

How Open Source Supports the Largest Computers on the Planet

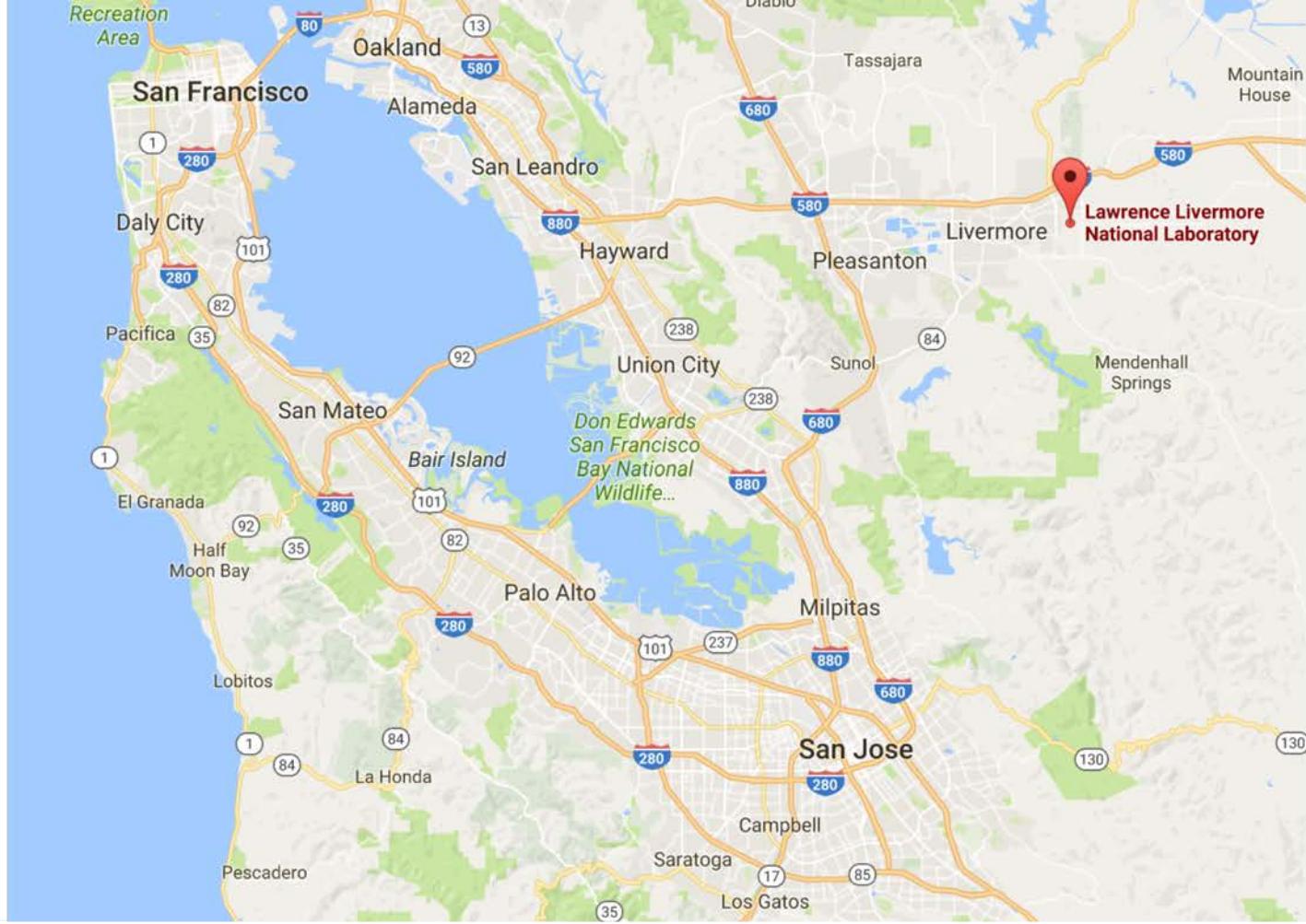
Best Practices for HPC Software Developers

