



Enabling painless reuse of shared research data and code: a case study on computational reproducibility

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25/08/2020

Agenda

- ▶ Short introduction (5 mins)
- ▶ Talk #1 (20 mins):
 - ▶ Enabling Painless Reuse of Shared Research Data and Code in data repository Dataverse, by Ana Trisovic
- ▶ Talk #2 (20 mins):
 - ▶ Enabling Painless Reuse of Shared Research Data and Code for HPC-driven computational reproducibility of research, by Qian Zhang
- ▶ Q&A and open discussion (15 mins)

Acknowledgements

- ▶ Our research is funded or supported by:
 - ▶ Council on Library and Information Resources (CLIR)
 - ▶ Portage Network
 - ▶ The Alfred P. Sloan Foundation
 - ▶ The AWS Cloud Credits for Research program
 - ▶ Institute for Quantitative Social Science
 - ▶ David R. Cheriton School of Computer Science & University Library, University of Waterloo



Enabling Painless Reuse of Shared Research Data and Code in data repository Dataverse

Ana Trisovic,

Sloan postdoctoral fellow at IQSS,

Harvard University

Agenda of this talk

- ▶ Introduction
- ▶ Quality of shared data & code
 - ▶ How do we ensure it?
- ▶ Code execution experiments
 - ▶ What happens when we automatically re - execute R or Python code?
 - ▶ What are the most common errors?
- ▶ Painless research reproducibility and reuse
 - ▶ Toward enabling painless reproducibility and reuse in Dataverse

Introduction

- ▶ "Reproducibility (computational) is obtaining consistent results using the *same* input data, computational steps, methods and code"
- ▶ "Replicability is obtaining consistent results across studies aimed at answering the *same scientific questions*, each of which has obtained its own data"

~ *National Academies of Sciences, Engineering, and Medicine. 2019.*
<https://doi.org/10.17226/25303>

Introduction

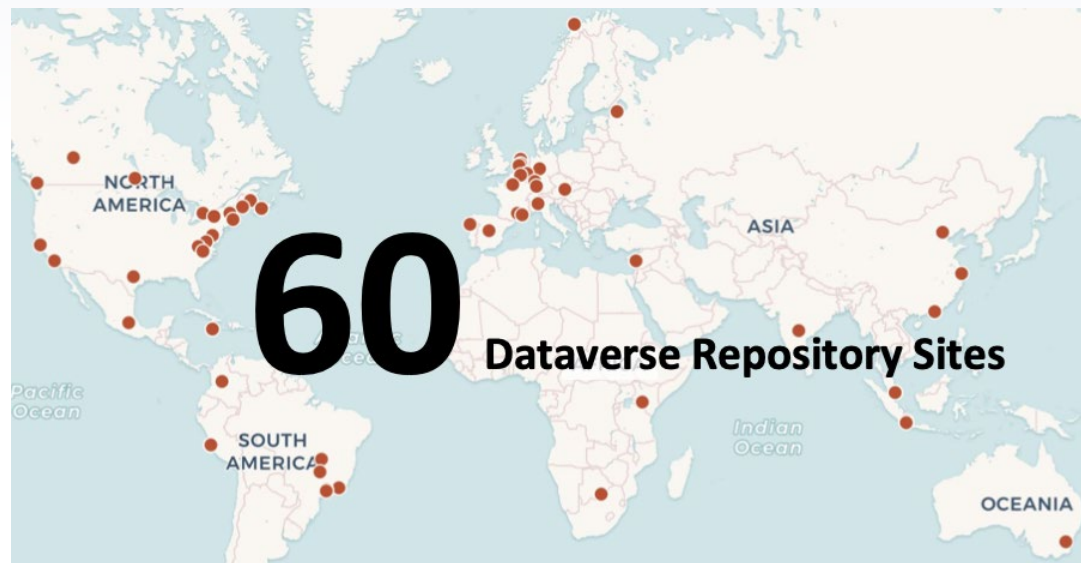
- ▶ Enabling research reproducibility and reuse in practice:
 - ▶ Researchers collect, create, process, analyze and interpret data
 - ▶ They publish their findings through journal publication
 - ▶ They share their data and code (when possible) typically through data repositories
 - ▶ Researchers often face numerous degrees of freedom and lack of guidance when sharing data, which later hinder reproducibility and reuse



Figure credit: NTU Libraries

Introduction

- ▶ Dataverse is a free and open-source software platform to archive, share, and cite research data
- ▶ 60 institutions around the globe run Dataverse instances as their data repository



Introduction

The screenshot shows the top of the Harvard Dataverse website. On the left is the Harvard Dataverse logo. On the right are navigation links: "Add Data", "Search", and "About". Below the navigation is a large red banner with the text "POLITICAL ANALYSIS" in white serif font. Underneath the banner, it says "Political Analysis Dataverse (Cambridge University Press)".

Harvard Dataverse > Political Analysis Dataverse

Political Analysis is the official journal of the Society for Political Methodology. We publish articles that provide original and significant methodology, including both quantitative and qualitative methodological approaches.


Search this dataverse... [Advanced Search](#)

- [Dataverses \(0\)](#)
- [Datasets \(421\)](#)
- [Files \(5,320\)](#)

Publication Year
2010 (102)
2018 (43)
2019 (39)

1 to 10 of 421 Results

Replication Data for: Generalized full matching
Jun 23, 2020

 Sävje, Fredrik; Higgins, Michael; Sekhon, Jasjeet, 2020, "Replication Data for: <https://doi.org/10.7910/DVN/1YIX0D>, Harvard Dataverse, V1

Replication code for simulation and application presented in the paper.

Introduction

HARVARD
Dataverse

Add Data ▾ Search ▾ About

POLITICAL ANALYSIS

Political Analysis Dataverse (Cambridge University Press)

Harvard Dataverse > Political Analysis Dataverse

Political Analysis is the official journal of the Society for Political Methodology. We publish articles that provide original and significant methodology, including both quantitative and qualitative methodological approaches.

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HARVARD
Dataverse

Add Data ▾ Search ▾ About User Guide Support

AJPS AMERICAN JOURNAL of POLITICAL SCIENCE

American Journal of Political Science (AJPS) Dataverse (Midwest Political Science Association) ajps.org

Harvard Dataverse > American Journal of Political Science (AJPS) Dataverse

The *American Journal of Political Science* is committed to significant advances in knowledge and understanding of citizenship, politics, and to the public value of political science research. To find out more about our data integrity policies, please visit our [web](#).

