ENCORE. A practical implementation to improve reproducibility and transparency of computational research

Antoine H.C. van Kampen[1,2*#], Utkarsh Mahamune[1#], Aldo Jongejan[1], Barbera D.C. van Schaik[1], Daria Balashova[1], Danial Lashgari[1], Mia Pras-Raves[1], Eric J.M. Wever[1,3], Adrie D. Dane[1,4], Rodrigo García-Valiente[1], Perry D. Moerland[1]

[1]Amsterdam UMC location University of Amsterdam, Epidemiology and Data Science, Meibergdreef 9, Amsterdam, Netherlands. Amsterdam Public Health, Methodology, Amsterdam, The Netherlands. Amsterdam Institute for Immunology and Infectious Diseases, Amsterdam, The Netherlands.

[2]Biosystems Data Analysis, Swammerdam Institute for Life Sciences, University of Amsterdam, Amsterdam, the Netherlands

[3]Amsterdam UMC location University of Amsterdam, Department of Clinical Chemistry; Laboratory Genetic Metabolic Diseases, Department of Pediatrics; Emma Children's Hospital, Meibergdreef 9, Amsterdam, The Netherlands

[4]Core Facility Metabolomics, Amsterdam UMC location University of Amsterdam, Amsterdam, The Netherlands

# Equally contributed

*Corresponding author:
Antoine H.C. van Kampen
Bioinformatics Laboratory
Epidemiology and Data Science
Amsterdam University Medical Centers
Meibergdreef 9, 1105 AZ Amsterdam, the Netherlands
a.h.vankampen@amsterdamumc.nl
tel. +31-20-5667096

Abstract

Outcomes of computational approaches are occasionally difficult to reproduce despite ongoing (open science) initiatives that resulted in guidelines and best practices to improve reproducibility. However, their translation and application in practice still is an obstacle. We propose ENCORE (ENhancing COmputational REproducilbity) to improve reproducibility and transparency through integration of all project components (e.g., data, code, results, concepts, documentation) in a standardized file system structure. The approach makes use of pre-defined (template) files to guide documentation, a GitHub repository for software versioning, a HTML-based navigator, and ENCORE user documentation. ENCORE is agnostic to the type of computational project, data, programming language, and ICT infrastructure and does not depend on any software tool. ENCORE improved reproducibility and transparency of computational projects in our group. Perhaps the most significant challenge to overcome for routine usage of initiatives such as ENCORE is the lack of incentives to sufficiently motivate researchers to spend sufficient time and effort on reproducibility. We expect ENCORE to contribute to the further development of approaches increasing transparency and reproducibility of computational research.

Keywords: Computational research, Reproducibility, Transparency, Open-Science.

Introduction

Reproducibility of research outcomes has become increasingly important within all research fields, including the (bio)medical domain (Ioannidis, 2005; Stupple et al., 2019). The scientific community is increasingly concerned about the so-called 'reproducibility crisis', which includes but is not limited to the failure to reproduce results of published studies and lack of transparency and completeness (Fidler & Wilcox, 2021). Research transparency importantly contributes to reproducibility and refers to the degree to which methodologies, data, and results are accessible and understandable to others and, consequently, contributes to the overall credibility and trustworthiness of a study (Diaba-Nuhoho & Amponsah-Offeh, 2021). Increased data size, increased complexity of experimental and computational methods, and multi-disciplinarity, make reproducibility increasingly challenging. Scientist-driven efforts complemented with pressure from research institutes, funders, and journals have resulted in various initiatives and approaches, covering the different stages of the research lifecycle, to increase reproducibility of scientific findings (Turkyilmaz-van der Velden et al., 2020) (**Figure 1**). Typically, this cycle starts (stage 1) with a careful preparation of the study, which includes planning in terms of research objectives, funding, data management, ethics, experimental design, experimental and computational approaches, publishing, and study archiving. Stage 2 concerns the collection and processing of (patient) samples, and the generation of data. Once data has been collected, it is analyzed using statistical or other computational methods (stage 3). Mathematical modelling and simulations can be part of the computational phase. Alternatively, one may solely or partially rely on existing data from (public) repositories or conduct studies that are based on computer simulations (Lashgari et al., 2022; Merino Tejero et al., 2020). Stage 4 (publication and archiving) is increasingly driven by initiatives aiming for open-access publications and data (Pulverer, 2018; van der Heyden & van Veen, 2018) and open-source software (Garijo et al., 2022; Open Source Initiative, 2023). Research findings are published in open-access preprint repositories (e.g., bioRxiv, medRxiv) and/or peer-reviewed (open-access) journals, while additional output (e.g., data, code) can be archived in, for example, the major omics repositories (Rigden & Fernandez, 2023), figshare (Figshare, 2023) and Zenodo (CERN & OpenAIRE, 2023).

[FIGURE 1]

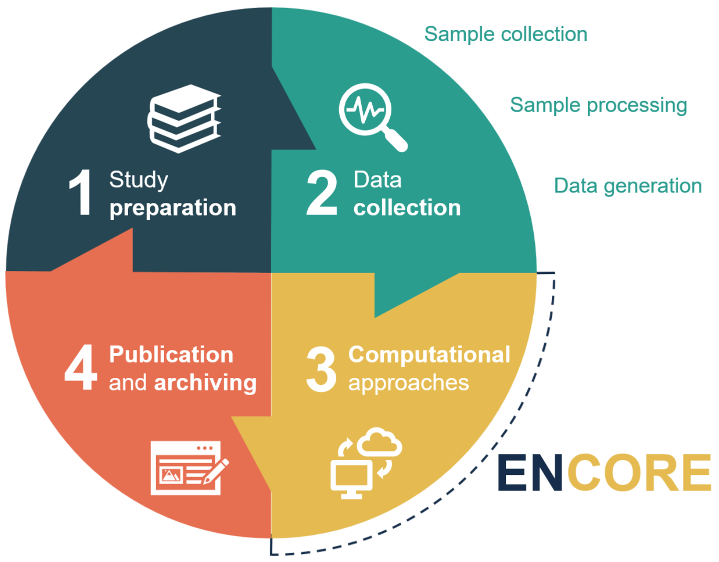


Figure 1. Research lifecycle. Most (biomedical) studies go through the stages of (1) study preparation, (2) data collection (involving sample collection and processing, and data generation), (3) computational approaches for data analyses, modelling and/or simulations, and (4) (open-access/open-source) publication & archiving. Published research findings will drive new studies. ENCORE focuses on computational reproducibility (stage 3).

Despite ongoing initiatives to improve computational reproducibility, results from computational analyses, including from our group, often remain difficult to reproduce even if data and code are available (Mendes, 2018; Papin et al., 2020; Stodden et al., 2018; Tiwari et al., 2021). Irreproducibility of computational research has well-known causes, including undocumented manual processing steps, unavailability of software or data, changes in software libraries, incomplete software documentation, and unspecified parameters. Guidelines to improve computational reproducibility have been suggested by several groups (e.g., (Sandve et al., 2013; Wilson et al., 2017; Ziemann et al., 2023)) but their translation and application in research practice seems to be a bottleneck given that computational studies do not always (fully) adhere to these guidelines. Reproducibility may also be compromised if software is not transparent and, consequently, is not easy to run, understand, test, or modify. This problem typically arises in software developed by (biomedical) researchers without formal training in software engineering (Deardorff, 2020; Hunter-Zinck et al., 2021). Such software might even contain undetected (conceptual) errors although this does not necessarily result in irreproducible results. Nevertheless, training researchers with best practices in software engineering is expected to improve reproducibility. Moreover, making software available as open-source (Margan & Čandrlić, 2015), allows peers to inspect, use, verify, correct, and/or extend the software. This prompts for the use of code versioning systems like Git and GitHub (Blischak et al., 2016), which also facilitate code hosting and sharing, and allow collaborative software development thereby contributing to transparency and reproducibility of computational research (Perez-Riverol et al., 2016; Ram, 2013).

Over the last decade, FAIR data management has been introduced to ensure availability and reusability of experimental data (Wilkinson et al., 2016) while newly developed software is increasingly made available on GitHub and other dedicated software repositories (Di Cosmo, 2020; Garijo et al., 2022). However, in our view, the separation of data and software in different repositories is another potential cause for irreproducibility since manual steps may be required to link data and software. Since such steps are general not described in published papers, it is left to the researcher to reconstruct the precise computational workflow. Moreover, by storing code and data in different repositories, a direct connection with (published) results is also lost. Lack of detailed project documentation further impedes transparency and reproducibility. Therefore, we believe that computational reproducibility is improved if data, code, and results are more tightly integrated and well-documented. Such a self-contained project bundle could also more easily be shared with peers and reviewers.

