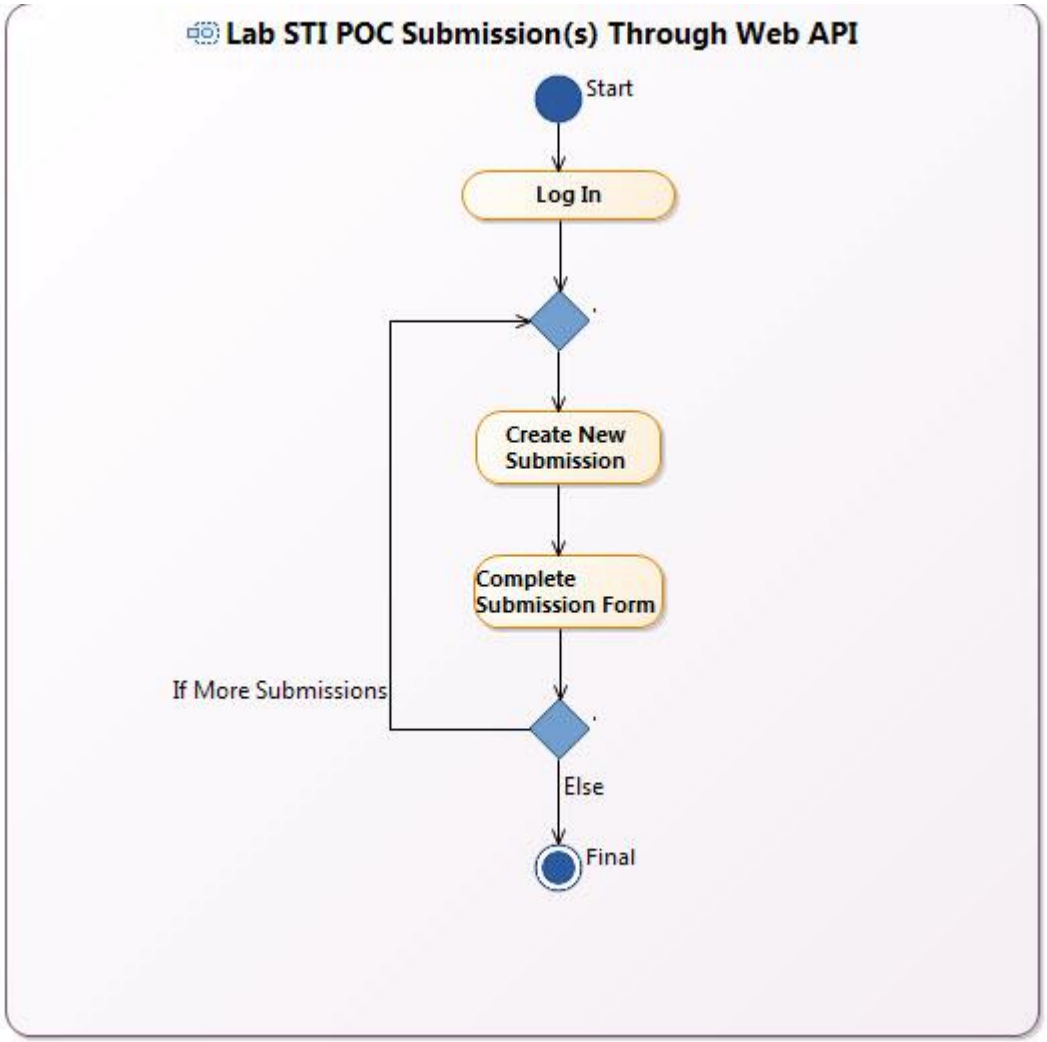
- What must change?
- What ought to change?
- What should our metadata look like?
- What's the new process for submitting software?

Both: *What do users want?*

What does this process look like?

1. The policy teams ask a question and answers it with a model.
2. The tech team responds with more questions, models or wireframes.