Search this dataverse... [Advanced Search](#)

[Dataverses \(0\)](#)

[Datasets \(451\)](#)

[Files \(7,708\)](#)

Publication Year

2019 (72)

2014 (67)

2013 (64)

1 to 10 of 451 Results

Replication Data for: Do Politicians Discriminate Against Internal Migrants? Evidence from Field Experiments in India

Jun 23, 2020



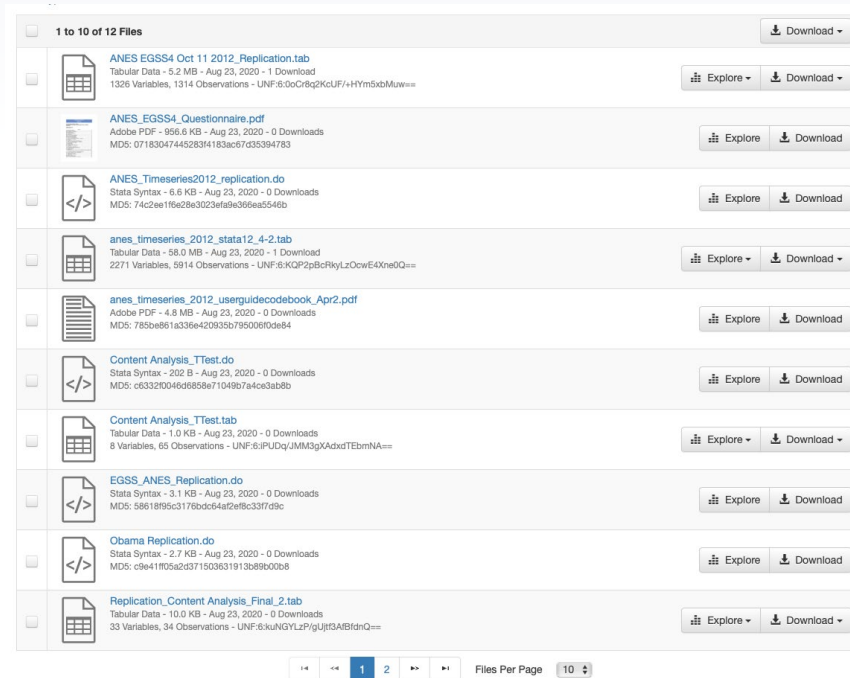
Gaikwad, Nikhar; Nellis, Gareth, 2020, "Replication Data for: Do Politicians Discriminate Migrants? Evidence from Nationwide Field Experiments in India", <https://doi.org/10.7910/DVN/1YIX0D>, Harvard Dataverse, V1, UNF:6:2o5/ifuGeg5olyLtCvndsw== [fileUNF]

Quality of shared research data & code

- ▶ Data quality is determined by its **fitness-for-use** for a given community. Data accuracy, precision, consistency, and completeness are valued across all user communities.
- ▶ Before data is published and disseminated, there is a **high potential** in developing its documentation that can improve its fitness for future use.
- ▶ After data is deposited, measuring reuse is one way to understand researchers' perceived quality of data products.
 - ▶ For example, Harvard Dataverse measures dataset view, downloads, and citations.

Computational metrics: research code completeness

- ▶ Necessary component for reproducibility:
 - ▶ Input data
 - ▶ Research code
 - ▶ Code dependencies (libraries, system dependencies, etc.)
 - ▶ Research workflow (i.e., a sequence of analysis steps)
 - ▶ Other (computational infrastructure, OS, contextual information etc.)



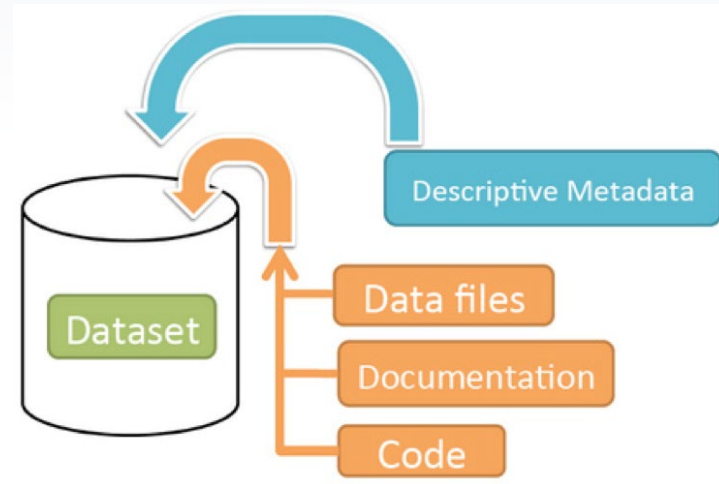
The screenshot displays a file explorer interface with a list of 12 files. The files are organized into a table with columns for file type, name, details, and actions. The files include:

File Type	File Name	Details	Actions
Table	ANES EGSS4 Oct 11 2012_Replication.tab	Tabular Data - 5.2 MB - Aug 23, 2020 - 1 Download 1328 Variables, 1314 Observations - UNF:6:0ocBq2KUF/+HYm5xbMw==	Explore, Download
PDF	ANES_EGSS4_Questionnaire.pdf	Adobe PDF - 956.6 KB - Aug 23, 2020 - 0 Downloads MD5: 07183047445283f4183ac67d35394783	Explore, Download
Code	ANES_Timeseries2012_replication.do	Stata Syntax - 6.6 KB - Aug 23, 2020 - 0 Downloads MD5: 74c2ee1f6e28e3023efa9e366ea546b	Explore, Download
Table	anes_timeseries_2012_stata12_4-2.tab	Tabular Data - 58.0 MB - Aug 23, 2020 - 1 Download 2271 Variables, 5914 Observations - UNF:6:KQP2pBcRkylzCocE4kne0Q==	Explore, Download
PDF	anes_timeseries_2012_userguidecodebook_Apr2.pdf	Adobe PDF - 4.8 MB - Aug 23, 2020 - 0 Downloads MD5: 7856be891a336e420935b795006f0de84	Explore, Download
Code	Content Analysis_TTest.do	Stata Syntax - 202 B - Aug 23, 2020 - 0 Downloads MD5: c5322f0046d8559e71049b7a4ce3ab2b	Explore, Download
Table	Content Analysis_TTest.tab	Tabular Data - 1.0 KB - Aug 23, 2020 - 0 Downloads 8 Variables, 65 Observations - UNF:6:JPUDqJMM3gXAdxdTEbrNA==	Explore, Download
Code	EGSS_ANES_Replication.do	Stata Syntax - 3.1 KB - Aug 23, 2020 - 0 Downloads MD5: 58618f95c3176bdc54a2ef8c337d9c	Explore, Download
Code	Obama_Replication.do	Stata Syntax - 2.7 KB - Aug 23, 2020 - 0 Downloads MD5: c9e41f05a2d371503631913b8990008	Explore, Download
Table	Replication_Content Analysis_Final_2.tab	Tabular Data - 10.0 KB - Aug 23, 2020 - 0 Downloads 33 Variables, 34 Observations - UNF:6:kUNGYLzPjgUjR3A8fIdnQ==	Explore, Download

