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The Next Frontier: Making Research More Reproducible

David E. Rosenberg Utah State University

Yves Fillion Queen's University

Rebecca L. Teasley University of Minnesota - Duluth

Samuel Sandoval-Solis University of California, Davis

Jory S. Hecht United States Geological Survey

Jakobus E. van Zyl University of Auckland

See next page for additional authors

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| Authors David E. Rosenberg, Yves Fillion, Rebecca L. Teasley, Samuel Sandoval-Solis, Jory S. Hecht, Jakobus van Zyl, George F. McMahon, Jeffery S. Horsburgh, Joseph R. Kasprzyk, and David G. Tarboton | | | | | |
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The Next Frontier: Making Research More Reproducible Editorial submitted to *Journal of Water Resources Planning and Management*

November 27, 2019

David E. Rosenberg, Yves Filion, Rebecca Teasley, Samuel Sandoval-Solis, Jory S. Hecht, Jakobus E. van Zyl, George F. McMahon, Jeffery S. Horsburgh, Joseph R. Kasprzyk, David G. Tarboton

David E. Rosenberg, Associate Professor, Department of Civil and Environmental Engineering and Utah Water Research Laboratory, 8200 Old Main Hill, Utah State University, Logan, UT 84322-8200, ORCID 0000-0003-2163-2907, A.M. ASCE, david.rosenberg@usu.edu

Yves Filion, Professor, PhD, PEng, ing., Department of Civil Engineering, Queen's University, 58 University Avenue, Kingston, Ontario, Canada, K7K0B9. Email: yves.filion@civil.queensu.ca.

Rebecca L. Teasley, Associate Professor, Department of Civil Engineering, University of Minnesota Duluth, 1405 University Drive, Duluth, Minnesota 55812, A.M. ASCE, rteasley@d.umn.edu

Samuel Sandoval-Solis, Associate Professor, Department of Land, Air, and Water Resources, University of California, Davis, 1 Shields Ave, Davis, California, 95616. ORCID: 0000-0003-0329-3243 Email: samsandoval@ucdavis.edu

Jory S. Hecht, Hydrologist, United States Geological Survey, 12201 Sunrise Dr., Reston, VA, 20192, ORCID 0000-0002-9485-3332, jhecht@usgs.gov

Jakobus E. van Zyl, Watercare Chair in Infrastructure, Department of Civil and Environmental Engineering, University of Auckland, 20 Symonds Street, Auckland, 1010, New Zealand, MASCE. Email: k.vanzyl@auckland.ac.nz

George F. McMahon, Ph.D., PE, D.WRE, PH, BCEE, ENV SP, Vice President, National Expert, Water Management, Arcadis, 2839 Paces Ferry Road, Suite 900, Atlanta GA 30339. Email:george.mcmahon@arcadis.com

Dr. Jeffery S. Horsburgh, Associate Professor, Department of Civil and Environmental Engineering and Utah Water Research Laboratory, Utah State University, 8200 Old Main Hill, Logan, UT 84322-8200, ORCID: https://orcid.org/0000-0002-0768-3196, jeff.horsburgh@usu.edu

Joseph R. Kasprzyk, PhD, AMASCE. Assistant Professor, Department of Civil, Environmental, and Architectural Engineering, University of Colorado Boulder. UCB 607, Boulder, CO 80309. ORCID: https://orcid.org/0000-0002-6344-6478

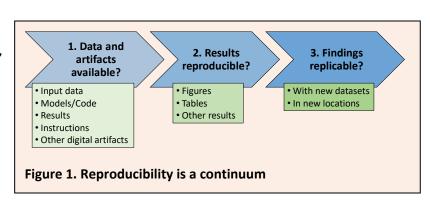
David G. Tarboton, Sc.D., PE, M.ASCE, Professor, Director Utah Water Research Laboratory, Department of Civil and Environmental Engineering, Utah State University, 8200 Old Main Hill, Logan, UT 84322-8200, ORCID: https://orcid.org/0000-0002-1998-3479, david.tarboton@usu.edu

The Next Frontier: Making Research More Reproducible

Science and engineering rest on the concept of reproducibility. An important question for any study is: are the results reproducible? Can the results be recreated independently by other researchers or professionals? Research results need to be independently reproduced and validated before they are accepted as fact or theory. Across numerous fields like psychology, computer systems, and water resources there are problems to reproduce research results (Aarts et al. 2015; Collberg et al. 2014; Hutton et al. 2016; Stagge et al. 2019; Stodden et al. 2018). This editorial examines the challenges to reproduce research results and suggests community practices to overcome these challenges. Coordination is needed among the authors, journals, funders and institutions that produce, publish, and report research. Making research more reproducible will allow researchers, professionals, and students to more quickly understand and apply research in follow-on efforts and advance the field.

