Kitware's Software Sustainability Matrix

Building Vital Computing Infrastructure

Best Practices for HPC Software Developers
August 2024
Bill Hoffman, CTO
Will Schroeder, Opportunity Catalyst

Introduction

Bill Hoffman, CTO Kitware Inc.

Bill Hoffman

- **CTO, Kitware**
- **One of five founders of Kitware**
- **Short boring list of jobs**
  - GE CRD 1990-1999
  - Kitware 1999-2023
- **Personas**
  - CMake guy
  - Kitware guy
  - Sandal runner guy

Will Schroeder

- **Opportunity Catalyst, Kitware**
- **One of five founders of Kitware**
- **Former CEO (18 yrs)**
- **Short boring list of jobs**
  - GE Power Systems
  - GE Research
- **Sidelines**
  - VTK Developer / VTK Book author
  - Open Source / Science Advocate
  - Sea kayaking

Center for Open-Source Research Software Stewardship and Advancement (CORSA)

- Kitware is part of the CORSA team working on Metrics and Sustainability Scorecards

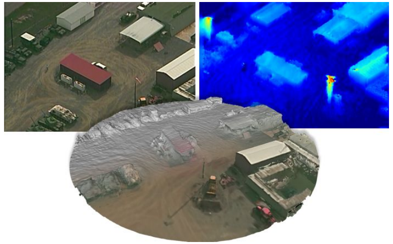
https://corsa.center/

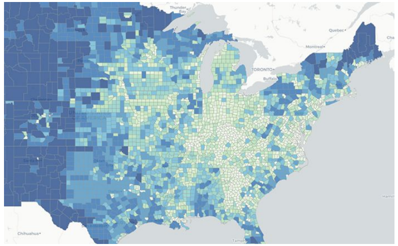
Consortium for the Advancement of Scientific Software

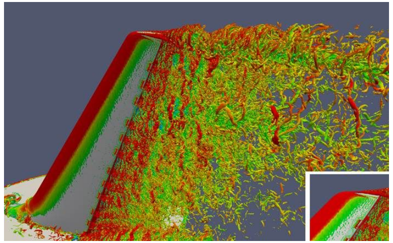
Fostering collaboration across a diverse collection of Software Stewardship Organizations (SSOs)

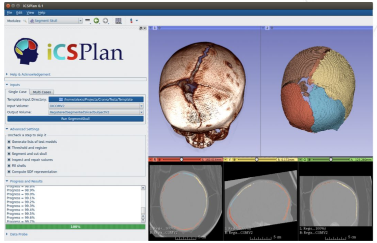
https://cass.community/

Kitware Areas of expertise / Built on open source









Computer Vision

Data and Analytics

Scientific Computing

Medical Computing

Software Solutions

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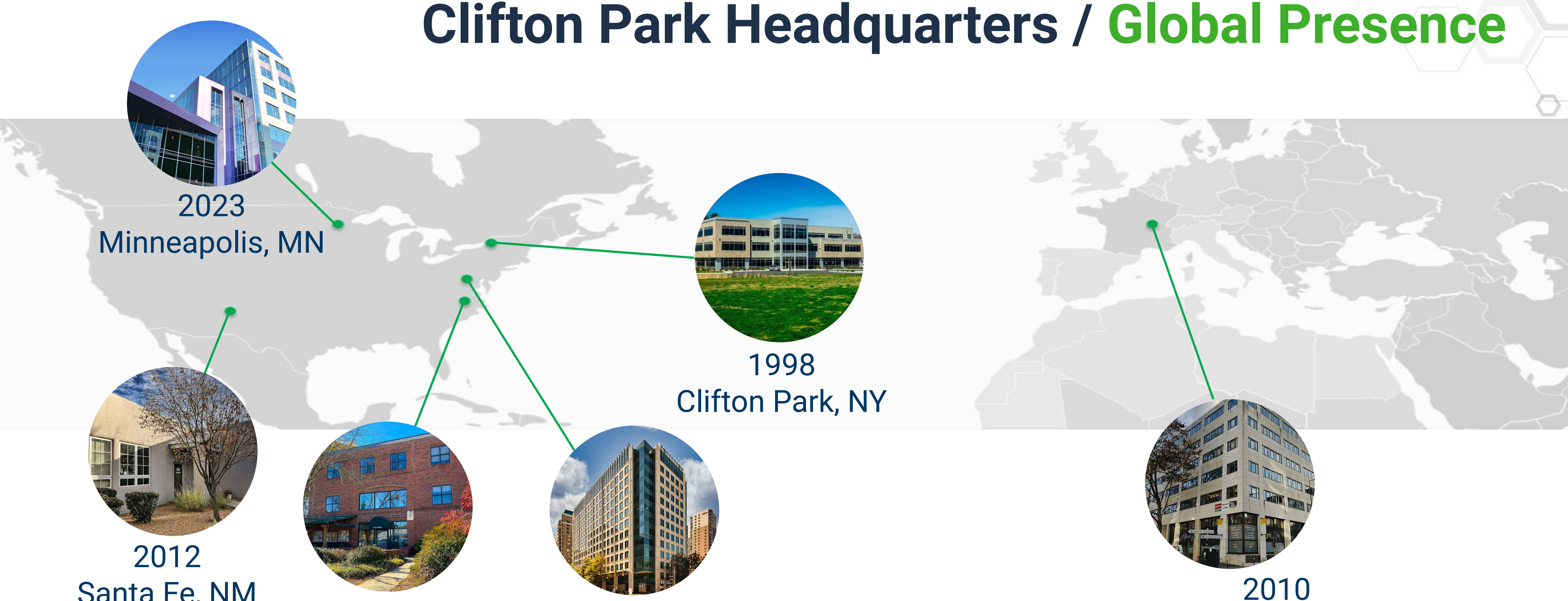
Clifton Park Headquarters / Global Presence



2023
Minneapolis, MN

1998
Clifton Park, NY

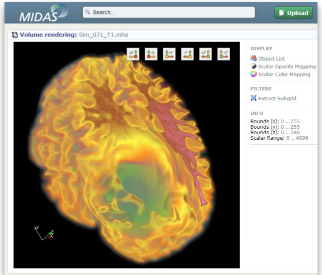
2012
Santa Fe, NM

2006
Carrboro, NC

2018
Arlington, VA

2010
Lyon, France

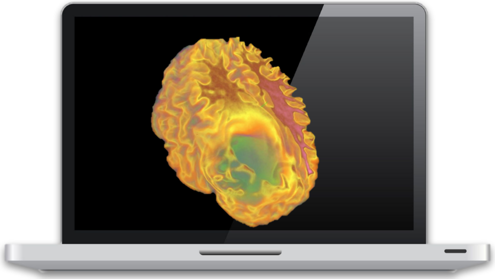
Applications / Universal Platforms



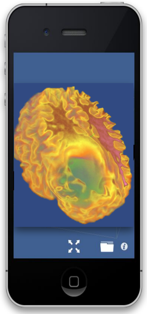
Volume rendering: Sim_071_T1.mha

Bounds (x): 0 .. 255
Bounds (y): 0 .. 255
Bounds (z): 0 .. 180
Scalar Range: 0 .. 4096

Web



Desktop



Mobile

Cloud /HPC

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Platforms

3D Slicer
ParaView
KWIVER
imstk
VTK
Pulse Physiology Engine
CMake
Resonant
tomviz
ITK

What Is Sustainability?

“...the expectation that the software used today will be available into the future.”

Corollary (Open Science): Published computational results can be reproduced

Related: Data is available into the future

Sustainability: It’s not that simple…….

What does it mean to be available in the future? In the face of:

- Platform (hardware / software) changes
- Compiler / interpreter changes
- New / obsoleted programming languages
- API changes
- Build / test process
- Technical innovation

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Alternate Meaning of Sustainability

Reduce the cost of developing and using software

- Energy efficient computing infrastructures
- Energy efficient software / algorithms
- Virtualization / containerization - reduce server loads
- Efficient testing processes

Why Sustainability?