Ian Lee

Lawrence Livermore National Laboratory

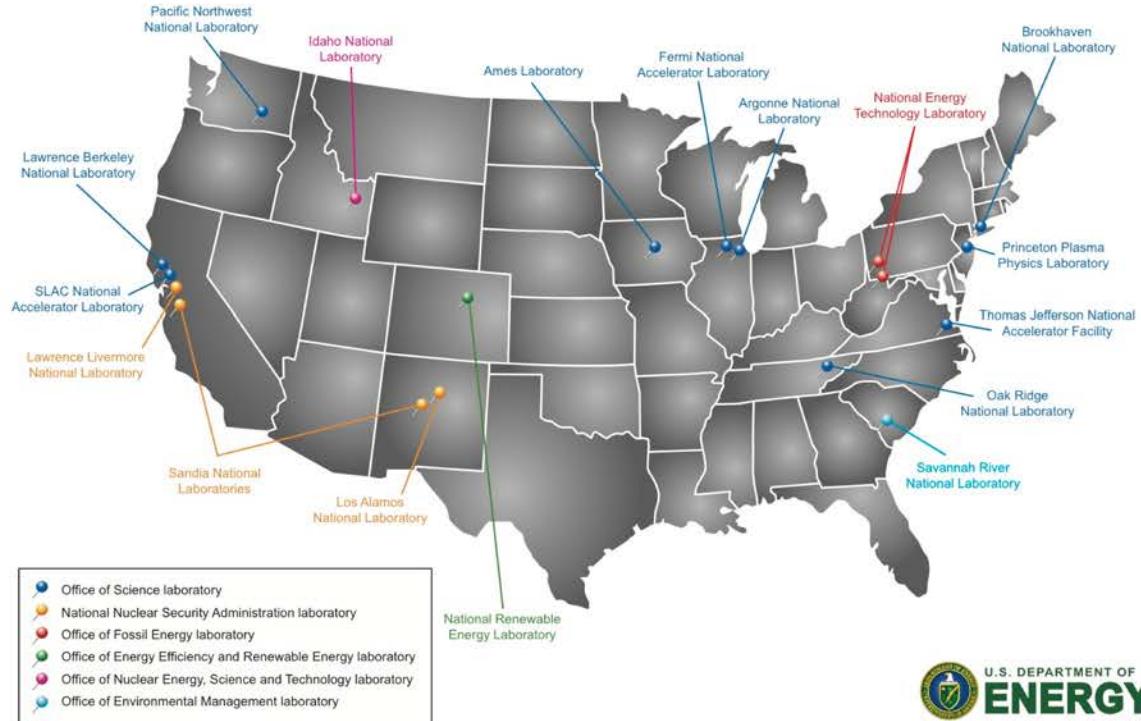
July 18, 2018

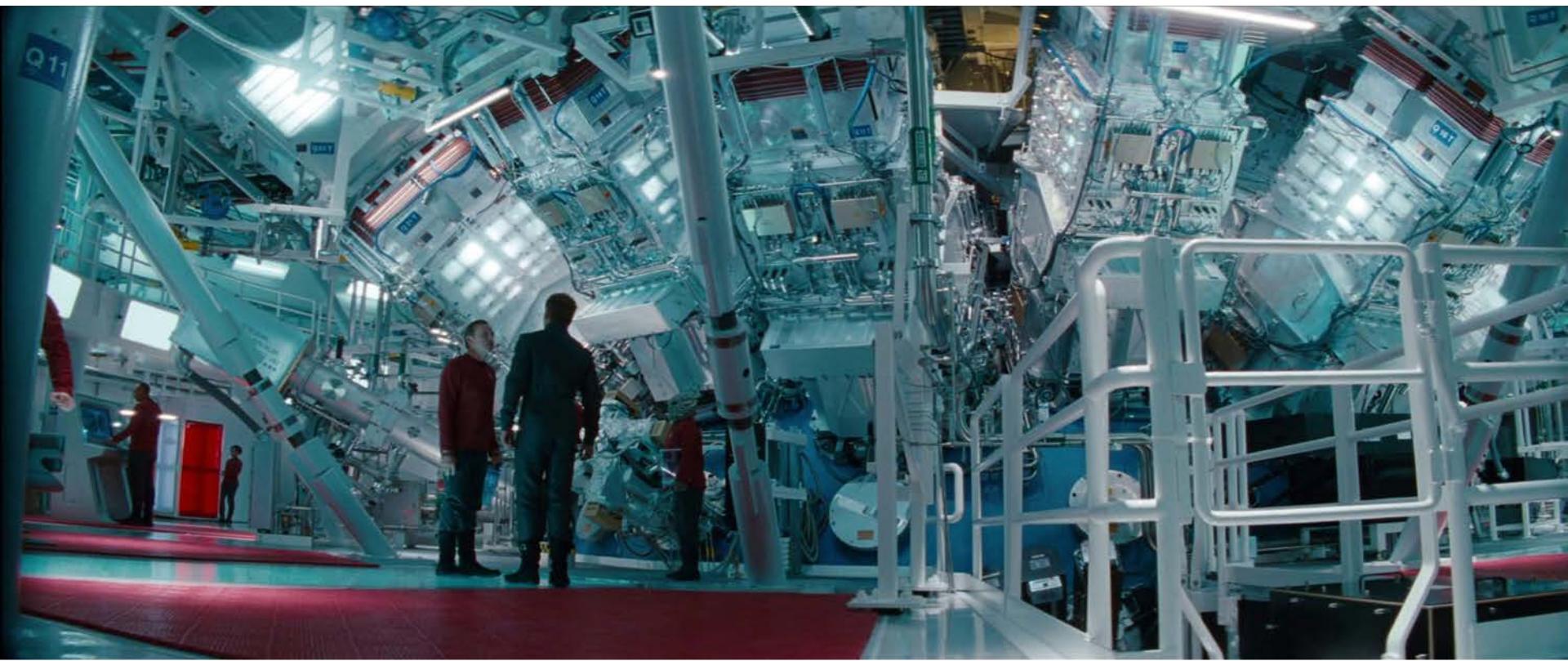






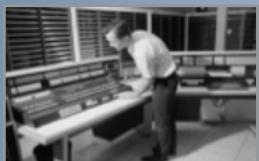
Department of Energy National Laboratories