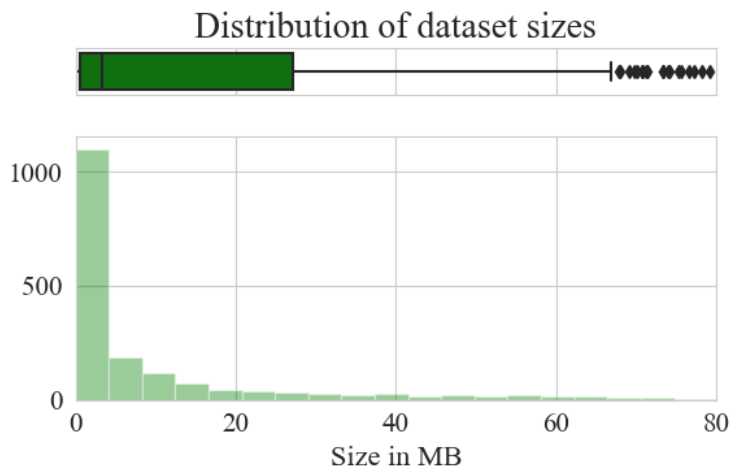
At the bottom of the interface, there is a navigation bar showing page 1 of 2, and a 'Files Per Page' dropdown set to 10.

Code execution experiments from Dataverse

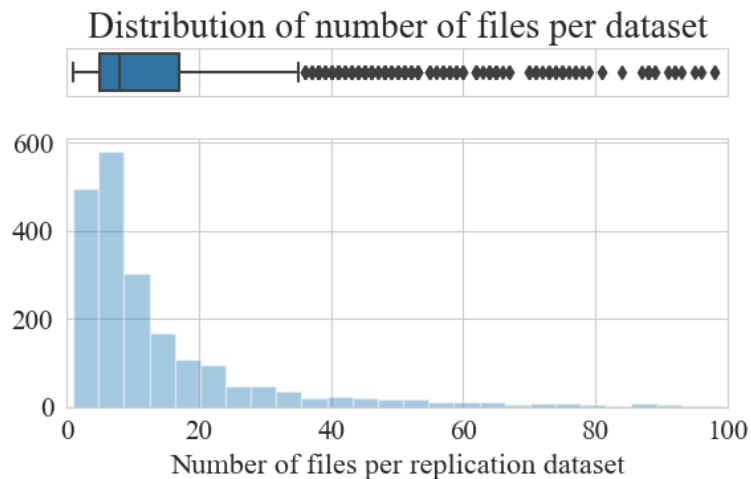
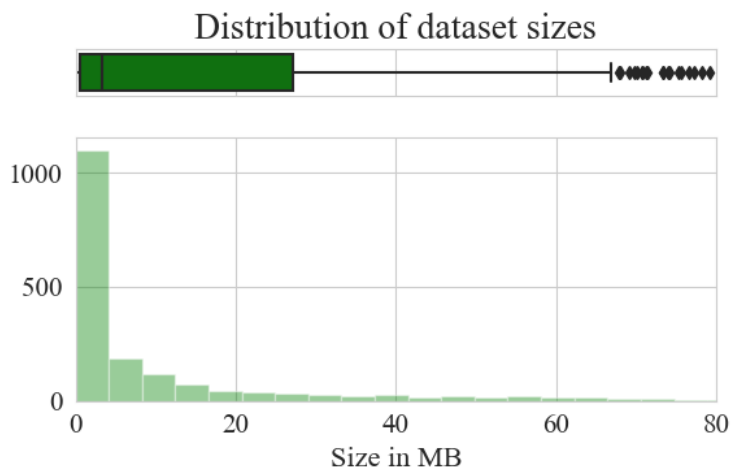
- ▶ The experiment is implemented on **AWS Batch**
- ▶ A replication dataset contains: R (or Python) code, data and documentation
- ▶ Allocated time to run each R file is 1 hour (we also ran experiments with 10 minutes per R file)
- ▶ We studied over 2091 datasets, containing over 8178 R files.



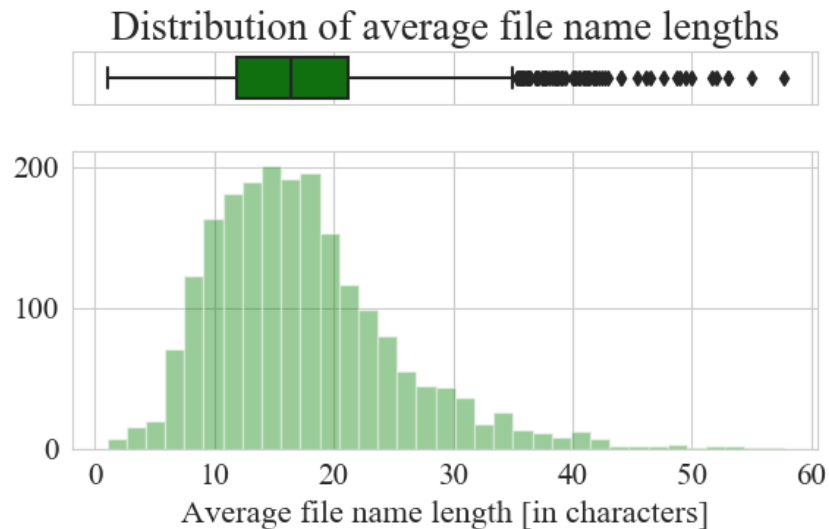
How do datasets with R code look like?