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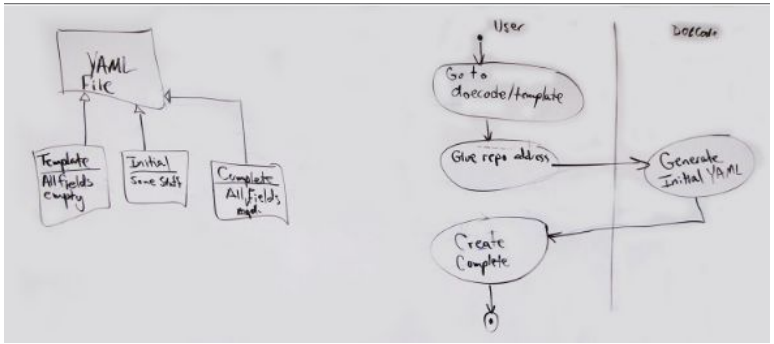
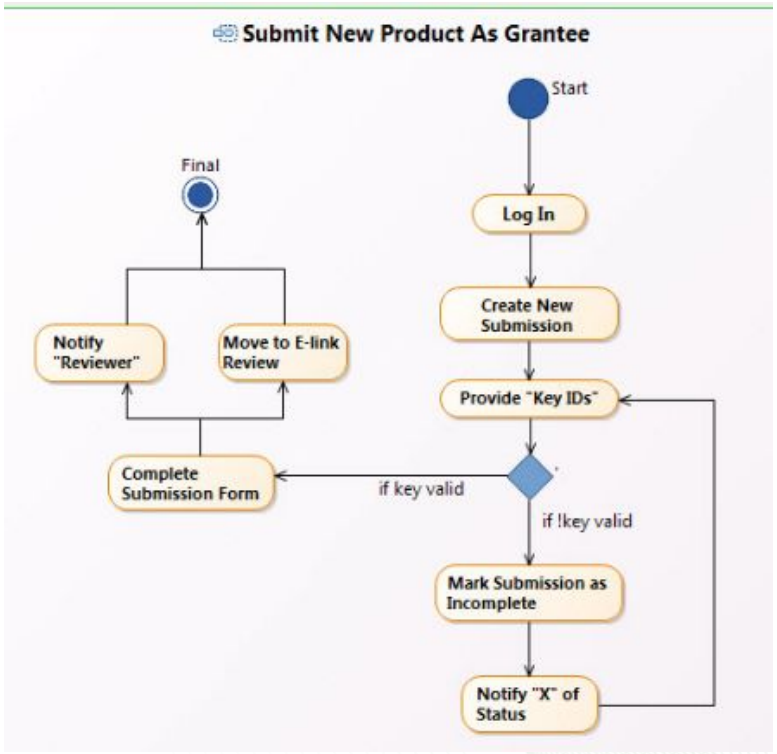
Managing Requirements, pt 1

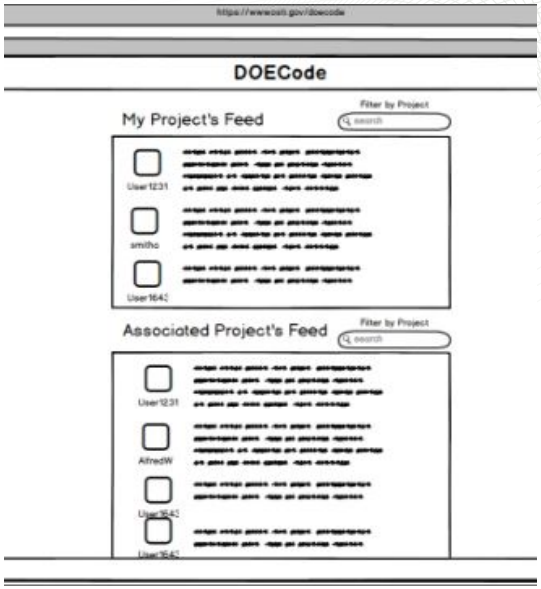
Includes high-level requirements and features captured as...

