

# Package: Capsule (via r-universe)

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**Type** Package

**Title** Comprehensive Reproducibility Framework for R and Bioinformatics Analysis

**Version** 0.2.0

**Description** A comprehensive reproducibility framework designed for R and bioinformatics workflows. Automatically captures the entire analysis environment including R session info, package versions, external tool versions (Samtools, STAR, BWA, etc.), conda environments, reference genomes, data provenance with smart checksumming for large files, parameter choices, random seeds, and hardware specifications. Generates executable scripts with Docker, Singularity, and renv configurations. Integrates with workflow managers (Nextflow, Snakemake, WDL, CWL) to ensure complete reproducibility of computational research workflows.

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**Suggests** testthat (>= 3.0.0)

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---

capture\_environment    *Capture Environment State*

---

### Description

Captures the current global environment state including objects and their types

**Usage**

```
capture_environment(  
  output_file = NULL,  
  include_values = FALSE,  
  max_size = 1024 * 1024  
)
```

**Arguments**

`output_file` Character. Path to save environment info. If NULL, returns as list.  
`include_values` Logical. Whether to include object values (for small objects). Default FALSE.  
`max_size` Numeric. Maximum object size (in bytes) to include values. Default 1MB.

**Value**

A list containing environment information

**Examples**

```
## Not run:  
x <- 1:10  
y <- "test"  
capture_environment("env_state.json")  
  
## End(Not run)
```

---

captureHardware	<i>Capture Hardware Information</i>
-----------------	-------------------------------------

---

**Description**

Capture hardware specifications including CPU, RAM, and GPU information. Useful for documenting computational resources used in analysis.

**Usage**

```
captureHardware(output_file = NULL)
```

**Arguments**

`output_file` Character. Path to save hardware info. If NULL, returns as list.

**Value**

List containing hardware information

## Examples

```
## Not run:
capture_session("hardware_info.json")

## End(Not run)
```

---

capture_session	<i>Capture Complete Session Information</i>
-----------------	---

---

## Description

Captures comprehensive R session information including R version, platform, loaded packages, system information, and locale settings.

## Usage

```
capture_session(output_file = NULL, format = c("json", "yaml", "rds"))
```

## Arguments

output_file	Character. Path to save the session info. If NULL, returns as list.
format	Character. Output format: "json", "yaml", or "rds". Default is "json".

## Value

A list containing session information, invisibly returned

## Examples

```
## Not run:
# Capture session info to JSON
capture_session("session_info.json")

# Capture and return as list
info <- capture_session()

## End(Not run)
```

---

`capture_system_libraries`*Capture System Libraries*

---

**Description**

Capture version information for system libraries that R packages depend on (e.g., libcurl, libxml2, BLAS/LAPACK implementations)

**Usage**

```
capture_system_libraries(output_file = NULL)
```

**Arguments**

`output_file`      Character. Path to save library info. If NULL, returns as list.

**Value**

List containing system library information

**Examples**

```
## Not run:  
capture_system_libraries("system_libs.json")  
  
## End(Not run)
```

---

`compare_snapshots`*Compare Two Workflow Snapshots*

---

**Description**

Compare two Capsule snapshots to identify differences in packages, parameters, data files, and other tracked components

**Usage**

```
compare_snapshots(snapshot1, snapshot2, output_file = "snapshot_comparison.md")
```

**Arguments**

`snapshot1`      Character. Name of first snapshot  
`snapshot2`      Character. Name of second snapshot  
`output_file`     Character. Path to save comparison report. Default "snapshot\_comparison.md"

**Value**

List containing comparison results

**Examples**

```
## Not run:  
compare_snapshots("analysis_v1", "analysis_v2")  
  
## End(Not run)
```

---

create\_renv\_lockfile *Create renv Lockfile*

---

**Description**

Generate an renv-compatible lockfile for package reproducibility

**Usage**

```
create_renv_lockfile(output_file = "renv.lock", project_path = ".")
```

**Arguments**

output\_file     Character. Path to save lockfile. Default "renv.lock".  
project\_path    Character. Path to project. Default is current directory.