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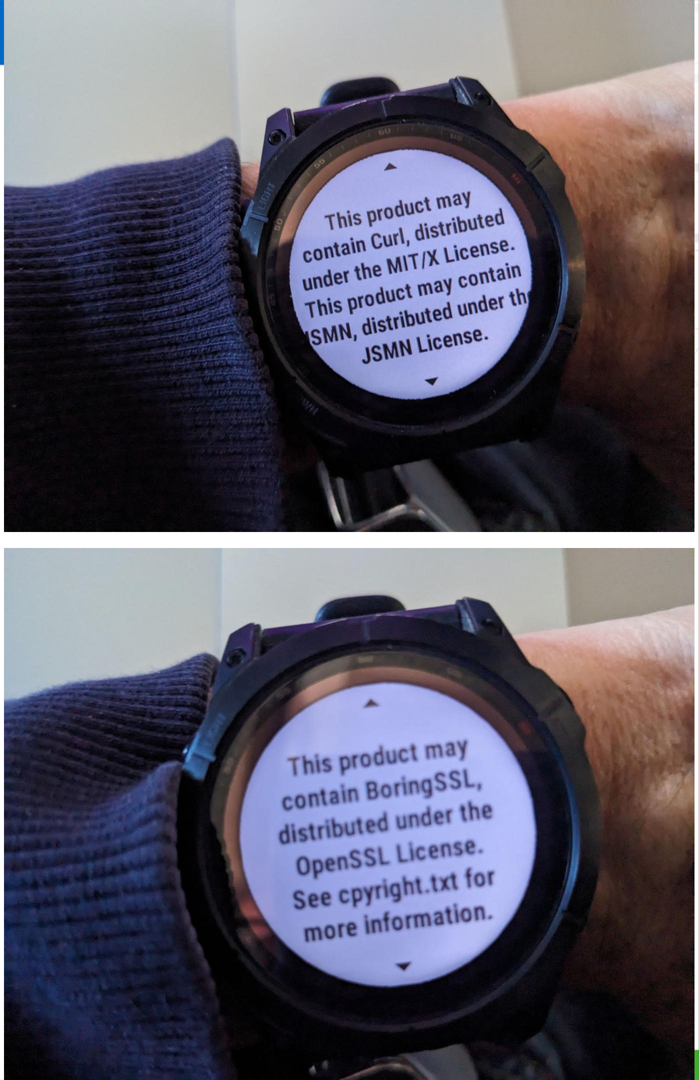
The Importance of Software

- The scientific method / innovation is increasingly dependent on software (and data)
- Modern societies increasingly rely on software
- A throw-away mentality is no longer viable for large, complex software systems



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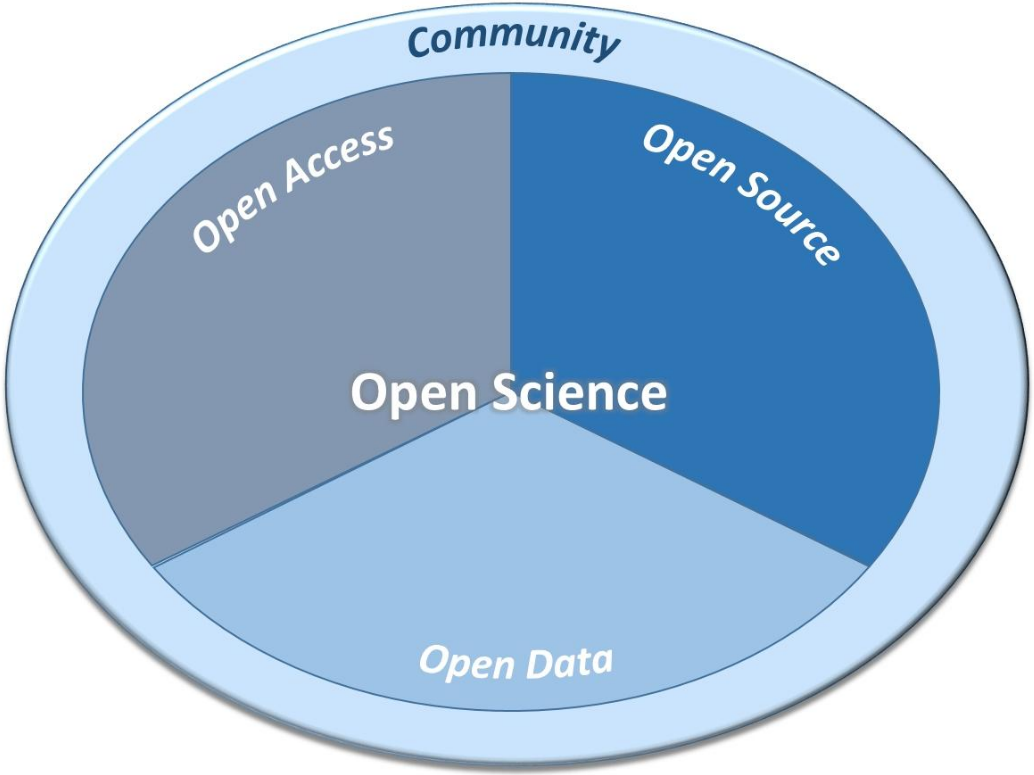
This product may contain BoringSSL, distributed under the OpenSSL License. See cpyright.txt for more information.

Bill's running watch

Sustainability for Open Science - Reproducibility



If it’s not reproducible, it’s not Science

Nullius in Verba

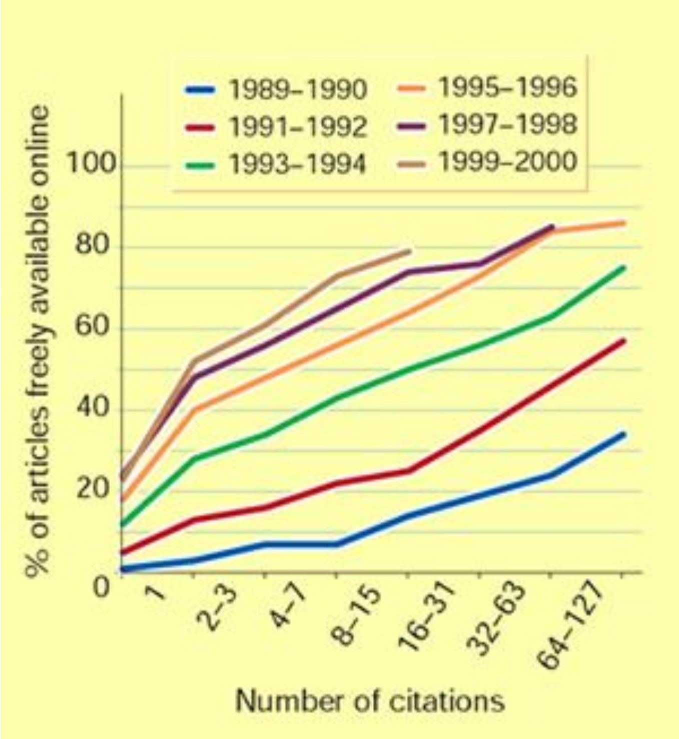
“take nobody's word for it”
Royal Society 1660

Failure of Reproducibility (350 years later)

- ***Nature*** **(March 2012)**
  - Glenn Begley, former head of cancer research at pharma giant Amgen
  - Lee M. Ellis, cancer researcher at the University of Texas

Found that more than 90% of papers published in science journals describing "landmark" breakthroughs in preclinical cancer research, are not reproducible, and are thus just plain wrong.