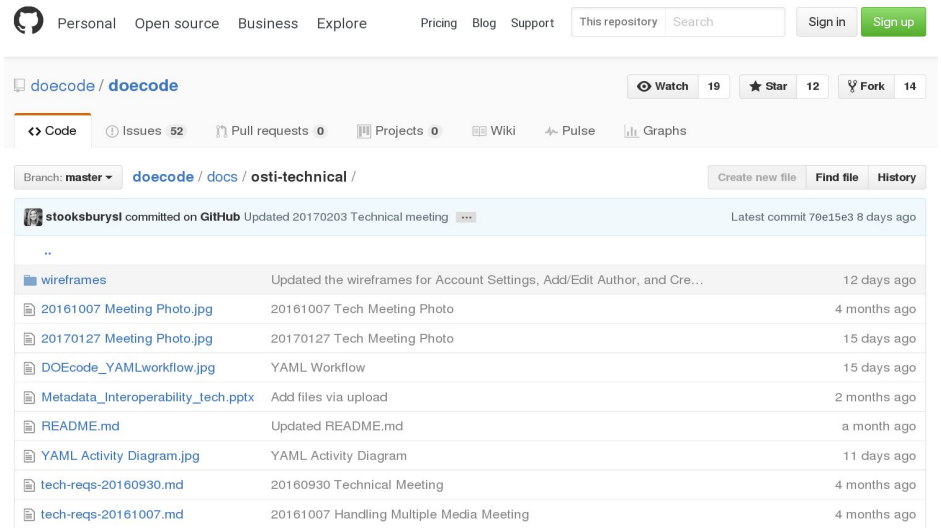
- –activity/workflow diagrams
- –wireframes
- –metadata schemas





Managing Requirements, pt 2





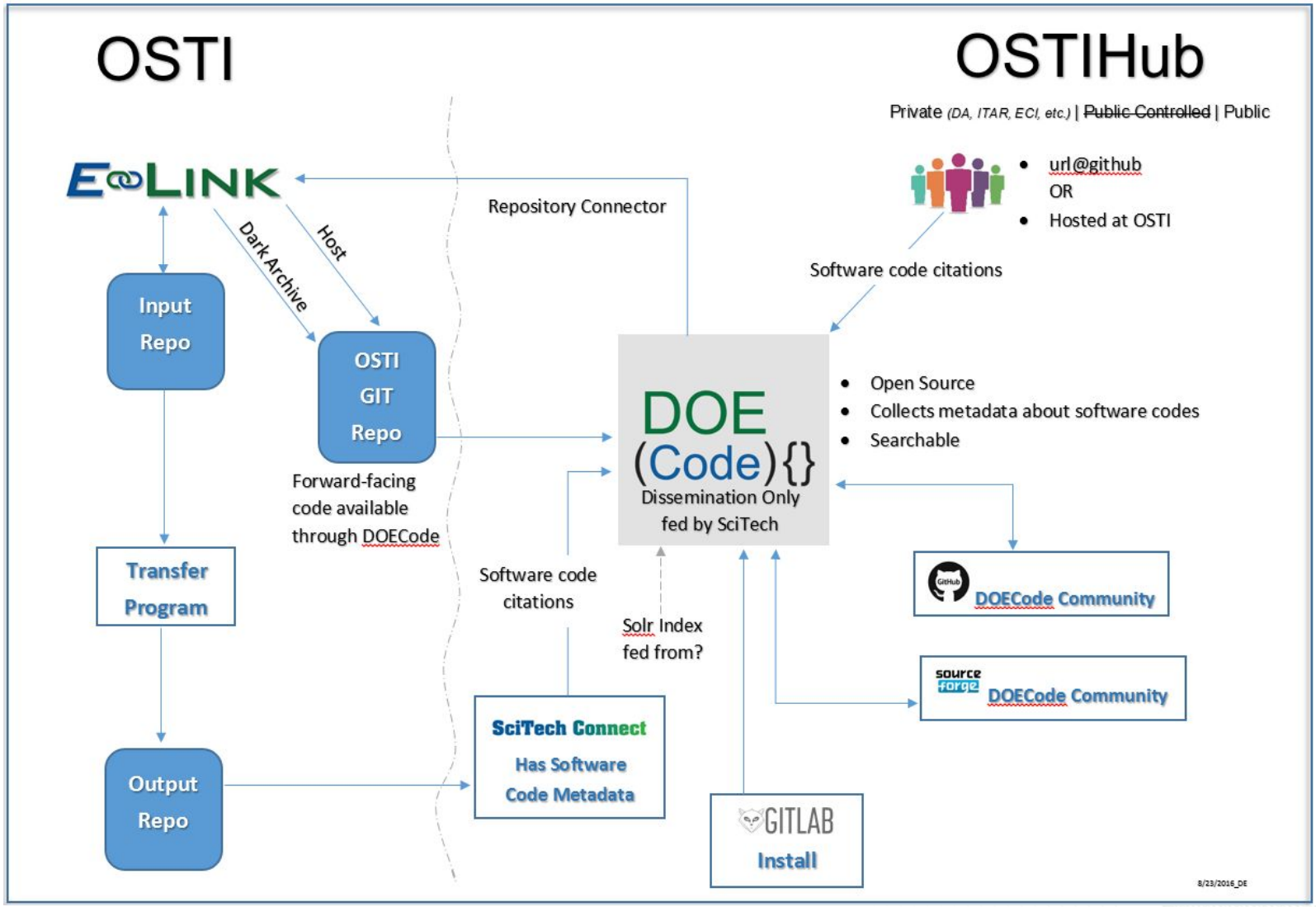
Strong engagement in detailed analysis and tracking from team **AND** community.

