LIME TOOLBOX USER GUIDE

ABSTRACT

This document provides the LIME Toolbox user guide.

Javier Gatón
Ramiro González
Carlos Toledano
Pieter De Vis
Stefan Adriaensen

UVa, NPL, VITO

12 June 2025

This document was produced as part of the ESA-funded project "Improving the Lunar Irradiance Model of ESA" under ESA contract number:

Signatures and version history

	Name	Organisation	Date
Written by	Javier Gatón	UVa	12 June 2025
Reviewed by (consortium)		UVa, NPL, VITO	
Approved by (ESA)		ESA	

Version history

Version	Date	Publicly available or private to consortium?
0.1	21/12/2023	
0.2	08/01/2024	
0.3	05/03/2025	
0.4	21/04/2025	
0.5	12/06/2025	

Contents

1. Introduction

1.1 Purpose and Scope

This document provides the LIME Toolbox (TBX) user guide, therefore all the auxiliar information of the software of the toolbox itself. The scope is to ensure that the user knows how to correctly operate the LIME TBX and the LIME model.

1.2 Applicable and reference documents

1.2.1 Applicable Documents

The following applicable documents are those specification, standards, criteria, etc. used to define the requirements of this task.

Number	Reference
[AD0]	ESA-EOPG-EOPGMQ-SOW-24. Improving the Lunar Irradiance Model of ESA.

1.3 Glossary

Abbreviation	Stands For	Notes
AOLP	Angle of Linear Polarisation	
ASD	Analytical Spectral Devices - Instrument manufacturer	Also refers to the instrument itself
Cimel	(Not an abbreviation) Instrument manufacturer	Also refers to the instrument itself
CSV	Comma-Separated Values	
CLI	Command Line Interface	
DOLP	Degree of Linear Polarisation	
EO	Earth Observation	
EO-CFI	Earth Observation CFI Software	
ESA	European Space Agency	Project client
FOV	Field of View	
GIRO	GSICS Implementation of the ROLO Model	
GLOD	GSICS Lunar Observation Dataset	
GSICS	Global Space Based Inter-calibration System	

GUI	Graphical User Interface	
KO	Kick-off meeting	
LGLOD	LIME-GLOD	Former term, now deprecated
LIME	Lunar Irradiance Model of ESA	
MARD	Mean Absolute Relative Difference	
MPD	Mean Percentage Difference	
MRD	Mean Relative Difference	
NPL	National Physical Laboratory	Project partner
OSF	Orbit Scenario File	
ROLO	RObotic Lunar Observatory	
SoW	Statement of Work	
TBX	Toolbox	
TLE	Three-Line Element Set	Also known as 3LE
TOA	Top of Atmosphere	
UVa	University of Valladolid	Project partner
VITO	Vlaamse Instelling voor Technologisch Onderzoek; Flemish Institute for Technological Research	Project partner

2. Overview

2.1 Simulation & Comparison Workflow

LIME Toolbox follows a structured process to compute lunar reflectance and irradiance based on precomputed coefficients and user-defined settings. The computed irradiance can then be compared against real instrument observations. This process is described in (Figure 1).

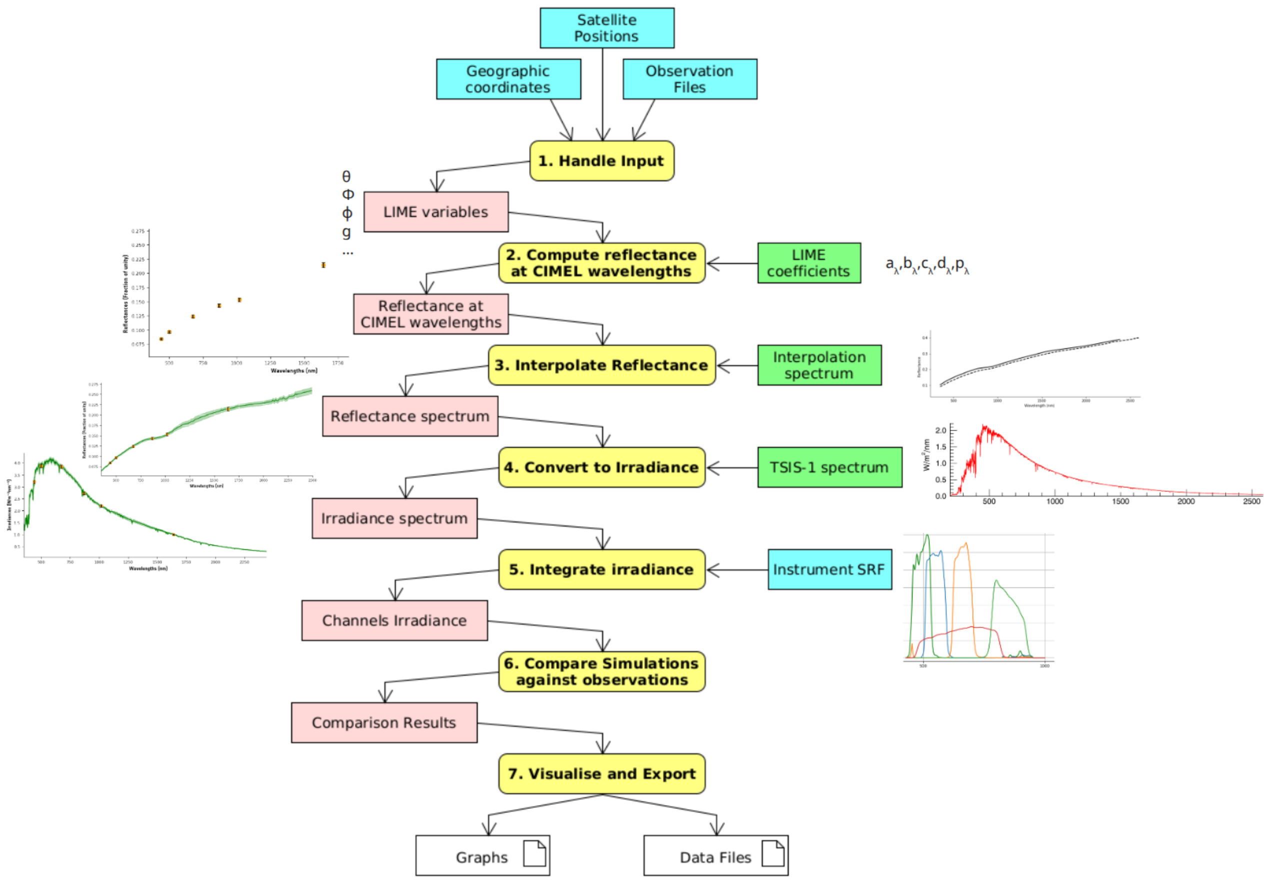


Figure 1: Activity diagram of the Simulation & Comparison Workflow.

Summary of the Process

1. **Handle input** obtaining **LIME variables**.
2. **Compute LIME reflectance at CIMEL wavelengths** using LIME **coefficients**.
3. **Interpolate reflectance** using **ASD** or **Apollo 16 + Breccia** spectrum.
4. **Convert reflectance to irradiance** using the **selected TSIS-1 SRF instance**.
5. **Integrate irradiance over the instrument SRF** to compute **channel-specific values**.
6. **Compare simulated irradiance against real instrument observations**.
7. **Visualise and export results**.

2.1.1 Input Handling

Before computing simulations or comparisons, LIME Toolbox must extract the necessary input parameters. These include key **LIME model variables**, such as:

- **Selenographic latitude and longitude of the observer**
- **Distance between the Sun and the Moon**
- **Distance between the observer and the Moon**
- **Selenographic longitude of the Sun**
- **Moon phase angle**

LIME Toolbox retrieves these parameters from one of two sources:

1. **Direct Input** – Users can provide **geographic, selenographic, or satellite coordinates**.
2. **Observation Files** – Provide precise **geographic coordinates** but can also be used with selenographic or satellite-based simulations.

To ensure accuracy, LIME Toolbox computes missing parameters using:

- **SPICE** for orbital and positional data. Used to compute LIME variables from geographic coordinates.
- **EO-CFI** when processing satellite-based observations.

2.1.2 Computing LIME for CIMEL Wavelengths

- The first step in the simulation is to **compute the LIME model for the predefined CIMEL wavelengths**.
- These computations are based on **LIME coefficients**.
- The result of this step is a set of **lunar reflectance values** at the specific CIMEL wavelengths.

2.1.3 Spectral Interpolation

- Since LIME coefficients provide **values only for CIMEL wavelengths**, the next step is **spectral interpolation**.
- **The interpolation uses a reference spectrum**, which is selected by the user:
    - **ASD Spectrum** (*default and preferred choice*), derived from Izaña ground-based observations.
    - **Apollo 16 + Breccia Spectrum**, a ROLO-based composite spectrum.
- Using the selected spectrum, LIME **interpolates reflectance values** across the entire **wavelength range** (typically 350–2500 nm).

2.1.4 Conversion to Irradiance Using the Solar Spectrum

- Once reflectance values are interpolated, **LIME converts them into lunar irradiance**.

- This transformation involves multiplying reflectance by the **selected TSIS-1 solar spectrum instance**.
- The available **TSIS-1 Spectral Response Function (SRF) instances** include:
    - **ASD SRF** (*corresponding to the ASD spectroradiometer*).
    - **Gaussian SRF** (*1nm spectral sampling, 3nm resolution*).
    - **Triangular SRF** (*1nm spectral sampling, 1nm resolution*).
- The selected **TSIS-1 SRF determines how much sunlight radiance reaches the Moon at each wavelength**.

2.1.5 Spectral Response Function (SRF) Integration

- The computed irradiance values **must be adjusted based on the instrument response**.
- Each instrument has a **Spectral Response Function (SRF)** that weights different wavelengths differently.
- LIME integrates the simulated **irradiance over the instrument SRF**, producing an **integrated irradiance value per spectral channel**.

2.1.6 Compare Simulations against Observations

Once the simulated **irradiance values per channel** have been computed, they can be **compared against real instrument observations**.

2.1.6.1. Align Simulations and Observations

- LIME matches **timestamps** between observations and simulations.
- Observed irradiance is **compared to the simulated values**.
- If needed, LIME **recomputes distances and normalisation factors**.

2.1.6.2. Computing Comparison Metrics

Once observations and simulations are aligned, LIME computes **comparison metrics**:

- **Relative Difference (%)**: `100 * ((irr_obs - irr_sim) / irr_sim)`
- **Percentage Difference (%)**: `100 * abs(irr_sim - irr_obs) / ((irr_sim + irr_obs) / 2)`
- **Statistical Metrics** per channel:
    - **Mean Relative Difference (MRD)**
    - **Mean Absolute Relative Difference (MARD)**
    - **Mean Percentage Difference (MPD)**
    - **Standard Deviation of MRD**
    - **Number of Observations per Channel**

2.1.7 Visualisation and Data Export

Once simulations and comparisons are computed, users can:

- **Visualise Data**:
  - **Time-series plots** of irradiance and difference.
  - **Boxplots** for spectral variability.
  - **Comparison graphs based on**:
    - **Timestamp**
    - **Moon Phase Angle**
    - **Wavelength**
- **Export Results**:
  - **Graphs** (*PNG, JPG, PDF*).
  - **Raw Data** (*CSV, NetCDF for future reloading*).