Real and perceived challenges to reproduce research results include: 1) The skill and effort required for authors to prepare, organize and share their data, models, code, and directions to reproduce article figures, tables and other results; 2) Some authors fear that other researchers will scoop them on follow-up studies, they cannot support their materials after publication, or materials will never be used; 3) Authors cannot share proprietary or sensitive materials or materials containing protected intellectual property; 4) Some workflows use stochastic, high performance computing, big data, or methods with long run times that are too big to share or reproduce bit for bit; 5) It takes time and expertise to reproduce others' results, and users may encounter unclear directions or missing materials; 6) Funders and universities value publication of novel, peer-reviewed journal articles rather than datasets, documentation, or reproducing others' efforts; and 7) Promoting and rewarding reproducibility may unintentionally push researchers towards simpler, easier to reproduce methods, rather than studies that are more complex and far reaching, but harder to reproduce.

Recent guidance by the
National Academy of Sciences,
Engineering, and Medicine
(NAS 2019), Institute of
Education Sciences, U.S.
Department of Education, and
U.S. National Science
Foundation (IES et al. 2018)
describe reproducibility as a
continuum (Figure 1). The



goal is to push work up the continuum to (a) make data, models, code, directions, and other digital artifacts used in the research available for others to reuse (availability). Then, (b) use shared artifacts to exactly reproduce published results (reproducibility, sometimes called bit or computational reproducibility). Finally, (c) use artifacts with existing and new datasets to replicate findings across sites or domains (replicability). For example, the *Journal of Water Resources*, *Planning and Management* policy to specify the availability of data, models, and

code (Rosenberg and Watkins 2018) primarily targets availability in the reproducibility continuum. This policy has subsequently been adopted by nearly all of the 30+ journals published by the American Society of Civil Engineers.

We must also emphasize benefits to making materials available and organizing materials so others can reproduce the results:

- Increasing impact by increasing the number of persons who can access, use, and extend work,
- Improving trust in the outcomes and findings from work,
- Benchmarking and comparing new proposed methods and models with existing methods,
- Organizing research materials in perpetuity for oneself and future users, including future students who will later extend prior research,
- Reducing and streamlining effort authors spend to respond to individual user requests for article materials, and
- Transforming the experience of reading science articles into opportunities to learn by doing. Engaging with article data, models, code, and directions lets users more fully comprehend, experiment, extend, remember, and eventually cite materials.

Each benefit also provides professionals better access to published research and can help narrow the gap between research and practice.

We should also look for ideas in the very small number of journals—such as *Biostatistics*, *ACM Transactions on Mathematical Software*, *Journal of the American Statistical Association*, and *American Journal of Political Science*—that already have reproducibility policies. Many of these journals created a new role of associate editor of reproducibility (AER). The AER has the responsibility to either reproduce manuscript results themselves or invite an external person to reproduce results. The AER can describe the value of reproducing a study and recommend how authors can make their results more reproducible. New roles of AER and reproducibility reviewers provide opportunities to engage more people in the journal peer-review process and to improve the quality of results.

Researchers and professionals use varied experimental, modeling, open-source, proprietary, deterministic, stochastic, local, cloud, and computationally intensive methods whose results may not be reproduced using today's tools. Below, we provide a checklist of recommended practices for authors, journals, funders, and institutions to push their research up the reproducibility continuum. Box 1 lists our favorite practices.

