EESSD - ESS Cyberinfrastructure Working Groups

Software Engineering and Interoperability

Leads: David Moulton (LANL/acting)   Ethan Coon (ORNL)

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Interests and Scope

*A high quality community driven **open-source software ecosystem of interoperable components** that can be assembled in flexible configurations within a common framework **supporting ModEx and the Virtual Laboratory:***

- integration of legacy and new capabilities across projects
- rigorous – but rapid – testing and validation of model-data integration capabilities
- changing architectures and programming models
- complex multiscale models (coupling, interoperability)
- performing quantitative and formalized UQ
- diverse interdisciplinary teams, and training
- increased scientific productivity

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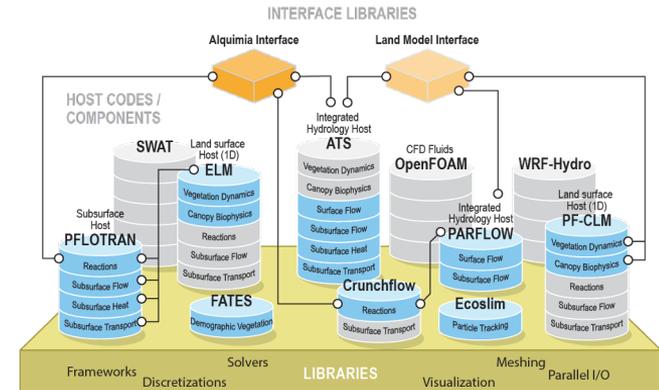
Progress and Related Goals

- Existing codes have been released under an Open Source License and increasingly are adopting an Open Development Model
  - Transparency – issues and feature branches are generally open
  - Broader community can submit fixes/features via pull/merge request.
- Software Ecosystem codes are developing ***Software Productivity and Sustainability Improvement Plans*** (roadmap concept from IDEAS)
  - Leverage and extend "policies" work in the xSDK
- Participate in the broader community, e.g.,
  - CSDMS annual meeting, modeling clinics
  - International Soil Modelling Consortium (ISMC) workshop
  - CUAHSI Community Modeling Working
- Co-lead/participate in Model Intercomparison studies

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Software Productivity and Sustainability Improvement Plans (S-PSIPs)

Derived from the IDEAS-Classic Project

Proposal Review Criterion applicable to:

- **SBR SFAs and university applicants, ICoM, InteRFACE, Coastal proposal**
- **"New" Scientific Software (developed, enhanced, modified)**
  - Requires a Software Productivity and Sustainability Improvement Plan (S-PSIP)
  - S-PSIP expected to outline plans for releasing the code open source and making the software available to the broader community
  - Plans for incorporating best practices for development/enhancement
  - How the source code will be managed and issues tracked
  - Whether there are mechanisms for recognizing the value of the individual developing/enhancing the code
  - Whether there is a long-term plan for sustaining and continuing to improve the developed code

DOE (ASCR) Open Source Software (OSS) Guidance   2003

TO: DEPARTMENT OF ENERGY NATIONAL LABORATORIES

FROM: WILLIAM H. REED ACTING DIRECTOR
OFFICE OF ADVANCED SIMULATION AND COMPUTING

CARL E. OLIVER ASSOCIATE DIRECTOR
OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH

SUBJECT: POLICY GUIDANCE – OSS LICENSE RELEASE OF SOFTWARE DEVELOPED WITH ASC AND OASCR FUNDING

POLICY:
The U.S. Department of Energy (DOE) Office of Science/Office of Advanced Scientific Computing Research (OASCR) and the Office of Defense Programs/Office of Advanced Simulation and Computing (historically known as ASCI) are establishing the following policy:
All publicly released DOE Laboratory software, which is developed using funding from OASCR and/or ASCI, shall be either:
designated and distributed to the public as Open Source Software (OSS); or
designated as an unrestricted releasable software to the public by delivering the software to DOE's Energy Science and Technology Software Center (ESTSC) for sole distribution using DOE standard software licenses.
HQ Program approval will be required for software to be restrictively licensed when:
Laboratory successfully demonstrates that extraordinary circumstances exist such that commercialization of software through restrictive licensing is necessary; or
the software is subject to export control, classification or contractual requirements.
The DOE Laboratories will ensure that subcontracts to contractors working directly for Laboratory code development will include provisions consistent with this policy.