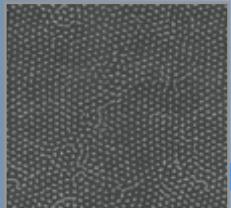




1960s



CDC 3600

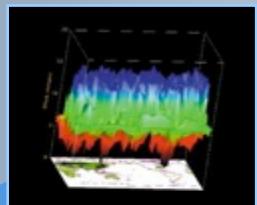


Pioneering
simulations of
particle tracking

1970s



CDC 7600



Ozone mixing
models

1980s



CRAY 1

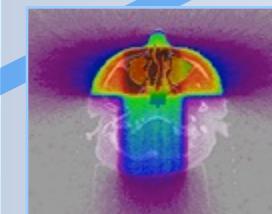


Dynamics in three
dimensions

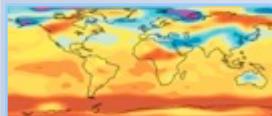
1990s



ASCI Blue-Pacific



Helping the medical
community plan
radiation treatment

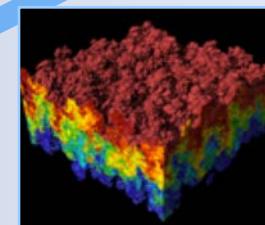


Global climate
modeling

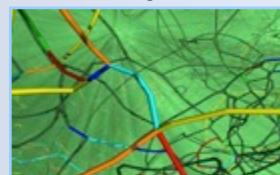
2000s



BlueGene



Breakthrough
visualizations of
mixing fluids

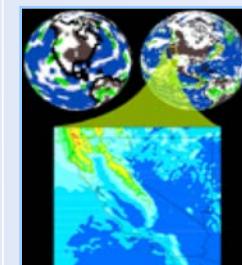


Unprecedented
dislocation dynamics
simulations

2010s



Petascale
and exascale
computing



Detailed
predictions
of ecosystems

- 3 out of 16 #1 systems over last 20 years

ASCI White
Nov 2000 – Nov 2001



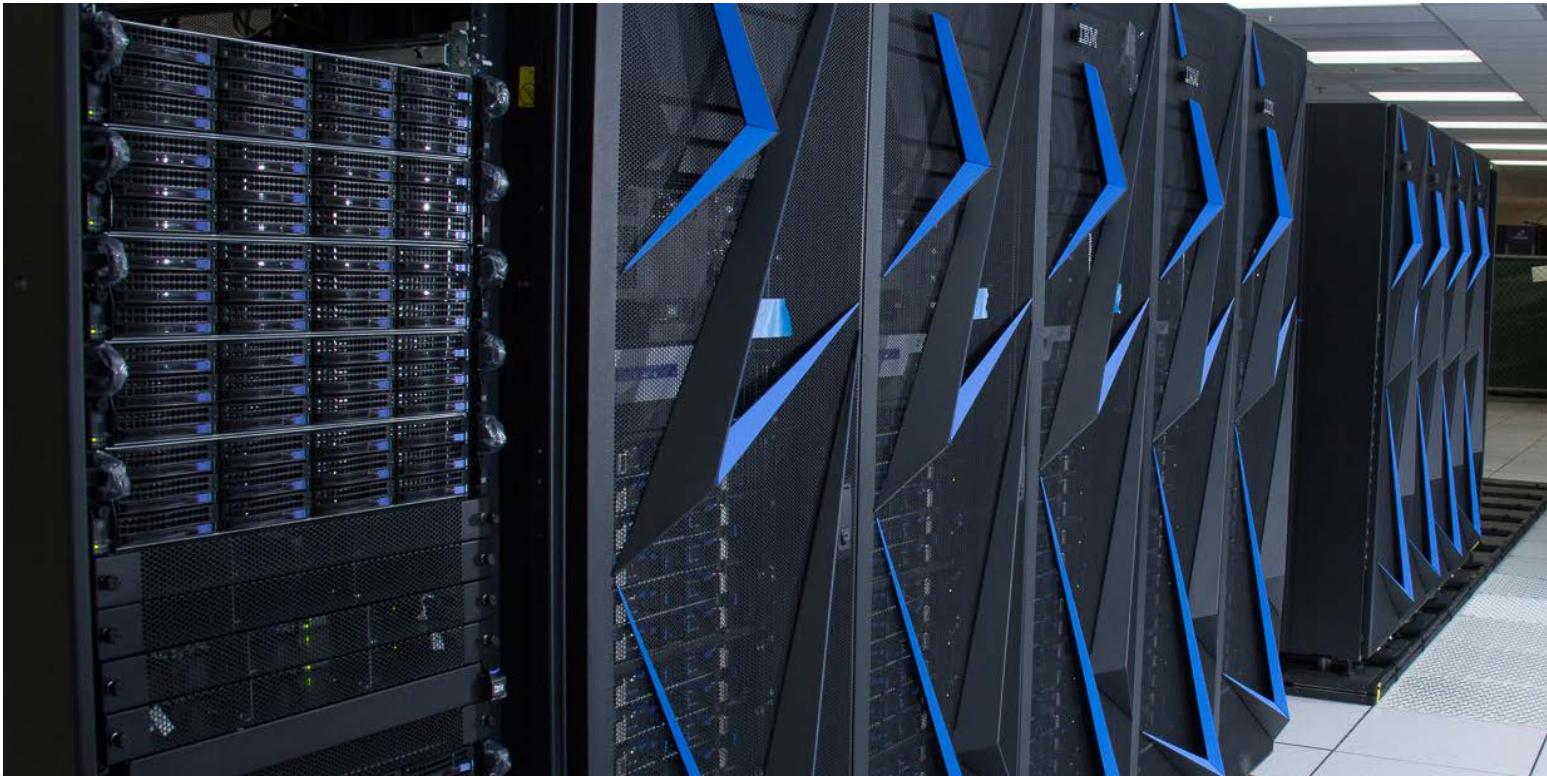
BlueGene/L
Nov 2004 – Nov 2007



Sequoia
June 2012

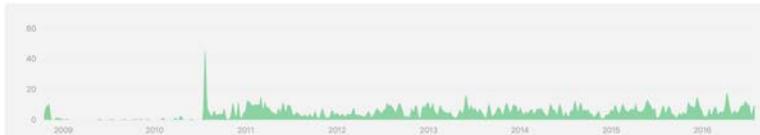


Sierra

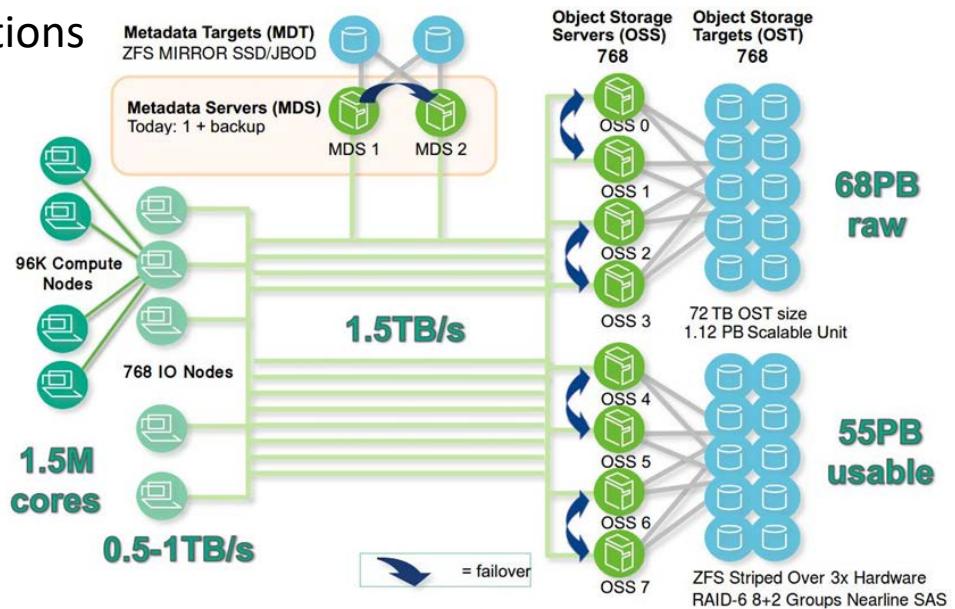




ZFS on Linux



- ZFS is an open source filesystem and volume manager designed to address the limitations of existing storage solutions
- 2011: Available for Linux
- Ten LLNL filesystems, totaling ~ 100PB
- Ships in Ubuntu 16.04



Screenshot of a GitHub repository page for `zfsonlinux/zfs`. The page shows the Issues tab selected, displaying 938 open issues.

Key statistics at the top:

- Watch: 381
- Star: 2,955
- Fork: 706

Navigation and search:

- Code
- Issues 938 (selected)
- Pull requests 40
- Projects 2
- Wiki
- Insights

Filters and search bar:

- Filters: is:issue is:open
- Labels
- Milestones
- New issue

Issue list:

Count	Label	Title	Comments
938	Open	zfs iostat: zfs send does not seem to affect bandwidth rates #7076 opened 3 days ago by voidzero	3
3,464	Closed	scrub found mirrored file with checksum error on both copies #7075 opened 3 days ago by array42	1
		"fg: no job control" error on installing zfs .deb #7074 opened 3 days ago by darrenfreeman	1
		selinux messages, invalid context, relabel inode or filesystem in question? #7073 opened 3 days ago by array42	1
		Suspend to disk does not work with zfs/spl 0.7.5 #7071 opened 4 days ago by jhyeon	4
		Silent drive failures with kernel debug messages #7070 opened 5 days ago by darrenfreeman	4
		Compilation error kernel 4.14.13 and zfs 0.7-release #7069 opened 5 days ago by voidzero	8

GitHub, Inc. github.com/zfsonlinux/zfs/blob/master/.github/CONTRIBUTING.md

zfs/CONTRIBUTING.md at master · zfsonlinux/zfs

This repository Search Pull requests Issues Marketplace Explore

 zfs/zfsonlinux / zfs Watch 381 Star 2,956 Fork 706

Code Issues 938 Pull requests 40 Projects 2 Wiki Insights

Branch: master → [zfs/.github/CONTRIBUTING.md](#) Find file Copy path

 [dinatale2](#) commitcheck: Multiple OpenZFS ports in commit 69b229b on Oct 26, 2017

3 contributors 

291 lines (230 sloc) | 11.6 KB Raw Blame History

Contributing to ZFS on Linux



First of all, thank you for taking the time to contribute!

By using the following guidelines, you can help us make ZFS on Linux even better.

Table Of Contents

[What should I know before I get started?](#)

- [Get ZFS](#)
- [Debug ZFS](#)
- [Where can I ask for help?](#)

[How Can I Contribute?](#)

- [Reporting Bugs](#)
- [Suggesting Enhancements](#)
- [Pull Requests](#)
- [Testing](#)

[Style Guides](#)

- [Coding Conventions](#)
- [Commit Message Formats](#)
 - [New Changes](#)
 - [OpenZFS Patch Ports](#)
 - [Coverity Defect Fixes](#)
 - [Signed Off By](#)

```
12  
13 The latest stable and development versions of this port can be downloaded  
14 from the official ZFS on Linux site located at:  
15  
16 http://zfsonlinux.org/  
17  
18 This ZFS on Linux port was produced at the Lawrence Livermore National  
19 Laboratory (LLNL) under Contract No. DE-AC52-07NA27344 (Contract 44)  
20 between the U.S. Department of Energy (DOE) and Lawrence Livermore  
21 National Security, LLC (LLNS) for the operation of LLNL. It has been  
22 approved for release under LLNL-CODE-403049.  
23  
24 Unless otherwise noted, all files in this distribution are released  
25 under the Common Development and Distribution License (CDDL).  
26 Exceptions are noted within the associated source files. A few notable  
27 exceptions and their respective licenses include:  
28  
29 Skein Checksum Implementation: module/icp/algs/skein/THIRDPARTYLICENSE  
30 AES Implementation: module/icp/asm-x86_64/aes/THIRDPARTYLICENSE.gladman  
31 AES Implementation: module/icp/asm-x86_64/aes/THIRDPARTYLICENSE.openssl
```