**Value**

Path to created lockfile

**Examples**

```
## Not run:  
create_renv_lockfile("renv.lock")  
  
## End(Not run)
```

---

create\_repro\_report     *Create Reproducibility Report*

---

**Description**

Generate a comprehensive markdown report documenting all reproducibility information

**Usage**

```
create_repro_report(  
  output_file = "reproducibility_report.md",  
  analysis_name = NULL,  
  include_package_list = TRUE  
)
```

**Arguments**

output\_file     Character. Path to save the report. Default "reproducibility\_report.md"  
analysis\_name    Character. Name of the analysis  
include\_package\_list  
                 Logical. Include full package list. Default TRUE.

**Value**

Path to generated report

**Examples**

```
## Not run:  
create_repro_report("report.md", "main_analysis")  
  
## End(Not run)
```

---

export\_for\_cwl             *Generate CWL (Common Workflow Language) Input*

---

**Description**

Export Capsule data in YAML format suitable for CWL workflows

**Usage**

```
export_for_cwl(output_file = "capsule_cwl_inputs.yml")
```

**Arguments**

output\_file      Character. Path to save inputs. Default "capsule\_cwl\_inputs.yml"

**Value**

List containing input data

**Examples**

```
## Not run:  
export_for_cwl("reproflow_cwl_inputs.yml")  
  
## End(Not run)
```

---

export\_for\_nextflow      *Export Capsule Data for Nextflow*

---

**Description**

Export all Capsule tracking data in a format suitable for Nextflow pipelines

**Usage**

```
export_for_nextflow(  
  output_file = "capsule_manifest.json",  
  include_checksums = TRUE  
)
```

**Arguments**

output\_file      Character. Path to save manifest. Default "capsule\_manifest.json"  
include\_checksums      Logical. Include file checksums. Default TRUE.

**Value**

List containing manifest data

**Examples**

```
## Not run:  
export_for_nextflow("reproflow_manifest.json")  
  
## End(Not run)
```

---

export\_for\_snakemake    *Export Capsule Data for Snakemake*

---

### Description

Export all Capsule tracking data in YAML format for Snakemake pipelines

### Usage

```
export_for_snakemake(  
  output_file = "capsule_config.yaml",  
  include_checksums = TRUE  
)
```

### Arguments

output\_file    Character. Path to save config. Default "capsule\_config.yaml"  
include\_checksums    Logical. Include file checksums. Default TRUE.

### Value

List containing config data

### Examples

```
## Not run:  
export_for_snakemake("reproflow_config.yaml")  
  
## End(Not run)
```

---

export\_for\_wdl    *Create WDL (Workflow Description Language) Config*

---

### Description

Export Capsule data in JSON format suitable for WDL workflows

### Usage

```
export_for_wdl(output_file = "capsule_inputs.json")
```

### Arguments

output\_file    Character. Path to save config. Default "capsule\_inputs.json"

**Value**

List containing config data

**Examples**

```
## Not run:
export_for_wdl("reproflow_inputs.json")

## End(Not run)
```

---

generate_docker	<i>Generate Docker Configuration</i>
-----------------	--------------------------------------

---

**Description**

Generate a Dockerfile and docker-compose.yml for complete environment reproducibility

**Usage**

```
generate_docker(
  output_dir = ".",
  r_version = NULL,
  base_image = "rocker/r-ver",
  system_deps = NULL,
  project_name = "reproflow-project",
  include_rstudio = FALSE
)
```

**Arguments**

output_dir	Character. Directory to save Docker files. Default is current directory.
r_version	Character. R version to use. Default is current R version.
base_image	Character. Base Docker image. Default "rocker/r-ver"
system_deps	Character vector. System dependencies to install
project_name	Character. Name for the project
include_rstudio	Logical. Include RStudio Server. Default FALSE.

**Value**

List of generated file paths

## Examples

```
## Not run:
generate_docker(
  output_dir = ".",
  project_name = "my_analysis",
  system_deps = c("libcurl4-openssl-dev", "libxml2-dev")
)

## End(Not run)
```

---

generate\_repro\_script *Generate Reproducible Script*

---

## Description

Generate an executable R script that includes all reproducibility information including package versions, seeds, parameters, and data verification.