2.2 Polarisation Computation

While LIME Toolbox primarily computes reflectance and irradiance, it can also estimate **polarisation** using precomputed polarisation coefficients.

- **Degree of Lunar Polarisation (DoLP)** and **Angle of Linear Polarisation (AoLP)** are derived using **LIME polarisation coefficients**.
- **Polarisation calculations follow the same interpolation process** but do not influence irradiance computation.
- The **polarisation interpolation spectrum is fixed** (users cannot select it).

Polarisation results are computed separately and are available in **dedicated output files**.

3. Installation

3.1 Prerequisites

The LIME Toolbox is only compatible with the following operating systems and architectures:

- Windows 10 (x86_64).
- Linux (x86_64, GLIBC >= 2.23)
- Mac (x86_64)
- Mac (ARM64 with Rosetta interpreter)

3.2 Installation Steps

3.2.1 Windows

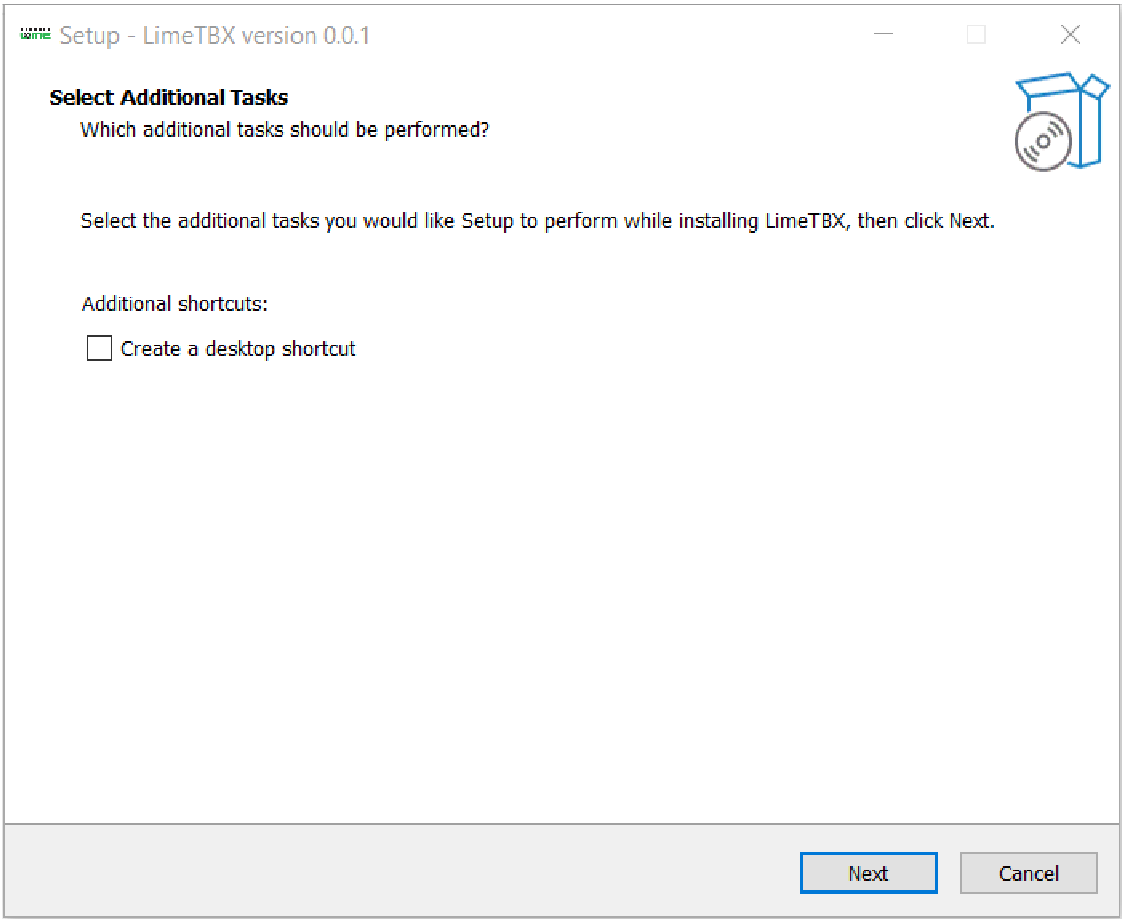


Figure 2: Windows installation wizard.

1. Download the Windows install wizard.
2. Run it.
3. Follow the wizard instructions to complete the installation (Figure 2).

3.2.2 Mac

1. Download the .pkg installer for macOS.
2. Run the .pkg file.
3. Follow the installation wizard instructions (Figure 3).

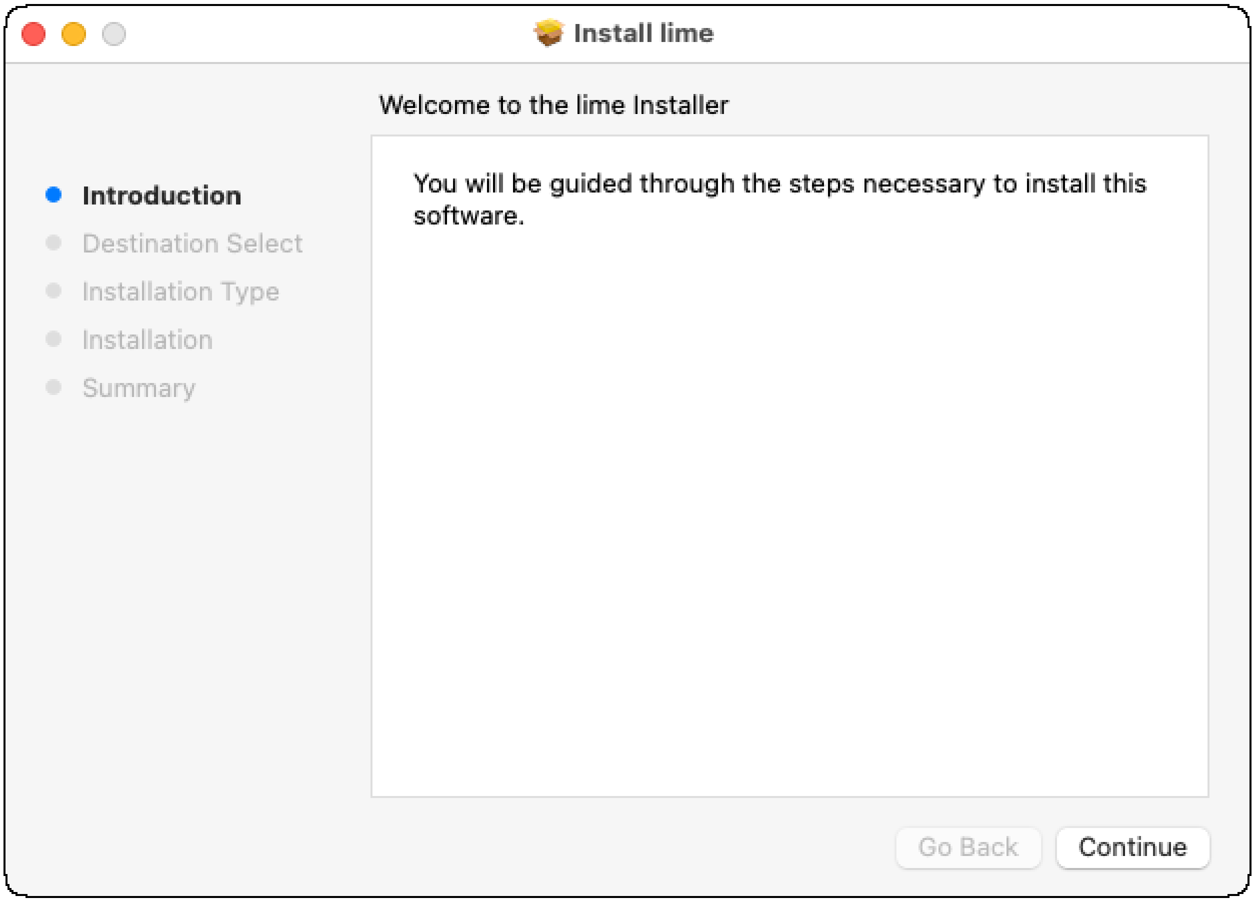


Figure 3: Mac installation wizard.

3.2.3 Debian (Ubuntu)

1. Download the .deb package
2. Install it by running:

```
sudo dpkg -i <package>
```

3.2.4 Linux

1. Download the Linux .zip installer.
2. Extract the files into a directory.
3. Run the installer inside that directory:

```
sudo ./lime_installer.sh
```

4. Cleanup (optional): You can delete the `.zip` file and extracted data after installation.

4. Configuration

4.1 Interpolation Settings

LIME Toolbox allows users to modify five settings that customize interpolation behavior and output visualization.

4.1.1 Available Interpolation Settings

- **Interpolation Reference**: Defines the reference spectrum for reflectance interpolation. Options:
    - **ASD**: Uses the lunar reflectance spectrum obtained with the ASD spectroradiometer at Izaña as part of the LIME project.
    - **Apollo 16 + Breccia**: Uses ROLO's composite spectrum based on Apollo 16 Soil and Breccia samples.
- **TSIS-1 Solar Spectrum SRF**: Specifies the spectral response function of the TSIS-1 Hybrid Solar Reference Spectrum. Options:
    - **ASD**: Use the ASD spectroradiometer spectral response function.
    - **Interpolated Gaussian**: Gaussian SRF with 1nm spectral sampling and 3nm resolution.
    - **Interpolated Triangle**: Triangular SRF with 1nm spectral sampling and 1nm resolution.
- **Show CIMEL anchor points**: Enables/disables the plotting of CIMEL anchor points.
- **Show interpolation spectrum**: Controls whether the interpolation reference spectrum appears in the output plot.
- **Skip Uncertainty Calculations**: Disables uncertainty computations.

Note: Uncertainty calculations are the primary **performance bottleneck** in LIME Toolbox simulations. Disabling them significantly improves speed.

4.1.2 Modifying Interpolation Settings

Interpolation settings can be modified through the interpolation settings window.

1. Go to the action menu bar and navigate to "Settings → Interpolation options" (Figure 4).

Figure 4: Opening the Interpolation Settings Window.

2. The **Interpolation Settings** window (Figure 5) will appear.
    a. The first two settings are dropdowns.
    b. The remaining three settings are checkboxes.
    c. Click "Save" to apply changes or "Cancel" to close without saving.

