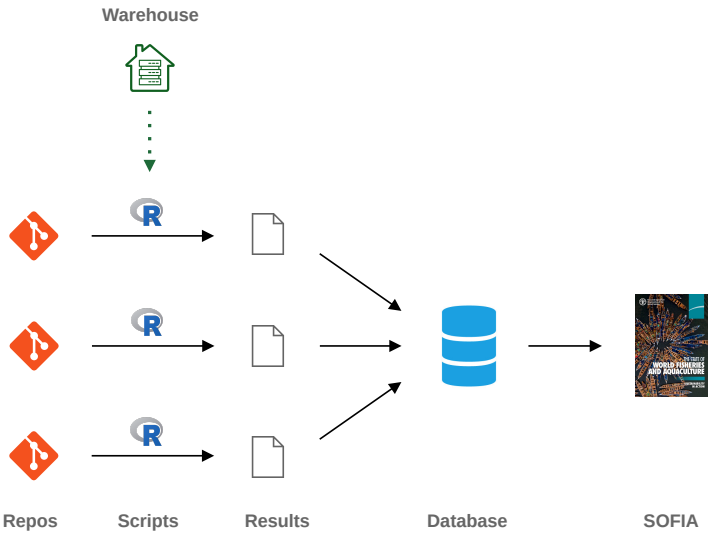
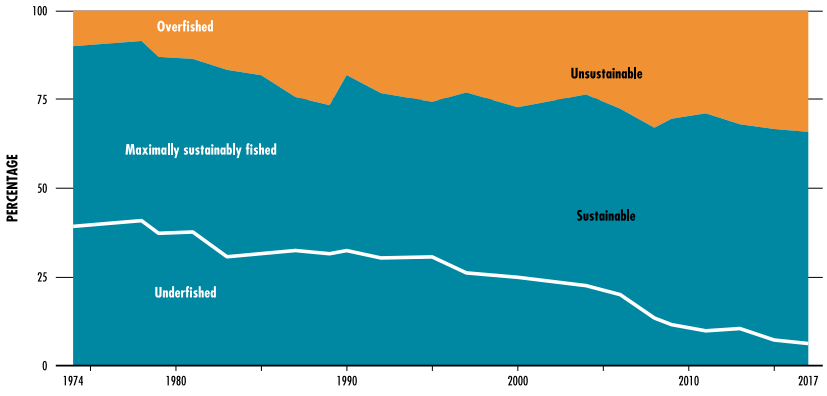
SOFIA Transparent Analytical Framework

Design and development progress





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1 Executive summary

This report gives a brief overview of the design and development progress of the new SOFIA Transparent Analytical Framework (SOFIA-TAF). The overall framework consists of four components:

- SOFIA-TAF repositories, where each repository contains one analysis, calculating the status of stocks in a given area.
- Input data warehouse, with fisheries data for all areas and stocks.
- R package, a collection of utilities that are commonly used in SOFIA-TAF analyses.
- Database, storing the results from all SOFIA-TAF analyses.

This report uses a similar structure as the previous report on SOFIA-TAF design and development progress report (Magnusson 2021), updating each section to reflect the current state of SOFIA-TAF. The main activities and milestones achieved in 2022 are listed in Table 1.

Table 1. Overview of main activities and milestones in 2022.

Jan 2022	SOFIA package version 1.0 released.
Feb 2022	SOFIA package versions 1.1 and 1.2 released.
May 2022	Workshop with experts in Area 37 (Mediterranean and Black Sea), based on 2022Area37Demo and other repositories.
Aug 2022	GitHub organization renamed from `sofia-tsaf` to `sofia-taf`.
—	SOFIA package version 2.0 released.
Oct 2022	SOFIA-TAF launch event at CAPAM Good Practices conference in Rome, with presentations by Rishi Sharma and Arni Magnusson.
Nov 2022	SOFIA package version 2.1 released.
—	Workshop with experts in Area 31 (W Central Atlantic), based on 2022Area31DemoEffortShared, 2022Area31DemoEffortByStock, 2022Area31DemoIndex, and other repositories.
—	Workshop with experts in Area 41 (SW Atlantic), based on 2022Area37DemoPriorsByStock and other repositories.
Dec 2022	SOFIA-TAF repositories developed in 2022 are in Areas 31, 37, 41, and 57.
—	Alternative GitHub site `https://github.com/sofia-taf-dev` created.
—	Progress report summarizes the overall design and the current development status.

