Reducing Technical Debt with Reproducible Containers

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WhoamI

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My expertise is:
Databases and distributed computing
Data provenance: history and lineage of data and software
Computational reproducibility: Repeating and recreating some one else's work

Systems built: http://sciunit.run

I want to know more about:
Reproducibility case studies in HPC and how containers are used.

Problems I'm currently working on:
Provenance alignment: Using provenance to highlight sources of irreproducibility
State maintenance in lineage graphs: Making Jupyter Notebooks reproducible

Outline

PART 1: How technical debt affects reproducibility?

PART 2: If reproducible containers provide a start?

PART 3: Guidance and summary

PART 1: How technical debt affects reproducibility?

Monetary debt

Monetary debt meets the objective "sooner"

Technical debt[1] is no different

[1]A metaphor introduced by Ward Cunningham in 1992.

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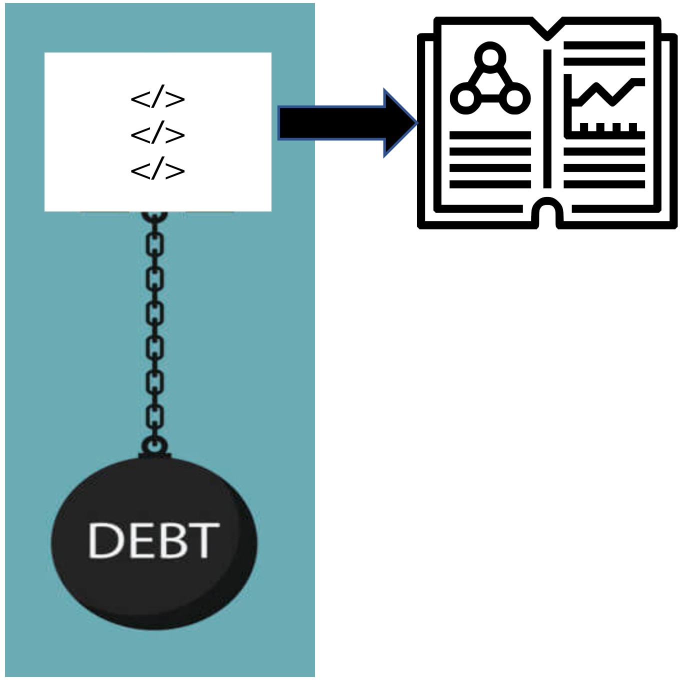
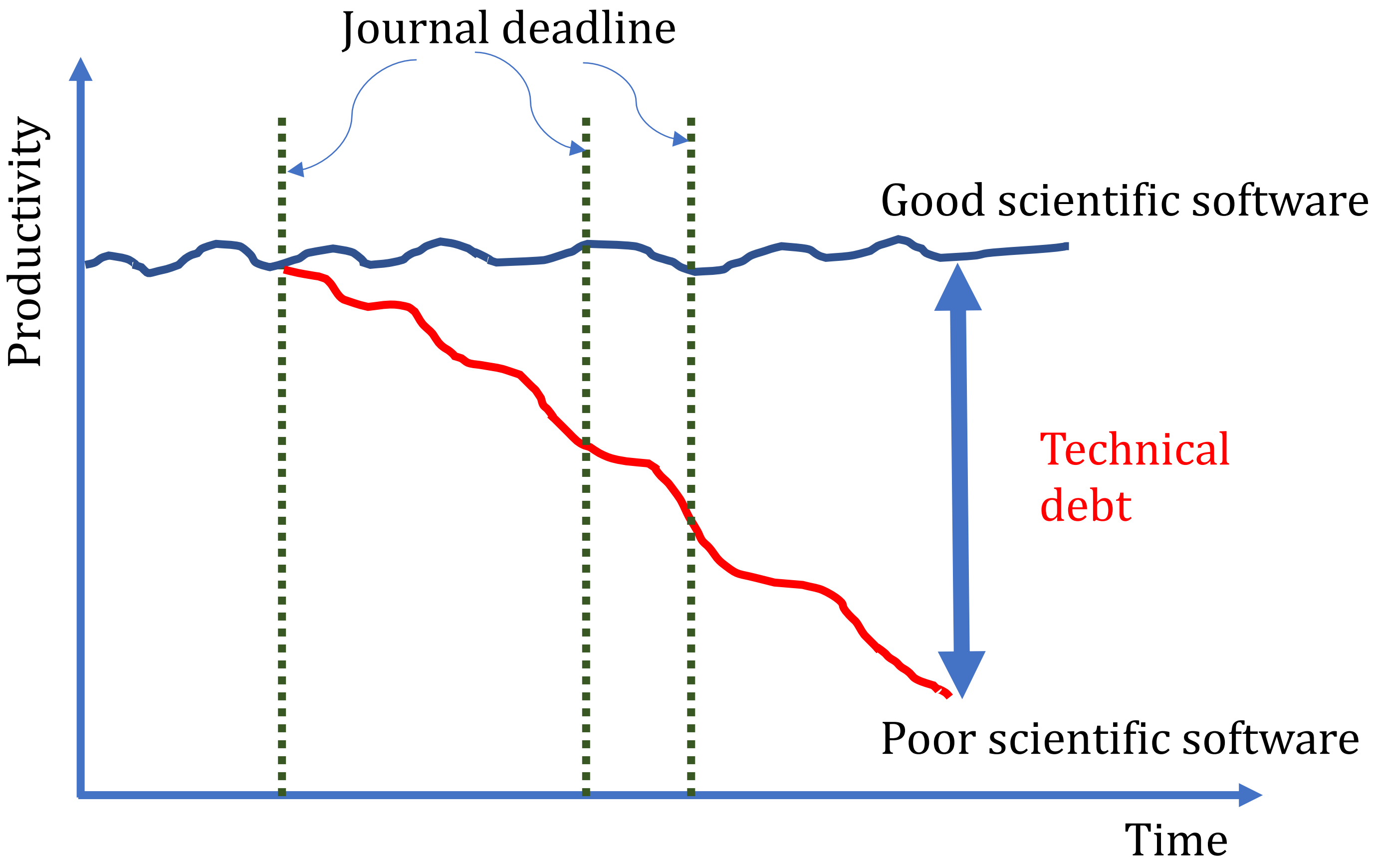


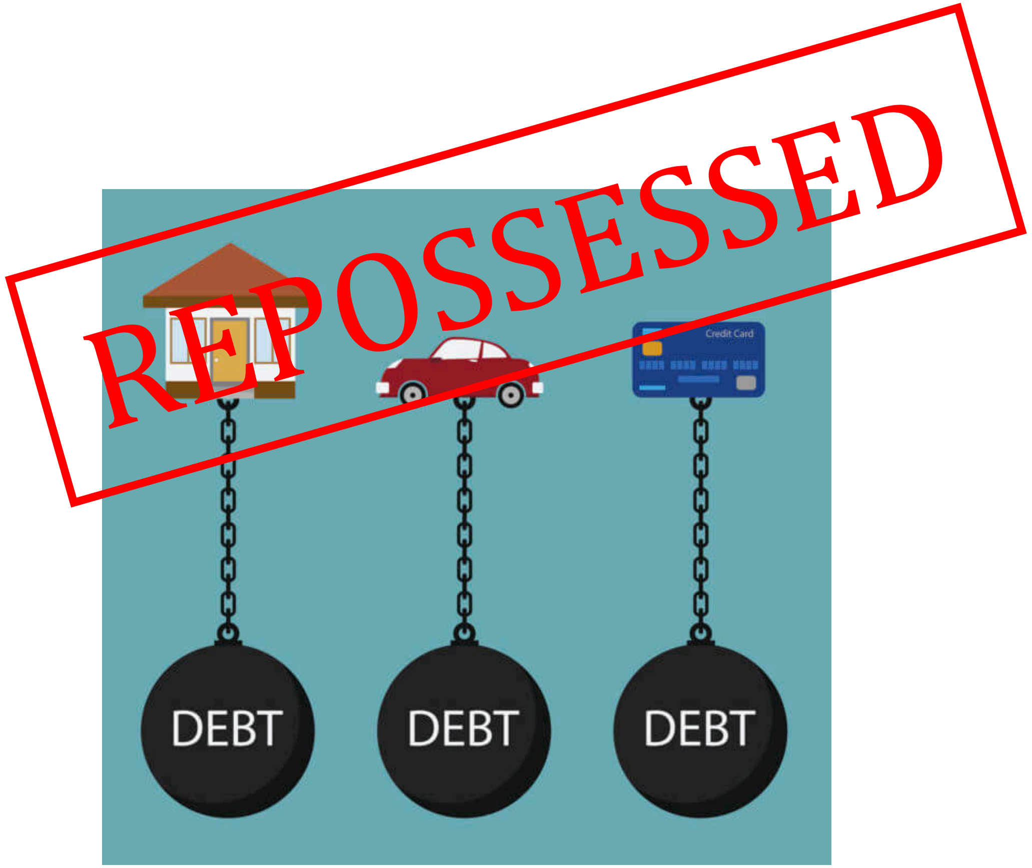
Technical debt is no different.



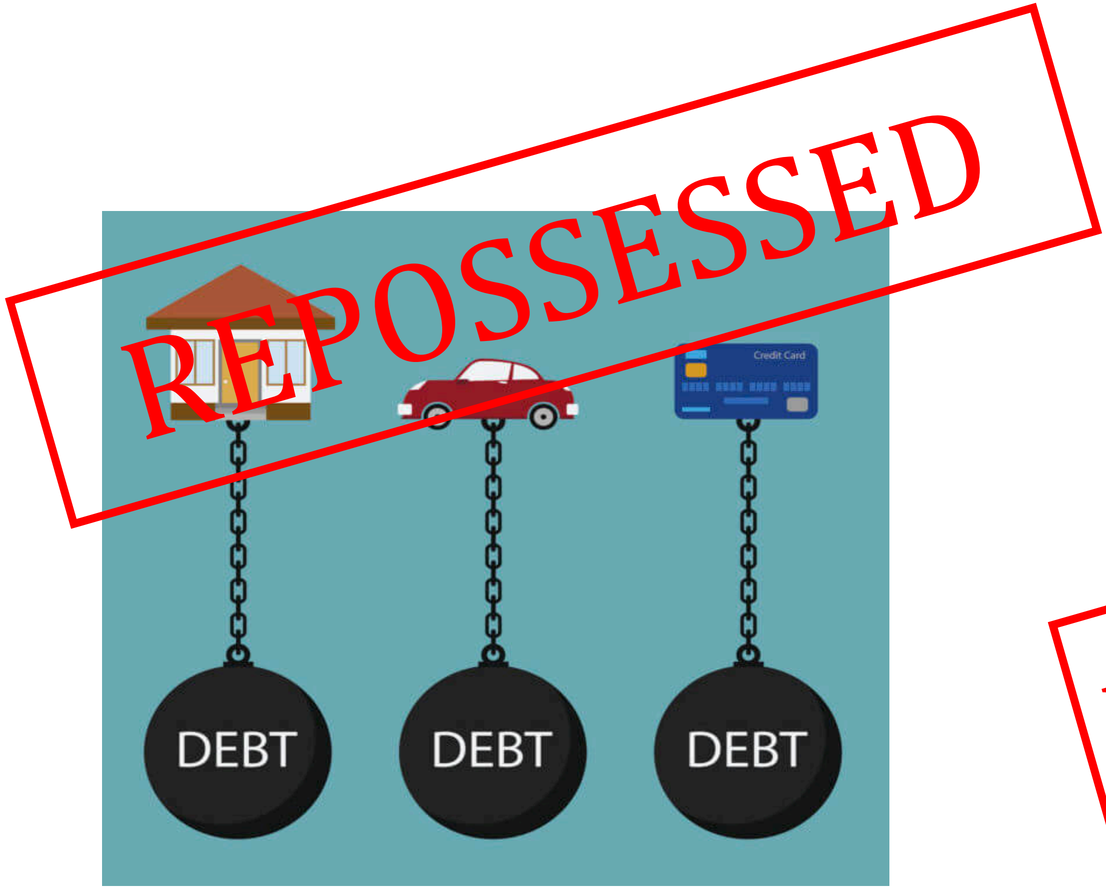
Dimensions of Technical Debt

- Poor quality code
- Poor design
- Environment debt
- Documentation debt
- Testing debt

Consequence of Mismanaged Debt



Consequence of Mismanaged Debt



Dimensions of Scientific Technical Debt

- Poor quality code
- Poor design
- Environment debt
- Documentation debt
- Testing debt

[1]E. Tom, A. Aurum, R. Vidgen, An exploration of technical debt, Journal of Systems and Software, Volume 86, Issue 6, 2013, Pages 1498-1516, ISSN 0164-1212, https://doi.org/10.1016/j.jss.2012.12.052.