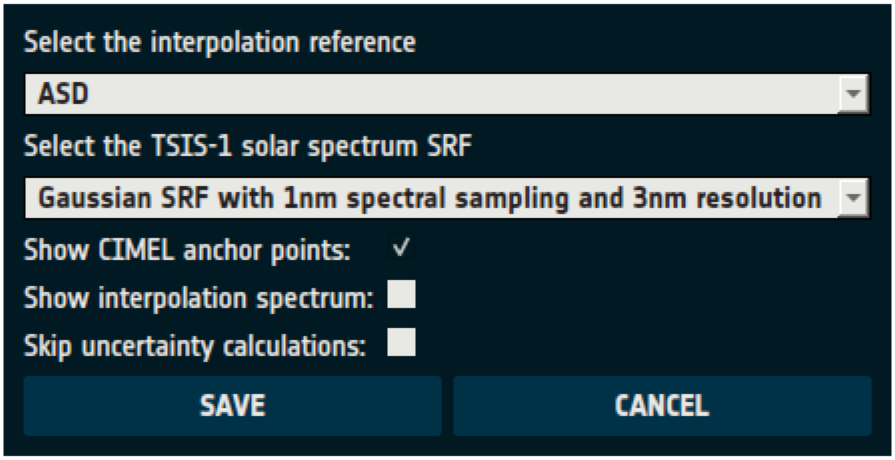


Figure 5: Interpolation Settings Window.

4.1.3 Command-Line Interface (CLI)

Interpolation settings can also be modified via the CLI using the `-i` or `--interpolation-settings` option.

The option must be followed by a string in JSON-formatted string, including any of the attributes in Table 1.

Attribute	Related Setting	Valid Values
`interp_spectrum`	Interpolation Reference	ASD or `Apollo 16 + Breccia`
`interp_srf`	TSIS-1 Solar Spectrum SRF	asd, `interpolated_gaussian` or `"interpolated_triangle"`
`show_cimel_points`	Show CIMEL anchor points	`False` or `True`
`show_interp_spectrum`	Show interpolation spectrum	`False` or `True`
`skip_uncertainties`	Skip Uncertainty Calculations	`False` or `True`

Table 1: Description of CLI's Interpolation settings JSON attributes.

Example usage:

```
lime -i '{"interp_spectrum": "ASD", "skip_uncertainties": "False",
"show_interp_spectrum": "False", "interp_srf": "interpolated_gaussian"}'
```

- Running this alone changes settings for subsequent runs.

- Running it with a simulation/comparison option updates settings for the current run and future runs.
- **Note**: When running multiple instances concurrently, they must share the same settings. Otherwise, behavior is undefined and may lead to crashes or wrong results.

4.1.4 Logging

LIME Toolbox logs error, warning and debug messages, that range from trivial information to error descriptions. This messages are written into text files within the logging directory which location varies depending on the operating system:

- Windows: `%appdata%\LimeTBX\`
- Mac: `~/Library/Application Support/LimeTBX/`
- Linux: `~/.LimeTBX/`

By default, LIME Toolbox logs at the `INFO` level. This means that all messages except DEBUG-level ones are included in the log files. If they were included they would bloat the log files with mostly useless information. Nevertheless, that information can be useful in case the software malfunctions. To enable DEBUG logging, set the environment variable `LIME_DEBUG` to DEBUG.

```
export LIME_DEBUG=DEBUG  # Linux/Mac
set LIME_DEBUG=DEBUG     # Windows (cmd)
$env:LIME_DEBUG="DEBUG"  # Windows (PowerShell)
```

If the LIME Toolbox suddenly crashes without generating any information in the standard logs, a detailed crash report is automatically saved to a file named `crash.log` located in the appdata directory. This file can be useful for troubleshooting and should be included when reporting issues.

5. Simulations

LIME Toolbox allows users to simulate lunar reflectance, irradiance, the degree of linear polarisation (DoLP) and the angle of linear polarisation (AoLP). Simulations are performed using the Simulation page (Figure 6), which is the default view when launching LIME Toolbox.

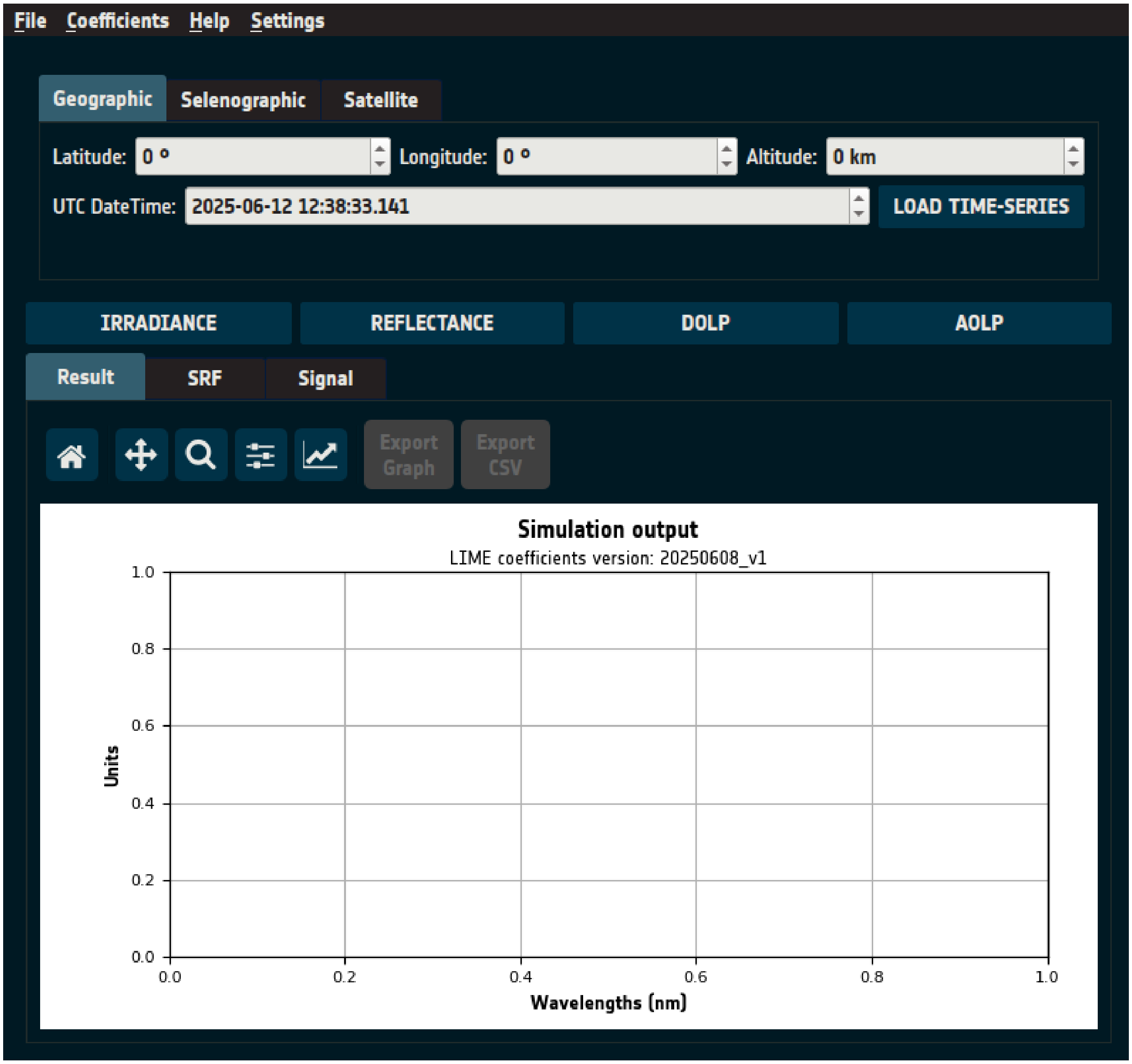


Figure 6: Simulation page.

Users can select one of three simulation methods:

- **Geographic Coordinates** – Based on an Earth-based location.
- **Selenographic Coordinates** – Based on a location on the Moon.
- **Satellite Position** – Based on an orbiting satellite's position.

5.1 Simulation Using Geographic Coordinates

Selecting the "Geographic" tab allows users to perform simulations based on Earth coordinates (Figure 7). Users must provide:

- **Latitude & Longitude** (in decimal degrees)

- **Altitude** (in kilometers)
- **UTC Date & Time**

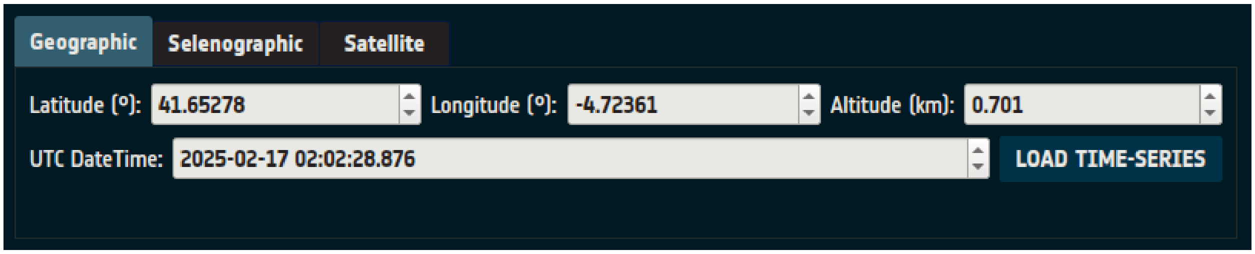


Figure 7: Geographic coordinates input.

5.1.1 Time-Series Input

For multiple timestamps, click "LOAD TIME-SERIES", which enables time-series file input (Figure 8).

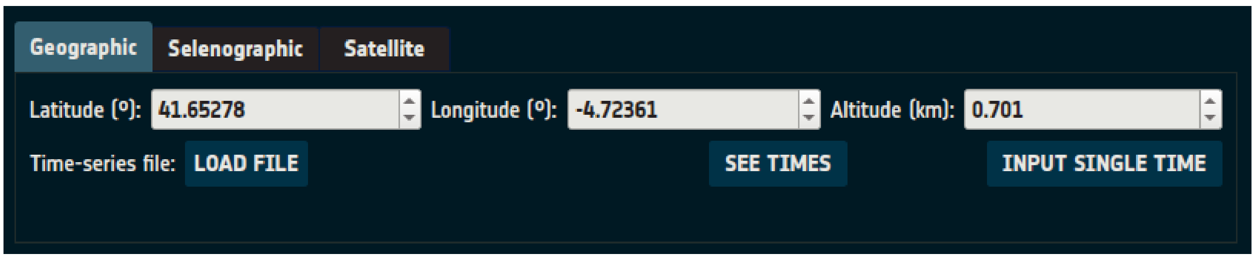


Figure 8: Geographic coordinates input for multiple timestamps.

5.1.1.1 Loading Time-Series Data

1. Click "LOAD FILE" to open a file selection dialog.
2. Select a file containing timestamps in one of the following formats:
   a. **ISO 8601 format**
   b. **Comma-separated values (CSV)**:
      i. `yyyy,mm,dd,HH,MM,SS`
      ii. `yyyy,mm,dd,HH,MM,SS,microseconds`

5.1.1.2 Example Valid File

```
2022,01,17,02,02,04
2023,01,17,02,02,04,123545
2020-01-12 00:22:43.124
```

Additional options:

- **"SEE TIMES"** – Opens a window displaying imported timestamps.
- **"INPUT SINGLE TIME"** – Switches back to single timestamp mode.