 GitHub, Inc. github.com/zfsonlinux/zfs/pull/7079

OpenZFS 8731 - ASSERT3U(nui64s, <=, UINT16_MAX) fails for large blocks by dinatale2 · Pull Request #7079 · zfsonlinux/zfs

 **Review required** [Add your review](#)

At least one approved review is required by reviewers with write access. [Learn more.](#)

 **Some checks haven't completed yet** [Hide all checks](#)

1 failing, 1 pending, and 22 successful checks

 buildbot/CentOS 7 x86_64 Mainline (TEST)	— Build done.	Required	Details
 buildbot/Ubuntu 17.04 x86_64 Coverage (TEST)	— Build started.	Required	Details
 buildbot/Amazon 2 x86_64 (BUILD)	— Build done.	Required	Details
 buildbot/Amazon 2 x86_64 Release (TEST)	— Build done.	Required	Details
 buildbot/CentOS 6 x86_64 (BUILD)	— Build done.	Required	Details

 **Merging is blocked**

Merging can be performed automatically with one approved review.

 [Merge pull request](#) You're not [authorized](#) to merge this pull request.

GitHub, Inc. GitHub.com/LLNL/hypre

LLNL/hypre: Parallel solvers for sparse linear systems featuring multigrid methods. This repository houses releases and test releases. Pull requests can still be addressed. LLNL users should use the main repository on MyBitbucket.

This repository Search Pull requests Issues Marketplace Explore

Watch 18 Star 55 Fork 28

Code Issues 5 Pull requests 0 Projects 0 Wiki Insights Settings

Parallel solvers for sparse linear systems featuring multigrid methods. This repository houses releases and test releases. Pull requests can still be addressed. LLNL users should use the main repository on MyBitbucket. <https://www.llnl.gov/casc/hypre/>

Add topics

39 commits 1 branch 31 releases 3 contributors LGPL-2.1

Branch: master New pull request Create new file Upload files Find file Clone or download

rfgalgot Release v2.13.0-28-g42e267b Latest commit dea490d on Dec 5, 2017

	AUTOTEST	Release v2.13.0-28-g42e267b
	docs	Release v2.13.0-28-g42e267b
	src	Release v2.13.0-28-g42e267b
	CHANGELOG	Release v2.13.0
	COPYING.LESSER	Checkin of Hypre 2.4.0b
	COPYRIGHT	Checkin of Hypre 2.8.0b
	INSTALL	Checkin of Hypre 2.10.0b

GitHub, Inc. github.com/llnl/hYPRE/issues

Issues - LLNL/hYPRE

This repository Search Pull requests Issues Marketplace Explore

Watch 18 Star 55 Fork 28

LLNL / hYPRE

Code Issues 5 Pull requests 0 Projects 0 Wiki Insights Settings

Filters is:issue is:open Labels Milestones New issue

5 Open ✓ 12 Closed

Author Labels Projects Milestones Assignee Sort

ⓘ HYPRE Parallel Scaling Problem #25 opened 2 days ago by shahaneshtantanu 1

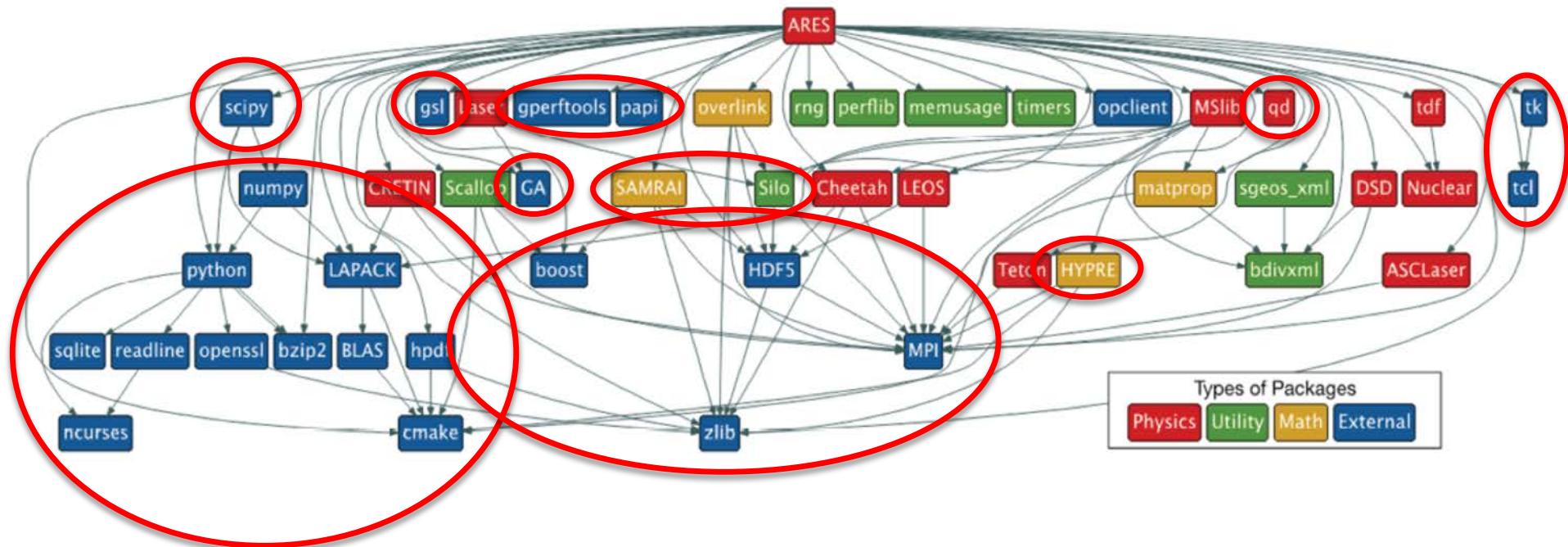
ⓘ Does HYPRE StructVectorGetValue support getting values at the other cpu? #23 opened 25 days ago by ztdepztdep 6

ⓘ SStructSet/GetBoxValues not working as expected #22 opened on Dec 4, 2017 by nncarlson 15

ⓘ Small bug in hypre_BoomerAMGBuildCoarseOperator? #18 opened on Oct 10, 2017 by IdoAkkerman 1

ⓘ hypre_ParCSRMatrixPrintIJ / hypre_ParCSRMatrixReadIJ #6 opened on Jun 10, 2016 by mlstowell 1

💡 ProTip! Type **g** **p** on any issue or pull request to go back to the pull request listing page.