Be Selfish and Share, increase your impact



Sustainability for Innovation

- Open infrastructure as a springboard
- Avoid reinventing the wheel
- Reduce technical debt / bankruptcy

Takeaways so far

- Scientific research depends on software, lots of complex software
- Research and Software needs to be reproducible
- Agile innovation relies on reliable, computational foundations

Measuring Software Sustainability

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Ins & Outs of Measuring Software

- **Improve software quality**
- **Build healthy communities**
- **Monitor and increase impact**

Identify areas for improvement

- **Balancing *Objective* measures vs. *Subjective* measures**
- **Claim: Software Quality ≠ Software Sustainability**
  - Claim: Sustainability requires ongoing interest in, and support from, a community
  - Community depends on squishy characteristics like:
    - Usefulness
    - Technological artistry
    - Market forces
    - Cultural influences

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Early Approaches

- **GE Six Sigma (1995) - Measure and improve quality**
- **CMake / CTest / CDash - conceived at GE Research: a direct response to Six Sigma applied to software**
- **Measuring software quality**
  - Identify areas for improvement
  - Software quality: necessary but not sufficient for sustainability

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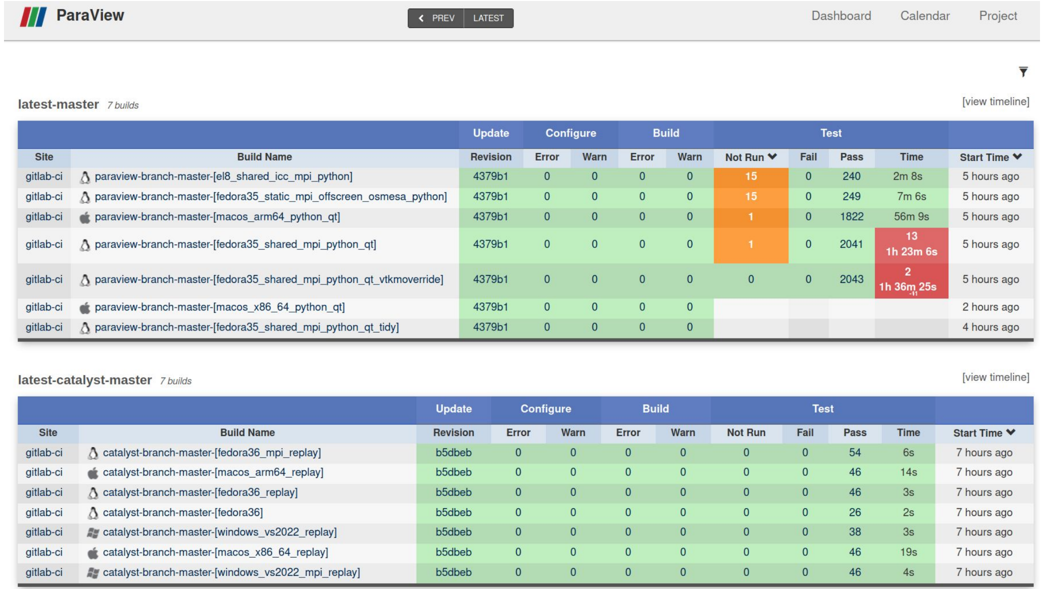
CMake / CTest / CDash

Computing metrics since 1995!

- # Warnings
- # Errors
- # Failed tests
- Static analysis
- Dynamic analysis
- Code coverage
- etc.



latest-master *7 builds* [view timeline]

		Update	Configure		Build		Test				
Site	Build Name	Revision	Error	Warn	Error	Warn	Not Run	Fail	Pass	Time	Start Time
gitlab-ci	paraview-branch-master-[el8_shared_icc_mpi_python]	4379b1	0	0	0	0	15	0	240	2m 8s	5 hours ago
gitlab-ci	paraview-branch-master-[fedora35_static_mpi_offscreen_osmesa_python]	4379b1	0	0	0	0	15	0	249	7m 6s	5 hours ago
gitlab-ci	paraview-branch-master-[macos_arm64_python_qt]	4379b1	0	0	0	0	1	0	1822	56m 9s	5 hours ago
gitlab-ci	paraview-branch-master-[fedora35_shared_mpi_python_qt]	4379b1	0	0	0	0	1	0	2041	13 1h 23m 6s	5 hours ago
gitlab-ci	paraview-branch-master-[fedora35_shared_mpi_python_qt_vtkmoverride]	4379b1	0	0	0	0	0	0	2043	2 1h 36m 25s	5 hours ago
gitlab-ci	paraview-branch-master-[macos_x86_64_python_qt]	4379b1	0	0	0	0					2 hours ago
gitlab-ci	paraview-branch-master-[fedora35_shared_mpi_python_qt_tidy]	4379b1	0	0	0	0					4 hours ago

latest-catalyst-master *7 builds* [view timeline]

		Update	Configure		Build		Test				
Site	Build Name	Revision	Error	Warn	Error	Warn	Not Run	Fail	Pass	Time	Start Time
gitlab-ci	catalyst-branch-master-[fedora36_mpi_replay]	b5dbeb	0	0	0	0	0	0	54	6s	7 hours ago
gitlab-ci	catalyst-branch-master-[macos_arm64_replay]	b5dbeb	0	0	0	0	0	0	46	14s	7 hours ago
gitlab-ci	catalyst-branch-master-[fedora36_replay]	b5dbeb	0	0	0	0	0	0	46	3s	7 hours ago
gitlab-ci	catalyst-branch-master-[fedora36]	b5dbeb	0	0	0	0	0	0	26	2s	7 hours ago
gitlab-ci	catalyst-branch-master-[windows_vs2022_replay]	b5dbeb	0	0	0	0	0	0	38	3s	7 hours ago
gitlab-ci	catalyst-branch-master-[macos_x86_64_replay]	b5dbeb	0	0	0	0	0	0	46	19s	7 hours ago
gitlab-ci	catalyst-branch-master-[windows_vs2022_mpi_replay]	b5dbeb	0	0	0	0	0	0	46	4s	7 hours ago

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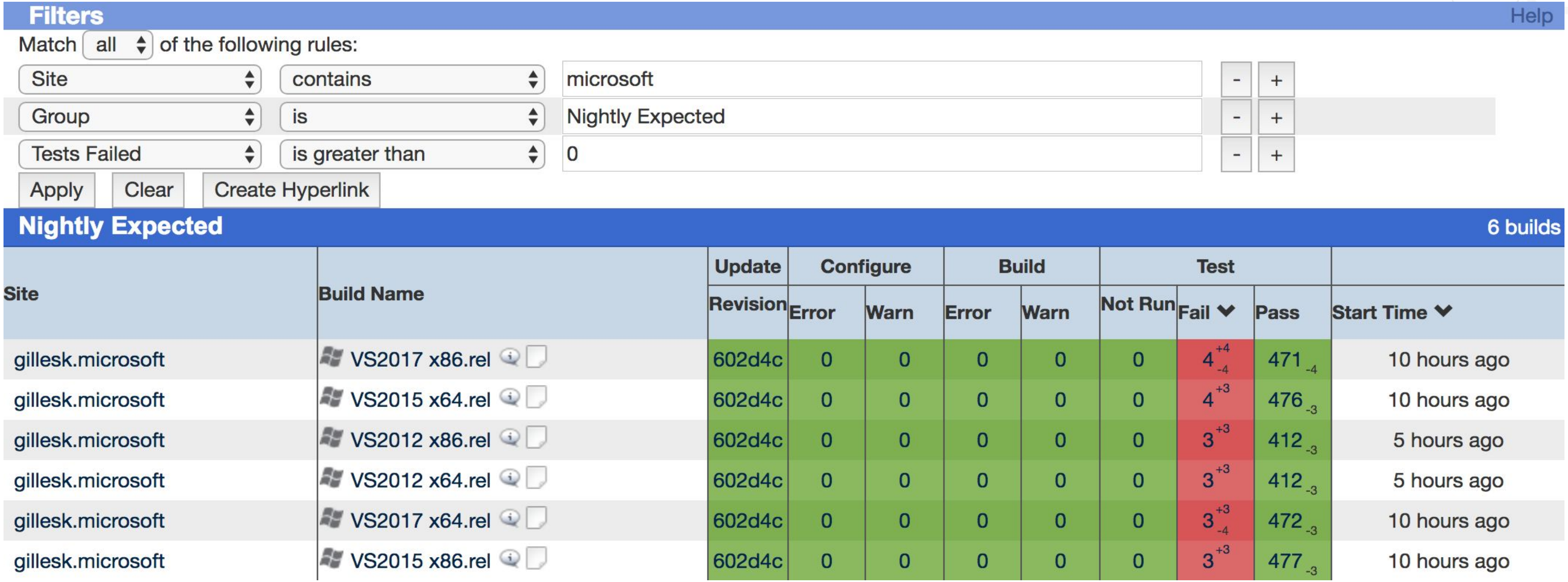
CTest/CDash: Search for Relevant Results