At the end of this report is an appendix, listing Arni Magnusson's contributions in 2022 to SOFIA-TAF design and development.

2 Introduction

2.1 Background

To provide context behind the activities and milestones from SOFIA-TAF development in 2022, it is worthwhile to quickly review the 2021 timeline (Table 2). See Magnusson (2021) for details.

Table 2. Review of main activities and milestones in 2021.

Mar 2021	Initial design discussions.
—	Development begins by converting monolithic R Markdown document into modular TAF scripts in Area 37.
Apr 2021	Prototype analysis of Area 37 presented to the FAO team overseeing the SOFIA analysis.
Aug 2021	Presentation at NOAA National Stock Assessment seminar series.
Oct 2021	Regular development team meetings begin.
Nov 2021	Initial development of the SOFIA package.
Dec 2021	Total of 12 SOFIA-TAF repositories under development on GitHub.
—	Progress report summarizes the overall design and the current development status.

2.2 Objectives

It is not for this author to define or prioritize the objectives of SOFIA-TAF to support the overall analysis behind SOFIA. However, the following topics are worth mentioning, as a context for some of the design decisions and features that are being developed.

Efficiency is the ability to edit code in a single place to modify a large number of analyses, and to calculate top-level summary statistics from a large number of analyses.

Clarity is the ability to easily navigate to a specific part of the analysis of a particular stock group and area, and to look up a specific result from one or more analyses.

Traceability is the ability to backtrack exactly how a specific result was calculated, such as the status of a particular stock group in a given area.

Open science is the ability to make the R scripts available online, along with the input data required for the scripts to run, inviting peer review of methodology and scientific collaboration.

Reproducibility is the ability to run analyses on a variety of computers, e.g., a personal Windows laptop or a high-performance Linux cluster, to get the exact same result — also when the analysis is rerun months or years later.

Quality assurance is the design and adoption of a workflow that reduces the probability of making human mistakes when preparing, modifying, running, and postprocessing the results from analyses.

Quality control is the ability to identify where a human mistake has been made in a given analytical process, so the mistake can be located and corrected.

The initial development of SOFIA-TAF has focused especially on Tier 2 cases of SOFIA analyses, where official stock assessments are not available, but catch, effort, and survey index data exist as a basis for estimating stock status using data-limited methods.

The SOFIA-TAF design also aims to serve as a platform to organize Tier 1 analyses (deriving stock status from official stock assessments) as well as Tier 3 analyses (deriving stock status estimates from expert elicitation). These tiers will require less R code than Tier 2 but use the same structure for R scripts and data provenance to document exactly how the stock status was calculated.

3 Design

The SOFIA-TAF design (Figure 1) is based on repositories containing R scripts that read input from a data warehouse to estimate stock status. These results are then stored in a dedicated SOFIA-TAF database, which serves as the foundation for calculating summary statistics for the final SOFIA report.