5.1.2 Command-Line Interface (CLI)

Use the `-e` or `--earth` option:

```
lime -e latitude_deg,longitude_deg,height_km,datetime_isoformat
```

5.1.2.1 Example

For a simulation of 35° of latitude, -25.2° of longitude, 400 meters of altitude, and at the date and time of 2022-01-20 02:00:00 UTC:

```
lime -e 35,-25.2,0.4,2022-01-20T02:00:00
```

For time-series input:

```
lime -e 35,-25.2,0.4 -t timeseries.txt
```

5.2 Simulation Using Selenographic Coordinates

Selecting the "Selenographic" tab enables simulations using Moon-based coordinates (Figure 9). Users must provide:

- **Sun-Moon Distance** (AU)
- **Observer-Moon Distance** (km)
- **Selenographic Latitude & Longitude of Observer** (decimal degrees)
- **Selenographic Longitude of the Sun** (radians)
- **Moon Phase Angle** (decimal degrees)

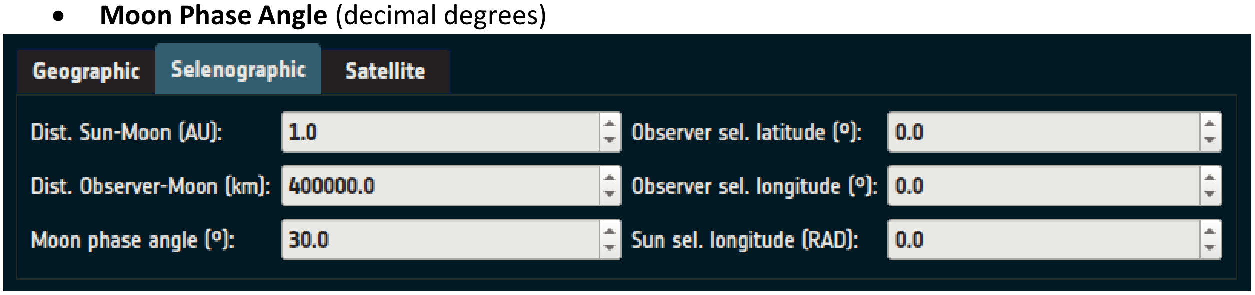


Figure 9: Selenographic coordinates input.

5.2.1 Command-Line Interface (CLI)

Use the `-l` or `--lunar` option:

```
lime -l
distance_sun_moon,distance_observer_moon,selen_obs_lat,selen_obs_lon,selen_
sun_lon,moon_phase_angle
```

5.2.1.1 Example

For a simulation for 0.98 AU of Sun-Moon Distance, 420000 km of Observer-Moon Distance, 20.5° and -30.2° as the selenographic latitude and longitude of the observer, 0.69 radians as the selenographic longitude of the Sun, and 15º as the moon phase angle:

```
lime -l 0.98,420000,20.5,-30.2,0.69,15
```

5.3 Simulation Using Satellite Positions

Selecting the **"Satellite"** tab enables simulation based on **orbiting satellites** (Figure 10).

Users must:

- **Select a satellite** from the available list.
- **Provide a UTC Date & Time**.

Note: Time-series input works the same as in Geographic Coordinates.

Selecting the "Satellite" tab enables simulations based on orbiting satellite (Figure 10). Users must:

- **Select a satellite** from the available list.
- **Provide a UTC Date & Time**.

Note: Time-series input works the same as in Geographic Coordinates.

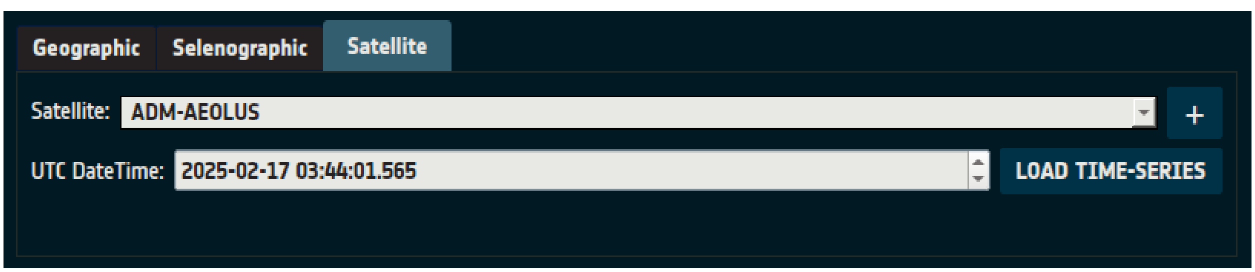


Figure 10: Satellite position input.

5.3.1 Adding a New Satellite

It's possible to add user-defined satellites to the list of available satellites.

1. Click the button with a plus (+) sign on the right of the dropdown.

2. The user will be prompted with the *Add Satellite Data* window (Figure 11).
3. Click "LOAD FILE" which opens a file selection dialog where users can load Orbit Scenario Files (OSF) or Three-Line Element Set files (TLE/3LE).
4. The *Add Satellite Data* window will now display information of the loaded file, and the user must fill the last details.
    a. **Satellite Name**: Only editable for OSF files. Name that will be displayed in the satellite list.
    b. **Start time**: Date when the file validity starts.
    c. **End time**: Date when the file validity stops.
5. Click "SAVE SATELLITE DATA" to store the loaded data in the local LIME Toolbox system.

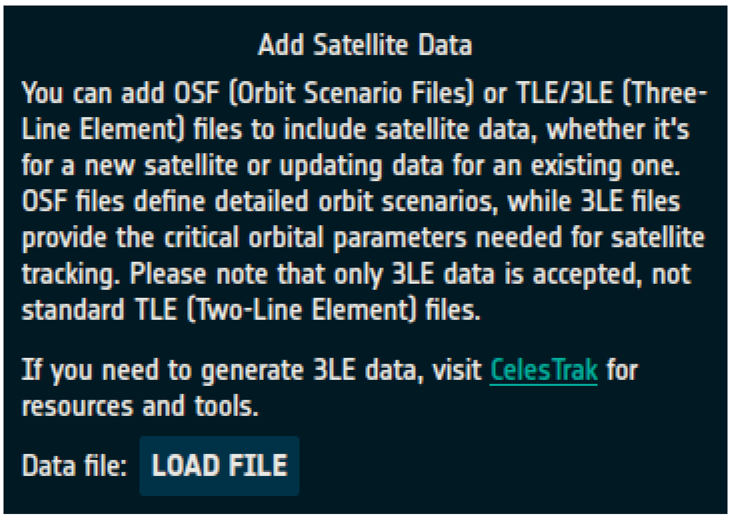


Figure 11: Add Satellite Data window.

5.3.2 Command-Line Interface (CLI)

Use the `-s` or `--satellite` option:

```
lime -s sat_name,datetime_isoformat
```

5.3.2.1 Example

To perform a simulation for the satellite PROVA-B at the date and time of 2020-01-20 02:00:00h:

```
lime -s PROBA-V,2020-01-20T02:00:00
```

As in Geographic Coordinates, one can use time-series input:

```
lime -s PROBA-V -t timeseries.txt
```

It's not possible to add a user-defined satellite throught the CLI at the moment.

5.4 Simulation output

The simulation results are displayed below the input section. Users can select one of the following button to run simulations and view results:

- **"IRRADIANCE"** – Displays irradiance results.
- **"REFLECTANCE"** – Shows reflectance results.
- **"DOLP"** – Visualises the Degree of Linear Polarisation (DoLP).
- **"AOLP"** – Visualises the Angle of Linear Polarisation (AoLP).

These buttons are positioned between the input and the output, as shown on top of Figure 12.

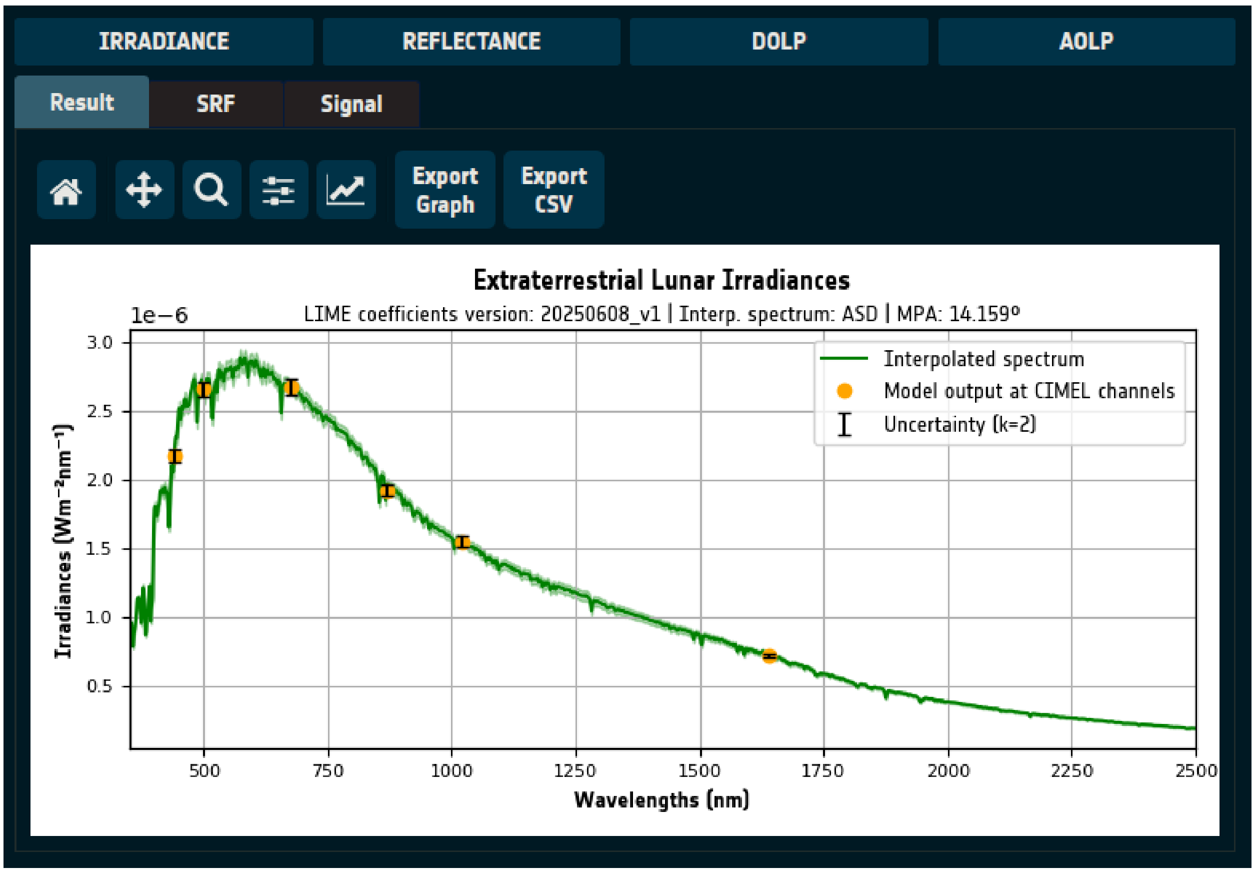


Figure 12: Simulation output.