Dimensions of Scientific Technical Debt

- ~~Poor quality code~~
- ~~Poor design~~

✓Environment debt

✓Documentation debt

- ~~Testing debt~~

Bad bugs: The worst disasters caused by software fails

5 June 2013

Clever software can make our lives easier but a glitch can have disastrous consequences. In the past decades, computer bug catastrophes have caused deaths and disrupted lives on a large scale. **Sally Adee** takes us through six major software fails.

https://www.newscientist.com/gallery/software-bugs

A Scientist's Nightmare: Software Problem Leads to Five Retractions

Greg Miller

+ See all authors and affiliations

Science 22 Dec 2006:
Vol. 314, Issue 5807, pp. 1856-1857
DOI: 10.1126/science.314.5807.1856

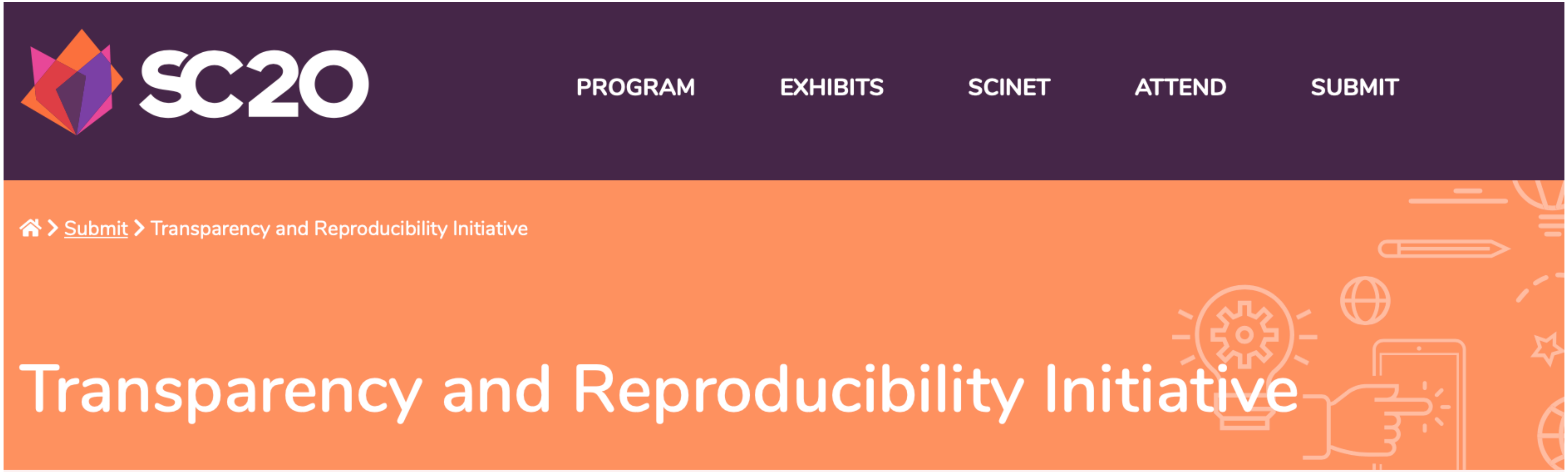
Critiqued coronavirus simulation gets thumbs up from code-checking efforts

Influential model judged reproducible – although software engineers called its code 'horrible' and 'a buggy mess'.

https://www.nature.com/articles/d41586-020-01685-y

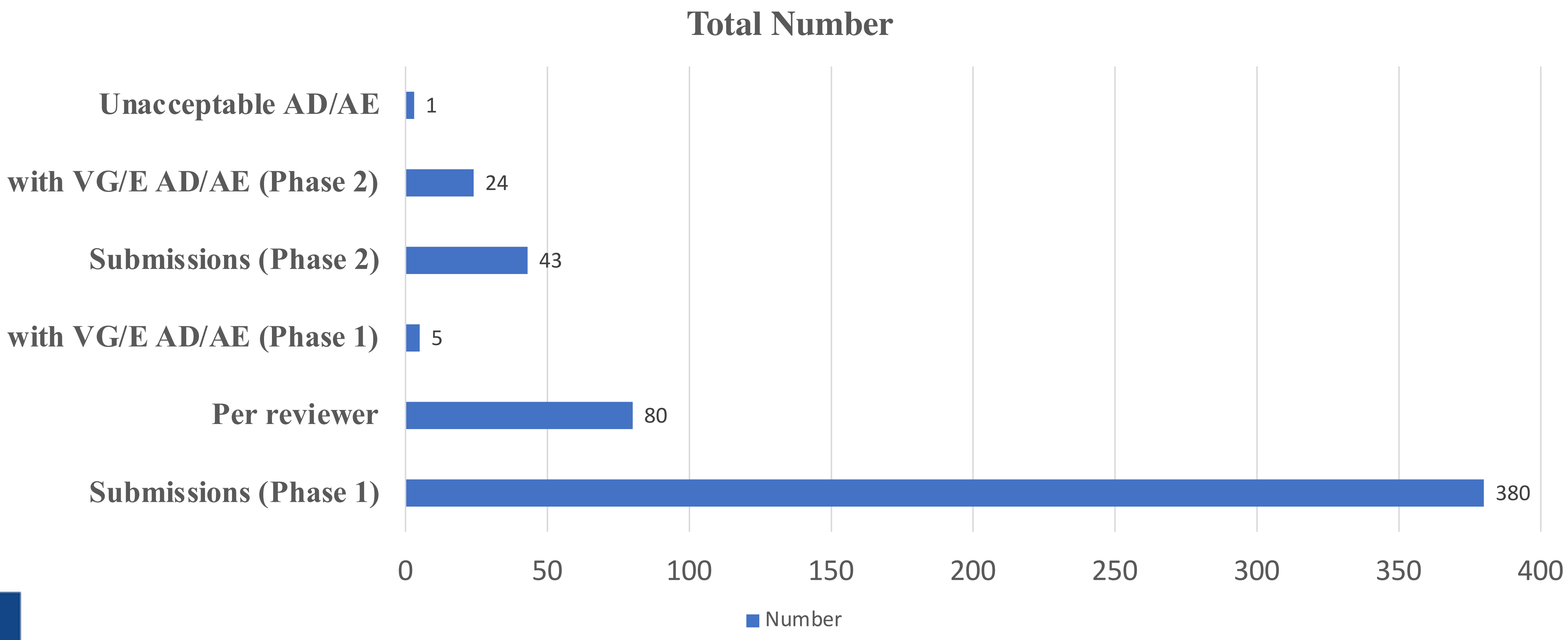
Cost of Scientific Technical Debt

Supercomputing Artifact Description and Evaluation Initiative



https://sc20.supercomputing.org/planning-committee/

Lack of artifacts will reject a paper



Technical debt incurs burden

- Reproducibility is an after thought.
- Identifying files for an application is a challenge
- Missing workflows
  - Really, that data/algorithm should be part of the bundle?
- “Sticks” from reviewers work
  - Authors who have not taken AD/AE process seriously do submit additional work
- Time consuming task
  - No tools to check if everything relevant for the publication is submitted
- No mapping of experiments to content in the paper.
  - No infrastructure for efficiently verifying claimed results

PART 2: Do reproducible containers provide a start?

Reproducibility ecosystem

Zenodo.org

Github

OpenData.gov

Package managers

Figshare

Sharing images via the cloud

Docker.com

[An introduction to **Docker** for **reproducible research**]
[C Boettiger] - ACM SIGOPS Operating Systems Review, 2015 - dl.acm.org

Docker: Using containers from build to run

Build

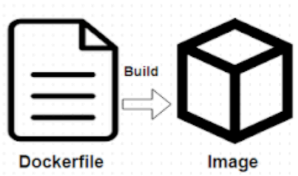
- Build images that captures applications requirements.
- Manually commit or use a recipe file.

Ship

- Push an image to DockerHub, a hosted registry, or a private Docker Registry.
- Share Images

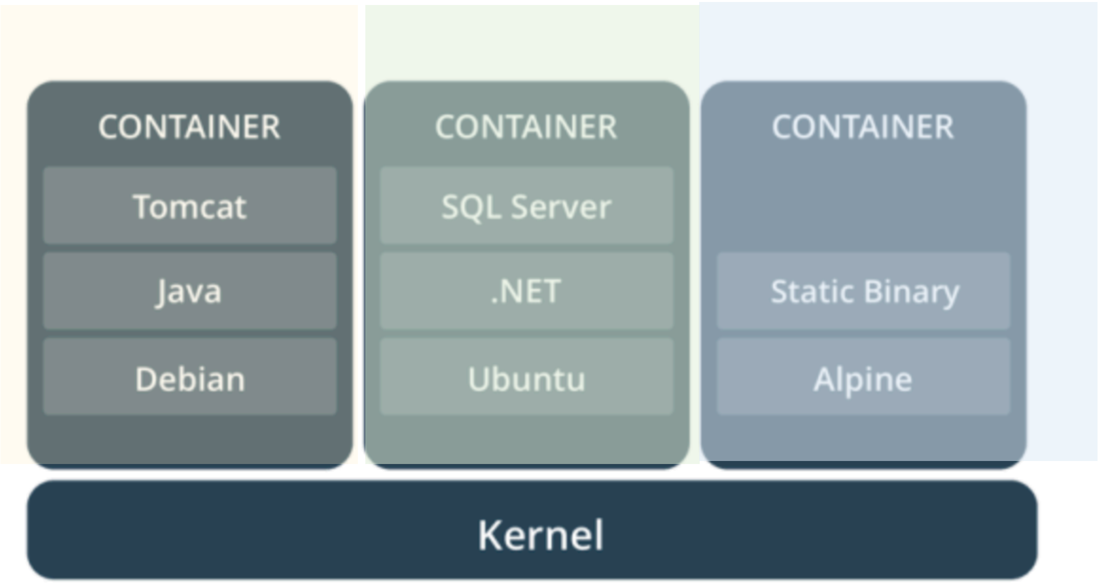
Run

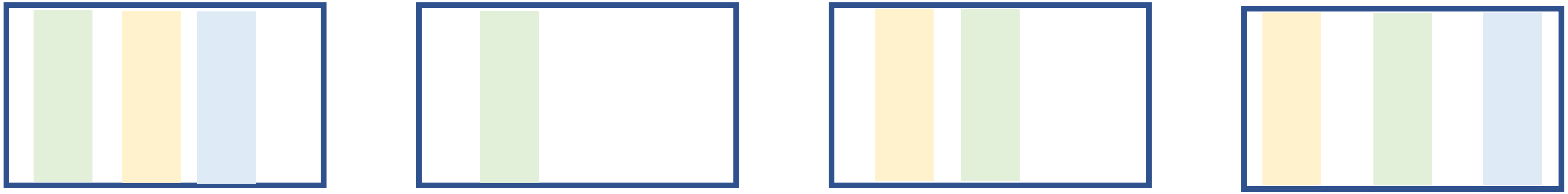
- Use Docker Engine to pull images down and execute a container from the image.