## Usage

```
generate_repro_script(
  script_file,
  source_script = NULL,
  analysis_name = "analysis",
  include_renv = TRUE,
  include_data_check = TRUE,
  include_session_info = TRUE
)
```

## Arguments

`script_file` Character. Path to save the generated script

`source_script` Character. Original analysis script to include

`analysis_name` Character. Name for this analysis

`include_renv` Logical. Include renv initialization. Default TRUE.

`include_data_check` Logical. Include data verification. Default TRUE.

`include_session_info` Logical. Include session info at end. Default TRUE.

## Value

Path to generated script

## Examples

```
## Not run:
generate_repro_script(
  "analysis_reproducible.R",
  source_script = "analysis.R",
  analysis_name = "main_analysis"
)

## End(Not run)
```

---

generate\_singularity *Generate Singularity Definition File*

---

## Description

Generate a Singularity/Aptainer definition file for HPC environments. Singularity is commonly used in HPC clusters where Docker is not available.

## Usage

```
generate_singularity(
  output_dir = ".",
  r_version = NULL,
  base_image = "rocker/r-ver",
  conda_env = NULL,
  system_deps = NULL,
  project_name = "reproflow-project"
)
```

## Arguments

output_dir	Character. Directory to save Singularity files. Default "."
r_version	Character. R version to use. Default is current R version.
base_image	Character. Base Docker image. Default "rocker/r-ver"
conda_env	Character. Path to conda environment file. Optional.
system_deps	Character vector. System dependencies to install
project_name	Character. Name for the project

## Value

List of generated file paths

**Examples**

```
## Not run:
generate_singularity(
  output_dir = ".",
  project_name = "my_analysis",
  system_deps = c("samtools", "bwa")
)

## End(Not run)
```

---

get\_conda\_env\_info      *Get Conda Environment Info*

---

**Description**

Retrieve information about tracked conda environments

**Usage**

```
get_conda_env_info(
  env_name = NULL,
  registry_file = ".capsule/conda_registry.json"
)
```

**Arguments**

env\_name            Character. Specific environment name, or NULL for all  
registry\_file      Character. Path to conda registry

**Value**

List of environment information

---

get\_data\_lineage      *Get Data Lineage*

---

**Description**

Retrieve complete lineage information for tracked data

**Usage**

```
get_data_lineage(
  data_path = NULL,
  registry_file = ".capsule/data_registry.json"
)
```

**Arguments**

data\_path        Character. Path to data file. If NULL, returns all lineage.  
registry\_file    Character. Path to provenance registry.

**Value**

List containing lineage information

**Examples**

```
## Not run:  
# Get lineage for specific file  
lineage <- get_data_lineage("data/mydata.csv")  
  
# Get all lineage  
all_lineage <- get_data_lineage()  
  
## End(Not run)
```

---

get\_param\_history        *Get Parameter History*

---

**Description**

Retrieve parameter tracking history

**Usage**

```
get_param_history(  
  analysis_name = NULL,  
  registry_file = ".capsule/param_registry.json"  
)
```

**Arguments**

analysis\_name    Character. Specific analysis name, or NULL for all  
registry\_file    Character. Path to parameter registry

**Value**

List of parameter records

---

get\_reference\_info      *Get Reference Genome Information*

---

**Description**

Retrieve information about tracked reference genomes

**Usage**

```
get_reference_info(  
    genome_build = NULL,  
    registry_file = ".capsule/reference_registry.json"  
)
```

**Arguments**

genome\_build      Character. Specific genome build, or NULL for all  
registry\_file      Character. Path to reference registry

**Value**

List of reference genome information

**Examples**

```
## Not run:  
# Get all tracked references  
get_reference_info()  
  
# Get specific reference  
get_reference_info("GRCh38")  
  
## End(Not run)
```

---

get\_seed\_history      *Get Seed History*

---

**Description**

Retrieve seed tracking history

**Usage**

```
get_seed_history(  
    analysis_name = NULL,  
    registry_file = ".capsule/seed_registry.json"  
)
```

**Arguments**

analysis\_name Character. Specific analysis name, or NULL for all  
registry\_file Character. Path to seed registry

