February 8, 2024 | 1:30-3pm Virtual Workshop

Best Practices for Managing Your Code & Scripts You Use to Generate Your Research

u.mcmaster.ca/scds-events



Best Practices for Managing Your Code and Scripts to Generate Your Research

Research Software Development

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- Ola Hejazi
- David Beardwood

Research Data Management

- Emilie Altman
- Danica Evering







McMaster University is located on the traditional Territories of the Mississauga and Haudenosaunee Nations, and within the lands protected by the "Dish With One Spoon" wampum agreement.

Laslovarga, "Webster Falls in Winter, Waterdown, Hamilton, Ontario, Canada - Spencer Gorge / Webster's Falls Conservation Area," 23 January 2011, Wikimedia Commons - <u>https://commons.wikimedia.org/wiki/File:Waterdawn Webster Falls in Winter8.jpg</u>

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Questions asked via the chat box will be read by the facilitator without identifying you. Note that you may be identifiable when asking a question during the session in an audio or visual format.





Certificate Program

The Sherman Centre offers a Certificate of Attendance that rewards synchronous participation at 7 workshops. We also offer concentrations in Data Analysis and Visualization, Digital Scholarship, and Research Data Management.

Learn more about the Certificate Program: <u>https://scds.ca/certificate-program</u> Verify your participation at a session: <u>https://u.mcmaster.ca/verification</u> At an unspecified point during the workshop, a code will be read aloud. This is the answer to the third question of the form.





FAIR Principles

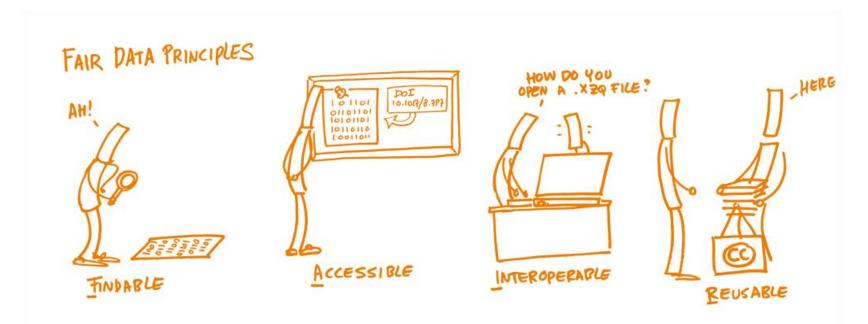


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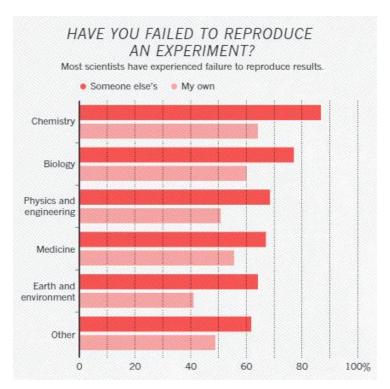
Library



Open Research and Reproducibility

- Reproducibility is essential for research verification and integrity
- The Reproducibility Crisis
 - In recent years, many researchers have failed to replicate previous scientific experiments
 - The Replication Project replicated 100 prominent psychology studies and succeeded in only 39% of attempts¹
 - Baker surveyed 1500 scientists high replication failure rates²
 - While contextual reasons may be a factor, it makes clear the importance of replication in science

[1] Open Science Collaboration. (2015). Estimating the reproducibility of psychological science. Science, 349(6251), aac4716. Doi: 10.1126/science.aac4716



[2] Baker M .1,500 scientists lift the lid on reproducibility. NatureNews. 2016; 533:452





Open Research and Reproducibility

• How can we make our research reproducible?

1. Open Data

- Increases the reliability of the study replicable
- o Increases opportunities for collaboration
- Increases citations
- o Often required by journals and funding agencies

2. Documentation

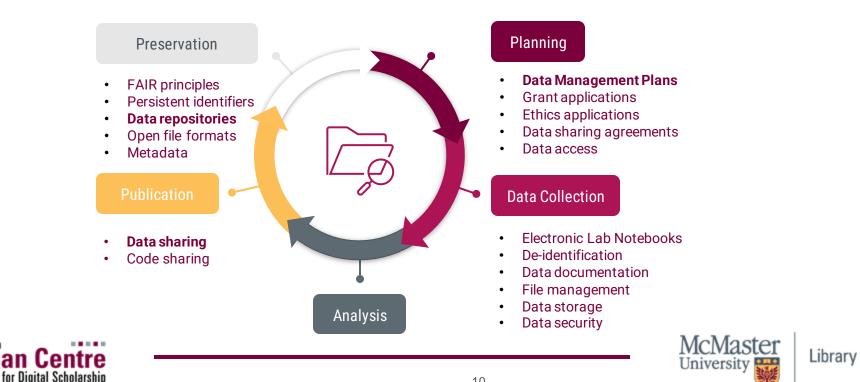
- Good documentation is needed for data to be useful!
- Will you understand your own data in 5 years? What about someone who has never seen your data before?