Filters Help

Match all of the following rules:

Site	contains	microsoft	-	+
Group	is	Nightly Expected	-	+
Tests Failed	is greater than	0	-	+

Nightly Expected 6 builds

Site	Build Name	Update	Configure		Build		Test			
		Revision	Error	Warn	Error	Warn	Not Run	Fail	Pass	Start Time
gillesk.microsoft	VS2017 x86.rel	602d4c	0	0	0	0	0	4 $^{+4}_{-4}$	471 $_{-4}$	10 hours ago
gillesk.microsoft	VS2015 x64.rel	602d4c	0	0	0	0	0	4 $^{+3}$	476 $_{-3}$	10 hours ago
gillesk.microsoft	VS2012 x86.rel	602d4c	0	0	0	0	0	3 $^{+3}$	412 $_{-3}$	5 hours ago
gillesk.microsoft	VS2012 x64.rel	602d4c	0	0	0	0	0	3 $^{+3}$	412 $_{-3}$	5 hours ago
gillesk.microsoft	VS2017 x64.rel	602d4c	0	0	0	0	0	3 $^{+3}_{-4}$	472 $_{-3}$	10 hours ago
gillesk.microsoft	VS2015 x86.rel	602d4c	0	0	0	0	0	3 $^{+3}$	477 $_{-3}$	10 hours ago

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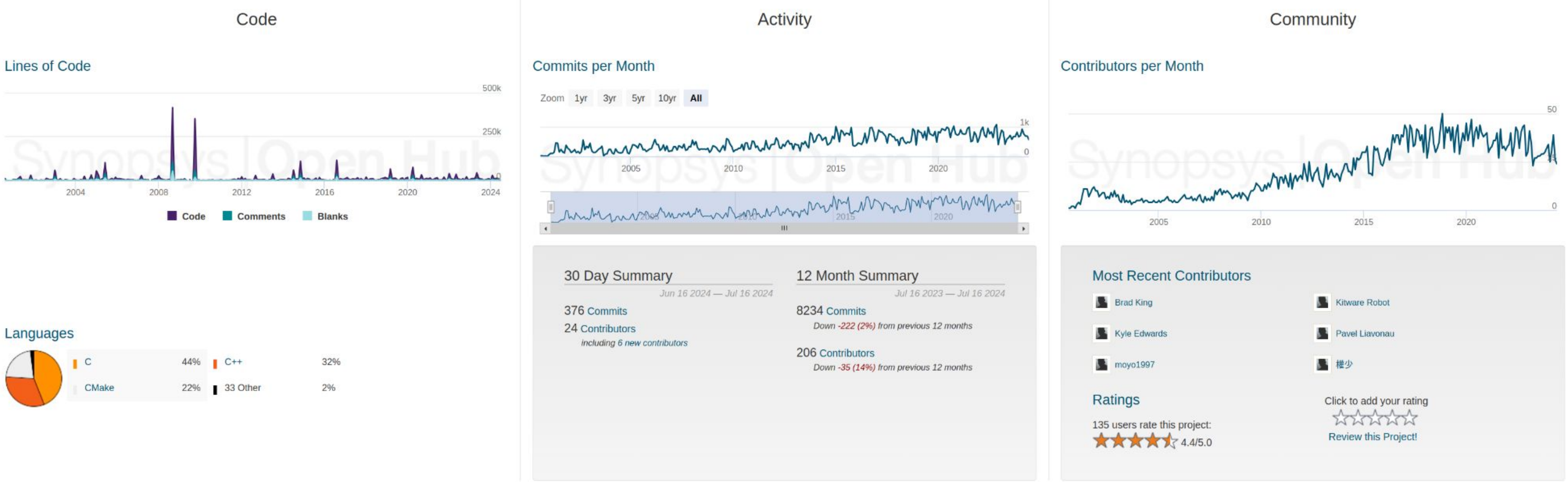
Examples of Measurement Metrics

- CMake / CTest / CDash
- OpenHub.net
- Repo-Review from Scientific Python
- Open Source Security Foundation (OpenSSF) Scorecard
- Linux Foundation’s CHAOSS community analytics
- Oak Ridge National Lab Scientific Software Excellence Assessment
- Kitware’s Sustainability Matrix

OpenHub.net



Languages

C	44%	C++	32%
CMake	22%	33 Other	2%

30 Day Summary

Jun 16 2024 — Jul 16 2024

376 Commits

24 Contributors

including 6 new contributors

12 Month Summary

Jul 16 2023 — Jul 16 2024

8234 Commits

Down -222 (2%) from previous 12 months

206 Contributors

Down -35 (14%) from previous 12 months

Most Recent Contributors

Brad King	Kitware Robot
Kyle Edwards	Pavel Liavonau
moyo1997	權少

Ratings

135 users rate this project:

★★★★☆ 4.4/5.0

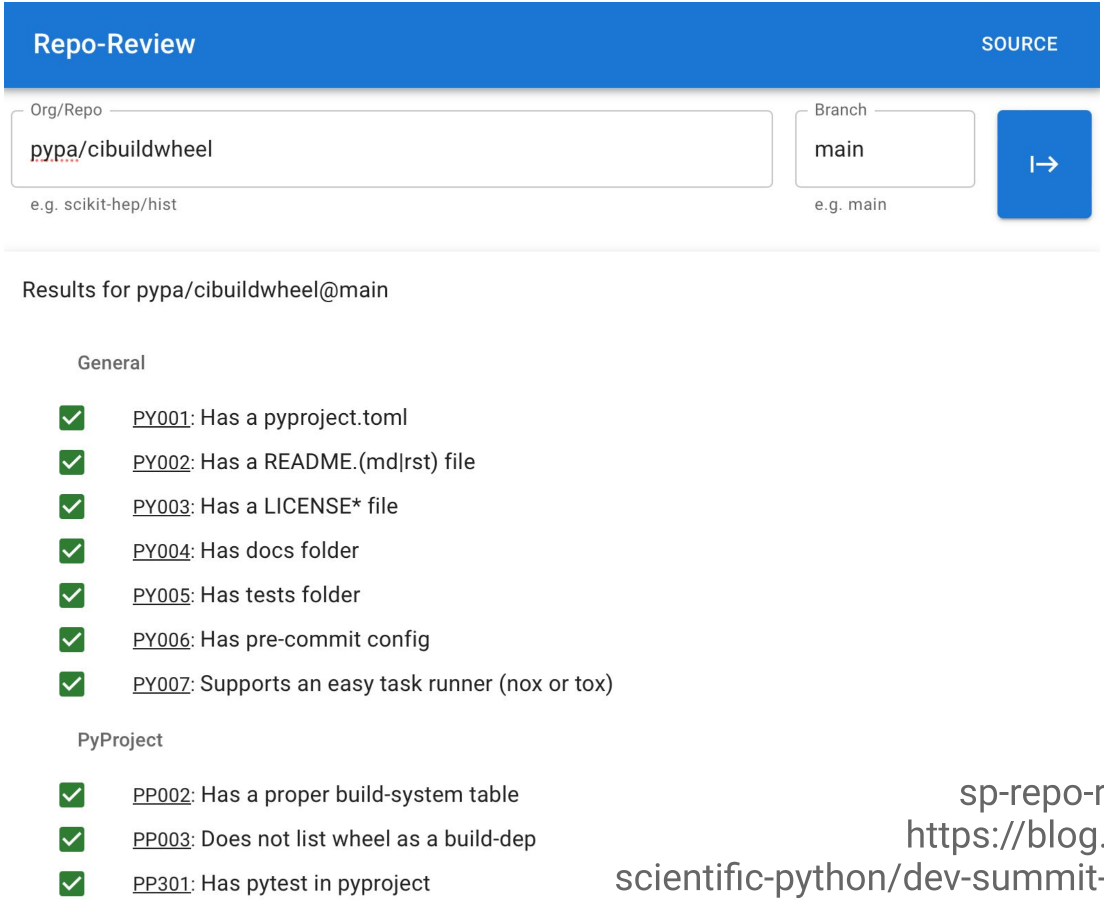
Click to add your rating

☆☆☆☆☆

Review this Project!