BACKGROUND:
OASCR and ASCI have strategic interests in the software products produced at DOE Laboratories to be released to the public. The open-source model for software development and release in the high-performance computing (HPC) community is well established and provides the following benefits:

OSS provides HPC sites the opportunity to identify and fix bugs quickly;
The OSS model yields important contributions to the global state of the art, thus providing significant leverage of Government investments;
The OSS model provides a hedge against "change in support" status for software required to execute the missions of these Programs. This yields protection for the investments made in the software; and
Access to source code of OSS can enhance cyber security by facilitating rapid identification and repair of security vulnerabilities.

To: All DOE Patent Counsel Da : April 29, 2010

Re: DOE LABORATORY OPEN SOURCE SOFTWARE: ADVANCE DOE PROGRAM APPROVAL AND OTHER OSS LICENSING ISSUES

INTRODUCTION

On Feb 1, 2002, DOE Patent Counsel issued an IPI-II-1-01 for "Development and Use of Open Source Software." A year later, subparagraph (f) of the Rights in Data clause of the M&O Contract (DEAR 970.5227-2) was developed to incorporate the IPI into the M&O Contract. Before this change, a DOE laboratory was required to seek DOE approval from both the patent counsel and the cognizant funding program before asserting copyright in any software . The new OSS clause was developed because it was not necessary for DOE patent counsel to review each OSS request before a laboratory could assert copyright. Program approval for release of the software as OSS is still required. However, the clause provides that DOE patent counsel may provide sole approval if program approval is not practicable. The new clause has been incorporated into many M&O Contracts by the DOE Contracting Officers . It is currently pending to be included in the DEAR.

In 2003, and the Office of Science/Office of Advanced Scientific Computing Research (OASCR) and the Office of Defense Programs/Office of Advanced Simulation and Computing (ASCI) issued a policy (Policy Guidance-OSS License Release of Software Developed with ASCI and OASCR Funding) that directs the DOE national laboratories to release all publicly releasable software, which is created from funding by its programs, as either OSS or Government software distributed by DOE's Energy Science and Technology Software Center (ESTSC) . If a laboratory wants to commercialize the software with royalty-bearing licenses, a laboratory must seek OASCR/ASCI approval. This policy is still in effect and is not altered by this IPL.

Several DOE laboratories have had difficulty in getting DOE Program approval for release of OSS over the last eight years. This was due to funding program confusion over the OSS approval process. This is more evident with funding from other government agencies because statutes and rules governing these agencies automatically allow the recipient of funds to assert copyright in software without agency approval.

In addition, DOE and its laboratories have encountered additional issues regarding OSS over the last eight years when DOE first granted the OSS authority to its laboratories. The last section of this IPI will address some of these recent issues .

CANCELLATION OF PREVIOUS IPI

IPI-II-1-01 had two major sections. First, the IPI established the authority of OSS at the laboratories that was later amended into the M&O Contracts and codified in the DEAR. Second, the IPI outlined guidance for using OSS at a laboratory. Some of this guidance is included in this IPL Therefore, IPI-II-1-01 is hereby cancelled.

DOE PROGRAM BLANKET APPROVAL :

At present, only the OASCR/ ASCI programs have issued a blanket approval of all software to be licensed as OSS. As for other DOE Programs, it is recommended to have a blanket approval from all DOE programs to issue software as OSS. Over the last eight years, the laboratories have requested DOE

ESS - Open Source Software Review/Approval

OSS Release Approval Requests

- Release requests submitted to funding program for approval
- Most often submitted by DOE lab Intellectual Property Office on behalf of the lead software developer
- Rarely have any supporting information that outlines any details of what would be approved
- ESS Program Managers need to understand what we are being asked to approve (not only for Export Control but from a programmatic standpoint)
- ESS developed a Software Disclosure, Abstract and Export Control Form
- Posted on the Google Docs for comment from the ESS community

Software Disclosure, Abstract and Export Control
Review Form for DOE-BER Sponsor

Software Title and Version Number:
Name of the software and version number.

Category of Invention:
Software – (*Earth science, Geoscience, Bioscience, etc.*)

Abstract:
1-2 paragraphs on what the software is, what it does, what area(s) or science it might be used for, and why it's development should be important to the DOE/BER funding program. If it is an enhancement/new version additionally provide what the enhancement is and why the enhancement should be useful for the scientific community and the DOE/BER funding program.