Data Management Plans are an integral part of good research data management practices. This lays out your plan to create, store, organize, document, secure, preserve, and share your research data. It's an essential part of the research data lifecycle and good data management practices.



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Lewis & Ruth

Data Management Plan (DMP)

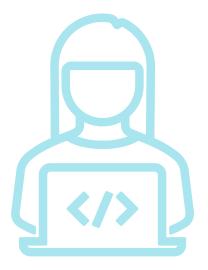
- A tool to help you plan to create, store, organize, document, secure, preserve, and share your research data.
- A **living document –** something you'll work with, adapt, and change through your research.
- Create it at the start of your research avoid pitfalls and problems before they occur.
- Prepare for future stages of research including potential data sharing (if desired) and preservation.
- Research is a team effort collaborate on your DMP.
- Many research funders require grant applicants to submit a DMP including the Tri-Agencies (NSERC, CIHR, SSHRC started 2022), NIH, and others.







Best Practices for Managing Your Code and Scripts You Use to Generate Your Research *through* Software Management Plans

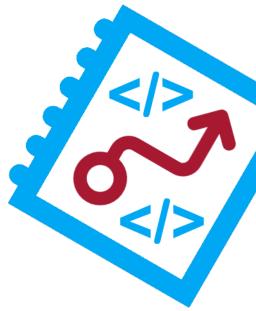






Data Software Management Plan (DMP SMP)

- A tool to help you plan to create, store, organize, document, secure, preserve, and share your research data software.
- A **living document** something you'll work with, adapt, and change through your research.
- Create it at the start of your research avoid pitfalls and problems before they occur.
- Prepare for future stages of research including potential data sharing (if desired) and preservation.
- Research is a team effort collaborate on your SMP.
- Many research funders are evaluating SMP requirements Tri-Agency Research Data Management Policy: deposit alongside research data any "code that directly support the research conclusions in journal publications and pre-prints that arise from agency-supported research."

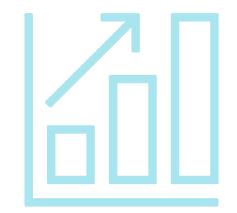






Why include software in my management plans?

- Researchers increasingly rely on software in their research.
- A survey by the Software Sustainability Institute, carried out among UK researchers, found that 92% of academics use research software, and 7 out of 10 researchers deemed it impossible to conduct their research without it.¹



That's a lot of research software!



[1] Netherlands eScience Center. (2023). Practical guide to Software Management Plans. Martinez-Ortiz, C., et al. Doi: 10.5281/zenodo.7589725



What is "Research Software"?

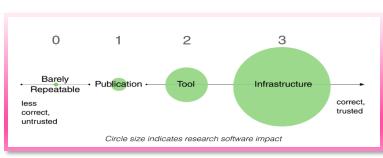
- Software that is itself a research activity or experiment, a scholarly object worthy to be published
- Code that directly support the research conclusions in journal publications and pre-prints that arise from agency-supported research. (<u>Tri-Agency</u> <u>Research Data Management Policy</u>, §3.3 Data Deposit)
- Software that supports research, such as **tools** and **infrastructure systems**
- Anything in between





Reproducibility Goals

- Criteria of different levels of reproducibility suggested by <u>How reproducible should research software be?</u>
- Level 0 The script you downloaded that one time from the internet
 - Shared code snippets, functions, single operations from the internet
 - Simple code intended for single or occasional use
 - Needs to be verified for correctness and appropriateness

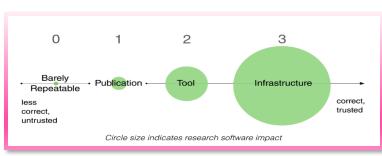






Reproducibility Goals

- Criteria of different levels of reproducibility suggested by <u>How reproducible should research software be?</u>
- Level 1 Research software for publication
 - o Code that directly support the research conclusions
 - E.g. data processing, analysis, and visualization scripts specific to the project or data
 - Facilitate trust in the published results obtained from research software