**Value**

List of seed records

---

get\_tool\_versions      *Get External Tool Versions*

---

**Description**

Retrieve version information for previously tracked external tools

**Usage**

```
get_tool_versions(  
    tool_name = NULL,  
    registry_file = ".capsule/tools_registry.json"  
)
```

**Arguments**

tool\_name Character. Specific tool name, or NULL for all tools  
registry\_file Character. Path to tools registry

**Value**

List of tool version information

**Examples**

```
## Not run:  
# Get all tracked tools  
get_tool_versions()  
  
# Get specific tool  
get_tool_versions("samtools")  
  
## End(Not run)
```

---

init_capsule	<i>Initialize Capsule in Project</i>
--------------	--------------------------------------

---

### Description

Initialize Capsule reproducibility framework in the current project. Creates necessary directory structure and configuration files.

### Usage

```
init_capsule(  
  project_path = ".",  
  use_renv = TRUE,  
  use_git = TRUE,  
  create_gitignore = TRUE  
)
```

### Arguments

project_path	Character. Path to project directory. Default is current directory.
use_renv	Logical. Initialize renv for package management. Default TRUE.
use_git	Logical. Initialize git if not already present. Default TRUE.
create_gitignore	Logical. Create/update .gitignore. Default TRUE.

### Value

Invisible NULL

### Examples

```
## Not run:  
# Initialize Capsule in current directory  
init_capsule()  
  
# Initialize without renv  
init_capsule(use_renv = FALSE)  
  
## End(Not run)
```

---

`list_reference_sources`*List Common Reference Genome Sources*

---

**Description**

Display a helpful list of common reference genome sources

**Usage**

```
list_reference_sources()
```

**Examples**

```
list_reference_sources()
```

---

`list_snapshots`*List Available Snapshots*

---

**Description**

List all available snapshots with basic metadata

**Usage**

```
list_snapshots()
```

**Value**

Data frame with snapshot information

**Examples**

```
## Not run:  
list_snapshots()  
  
## End(Not run)
```

---

restore_conda_env	<i>Restore Conda Environment</i>
-------------------	----------------------------------

---

## Description

Restore a conda environment from a previously exported environment file

## Usage

```
restore_conda_env(  
  env_file = "conda_environment.yml",  
  env_name = NULL,  
  use_mamba = FALSE,  
  force = FALSE  
)
```

## Arguments

env_file	Character. Path to environment YAML file. Default "conda_environment.yml"
env_name	Character. Name for the new environment. If NULL, uses name from file.
use_mamba	Logical. Use mamba instead of conda. Default FALSE.
force	Logical. Remove existing environment if it exists. Default FALSE.

## Value

Logical. TRUE if successful, FALSE otherwise

## Examples

```
## Not run:  
# Restore environment from file  
restore_conda_env("conda_environment.yml")  
  
# Use mamba for faster installation  
restore_conda_env("conda_environment.yml", use_mamba = TRUE)  
  
# Force recreate if exists  
restore_conda_env("conda_environment.yml", force = TRUE)  
  
## End(Not run)
```

---

restore_seed	<i>Restore Random Seed</i>
--------------	----------------------------

---

**Description**

Restore a previously tracked random seed

**Usage**

```
restore_seed(analysis_name, registry_file = ".capsule/seed_registry.json")
```

**Arguments**

analysis\_name Character. Name of analysis to restore seed from  
registry\_file Character. Path to seed registry

**Value**

The seed value (invisibly)

**Examples**

```
## Not run:  
# Restore previously tracked seed  
restore_seed("simulation_1")  
  
## End(Not run)
```

---

set_seed	<i>Set and Track Random Seed</i>
----------	----------------------------------

---

**Description**

Set a random seed and track it for reproducibility

**Usage**

```
set_seed(  
  seed = NULL,  
  kind = NULL,  
  normal.kind = NULL,  
  sample.kind = NULL,  
  analysis_name = NULL,  
  registry_file = ".capsule/seed_registry.json"  
)
```

**Arguments**

seed	Numeric. Random seed to set. If NULL, generates random seed.
kind	Character. RNG kind (see ?set.seed). Default NULL uses current.
normal.kind	Character. Normal RNG kind. Default NULL uses current.
sample.kind	Character. Sample RNG kind. Default NULL uses current.
analysis_name	Character. Name to associate with this seed
registry_file	Character. Path to seed registry

**Value**

The seed value (invisibly)

**Examples**

```
## Not run:
# Set and track a specific seed
set_seed(12345, analysis_name = "simulation_1")

# Generate and track a random seed
set_seed(analysis_name = "bootstrap_analysis")

## End(Not run)
```

---

snapshot\_packages      *Track Package Versions and Dependencies*

---

**Description**

Creates a comprehensive snapshot of all installed packages, their versions, dependencies, and sources for reproducibility.