A Checklist of Practices to Improve Reproducibility **Box 1. Our Favorite Practices to Make Results** more Reproducible Build reproducibility into the project from the start 1. Build reproducibility into the project ☐ Budget time, money, local or cloud storage, from start - budget time, money, and other resources to make results storage, and tools 2. Make all materials available in a reproducible. ☐ Select tools such as version control (Git or repository 3. Ask someone to verify your results are GitHub) and containerization (e.g., Docker, reproducible Sciunit) to make reproducibility practices 4. Train students and employees in easier and less time-consuming. reproducible practices ☐ Where possible, choose open-source tools to reduce the financial and time costs for others to reproduce results. ☐ Prepare data licensing agreements or IRB protocols to allow for the future release of anonymized versions of proprietary or private data. ☐ When possible, set up repository materials to run on a cloud-based system (e.g., using a Jupyter Hub) so users can run code and reproduce results directly on the web rather than download, setup, and execute on a local machine. Choose a repository □ When possible, choose a single open repository common for your field. Example repositories for water resources work include an institutional repository, HydroShare, Harvard Dataverse, Figshare, Dryad, GitHub, etc. Choose a repository that is consistent with the content you are sharing. For example, GitHub is well suited for sharing source code, whereas HydroShare is better-suited for data and models. Choose a repository that meets funder requirements and applicable data sharing laws. □ Where possible, bundle all contents—input data, models, code, results, directions, requirements, and other materials—in a single repository rather than spread across multiple repositories. State the level of reproducibility users should expect and list requirements

□ State the level of reproducibility the user should expect.

☐ List all required hardware needed to reproduce results.

List the skills/training needed by a person to reproduce work.

☐ List which portions of the workflow can be reproduced and which cannot.

to reproduce results. Specify software that requires a license to purchase.

☐ List all required software and code library dependencies (packages and versions) needed

Make all materials available in the repository Provide all data, model(s), and code(s) for the workflow needed to reproduce the results in a publicly accessible repository. □ Provide directions to install and run code and use materials to generate study results. Use a human-readable format that will persist through time (e.g., plain, ASCII, or rich text). □ Write directions assuming people who will use the content are technically proficient in the field but not familiar with the data, models, code, software, programming language, methods, or study materials. □ Provide metadata and describe the structure of the content (e.g., folder and file structure) and supplemental materials. □ Describe all tabular data (comma separated value (csv), Excel, text, etc. files). Describe columns and units of measurement. Specify which code segments produce each figure, table, or other results in the article. Remove (or indicate) code references to local paths that are machine (user) specific. Where possible, use relative path names rather than local paths. ☐ Provide links to download all software, libraries, or platforms. Provide the input data to and results from each step that uses proprietary (licensed) software or data. Provide directions for how the software was used to generate the results. Write code to automate manual computation steps Automate manual computation steps with code and scripts to increase the likelihood that others can reproduce results and reduce their time to complete those steps. Comment each step of the code or script to make materials readable and easy to follow. Follow coding standards and conventions for the language used (e.g., indentation, commenting, declarations, statements, white space, etc.). Make proprietary, private, sensitive, computationally intensive, and stochastic data, models, and code more reproducible □ Where possible, make available the input and output data from every step of a workflow that uses proprietary software or is data intensive, requires a long run time, or cannot be rerun by other users. Provide inputs and outputs for each step so that a user who cannot access the underlying materials can still complete the workflow and reproduce overall results. For example, for an optimization study using the proprietary General Algebraic Modeling System (GAMS; Brooke et al. 1998), make the input data

□ Note the underlying random seeds for steps that include randomness (stochasticity).
 □ Make copies of proprietary data and results available in commonly-used file formats (e.g., .gdx in Figure 2 to .xlsx, CSV, etc.).

(.csv), model text file (.gms), output (.gdx and .xlsx) and post processing (.r) files

available (Figure 2).

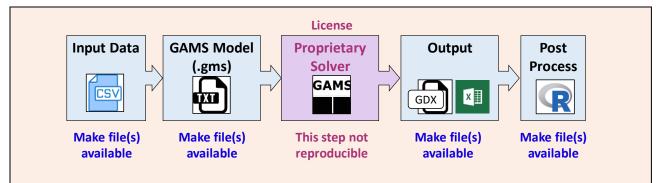


Figure 2. Make a proprietary work flow more reproducible. Example with General Algebraic Modeling System (GAMS) optimization model

- Anonymize proprietary, private, or sensitive data sets (e.g., datasets containing personally identifiable information or data protected by Institutional Review Board (IRB) requirements) so you can share.
- ☐ Indicate where and how the user can obtain copies of proprietary or private data.
- ☐ Where proprietary or big datasets cannot be shared, provide an additional example of the workflow with a non-proprietary or illustrative dataset.