In this paper we focus on computational reproducibility, that is the reanalysis of the same data using the same computational methods. We propose ENCORE (ENhancing COmputational REproducibility) as a practical approach to improve transparency and reproducibility. The development of ENCORE started in 2018 and is based on existing ideas and initiatives e.g., (Brito et al., 2020; Gruning, Chilton, et al., 2018; Lee, 2018; Markowetz, 2015; Noble, 2009; Perez-Riverol et al., 2016; Sandve et al., 2013; Spreckelsen et al., 2020; Stodden & Miguez, 2014; Taschuk & Wilson, 2017; Turkyilmaz-van der Velden et al., 2020; Wilson et al., 2014; Ziemann et al., 2023), discussions within our research group, and improvements made over a five-year period. It aims to integrate all project components in a single project bundle. ENCORE guides researchers to structure and document the computational part of a research project to substantially improve computational reproducibility. It also harmonizes the approach towards reproducibility if adopted by a whole research group, which brings additional advantages. ENCORE does not specifically address stages 1, 2 and 4 of the research lifecycle (**Figure 1**). However, (parts of) the documentation resulting from these stages will generally be included in the project bundle for completeness but also to correctly design and perform the computational analyses (Stodden, 2015). This includes but is not limited to information about hypotheses to be tested, experimental design, descriptions of (patient) samples and the physical experiment, and the (FAIR) data. Conversely, the ENCORE documentation of computational protocols provides information for annotating the (pre)processed data to meet the FAIR requirements. The ENCORE bundle can be provided as supplementary information for research papers. It is, however, important to recognize that ENCORE will generally contain much more information than published in a research paper. Here, we describe the design of ENCORE, our experiences, and results from internal evaluations. ENCORE improved reproducibility and transparency of our computational projects but, at the same time, made clear that achieving full reproducibility will require further steps. Perhaps the most significant challenge to overcome for routine usage of initiatives such as ENCORE is the lack of incentives to sufficiently motivate researchers to spend sufficient time and effort on reproducibility. We expect ENCORE to contribute to the further development of approaches increasing transparency and reproducibility of computational research.

Methods

ENCORE comprises a standardized file system structure (sFSS), pre-defined (Markdown) files for documentation, a GitHub repository for software version control, a HTML-based sFSS browser (sFSS Navigator), and ENCORE documentation to initiate a self-contained project bundle and support the researcher to use ENCORE in a consistent manner. The sFSS template can be retrieved from the ENCORE GitHub repository (https://github.com/EDS-Bioinformatics-Laboratory/ENCORE). In principle, ENCORE can be used for any type of (research) project and is not domain-specific.

The ENCORE approach was driven by the following main requirements:

1. **Consist of a single self-contained project bundle**. The computational project should be organized and available as a self-contained and integrated package of data, code, results, and (concept) documentation, stored at a single location. It should also be easily transferable to other researchers or reviewers without breaking its internal consistency.
2. **Facilitate transparency and documentation**. ENCORE should facilitate transparency and a deep understanding (e.g., addressing why specific methods were selected and how these were applied) of the project through its standardized structure and documentation of concepts, methodology, data, code, and results.
3. **Enable reproducibility**. The project bundle should enable an external researcher to autonomously execute and understand the computational techniques and recreate the (published) outcomes.
4. **Adhere to proposed guidelines**. ENCORE should follow published guidelines for computational reproducibility as much as possible (e.g., (Brito et al., 2020; Lee, 2018; Noble, 2009; Sandve et al., 2013)).
5. **Enable version control**. ENCORE should allow version control of code and code documentation.
6. **Facilitate harmonization**. The ENCORE approach itself should be standardized and well-documented such that it can easily be adopted by any researcher. This allows harmonization within research groups, enabling the further joint development of best practices within the

ENCORE framework. Moreover, harmonization also facilitates checking transparency and reproducibility prior to publication by direct colleagues.

7. **Provide a generic approach.** ENCORE should be agnostic to the type of computational project (e.g., statistical analysis, mathematical modelling), data, programming language, and ICT infrastructure (e.g., operating system and computer hardware). It should not depend on (project management) tools that are not freely available.
8. **Allow adaptation to different styles of work**. ENCORE should leave sufficient flexibility to accommodate different styles of work. The underlying sFSS should be accessible from any software tool the researcher might be using.

The sFSS in context

The sFSS is the project's entry point (**Figure 2**) and, therefore, should be self-contained, which is the responsibility of the project team. The software developed in the project and the external software documentation are additionally managed through Git and the project's GitHub repository to enable version control and joint development. The principled decision to only make code and code documentation available on GitHub and exclude other project components such as data and results, is motivated by the requirement to create a self-contained sFSS project bundle while GitHub is not a universal storage platform. In addition, the size of the data and results may be too large to host on GitHub. Consequently, in practice, an sFSS contains only the software version that will be shared, while the GitHub repository may also contain older or alternative versions not required to reproduce the computational results. The complete project bundle can be shared with other researchers or reviewers or submitted to public repositories such as Zenodo for archiving, in which case a DOI can be assigned. Providing third-parties access to the GitHub repository is optional.

[FIGURE 2]

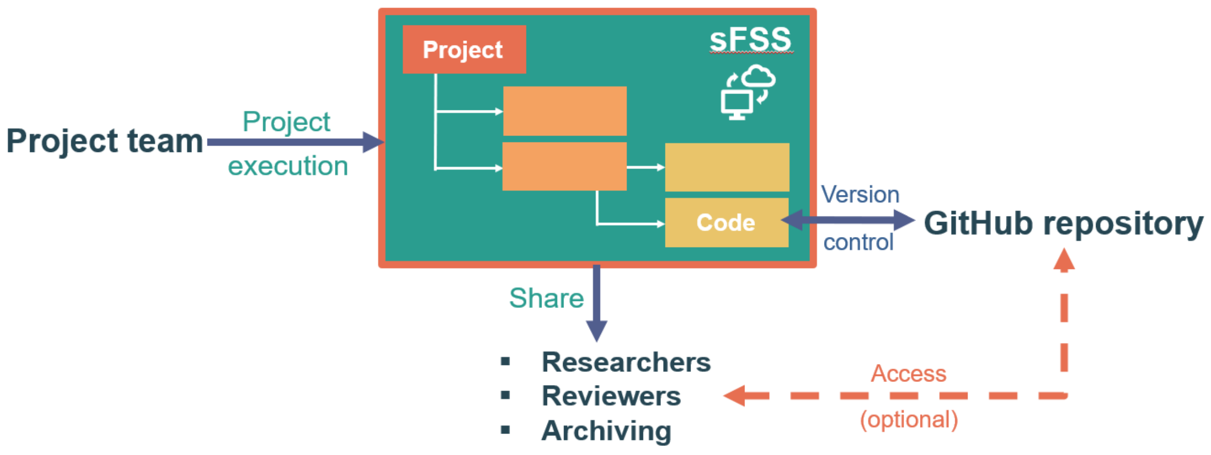


Figure 2. The sFSS and its environment. The green box denotes the sFSS with small part of the directory structure shown. The sFSS is the central point of entry for a project. The project team is responsible for the organization and documentation of the project. Only the code and code documentation are synchronized to the project's GitHub repository. An sFSS project bundle can be shared (in the cloud) or archived in a public repository.

Instantiation of a new ENCORE-based project

ENCORE enables several approaches to set up a new project. The approach used for most research projects is to first copy and initialize the sFSS template from the ENCORE GitHub repository. Subsequently, one creates a new project GitHub repository and connects it to the new project. Finally, one starts documenting the project. This approach is documented in detail in the ENCORE Step-by-Step guide (**Supplementary File 1**) and takes less than 30 minutes to complete. Another option is to generate a small program (script) that retrieves the sFSS template from the ENCORE GitHub repository and automatically fills in certain portions of the required documentation, which is particularly useful if one conducts projects with a certain degree of similarity. For specific cases, one may also write software that does not use the sFSS GitHub template but generates the structure and files itself. However, this is not recommended since such software can easily get outdated with further modifications to the sFSS template.