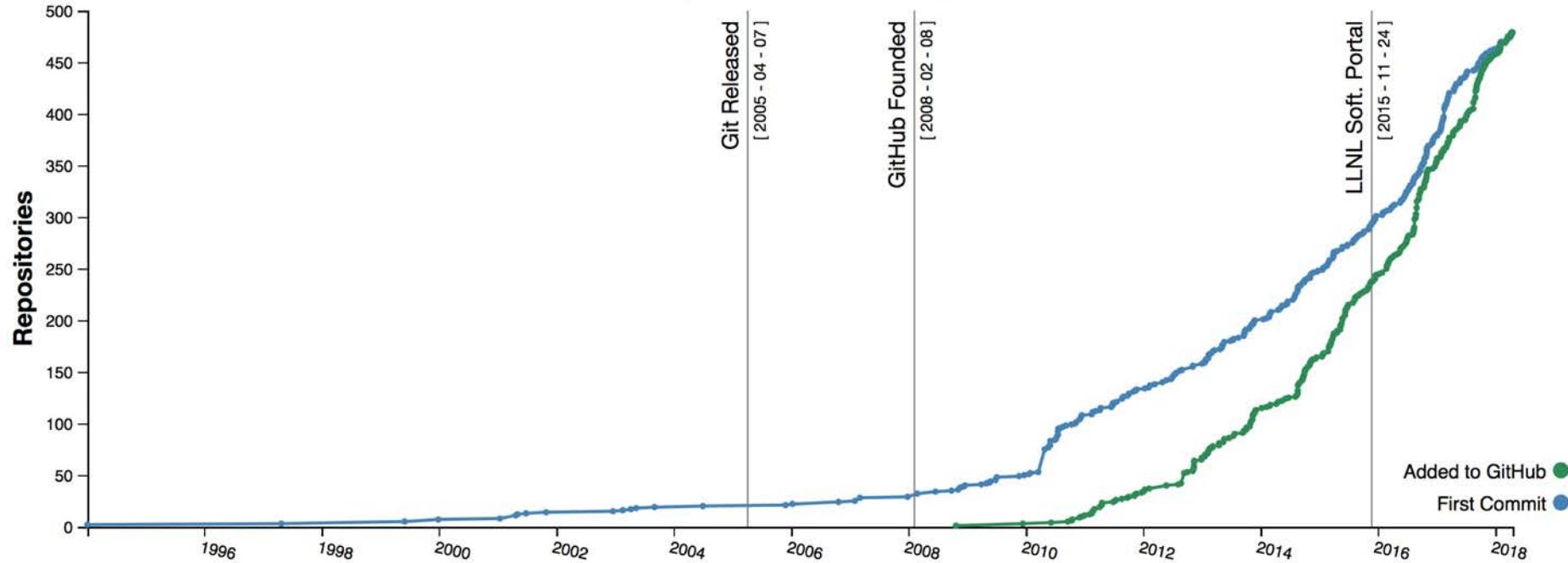
The screenshot shows a web browser window displaying the LLNL Software Catalog. The page title is "LLNL Software Portal". A banner at the top right says "Fork me on GitHub". The main heading is "432 Software Repositories". A search bar labeled "Filter Repositories" is present. Below are nine software repository cards:

- zfs** | zfsonlinux | C
ZFS on Linux - the official OpenZFS implementation for Linux.
0 ⭐ 3316 ⚡ 699
- spack** | spack | Python
A flexible package manager that supports multiple versions, configurations, platforms, and compilers.
0 ⭐ 571 ⚡ 417
- zfs-auto-snapshot** | zfsonlinux | Shell
ZFS Automatic Snapshot Service for Linux
0 ⭐ 373 ⚡ 104
- spl** | zfsonlinux | C
A shim layer which adds the core interfaces required for OpenZFS.
0 ⭐ 284 ⚡ 168
- pkg-zfs** | zfsonlinux | -
Native ZFS packaging for Debian and Ubuntu
0 ⭐ 262 ⚡ 34
- mfem** | mfem | C++
Lightweight, general, scalable C++ library for finite element methods
0 ⭐ 199 ⚡ 79
- rose** | rose-compiler | C
A release version of ROSE that passes all regression tests
0 ⭐ 167 ⚡ 59
- pdsh** | chaos | C
A high performance, parallel remote shell utility
0 ⭐ 162 ⚡ 27
- dcp** | hpc | Shell
dcp is a distributed file copy program that automatically distributes and dynamically balances work equally across nodes in a large distributed system without centralized state.
0 ⭐ 154 ⚡ 10
- diiod** | chaos | C
Distributed I/O Daemon - a 9P file server
0 ⭐ 145 ⚡ 29
- zfp** | LLNL | C
Library for compressed numerical arrays that support high throughput read and write random
- magpie** | LLNL | Shell
Magpie contains a number of scripts for running Big Data software in HPC environments,

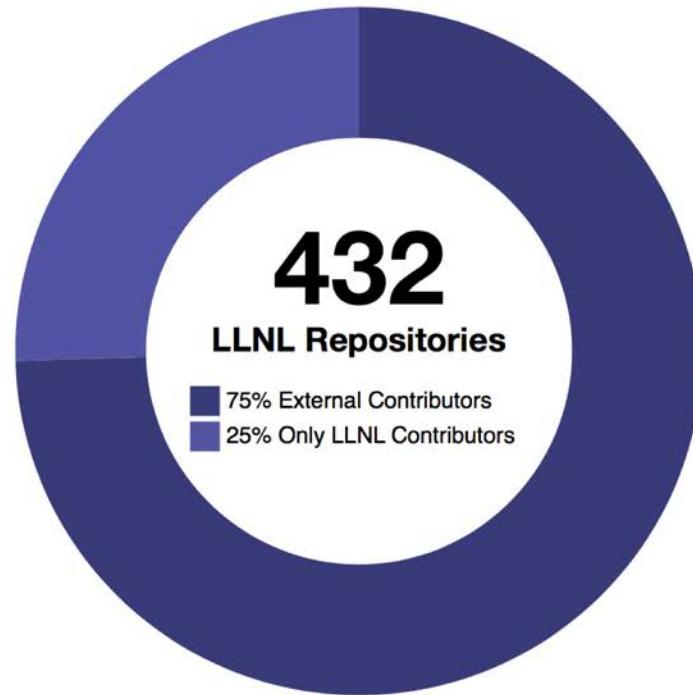
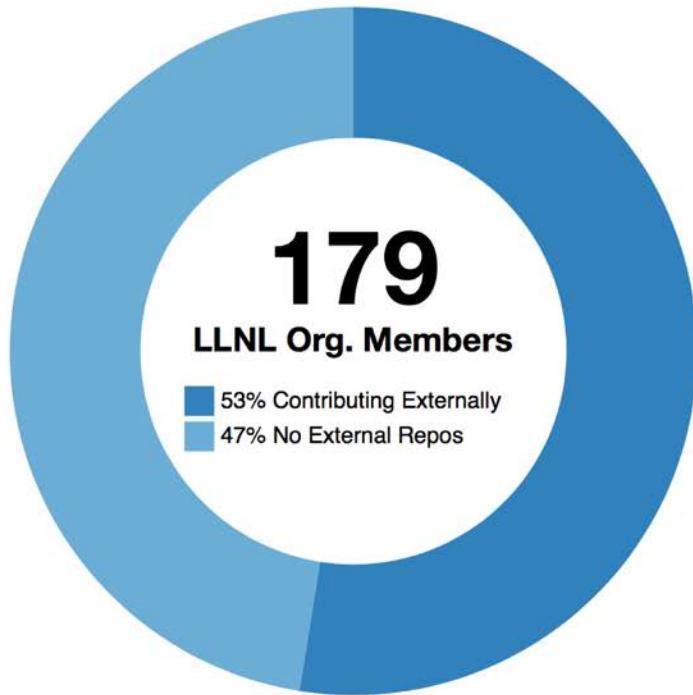