Results are plotted with:

- **X-axis** → Wavelengths.
- **Y-axis** → Computed values.

5.4.1 Exporting Simulation Results

Users can export the results in multiple formats:

5.4.1.1 Graphical Export (Image/PDF)

- Click "EXPORT GRAPH" (top-center) to save the graph as an image or PDF.
- A file system dialog will prompt the user to select the location, filename, and format.
- Supported formats include JPG, PNG, PDF, and other common image formats.

5.4.1.2 Data Export (CSV File)

- Click "EXPORT CSV" (top-right) to save the simulation data as a comma-separated values (CSV) file.
- The user will be prompted to choose the location and filename.

5.4.1.3 NetCDF Export

- Go to the action menu bar and navigat to "File → Save as a netCDF file" to save results as a netCDF file.

Why use netCDF?

- Unlike CSV, netCDF allows LIME Toolbox to reload previous simulations for visualization.
- This format enables efficient data storage and retrieval.

5.4.2 Command-Line Interface (CLI) Export Options

In the CLI, results are only accessible by exporting them to data files. To do this, users must utilize the `-o` or `--output` option, with the argument varying based on the desired output type.

5.4.2.1 Graphical Export (Image/PDF)

Specify the image type, paths and filenames of each graph:

```
-o
graph,(pdf|jpg|png|svg),reflectance_path,irradiance_path,dolp_path,aolp_pat
h
```

For example:

```
-o graph,jpg,reflectance.jpg,irradiance.jpg,dolp.jpg,aolp.jpg
```

5.4.2.2 Data Export (CSV File)

Specify paths and names of each file:

```
-o
csv,reflectance_path,irradiance_path,dolp_path,aolp_path,integrated_irradia
nce_path
```

For example:

```
-o
csv,reflectance.csv,irradiance.csv,dolp.csv,aolp.csv,integrated_irradiance.
csv
```

5.4.2.3 NetCDF Export

Specify the netCDF file path:

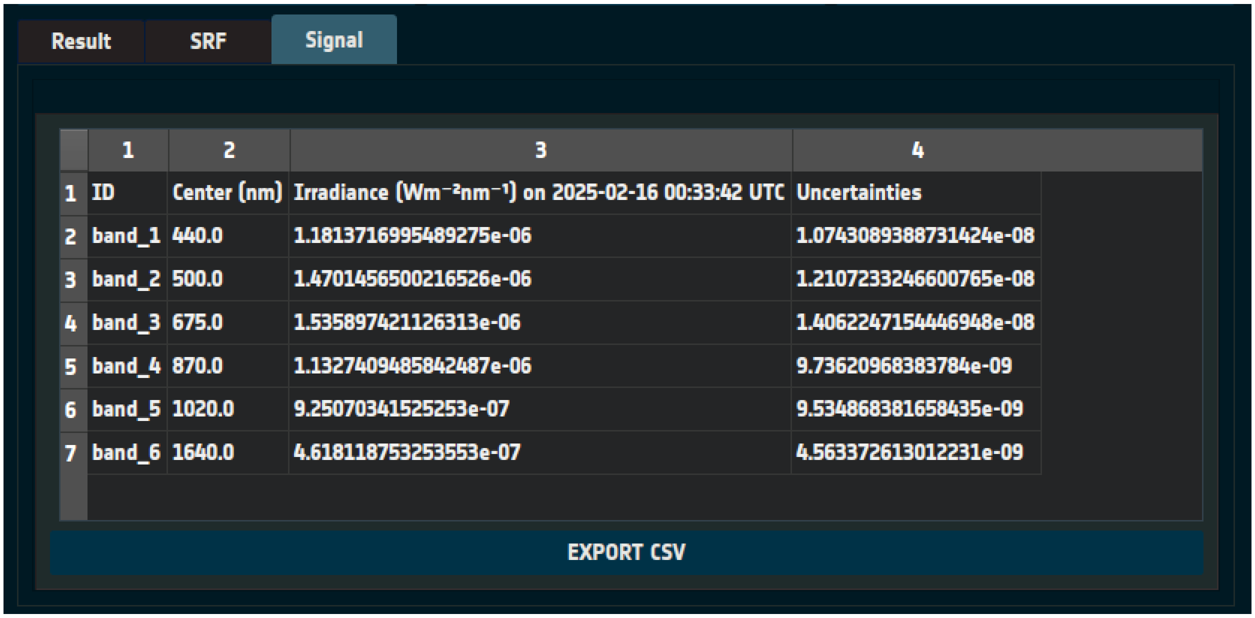
```
-o nc,output_path
```

For example:

```
-o nc,output.nc
```

5.5 Integrated Irradiance

LIME Toolbox integrates the calculated irradiance over the selected spectral response function (SRF). These values appear in the "Signal" tab (Figure 13), showing one value per SRF channel, and can be exported as CSV.



	1	2	3	4
1	ID	Center (nm)	Irradiance ($Wm^{-2}nm^{-1}$) on 2025-02-16 00:33:42 UTC	Uncertainties
2	band_1	440.0	1.1813716995489275e-06	1.0743089388731424e-08
3	band_2	500.0	1.4701456500216526e-06	1.2107233246600765e-08
4	band_3	675.0	1.535897421126313e-06	1.4062247154446948e-08
5	band_4	870.0	1.1327409485842487e-06	9.73620968383784e-09
6	band_5	1020.0	9.25070341525253e-07	9.534868381658435e-09
7	band_6	1640.0	4.618118753253553e-07	4.563372613012231e-09

Figure 13: Signal tab showing some results for the CIMEL SRF.

5.5.1 Spectral Response Functions (SRF)

Users can visualise, load, and switch between different SRFs in the "SRF" tab (Figure 14). This tab presents:

- A graph of the currently selected SRF, where:
  - X-axis represents wavelengths.
  - Y-axis represents the spectral response.
- Two vertical black lines marking the lower and upper simulation limits of LIME Toolbox.

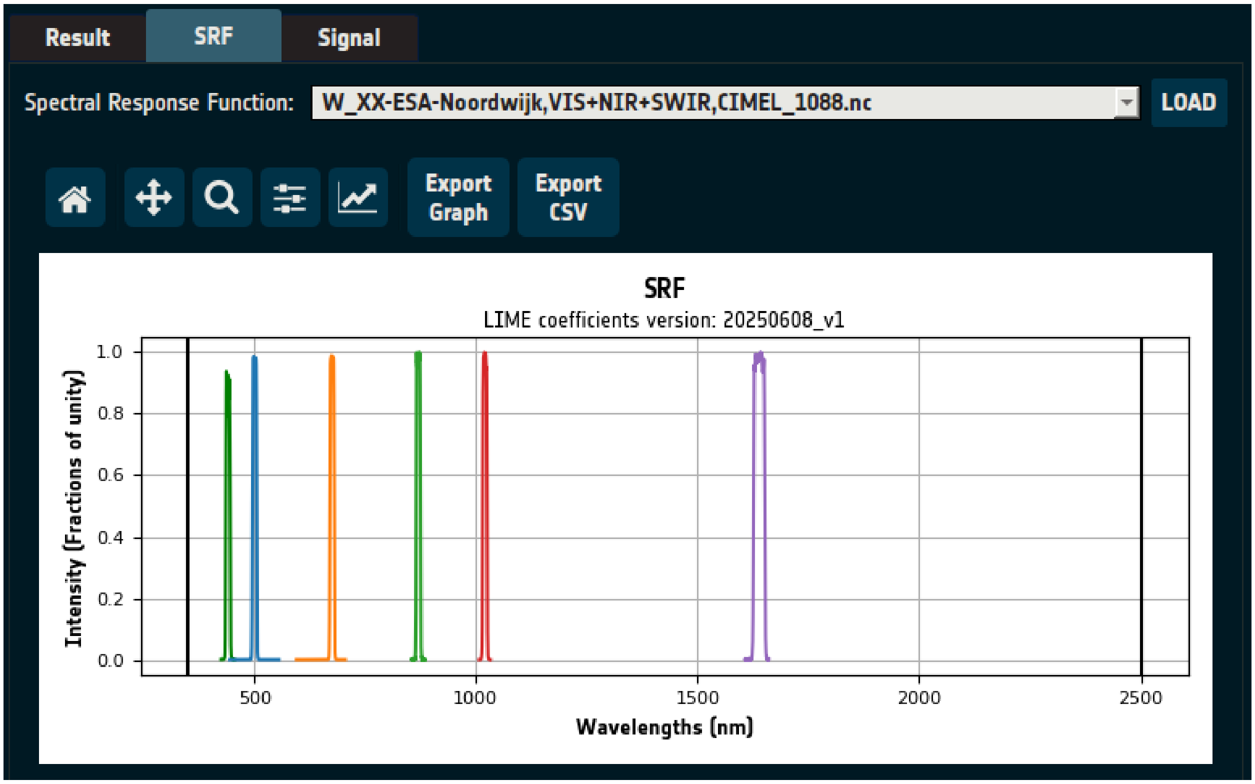


Figure 14: SRF tab showing CIMEL SRF.

By default, LIME Toolbox includes a default SRF that encompasses the entire LIME spectrum, named "Default".

5.5.1.1 Loading a New SRF

1. Click "LOAD" (top-right corner in Figure 14).
2. Select a netCDF SRF file in GLOD format (explained in the File Formats section).
3. Once loaded, use the dropdown menu next to the "LOAD" button to switch between SRFs.

This can also be done in the CLI using the `-f` or `--srf` option followed by the SRF path:

```
-f srf_path
```

5.5.1.2 Exporting SRF Data

- Graphs can be exported as images or PDFs.
- SRF data can be exported as CSV files.

6. Comparisons

Users must switch to the comparison page. Go to the action menu bar and navigate to "File → Perform comparisons from a remote sensing instrument" as seen in Figure 15.

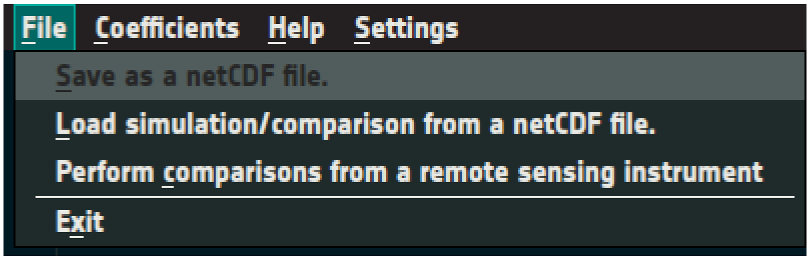


Figure 15: Action menu option to switch to the comparisons page.