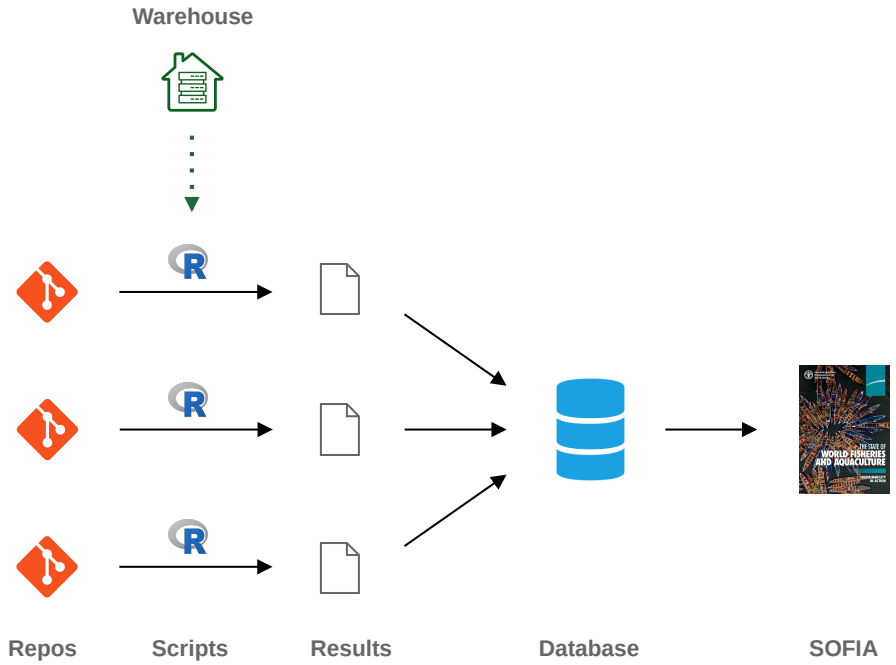

Figure 1. SOFIA-TAF diagram, showing the flow of information from individual repositories (analyses of stocks and areas) to the final SOFIA report.

The scripts use a dedicated R package called SOFIA. The next sections describe each component of the SOFIA-TAF design in some detail: repositories, input data warehouse, R package, and the database.

3.1 SOFIA-TAF repositories

3.1.1 Repository features

Each SOFIA-TAF repository is a unit of analysis, corresponding to a specific area and a set of stocks. A GitHub repository, sometimes abbreviated as 'repo', is an online directory that is especially convenient for organizing text files, such as scripts and data files. GitHub repository features relevant for SOFIA-TAF include:

- Ability to make scripts available online, for browsing and downloading, along with the input data required for the scripts to run.
- Automatic backup of all files with the ability to return to previous saved states.

- Tracked changes showing who changed what and when, supporting online teamwork.
- Ability to tag specific saved states of the analysis and give them descriptive names, such as 'starting point', '2021 data' or 'results imported to database'.
- Ability to upload large attachments (>100 MB) to accompany tagged states.
- Online facilities to compare text files and view changes, line by line.

3.1.2 R scripts

The analysis inside each repository consists of a set of R scripts that are organized in TAF format (Magnusson and Millar 2021). This means there are four standard scripts (Table 3) that conduct and document the analysis:

Table 3. Standard TAF scripts for a given analysis.

Script	Purpose
`data.R`	Preprocess data, write TAF data tables
`model.R`	Run analysis, write model results
`output.R`	Extract results of interest, write TAF output tables
`report.R`	Prepare plots and formatted tables

The TAF scripts are run sequentially, each reading files that were created in a previous step. The first script, `data.R`, reads data files that were declared and documented in a `DATA.bib` text file. A similar `SOFTWARE.bib` file can be used to declare specific versions of software used in the analysis, to strengthen reproducibility.

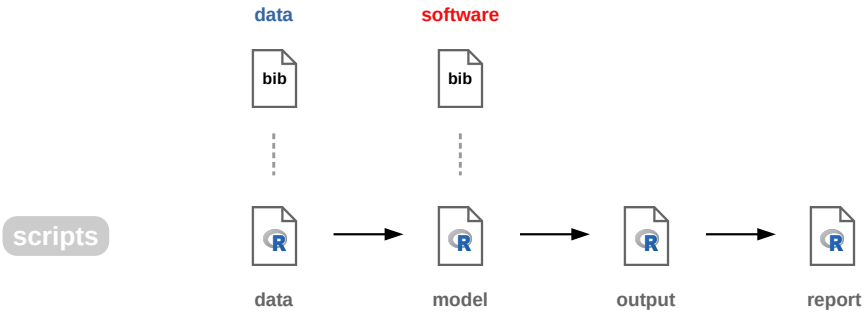

Figure 2. TAF scripted workflow. Each SOFIA-TAF repository/analysis contains four standard R scripts that are run sequentially. The initial data and software are declared in so-called bib files.