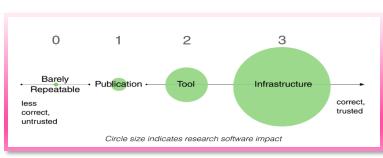






Reproducibility Goals

- Criteria of different levels of reproducibility suggested by <u>How reproducible should research software be?</u>
- Level 2 Research software as a tool
 - Code that is intended to be applied to different inputs or scenarios over a modest period of time
 - E.g. Scientific software packages, web development frameworks
 - Either the original developer, or somebody else with the skills to understand and maintain or modify the code themselves

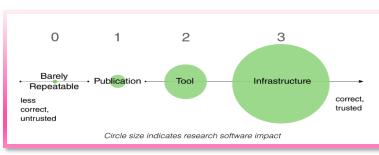






Reproducibility Goals

- Criteria of different levels of reproducibility suggested by <u>How reproducible should research software be?</u>
- Level 3 Research software as infrastructure
 - Software that is used by a broader community
 - E.g. web systems, management systems
 - Fundamental aspects include correctness, reusability, and documentation

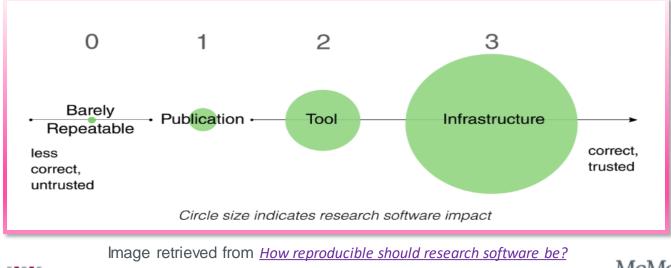






Reproducibility Goals

- Reproducibility goals are proportionate to the size, complexity and audience of the software
- Relates to the expected re-usability of the code and reproducibility of the results
- Level of documentation is proportionate to the reproducibility goals





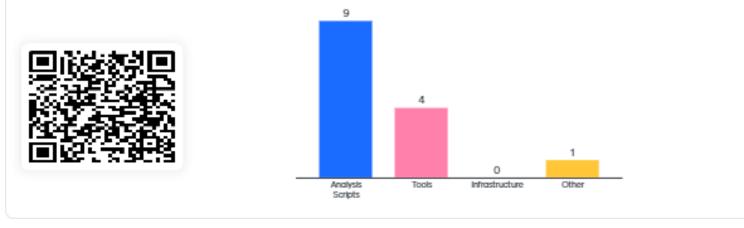
Sherman Centre Certificate Program

- Certificate you can add to your CV or ORCiD
- Attend 7 RDM workshops to receive a certificate!
- Go to this website to verify today's session: https://u.mcmaster.ca/verification
- Learn more about the Certificate Program: https://scds.ca/certificate-program

Image by Markus Spiske on Unsplash.

Join at menti.com | use code 9314 3691

What kind of Research Software do you create?







Mentimeter

Software Management Plan (SMP)

- For project stakeholders to reference at anytime
- A living document, periodically review during the research process
 - Allow you to consider and define your **reproducibility goal**
 - Provide your research team a **general guideline** to FAIR principle and reproducibility
- Outlines the **strategies** and **practices** for effectively managing software throughout the research process
- Ensures the **continuity of operations** by implementing plans for knowledge retention and knowledge transfer
- Proactively **identifies** and **mitigates** any ethical, licensing and legal risks and liabilities in the project





Software Management Plan (SMP)

SMP typically includes plans for the following considerations:

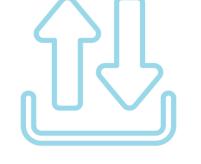
- Assets used and produced (input and output)
- Documentation
- Version control protocol
- Preservation and sustainability
- Roles and responsibilities
- Ethics, licensing and legal compliance





Assets Used and Produced

- A.K.A. inputs and outputs
- Input assets used like research data and third-party software libraries
- These inputs produce the software source code/executable, documentation, licenses and research outputs
- Identifies project components to project team, stakeholders and future maintainers
- Plans for **compliance with the terms of use** for any third-party data or software libraries integrated into project







Documentation

- A software management plan should include explanation of how the research software will be documented
- A research software project commonly includes guides for both users and developers
- This documentation helps others understand how to use the software and what it can or should do, as well as how to maintain and extend it







Documentation

• User guide

- Assist user in understanding the features
- Provides instructions, information, and guidance on how to use the software
- Serves a reference guide during troubleshooting
- "I'm not getting the expected results. Am I using it correctly, or is there a problem in the code?"