6.1 Comparison Input

The comparison page (Figure 16) contains the user input fields at the top:

- **Lunar Observation Files**:
  - Instrument observation netCDF files in GLOD format to be compared.
    - The format is explained in the File Formats section.
  - "LOAD FILES": Opens a file selection dialog for loading observation files.
  - "UNLOAD FILES": Clears all loaded observation files.
- **SRF File**:
  - SRF netCDF file in GLOD format.
    - Must contain channels matching those in the observation files.
  - "LOAD FILE": Opens a file selection dialog for selecting the SRF file.
- **Compare Button**:
  - Initiates the comparison processing, displaying a progress indicator (as shown in Figure 17).
  - This button is enabled once valid observations and an SRF file are loaded.

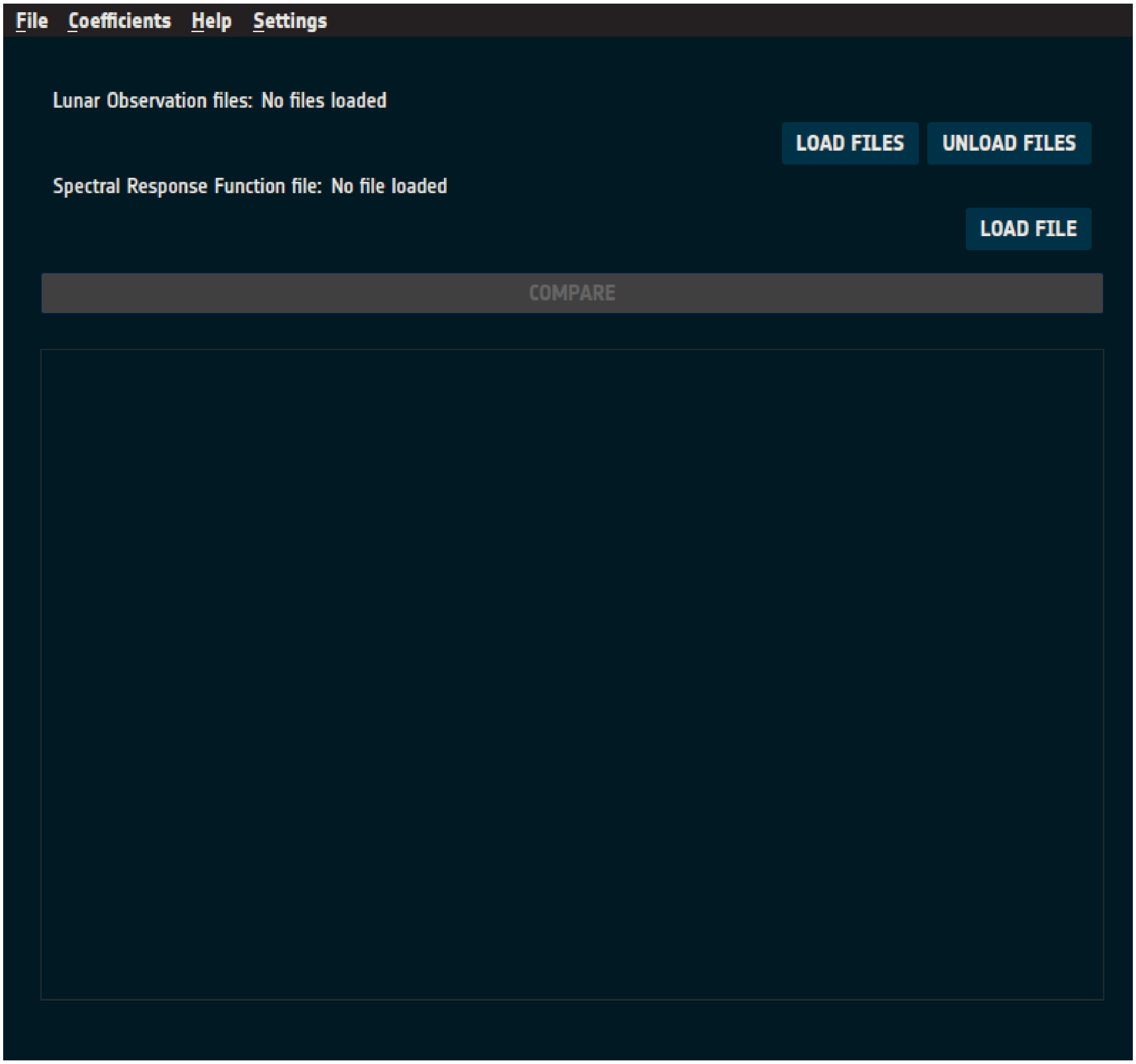


Figure 16: Initial view of the comparison page.

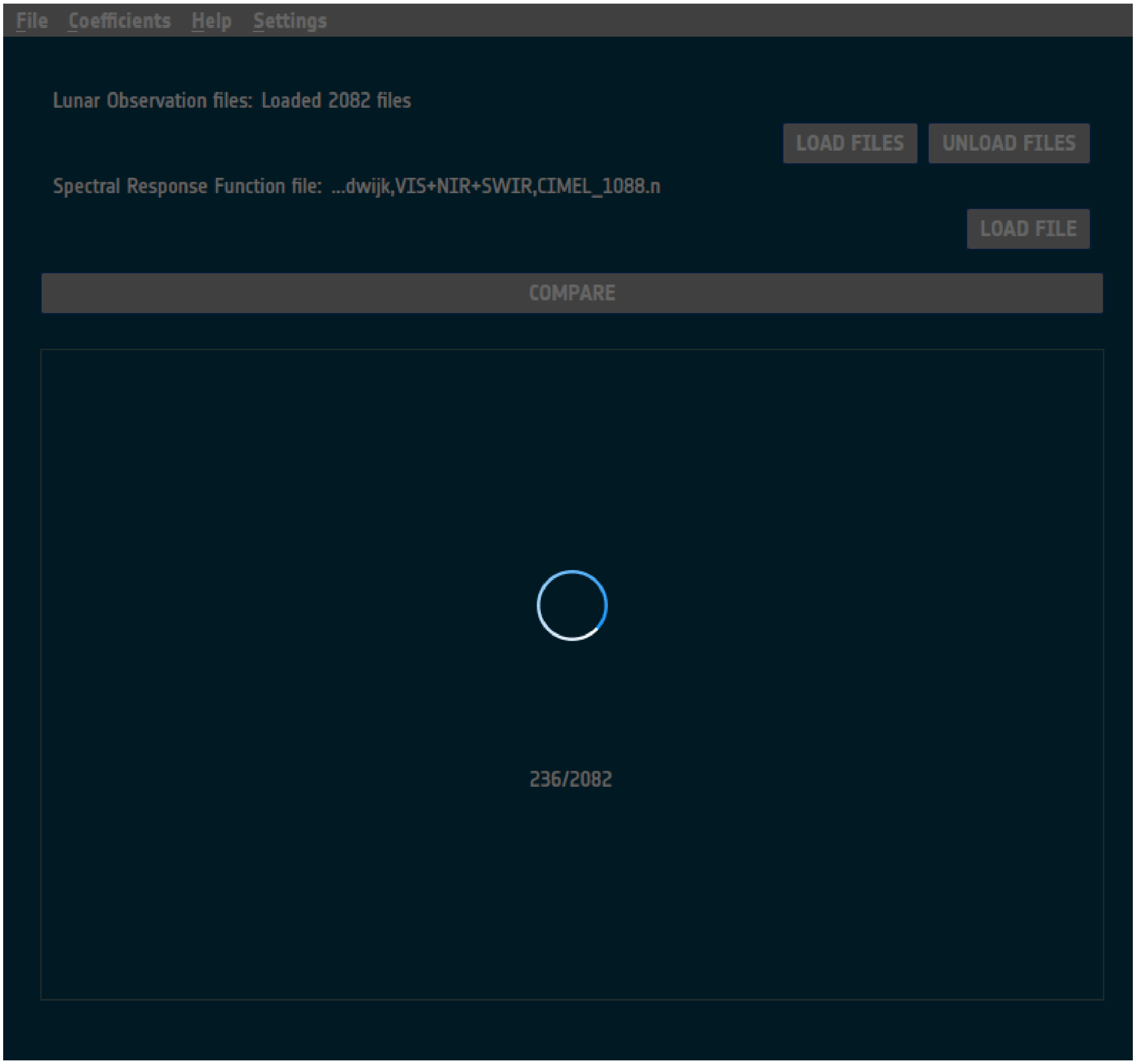


Figure 17: Comparison page processing comparisons.

6.2 Comparison Output

Once comparisons are computed, the comparison page presents the results and provides tools for exploring the data, as shown in Figure 18.

Figure 18: Comparison page after comparisons are computed.

6.2.1 Default View

- The **instrument's first-channel irradiance observations** (blue) are plotted alongside **LIME simulations** (orange) for the same channel.
- The **x-axis** represents the **comparison variable** (default: **Date**).
- The **primary y-axis** represents **irradiance values**.
- The **secondary y-axis** (right) represents the **relative difference (%)** (gray).

6.2.2 User Options

- **Channel Selection**: Switch between instrument channels via the "Channels" tab (above the graphs).
- **Difference Metric**: Adjust the displayed difference via the "Difference" dropdown (top-right), selecting:
    - **Relative difference**
    - **Percentage difference**
    - **No difference**
- **Comparison Method**: Change the comparison basis via the "Comparison by" dropdown (top-center) from **Date** to:
    - **Moon phase angle**
    - **Wavelength**, with two visualization options:
        - **Mean-based Comparison**: Computes the mean of all observations and simulations for each channel.
        - **Boxplot Visualization**: Displays the distribution of values per channel, as explained in Figure 19.
- **New Comparison**: Click "NEW" (top-left) to clear results and start a new comparison.
    - A **confirmation dialog** appears, as shown in Figure 20.