The R scripts conducting SOFIA-TAF analyses rely especially on three R packages:

- SOFIA – a dedicated package to support SOFIA-TAF (Sharma and Magnusson 2022)
- TAF – utilities to manage scripts, data files, metadata, and R data objects (Magnusson and Millar 2021)
- sraplus – biomass dynamics model with Bayesian priors (Ovando 2022)

3.1.3 Repository names and directory structure

GitHub repositories are given descriptive names, such as

`https://github.com/sofia-taf/2021Area37Coastal`

for the analysis conducted in 2021 of coastal stocks in Area 37.

On a personal laptop or a high-performance cluster, the SOFIA-TAF repositories are organized in a hierarchical directory structure (Figure 3), similar to the repository name as year/area/stock group.

Figure 3. SOFIA-TAF local directory structure, showing the similarity between the remote repository name and the local directory names.

This hierarchical directory structure is practical to navigate and run the analyses, access results, and run top-level summary calculations across a large number of analyses.

3.2 Data collection templates

SOFIA-TAF input data are collected and prepared in a collaborative process between FAO and regional experts. The data used within a Tier 2 analysis are organized in files such as `catch.csv`, `effort.csv`, and `index.csv`, containing multiple stocks in each file. Data provided by regional experts, however, are termed *primary* data files and are organized as one file per stock, using filenames such as `Yellowtail_snapper_Mexico.csv`. The conversion from primary data files to Tier2 input data files is handled by the SOFIA package.

3.3 Input data warehouse

The input data warehouse contains fisheries data for all areas and stocks. Catch and effort data for Tier 2 stocks are organized in two GitHub repositories:

https://github.com/sofia-taf/catches

https://github.com/sofia-taf/effort

Individual SOFIA-TAF analyses start by reading catch and effort data from the data warehouse. In this way, the input data for all analyses are stored in one central place, where they can be updated, documented, and quality checked.

3.4 R package

The SOFIA package (Sharma and Magnusson 2022) contains utilities that are commonly used in SOFIA-TAF analyses. It is developed in a dedicated GitHub repository:

https://github.com/sofia-taf/SOFIA

The SOFIA package provides a single place to modify a large number of SOFIA-TAF analyses. Incremental improvements become more manageable, e.g., changing the format of a specific plot, without having to edit each and every SOFIA-TAF analysis. It also makes the R scripts for each analysis shorter and thus easier to read, write, and maintain.

3.5 Database

The SOFIA-TAF database will contain the results from all the individual SOFIA-TAF analyses. The primary focus of the database is on stock status, both in numerical terms and in categorical terms: underfished, fully fished, and overfished.

The database is the central node and key component of the SOFIA-TAF design. The only way to enter data into the database is via SOFIA-TAF analyses, as indicated in the SOFIA-TAF diagram (Figure 1), and when SOFIA-TAF analyses of a specific areas and stocks are updated, the database is automatically updated. Furthermore, the top-level analysis for the final SOFIA report, aggregating a large number of SOFIA-TAF analyses, should be based on queries to the database.

The above design guarantees the traceability of SOFIA results, all the way from the individual datasets and analyses to the final published report.

The database is also a convenient stage in the pipeline to apply quality control. Examples of quality checks could include referential integrity of species and stock names, summary statistics at different levels of aggregation, counting stocks in each area, plotting the distribution of numerical stock status, etc. This will ensure that all stocks are accounted for, and reveal any inconsistencies or issues that should be checked in the underlying analyses.

4 Development status and next steps

4.1 SOFIA-TAF repositories

4.1.1 Current status

As of end of December 2022, the GitHub site https://github.com/sofia-taf contains 32 SOFIA-TAF repositories, 12 that were created in 2021, and 20 created in 2022 (Table 4).

Table 4. Overview of SOFIA-TAF repositories.