The ENCORE components

ENCORE comprises five main components (**Figure 3**) to structure, integrate, control code and documentation versions, and to improve transparency and reproducibility of a project.

[FIGURE 3]

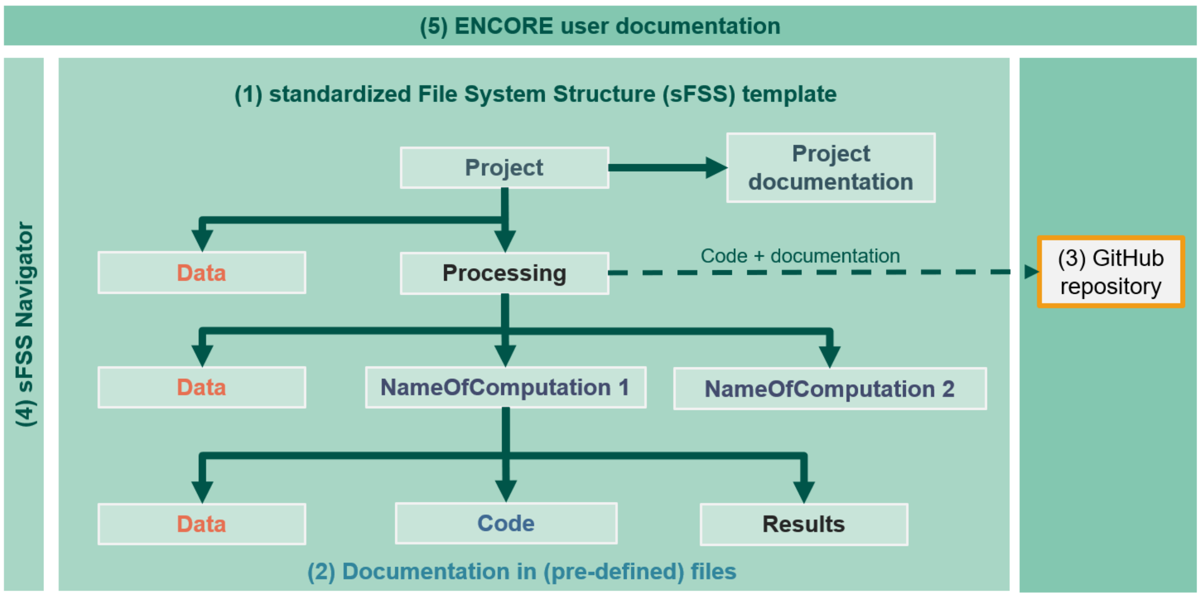
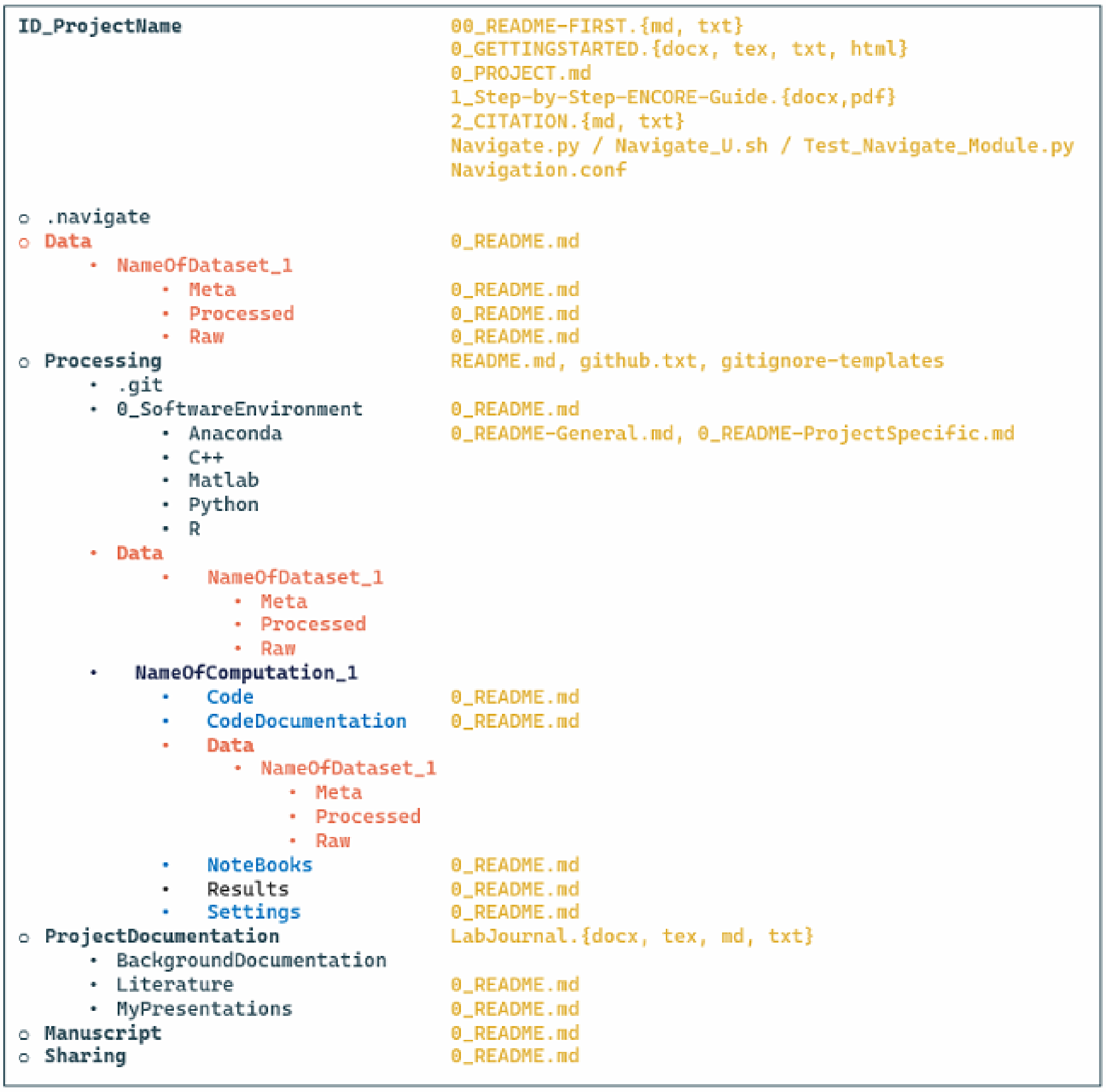


Figure 3. Five components of ENCORE. The main component comprises the sFSS template (1) that organizes all parts of the project. 'Project' corresponds to the root directory of the template. The blocks represent project dependent sub-directories (**Figure 4**). Project documentation resides in (pre-defined) files (2) that are found in all subdirectories of the sFSS template. The pre-defined files contain instructions about the minimum information that needs to be provided in terms of documentation for the different parts of a project. Each project is complemented with a GitHub repository (3) for version control of the code and documentation in the 'Processing' (sub-)directories. The sFSS Navigator (4) allows (end) users to browse the main contents of the project. The external ENCORE user documentation (5) provides instructions for new users on how to instantiate a new project.

Component 1. The standardized File System Structure (sFSS) template

The sFSS provides a standardized, yet flexible, template to organize conceptual information, data, code, documentation, and (intermediate) results (e.g., tables, figures, text files). In essence, it is a standardized directory structure containing pre-defined files, which can be used with any operating system (**Figure 4**) and can be used with any data analysis software that reads from and writes to a file system. Conceptual information includes any information considered relevant to correctly setup the computations, but also information that helps peers to understand the (background of the) project and information that documents why specific choices were made. This includes information about the research question, experimental design, samples used, wet-lab experiments, description of computational (for example, statistical or mathematical modelling) approaches, interpretation of results, relevant literature, presentations about the project, and summaries from (email) discussions during the project. Files within the sFSS may exist as different versions if, for example, new data was generated, code was modified, or figures were updated based on different settings for the computations. The information within the sFSS is implicitly and explicitly integrated. Implicit links correspond to relations that are imposed due to the hierarchical structure of the sFSS. Explicit links are made in the (code) documentation, for example, by linking a particular computation to a specific subset of the data. The sFSS allows a certain degree of flexibility to accommodate different types of projects or different ways of working. For example, data can be organized at different levels in the sFSS (**Figure 3**). This allows, for example, to organize the data directly within the subdirectory of a specific computation, if that data is not used by other computations. Similarly, if a project involves the (pre)processing of data, then the outcome of these steps may either be considered as a 'Result' in a 'NameOfComputation' directory, or as 'Processed data' in a 'Data' directory (**Figure 4**). The 'LabJournal' can be copied to other directories to accommodate more specific documentation. Markdown README files for project documentation may be replaced with other file types (e.g. LaTeX) if one prefers. Pre-defined sFSS directories and files that are not used can be removed. Detailed information about specific structure of the sFSS directory structure can be found in **Supplementary File 2**.