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Documentation

- Developer guide
 - Targeted at other research software developers who may be involved in the development, customization or future maintenance of the software.
 - Provides comprehensive technical documentation
 - Ensures the long-term sustainability of the software project

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Documentation

poly = PolynomialFeatures(degree=2, include_bias=False)

- **Documentation** can be simple
 - o Just a README file with instructions to build/run the software
 - o Example: OpenAI/Whisper, MakeAReadme.com
 - o Or exist as comments in the source code
- Code commenting is the practice of adding short notes throughout your code
- The goal is to publish code that can be **understood** by others
- Publish well-documented, well-commented code
- There are tools to assist with code commenting, e.g. GitHub Copilot





tokens to be predicted by the decoder, allowing a single model to replace many stages of a traditional speech-processing pipeline. The multitask training format uses a set of special tokens that serve as task specifiers or classification targets.

Setup

We used Python 3.9.9 and <u>PyTorch</u> 1.10.1 to train and test our models, but the codebase is expected to be compatible with Python 3.8-3.11 and recent PyTorch versions. The codebase also depends on a few Python packages, most notably <u>OpenAl's tiktoken</u> for their fast tokenizer implementation. You can download and install (or update to) the latest release of Whisper with the following command:

pip install –U openai—whisper	G
Alternatively, the following command will pull and install the latest commit from this repository, along with its Python dependencies	
pip install git+https://github.com/openai/whisper.git	J
To update the package to the latest version of this repository, please run:	
pip installupgradeno-depsforce-reinstall git+https://github.com/openai/whisper.git	J
It also requires the command-line tool <u>ffmpeg</u> to be installed on your system, which is available from most package managers:	
# on Ubuntu or Debian sudo apt update 💩 sudo apt install ffmpeg	J
# on Arch Linux sudo pacman -S ffmpeg	
<pre># on MacOS using Homebrew (https://brew.sh/)</pre>	
brew install ffmpeg	
<pre>brew install ffmpeg # on Windows using Chocolatey (https://chocolatey.org/) choco install ffmpeg</pre>	

You may need <u>rust</u> installed as well, in case <u>tiktoken</u> does not provide a pre-built wheel for your platform. If you see installation errors during the <u>pip install</u> command above, please follow the <u>Getting started page</u> to install Rust development environment. Additionally, you may need to configure the <u>PATH</u> environment variable, e.g. <u>export PATH="\$HOME/.cargo/bin:\$PATH"</u>. If the installation fails with <u>No</u> module named 'setuptools_rust', you need to install setuptools_rust, e.g. by running:

in inchail contracts and

Version Control Protocol

- Version control protocol provides a systematic approach to manage development and collaboration
- Audit trail of changes with reasons
- Version control helps keep your code base transparent and accessible.
- Exist cloud services to make all of this easier, e.g. GitHub, which can provide:
 - o Automated change/difference identification
 - Backups of each change and version
 - Shared public and private remote access for collaborators
 - o Conflict resolution when editing the same file





Version Control Protocol

) 위 master 👻 linux / fs / sync.c 다

)lder	Newer			
7 years ago 🛛 🌍	License cleanup: add SPDX GPL	(1	// SPDX-License-Identifier: GPL-2.0
19 years ago	[PATCH] sys_sync_file_range()		2	/*
, ,			3	* High-level sync()-related operations
			4	*/
			5	
3 years ago	block: removesync_blockdev	(6	<pre>#include <linux blkdev.h=""></linux></pre>
19 years ago	[PATCH] sys sync file range()		7	<pre>#include <linux kernel.h=""></linux></pre>
is years ago	[8	<pre>#include <linux file.h=""></linux></pre>
			9	<pre>#include <linux fs.h=""></linux></pre>
14 years ago 🛛 😡	include cleanup: Update gfp.h a	(10	<pre>#include <linux slab.h=""></linux></pre>
13 years ago 🛛 🕷	fs: reduce the use of module.h w	(11	<pre>#include <linux export.h=""></linux></pre>
13 years ago 🛛 🔮	introduce sys_syncfs to sync a si	(12	<pre>#include <linux namei.h=""></linux></pre>
18 years ago	[PATCH] severing fs.h, radix-tree	(13	<pre>#include <linux sched.h=""></linux></pre>
19 years ago	[PATCH] sys sync file range()		14	<pre>#include <linux writeback.h=""></linux></pre>
			15	<pre>#include <linux syscalls.h=""></linux></pre>
			16	<pre>#include <linux linkage.h=""></linux></pre>
			17	<pre>#include <linux pagemap.h=""></linux></pre>
18 years ago 🛛 💼	[PATCH] BLOCK: Move functions	(18	<pre>#include <linux quotaops.h=""></linux></pre>