https://www.exascaleproject.org/event/conthpc

Containers provide constrained resource isolation





CPU Memory Filesystem Network

Authors must program a Dockerfile

```
# fetch node v4 LTS codename argon
FROM node:argon

# Request samplename build argument
ARG samplename

# Create app directory
RUN mkdir -p /usr/src/spfx-samples
WORKDIR /usr/src/spfx-samples

#Install app dependencies
RUN git clone https://github.com/SharePoint/sp-dev-fx-webparts.git .
WORKDIR /usr/src/spfx-samples/samples/$samplename

# install gulp on a global scope
RUN npm install gulp -g

# RUN ["npm", "install", "gulp"]
RUN npm install
RUN npm cache clean

# Expose required ports
EXPOSE 4321 35729 5432

# Run sample
CMD ["gulp", "serve"]
```

```
FROM buildkit-export AS buildkit-buildkitd.oci_only
COPY --from=buildkitd.oci_only /usr/bin/buildkitd.oci_only /usr/bin/
COPY --from=buildctl /usr/bin/buildctl /usr/bin/
ENTRYPOINT ["buildkitd.oci_only"]

# Copy together all binaries for containerd worker mode
FROM buildkit-export AS buildkit-buildkitd.containerd_only
COPY --from=runc /usr/bin/runc /usr/bin/
COPY --from=buildkitd.containerd_only /usr/bin/buildkitd.containerd_only /usr/bin/
COPY --from=buildctl /usr/bin/buildctl /usr/bin/
ENTRYPOINT ["buildkitd.containerd_only"]

FROM alpine AS containerd-runtime
COPY --from=runc /usr/bin/runc /usr/bin/
COPY --from=containerd /go/src/github.com/containerd/containerd/bin/containerd* /usr/bin/
COPY --from=containerd /go/src/github.com/containerd/containerd/bin/ctr /usr/bin/
VOLUME /var/lib/containerd
VOLUME /run/containerd
ENTRYPOINT ["containerd"]

FROM buildkit-${BUILDKIT_TARGET}
```

Containers do not reduce technical debt

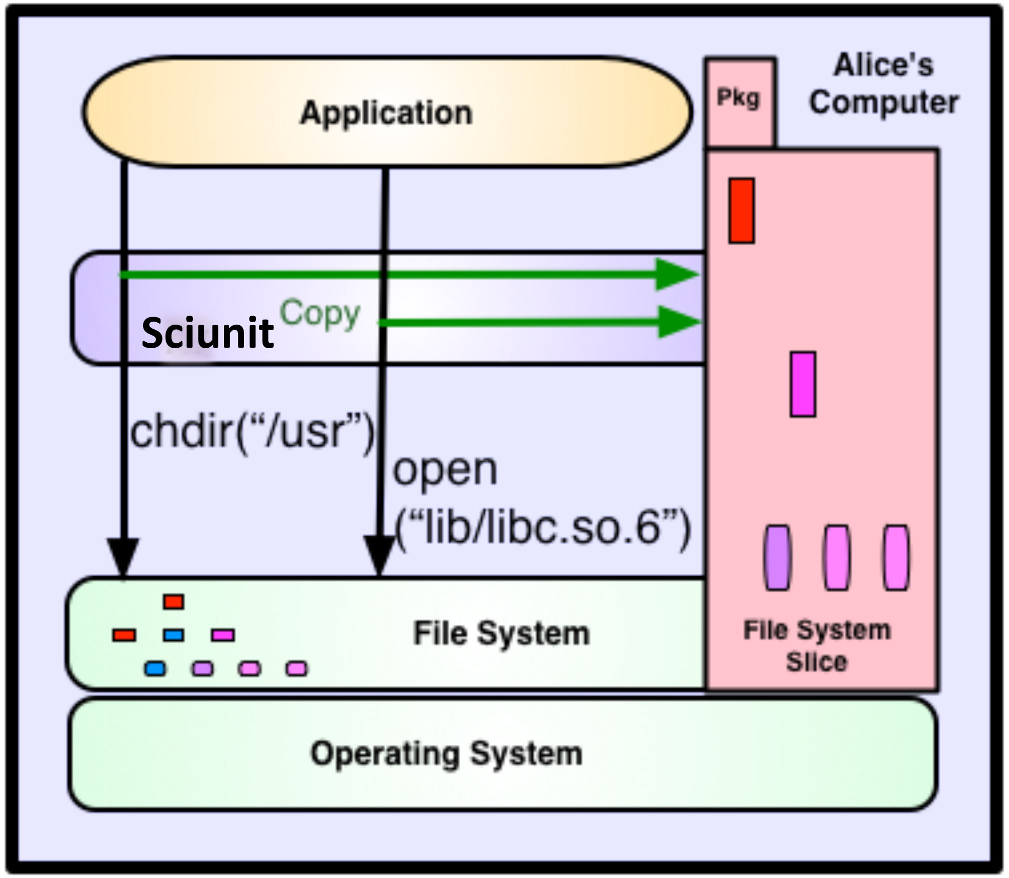
- Declarative encapsulation of dependencies for isolated execution
  - E.g. various shell utilities and library versions unknown to user

Automatic Encapsulation of Dependencies: The Sciunit

Key Idea: Identify dependencies during program execution

- Captures application dependencies during executions
- Repeats executions (with guarantees) within isolated environments

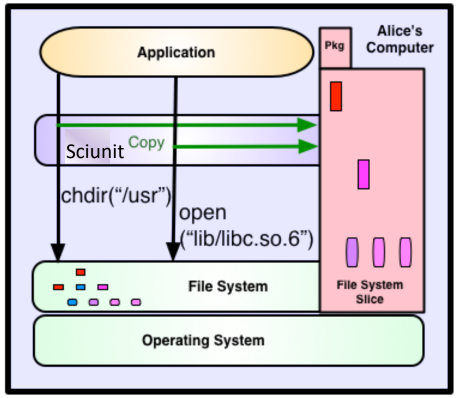
Sciunit: Audit

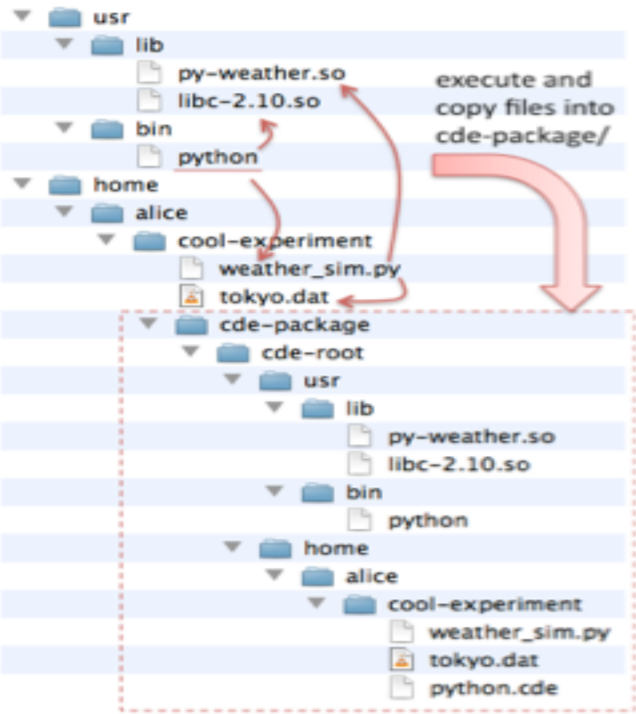


- Audit uses *ptrace* to observe dependencies and environment variables
  - Identifies binaries, libraries, scripts, and environment variables that application is dependent on.
- Dependencies are copied into a directory in the filesystem
- Inclusion of data files is optional
  - user may or may not want to package based on the size of the dataset.

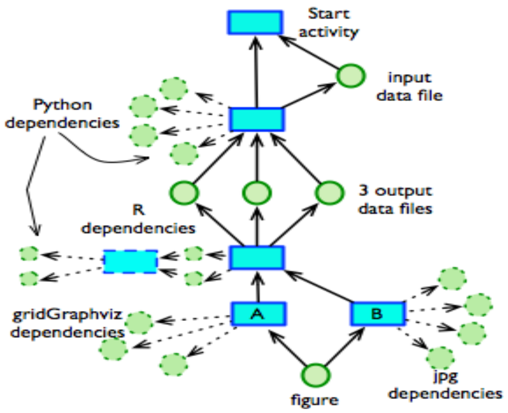
D.H. Ton That, G. Fils, Z. Yuan, T. Malik. Sciunits: Reusable Research Objects. In *IEEE eScience Conference* (eScience), 374-383, 2017

Audits provenance during execution time



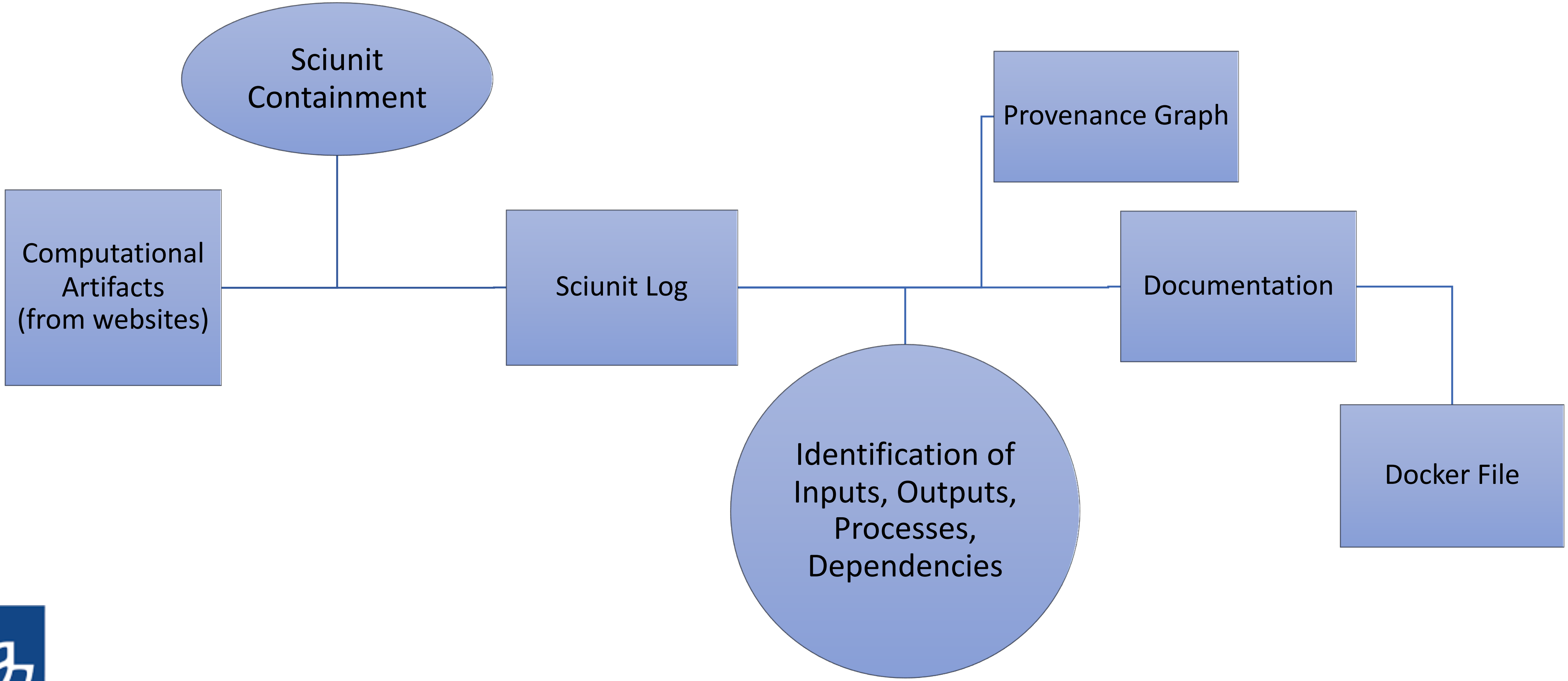



```
1542206708 2617 EXECVE 2623 /usr/bin/python3 /home/ubuntu/scripts/pysumma ["python3", "python_script.py"]
1542206708 2623 READ /etc/ld.so.cache
1542206708 2623 READ /lib/x86_64-linux-gnu/libpthread.so.0
1542206708 2623 READ /usr/lib/locale/locale-archive
1542206708 2623 READ /usr/lib/python3.6/__pycache__/_sysconfigdata_m_linux_x86_64-linux-gnu.cpython-36.pyc
1542206708 2623 READ /usr/lib/python3.6/collections
1542206708 2623 READ /home/ubuntu/scripts/pysumma/python_script.py
1542206708 2623 READ /etc/localtime
1542206708 2623 READ /home/ubuntu/.local/lib/python3.6/site-packages/dateutil
1542206709 2623 READ /home/ubuntu/.local/lib/python3.6/site-packages/numpy
1542206709 2623 READ /home/ubuntu/.local/lib/python3.6/site-packages/numpy/core
1542206709 2623 READ /home/ubuntu/.local/lib/python3.6/site-
1542206709 2623 READ /usr/lib/python3.6/unittest
```