[FIGURE 4]



```
ID_ProjectName                           00_README-FIRST.{md, txt}
                                         0_GETTINGSTARTED.{docx, tex, txt, html}
                                         0_PROJECT.md
                                         1_Step-by-Step-ENCORE-Guide.{docx,pdf}
                                         2_CITATION.{md, txt}
                                         Navigate.py / Navigate_U.sh / Test_Navigate_Module.py
                                         Navigation.conf

o .navigate
o Data                                   0_README.md
    • NameOfDataset_1
        • Meta                           0_README.md
        • Processed                      0_README.md
        • Raw                            0_README.md
o Processing                             README.md, github.txt, gitignore-templates
    • .git
    • 0_SoftwareEnvironment              0_README.md
        • Anaconda                       0_README-General.md, 0_README-ProjectSpecific.md
        • C++
        • Matlab
        • Python
        • R
    • Data
        •  NameOfDataset_1
            • Meta
            • Processed
            • Raw
    •  NameOfComputation_1
        •  Code                          0_README.md
        •  CodeDocumentation             0_README.md
        •  Data
            • NameOfDataset_1
                • Meta
                • Processed
                • Raw
        •  NoteBooks                     0_README.md
        •  Results                       0_README.md
        •  Settings                      0_README.md
o ProjectDocumentation                   LabJournal.{docx, tex, md, txt}
    • BackgroundDocumentation
    • Literature                         0_README.md
    • MyPresentations                    0_README.md
o Manuscript                             0_README.md
o Sharing                                0_README.md
```

Figure 4. The standardized File System Structure (FSS) and associated pre-defined files. Standardized directory structure of the sFSS containing pre-defined files (brown), which include README files (in Markdown format) that provide a documentation template and instructions. Note that the pre-defined files in the 'Data' directories (red) and the '0_SoftwareEnvironment' subdirectories are only shown once. The names of the directories 'NameOfDataset_1' and 'NameOfComputation_1' are placeholders and should be replaced with more descriptive names. These directories can be replicated if multiple datasets are used or if different computation procedures are performed. Subdirectories shown in light blue are under version control using Git/GitHub. The '0' prefix ensures that the corresponding files/directories are always on top of the file list when using lexicographic ordering. The README.md in 'Processing' is the default GitHub repository README file and therefore does not have the '0' prefix.

Component 2. Pre-defined files

The sFSS contains many pre-defined files that should be used directly from the start of the project and maintained throughout the project (**Figure 4**). Most files are Markdown files, which was chosen as a file format because Markdown is the default for the README file of a GitHub repository. Markdown is a markup language, which enables adding formatting elements to plain text (Markdown, 2023) and requires a compatible editor. However, if preferred, these may be replaced by other file formats (e.g., LaTeX, HTML, Microsoft Word). In the sFSS root directory, the *0_PROJECT.md* file should provide basic project details, including the project name, start date, a short description, and project team. In addition, the *0_GETTINGSTARTED* template (HTML, tex, docx, txt) should describe the most important aspects of the project and should provide links to the relevant sub-directories and files. This final template is then saved as a HTML file and together with *0_PROJECT.md* used by the sFSS Navigator (see below). The *LabJournal* template (tex, docx, md, txt) in *ProjectDocumentation* should contain general project documentation including but not limited to an explanation of the project's background and concepts, computational approaches, summaries of project discussions, new research ideas, and to-do lists. Preferably, the lab journal should contain pointers to relevant sub-directories and files whenever needed. Alternatively, one may maintain multiple lab journals in different directories containing documentation for specific parts of the project. The lab journal is important for the scientific legacy of the research group by ensuring that others can replicate what the original researcher(s) has done. We decided to deviate from standard practice and to also use the lab journal to record new ideas, provide summaries of (email) discussions, and to-do lists, since it is important to have a record of these for the supervision of the projects and for follow-up projects. Consequently, not all information in the lab journal can be shared with others (see Discussion). Each directory also contains a Markdown README file that is specific for the directory in which it is located. In general, these README files contain an explanation of the information found in that specific directory, instructions, and a documentation template specifying the minimum required documentation that a researcher should provide (**Supplementary File 3)**. The instructions and templates are basically a translation of a selection of published guidelines to enhance reproducibility of computational projects. This is an essential part of ENCORE since following the instructions and templates will likely improve the reproducibility of the project while preventing the researcher from reading the many publications about computational reproducibility to deduce what should be documented and why. The instructions and templates also enforce internal consistency of the sFSS and promote consistency between different ENCORE projects within the same research group. One decision to be made by the project team is how to distribute the documentation over the various README files and the lab journal(s). However, as a rule one should document any project file (code, data, results) in the directories in which these are located. The lab journal can then be used for more general documentation.

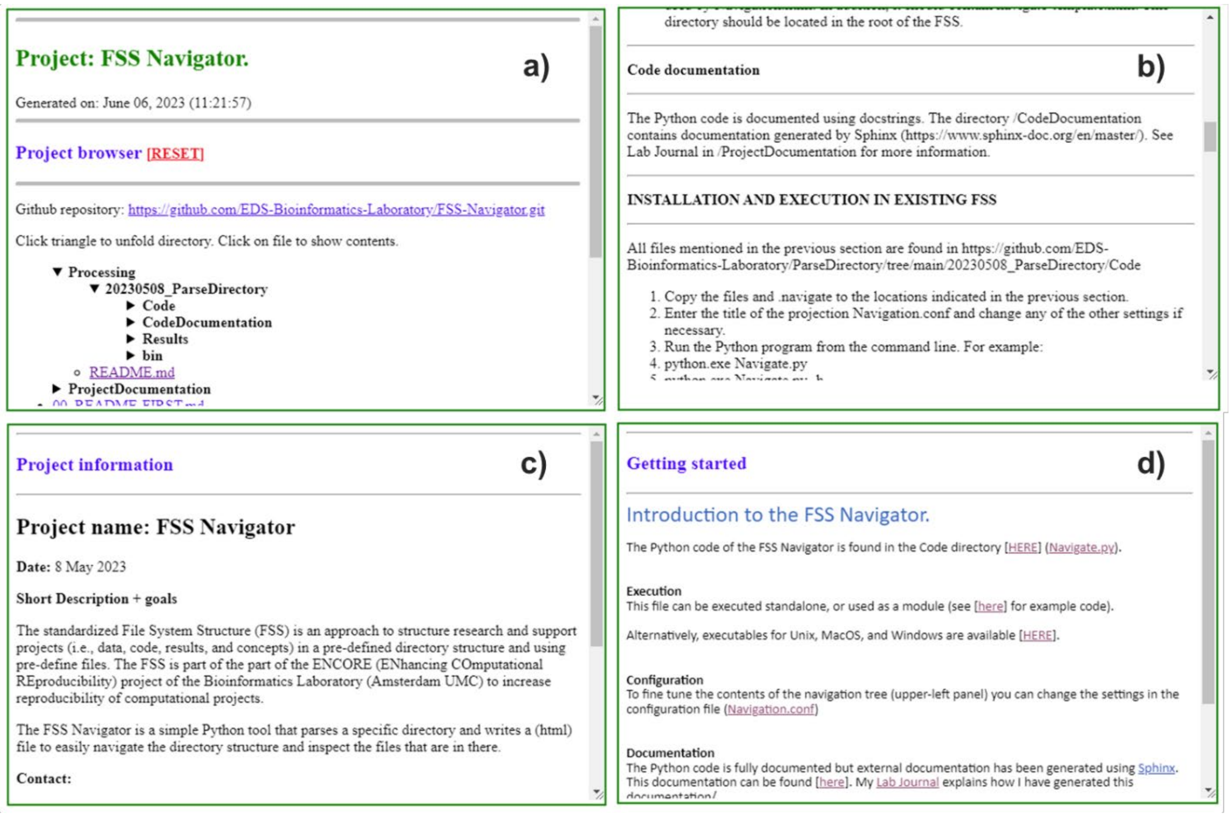
Component 3. The GitHub repository

ENCORE utilizes Git and GitHub for version control of software and its documentation, and to collaborate on software development. Since the sFSS project bundle contains all information of a project, it is not necessary to also share the GitHub repository. However, the project team may still share this repository or make it public in case of joint code development or if access to previous code versions is requested or required. To ensure that only code, (Jupyter) notebooks, software settings, and documentation is managed by Git, the project owner needs to configure the so-called '.ignore' file of which templates are provided in the sFSS (**Supplementary File 1**) (GitHub, 2023).