Year	Area	Number of analyses	Specifically
2021	Area 31	1	Test
	Area 37	11	ClamsOK, Coastal, Cods, Demersal, Flounder, Herring, Other, Shads, Shimps, Squid, Test
2022	Area 31	10	CatchEffortGlobalv2JM, CatchOnly, DemoEffortByStock, DemoEffortShared, DemoIndexByStock, EffortJMstcks, effortlocalcatchlocalv2JM, IndexMethodv2JM, Indexstocks, Testnewstocks
	Area 37	2	Clams, Demo
	Area 41	3	DemoPriorsByStock, RelevantStocks
	Area 57	4	Efforttest, EffortTestNoPriornew70yrstocks, Tier2FAOMonitored31withdepPrior, Tier2FAOMonitorednodepPrior
	Deep Seas	1	CCAMLR

The status of all of these analyses is exploratory for development purposes, as opposed to production analyses for a final SOFIA report. As development progresses, some of the early exploratory repositories are left behind and will only run with older versions of the SOFIA package. Repositories under current development have been updated to the current SOFIA-TAF version 2 format.

Five demo repositories were developed for regional SOFIA-TAF workshops that were held in 2022:

- 2022Area37Demo
- 2022Area31DemoEffortShared
- 2022Area31DemoEffortByStock
- 2022Area31DemoIndex
- 2022Area37DemoPriorsByStock

These five demos serve as a reference for SOFIA-TAF, demonstrating standardized scripts for analyzing various combinations of effort data, survey index data, and priors. As reference analyses, they will be updated and synchronized when changes and improvements are introduced in the SOFIA package and other components of the SOFIA-TAF framework.

To strengthen the reproducibility aspect of running SOFIA-TAF, analyses created in 2022 have used the `SOFTWARE.bib` file to declare the version of the SOFIA package that is required to run a given analysis. This has been especially useful after the release of version 2 of the SOFIA package in August 2022.

Near the end of 2022, a new GitHub site https://github.com/sofia-taf-dev was created, as an alternative place from https://github.com/sofia-taf to store repositories. One approach to manage SOFIA-TAF would be store experimental analyses on the 'dev' site and production analyses on the main site.

4.1.2 Next steps

Read from input data warehouse

Currently, the SOFIA-TAF analyses read catch and effort data from a local data directory, specific to each analysis. This means that data are repeated between analyses, especially the effort data. Furthermore, to update catch and effort data, one would have to modify a large number of SOFIA-TAF repositories. The input data warehouse offers a more efficient, traceable, and quality-controlled workflow.

Categorical status by stock and year

SOFIA-TAF analyses produce an output file called `stock_timeseries.csv` with numerical B/B_{MSY} and F/F_{MSY} by stock and year. For the subsequent analysis, it would be beneficial if the categorical stock status (underfished, fully fished, overfished) by year is also included in this file. This improvement will require modifications to the `output.R` script of all SOFIA-TAF analyses.

Managing repositories

During the development of SOFIA-TAF, a number of experimental analyses have been created as repositories on the main https://github.com/sofia-taf site. Some analyses can be considered will become production analyses for a final SOFIA report, whose results should be imported into the SOFIA-TAF database, while other analyses should probably be migrated to the development area on https://github.com/sofia-taf-dev. Some older experimental analyses could be deleted, if they have been superseded by more recent analyses.

When importing results from analyses into the SOFIA-TAF database, the relevant analyses could be defined as all repositories on https://github.com/sofia-taf whose name begins with year and area.

Managing output files

A significant challenge in SOFIA-TAF is that each analysis takes considerable time to run (>1 hr) and produces large output files (>100 MB). Every time a small update is made to the scripts or underlying data, a new run is required and the output files are likely to change. SOFIA-TAF development so far has explored two approaches to store the output files.

Approach 1. Initial development (e.g., `area37`) kept the output files outside of the repository. Instead of uploading the output files along with the R scripts, output files were uploaded as GitHub 'release assets'. The advantage of this approach is that the repository remains very light and easy to work with, and takes much less space on the hard drive of a personal laptop.

Approach 2. Later development (e.g., `2021Area37Coastal`) has the output files stored inside the repository. The advantage of this approach is that it reduces the need to manage tags and GitHub releases, and makes it slightly less likely to have mismatching R scripts and output files.