Utilizing Provenance in Reusable Research Objects, In *Special Issue on Using Computational Provenance*, MDPI Informatics, Vol 5(1), 2018.
Light-weight Database Virtualization. In *IEEE International Conference on Data Engineering*, ICDE, 2015.
Auditing and Maintaining Provenance in Software Packages. In *International Provenance and Annotation Workshop* (IPAW), 97-109, 2014

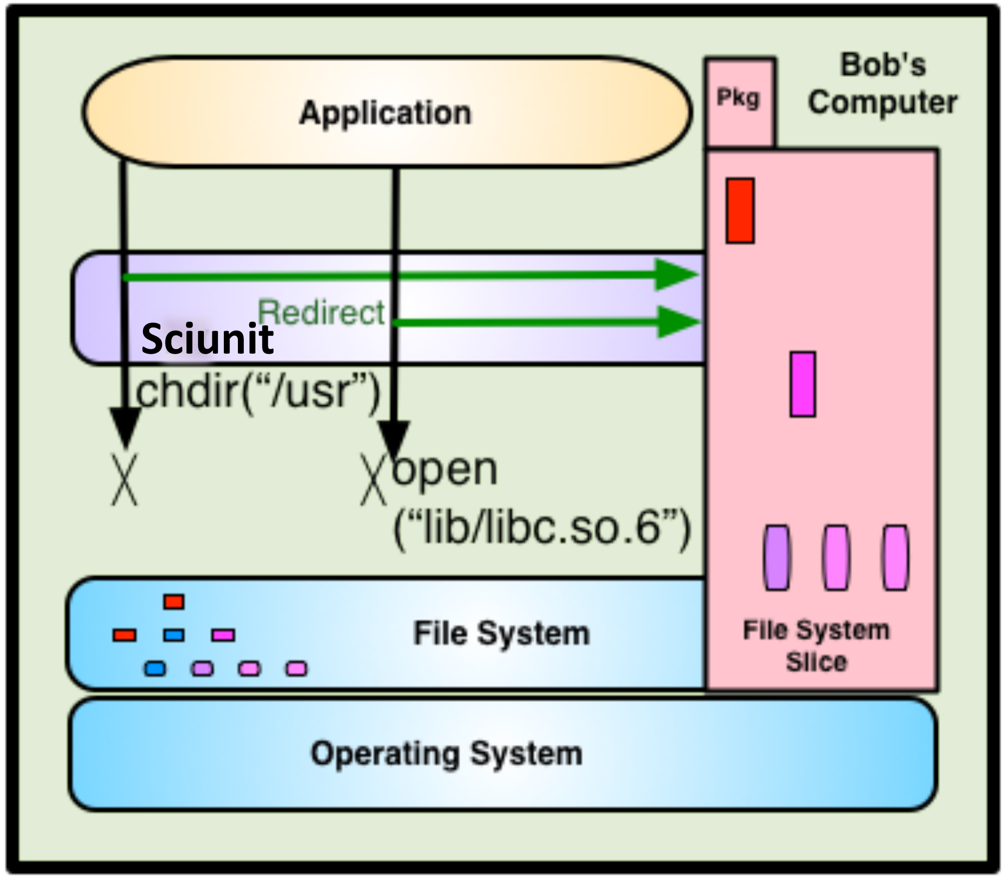
Sciunit: Share as a Zip file or Docker container



Documenting Computing Environments for Reproducible Experiments, In *Parallel Computing: Technology Trends, 756-765, 2020*

Sciunit: Repeat

- Sciunit uses namespace isolation during repeat
- Redirection of each call into the package



Efficient Provenance Alignment in Reproduced Executions, In *Theory and Practice of Provenance*, 2020.
SciInc: A Container Runtime for Incremental Recomputation", In*IEEE 15th International Conference on eScience* (eScience), 291-300, 2019, *doi:* 10.1109/eScience. 2019.00040.

Sciunit steps and external requirements

1. Create

2. Share

3. Repeat

figshare

HYDROSHARE

XSEDE
Extreme Science and Engineering Discovery Environment

CloudLab

C/C++

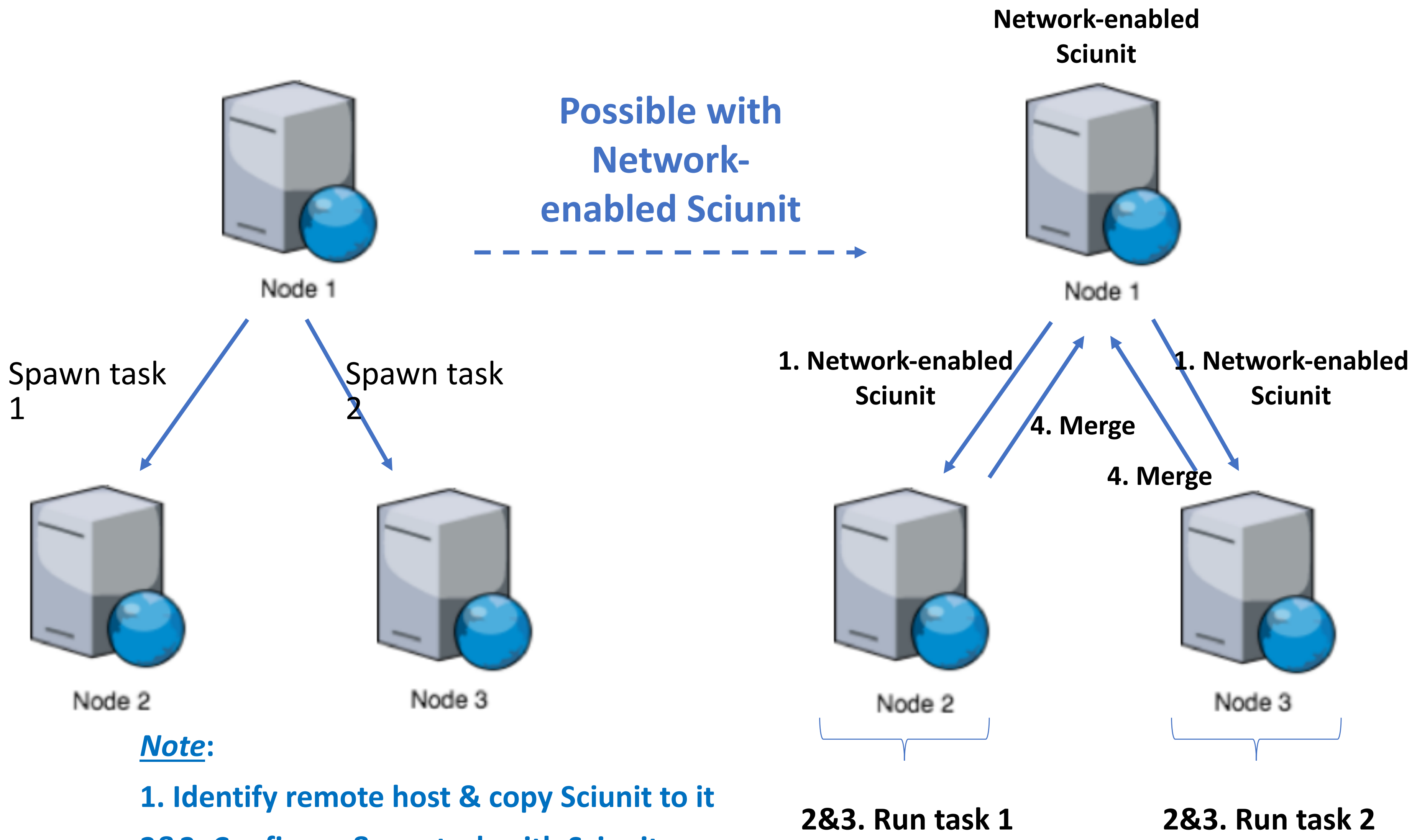
fortran
THE ORIGINAL HANGING CHAD

julia

jupyter

OPEN MPI

Network-enabled Sciunit: Audit



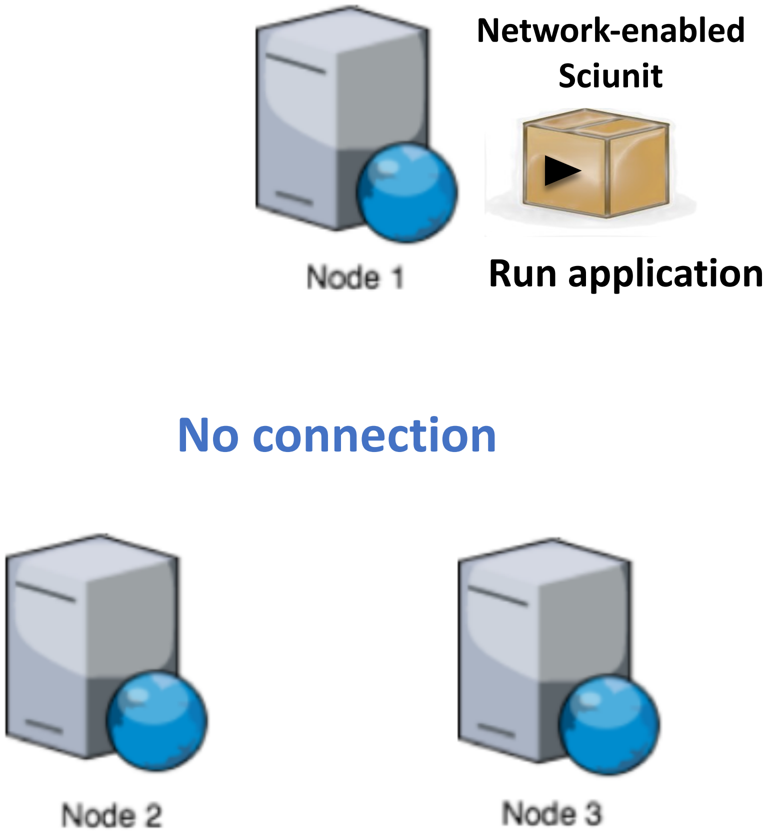
Note:

1. Identify remote host & copy Sciunit to it

2&3. Configure & run task with Sciunit

4. Retrieve & manually merge

Network-enabled Sciunit: Repeat on single node



***Note*:**

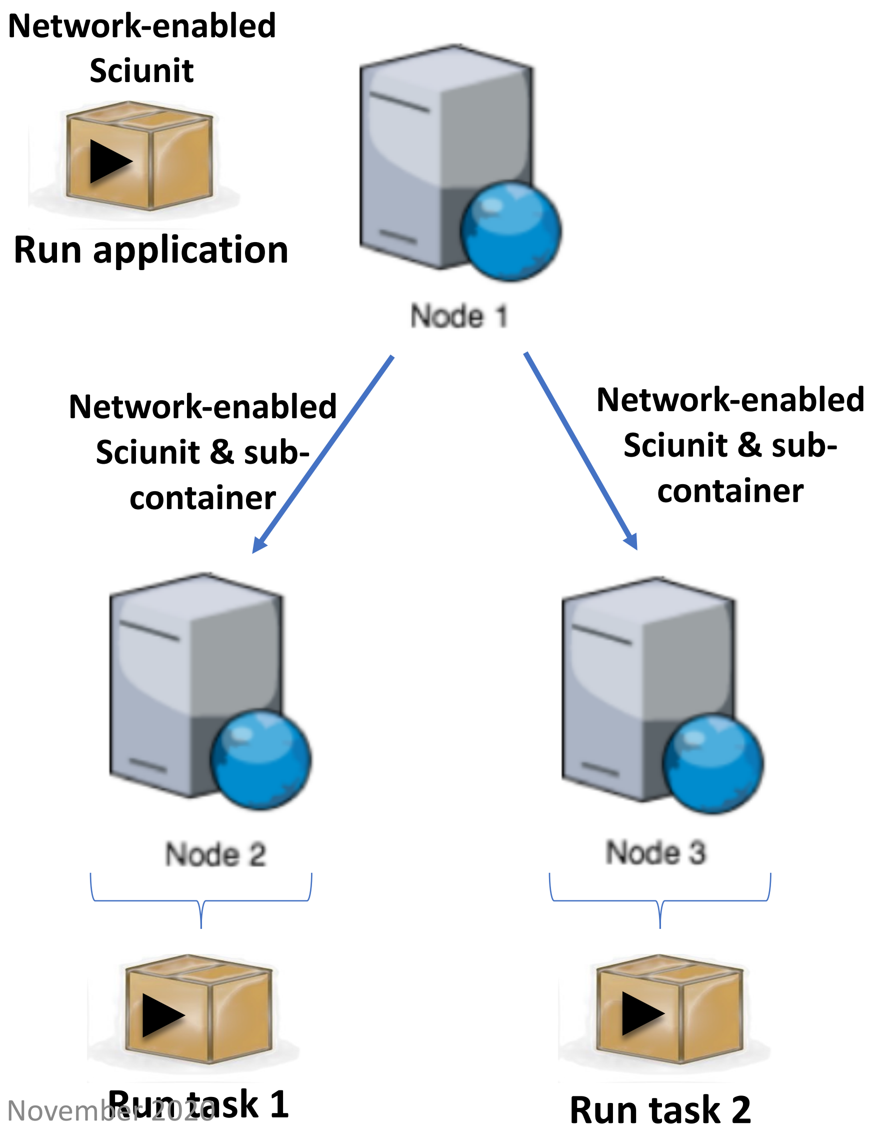
1. Repeat all computations at root node.

2. Network system calls are supplied through the content data captured during the original audit.

Network-enabled Sciunit: Repeat on multiple nodes

Requirements:

1. Identical number of nodes
2. Descriptions of new hostnames or IP addresses



Usecases

TABLE I: Usecases descriptions.

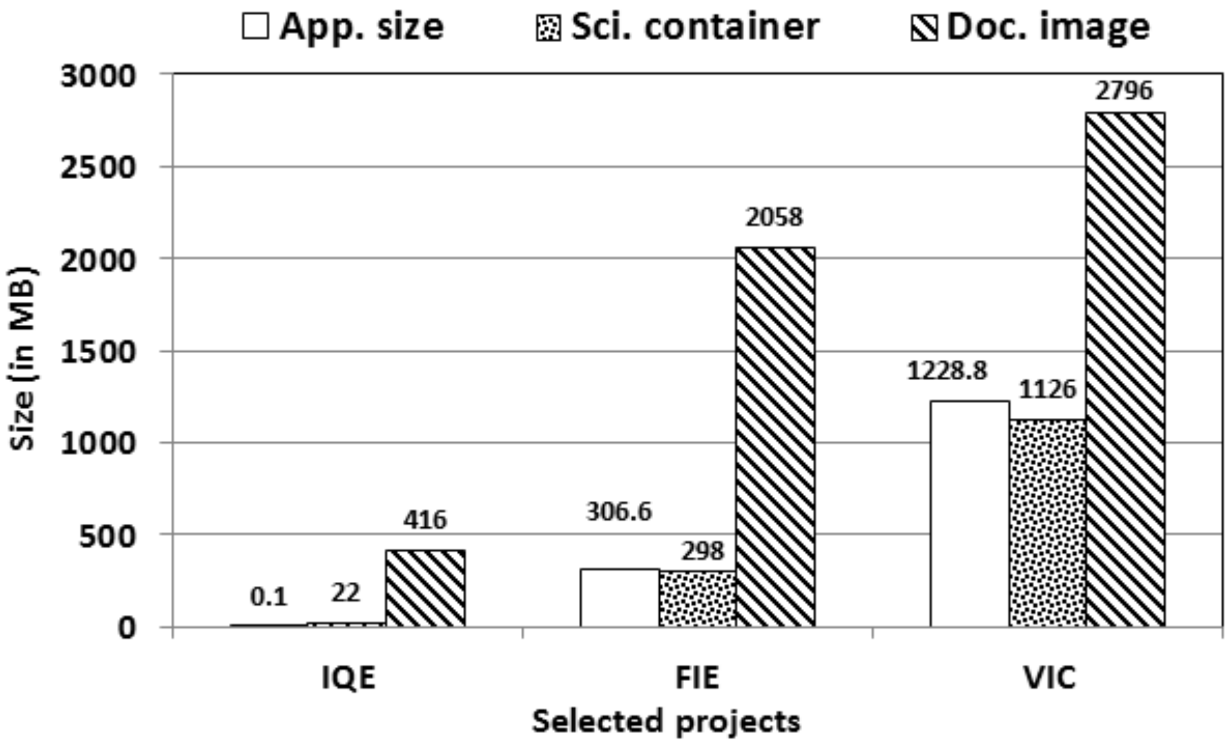
	FIE [16]	**VIC [17]**	**IQE [18]**
Source code languages	R, Bash	C, C++, Python, C shell script, Fortran	Python
Source code files	29	97	5
Data files	14	11,481	5
Dependency files	659	357	112
Size of all files	306.6 MB	1.2 GB	22 MB
Normal run time	286.756 s	40.259 s	5.226 s

[16[City of Chicago, "Food Inspection Evaluation," https://chicago.github. io/food-inspections-evaluation/, 2017, [Online; accessed 7-May-2017].

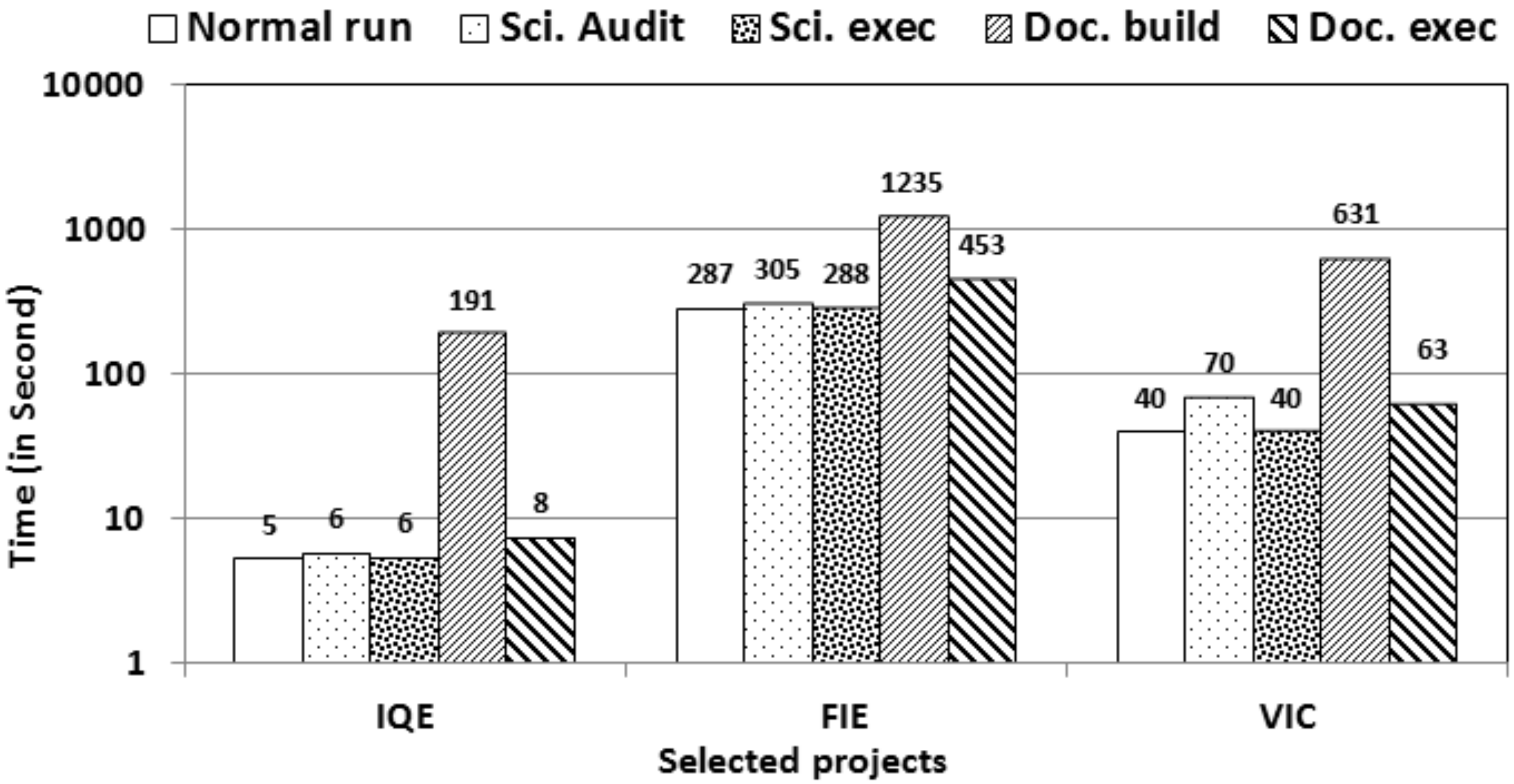
[17] M. M. Billah, J. L. Goodall *et al.*, "Using a data grid to automate data preparation pipelines required for regional-scale hydrologic modeling," *Environmental Modelling & Software*, vol. 78, 2016.