**Usage**

```
snapshot_packages(
  output_file = NULL,
  include_dependencies = TRUE,
  only_attached = FALSE
)
```

**Arguments**

output_file	Character. Path to save package info. If NULL, returns as list.
include_dependencies	Logical. Include dependency tree. Default TRUE.
only_attached	Logical. Only track attached packages. Default FALSE.

**Value**

A list containing package information

**Examples**

```
## Not run:
# Track all installed packages
snapshot_packages("package_manifest.json")

# Track only attached packages
snapshot_packages("packages.json", only_attached = TRUE)

## End(Not run)
```

---

snapshot_workflow	<i>Create Complete Workflow Snapshot</i>
-------------------	--

---

**Description**

Create a comprehensive snapshot of the entire workflow including session info, packages, data, parameters, and generate all reproducibility artifacts.

**Usage**

```
snapshot_workflow(
  snapshot_name = NULL,
  analysis_name = "analysis",
  source_script = NULL,
  description = NULL,
  generate_docker = TRUE,
  generate_script = TRUE,
  generate_report = TRUE
)
```

**Arguments**

snapshot_name	Character. Name for this snapshot. Default is timestamp.
analysis_name	Character. Name of the analysis
source_script	Character. Path to main analysis script
description	Character. Description of this workflow
generate_docker	Logical. Generate Docker configuration. Default TRUE.
generate_script	Logical. Generate reproducible script. Default TRUE.
generate_report	Logical. Generate reproducibility report. Default TRUE.

**Value**

List containing paths to generated files

**Examples**

```
## Not run:
# Create complete workflow snapshot
snapshot_workflow(
  snapshot_name = "analysis_v1",
  analysis_name = "main_analysis",
  source_script = "analysis.R",
  description = "Initial analysis run"
)

## End(Not run)
```

---

track_conda_env	<i>Track Conda Environment</i>
-----------------	--------------------------------

---

**Description**

Export and track a conda environment specification for reproducibility. Works with both conda and mamba.

**Usage**

```
track_conda_env(
  env_name = NULL,
  output_file = "conda_environment.yml",
  use_mamba = FALSE,
  registry_file = ".capsule/conda_registry.json"
)
```

**Arguments**

env_name	Character. Name of conda environment. If NULL, uses active environment.
output_file	Character. Path to save environment file. Default "conda_environment.yml"
use_mamba	Logical. Use mamba instead of conda. Default FALSE.
registry_file	Character. Path to conda registry

**Value**

List containing environment information

**Examples**

```
## Not run:
# Track currently active conda environment
track_conda_env()

# Track specific environment
track_conda_env(env_name = "bioinfo_env")

# Use mamba instead
track_conda_env(use_mamba = TRUE)

## End(Not run)
```

---

track\_data

*Track Data Provenance*


---

**Description**

Records comprehensive provenance information for data files including checksums, sources, timestamps, and metadata. Supports fast hashing for large files.

**Usage**

```
track_data(
  data_path,
  source = c("downloaded", "generated", "manual", "reference", "other"),
  source_url = NULL,
  description = NULL,
  metadata = NULL,
  fast_hash = TRUE,
  size_threshold_gb = 1,
  registry_file = ".capsule/data_registry.json"
)
```

**Arguments**

data_path	Character. Path to data file or directory.
source	Character. Source of the data (e.g., "downloaded", "generated", "manual", "reference").
source_url	Character. URL if data was downloaded. Optional.
description	Character. Description of the data. Optional.
metadata	List. Additional metadata. Optional.
fast_hash	Logical. Use faster xxHash for large files (>1GB). Default TRUE.
size_threshold_gb	Numeric. Size threshold (GB) for using fast hash. Default 1.
registry_file	Character. Path to provenance registry. Default ".capsule/data_registry.json".