Component 4. The sFSS Navigator

At later stages of a project, the sFSS may contain a large amount of information potentially making it difficult for peers to determine the best point of entry. Therefore, we developed the sFSS Navigator to provide a first overview of the project. It also provides a convenient tool to, for example, browse and show results while the project is still active. The sFSS Navigator itself was developed following the ENCORE approach, and the project bundle can be found in Zenodo (Van Kampen et al., 2023). The Navigator is a Python program, which scans the sFSS and generates a web page (Navigate.html) that can be opened in any web browser. In addition to the Python code (Navigate.py), executables for

Windows, macOS (for both Intel- and silicon-based chips) and shell scripts for Linux/Unix using Python v3 are provided to ensure the Navigator can be used if the Python interpreter is not installed. The generated web page consists of four panels (**Figure 5**). The content of the panels is configured by the project owner to guide peers to the important parts of the project.



Project: FSS Navigator.

Generated on: June 06, 2023 (11:21:57)

Project browser [RESET]

Github repository: https://github.com/EDS-Bioinformatics-Laboratory/FSS-Navigator.git

Click triangle to unfold directory. Click on file to show contents.

- ▼ Processing
  - ▼ 20230508_ParseDirectory
    - ▶ Code
    - ▶ CodeDocumentation
    - ▶ Results
    - ▶ bin
  - README.md
- ▶ ProjectDocumentation

directory should be located in the root of the FSS.

Code documentation

The Python code is documented using docstrings. The directory /CodeDocumentation contains documentation generated by Sphinx (https://www.sphinx-doc.org/en/master/). See Lab Journal in /ProjectDocumentation for more information.

INSTALLATION AND EXECUTION IN EXISTING FSS

All files mentioned in the previous section are found in https://github.com/EDS-Bioinformatics-Laboratory/ParseDirectory/tree/main/20230508_ParseDirectory/Code

1. Copy the files and .navigate to the locations indicated in the previous section.
2. Enter the title of the projection Navigation.conf and change any of the other settings if necessary.
3. Run the Python program from the command line. For example:
4. python.exe Navigate.py

Project information

Project name: FSS Navigator

Date: 8 May 2023

Short Description + goals

The standardized File System Structure (FSS) is an approach to structure research and support projects (i.e., data, code, results, and concepts) in a pre-defined directory structure and using pre-define files. The FSS is part of the part of the ENCORE (ENhancing COmputational REproducibility) project of the Bioinformatics Laboratory (Amsterdam UMC) to increase reproducibility of computational projects.

The FSS Navigator is a simple Python tool that parses a specific directory and writes a (html) file to easily navigate the directory structure and inspect the files that are in there.

Contact:

Getting started

Introduction to the FSS Navigator.

The Python code of the FSS Navigator is found in the Code directory [HERE] (Navigate.py).

Execution
This file can be executed standalone, or used as a module (see [here] for example code).

Alternatively, executables for Unix, MacOS, and Windows are available [HERE].

Configuration
To fine tune the contents of the navigation tree (upper-left panel) you can change the settings in the configuration file (Navigation.conf)

Documentation
The Python code is fully documented but external documentation has been generated using Sphinx. This documentation can be found [here]. My Lab Journal explains how I have generated this

Figure 5. The sFSS Navigator. (a) Expandable sFSS directory tree and link to the project's GitHub repository. The project owner can configure, which directories and files to show. (b) Content of a selected file. In this example, the panel shows the content of the default GitHub Markdown README file. (c) General project description, contact person, and collaborators (0_PROJECT.md). (d). Getting started explains the project and includes links to the various files and directories in the sFSS (0_GettingStarted.html).

Component 5. User documentation

ENCORE is complemented with extensive documentation to guide the user in setting up a new project and maintaining documentation throughout the project. In addition to the documentation already present in the pre-defined files, we have created a comprehensive 'Step-by-Step ENCORE Guide' (**Supplementary File 1**). This guide offers a brief introduction to the ENCORE principles and components and provides a recipe for instantiating an sFSS for a specific project, a corresponding GitHub repository, and the sFSS Navigator. It also includes a basic introduction to Git and GitHub for troubleshooting purposes.

General ENCORE guidelines

The initialization of an ENCORE-based project is straightforward and does not take much time. However, it is important to keep working according to the provided instructions and to keep the documentation continuously up to date. Recollecting (from memory) all important details at the end of a project is virtually impossible. Moreover, this will take significantly more time than gradually adding documentation during the project. While organizing and documenting a project, one should assume that at some stage the project is going to be shared with a peer who is initially unfamiliar with the project, the computational concepts, the type of data, and the programming language. Although it may be tempting to document all aspects of the project in a single document eventually evolving into a manuscript to be submitted for peer review, we advise not to do so for several reasons. First, it breaks the connection between the documentation and the files (e.g., code or data) being documented. Second, the level of documentation in an sFSS is likely to be much more detailed than what is provided in a typical research paper. Even the manuscript's supplementary information may not provide the same level of detail. Third, since ENCORE is used right from the start of a project, it is likely that not all parts of the project end up in a publication. For example, not all (intermediate) results will become part of a publication. In addition, documenting specific approaches that failed may be equally important. Fourth, keeping the documentation modular and in the directories where it belongs helps in its maintenance. Once the manuscript will be written then the parts of the documentation that are needed can easily be incorporated. We also recommend that the overall sFSS structure, names of directories (with exceptions mentioned earlier), and names of pre-defined files are not changed. This holds in particular for research groups that embrace this approach to achieve harmonization. Additional directories may be added if this does not effectively change the overall sFSS structure. For example, within the *Results* directory, one may create separate sub-directories for figures and tables, but one should not move *Results* to the root of the sFSS. As mentioned earlier, unused directories and files should be removed. Since an sFSS should be self-contained, any directory path used within the code or in any of the pre-defined files should be relative to the top-level directory.

Results

Initial discussions and review of publications to improve reproducibility of research projects in our group started in 2018 (**Figure 6**), and consistently involved all group members (i.e., staff, postdocs, PhD students, and internship students). This led to the aims specified in the introduction (transparency, reproducibility, harmonization) and to a first version of ENCORE in October 2020. At the same time, we initiated a GitHub organization account (GitHub accounts, 2023) to host all ENCORE repositories from our group. The use of ENCORE was made mandatory for all new research projects and for everyone in our group. This initial step led to the harmonization of project organization within our group. Currently, we have over 20 ENCORE research projects. In addition, we have over 50 ENCORE projects for data analysis services provided to other groups.