18] D. DBGroup, "Incremental Query Execution," 2019, [Online; accessed 3-April-2019]. [Online]. Available: https://TonHai@bitbucket. org/TonHai/iqe.git

Sciunit (native) versus Docker sizes



Sciunit audit and repeat times



Experiments

- NASA Parallel Benchmark:
  - Data transferred (~524 KB (class A) & ~268 KB (class B))

	Normal	#Calls	Meta Audit	Content Audit
NPB BT-MZ.A.2	20.30			
NPB LU-MZ.A.2	15.74	190	$\sim 2.1\%\uparrow$	$\sim 5.3\%\uparrow$
NPB SP-MZ.A.2	14.84			
NPB BT-MZ.B.2	83.95			
NPB LU-MZ.B.2	71.02	190	$\sim 0.8\%\uparrow$	$\sim 3.2\%\uparrow$
NPB SP-MZ.B.2	59.12			

- VIC

	Normal	Meta Audit	Content Audit	Replay
Data retrieval	146.5±1.8	$0.2\%\uparrow$	$134.5\%\uparrow$	53.0±3.0
Other steps	varies	2% - 30% ↑ overhead		

Sample Interaction of Sciunit

```
1. > sciunit create FIE
2. > sciunit exec ./FIE.sh ./DATA/weather_201710.Rds
     0. Download…
     1. Calculate violation matrix…
     2. Calculate heat map…
     3. Generate model data with ./DATA/weather_201710.Rds…
     4. Apply random forest model…
     5. Evaluation…
3. > sciunit list
     e1 Dec 4 12:44 ./FIE.sh ./DATA/weather_201710.Rds
4. > sciunit show
     id: e1
     sciunit: FIE
     command: ./FIE.sh ./DATA/weather_201710.Rds
     size: 306.6 MB
     started: 2017-12-04 12:44
5. > sciunit push
     …
     Title for the new article: FIE
     new: 306.6 MB [01:05, 4.72MB/s]
6. > sciunit copy
     mSLLTj#
```

Alice's Computer

```
1. > sciunit open mSLLTj#
     Opened Sciunit FIE
2. > sciunit list
     e1 Dec 4 12:44 ./FIE.sh ./DATA/weather_201710.Rds
3. > sciunit repeat e1
     …
     0. Download…
     1. Calculate violation matrix…
     2. Calculate heat map…
     3. Generate model data with ./DATA/weather_201710.Rds
     4. Apply random forest model…
     5. Evaluation…
4. > sciunit given '/tmp/weather_201801.Rds' e1 %
     …
     1. Generate model data with '/tmp/weather_201801.Rds
     2. Apply random forest model…
     3. Evaluation…
5. > sciunit list
     e1 Dec 4 12:44 ./FIE.sh ./DATA/weather_201710.Rds
     e2 Dec 14 2:44 ./FIE.sh ./tmp/weather_201801.Rds
```

Bob's Computer

Container Limitations

- Container either include the data or exclude the data
  - The decision is binary but does not consider necessary and sufficient data

Container Debloating: MiDAS

Example

```
void file_read(int bytes) {
        int fd, sz;
        char *c = (char *) calloc(bytes, sizeof(char));
        fd = open("test.txt", O_RDWR);
        lseek(fd,100,SEEK_SET);
        sz = read(fd, c, bytes);
}
```

```
test.txt, 100, 150
test.txt, 100, 190
test.txt, 100, 230
test.txt, 100, 450
```

Example

```
void file_read(int bytes) {
	int fd, sz;
	char *c = (char *) calloc(bytes, sizeof(char));
	fd = open("test.txt", O_RDWR);
	lseek(fd,100,SEEK_SET);
	sz = read(fd, c, bytes);
}
```

```
test.txt, 100, 150
test.txt, 100, 190
test.txt, 100, 230
test.txt, 100, 450
```

MiDAS: Minimizing DAtasetS

WHAT

Automatically identify & include **ONLY relevant data chunks** with application

HOW

Map **high level user inputs** to **file offsets**

Partial Evaluation & LLVM

- **Partial Evaluation**→optimization technique to **prune codebase**
  - Uses static inputs to generate a **specialized program** to accept remaining dynamic inputs

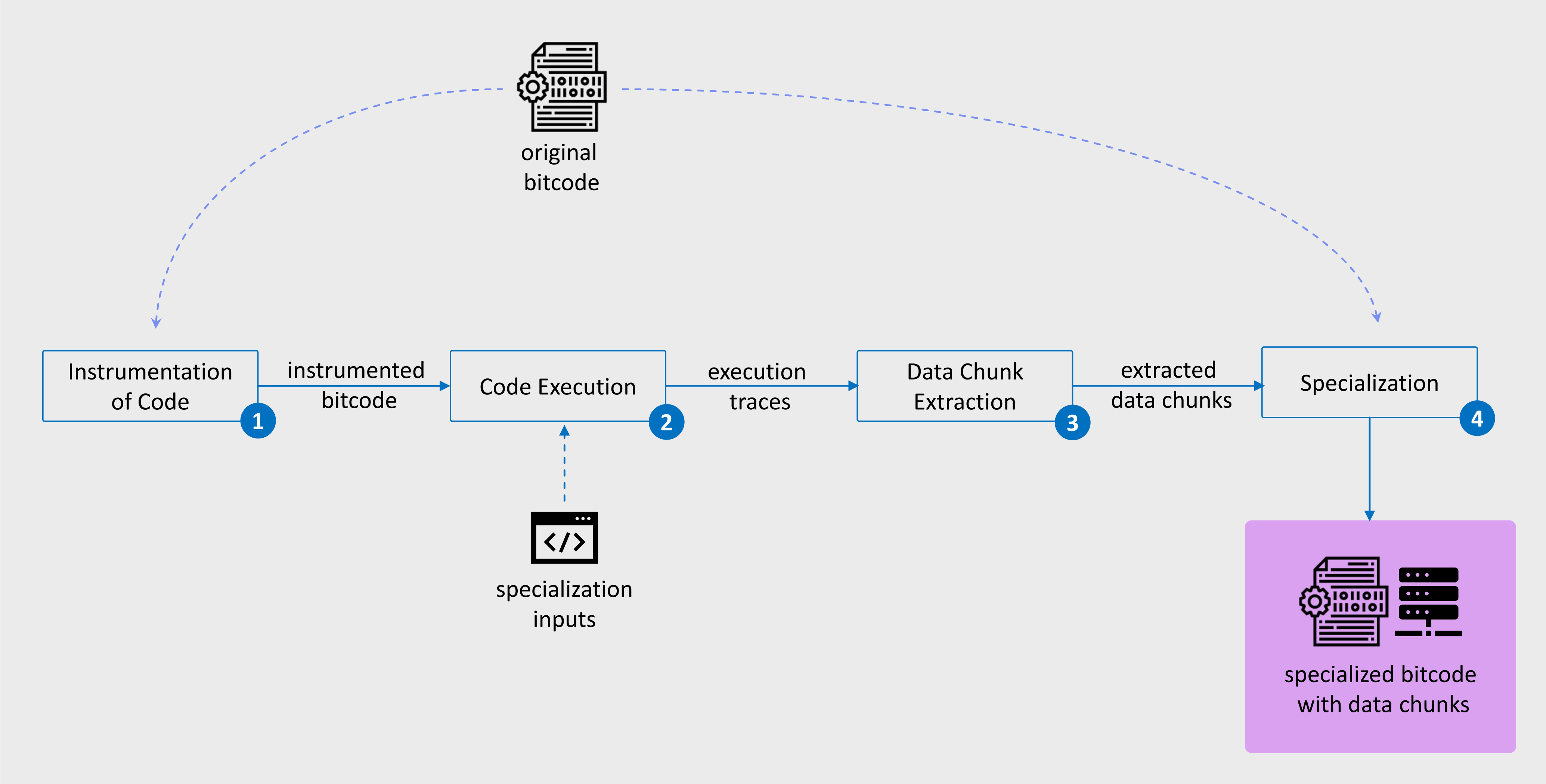
```
#include <math.h>
float compute_building_height(float building_distance){
        float viewing_angle = pi/4;
        float building_height =
          compute_opposite(building_distance,
            viewing_angle);
        return building_height;
}
float compute_opposite(float adjacent, float angle){
        float opposite = adjacent * tan(angle);
        return opposite;
}
```

(a) Original code

```
float compute_building_height(float building_distance){
        float building_height =
          compute_opposite_specialized(building_distance);
        return building_height;
}
float compute_opposite_specialized(float adjacent){
        float opposite = adjacent * 1;
        return opposite;
}
```

(b) Specialized code

MiDAS



original bitcode
Instrumentation of Code
1
instrumented bitcode
Code Execution
2
execution traces
Data Chunk Extraction
3
extracted data chunks
Specialization
4
specialization inputs
specialized bitcode with data chunks

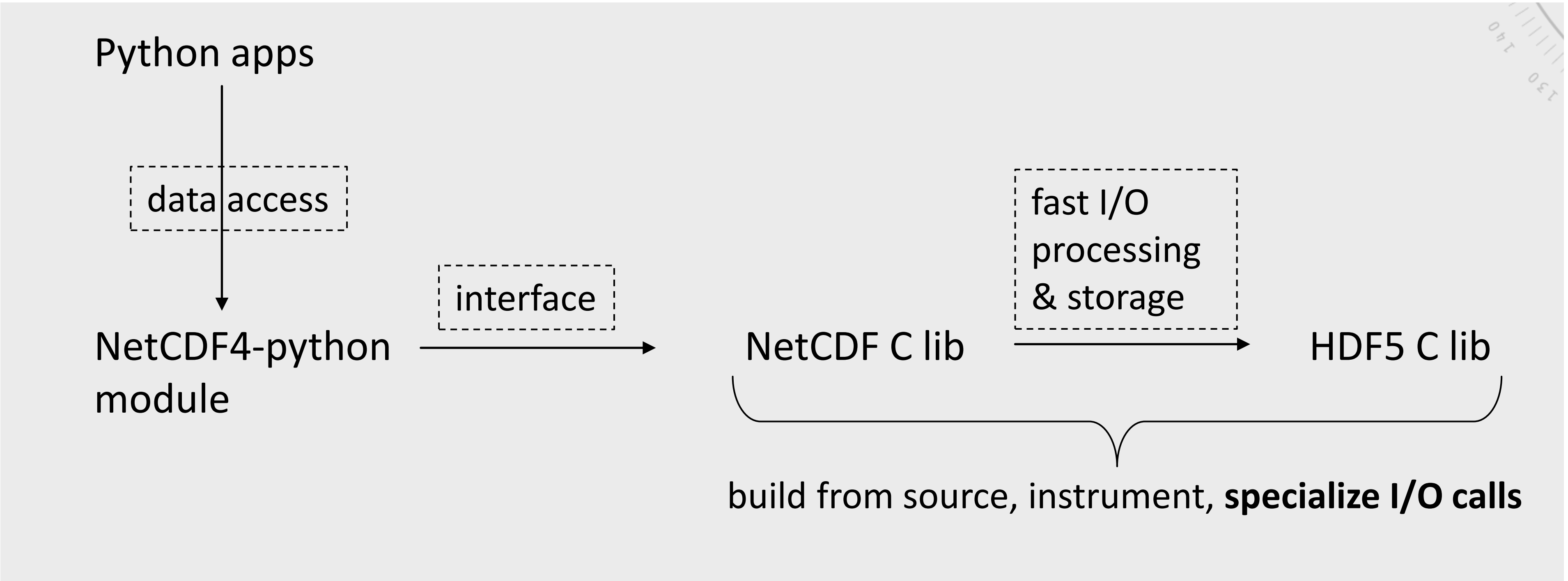
I/O Specialization

- **Replace I/O call & *preserve functionality***
  - Extracted file data in global variable→ fileData
  - Copy from global variable to *read* buffer → *memcpy*
  - Update all I/O call variables→return value of *read*
  - I/O call instruction removed → read

```
%94 = load i32, i32* %9, align 4
%95 = sext i32 %94 to i64
%96 = call i64 @read(i32 %92, i8* %93, i64 %95)
%97 = trunc i64 %96 to i32
store i32 %97, i32* %13, align 4
%98 = load i32, i32* %12, align 4
```

```
%94 = load i32, i32* %9, align 4
%95 = sext i32 %94 to i64
%96 = bitcast [17 x i8]* @fileData to i8*
call void @llvm.memcpy.p0i8.p0i8.i64(i8* %93,
        i8* %96, i64 %95, i32 1, i1 false)
%97 = alloca i64
store i64 %95, i64* %97
%loadRetVal = load i64, i64* %97
%98 = trunc i64 %loadRetVal to i32
store i32 %98, i32* %13, align 4
%99 = load i32, i32* %12, align 4
```

Specializing I/O Calls in Scientific Libraries



Results | Percentage of File Accessed

- Larger files generated from 30 MB NetCDF data file
- Rewriting data for multiple timesteps
- Data accessed corresponding to *temperature* attribute

Total Size	Accessed Size
30 MB	6.6 MB
700 MB	154 MB
1.4 GB	0.3 GB
9 GB	1.98 GB
12.8 GB	2.82 GB

APPLICATIONS OFTEN ACCESS
ONLY A SUBSET
OF A LARGE DATASET

PART 3: Summary and Guidance

Summary

- Technical debt affects reproducibility of scientific claims.
  - Process for evaluation of scientific claims is being rethought.
  - Artifact description and evaluation are becoming part of conferences
- Better reliability is needed.
  - Containers will be a prominent choice but their reliability is poor
    - Dependencies must be specified
    - Inefficient to use
    - No guarantees for execution verification
    - Not meant for interactive programs
- New light-weight methods: Sciunit, MiDAS

Use Sciunit for your next paper submission!

