

# Integration of Reproducible Methods into Community Cyberinfrastructure

**Integration of Reproducible Methods into Community Cyberinfrastructure**  
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**Problem**

- Reproducible Crisis: Considerable research has documented difficulties in research reproducibility (Stokes, 2016a,b; Stigge et al., 2016).
- Not for Scientists to Reliably Support New Discoveries: As results must be reproducible.
- Reproducibility of computational studies is particularly difficult because they require open, documented sharing of data and models, and careful control of underlying hardware and software dependencies so that computational procedures executed by the original researcher are portable and can be run on different hardware or software and produce consistent results.

**Goals of ReproBench EarthCube Project**

- Advance computational reproducibility and make it easier and more efficient for geoscientists to preserve, share, reuse and replicate scientific computations.
- Advance the use of cloud software which encapsulates application dependencies (operating system, libraries, code, data, environment) and application provenance so that the resulting computational research object can be shared and re-executed on different platforms.
- Deploy cloud within the HydroShare supported platform operated by the Consortium of Universities for the Advancement of Hydrologic Science in a global context for the hydrologic research community and demonstrate how to preserve, share, reuse and replicate scientific results from the field of hydrologic modeling.

**An Actionable Approach to Reproducible Research**

**Computational Reproducibility**

Computational Reproducibility requires establishing a progression from Reproducibility through Reusability, Reproducibility, and Replicability, demanding increased time and effort.

**Repository and Compute**

HydroShare is the context of hydrology, the platform that links repository and compute capabilities and the methods and tools developed as part of this project have the potential to be extended to other geoscientific domains. They also have the potential to return the reproducibility evaluation process to currently underused by journals and publishers.

**Automatic Containerization of Execution Dependencies**

HydroShare Client

Scientist Client observes the repository made to the host OS using a run of an experiment

1. Client Scientist

2. Shared Scientist

**Cyberinfrastructure Requirements**

- Provenance input data and results
- Provenance Code
- Provenance the computational environment

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PRESENTED AT:



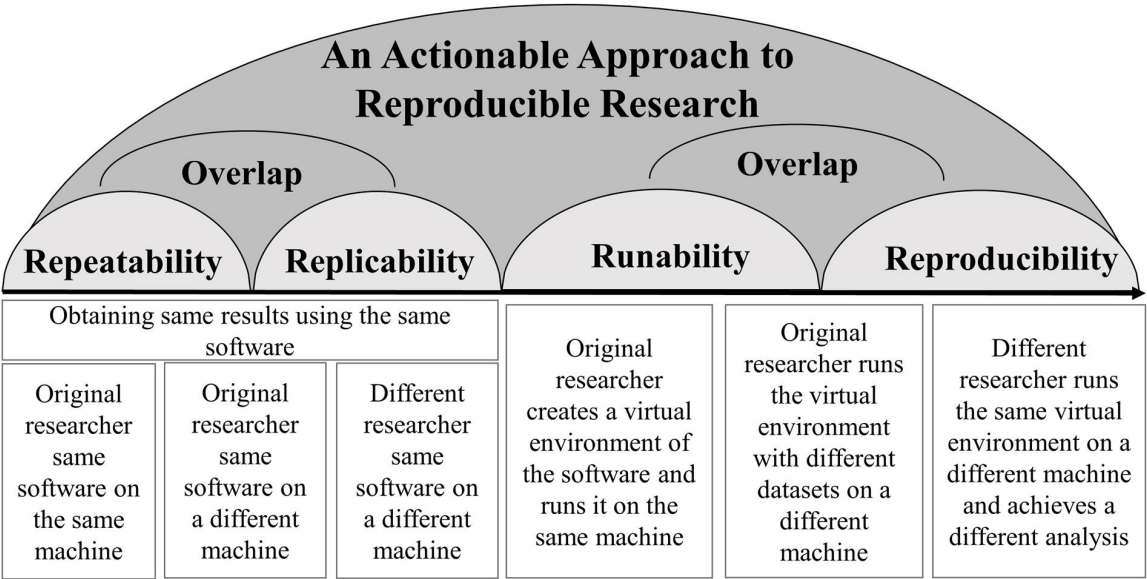
2020 EarthCube Annual Meeting  
Virtual – June 18, 2020

# PROBLEM

- Reproducibility Crisis. Considerable research has documented difficulties in research reproducibility (Baker, 2016a,b; Stagge et al., 2019).
- Yet, for science to reliably support new discoveries, its results must be reproducible.
- Reproducibility of computational studies is particularly difficult because they require open, documented sharing of data and models and careful control of underlying hardware and software dependencies so that computational procedures executed by the original researcher are portable and can be run on different hardware or software and produce consistent results.