Label	*Version*
Definition	The described resource is a version, edition, or adaptation of the referenced resource. Changes in version imply substantive changes in content rather than differences in format.
Scheme	n/a
Property	dcterms:hasVersion / dcterms:isVersionOf
Usage	Potential use for multiple versions is the standard rdf:Alt container (or rdf:Seq or rdf:Bag) as a blank node containing the ordered or unordered versions
Cardinality	0 - n

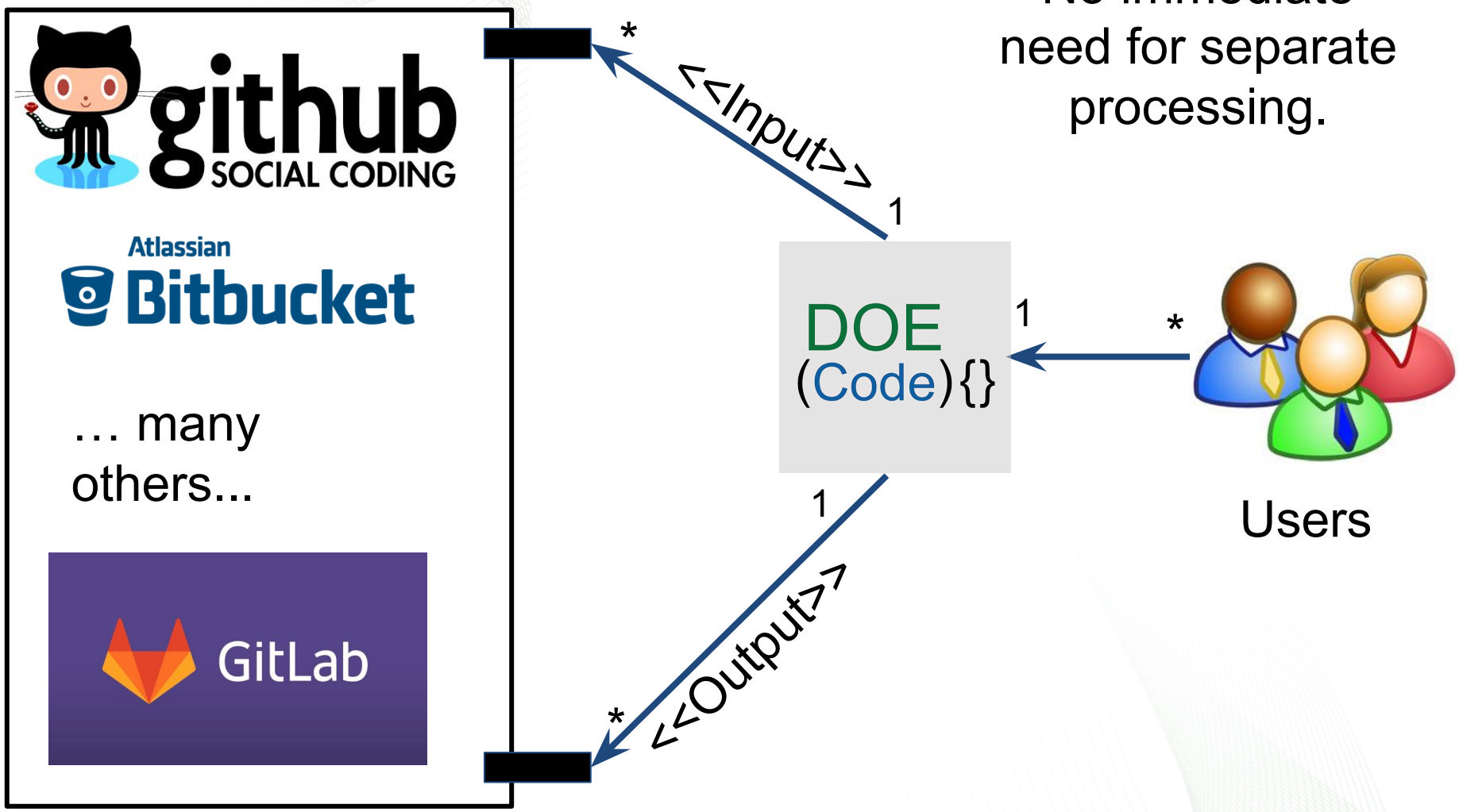
Example:

```
<dcterms:hasVersion>
<rdf:Alt rdf:about="http://www.github.com/Software">
    <rdf:_1 rdf:resource="github.com/Version2">
    <rdf:_2 rdf:resource="github.com/Version3">
    <rdf:_3 rdf:resource="github.com/Version4">
```