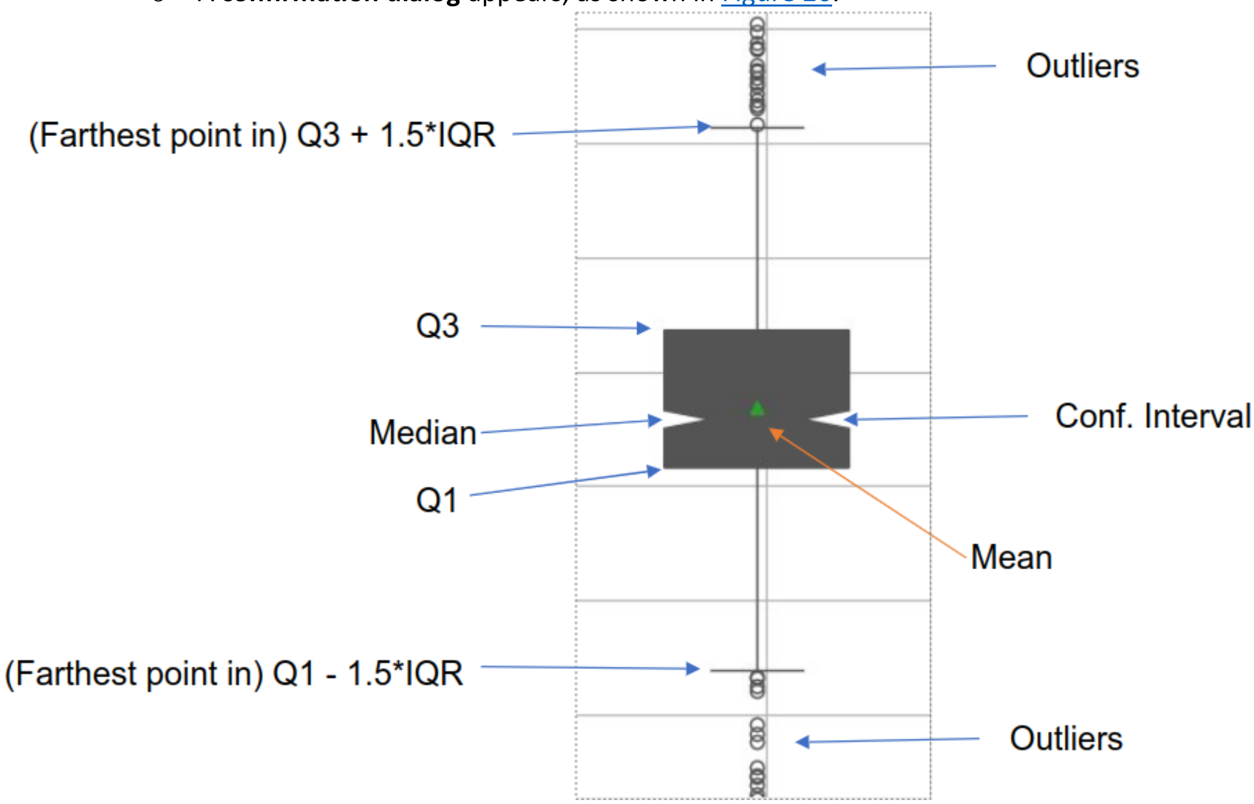


Figure 19: Breakdown of LIME comparison boxplots.

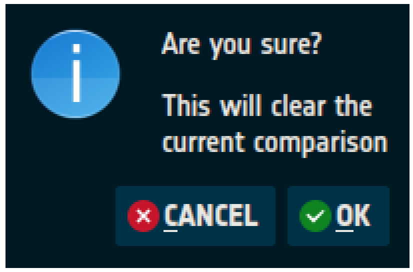


Figure 20: Dialog asking for confirmation after clicking "NEW"

6.2.3 Exporting Data

- Graphs can be exported as images (JPG, PNG, PDF, etc.) or CSV files.
- The full comparison dataset can be saved as a netCDF file, allowing it to be reloaded in LIME Toolbox for future analysis.

6.3 Comparing throught the Command-Line Interface (CLI)

6.3.1 CLI Comparison Input

To perform comparisons via CLI, use the `-c` or `--comparison` option along with `-f` or `--srf`:

```
lime -c "path_observation_1 path_observation_2 ... path_observation_n" -f
path_srf
```

Example: To compare `input_1.nc`, `input_2.nc` and `input_3.nc`, using the spectral response function defined in `srf.nc`:

```
lime -c "input_1.nc input_2.nc input_3.nc" -f srf.nc
```

Users can also use glob patterns to load multiple files. For example to compare all `.nc` files in the `files` directory:

```
lime -c "files/*.nc"
```

6.3.2 CLI Comparison Output

As with simulations, comparison results must be be exported in order to be able to interact with them. Append the `-o` or `--output` option for this.

6.3.2.1 Graphical Export (Image/PDF)

Specify the image type, comparison variable, difference metric, and file paths for each channel:

```
-o
graph,(pdf|jpg|png|svg),(DT|MPA|BOTH|CHANNEL|CHANNEL_MEAN),(rel|perc|none),
comparison_channel_1,comparison_channel_2,...,comparison_channel_n
```

To simplify, export all channels to a directory using `graphd`:

```
-o
graphd,(pdf|jpg|png|svg),(DT|MPA|BOTH|CHANNEL|CHANNEL_MEAN),(rel|perc|none)
,output_directory
```

Examples:

```
-o graph,jpg,DT,rel,comparison1.jpg,comparison2.jpg
```

Using `graphd`:

```
-o graphd,jpg,DT,rel,comparison_dir
```

6.3.2.2 Data Export (CSV File)

Specify the comparison variable, difference metric, and file paths for each channel:

```
-o
csv,(DT|MPA|BOTH|CHANNEL|CHANNEL_MEAN),(rel|perc|none),comparison_channel_1
,comparison_channel_2,...,comparison_channel_n
```

To export all channels to a directory, use `csvd`:

```
-o csvd,(DT|MPA|BOTH|CHANNEL|CHANNEL_MEAN),(rel|perc|none),output_directory
```

Examples:

```
-o csv,DT,rel,comparison1.csv,comparison2.csv
```

Using `csvd`:

```
-o csvd,DT,rel,comparison_dir
```

6.3.2.3 NetCDF Export

Specify the netCDF file path:

```
-o nc,output_path
```

Example:

```
-o nc,output.nc
```

7. Coefficients

LIME Toolbox requires coefficients to run its LIME model equations for reflectance (and consequently irradiance) and for the Degree of Lunar Polarisation (DoLP).

These models are continuously updated, improving their accuracy with each new coefficient release.

7.1 Updating the Coefficients

To update the coefficients, navigate to "Coefficients → Download updated coefficients" in the action menu bar.

A window will appear indicating that the coefficient download is in progress, as shown in Figure 21.

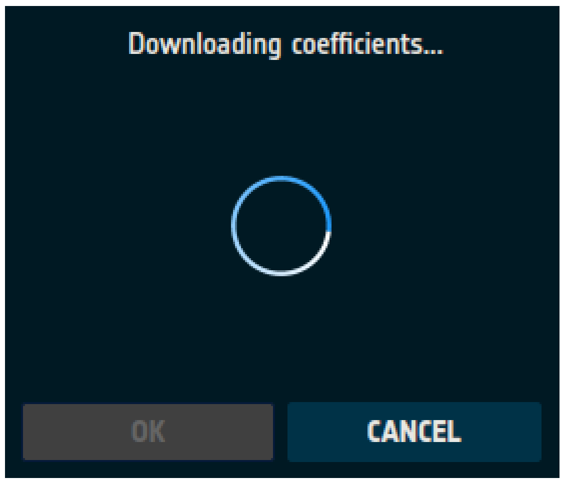


Figure 21: Coefficients download in progress.

Once the process is complete, the window will display:

- The number of new coefficient versions downloaded.
- Any errors encountered during the download.

The result may indicate that new coefficients were downloaded (Figure 22) or that no new updates were available (Figure 23). If there was an issue connecting to the coefficients server, an error message will be displayed (Figure 24).

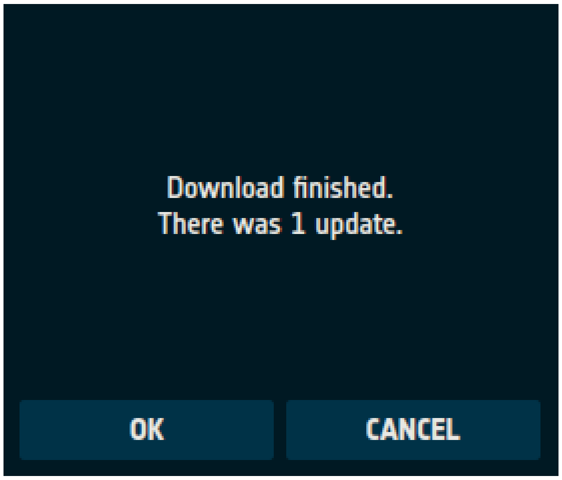


Figure 22: One new coefficient version.

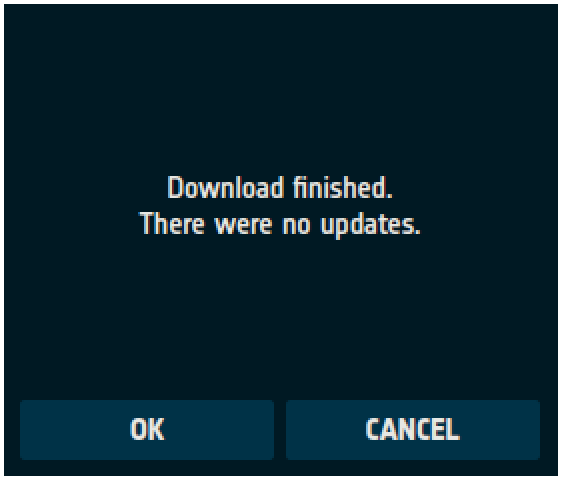


Figure 23: No new coefficient updates available.

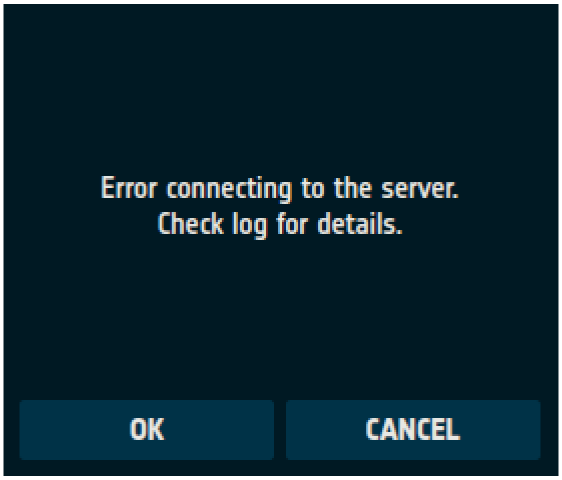


Figure 24: Error downloading the coefficients.

7.1.1 Updating the Coefficients via CLI

Users can also update coefficients via the command-line interface (CLI) using the `-u` or `--update` option:

```
lime -u
```

7.2 Selecting a Coefficients Version

To use a specific coefficient version, navigate to "Coefficients → Select coefficients" in the action menu bar.

A window will appear, displaying a dropdown menu containing all available coefficient versions (Figure 25). To change the version:

1. Open the dropdown menu.
2. Select the desired coefficient version.
3. Click "SAVE" to confirm the selection.

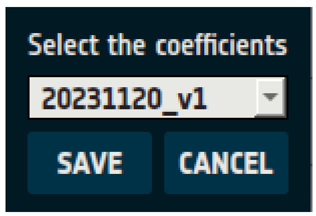


Figure 25: Selecting a coefficient version.

7.2.1 Choosing the Coefficients Version via CLI

To choose a different coefficient version through the CLI, use the `-C` or `--coefficients` option:

```
lime -C SELECTED_COEFF_VERSION_NAME
```

This updates the coefficient version for all subsequent simulations and applies immediately to the current simulation if used alongside any simulation or comparison option.