Unfortunately, neither of the above approaches can guarantee a correct match between the R scripts and the output files. In other words, when a change is made to an R script and uploaded to the repository, it's easy to forget or omit running the entire analysis and uploading new output files.

A 3rd approach worth exploring would be not to upload output files to the GitHub repository at all. Instead, the database server would run all analyses locally. Specifically, a GitHub webhook could be developed, so that whenever a change is uploaded to the GitHub repository, the database server pulls the changes, runs the analysis and imports the results into the database. This would guarantee a strong linkage between the SOFIA-TAF repositories and the database.

4.2 Data collection templates

4.2.1 Current status

The data collection templates are under development. For Tier 2, a prototype of the conversion process from primary data files (provided by regional experts) to SOFIA-TAF format has been implemented in the SOFIA package, where `groupData` organizes primary data files into subdirectories and `convertData` converts them to SOFIA-TAF format.

The Tier 2 prototype functions `groupData` and `convertData` perform quality control and raise descriptive error messages if a primary data file does not meet the criteria required for data conversion to SOFIA-TAF format.

4.2.2 Next steps

Data collection templates for Tiers 1, 2, and 3 will be further developed in 2023. For Tier 2, the primary data files should be in a format that meets the criteria of the `groupData` and `convertData` functions.

4.3 Input data warehouse

4.3.1 Current status

The https://github.com/sofia-taf/catches repository currently contains the following file with catch data:

`cap_2021-10-17_193245.csv`

The https://github.com/sofia-taf/effort repository has been created but is still empty.

4.3.2 Next steps

The data in the `catches` repository data are ready for exploratory use, testing the ability of R scripts to read catch data from the central warehouse instead of a local data directory.

Data can be added to the `effort` repository in CSV format. Alternative structures of the data will be evaluated, before deciding how to organize the effort data from different areas and stocks.

For SOFIA-TAF analyses of Tier 1 and 3, the data warehouse can incorporate the underlying numerical and categorical data from official stock assessments and expert elicitation. This could further increase the clarity and traceability of the overall SOFIA analysis of stock status.

4.4 R package

4.4.1 Current status

Version 2.1.1 of the SOFIA package was released on 15 Nov 2022. The package help page that comes with SOFIA lists the following functions, categorized by functionality.

Prepare data:

`addDriors`	add driors column to stocks object
`addEffort`	add effort column to catch data
`addIndex`	add index column to catch data
`convertData`	convert primary data to combined data
`groupData`	group primary data in subdirectories

Calculate:

`calcCat`	stock status categories

Plot:

`plotCat`	summary of stock status categories

Repositories:

`gitRepos`	list GitHub repositories
`gitClone`	clone GitHub repository
`gitCloneAll`	clone all SOFIA-TAF repositories

The current status of the package is stable and fully documented, passing a strict `R CMD --as-cran` quality check. Table 5 shows the complete release history.

Table 5. SOFIA package release history.

Version	Date	New functions
2.1.1	2022-11-15	
2.1.0	2022-11-11	`addIndex`.
2.0.0	2022-08-08	`gitRepos`, `gitClone`, `gitCloneAll`.
1.2.1	2022-05-21	
1.2.0	2022-02-25	`convertData`.
1.1.0	2022-02-20	`groupData`.
1.0.3	2022-02-14	
1.0.2	2022-01-24	`addDriors`, `addEffort`, `calcCat`, `plotCat`.

A more detailed list of changes introduced in each version of the SOFIA package can be found online at https://github.com/sofia-taf/SOFIA/blob/main/NEWS.md.

4.4.2 Next steps

One area of the SOFIA package that can be developed is the creation of QC functions to apply quality control for SOFIA-TAF analyses, identifying possible mistakes in the analyses that can then be fixed.

4.5 Database

4.5.1 Current status

The database of SOFIA results is implemented in MySQL. Its development is organized in a GitHub repository:

`https://github.com/sofia-taf/database`

Database import and export is managed using Bash shell scripts, which are found in the GitHub repository.