# GOALS OF REPROBENCH EARTHCUBE PROJECT

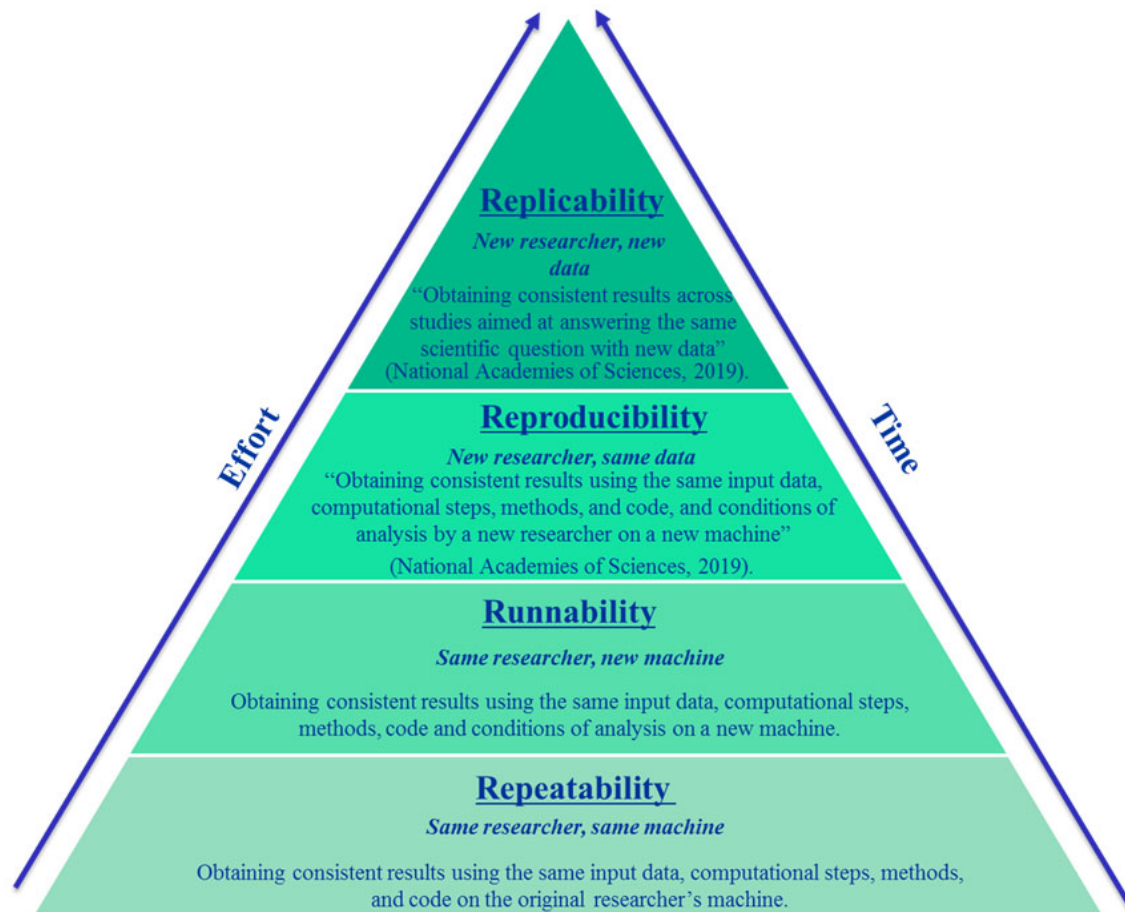
- Advance computational reproducibility and make it easier and more efficient for geoscientists to preserve, share, repeat and replicate scientific computations.
- Advance the use of Sciunit software which encapsulates application dependencies composed of system binaries, code, data, environment and application provenance so that the resulting computational research object can be shared and re-executed on different platforms.
- Deploy Sciunit within the HydroShare JupyterHub platform operated by the Consortium of Universities for the Advancement of Hydrologic Science Inc. (CUAHSI) for the hydrology research community and demonstrate how to preserve, share, repeat and replicate scientific results from the field of hydrologic modeling



Actionable approach for moving geoscience workflows from the Runability to Reproducibility level.