1. Tools downloaded ~850 times (tracked using pip)
2. 8 active contributors to the project
3. Actively used in geoscience disciplines that develop computational models and data-analytic pipelines

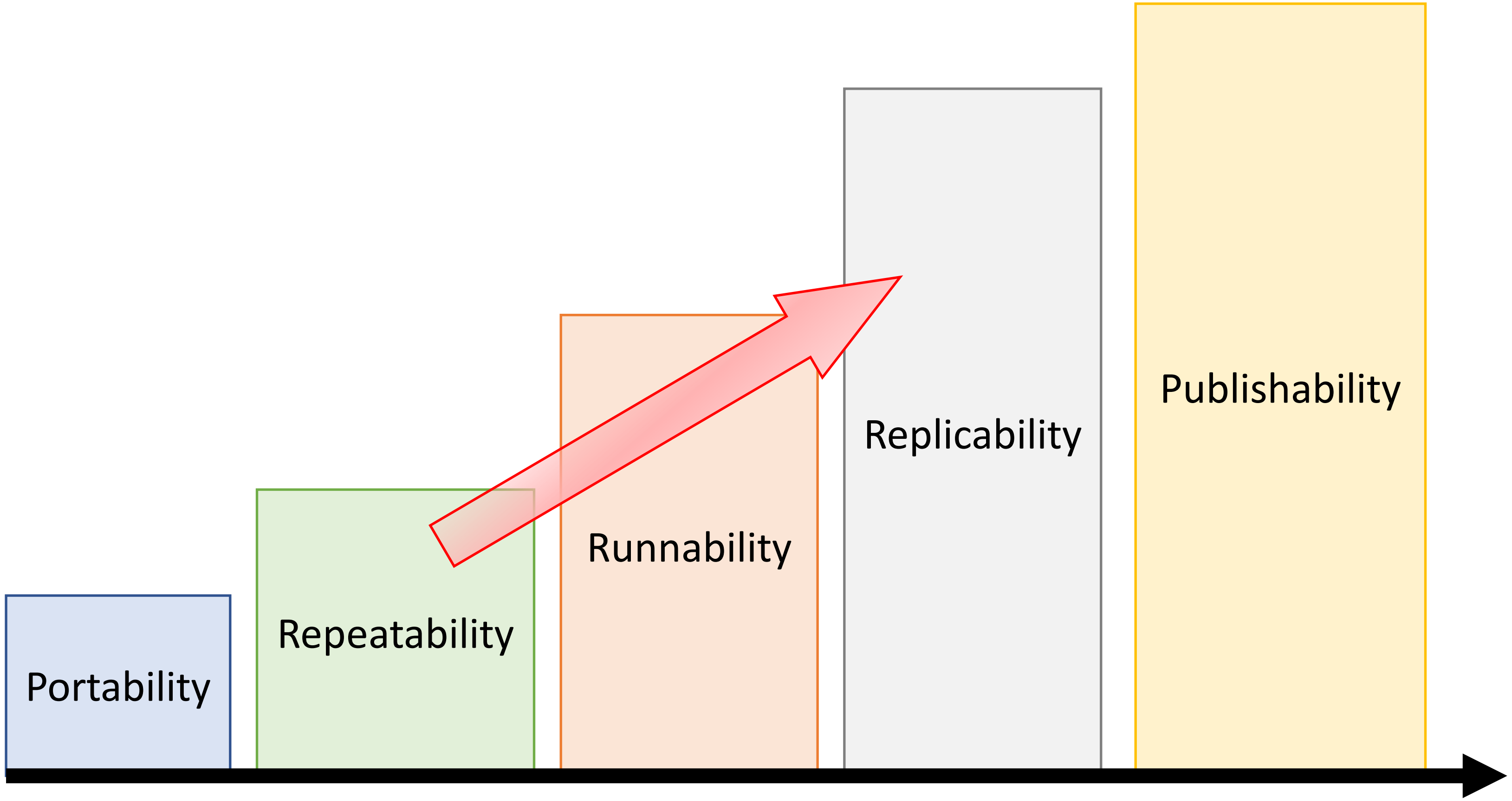
Website: http://sciunit.run

Issues and contribution: pr@sciunit.run

Guidance for Improving Reproducibility

Guidance for Improving Reproducibility

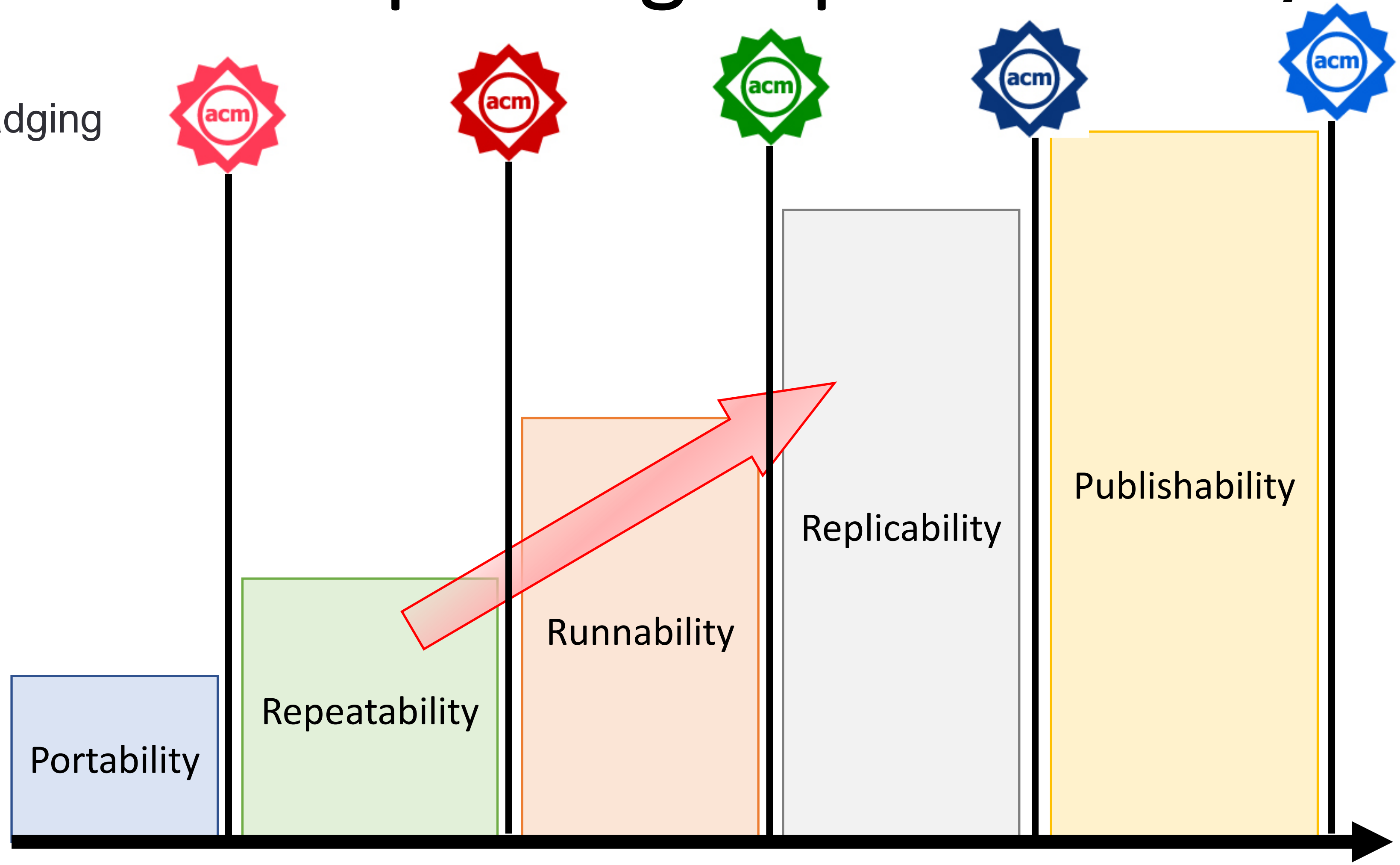
https://bssw.io/items?topic=reproducibility



1. J. Freire, N. Fuhr, and A. Rauber. *Reproducibility of data-oriented experiments in e-science* (Dagstuhl seminar 16041) Dagstuhl reports. 6(1):108–159, 2016. [Online; accessed 10-Sep-2017].