Preservation & Sustainability

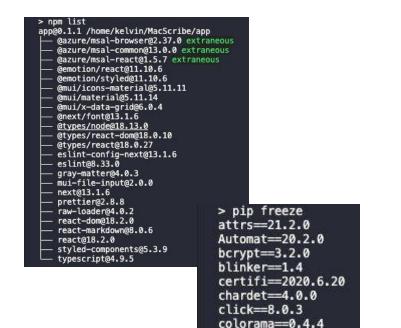
- Involves measures to address technological, organizational and environmental factors
 - **Technological**: Advances in hardware technology or changes in host systems can impact software compatibility
 - **Organizational**: Project stakeholders (e.g. staff, developers) changes
 - Environmental: Changes in regulatory compliance, e.g. AODA
- Long-term Availability, Usability, and Maintenance of software beyond project's duration
- Continuity of Operations
 - Knowledge Retention
 - Knowledge Transfer
 - Preservation allows future maintainers to understand the software's history and decision-making processes





Preserving Software and Dependencies

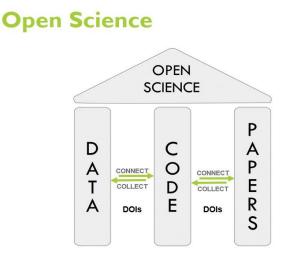
- Store your source code with dependencies
 - Package manager to install, manage and document (e.g. pip, conda, npm)
- Building and sharing software as container images
 - Via Docker Hub or self-hosted container image repository







Preserving Software with Persistent Identifiers



Courtesy of Jeffrey Demaine



- Generating (persistent) Digital Object
 Identifiers for your software and source code
 - DOIs allow software to be easily referenced in publication
 - DOIs will improve findability of the software in the research community
- Using Zenodo and GitHub
 - Zenodo example: <u>QSM</u>
 - GitHub example: QSM



Preserving Software with Persistent Identifiers

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Zenodo Search records.	Q. Communities My dashboard		a +• Lihjebine •	Refactored code and added more deployment instruction		hykelvinlee42 added more	informa fe54914 · 6 minutes ag	o 🕚 16 Commits
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McMaster

University

Library



Software Testing

- Testing aids in managing dependencies by verifying the software works correctly and provides a shared understanding of the software's behaviour
- A test plan should be well-documented, well-commented
- Formal test plan includes:
 - Unit Testing (test a function works as intended)
 - Regression Testing (re-run old tests to make sure nothing else changed)
 - Integration Testing (test system, i.e. all of the functionality together)
- Using Continuous Integration (CI) Automation Tools
 - GitHub Actions
 - Travis CI





Ethics, Licensing & Legal Compliance

- Consider potential ethical biases in software (algorithms) developed/used to process your data
 - Does your software handle data in a way that respects privacy rights and maintains confidentiality
 - o Does your software provide results from an unbiased perspective
- Consider software licensing as early as possible
 - Consider how others may use your software
 - Your software dependencies (assets used) may have licenses restricting how or others can share or reuse your software, which can have license requirements for your work
 - If you don't include a software license, nobody else can copy, distribute, or modify your work





Ethics, Licensing & Legal Compliance

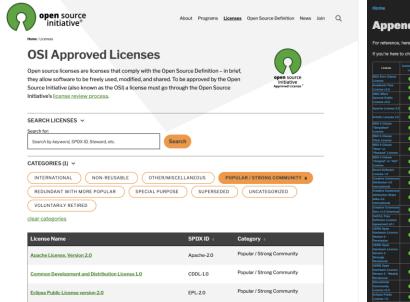
- Where possible, use existing licenses, rather than creating custom terms of use
 - Common OSS Licenses like GNU GPL, MIT, Mozilla and Apache
 - Existing licenses are designed to be (mostly) compatible with other commonly used licenses
 - Creating custom licenses requires careful consideration of legal and licensing issues
- Web tools to help:
 - Choose-a-license (choosealicense.com)
 - Open Source Initiative (opensource.org/licenses)