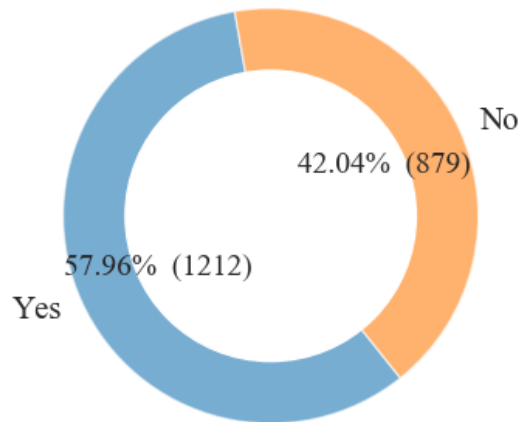
How do datasets with R code look like?



How do datasets with R code look like?



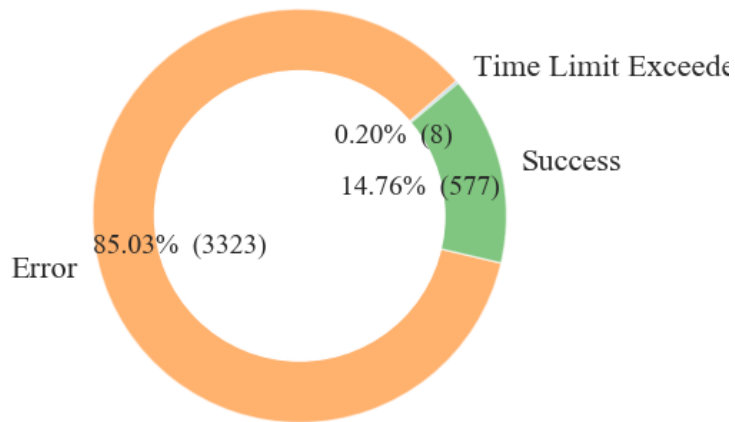
Replication package contains documentation (readme or instructions)?



Execution of R code

Without code cleaning:

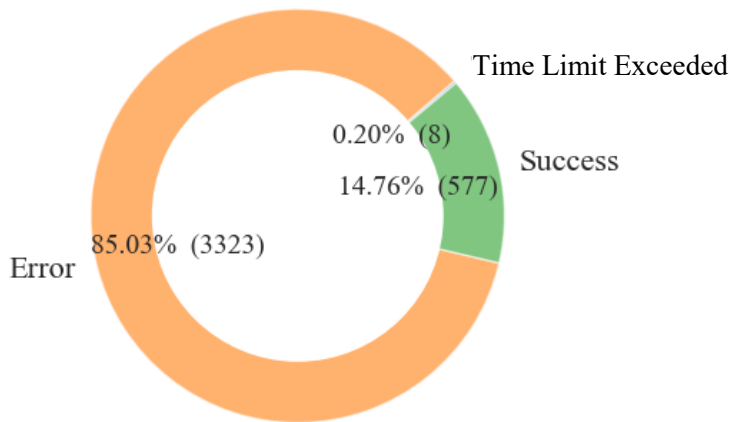
Re-execution rate with R3.6 and no code cleaning



Execution of R code

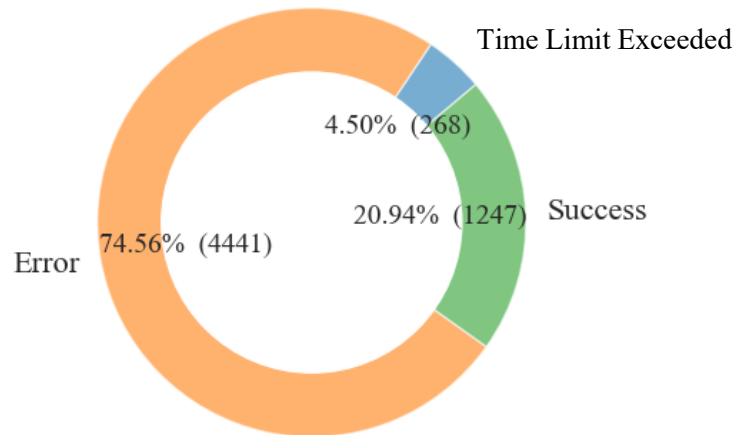
Without code cleaning:

Re-execution rate with R3.6 and no code cleaning



With code cleaning:

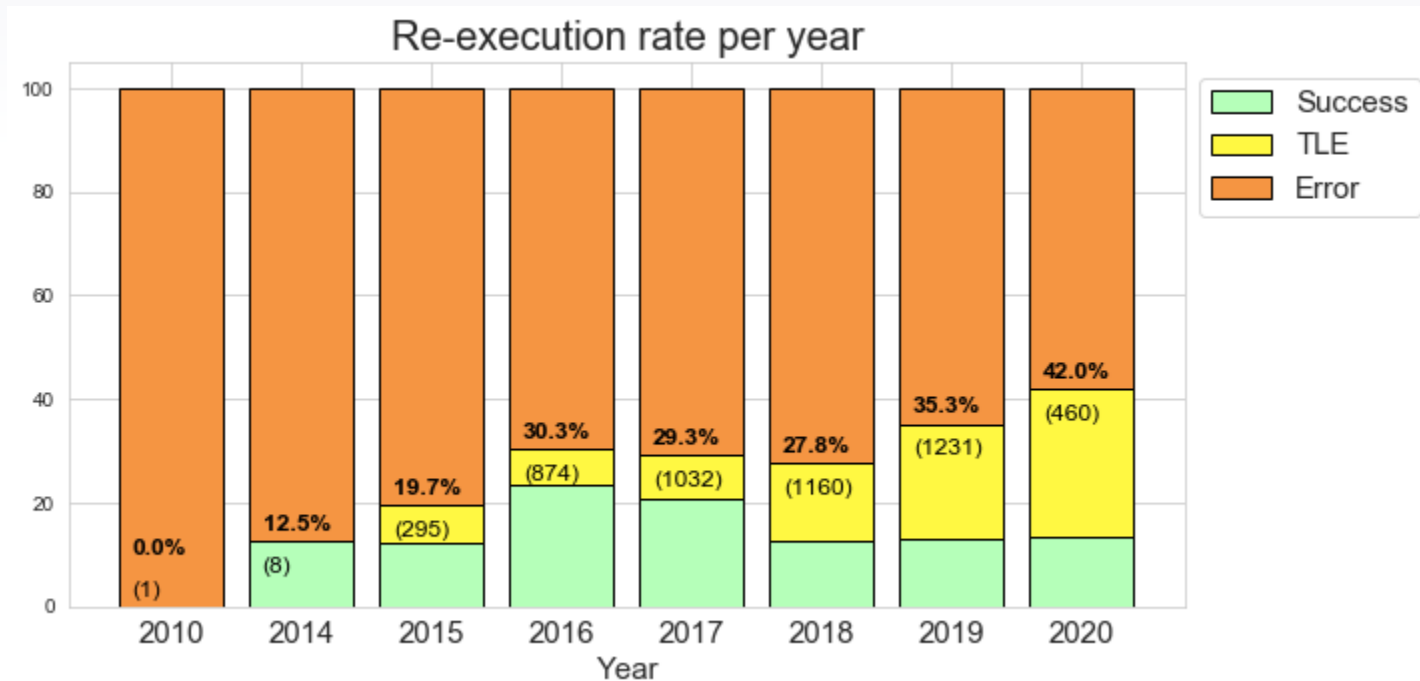
Re-execution rate with R3.6 & code cleaning