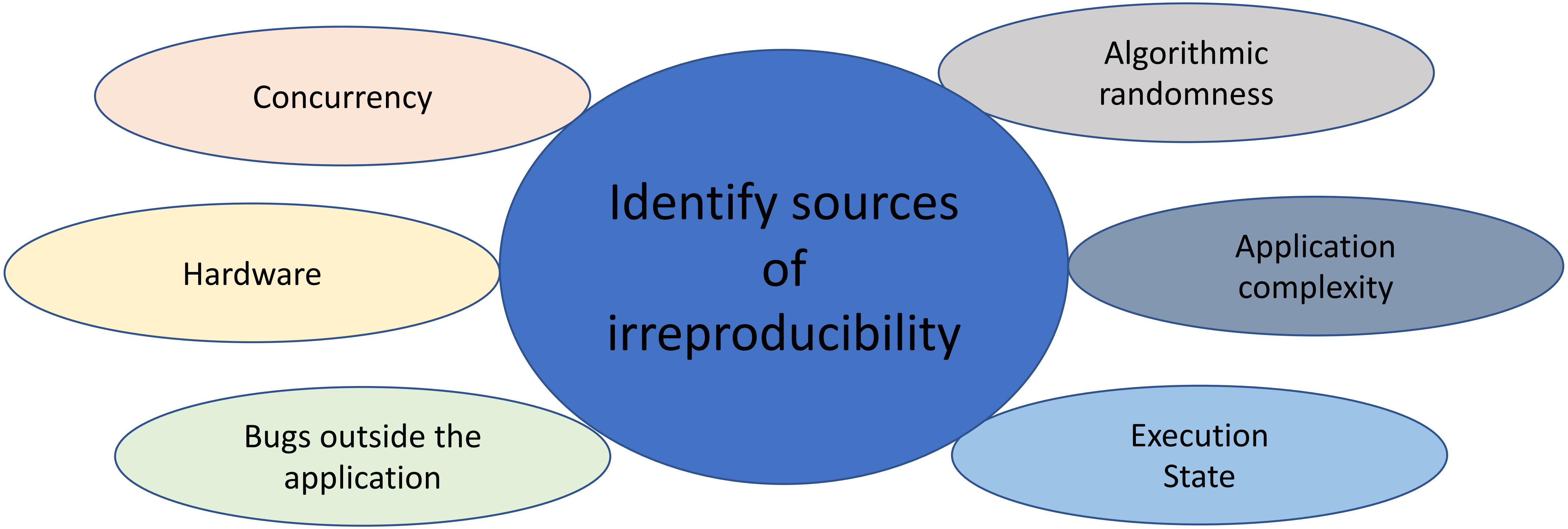
Guidance for Improving Reproducibility

Artifact Review and Badging

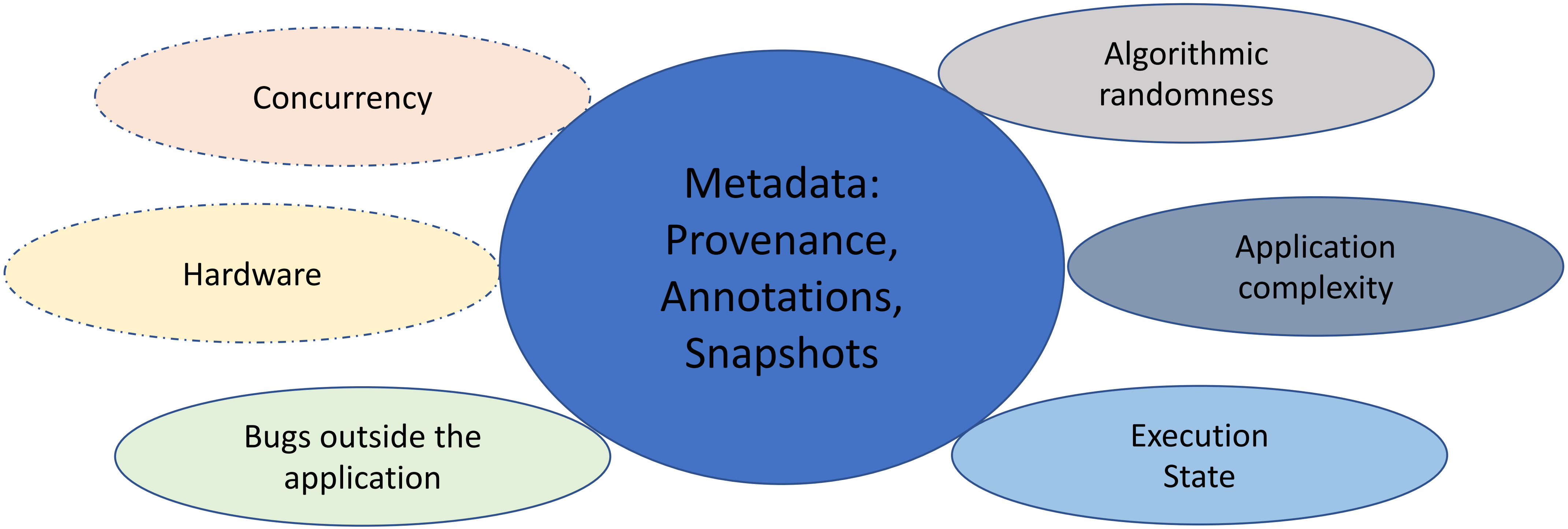


1. J. Freire, N. Fuhr, and A. Rauber. *Reproducibility of data-oriented experiments in e-science* (Dagstuhl seminar 16041) Dagstuhl reports. 6(1):108–159, 2016. [Online; accessed 10-Sep-2017].

Guidance for Improving Reproducibility

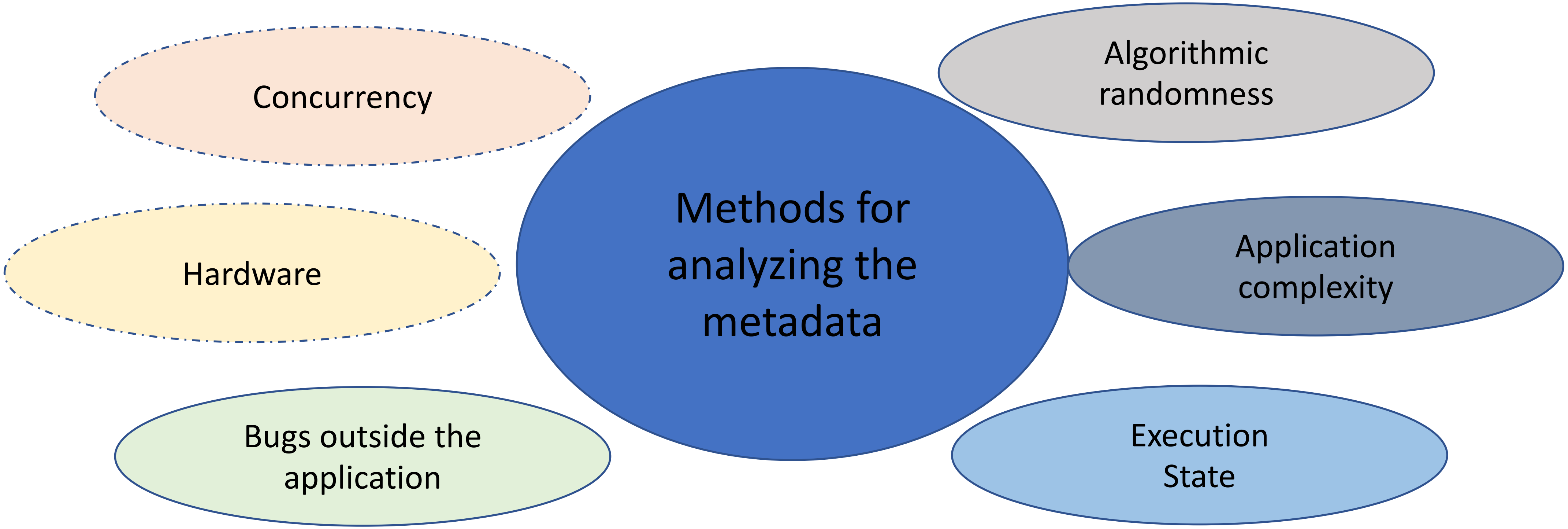


Guidance for Improving Reproducibility



https://bssw.io/items?topic=reproducibility

Guidance for Improving Reproducibility



https://bssw.io/items?topic=reproducibility

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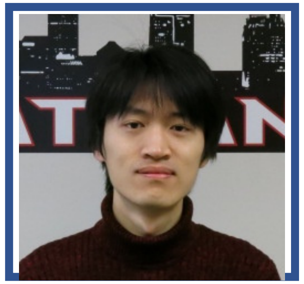

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Questions

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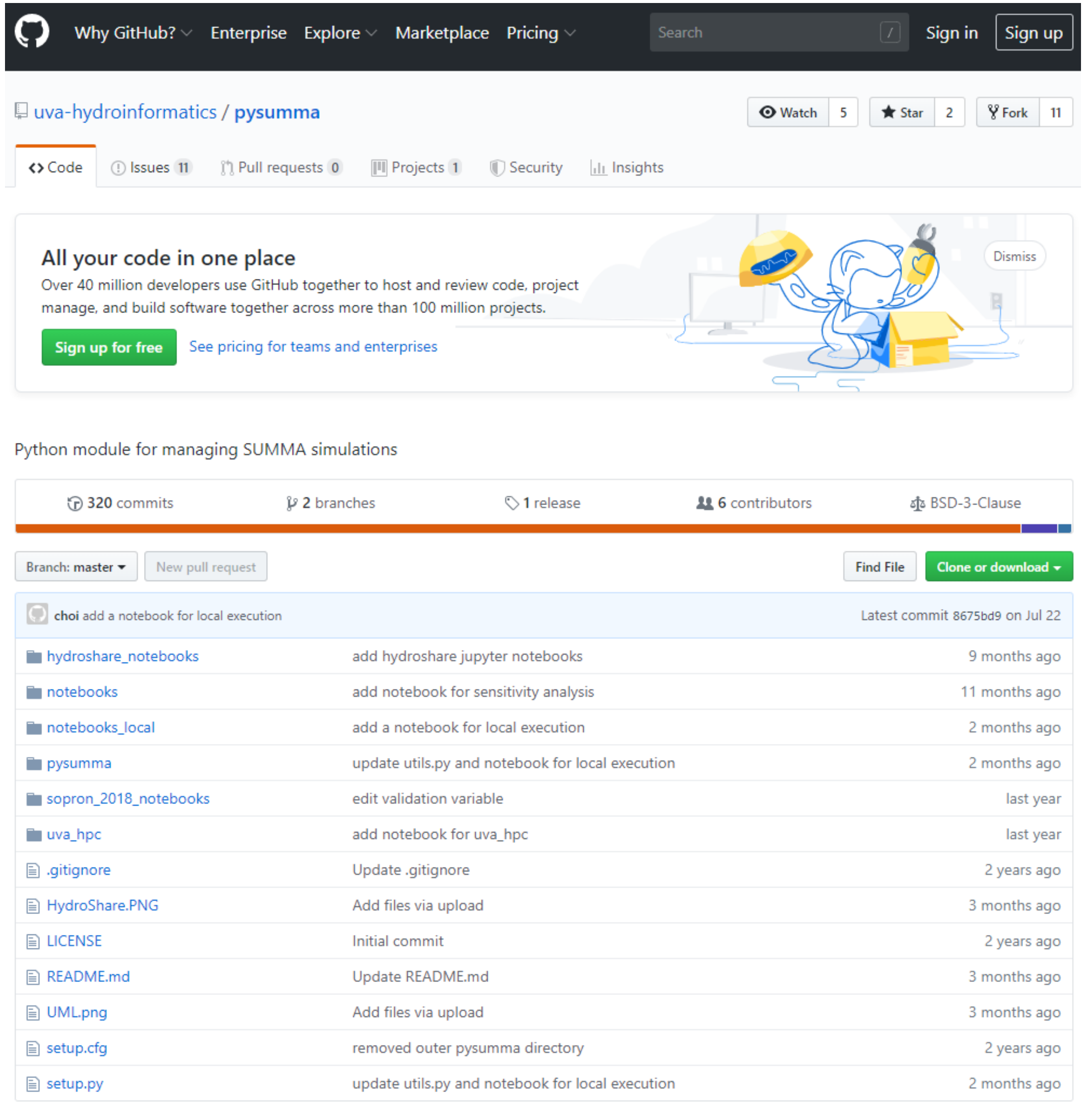
Example



How to run pySUMMA locally

Installation and Usage

pySUMMA requires Python 3.6 and following packages :

- xarray 0.10.7 : N-D labeled arrays and datasets in python
- numpy 1.16.1 : the fundamental package for scientific computing with Python
- matplotlib 3.0.2 : a Python 2D plotting library
- seaborn 0.9.0 : statistical data visualization
- jupyterthemes 0.20.0 : select and install a Jupyter notebook theme
- hs-restclient 1.3.3 : HydroShare REST API python client library
- ipyleaflet 0.9.2 : A jupyter widget for dynamic Leaflet maps
- Linux Environment (VirtualBox 5.2.8)
  - lubuntu-16.10 executable
  - lubuntu-16.04.4 executable

Download and Install pySUMMA:

1.) Download pySUMMA

```
~/Downloads$ git clone https://github.com/uva-hydroinformatics/pysumma.git
```

Result

Listed Packages	Identified Packages
xarray{0.10.7} numpy{1.16.1} matplotlib{3.0.2} hs-restclient{1.3.3} ipyleaflet{0.9.2} seaborn{0.9.0} jupyterthemes{0.20.0}	xarray{0.10.7} numpy{1.16.1} matplotlib{3.0.2} hs-restclient{1.3.3} ipyleaflet{0.9.2}
Identified Sub-Packages	
Pygments{2.2.0} asyncio backcall{0.1.0} blinker{1.3} certifi{2018.10.15} cftime{1.0.2.1} geopandas{0.4.0} html http ipykernel{5.1.0} ipython-genutils{0.2.0} ipython{7.1.1} ipywidgets{7.4.2} jedi{0.13.1} jupyter-core{4.4.0} netCDF4{1.4.2} pandas{0.23.4} parso{0.3.1} pexpect{4.6.0} prompt-toolkit{2.0.7} ptyprocess{0.6.0} pyparsing{2.3.0} pysumma{0.1} pytz{2018.7} pyzmq{17.1.2} requests-oauthlib{1.0.0} requests-toolbelt{0.8.0} tornado{5.1.1} traitlets{4.3.2} traittypes{0.2.1} wcwidth{0.1.7}	
Python Built-In Packages	
chardet collections concurrent ctypes dateutil distutils email encodings idna importlib jinja2 json logging markupsafe multiprocessing oauthlib pkg_resources pydoc_data requests sqlite3 unittest urllib urllib3 xml	

Current and Future Work

- Developing Sciunit audit and repeat with checkpoint-restart
  - Compute- and data-analytic models that vary several parameters and are reexecuted multiple times to test their reproducibility.
  - Useful for Jupyter Notebooks

- Sciunit for reproducibility will provide provenance-based guarantees
  - Several cyberinfrastructure for Artifact Evaluation (OCCAM, CKFoundation)
  - Provenance-based guarantees are missing

- Developing MiDAS for different inputs