4.5.2 Next steps

Strong link between repositories and database

The link between SOFIA-TAF repositories and the database of results (Figure 1) is essential for traceability and the fundamental purpose of SOFIA-TAF. The very basis of the SOFIA-TAF design is that the results found in the database should match exactly the results produced by the SOFIA-TAF repositories.

One database script under development loops through the list of repositories and pulls down the `current_status.csv` file to ingest to the database.

The design and development of this linkage is still ongoing, including automatic detection of which analyses contain results that should be imported into the database. The separation of repositories into production analyses on sofia-taf and experimental analyses on sofia-taf-dev (Section 4.1.2 on 'Managing repositories') is related to designing a strong link between repositories and the database of SOFIA-TAF results.

Database server managing SOFIA-TAF output files

One design possibility is to have a dedicated SOFIA-TAF database server as the main platform to run SOFIA-TAF analyses and manage output files, in addition to importing the results into the database.

The development goal 'Managing output files' (Section 4.1.2) elaborates on this possible approach, which could involve a GitHub webhook to establish a reliable pipeline of information from SOFIA-TAF repositories to the database.

5 Acknowledgements

Working with Rishi Sharma and Nicole Tursich on this project is a privilege and joy. Our domains of expertise complement each other, and we share a common vision and enthusiasm to enhance the FAO infrastructure and analytical workflows for estimating the state of the world's fisheries. I would like to acknowledge Colin Millar for our collaboration in creating TAF (Magnusson and Millar 2021), which has served as an inspiration and basis for the SOFIA-TAF design. Last but not least, I am grateful to Pedro Barros and colleagues at FAO for their guidance and vote of confidence for this technical development project.

6 References

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A Arni's contributions in 2022

SOFIA-TAF design

The work on this project is divided been design and development. The design part takes place largely during online technical meetings of the SOFIA-TAF development team, and is the product of dynamic teamwork and discussions. As the SOFIA-TAF design borrows both ideas and technical components from TAF (Magnusson and Millar 2021), Arni has served in a lead role in the design of many aspects of SOFIA-TAF, especially the structure of SOFIA-TAF repositories, input data warehouse, and the R package.

SOFIA-TAF repository development

On the development front, Arni has created and updated five demo repositories that serve as serve as a reference, demonstrating the current and recommended format for SOFIA-TAF analyses.

Teaching and documenting

For the regional workshops in 2022, Arni gave presentations and participated in discussions to explain the overall design of SOFIA-TAF and how data files and R scripts perform the analysis of stock status. The goal is to enable regional experts to contribute the best data available to SOFIA-TAF.

For the SOFIA-TAF launch event at the CAPAM conference, Arni gave a presentation describing the importance of open and reproducible analyses in fisheries science, and how the SOFIA-TAF design is centered on those objectives.

All functions of the SOFIA package are fully documented and updated with each release. Arni has also analyzed the extent of package dependencies of the sraplus package, which is especially relevant for the reproducibility aspect of SOFIA-TAF analyses.

R package

Arni maintains the SOFIA package, acting as a single place of analytical methods used in all SOFIA-TAF analyses. This greatly improves the ability to manage and maintain the large number of SOFIA-TAF analyses behind SOFIA.

Contributions to project management

With this report, updated annually, Arni has aimed to describe the current status and next steps in the development of SOFIA-TAF, especially the aspects relating to the analyses (data, scripts, and results) and the underlying SOFIA package. This conveys a design manifesto and has helped to track progress, set objectives, and provide an up-to-date documentation of how the SOFIA-TAF components work together.

Links to deliverables

- Demo analyses:
  - 2022Area37Demo
  - 2022Area31DemoEffortShared
  - 2022Area31DemoEffortByStock
  - 2022Area31DemoIndex
  - 2022Area37DemoPriorsByStock
- Presentations:
  - Area 31 (overview, demo)
  - Area 41 (overview, demo)
  - CAPAM conference
- Documentation page, including sraplus dependencies and history
- SOFIA package
- This current report