Ethics, Licensing & Legal Compliance

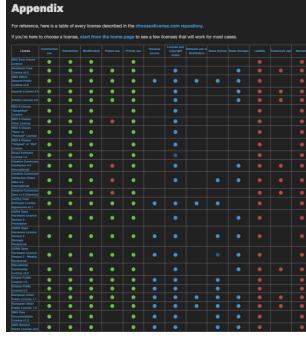


GPL-2.0

GPL-3.0-only

Popular / Strong Community

Popular / Strong Community





GNU General Public License version 2

GNU General Public License version 3



Software Management Plan (SMP)

Elements of an SMP:

- Assets used and produced (input and output) ✓
- Documentation ✓
- Version control protocol \checkmark
- Preservation and sustainability ✓
- Roles and responsibilities (same as DMP)
- Ethics, licensing and legal compliance \checkmark

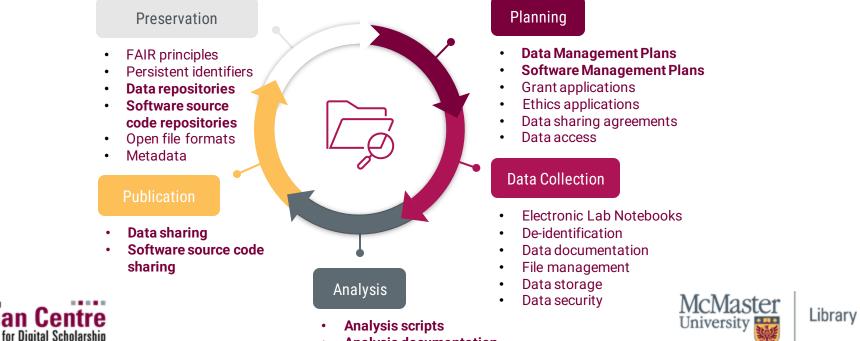




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Software and Data Management Plans are an integral part of good research data management practices. They lay out your plan to create, store, organize, document, secure, preserve, and share your research software and data. It's an essential part of the research data lifecycle and good data management practices.



Analysis documentation

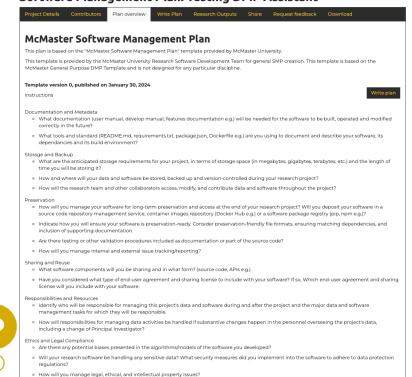
Software Management Plan Templates

Samples and Templates

- Our McMaster Software Management
 Plan template on DMP Assistant
- DMP Assistant: <u>https://dmp-pgd.ca/</u>
- A Data Management Plan and a Software Management Plan can be used together to plan the management of these research assets



Software Management Plan: Testing DMP Assistant



Library

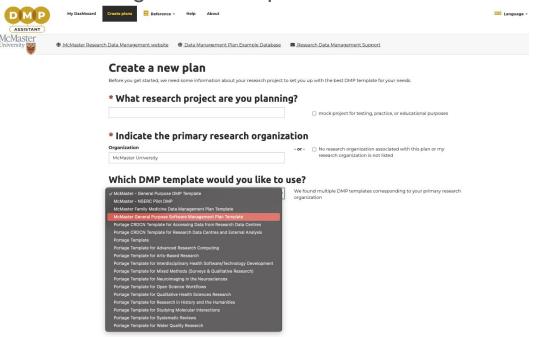
University



Software Management Plan Templates

McMaster General Purpose Software Management Template

 Create a new management plan on DMP Assistance



- Input "McMaster University" as the primary research organization
- You will then find

 "McMaster General Purpose Software Management Plan Template" in the template dropdown menu





Best Practices for Managing Your Code and Scripts to Generate Your Research

Please reach out to us if you have questions about the elements of Software Management Plans (RSD team) or Data Management Plans (RDM team).

- Research Software Development (RSD) Team
 - Email: <u>rsd@mcmaster.ca</u>
 - Website: <u>https://u.mcmaster.ca/rsd</u>
 - Join our community of practice: <u>https://u.mcmaster.ca/rsd-</u> <u>ms-team</u>
 - <u>Reproducible Research Software</u> <u>Learning Module</u>

- Research Data Management (RDM) Team
 - Email: rdm@mcmaster.ca
 - Website: htts://rdm.mcmaster.ca
 - Join our community of practice: <u>https://u.mcmaster.ca/rdmcommunity</u>







Thank You!

McMaster University Research Software Development and Research Data Management Teams