Scientific Python Repo-Review

- A repository-style checker
- A framework for building checks to see if a repository follows guidelines
- https://github.com/scientific-python/repo-review



pypa/cibuildwheel

e.g. scikit-hep/hist

main

e.g. main

Results for pypa/cibuildwheel@main

General

☑ PY001: Has a pyproject.toml

☑ PY002: Has a README.(md|rst) file

☑ PY003: Has a LICENSE* file

☑ PY004: Has docs folder

☑ PY005: Has tests folder

☑ PY006: Has pre-commit config

☑ PY007: Supports an easy task runner (nox or tox)

PyProject

☑ PP002: Has a proper build-system table

☑ PP003: Does not list wheel as a build-dep

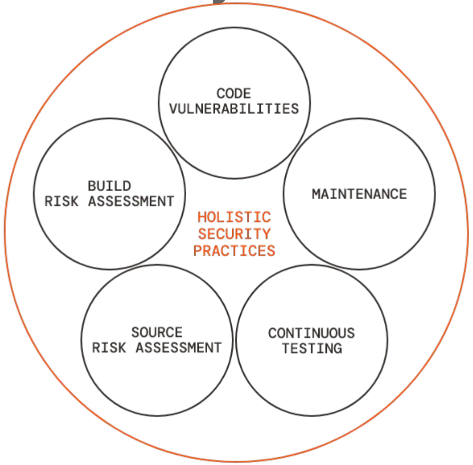
☑ PP301: Has pytest in pyproject

sp-repo-review on **cibuildwheel**
https://blog.scientific-python.org/-scientific-python/dev-summit-1-development-guide/

OpenSSF Scorecard

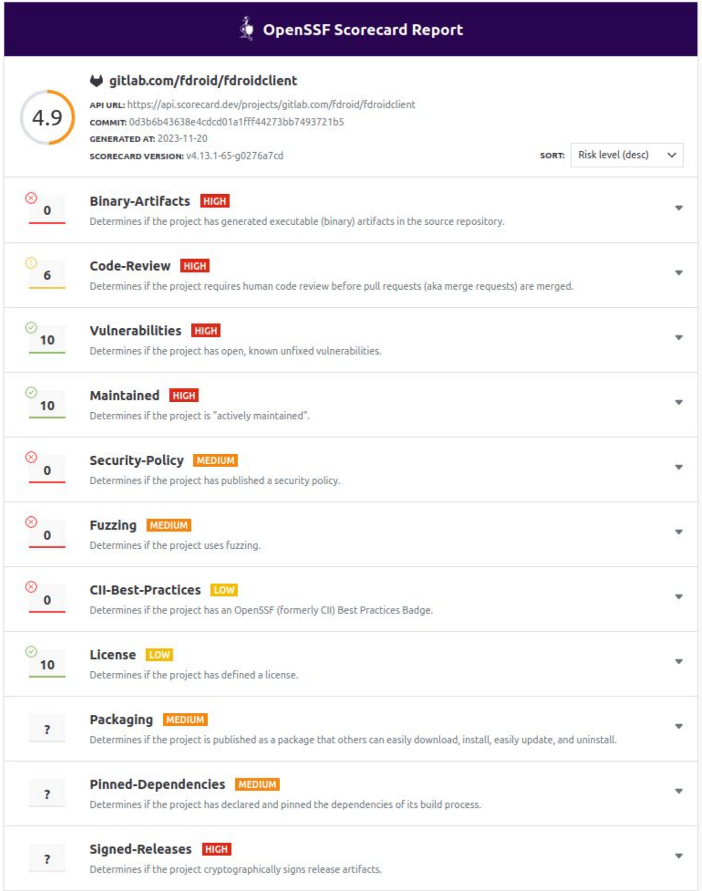
- Assess open source projects for security risks through a series of automated checks

- Automated evaluation covering five categories (20 tests)



- https://github.com/ossf/scorecard/tree/main

OpenSSF - Examples



OpenSSF Scorecard Report

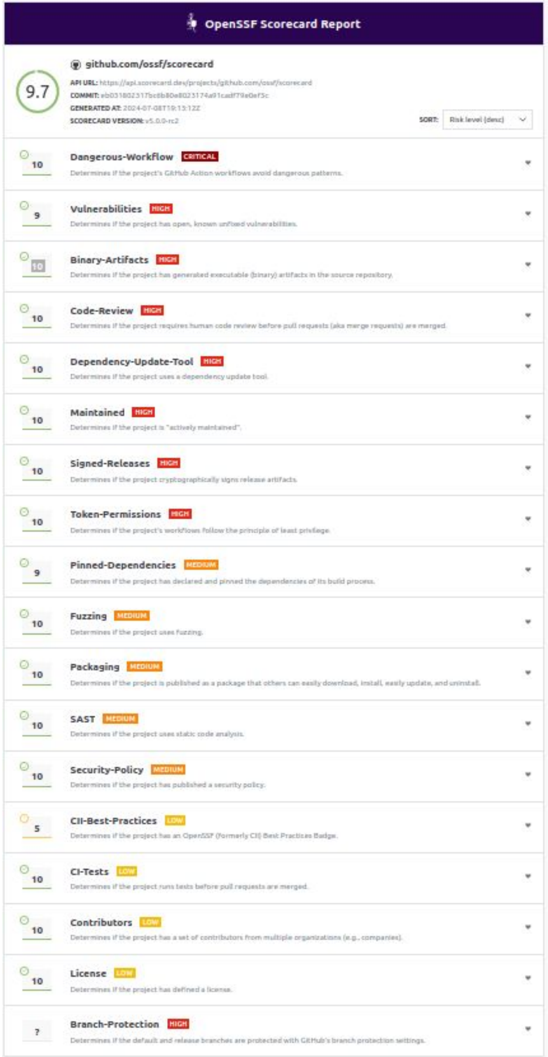
4.9

gitlab.com/fdroid/fdroidclient

API URL: https://api.scorecard.dev/projects/gitlab.com/fdroid/fdroidclient
COMMIT: 0d3b6b43638e4cdcd01a1fff44273bb7493721b5
GENERATED AT: 2023-11-20
SCORECARD VERSION: v4.13.1-65-g0276a7cd

SORT: Risk level (desc)

Score	Check	Risk	Description
0	Binary-Artifacts	HIGH	Determines if the project has generated executable (binary) artifacts in the source repository.
6	Code-Review	HIGH	Determines if the project requires human code review before pull requests (aka merge requests) are merged.
10	Vulnerabilities	HIGH	Determines if the project has open, known unfixed vulnerabilities.
10	Maintained	HIGH	Determines if the project is "actively maintained".
0	Security-Policy	MEDIUM	Determines if the project has published a security policy.
0	Fuzzing	MEDIUM	Determines if the project uses fuzzing.
0	CII-Best-Practices	LOW	Determines if the project has an OpenSSF (formerly CII) Best Practices Badge.
10	License	LOW	Determines if the project has defined a license.
?	Packaging	MEDIUM	Determines if the project is published as a package that others can easily download, install, easily update, and uninstall.
?	Pinned-Dependencies	MEDIUM	Determines if the project has declared and pinned the dependencies of its build process.
?	Signed-Releases	HIGH	Determines if the project cryptographically signs release artifacts.