Make it easy for people to find the content

- Provide a digital object identifier (DOI) encoded as a URL that links directly to your repository. Some repository hosts, such as ASCE or HydroShare, provide a DOI when publishing materials. For other hosts such as GitHub, use a service like Zenodo to create a snapshot of the content and then generate a DOI.
- In the manuscript, cite the repository directly in the text. Include full citation information, including the DOI, in the reference information.

Verify your results are reproducible

- Ask a colleague, student, or other person not affiliated with the study to reproduce study results. This person could be a new student who needs to get up to speed on the methods or someone else interested in the study or results.
- Ask this colleague, student, or other person to use a reproducibility survey tool (e.g., Stagge et al. 2019) to provide feedback on the repository, directions, and results that they reproduced.
- ☐ If the person can reproduce results, acknowledge their effort in the manuscript's "data availability" or "result reproducibility" section.
- ☐ If the person had difficulty reproduce results, make changes to the repository to address their difficulties.

Follow good examples

| | Adopt the practices of 6 articles that Stagge et al. (2019) awarded badges for full and partial reproducible results. For example, these papers: | | | |
|--------|---|--|--|--|
| | Provided all model and code in a Github (Buscombe 2017; Neuwirth 2017; Xu et al. 2017), institutional (Yu et al. 2017), or HydroShare (Horsburgh et al. 2017) repository. | | | |
| | Had an easy-to-find readme file that explained contents and gave directions to setup and run code (Buscombe 2017; Horsburgh et al. 2017; Neuwirth 2017; Xu et al. 2017). | | | |
| | Document workflows, make code reusable, and bundle code, data, and documentation (Hutton et al. 2016). | | | |
| Encour | rage journals to promote reproducible results | | | |
| | Develop policies to verify reproducible results and make these policies clear to editors, authors, and reviewers. | | | |
| | Encourage authors to self-assess the reproducibility of their work prior to submission (see Verify your results are reproducible section). | | | |
| | Assess reproducibility of submissions and provide feedback to authors. | | | |
| | Define what constitutes an article with reproducible results and recognize these articles | | | |
| | (e.g., with badges or other incentives). State the expected level of reproducibility of published articles. Track and report articles | | | |
| | with reproducible results over time. | | | |
| | Hold competitions to compare reproducible results across articles and synthesize best practices. | | | |
| | Create journal awards, such as for outstanding effort to make complex results more reproducible or outstanding effort to reproduce results. | | | |
| | Publish reproducible papers open-access free to the authors. | | | |
| Encour | rage funders to promote reproducible results | | | |
| | Determine and state the expected level of reproducibility in funder repositories. | | | |
| | Require reproducibility in requests for proposals. | | | |
| | Encourage authors to self-assess reproducibility prior to submission (see Verify your | | | |
| | results are reproducible section). Assess reproducibility of submissions and provide feedback to authors. | | | |
| | Verify work fulfills funder requirements for sharing data and results. | | | |
| | Support development of new tools to make it faster and easier for authors to make their research products more reproducible. | | | |
| | | | | |

Encourage universities, agencies, and institutions to promote reproducible results

| Train students and employees in reproducible practices (e.g., Software and Data |
|--|
| Carpentry workshops, Hydroinfomatics courses). |
| Determine and state the expected level of reproducibility in institutional repositories. |
| Require reproducible practices for theses, dissertations, and project reports. |
| Develop standards and initiatives for open data and open source code. |
| Recognize faculty, researchers, and students that reproduce and extend other's work. |

Reproducibility is a core principle of science and engineering. Making results more reproducible requires time and effort by authors, journals, funders, and institutions. The research community will benefit from tools that automate and speed those steps. We must also provide authors financial incentives and recognition to encourage them to make their work more available and results more reproducible. We look forward to including these reproducibility incentives and practices in a future reproducible results policy for the journal.

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Rosenberg wrote the first draft. The remaining authors provided feedback on subsequent drafts that Rosenberg merged into more final versions. Tanu Malik, William Farmer, Laura DeCicco, and 22 other Journal Associate Editors provided feedback that improved intermediate drafts.

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