LLNL Open Source Presence

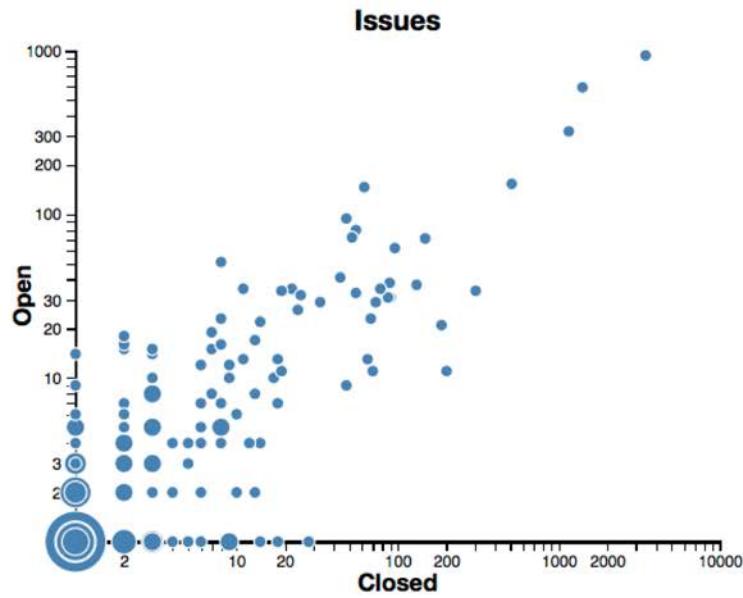
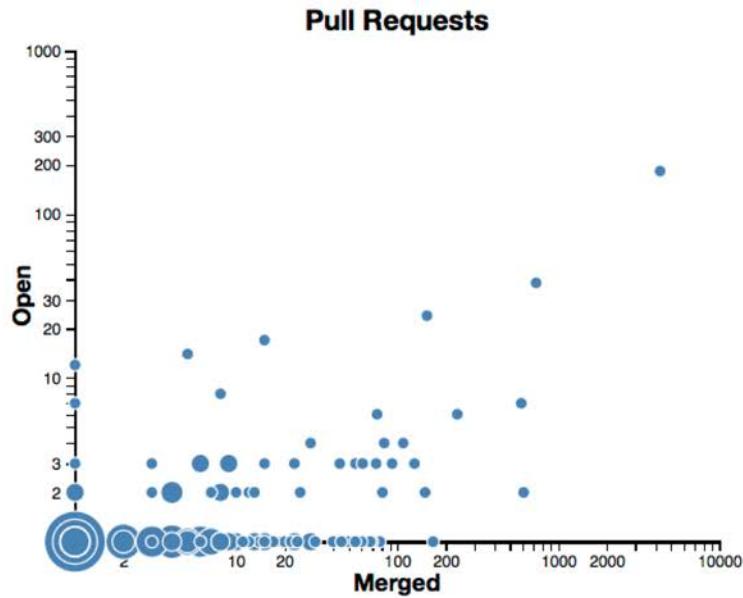
Repo Creation History



LLNL Open Source Engagement



LLNL Open Source Activities



Lawrence Livermore National Laboratory

January/February 2018

Science & Technology REVIEW



The magazine is open to several pages. One page features a large image of a supercomputer server rack. Another page shows a diagram of a network or system architecture. Other pages contain text articles and small images related to software development, space exploration, and scientific research.

Science & Technology Review

Commentary by Bruce Hendrickson



The High Value of Collaborative Software

“Our large collection of software is a precious Laboratory asset, one that benefits both Lawrence Livermore, and in many cases, the public at large.”

- Bruce Hendrickson

Associate Director, Computation

www.exascaleproject.org/more-on-the-software-that-underpins-the-exascale-computing-project

An Up-Close View of the Software that Underpins the Exascale Computing Project - Exascale Computing Project



FOCUS AREAS + NEWS AND MEDIA + TRAINING EVENTS

AN UP-CLOSE VIEW OF THE SOFTWARE THAT UNDERPINS THE EXASCALE COMPUTING PROJECT

08/30/17

When exascale systems become a reality, the Exascale Computing Project (ECP) will bring to those systems both existing high-performance computing (HPC) software and promising emerging research. Accordingly, one of the objectives of the ECP is to create a production-quality base—a software stack—to support the scientific applications that will run on these systems.

Scientists developing applications for exascale systems depend on an intricate set of software that makes the computing system usable and the job of the application developer easier. The broad services this software provides are often collectively referred to as the software stack.

Virtually all of the ECP software stack developed by the US Department of Energy (DOE) is composed of open-source code, which makes the software broadly available and appealing to other programmers to contribute when the base capabilities are established. Software provided by the platform vendors, however, often consists of a combination of open-source and

Federal Source Code Policy

- “Federal Source Code Policy: Achieving Efficiency, Transparency, and Innovation through Reuseable and Open Source Software”
 - “Agencies **shall make custom-developed code available for Government-wide reuse** and make their code inventories discoverable at <https://www.code.gov> (“Code.gov”) [...]”
 - “[...] establishes a pilot program that requires agencies, when commissioning new custom software, to **release at least 20 percent of new custom-developed code as Open Source Software (OSS)** [...]”

[&](https://code.gov) <https://sourcecode.cio.gov>

code_

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www.osti.gov/doecode/

DOE CODE: Your software services platform and search tool to easily submit, announce, and discover code funded by the U.S. Department of Energy

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U.S. Department of Energy
Office of Scientific and Technical Information

Search DOE CODE for submitted software entries

Q

Submit Software/Code

Repository Services

About

A screenshot of a web browser window showing the GitHub and Government homepage. The URL in the address bar is `government.github.com`. The page has a blue header with the GitHub logo and the text "GitHub and Government". Below the header are navigation links: "Who's using GitHub", "Peer Group", "Accessibility", and "Contact". The main content area features a large white title "How agencies build software" and a subtitle "Collaborate on code, data, policy, or procurement within your agency or with the public." Below this, there are two sections: "Collaborate on code" and "On your servers or in the cloud", each with a brief description.

GitHub and Government

Who's using GitHub Peer Group Accessibility Contact

How agencies build software

Collaborate on code, data, policy, or procurement within your agency or with the public.

Collaborate on code

Code collaboration and review are built into the development process with GitHub. Share work, discuss changes, and get feedback in one place to write quality code.

On your servers or in the cloud

Run GitHub Enterprise on your servers as a virtual appliance, on AWS GovCloud or Azure, or let us host the code for you on GitHub.com, whatever your security requires.

