

Understanding and Assessing Key Reasons for Computational Irreproducibility: Overlooked Social Drivers

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The Marvin Zelen Memorial Symposium

Advancing Reproducible Research: Principles, Practice, and Impact

Simmons University, Helen G. Drinan Hall

June 16, 2026

Agenda

1. Finding Consensus: Computational Reproducibility and Replication

~Work in Progress~

2. Understanding Sources of Irreproducibility:
 - **ReproReady Score**: Standards for Automated Reproducibility Assessment
 - **Human Factors**: A Structured Assessment of Influential Barriers to Computational Reproducibility
3. Conclusion



1. The Importance of Consensus

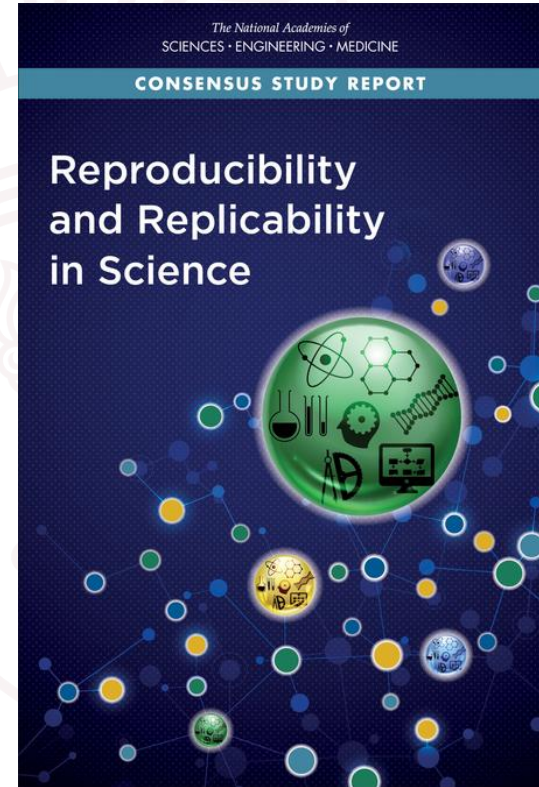
Computational Irreproducibility Results from Digital Abundance

- The previous two decades saw an explosion in both data gathering and storing, and in computational power and scale. These two changes have entirely disrupted science and discovery.
- Scientific communication e.g. journal and conference publication, is by and large unchanged since its inception in 1665: Relatively short and structured natural language descriptions of the scientific discovery process and outcome.
- Implication: Resolving computational reproducibility means researchers making code, data available along with the information needed to recompute their discoveries, separately from the traditional publication.

National Academies Consensus Report 2019

“Reproducibility and Replication in Science”

- 15 distinguished members (I was a committee member)
- Chair: Harvey Fineberg, President of Gordon and Betty Moore Foundation
- Stakeholder input: over 50 individuals representing a range of disciplines
 - ⇒ Produced key definitions and several recommendations.



Committee Charge

- Define reproducibility and replicability accounting for the diversity of fields in science and engineering.
- Examine state of contemporary science with regard to reproducibility and replication.
- Determine if lack of replication and reproducibility impacts the overall health of science and engineering as well as the public's perception of these fields.
- Make recommendations for improving rigor and transparency in scientific and engineering research.

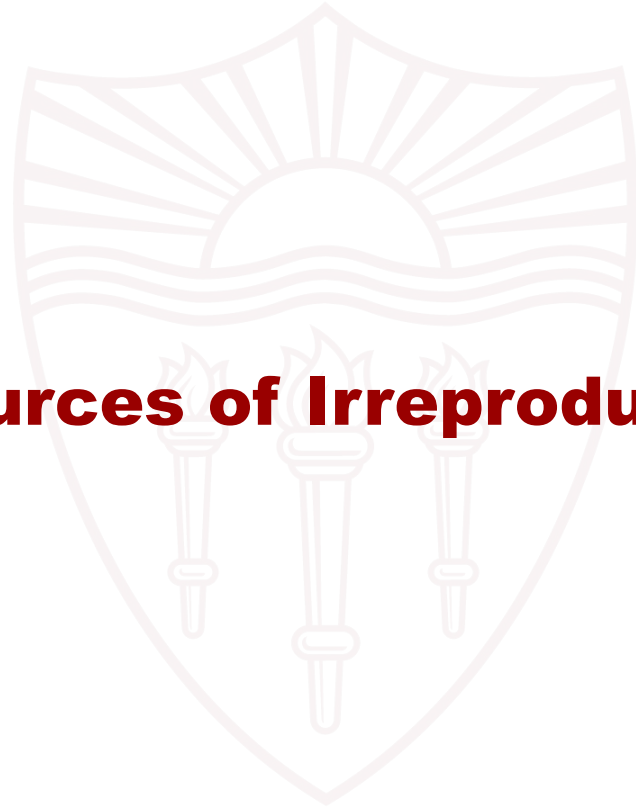
Reproducibility Definitions

- **Reproducibility** is obtaining consistent results using the same input data, computational steps, methods, and code, and conditions of analysis. This definition is synonymous with “**computational reproducibility**.”
- **Replicability** is obtaining **consistent results across studies** aimed at answering the same scientific question, each of which has obtained its own data. Two studies may be considered to have replicated if they obtain consistent results given the level of uncertainty inherent in the system under study.

Recommendation 4-1 (Transparency)

To help ensure the reproducibility of computational results, **researchers should convey clear, specific, and complete information about any computational methods and data products that support their published results** in order to enable other researchers to repeat the analysis, unless such information is restricted by non-public data policies. That information should include the data, study methods, and computational environment:

- **the input data** used in the study either in extension (e.g., a text file or a binary) or in intension (e.g., a script to generate the data), as well as intermediate results and output data for steps that are nondeterministic and cannot be reproduced in principle;
- **a detailed description of the study methods (ideally in executable form)** together with its computational steps and associated parameters; and
- **information about the computational environment** where the study was originally executed, such as operating system, hardware architecture, and library dependencies (which are relationships described in and managed by a software dependency manager tool to mitigate problems that occur when installed software packages have dependencies on specific versions of other software packages).



2. Understanding Sources of Irreproducibility

Standards for Computational Reproducibility

Recall: “Resolving computational reproducibility means researchers making code, data available along with the information needed to recompute their discoveries...”

- Requires standards so scientific communication can be understood within the community.
- Idea: Provide a tool that can assess the “readiness” of a publication (including supplementary material) for computational reproducibility.
- Such a tool embodies community standards and provides feedback to authors to improve “readiness.”



~ Work in Progress ~

Conclusion

1. Widely accepted standards are a key component in achieving community wide reproducibility.
2. We can understand where and why computational reproducibility fails, and automate assessments.
 - Example: *ReproReady Score*. Corollary: Such research provides an educational tool regarding community reproducibility standards.
 - Myth busting: Human factors (e.g. incentives, training, resources) are key to understanding and resolving reproducibility failures.