(*Lab Name*) Office of (*Technology Development/Deployment or Intellectual Property or Innovation Office, etc.*) Contact:
Name, telephone number and e-mail.

Inventor(s) and (*Lab Name*) Organization:
Name(s) of the originating lab organization (e.g., Office, Division, Program). Primary Contact Name, e-mail and telephone number.
Secondary Contact Names, e-mails and telephone numbers.

Funding:
A sentence that includes the name of the laboratory where the software was developed along with the name of contractor operating the laboratory and the contract number.

Review Form for DOE-BER Sponsor (sample)

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OSTI Code Repository: DOECODE

OSTI GitHub

- Developers can use the OSTI GitHub repository to develop or host open source projects.

DOE CODE's GitLab

- Developers can use the internal DOE CODE GitLab instance to develop or host projects needing controlled access.
- Ongoing work in ECP to use GitLab for CI testing on DOE computing facilities.
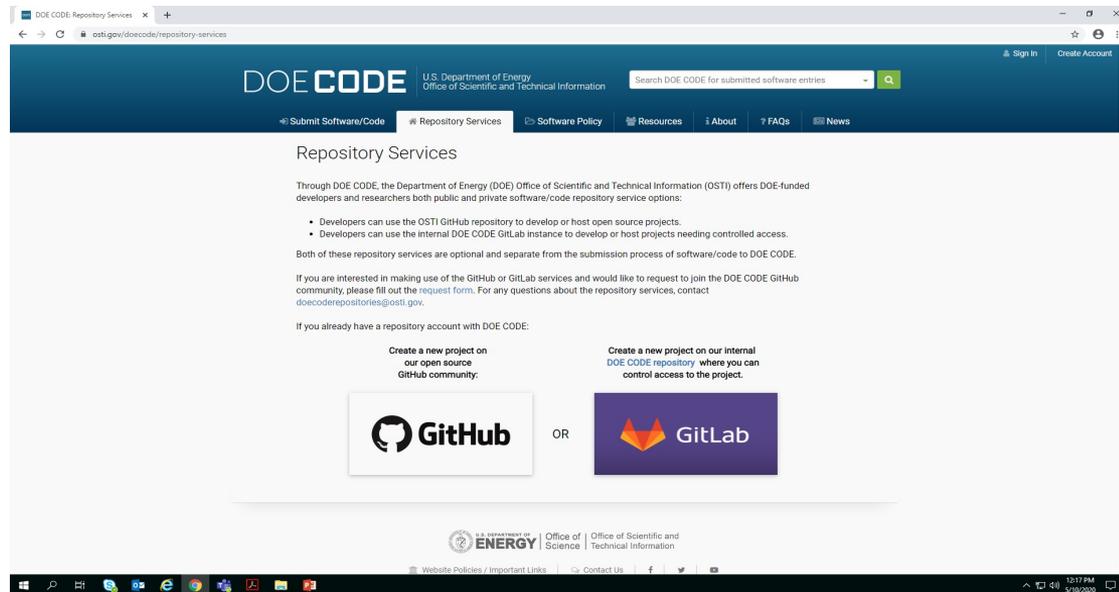
Near-Term Goals

Identify best practices for model-related data in repositories.
- Survey existing data practices, formats
- Determine how to **present, support, and ensure adoption** of identified best practices.

Identify the needs of the APIs and services in CESD applications.
- Inter-process (coupling) and model workflow communication
- Survey needs and existing capabilities of data mediators
- Survey existing interfaces used and identify targets based on immediate needs.

Publish/share high-resolution model output and analysis
- Reduce gap between HPC and Non-HPC modelers and domain scientists
- Develop Use Cases (approach, requirements, and prototype) for publishing large data sets arising from Integrated Hydrology simulations

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Contribute to SEI Challenges and Priorities

Contribute your challenges and priorities
Google doc: ESS-CI_SEIWG_ChallengesPriorities_Discussion

Plan:

- Collect challenges / resources in Google doc
- Complete Doodle Poll to set meeting this week to start prioritizing challenges
- May 18: Breakout session to
  - Review / modify / prioritize challenges
  - Flesh out details / resources
  - Identify writing teams / schedule

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