OpenSSF Scorecard Report

9.7

github.com/ossf/scorecard

API URL: https://api.scorecard.dev/projects/github.com/ossf/scorecard
COMMIT: eb031802317bc8b80e8023174a91cadf79e0ef5c
GENERATED AT: 2024-07-08T19:13:12Z
SCORECARD VERSION: v5.0.0-rc2

SORT: Risk level (desc)

Score	Check	Risk	Description
10	Dangerous-Workflow	CRITICAL	Determines if the project's GitHub Action workflows avoid dangerous patterns.
9	Vulnerabilities	HIGH	Determines if the project has open, known unfixed vulnerabilities.
10	Binary-Artifacts	HIGH	Determines if the project has generated executable (binary) artifacts in the source repository.
10	Code-Review	HIGH	Determines if the project requires human code review before pull requests (aka merge requests) are merged.
10	Dependency-Update-Tool	HIGH	Determines if the project uses a dependency update tool.
10	Maintained	HIGH	Determines if the project is "actively maintained".
10	Signed-Releases	HIGH	Determines if the project cryptographically signs release artifacts.
10	Token-Permissions	HIGH	Determines if the project's workflows follow the principle of least privilege.
9	Pinned-Dependencies	MEDIUM	Determines if the project has declared and pinned the dependencies of its build process.
10	Fuzzing	MEDIUM	Determines if the project uses fuzzing.
10	Packaging	MEDIUM	Determines if the project is published as a package that others can easily download, install, easily update, and uninstall.
10	SAST	MEDIUM	Determines if the project uses static code analysis.
10	Security-Policy	MEDIUM	Determines if the project has published a security policy.
5	CII-Best-Practices	LOW	Determines if the project has an OpenSSF (formerly CII) Best Practices Badge.
10	CI-Tests	LOW	Determines if the project runs tests before pull requests are merged.
10	Contributors	LOW	Determines if the project has a set of contributors from multiple organizations (e.g., companies).
10	License	LOW	Determines if the project has defined a license.
?	Branch-Protection	HIGH	Determines if the default and release branches are protected with GitHub's branch protection settings.

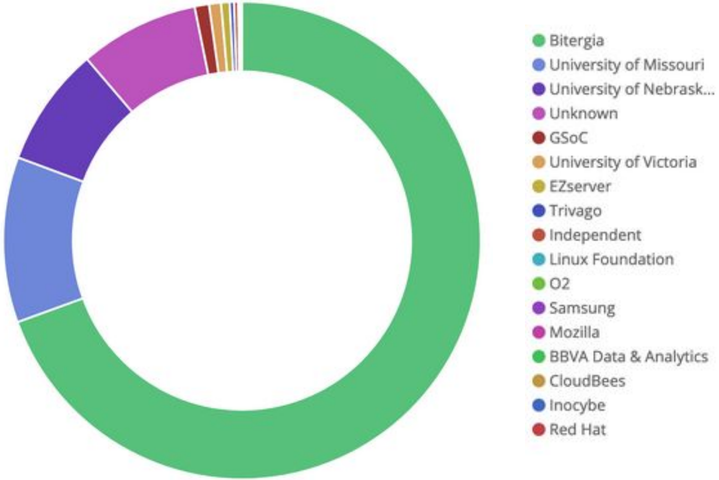
Linux Foundation CHAOSS community analytics

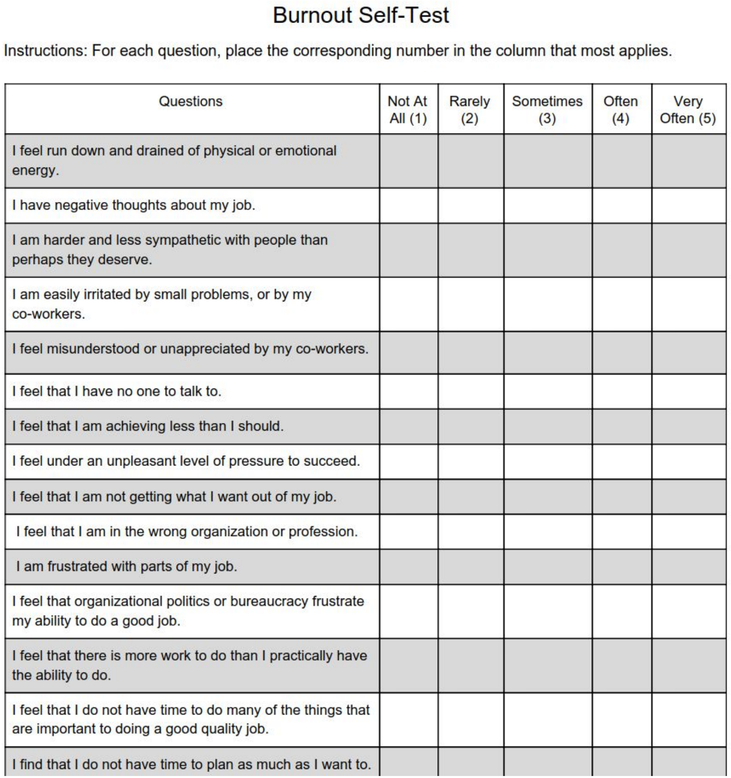
- **Focused on creating metrics, metrics models, and software to better understand open source community health**
- **89 metrics covering:**
  - Organization
  - Platform
  - Software
  - Contribution
  - Event
  - Governance & Leadership
  - Lifecycle
  - Contributor
  - Community
  - Ecosystem

CHAOSS - Metric Examples

Elephant Factor: *The distribution of work in the community across organizations*

E.g., the number of organizations contributing >50% of the project commits





Burnout Self-Test

Instructions: For each question, place the corresponding number in the column that most applies.

Questions	Not At All (1)	Rarely (2)	Sometimes (3)	Often (4)	Very Often (5)
I feel run down and drained of physical or emotional energy.					
I have negative thoughts about my job.					
I am harder and less sympathetic with people than perhaps they deserve.					
I am easily irritated by small problems, or by my co-workers.					
I feel misunderstood or unappreciated by my co-workers.					
I feel that I have no one to talk to.					
I feel that I am achieving less than I should.					
I feel under an unpleasant level of pressure to succeed.					
I feel that I am not getting what I want out of my job.					
I feel that I am in the wrong organization or profession.					
I am frustrated with parts of my job.					
I feel that organizational politics or bureaucracy frustrate my ability to do a good job.					
I feel that there is more work to do than I practically have the ability to do.					
I feel that I do not have time to do many of the things that are important to doing a good quality job.					
I find that I do not have time to plan as much as I want to.					

ORNL Scientific Software Excellence Assessment

- *“ORNL has developed a software excellence assessment survey that can be used to guide staff towards activities that would lead to beneficial improvements to a software project”*

- A. Malviya-Thakur, et al.,"Research Software Engineering at Oak Ridge National Laboratory" Computing in Science & Engineering

Kitware’s Software Sustainability Matrix

- **Practices KISS principle - keep it simple**
    - Avoid excessive number of, or overly complex, metrics

- **Four core values, each value scored according to combining multiple, simple metrics**
    - Impact
    - Risks
    - Community
    - Technology

Recipe for Sustainability Matrix

Impact (I)	Perceived value Business Model User Base	
Risks (R)	IP & License Bus Rule Security	Dependencies Competition
Community (C)	Culture Software Process	Governance Outreach
Technology (T)	Ubiquity Interoperability	Architecture Latest & Greatest

$$\text{Score} = \tfrac{1}{3} * I + \tfrac{1}{6} * R + \tfrac{1}{3} * C + \tfrac{1}{6} * T$$

$$0 \leq I,R,C,T \leq 1$$

Issues

- **Based on empirical approaches**
- **Metric set incomplete (and evolving)**
  - Is there a “minimal spanning set” of metrics?
- **Measuring software quality is *not* the same as measuring for sustainability**

Problems with “Objective” Metrics & Assessment

Evaluating CMake *Impact* *(measured by customer base)*:

- **# Downloads → ~100million/year Kitware servers**
  - Doesn’t count other distributions (e.g. Linux)
  - Cannot easily infer customer base

- **Alternative: CMake usage >50%** *(JetBrains study 2017-2021)*
  - C++ has 11.6million users *(SlashData)* →~6 million users?