**Value**

A list containing data provenance information

**Examples**

```
## Not run:
# Track a downloaded dataset
track_data("data/mydata.csv",
  source = "downloaded",
  source_url = "https://example.com/data.csv",
  description = "Customer data from API"
)

# Track generated data
track_data("results/simulation.rds",
  source = "generated",
  description = "Monte Carlo simulation results"
)

# Track large file with fast hashing
track_data("data/large_file.bam",
  source = "generated",
  fast_hash = TRUE
)

## End(Not run)
```

---

track\_external\_tools *Track External Bioinformatics Tools*

---

**Description**

Track versions of external command-line tools commonly used in bioinformatics pipelines (e.g., samtools, STAR, BWA, etc.)

**Usage**

```
track_external_tools(
  tools = NULL,
  registry_file = ".capsule/tools_registry.json"
)
```

**Arguments**

**tools** Character vector of tool names to track. If NULL, tracks common tools.  
**registry\_file** Character. Path to tools registry. Default ".capsule/tools\_registry.json"

**Value**

List containing tool version information

**Examples**

```
## Not run:  
# Track common bioinformatics tools  
track_external_tools()  
  
# Track specific tools  
track_external_tools(c("samtools", "bwa", "STAR"))  
  
## End(Not run)
```

---

track\_params

*Track Analysis Parameters*

---

**Description**

Record analysis parameters and configuration settings for reproducibility

**Usage**

```
track_params(  
  params,  
  analysis_name = NULL,  
  description = NULL,  
  registry_file = ".capsule/param_registry.json"  
)
```

**Arguments**

params	Named list of parameters to track
analysis_name	Character. Name/identifier for this analysis
description	Character. Description of what these parameters control
registry_file	Character. Path to parameter registry

**Value**

List containing parameter information

**Examples**

```
## Not run:
# Track model parameters
params <- list(
  learning_rate = 0.01,
  epochs = 100,
  batch_size = 32,
  model_type = "neural_network"
)
track_params(params, "model_training", "Deep learning model parameters")

## End(Not run)
```

---

track\_reference\_genome

*Track Reference Genome*


---

**Description**

Track reference genome files, annotations, and indices for reproducibility. This is critical for genomics/transcriptomics pipelines where the exact reference version affects results.

**Usage**

```
track_reference_genome(
  fasta_path,
  gtf_path = NULL,
  gff_path = NULL,
  genome_build = NULL,
  species = NULL,
  source_url = NULL,
  indices = list(),
  metadata = list(),
  registry_file = ".capsule/reference_registry.json"
)
```

**Arguments**

fasta_path	Character. Path to reference genome FASTA file
gtf_path	Character. Path to GTF annotation file. Optional.
gff_path	Character. Path to GFF annotation file. Optional.
genome_build	Character. Genome build identifier (e.g., "GRCh38", "mm10")
species	Character. Species name (e.g., "Homo sapiens", "Mus musculus")
source_url	Character. URL where reference was downloaded from
indices	Named list. Paths to aligner indices (STAR, BWA, etc.)
metadata	List. Additional metadata about the reference
registry_file	Character. Path to reference registry

**Value**

List containing reference genome information

**Examples**

```
## Not run:
track_reference_genome(
  fasta_path = "ref/GRCh38.fasta",
  gtf_path = "ref/gencode.v38.annotation.gtf",
  genome_build = "GRCh38",
  species = "Homo sapiens",
  source_url = "https://www.encodegenes.org/",
  indices = list(
    star = "ref/STAR_index/",
    bwa = "ref/bwa_index/GRCh38"
  )
)

## End(Not run)
```

---

verify\_data

*Verify Data Integrity*

---

**Description**

Verify that tracked data files have not been modified by comparing checksums

**Usage**

```
verify_data(data_path = NULL, registry_file = ".capsule/data_registry.json")
```

**Arguments**

`data_path` Character. Path to specific file, or NULL to verify all tracked files.  
`registry_file` Character. Path to provenance registry.

**Value**

Logical. TRUE if data is unchanged, FALSE otherwise

**Examples**

```
## Not run:
# Verify specific file
verify_data("data/mydata.csv")

# Verify all tracked files
verify_data()

## End(Not run)
```

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