Deployment Architecture for OSTI



Deployment Architecture for ORNL



No immediate need for separate processing.

Metadata Overview

Work done:

- Used “Software Fields” spreadsheet to map local fields to all established controlled vocabularies
- Met with stakeholders/teams to verify/discuss proposed mappings
- Drafted Metadata Application Profile, Data Map, and YAML files
- Appended initial “Software Fields” spreadsheet with controlled vocabulary mappings

Schemas used:

- ADMS, ORG, SKOS, FOAF, Dublin Core, Schema.org

Metadata Overview, pt 2

This will give OSTI **best-in-class metadata:**

- Make the data migratable/interoperable with other systems
- Make OSTI compliant with best practices described by:
  - ISO 23081-2:2009E
    - "Standardized metadata are an essential prerequisite for information system interoperability."
  - ISO/TC 46/SC11N800R1
    - "...discover and then analyse any existing relevant schemas to see if any can be implemented without further change"
    - "If possible, do not introduce any new elements"
  - The Government Linked Data Working Group (W3C).
    - "It is best practice to use or extend an existing vocabulary before creating a new vocabulary."

How can you help?

Tell us what YOU want from DOECode!
Join a requirements team!
Engage at the GitHub site!

Website: https://www.osti.gov/doecode/

GitHub: https://github.com/doecode

Email: doecode@osti.gov

Twitter: @ostigov or @jayjaybillings

We are very grateful for the support of the Oak Ridge Leadership Computing Facility + IDEAS!

Questions?

DOE(Code){}

Thank You!

Additional Authors from OSTI: Chris Augustus, Kim Buckner, Daphne Evans, Neal Ensor, Joy Fender, Susie Faust, Darel Finkbeiner, Judy Gilmore, Lorrie Johnson, Peter Lincoln, Mark Martin, Josh Nelson, Rebel Powell, Carly Robinson, Crystal Sherline, Andrew Smith, Shelby Stooksbury, Lance Vowell and others.

Please reach out by email!
Jay: billingsjj@ornl.gov
Mark Martin: martinm@osti.gov

Or social media!
Twitter Handles:
@jayjaybillings
@OSTIgov

Abstract

The U.S. Department of Energy's Office of Scientific and Technical Information (OSTI) is charged with cataloging and preserving the software artifacts, among other things, produced by the Department's researchers. The fast pace at which the software world changes - including the rise and dominance of Open Source Software - has presented OSTI with the opportunity to update and expand its Software Center. These updates will provide a platform for the research community that combines social coding with OSTI's vast database of papers, authors, data, and legacy software to provide an integrated, dynamic environment for scientific software developers. This talk will describe the on-going development effort around that platform, as well as the requirements that define it, and how OSTI is engaging the open research community at large in its development. This talk will also present a description of scientific software in a broader context to clarify further why such a platform is needed and the extremely great benefits expected from its deployment.