US Government Organizations on GitHub



Thank You!

ian@llnl.gov

@IanLee1521 // @LLNL_OpenSource

<https://speakerdeck.com/IanLee1521>

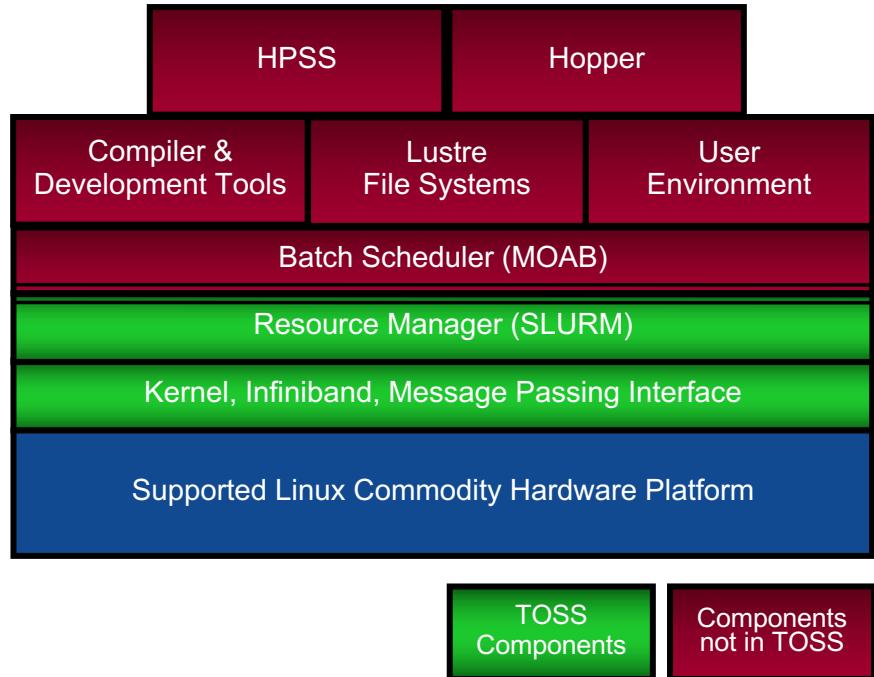


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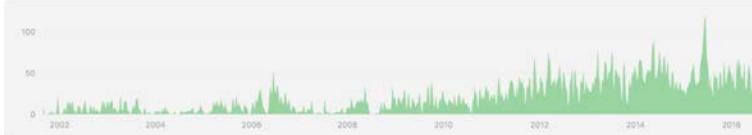


TOSS – Tri-Lab Operating System Software

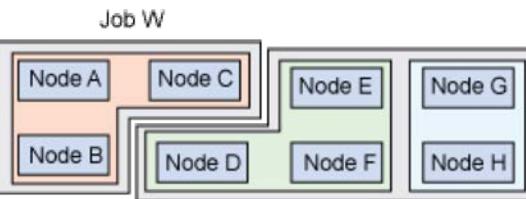
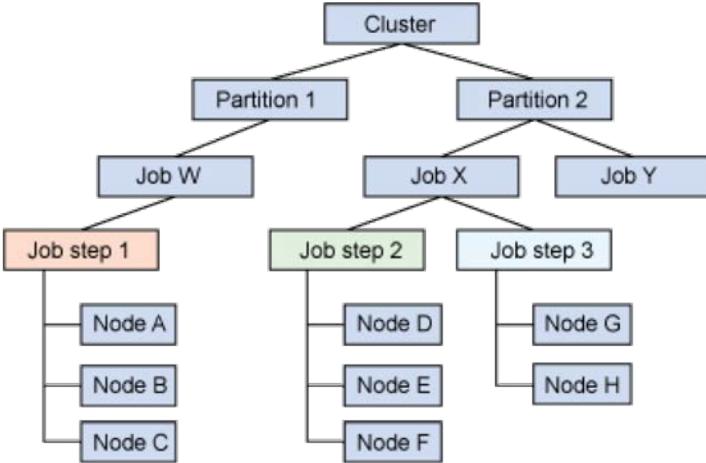
- Built on Red Hat Enterprise Linux
 - Not an HPC distribution
- Adds LLNL developed additions and patches to support HPC
 - Low Latency Interconnect: Infiniband
 - Parallel File System: Lustre
 - Resource Manager: SLURM
- Work closely with open communities



TOSS is a software stack for HPC – large, interconnected clusters!



- Began as simple resource manager
 - Now scalable to 1.6M+ cores (sequoia)
- Launch and manage parallel jobs
 - Large, parallel jobs, often MPI
- Queuing and scheduling of jobs
 - Much more work than resources



<http://slurm.schedmd.com>

[Watch](#)

13

[Star](#)

24

[Fork](#)

11



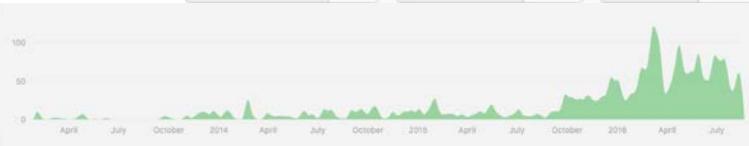
- Family of projects used to build site-customized resource management systems
- **flux-core**
 - Implements the communication layer and lowest level services and interfaces
- **flux-sched**
 - Consists of an engine that handles all the functionality common to scheduling
- **capacitor**
 - A bulk execution manager using flux-core, handles running and monitoring 1000's of jobs



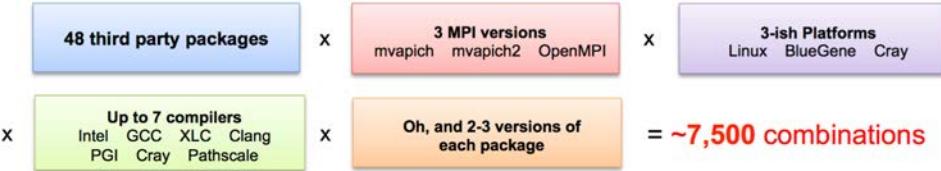


SPACK

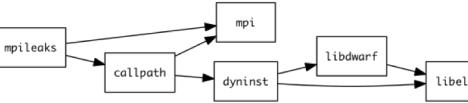
Watch 43 Unstar 150 Fork 134



- Handles combinatorial explosion of ABI-incompatible packages
- All versions coexist, binaries work *regardless of user's environment*
- Familiar syntax, reminiscent of brew, yum, etc



Dependency DAG

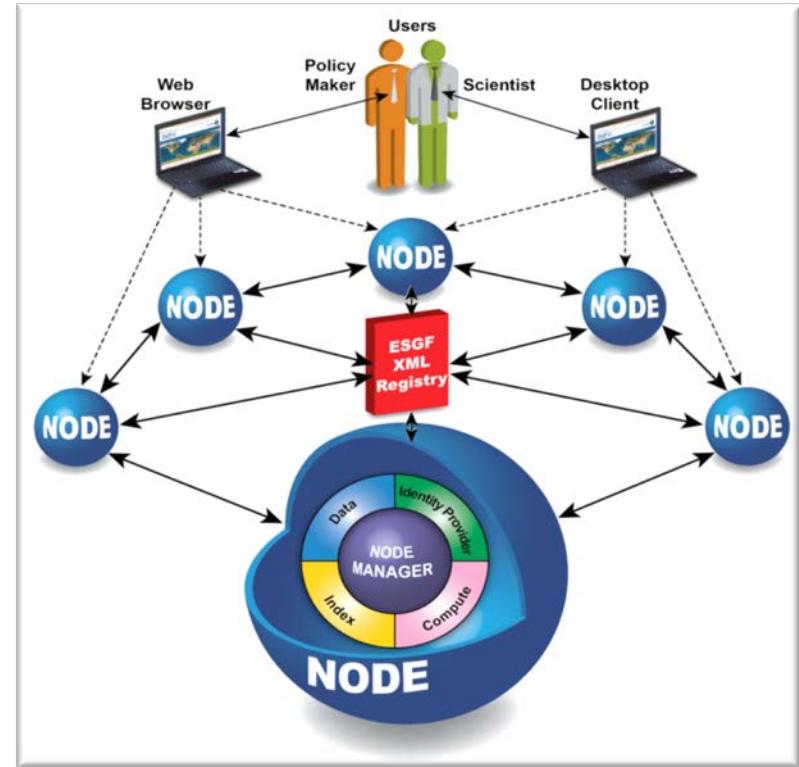


Installation Layout

```
spack/opt/
  linux-x86_64/
    gcc-4.7.2/
      mpileaks-1.1-0f54bf34cadk/
        intel-14.1/
          hdf5-1.8.15-lkf14aq3nqiz/
        bgq/
          xl-12.1/
            hdf5-1-8.16-fqb3a15abrx/
  ...
  ...
```