# COMPUTATIONAL REPRODUCIBILITY

Computational Reproducibility requires establishing a progression from Repeatability, through Runnability, Reproducibility, and Replicability, demanding increased time and effort.



The reproducibility taxonomy for complex computational studies (Essawy et al., 2020).

## Cyberinfrastructure Requirements

- Preserve input data and results
- Preserve Code
- Preserve the computational environment

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## Solution

- HydroShare platform for sharing and archiving data and models
- JupyterHub compute platforms linked to HydroShare for model execution
- Sciunit Software for encapsulating computational dependencies

## HydroShare Data and Model Repository

- Manage data (and models and workflows) throughout research life cycle
- Share data, models, and other research products
- Permanent publication of data and models with citable digital object identifiers (DOIs)
- Fulfill Findable, Accessible, Interoperable, Reusable (FAIR) open data mandate

The screenshot displays the HydroShare website interface. At the top, the navigation bar includes links for HOME, MY RESOURCES, DISCOVER, COLLABORATE, APPS, and HELP, along with a SIGN IN button. The main header states: "HydroShare is CUAHSI's online collaboration environment for sharing data, models, and code." Below this is a "Sign up now" button.

The "Discover" section features a large banner image of a snowy landscape with the text: "Discover content shared by your colleagues and other researchers. Access a broad range of data types used in hydrology." Below the banner, a sidebar on the left titled "How it works" shows a step "1 Create data" with the text: "Collect your data using the same methods you use now. HydroShare supports a broad set of hydrologic data types."

The main content area displays the details for the resource "TW Daniels Experimental Forest (TWDEF) Lidar". The resource information includes:

- Authors:** Michaela Teich | David G. Tarboton
- Owners:** Michaela Teich
- Resource type:** Generic
- Storage:** The size of this resource is 5.4 GB
- Created:** Nov 17, 2016 at 9:11 p.m.
- Last updated:** Nov 30, 2016 at 6:53 p.m. Michaela Teich
- DOI:** 10.4211/rs.36f3314971a547bc8c72dc60d6d03c
- Citation:** See how to cite this resource
- Sharing Status:** Published
- Views:** 251
- Downloads:** 11
- +1 Votes:** Be the first one to +1 this. (You need to be logged in to rate this.)
- Comments:** No comments (yet)

The "Abstract" section describes the resource: "This resource contains lidar data, collected at the TW Daniels Experimental Forest (TWDEF) on six separate flights in 2008 and 2009 measuring surface and canopy properties during snow-on and snow-off conditions. It was collected for the purposes of obtaining a digital elevation model (DEM) to characterize the area for snowmelt modeling, and by differencing between snow-on and snow-off observations to characterize the spatial distribution of snow depth. Canopy lidar returns also characterize the vegetation. The data was collected by the Utah State University (USU) Lidar-Assisted Stereo Imaging (LASSI) laboratory. The data was initially processed at USU shortly after collection and additionally processed by the Space Dynamics Laboratory (SDL) in support of Utah lidar efforts in 2016. The metadata report (sd16-1363.pdf) gives details about the hardware used for data collection, the flight plans and resulting data, the data processing steps, and a brief error analysis. Zip files are named by the collection date and contain: - Terra Scan Binary Files - LAS Files (one for each flight line and the combined file) - KML Files (one for each flight line) - ASC DEM file (1 m resolution) - PNG Hillshade file. A complete list can be found on pp. 17-22 of the metadata report."

The "Subject Keywords" section includes: "TW Daniels Experimental Forest", "TWDEF", "Lidar", "DEM", and "Snow Depth".

At the bottom left, the "Resource Level Coverage" section shows a map of the TW Daniels Experimental Forest in Utah, with coordinates: Longitude: -111.5002, Latitude: 41.8602, and temporal coverage from 03/28/2008 to 07/06/2009.

## CUAHSI and CyberGIS Jupyter for Water Gateways to computing

- Provide immediate value
  - What can I do now that I may not be able to easily do on my PC
- Model input data preparation
- Model execution
- Visualization and analysis (best of practice tools)
- Reduced needs for software installation and configuration (platform independence)
- Write and execute code in a Jupyter Notebook, acting on content of HydroShare resources and saving results back to HydroShare Repository
  - Collaboration
  - Access to enhanced computation (HPC, Big data)
- Enhanced trust in research through transparency, replicability and reproducibility

HYDROSHARE

HOMEMY RESOURCESDISCOVERCOLLABORATEAPPSHELP

Create

# Introduction to TauDEM

Authors:David Tarboton

Owners:David Tarboton

Resource type:Composite Resource

Storage:The size of this resource is 54.2 MB

Created:Dec 08, 2019 at 12:17 a.m.