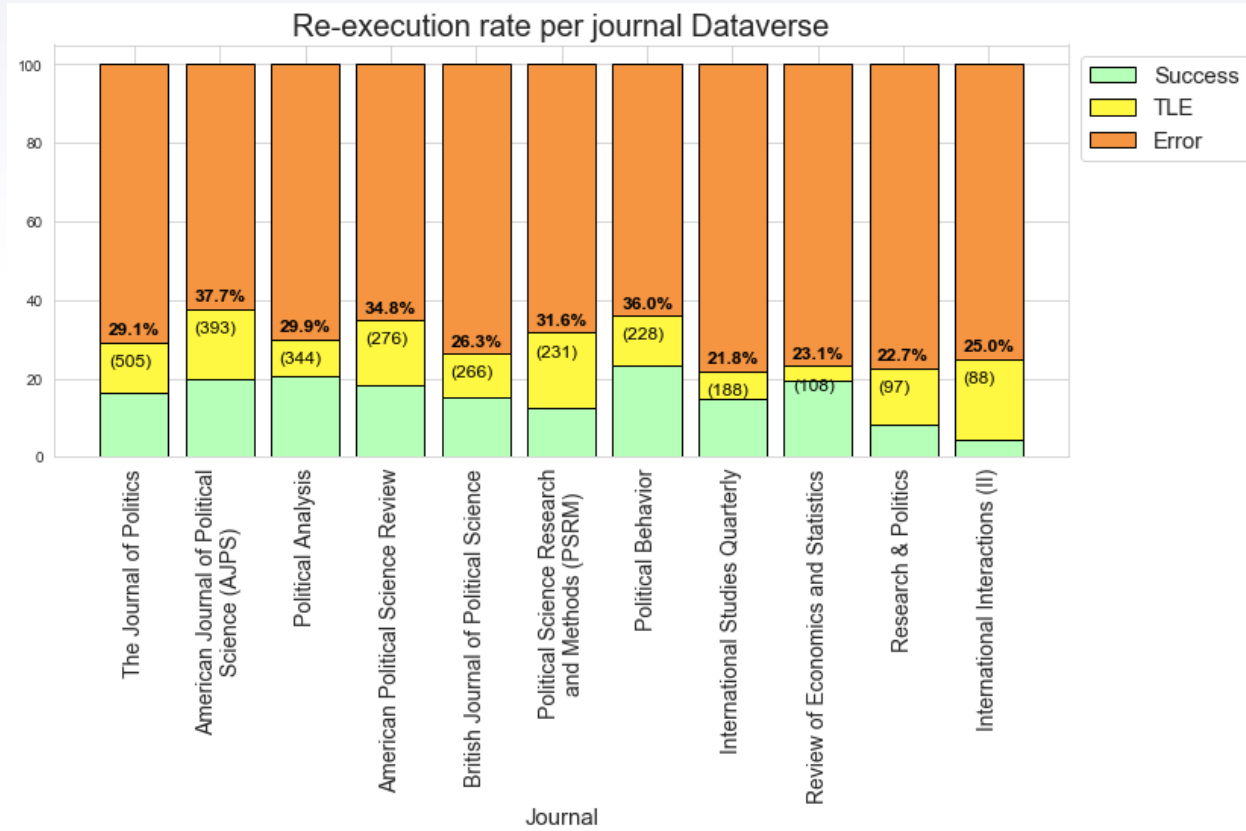
Execution of R code: errors

	Without code cleaning:	With code cleaning:
library	60%	25%
setwd	12%	0%
TLE	1%	15%
file	10%	10%
other	17%	50%

Execution rate of R 3.4 (with code cleaning) files per year of publishing



Execution rate per Dataverse journal

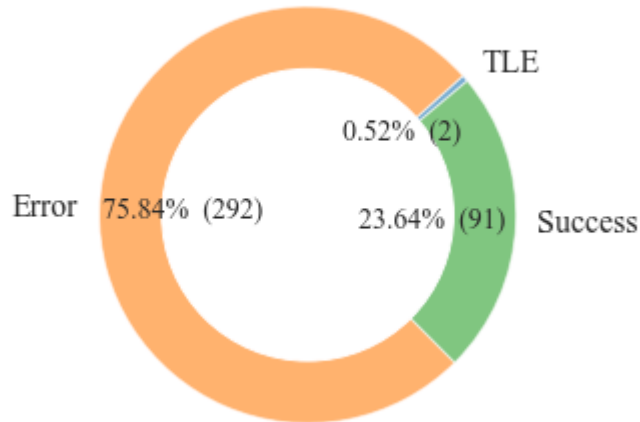


▶ Next steps

- ▶ We are analyzing re- execution rate for 3 different versions of R (3.2, 3.6 and 4.0)
 - ▶ With varied allocated time for execution (up to 1h per file)
 - ▶ Manuscript in preparation
- ▶ Also we want to prevent common execution mistakes before depositing code in Dataverse, possibly with an automatic CI (continuous integration)

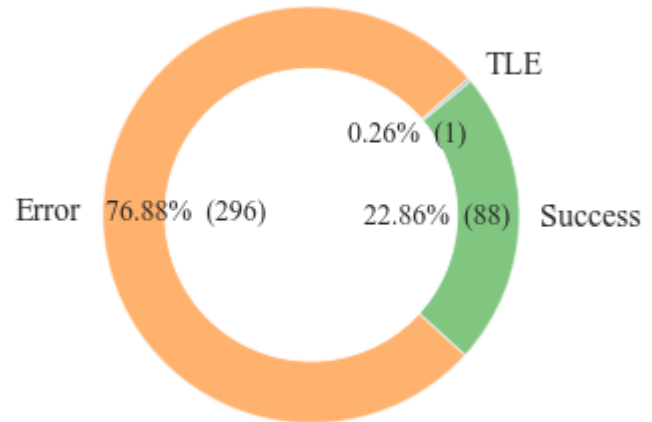
Execution of Python code with code cleaning