[FIGURE 6]

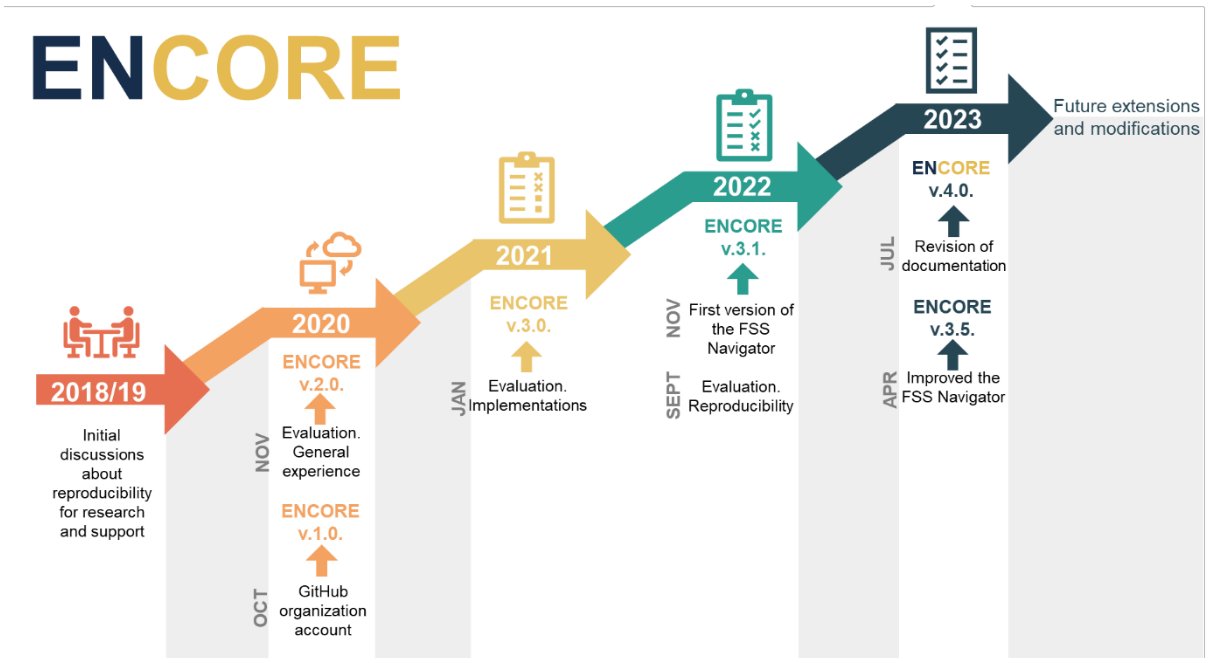

ENCORE
2018/19
Initial discussions about reproducibility for research and support
2020
ENCORE v.2.0.
NOV
Evaluation. General experience
ENCORE v.1.0.
OCT
GitHub organization account
2021
ENCORE v.3.0.
JAN
Evaluation. Implementations
2022
ENCORE v.3.1.
NOV
First version of the FSS Navigator
SEPT
Evaluation. Reproducibility
2023
ENCORE v.4.0.
JUL
Revision of documentation
ENCORE v.3.5.
APR
Improved the FSS Navigator
Future extensions and modifications

Figure 6. ENCORE evolution and evaluation. ENCORE evolved through different versions incorporating changes based on practical experiences, evaluations, and group discussions. This led to gradual improvements in the ENCORE approach and documentation, broader use for research projects, and Git/GitHub proficiency within our research group. In turn, this led to better and more transparent organization of projects and increased reproducibility. Further changes are expected in the future. l

Evolution and evaluation

Based on experience with an increasing number of projects, internal evaluations, and frequent discussions about the structure, pre-defined files, and usage guidelines, we gradually improved the initial setup. Overall, over the past three years, this led to a simplification of the sFSS structure, a reduced number of pre-defined files, and better ENCORE instructions and documentation.

A first evaluation was performed one month after introducing ENCORE 1.0 to exchange user experiences, which led to ENCORE 2.0. About three months later, in January 2021, we organized a second evaluation, during which each group member presented an ENCORE project. This evaluation made clear that most research projects adopted the sFSS structure, but that documentation (e.g., README files, lab journal) was occasionally incomplete or missing since keeping documentation up to date was perceived as overhead and time-consuming but also because it was often unclear what level of detail needed to be provided since no clear objectives were set. Some projects did not fully adhere to the sFSS naming and structure conventions, which was partially due to unclear or implicit ENCORE guidelines but also because some were still inclined to stick to old habits. Based on this evaluation we developed ENCORE 3.0, which comprised further simplifications of the directory structure (fewer directory levels), renaming of pre-defined files to improve consistency, and improved documentation (i.e., usage rules). In September 2022, we evaluated ENCORE 3.0 to test if ENCORE had indeed improved the reproducibility of our projects. We selected nine ENCORE projects, which were assigned to group members not involved in that project. Subsequently, each project was evaluated for the correct use of the sFSS, the pre-defined files and the level of documentation. In addition, each group member was asked to reproduce a specific subset of project results. The most important outcome of this evaluation was that only for about half of the selected projects the results could be reproduced. Various reasons prevented (full) reproducibility such as the use of different library versions used by the software, use of absolute directory paths that were not valid after transferring the sFSS to a different location, differences between operating systems, lack of instructions on which software to install and how to run the software, compilation problems, software errors, or difficulties in handling large datasets. In addition, some of the projects were difficult to understand due to lack of documentation (transparency) about goals and applied methodology. Some of these problems can easily be fixed such as changing absolute to relative directory paths. Other problems such as dealing with different library versions may require more effort to solve (see Discussion). Several other outcomes resulted from this evaluation. First, not being acquainted with a specific project, it sometimes was difficult to find the (core) information that is needed to reproduce and understand a project. This triggered the development of the sFSS Navigator, which was implemented as an R application in ENCORE 3.1 and later re-implemented in Python and extended in ENCORE 3.5. Second, despite more than two years of discussion and joint decision making about the structure of ENCORE, there was still debate about (how to use) the sFSS structure and the pre-defined files. The sFSS structure and files had been agreed upon by consensus, but still was a compromise of different structures previously used by individual group members. As a result, some parts of it seemed illogical to some members, who ideally still preferred a different setup. In addition, although the ENCORE user guidelines and their rationales had been discussed, agreed upon, and written down, it turned out to be difficult to memorize and apply all these rules. In our view this is also one of the main reasons that existing published guidelines are not consistently applied. At the same time, the user documentation was scattered over many files and lost consistency over the evolution of ENCORE. This prompted the changes incorporated in ENCORE 3.5 and 4.0. Specifically, these include the completion of the Step-by-Step ENCORE Guide (**Supplementary File 1**) and the merger of documentation and templates directly in the README files (e.g., **Supplementary File 3**). Third, the provided level of detail for the documentation of most projects was inadequate, partially caused by unclear guidelines. For example, it was not always clear how to run the software because our guidelines didn't make explicit how this should be documented and at what level of detail. One specific issue was that the lab journal often did not contain an adequate summary of (supervisory) meetings and email exchanges. It was therefore agreed that it is the responsibility of the project team to ensure that all relevant documentation is incorporated in the sFSS. Finally, it became clear that project organization and documentation often had lower priority than doing the actual research. For these reasons, most projects did not fully adhere to the ENCORE guidelines. Nevertheless, we decided to keep the approach mandatory and to only make minor changes to the current template to prevent delay in its further development.

Using remote computer systems with ENCORE

Most of our ENCORE projects reside in the cloud and are synchronized with the local computers (e.g., laptop) of the project participants. However, it is not uncommon to use dedicated compute infrastructure such as computer clusters to perform (part of) the computations. The sFSS is compatible with such scenario. One may simply transfer (part of) the sFSS to the remote system and, subsequently, perform the calculations there. Results can then be transferred back to the cloud and local computer (**Figure 7**).

[FIGURE 7]