- **Current impact vs. potential, future impact**
  - Maybe invest in innovative technologies?

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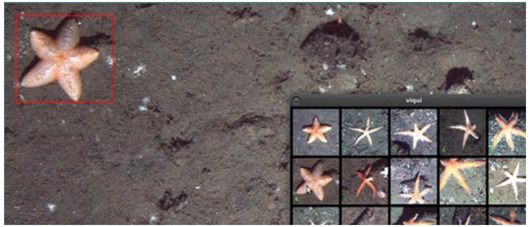
Measuring Impact: The Effects of Scale

Small:
VIAME
Video and Image Analytics for Marine Environments

100* downloads/month

<50K LOC



Medium:
VTK
The Visualization Toolkit

425,000* downloads/month

8M LOC**

Large:
CMake
Cross-Platform Make

8,500,000* downloads /month

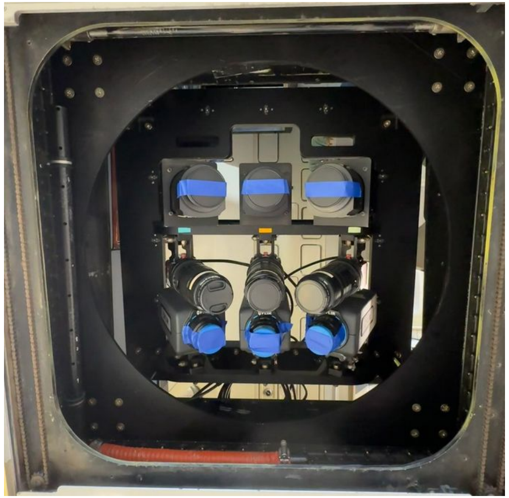
1.9M LOC**

** from Kitware servers*
*** openhub.net*

VIAME - NOAA Seal population census

(across three Arctic Seas: Bering, Beaufort, and Chukchi)

Adam Romlein (KW) is ready to go on NOAA's King Air



Takeaways so far

- Scientific research depends on software, lots of complex software
- Research and Software needs to be reproducible
- Agile innovation relies on reliable, computational foundations
- Use metrics to *improve* software, not *compare* software
- *Objective* metrics are quantifiable / reproducible
- *Subjective* metrics require human judgement
- Both objective and subjective metrics are prone to *biases*

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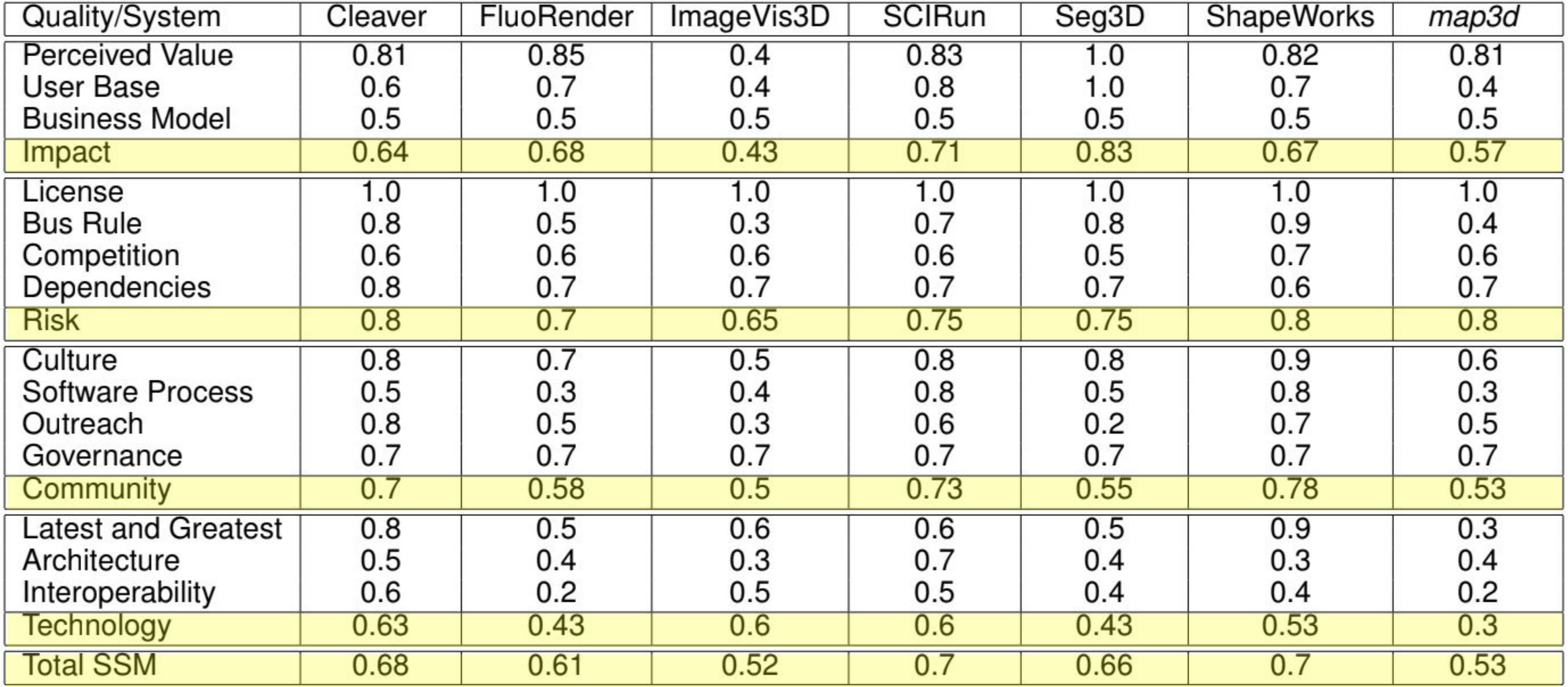
Case Studies

U Utah NIH R24

- **Utah SCI (Scientific Computing Institute)**
  - Aim: Improve sustainability of flagship software tools

- **Approaches**
  - Improve documentation ✅
  - Improved build process - support additional platforms ✅
  - Re-architected systems (extract reusable components) ✅
  - Replace OpenGL graphics engine with OS standard (VTK) ☒
  - Interoperability ✅✅

U Utah NIH R24: *Improving Interoperability increased Impact*



Quality/System	Cleaver	FluoRender	ImageVis3D	SCIRun	Seg3D	ShapeWorks	*map3d*
Perceived Value	0.81	0.85	0.4	0.83	1.0	0.82	0.81
User Base	0.6	0.7	0.4	0.8	1.0	0.7	0.4
Business Model	0.5	0.5	0.5	0.5	0.5	0.5	0.5
Impact	0.64	0.68	0.43	0.71	0.83	0.67	0.57
License	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Bus Rule	0.8	0.5	0.3	0.7	0.8	0.9	0.4
Competition	0.6	0.6	0.6	0.6	0.5	0.7	0.6
Dependencies	0.8	0.7	0.7	0.7	0.7	0.6	0.7
Risk	0.8	0.7	0.65	0.75	0.75	0.8	0.8
Culture	0.8	0.7	0.5	0.8	0.8	0.9	0.6
Software Process	0.5	0.3	0.4	0.8	0.5	0.8	0.3
Outreach	0.8	0.5	0.3	0.6	0.2	0.7	0.5
Governance	0.7	0.7	0.7	0.7	0.7	0.7	0.7
Community	0.7	0.58	0.5	0.73	0.55	0.78	0.53
Latest and Greatest	0.8	0.5	0.6	0.6	0.5	0.9	0.3
Architecture	0.5	0.4	0.3	0.7	0.4	0.3	0.4
Interoperability	0.6	0.2	0.5	0.5	0.4	0.4	0.2
Technology	0.63	0.43	0.6	0.6	0.43	0.53	0.3
Total SSM	0.68	0.61	0.52	0.7	0.66	0.7	0.53