Example: To select the coefficient version `20231120_v1`:

```
lime -C 20231120_v1
```

8. File Formats

LIME Toolbox reads various types of data from netCDF files, each following a specific format. These formats adhere as closely as possible to the GSICS Lunar Observation Dataset (GLOD) format standards.

8.1 Spectral Response Function (SRF)

Spectral Response Function files are structured with two dimensions:

- `channel`: A coordinate and dimension, where each value represents a different spectral channel.
- `sample`: A dimension without coordinates, which allows multiple wavelengths to be associated with each channel.

(This dimension may have different names depending on the dataset.)

These dimensions organise the mandatory data variables described in Table 2.

Variable	Dimensions	dtype	Description
`channel_id`	`channel`	str	Name of the channel
`wavelength`	`sample, channel`	float	Wavelengths present in each channel
`srf`	`sample, channel`	float	Spectral response of each wavelength per channel

Table 2: Mandatory variables of the Spectral Response Function netCDF file format.

Note: The variable `wavelength` must contain the attribute `units`, which value must be the variable unit symbol by the IS. For example, "nm".

8.2 Lunar Observation

Lunar Observation files format is a subset of the GLOD format for lunar observations. It's structured using three dimensions:

- `date`: A coordinate and dimension representing the time of the lunar observation.
  - Stored as a double precision float. Units: seconds since EPOCH.
- `chan`: A dimension without coordinates, where each value represents a different spectral channel.
- `sat_xyz`: A dimension without coordinates, representing the three spatial coordinates (x, y, z).
  - This dimension must have a fixed length of three.

These dimensions structure the required data variables outlined in Table 3.

Variable	Dimensions	dtype	Description
`channel_name`	`chan`	str	Name of the spectral channel
`irr_obs`	`chan`	float	Observed lunar irradiance per spectral channel
`sat_pos`	`sat_xyz`	float	Coordinates of the observer in `sat_pos_ref` reference frame
`sat_pos_ref`	None	str	Reference frame of the satellite position

Table 3: Mandatory variables of the Lunar Observation netCDF file format.

Note: The variable `sat_pos` must contain the attribute `units`, which value must be the variable unit symbol by the IS. For example, “km”.

In addition to these variables, the file must include the attribute:

- `data_source`: Specifies the origin of the observation data.

8.2.1 Lunar Observation Format Extension

Lunar Observation files should follow the subset of the GLOD format previously described. However, if the `sat_pos` variable is not available, LIME Toolbox will instead look for selenographic coordinates. In this case, the selenographic variables must follow the schema in Table 4, where all variables must have `date` as their dimension.

Variable Name	Mandatory	Description
`distance_sun_moon`	Yes	Distance between the Sun and the Moon (AU)
`sun_sel_lon`	Yes	Selenographic longitude of the Sun (radians)
`distance_sat_moon`	Yes	Distance between the satellite and the Moon (km)
`sat_sel_lon`	Yes	Selenographic longitude of the satellite (degrees)
`sat_sel_lat`	Yes	Selenographic latitude of the satellite (degrees)
`phase_angle`	Yes	Moon phase angle (degrees)
`sat_name`	No	Satellite name (used for handling missing data)

`geom_factor` or `geom_const`	No	Geometric constant used to normalize observed irradiance

Table 4: Data variables in the Lunar Observation netCDF file format representing selenographic coordinates.

8.2.1.1 Understanding `geom_factor`

The `geom_factor` (or `geom_const`) represents the geometric constant used in irradiance normalization.

- If a given, the toolbox will use this value to normalize its simulated irradiance.`normalised_irr = irr/geom_factor`

8.2.1.2 Handling Missing Data

If any mandatory variable is missing, LIME Toolbox will automatically compute them using:

- **SPICE library** → Computes `distance_sun_moon` and `sun_sel_lon`.
- **SPICE + EO-CFI libraries** → Compute `distance_sat_moon`, `sat_sel_lon`, `sat_sel_lat`, and `phase_angle`.

For these four latter variables, LIME Toolbox requires the satellite name (`sat_name`),

- It must be a string and must match a satellite in the LIME Toolbox satellite list.

8.2.1.3 Optional Attribute: `to_correct_distance`

- If present with a value of `1`, LIME Toolbox will normalise the observation's `irr_obs` value using the observation's distances.
- This is useful when the irradiance is not pre-normalized.

8.3 LIME Toolbox Simulations and Comparisons

LIME Toolbox allows exporting simulations and comparisons to netCDF format files, which can be reloaded within the toolbox for future visualization and analysis.

These files follow a structure similar to Lunar Observation files but contain multiple observation timestamps instead of just one. Additionally, they include more detailed data such as simulated irradiance, reflectance, and spectral values.

Both simulation and comparison files share a similar format but with distinct differences. This format is referred to as the LIME Toolbox netCDF format, previously known in documentation as LIME-GLOD (LGLOD) format.

8.3.1 File Attributes

LIME Toolbox netCDF format files include multiple attributes based on the GLOD format. The key attributes are:

- **data_source**: Indicates the origin of the data (LIME Toolbox).
- **reference_model**: Specifies the LIME coefficient version used.
- **not_default_srf**:
    - `0`: Default LIME Toolbox SRF was used.
    - `1`: A user-defined custom SRF was used.
- **spectrum_name**: Name of the spectrum used for reflectance interpolation.
- **is_comparison**:
    - `0`: Indicates a **simulation file**.
    - `1`: Indicates a **comparison file**.
- **skipped_uncertainties**:
    - `0`: Uncertainty computations were **performed**.
    - `1`: Uncertainty computations were **skipped**.
- **polarisation_spectrum_name**: Name of the spectrum used in polarization interpolation (*only present in simulation files*).

8.3.2 File Dimensions

All LIME Toolbox netCDF files are structured using four core dimensions:

- **chan**: Number of spectral channels in the data.
- **date**: Number of timestamps present.
- **number_obs**: Number of observation positions where simulations exist for at least one channel.
- **sat_xyz**: Fixed length of 3, representing the `(x, y, z)` coordinates of the satellite.

Simulations files contain two additional dimensions:

- **wlens**: Fixed length of `2151`, representing the number of wavelengths in full-spectrum simulations.
- **wlens_cimel**: Fixed length of 6, representing the number of CIMEL wavelengths.

8.3.3 File Variables

8.3.3.1 Common Data Variables

LIME Toolbox netCDF files share several core variables based on the GLOD format, described in Table 5.

Variable	Dimensions	dtype	Description
`date`	`date`	float64	Time of lunar observation, seconds since epoch.
`outside_mpa_range`	`number_obs`	int8	1 if the observation is outside the Moon phase angle valid range, 0 if inside.
`mpa`	`number_obs`	float64	Moon phase angle in degrees.
`channel_name`	`chan`	str	Channel/Sensor band identifier.
`sat_pos`	`number_obs`, `sat_xyz`	float64	Satellite position in (x, y, z) coordinates for `sat_pos_ref` frame.
`sat_pos_ref`	`number_obs`	str	Reference frame of the satellite position.
`sat_name`	None	str	Name of the satellite (or empty if it wasn't a satellite measure).
`irr_obs`	`number_obs`, `chan`	float64	Simulated integrated lunar irradiance for each channel.
`irr_obs_unc`	`number_obs`, `chan`	float64	Uncertainties of the simulated integrated lunar irradiance for each channel.

Table 5: Common data variables in all LIME Toolbox netCDF files.

8.3.3.2 Comparison Specific Variables

Comparison files contain additional variables that store observed and computed differences, detailed in Table 6.

Variable	Dimensions	dtype	Description

irr_comp	number_obs, chan	float64	Integrated lunar irradiance for each channel observed with the instrument, obtained from the user defined observation files.
irr_comp_unc	number_obs, chan	float64	Uncertainties of the integrated lunar irradiance for each channel observed with the instrument, obtained from the user defined observation files.
irr_diff	number_obs, chan	float64	Lunar irradiance comparison difference for each channel.
irr_diff_unc	number_obs, chan	float64	Uncertainties of the lunar irradiance comparison difference for each channel.
perc_diff	number_obs, chan	float64	Percentage difference in the lunar irradiance comparison for each channel.
perc_diff_unc	number_obs, chan	float64	Uncertainties of the percentage difference in the lunar irradiance comparison for each channel.
mrd	chan	float64	Mean relative difference.
mard	chan	float64	Mean absolute relative difference.
mpd	chan	float64	Mean percentage difference.
std_mrd	chan	float64	Standard deviation of the mean relative difference.
number_samples	chan	float64	Number of comparisons for each channel.

Table 6: Data variables in LIME Toolbox Comparison netCDF files.

8.3.3.3 Simulation Specific Variables

Simulation files contain additional variables that store spectral data, described in Table 7.

Variable	Dimensions	dtype	Description
wlens	wlens	float64	Wavelengths for irr_spectrum, refl_spectrum, and polar_spectrum.

irr_spectrum	number_obs, wlens	float64	Simulated lunar irradiance per wavelength.
irr_spectrum_unc	number_obs, wlens	float64	Uncertainties for the simulated lunar irradiance per wavelength.
refl_spectrum	number_obs, wlens	float64	Simulated lunar reflectance per wavelength.
refl_spectrum_unc	number_obs, wlens	float64	Uncertainties for the simulated lunar reflectance per wavelength.
polar_spectrum	number_obs, wlens	float64	Simulated lunar degree of linear polarization per wavelength.
polar_spectrum_unc	number_obs, wlens	float64	Uncertainties for the simulated lunar degree of linear polarization per wavelength.
aolp_spectrum	number_obs, wlens	float64	Simulated lunar angle of linear polarization per wavelength.
aolp_spectrum_unc	number_obs, wlens	float64	Uncertainties for the simulated lunar angle of linear polarization per wavelength.
cimel_wlens	wlens_cimel	float64	CIMEL wavelengths.
irr_cimel	number_obs, wlens_cimel	float64	Simulated lunar irradiance for the CIMEL wavelengths.
irr_cimel_unc	number_obs, wlens_cimel	float64	Uncertainties for the simulated lunar irradiance for the CIMEL wavelengths.
refl_cimel	number_obs, wlens_cimel	float64	Simulated lunar reflectance for the CIMEL wavelengths.
refl_cimel_unc	number_obs, wlens_cimel	float64	Uncertainties for the simulated lunar reflectance for the CIMEL wavelengths.
polar_cimel	number_obs, wlens_cimel	float64	Simulated lunar degree of linear polarization for the CIMEL wavelengths.

`polar_cimel_unc`	`number_obs, wlens_cimel`	float64	Uncertainties for the simulated lunar degree of linear polarization for the CIMEL wavelengths.
`aolp_cimel`	`number_obs, wlens_cimel`	float64	Simulated lunar angle of linear polarization for the CIMEL wavelengths.
`aolp_cimel_unc`	`number_obs, wlens_cimel`	float64	Uncertainties for the simulated lunar angle of linear polarization for the CIMEL wavelengths.

Table 7: Data variables in LIME Toolbox Simulation netCDF files.