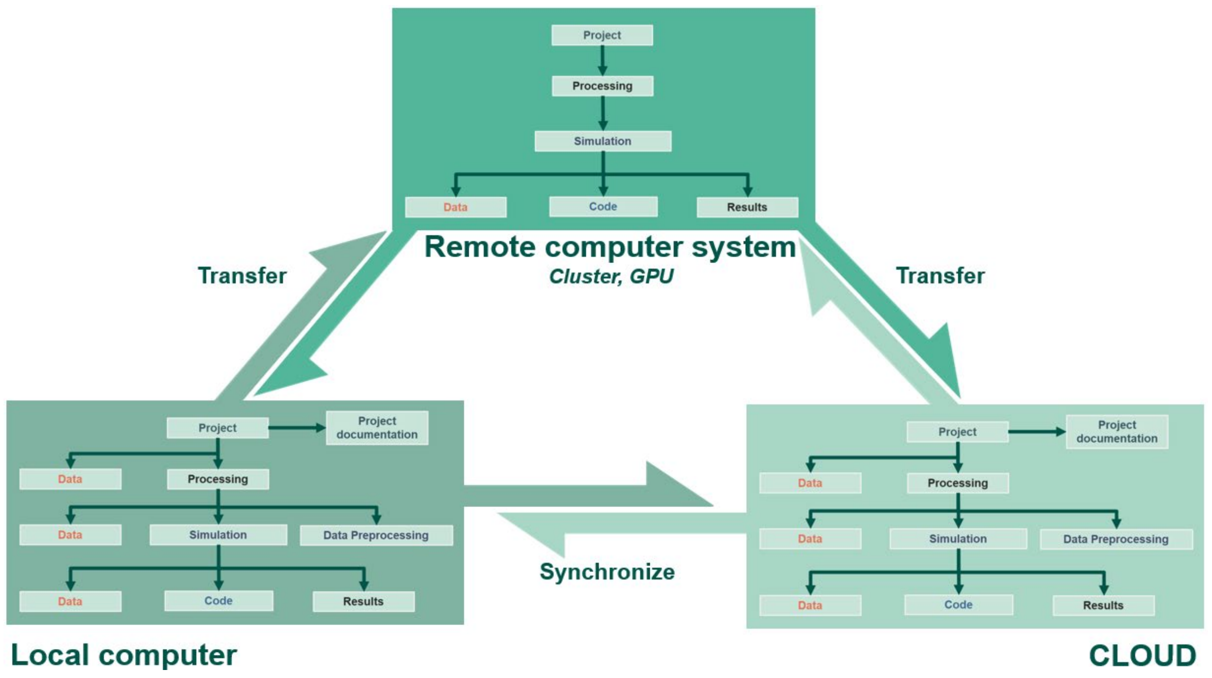


Figure 7. Using remote computer systems with ENCORE. A specific ENCORE project that contains code for data pre-processing and a simulation. The ENCORE project may reside in the cloud and/or on a local laptop or desktop computer to which it is synchronized. Specific computations that require dedicated hardware (e.g., computer cluster, GPU processors) can be performed on such system by temporarily transferring all or part of the sFSS between the local system and the remote computing system. In this example, only the simulation branch is transferred. To transfer files to the remote computer system one may use common data transfer tools, such as curl or rclone that support many data transfer protocols such as sFTP and SCP.

Discussion

We presented ENCORE as a practical implementation guiding researchers on how to structure and document computational projects according to published guidelines (Brito et al., 2020; Sandve et al., 2013; Spreckelsen et al., 2020; Turkyilmaz-van der Velden et al., 2020) in order to improve transparency and reproducibility, and to allow harmonization within a research group. ENCORE does not consider replicability (sometimes referred to as repeatability), which is about strengthening scientific evidence from replication studies by other research groups using independent data, and experimental and computational methods (Milkowski et al., 2018; National Academies of Sciences & Medicine, 2019; Patil et al., 2019; Plesser, 2017). An important aspect of ENCORE is the integration of all project information (concepts, data, code, results, documentation) in a single directory structure that can easily be shared and archived. Although we didn't have a pre-ENCORE baseline measurement for reproducibility in our group, ENCORE harmonized the way we work in a broad range of projects, and provided a big step forward in terms of the organization, transparency, and reproducibility of our projects. Integration and documentation to achieve transparency have also been referred to as the third dimension of open science (Lyon, 2016) and are in our view key to reproducibility of computational research.

ENCORE can be applied to virtually any type of computational project, it is agnostic to the computational infrastructure, and it can be used with any programming language or software tool the researcher is using. Over the past few years, we have experienced that it is crucial to use ENCORE from the start of a project and to have sufficient self-discipline to keep everything up to date. The ENCORE documentation is essential for introducing new ENCORE users to the underlying philosophy and approach and to provide background on the structure and desired level of project documentation.

Different areas of reproducibility are distinguished by Stodden (Stodden, 2015). (i) Empirical reproducibility refers to physical experiments and the (reporting) standards associated with these. (ii) Computational reproducibility is concerned with the reproduction of results using the same data and computational methodology. (iii) Statistical reproducibility focuses on the correct use of experimental design (including sample size calculations) and statistical analyses. (iv) Ethical reproducibility refers to reporting ethics methods in biomedical research (Anderson et al., 2013). ENCORE focuses on computational reproducibility and statistical reproducibility, at the same time taking into account that documentation about the physical experiments can be important for the computational analyses. Ethics reproducibility may come into play for specific (artificial intelligence) applications e.g., (Kulikowski & Maojo, 2021) but is not explicitly considered by ENCORE.

ENCORE promotes a pre-defined directory structure, integration of data, methods, and results, and detailed project documentation. This supports the continuity of research lines which are sometimes compromised by the continuous flux of scientific personnel in academic groups. ENCORE contributes to transparency and, as such, helps to detect software errors or conceptual methodological flaws by (external) researchers, supervisor(s), and reviewers. Transparency allows project supervisors to provide timely and more constructive feedback. Co-authors of a manuscript can more easily inspect details of the project before manuscript submission to, for example, comply with the ICMJE authorship rules (ICMJE, 2023). A recent editorial in Nature Human Behaviour (Editorial, 2021) proposed that software be part of the peer review process. ENCORE would facilitate such efforts since, in principle, it provides user documentation to install and use the software and datasets. Generally, it would be very time consuming and difficult to check the code itself, but reviewers could at least check if results presented in a paper can be reproduced by executing the software.

Increasing reproducibility, what is the problem?

The main hurdle to increase reproducibility of computational projects is neither the lack of guidelines nor substantial technical barriers. However, despite all discussions and initiatives concerning reproducibility, and our personal observation that many researchers agree on the importance of reproducibility, there still is a long way to go. Regularly, during the development of ENCORE, group members brought forward various arguments for not following (ENCORE) guidelines. For example, one argument being that it consumes time while we are virtually never asked by peers, reviewers, or funding agencies whether our research is reproducibility. In fact, there is often no penalty for being non-reproducible and, moreover, there also is no clear reward for being reproducible. Markowetz gives several examples of benefits of working in a reproducible manner (Markowetz, 2015), but he also encountered resistance from researchers when advocating reproducible research such as “I’d rather do real science than tidy up my data”. Indeed, an often-heard argument concerns the amount of overhead that comes along with (ENCORE) reproducibility approaches. However, for a typical research project, the time spent on following the ENCORE approach (e.g., documentation, structuring) is in our view negligible compared to the time spent on the actual research. There are clear advantages for working reproducibly as argued by other groups as well (e.g., (Diaba-Nuhoho & Amponsah-Offeh, 2021; Sandve et al., 2013; Stodden et al., 2012). For example, reproducibility is important for trust in science, it helps writing a publication, it will save time in the long run, and it supports the sustainability of the research. Although all true, for some researchers these arguments do not seem to provide enough incentives to improve their practices. Bottom line is that reproducibility requires intrinsic motivation, working attitude, and discipline, or otherwise can only be enforced with penalties and/or rewards. Indeed, it is well-recognized that the way in which we reward science should be changed. For example, the Declaration on Research Assessment (DORA) is a global initiative that proposes to change the evaluation of researchers and scholarly research output by funding agencies, academic institutions, and other parties (DORA, 2023). Complementary, at the national level similar initiatives emerged. For example, the Dutch public knowledge institutes and research funders wrote a position paper that, among others, encourages Open Science (VSNU et al., 2019). In addition, projects like Osiris aim to identify incentives for reproducibility by stakeholders, and embedding reproducibility in research design (Osiris, 2024). Due to such initiatives, we slowly witness a change in the reward system, and we expect that this will largely contribute to more reproducible research. Stodden and co-workers suggested to have journals and/or professional societies discern a yearly award for (young) investigators for excellent reproducible practice (Stodden et al., 2012). ENCORE perfectly matches with these suggestions and would contribute to building the researcher's scientific track record. An ENCORE project bundle can be shared through public repositories and assigned a DOI. We recently submitted the first ENCORE project to Zenodo (Van Kampen et al., 2023) and most of our future publications will be accompanied by an ENCORE project. In addition, we are preparing a publication describing specific challenges encountered when using ENCORE for a benchmark study for spatial transcriptomics deconvolution methods (Mahamune et al., In preparation).