Re-execution rate of Python files using Python 2.7



Errors: ImportError, SyntaxError

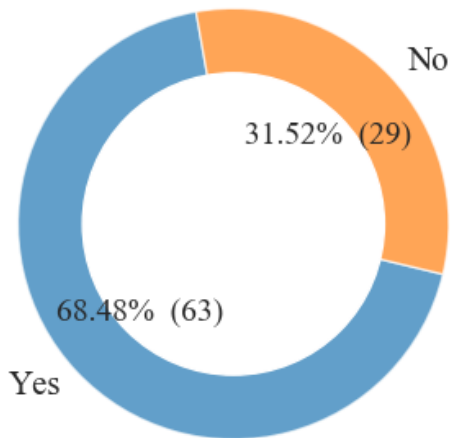
Re-execution rate of Python files using Python 3.5



TLE = time limit exceeded

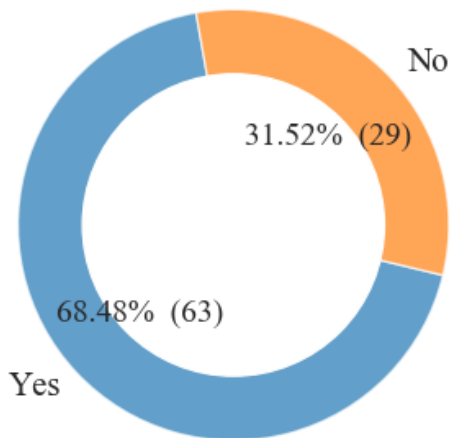
▶ Datasets with Python code

Packages contain documentation
(readme, codebook or instructions file)?



Datasets with Python code

Packages contain documentation
(readme, codebook or instructions file)?



File	Count (out of 92)
environment.yml	0
requirements.txt	6
Dockerfile	0

▶ Enabling reproducibility and painless reuse

- ▶ Container technology (or encapsulation) provides a way to virtualize an OS in a lightweight way and capture data, software and its dependencies
 - ▶ It is often used on the cloud
- ▶ Containers are becoming popular for preserving research data & code, as they can facilitate research reproducibility and reuse.
 - ▶ They are one of the best solutions to enable reproducibility
- ▶ There are different types of containers and they can describe research processes in a variety of computing infrastructures

Use of containers in research

- ▶ Many new tools encapsulate research data and code in a container “behind the scenes”, which capture computational environment that can be shared, reproduced and reused

- ▶ Examples:

- ▶ Code Ocean
- ▶ Whole Tale
- ▶ Renku
- ▶ ReProZip
- ▶ Stencila
- ▶ ...



CODE OCEAN



Stencila

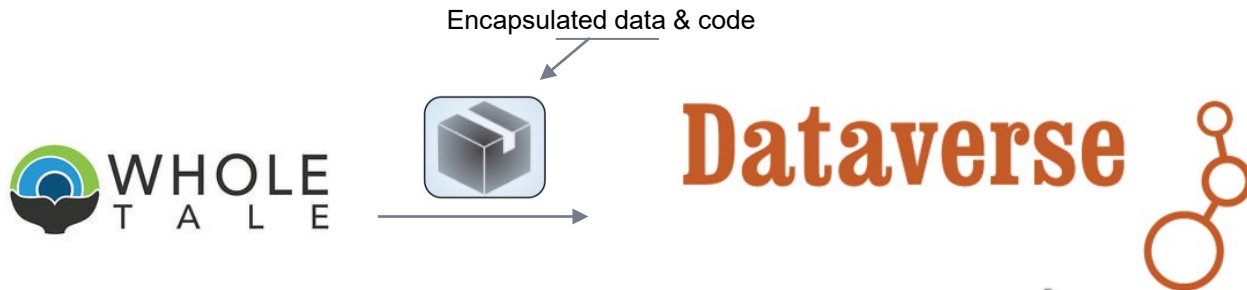


▶ Reproducibility platforms vs. data repositories

- ▶ Reproducibility platforms support
 - ▶ Research portability, reproducibility and reuse
 - ▶ However research data and code are not normally findable in data search engines, and there is no commitment for long-term preservation
- ▶ Data repositories often support
 - ▶ Findability through the use of standard metadata
 - ▶ Standardized persistent citation
 - ▶ Long-term accessibility of data and code
 - ▶ Troubles with enabling reproducibility

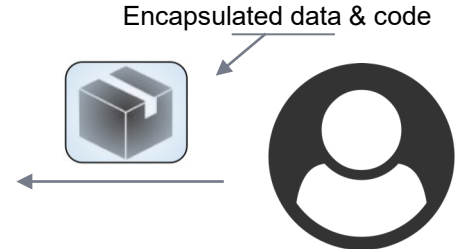
▶ Dataverse approach

- ▶ Dataverse data repository aims to improve reproducibility of deposited research data & code by developing new functionality to capture containers
- ▶ Ongoing integration with reproducibility platforms Code Ocean, Whole Tale, Renku and Binder, that would allow encapsulated data & code to be exported (deposited) in Dataverse



▶ Dataverse approach

- ▶ Dataverse data repository aims to improve reproducibility of deposited research data & code by developing new functionality to capture containers
- ▶ Ongoing integration with reproducibility platforms Code Ocean, Whole Tale, Renku and Binder, that would allow encapsulated data & code to be exported (deposited) in Dataverse
- ▶ Any user should be able to preserve their container based artifacts regardless of their use of the reproducibility platforms.



▶ Outlook

- ▶ How to enable painless reuse of shared research data and code?
 - ▶ Avoiding common mistakes
 - ▶ Including virtual environments in shared code
 - ▶ Better metadata to capture ever-more complicated computing infrastructures

Talk #2

**Enabling Painless Reuse of Shared Research Data and Code for
HPC-driven computational reproducibility of research**

Qian Zhang



Agenda of this talk

- ▶ What is HPC- driven:
 - ▶ computational research?
 - ▶ computational reproducibility?
 - ▶ Why is it important?
- ▶ HPC- driven computational reproducibility: A case study
 - ▶ Challenges & Opportunities
- ▶ Painless HPC- driven research reproducibility and reuse
- ▶ Outlook

What is the HPC-driven computational research?