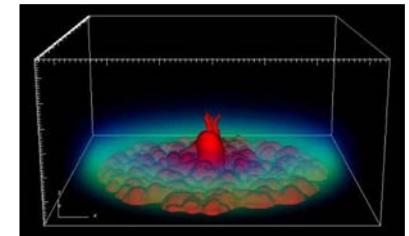
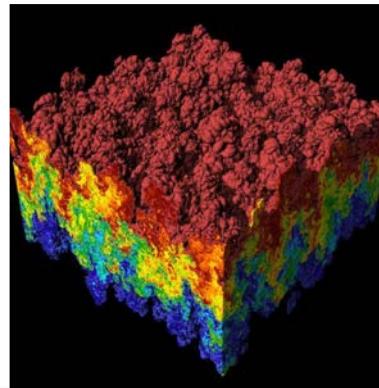
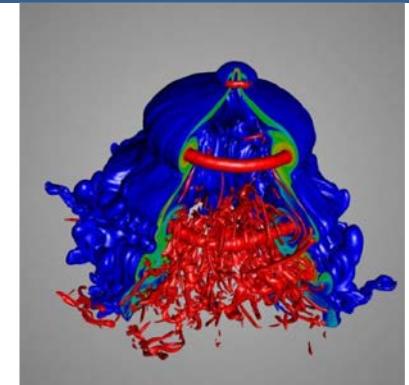
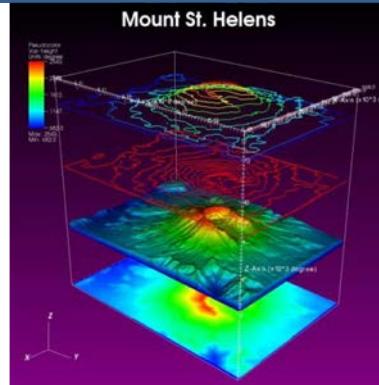
```
$ spack install mpileaks           unconstrained
$ spack install mpileaks@3.3       @ custom version
$ spack install mpileaks@3.3 %gcc@4.7.3   % custom compiler
$ spack install mpileaks@3.3 %gcc@4.7.3 +threads  +/- build option
$ spack install mpileaks@3.3 os=SuSE11    os=<frontend OS>
$ spack install mpileaks@3.3 os=CNL10     os=<backend OS>
$ spack install mpileaks@3.3 os=CNL10 target=haswell target=<cpu target>
```

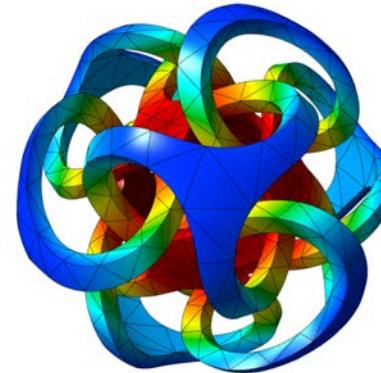
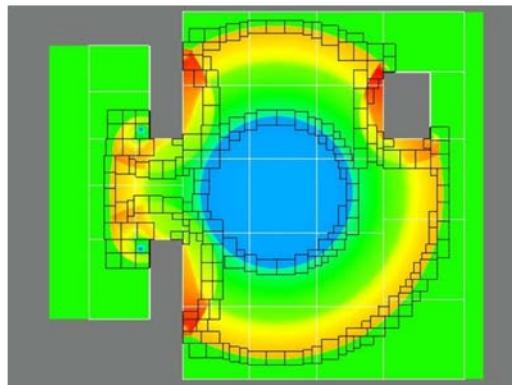
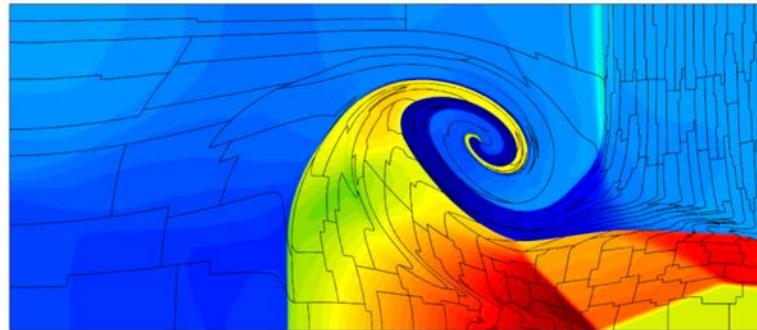
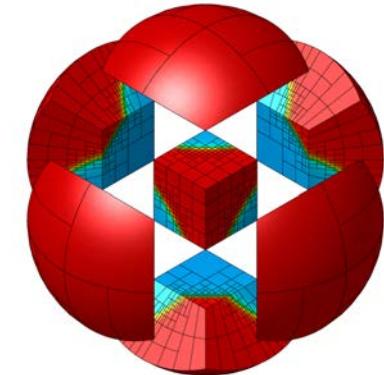
- Manages the first-ever decentralized database for handling climate science data
- Multiple petabytes of data at dozens of federated sites worldwide
- International collaboration for the software that powers most global climate change research



VisIt

- Originally developed to visualize and analyze the results of terascale simulations
- Interactive, scalable, visualization, animation and analysis tool
- Powerful, easy to use GUI
- Distributed and parallel architecture allows handling extremely large data sets interactively





code.gov/#/explore-code/agencies/DOE

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Department of Energy

877 Projects

[3D Torus Routing Engine Module for OFA OpenSM v.1.0](#)

This OpenFabrics Alliance (OFA) OpenSM routing engine module provides credit-loop-free routing while supporting two quality of service (QoS) levels for an InfiniBand fabric with a 3D torus topology. I...

 Open Source

[A Distributed, Parallel Visualization and Analysis Tool](#)

Visit is an interactive parallel visualization and graphical analysis tool for viewing scientific data on UNIX and PC platforms. Users can quickly generate visualizations from their data, animate them...

 Open Source

[A Grand Canonical Monte Carlo simulation program for computing ion distributions around biomolecules in hard sphere solvents](#)

The GIBS software program is a Grand Canonical Monte Carlo (GCMC) simulation program (written in C++) that can be used for 1) computing the excess chemical potential of ions and the mean activity coef...

 Open Source

[A Latency Tolerant Runtime System for Mass Market Computer Systems](#)

Grappa is a latency tolerant runtime system for mass market computer systems comprised of multiple nodes having x86 multicore processors and infiniband interconnect. Grappa is designed to enable in-me...

 Open Source

Public US Government GitHub Data Scrape

- 252 US Government Orgs
 - U.S. Federal (137)
 - U.S. Military and Intelligence (12)
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