Limitations of ENCORE

We consider ENCORE to be a step towards reproducible science, but it is not without several limitations and weaknesses. First, ENCORE is a compromise based on previous ways of working and, therefore, may not always fit the preferred way of working of an individual researcher. However, we believe ENCORE provides sufficient flexibility to accommodate most researchers and research practices. Second, the current sFSS Navigator has limited functionality, ways to present information, and possibilities to configure. We are in the process of improving the Navigator. Third, a shortcoming of ENCORE is the lack of and clear and easy approach to specify explicit links between results, code, data, and concepts. Currently, such links are imposed by the sFSS structure, the paths in the code, and/or manually added links specified in the documentation. The documentation has an important function in gluing the project parts together, but it requires effort from the researcher to specify relations between parts of the project, and to maintain this information. ENCORE would benefit from improved integration approaches to improve transparency and reproducibility. One possible approach is the use of YAML (YAML, 2023) as demonstrated by Spreckelsen and co-workers (Spreckelsen et al., 2020). Fourth, another challenge that is only partially addressed by ENCORE concerns the preservation of the full computing environment. This environment is defined by (interdependencies of) the operating system, software tools, versions and dependencies, programming language libraries, etc. Gruning and co-workers proposed a software stack of interconnected technologies to preserve the computing environment (Gruning, Chilton, et al., 2018). This stack comprises (i) (Bio)Conda (Anaconda Software Distribution, 2020; Gruning, Dale, et al., 2018) to provide virtual execution environments addressing software versions and dependencies, (ii) container platforms such as Docker (Nust et al., 2020) to preserve other aspects of the runtime environment, and (iii) virtual machines using cloud systems or dedicated applications such as VMware, to overcome the dependencies on the operating system and hardware. We are currently investigating how to best approach this within the context of ENCORE. Reproducibility can further be improved by using scientific workflow systems, which have been developed to modularize and execute steps in computations. Many workflow systems are available, including Galaxy (Galaxy, 2022), KNIME (Berthold et al., 2008), Snakemake (Molder et al.,

2021) and Nextflow (Di Tommaso et al., 2017). These workflow systems improve reproducibility and help to maintain and share computational analyses. They also allow incorporation of steps that otherwise would have been performed manually. Our group has used workflow systems in the past (e.g., (Boekel et al., 2015; Madougou et al., 2012)), but we decided not to make a workflow system an obligatory part of the ENCORE approach since we believe this may be too disruptive for some researchers. Yet, we encourage our group members to use a workflow system of choice. Fifth, ENCORE projects can easily be shared but currently we do not have a good mechanism to remove parts that should not be shared such as patient data, controlled access data obtained from public repositories, or PDF copies of copyright protected scientific publications. Finally, ENCORE requires that all data used by the computations are within the sFSS structure. For large datasets this implies that sufficient storage must be available. We encountered situations where sufficient storage was available in the cloud but not on a local computer (e.g., laptop; **Figure 7**) which may prohibit data inspection or data analyses. Moreover, also the (local) archiving of ENCORE projects requires sufficient storage space, which increases with the number of projects and the size of the datasets used.

Training, scientific computing, and software engineering

Over the past two decades, an increasing number of biomedical researchers have become involved in computational research. Many of these researchers have never been formally trained in scientific computing and software engineering (e.g., design, programming, documentation) (Hermann & Fehr, 2022; Martin, 2008), software version control (Blischak et al., 2016; Perez-Riverol et al., 2016), the use of high-performance computing infrastructures, the use of Unix/Linux which is still the major platform for scientific computing, algorithm design, the use of (Jupyter, R) notebooks (Rule et al., 2019), etc. Lack of such skills may negatively affect reliability and transparency of software and, consequently, reproducibility. For example, software may be poorly designed and documented, making it difficult to understand, use, modify, and debug. Software engineering is a discipline in its own and includes the design, implementation, documentation, testing and deployment of software. Following best practices for scripting, functional programming, or objective-oriented programming may significantly improve the quality of the code but requires training and experience. In addition, software documentation occasionally leaves much to desire. In a recent report, it was concluded that researchers are generally not aware for whom they write documentation and what documentation is required (Hermann & Fehr, 2022). Currently, ENCORE does not provide specific instructions for coding style (e.g., PEP 8 for Python and tidyverse for R; (Python Style Guide, 2024; Tidyverse Style Guide, 2024)) and documentation design because it is probably more effective to train scientist in the art of software engineering. Instead, general guidelines are provided in a README file (**Supplementary File 3**) Awareness of guidelines (e.g., (Karimzadeh & Hoffman, 2018)) and tools to (automatically) generate documentation such as Sphinx (Brandl, 2021) for Python, and r2readthedocs (r2readthedocs, 2023) and roxygen2 (Roxygen2, 2023) for R, will also help to improve reproducibility. We used Sphinx for the documentation of the sFSS Navigator (Van Kampen et al., 2023). Another useful resource is the software management plan developed by the Netherlands eScience Center and the Dutch Research Council (NWO) (Martinez-Ortiz et al., 2023). In general, appropriate training on reproducibility approaches could already significantly improve the current situation and will at least create awareness of the tremendous amount of literature about many aspects of sound scientific computing practices (Carey & Papin, 2018; Lapp et al., 2022; Larcombe et al., 2017; Toelch & Ostwald, 2018; Wilson et al., 2014; Wilson et al., 2017). In addition, senior researchers should strongly promote reproducibility and support, explain, and instruct junior researchers.

Complementary reporting guidelines and standards

To facilitate and improve reproducibility throughout the complete research lifecycle (**Figure 1**), numerous guidelines, policies, and standards have been developed (FAIRsharing.org, 2023) to guide and facilitate the detailed documentation of all steps. Many reporting guidelines provide structured tools specifying the minimum information required for specific study types and largely contribute to the transparency, understanding, and reproducibility of a study (EQUATOR Network, 2023). Examples include guidelines for clinical trials (CONSORT) (Schulz et al., 2010), diagnostic accuracy studies (STARD) (Bossuyt et al., 2015), and observational studies (STROBE) (von Elm et al., 2007). Virtually all these minimum information standards and reporting guidelines require the specification of statistical and computational methods that were used in a study. However, precise requirements to specify such methods are often lacking. In addition, an increasing number of scientific journals have their own guidelines. One example is the Nature Reporting Summary (Nature, 2023b) that partially relies on existing reporting guidelines and FAIR. Nature also has a specific software and algorithm policy with requirements about availability (e.g., using GitHub or Zenodo), use of an open-source license (Open Source Initiative, 2023), and code review (Nature, 2023a). Nature Computational Science and several other Nature journals have adopted Code Ocean, which is a cloud-based platform to share executable code to enable review (Editorial, 2018, 2022). The PLOS Computational Biology journal requires that editors and reviewers can access the software, reproduce the results, and run the software on a deposited dataset with provided control parameters (PLOS Computational Biology, 2023). The Science journal TOP guidelines require data and computer code to be available (Science, 2023). Interestingly, a study published in 2018 showed that despite these guidelines, many computational studies were not reproducible (Stodden et al., 2018). Clearly, computational projects require their own specific guidelines and standards to guarantee transparency and reproducibility. This was also recognized by the artificial intelligence community, which started initiatives to develop specific AI-oriented guidelines (Haibe-Kains et al., 2020; Ibrahim, Liu, & Denniston, 2021; Ibrahim, Liu, et al., 2021). To the best of our knowledge, there are not many (practical) reporting guidelines nor standards available for computational research that are routinely used in practice. Nevertheless, there are various initiatives to improve this situation. For example, recently detailed guidelines for a standardized file system structure for scientific data were published by Spreckelsen and co-workers (Spreckelsen et al., 2020), which inspired the sFSS used in ENCORE. However, they use a different organization, i.e., the top-level of their file system layout is not an individual project like in ENCORE but an experiment, simulation, data analysis, or publication. Recently, it has been suggested to apply the FAIR principles to software (Barker et al., 2022; Fair Software, 2023). Other examples include, the ICERM implementation and archiving criteria for software (Stodden et al., 2012), the Adaptive Immune Receptor Repertoire (AIRR) software guidelines (AIRR, 2023), the Software Ontology to describe software used to store, manage and analyze data (Malone et al., 2014), and the EDAM ontology to describe bioinformatics operations (Ison et al., 2013). For simulation-based research there are initiatives like the Minimum Information About a Simulation Experiment (MIASE) guidelines (Waltemath et al., 2011), the corresponding simulation experiment description markup language (SED-ML) (Smith et al., 2021), COMBINE/OMEX to share and reproduce modeling projects (Bergmann et al., 2014), and a range of others (Tatka et al., 2022). For the further development of ENCORE, we will need to consider which of these standards are relevant for ENCORE and how to incorporate them in the ENCORE approach.

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Author contributions.

AvK and PM led the development of ENCORE. UM made major contributions to improve ENCORE. All other authors contributed to the development, evaluation, and use of ENCORE. All authors contributed to this manuscript.

Competing interests.

No competing interests.

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