- ▶ *Not theoretical* : deductive mathematics
- ▶ *Not experimental* : empirical statistical analysis
- ▶ **Computational**: large- scale simulations / data- intensive computational science
 - ▶ **Big data**
 - ▶ High performance computing (**HPC**): Computational power, application of supercomputers, parallel computing
 - ▶ **Software & code** is persuasive in modern digital research landscape

▶ What is the HPC-driven computational reproducibility?

- ▶ ⇒ Same research results
 - ▶ Different team
 - ▶ Same experimental setup
 - ▶ Same artifacts
 - ▶ Same measurement procedure
 - ▶ *Same/different* operating conditions

Why does the HPC -driven computational reproducibility?

- ▶ “Reproducibility is a Process, not an Achievement” (Lin & Zhang, 2020)
- ▶ To root out the error
- ▶ Help to “frame the agenda of digital curation” ([Stodden, V., 2011. Reproducible Research: A Digital Curation Agenda](#))
- ▶ Central to scientific communication

HPC-driven computational reproducibility: A case study in Astrophysics

- ▶ We attempted to reproduce a study:
 - ▶ [IllinoisGRMHD: an open - source, user- friendly GRMHD code for dynamical spacetimes](#) (Etienne et al., 2015)

Class. Quantum Grav. 32 (2015) 175009 (33pp) doi:10.1088/0264-9381/32/17/175009


IllinoisGRMHD: an open-source, user-friendly GRMHD code for dynamical spacetimes

Zachariah B Etienne^{1,7}, Vasileios Paschalidis², Roland Haas³, Philipp Mösta⁴ and Stuart L Shapiro^{5,6}

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² Department of Physics, Princeton University, Princeton, NJ 08544, USA
³ Max-Planck-Institut für Gravitationsphysik, Albert-Einstein-Institut, D-14476 Golm, Germany
⁴ TAPIR, Mailcode 350-17, California Institute of Technology, Pasadena, CA 91125, USA
⁵ Department of Physics, University of Illinois at Urbana-Champaign, Urbana, IL 61801, USA
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Received 28 January 2015, revised 26 May 2015
Accepted for publication 23 June 2015
Published 10 August 2015



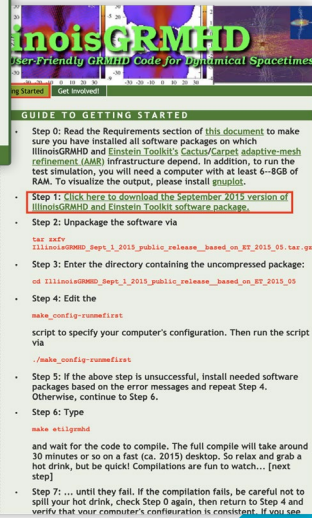
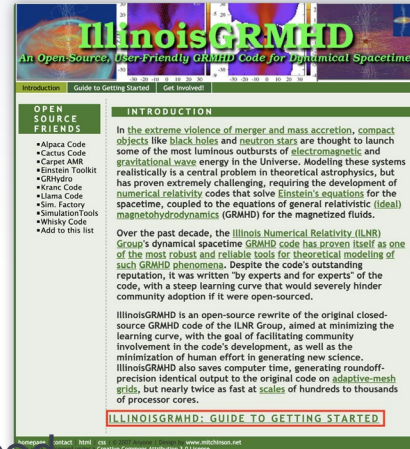
Abstract
In the extreme violence of merger and mass accretion, compact objects like black holes and neutron stars are thought to launch some of the most luminous outbursts of electromagnetic and gravitational wave energy in the Universe. Modeling these systems realistically is a central problem in theoretical astrophysics, but has proven extremely challenging, requiring the development of numerical relativity codes that solve Einstein's equations for the spacetime, coupled to the equations of general relativistic (ideal) magnetohydrodynamics (GRMHD) for the magnetized fluids. Over the past decade, the Illinois numerical relativity (ILNR) group's dynamical spacetime GRMHD code has proven itself as a robust and reliable tool for theoretical modeling of such GRMHD phenomena. However, the code was written 'by experts and for experts' of the code, with a steep learning curve that would severely hinder community adoption if it were open-sourced. Here we present IllinoisGRMHD, which is an open-source, highly extensible rewrite of the original closed-source

⁷ Author to whom any correspondence should be addressed.

0264-9381/15/175009+33\$33.00 © 2015 IOP Publishing Ltd Printed in the UK 1

HPC-driven reproducibility setup

- ▶ Link to the code: [IllinoisGRMHD](http://math.wvu.edu/~zetienne/ILGRMHD/)
 - ▶ “Instructions for downloading, compiling, and using IllinoisGRMHD may be found here: <http://math.wvu.edu/~zetienne/ILGRMHD/>”
- ▶ HPC resources: XSEDE
 - ▶ Stampede2's Skylake (SKX) @Texas Advanced Computing Center (TACC) & Comet @San Diego Supercomputer Center (SDSC)
- ▶ Download ⇒ compile ⇒ customize the parameter file ⇒ execute ⇒ post-analysis