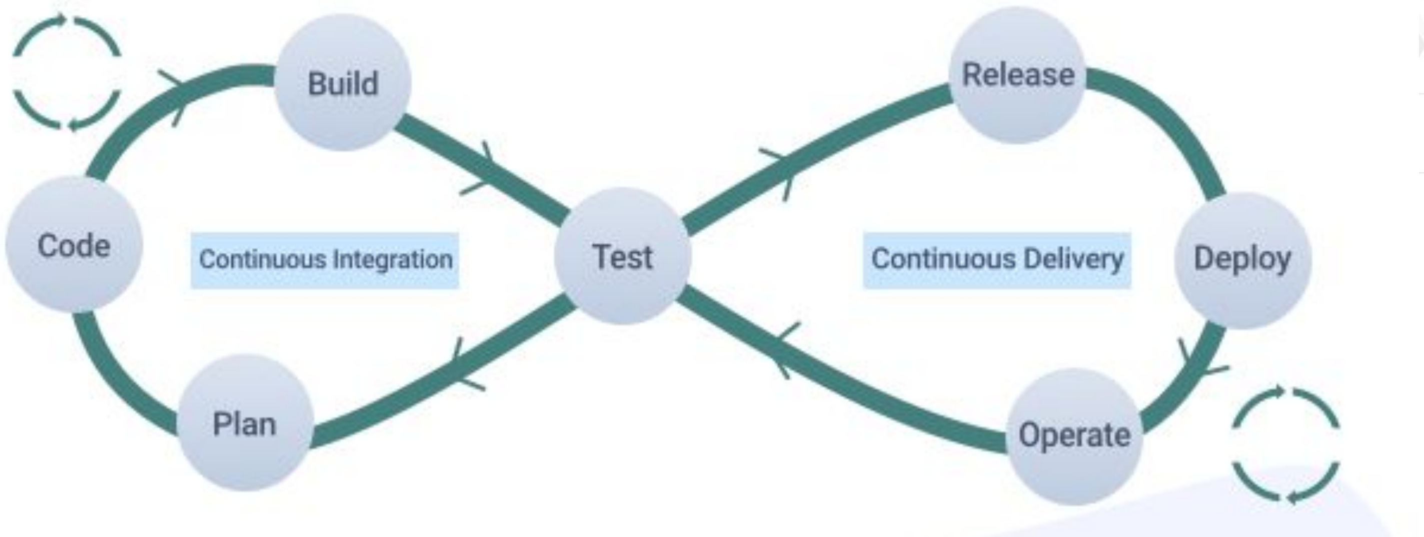
Major Focus on Interoperability → Cleaver Impact

- **Objective: Grow the community (i.e., increase impact)**
  - Users
  - Developers

- **Approach:** ***(improve Interoperability)***
  - Python integration via ***trame*** visual analytics platform
  - 3D Slicer extension

    (Cleaver downloads: 100/200 yr → 30,000 yr)

Path Forward

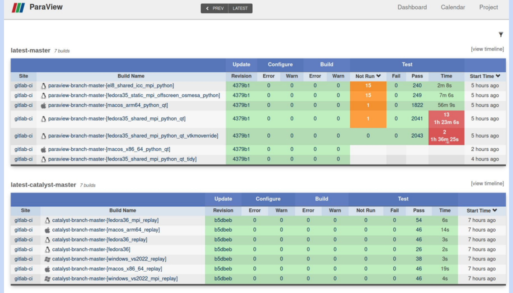


Identify spanning metrics

Integrate metrics into CI
(create a framework supporting plugin metrics)

Concept: *Software Sustainability Dashboard*

Software Quality



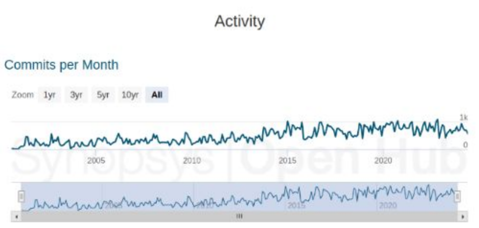
latest-master *7 builds* [view timeline]

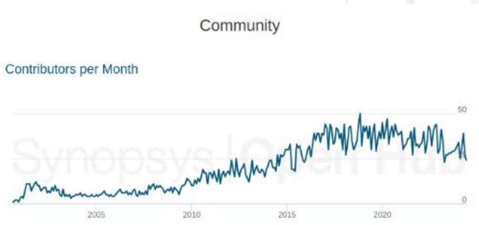
		Update	Configure		Build		Test				
Site	Build Name	Revision	Error	Warn	Error	Warn	Not Run	Fail	Pass	Time	Start Time
gitlab-ci	paraview-branch-master-[el8_shared_icc_mpi_python]	4379b1	0	0	0	0	15	0	240	2m 8s	5 hours ago
gitlab-ci	paraview-branch-master-[fedora35_static_mpi_offscreen_osmesa_python]	4379b1	0	0	0	0	15	0	249	7m 6s	5 hours ago
gitlab-ci	paraview-branch-master-[macos_arm64_python_qt]	4379b1	0	0	0	0	1	0	1822	56m 9s	5 hours ago
gitlab-ci	paraview-branch-master-[fedora35_shared_mpi_python_qt]	4379b1	0	0	0	0	1	0	2041	13 1h 23m 6s	5 hours ago
gitlab-ci	paraview-branch-master-[fedora35_shared_mpi_python_qt_vtkmoverride]	4379b1	0	0	0	0	0	0	2043	2 1h 36m 25s	5 hours ago
gitlab-ci	paraview-branch-master-[macos_x86_64_python_qt]	4379b1	0	0	0	0					2 hours ago
gitlab-ci	paraview-branch-master-[fedora35_shared_mpi_python_qt_tidy]	4379b1	0	0	0	0					4 hours ago

latest-catalyst-master *7 builds* [view timeline]

		Update	Configure		Build		Test				
Site	Build Name	Revision	Error	Warn	Error	Warn	Not Run	Fail	Pass	Time	Start Time
gitlab-ci	catalyst-branch-master-[fedora36_mpi_replay]	b5dbeb	0	0	0	0	0	0	54	6s	7 hours ago
gitlab-ci	catalyst-branch-master-[macos_arm64_replay]	b5dbeb	0	0	0	0	0	0	46	14s	7 hours ago
gitlab-ci	catalyst-branch-master-[fedora36_replay]	b5dbeb	0	0	0	0	0	0	46	3s	7 hours ago
gitlab-ci	catalyst-branch-master-[fedora36]	b5dbeb	0	0	0	0	0	0	26	2s	7 hours ago
gitlab-ci	catalyst-branch-master-[windows_vs2022_replay]	b5dbeb	0	0	0	0	0	0	38	3s	7 hours ago
gitlab-ci	catalyst-branch-master-[macos_x86_64_replay]	b5dbeb	0	0	0	0	0	0	46	19s	7 hours ago
gitlab-ci	catalyst-branch-master-[windows_vs2022_mpi_replay]	b5dbeb	0	0	0	0	0	0	46	4s	7 hours ago

Community Health





Impact

- # spack dependencies
- # downloads
- # references
- Community size

Challenges

- **Identify a (spanning) set of metrics**
  - Further reading: "How Sustainable is Your Software?"

- **Automate metrics scoring**

- **Software Engineering Research**
  - What metrics are important to real-world software quality?
  - What metrics are important to long-term sustainability?
  - Support CORSA / CASS

- **Balance the increased cost of testing / evaluating metrics**

May the Source Be With You