Last updated:Dec 08, 2019 at 3:52 p.m. David Tarboton

Citation:See how to cite this resource

Content types:

Geographic Feature Content

Geographic Raster Content

Sharing Status:Public

Views:69

Downloads:28

+1 Votes:Be the first one to +1 this resource

Comments:No comments (yet)

Open with...

HydroShare GIS

CUMSI JupyterHub

OPeNDAP

CyberGIS-Jupyter for Water

MATLAB Online

## Abstract

The Jupyter Notebook and data in this resource illustrate the use of Terrain Analysis Using Digital Elevation Model (TauDEM) software deployed on JupyterHub for watershed delineation.

js-168-155.jetstream-cloud.org/user/demo/tree/Downloads/18984997bf8f44dd99a246d4f8f903/18984997bf8f...

LogoutControl Panel

FilesRunningClusters

Select items to perform actions on them.

UploadNew

/ Downloads / 18984997bf8f44dd99a246d4f8f903 / 18984997bf8f44dd99a246d4f8f903 / data / contents

	Name	Last Modified	File size
		seconds ago	
	TauDEM.ipynb	Running 13 minutes ago	17.8 kB
	logan.tif	13 minutes ago	56.8 MB
	logan.vrt	13 minutes ago	1.73 kB

jupyter TauDEM (unsaved changes)

LogoutControl Panel

FileEditViewInsertCellKernelWidgetsHelp

Not TrustedHydro-Python3

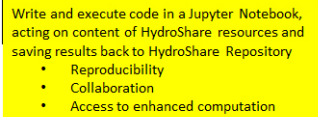
Run

Markdown

## Hydrologic Terrain Analysis Using TauDEM

The purpose of this notebook is to introduce **Terrain Analysis Using Digital Elevation Models (TauDEM)** software for Hydrologic Terrain Analysis in Jupyter. TauDEM is a free and open source set of Digital Elevation Model (DEM) tools for the extraction and analysis of hydrologic information from topography as represented by DEM. This software is developed at Utah State University (USU) for hydrologic digital elevation model analysis and watershed delineation.

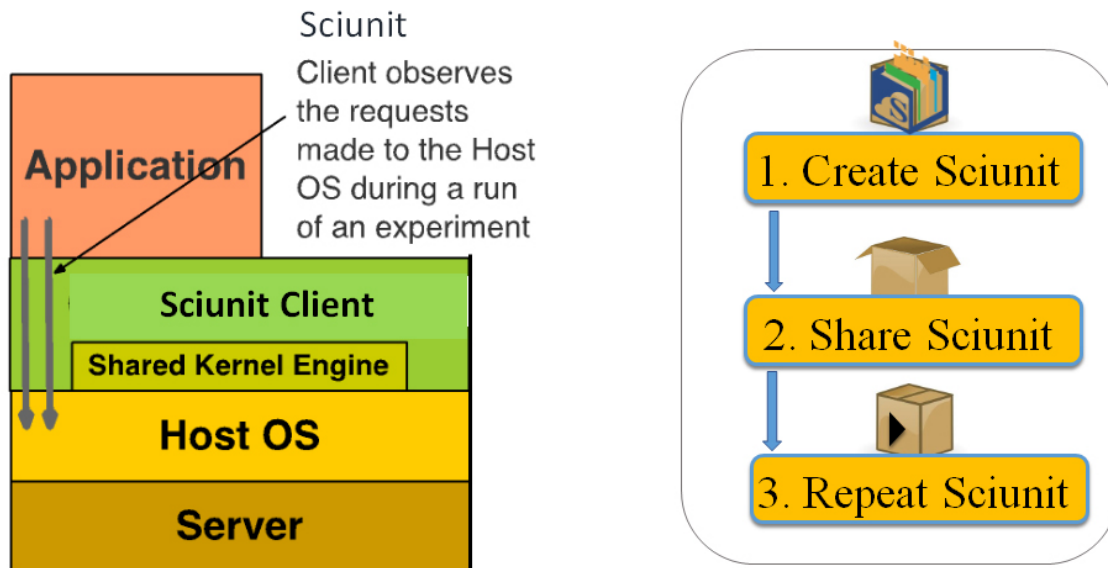
While illustrated in the context of hydrology, the pattern that links repository and compute capability and the methods and tools developed as part of this project have the potential to be extended to other geoscience domains. They also have the potential to inform the reproducibility evaluation process as currently undertaken by journals and publishers.