Preliminary results of the reproducibility case study

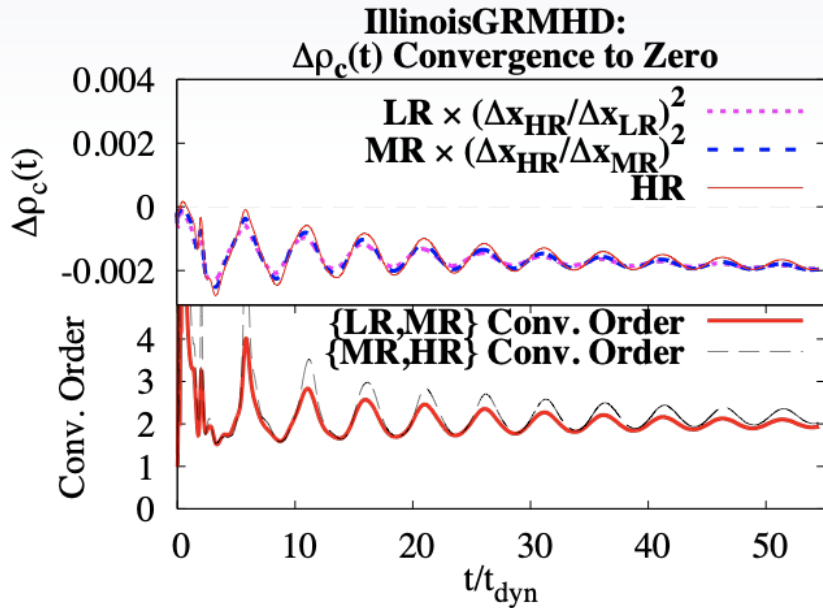
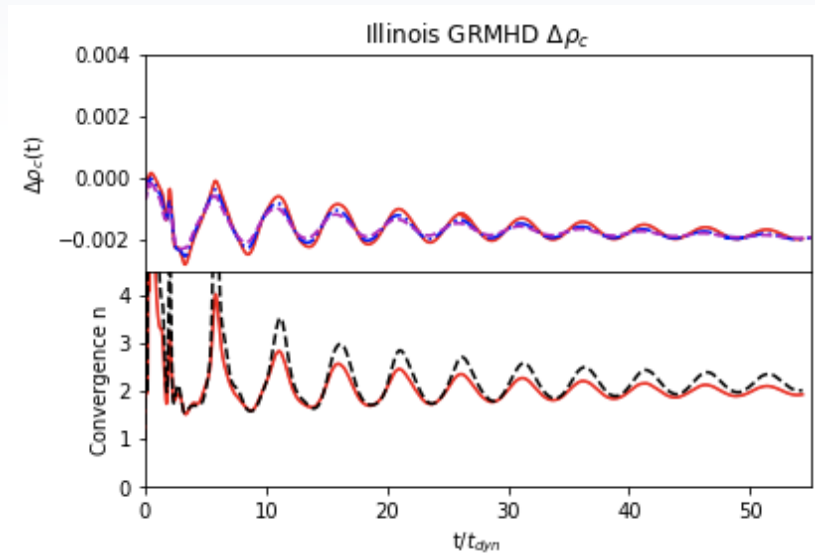


Figure in the paper



Reproducibility experiment result

Observations & lessons learned


- ▶ Insufficient data/code
 - ▶ Lack of documentation
 - ▶ Computational model compilation/execution errors
 - ▶ Unstoppable hardware upgrade
 - ▶ Link rot, software incompatibilities
 - ▶ Missing key parameter (file)

Observations & lessons learned (cont.)


- ▶ Installation issues
 - ▶ If installed on local laptops
 - ▶ Have to be clean slate
 - ▶ If installed on local institutional cluster platform
 - ▶ ⇒ Setup issues (next slide)
- ▶ ⇒ Provide instruction on installation
 - ▶ Documentation
 - ▶ Checklist
- ▶ Issues when submitting jobs (shell script) to queuing system
 - ▶ ⇒ Provide Human-readable info.


Next step (in progress)

- ▶ Develop *generic* setup template to configure a new machine
 - ▶ Machine definition
 - ▶ Option list: Compilers, Compilation and linking flags, Debugging, Optimisation, Profiling, OpenMP, Warnings, External Libraries (HDF5, MPI, Others)
 - ▶ Submission script
 - ▶ Run script
- ▶ Provide template & examples
 - ▶ XSEDE
 - ▶ Compute Canada
 - ▶ Perimeter Institute for Theoretical Physics
 - ▶ AWS





Why are HPC-
driven research
reproducibility
and reuse so
difficult?






Why are HPC-driven research reproducibility and reuse so difficult?

- ▶ Model
 - ▶ Model/code availability/ease of use
 - ▶ Platform/system availability
 - ▶ Where/how was this run?
 - ▶ Model re-usability (setup, etc.)
 - ▶ Human efforts
 - ▶ Data
 - ▶ Simulation inputs
 - ▶ Output usability
- 



Why are HPC-driven research reproducibility and reuse so difficult (cont.)?

- ▶ Accessibility
 - ▶ Conformance to open or established standards
 - ▶ Archival accessibility
 - ▶ Longevity of the technology
 - ▶ Cost
 - ▶ Computational cost
 - ▶ Storage cost
- 

Opportunities of HPC -driven research reproducibility and reuse

- ▶ Ensure **transparency, reproducibility** and **reusability** of research results
- ▶ Provide effective **communication** of research outputs (publication, data and code) and advanced research computing resources
- ▶ Promote enhanced **access** to research outputs and resources
 - ▶ Policies and strategies
 - ▶ Network and collaborative initiatives
 - ▶ Research infrastructures
 - ▶ Research software as a primary output of research

Opportunities of HPC -driven research reproducibility and reuse (cont.)

- ▶ Develop standards for reproducibility **badges**
 - ▶ [NISO's Draft Recommended Practice for Reproducibility Badging and Definitions](#)
 - ▶ ACM [Artifact Review and Badging Version 1.1 August 24, 2020](#)
- ▶ **Tools & platforms** for supporting computational science
 - ▶ Dissemination/reproducibility platforms ([code ocean](#), [Whole Tale](#))
 - ▶ Workflow tracking ([Kurator](#))
 - ▶ Better documentation ([Jupyter notebook](#))
- ▶ Practices & guidelines
- ▶ Training opportunities



<https://www.acm.org/binaries/content/gallery/acm/publications/large-replication-badges/all-badges.png>

Painless HPC-driven research reproducibility and reuse

- ▶ Accessioning, stabilizing, evaluating & describing digital objects
- ▶ Documenting and making documentation available
- ▶ Sharing resources
 - ▶ Data (& documentation) collected & used in analysis
 - ▶ Data output result(s) (& documentation) produced by analysis
 - ▶ Software (& documentation) in source code & human - readable formats
 - ▶ Software/hardware dependencies (technical details, system/software environments)
 - ▶ Computational research workflow and provenance
 - ▶ Software program(s) dependencies for replicating published results
 - ▶ Journal article
- ▶ Providing access

▶ Outlook

- ▶ Extensive re- use of data and code will become the norm
- ▶ Researcher competitiveness will be re-defined with multi-facet metrics
- ▶ Cultural change
 - ▶ Policy from publishers and funders
 - ▶ Author

Takeaways

- ▶ “Reproducibility is a Process, not an Achievement”
- ▶ Research community’s recommendations on good practices
- ▶ Greater clarity and guidance on dissemination of computational claims
- ▶ Code dissemination in data repositories:
 - ▶ Avoiding common mistakes by testing code in a clean environment
 - ▶ Including virtual environments in shared code
 - ▶ Better metadata to capture ever-more complicated computing infrastructures

Q & A

Questions for the audience

Questions for the audience

- ▶ How were your experiences with research reproducibility and reuse? What difficulties have you encountered?
- ▶ How do you disseminate data and code at your institution (or research field)? How do you document them?



▶ Thank you
for your
attention!