# AUTOMATIC CONTAINERIZATION OF EXECUTION DEPENDENCIES

<http://sciunit.run> (<http://sciunit.run>)



HydroShare Jupyter Notebook Resources that illustrate the use of Sciunit for reproducibility

- CHOI, Y. (2020). Sciunit SUMMA Result Reproduction Illustration, HydroShare, <http://www.hydroshare.org/resource/7d1403636fd3444c87e3c5b40b000b91> (<http://www.hydroshare.org/resource/7d1403636fd3444c87e3c5b40b000b91>) (This illustrates computational reproducibility using a model and computational environment encapsulated in a Sciunit stored in HydroShare. Details are described in Essawy et al., 2020)
- Choi, Y., J. Goodall, J. Sadler, A. M. Castronova, A. Bennett, T. Malik, B. Nijssen, Z. Li, S. Wang, M. Clark, D. Tarboton, M. Deeds (2020). EarthCube2020: An Approach for Open and Reproducible Environmental Modeling, HydroShare, <http://www.hydroshare.org/resource/75f31565dbd24c198450b9d37c6fcf74> (<http://www.hydroshare.org/resource/75f31565dbd24c198450b9d37c6fcf74>) (This illustrates the cycle involving the creation of a Sciunit container, saving to HydroShare and then re-execution of that container for computational reproducibility).



# ABSTRACT

For science to reliably support new discoveries, its results must be reproducible. This has proven to be a challenge in many fields including fields that rely on computational methods as a means for supporting new discoveries. Reproducibility in these studies is particularly difficult because they require open, documented sharing of data and models and careful control of underlying hardware and software dependencies so that computational procedures executed by the original researcher are portable and can be run on different hardware or software and produce consistent results. Despite recent advances in making scientific work more findable, accessible, interoperable and reusable (FAIR), fundamental questions in the conduct of reproducible computational studies remain: Can published results be repeated in different computing environments? If yes, how similar are they to previous results? Can we further verify and build on the results by using additional data or changing computational methods? Can these changes be automatically and systematically tracked? This presentation will describe our EarthCube project to advance computational reproducibility and make it easier and more efficient for geoscientists to preserve, share, repeat and replicate scientific computations. Our approach is based on Sciunit software developed by prior EarthCube projects which encapsulates application dependencies composed of system binaries, code, data, environment and application provenance so that the resulting computational research object can be shared and re-executed on different platforms. We have deployed Sciunit within the HydroShare JupyterHub platform operated by the Consortium of Universities for the Advancement of Hydrologic Science Inc. (CUAHSI) for the hydrology research community and will present use cases that demonstrate how to preserve, share, repeat and replicate scientific results from the field of hydrologic modeling. While illustrated in the context of hydrology, the methods and tools developed as part of this project have the potential to be extended to other geoscience domains. They also have the potential to inform the reproducibility evaluation process as currently undertaken by journals and publishers.

# REFERENCES

Baker, M., (2016a), "1500 scientists lift the lid on reproducibility," Nature News, 533(7604): 452-454, <https://doi.org/10.1038/533452a>.

Baker, M., (2016b), "Muddled meanings hamper efforts to fix reproducibility crisis," Nature News, <https://doi.org/10.1038/nature.2016.20076>

Essawy, B.T., Goodall, J.L., Voce, D., Morsy, M.M., Sadler, J.M., Choi, Y.D., Tarboton, D.G., Malik, T., 2020. A taxonomy for reproducible and replicable research in environmental modelling. Environ. Model. Softw. 104753. <https://doi.org/10.1016/j.envsoft.2020.104753>

Stagge, J. H., D. E. Rosenberg, A. M. Abdallah, H. Akbar, N. A. Attallah and R. James, (2019), "Assessing data availability and research reproducibility in hydrology and water resources," Scientific Data, 6: 190030, <https://doi.org/10.1038/sdata.2019.30>.