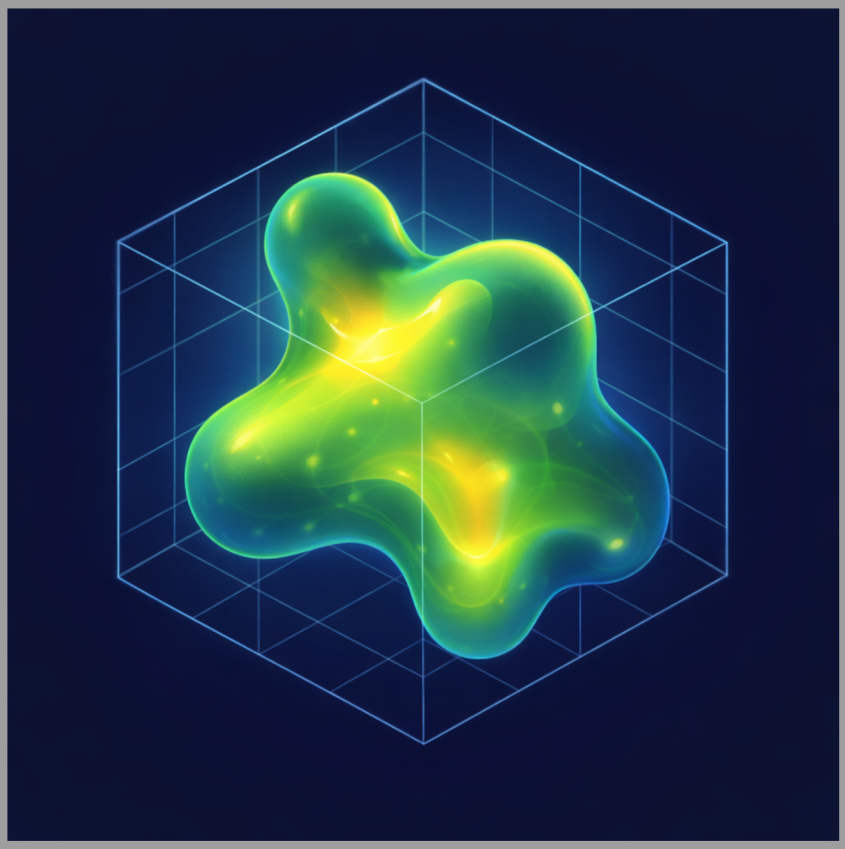
From Topological Data to Scientific Exploration

Toplso3D v2026 User Manual



Ary da Silva Maia

1st Edition

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TopIso3D v2026 User Manual

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Dados Internacionais de Catalogação na Publicação (CIP)
(Câmara Brasileira do Livro, SP, Brasil)

Maia, Ary da Silva
From topological data to scientific exploration [livro eletrônico] : TopIso3D v2026 user manual / Ary da Silva Maia. -- 1. ed. -- João Pessoa, PB : Ed. do Autor, 2026.
PDF

ISBN 978-65-02-29867-1

1. Dados - Estruturas (Ciência da computação) - Estudo e ensino 2. Tecnologia I. Título.

26-386735.0 CDD-005.73

Índices para catálogo sistemático:

1. Dados : Estruturas : Processamento de dados
005.73

Livia Dias Vaz - Bibliotecária - CRB-8/9638

To Deyse, my companion in life and adventure,
who has always made the unknown feel like an invitation.

And to my grandchildren — my three Anas (Beatriz, Gabriela, and Clara),
Ary Neto and Benício Luiz — may this book remind you that, for as long as we live,
we can always keep learning, exploring, and challenging ourselves.

About this manual

This manual explains how to install, configure, and use TopIso3D v2026 to manage, execute, organize, visualize, analyze, and export results from TOPOND-based topological investigations.

Manual philosophy

TopIso3D v2026 was conceived not to replace the researcher, but to augment the researcher's ability to explore, organize, correlate, and interpret topological information.

Document conventions

Explanatory sections describe the software and its scientific responsibilities in an objective style. Procedural sections speak directly to you and use imperative instructions such as “Choose”, “Select”, and “Click”.

- **Bold text** identifies interface elements and modules.
- `Monospaced text` identifies filenames, paths, and commands.
- Notes provide additional context.
- Important boxes highlight conditions that may affect a calculation or result.

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1 Introduction

1.1 Purpose of TopIso3D v2026

TopIso3D v2026 is a cross-platform scientific environment developed to support the management, execution, organization, exploration, and export of topological analyses produced through the TOPOND/PROPERTIES module of the CRYSTAL program suite [1, 2].

Its purpose is not to automate scientific reasoning, but to reduce the practical barriers that separate researchers from the topological information generated by TOPOND.

1.2 Who should use this manual?

This manual is intended for researchers, students, and collaborators who use TOPOND results in studies of periodic electronic structures, including crystalline materials, surfaces, interfaces, and adsorption systems.

1.3 System requirements

- Linux, Windows, or macOS.
- An official TopIso3D v2026 distribution for your operating system.
- The CRYSTAL `PROPERTIES` executable is strongly recommended for running new TOPOND analyses locally, but it is not required for exploring previously generated outputs.

2 Getting Started

2.1 Installation

Download the official binary distribution corresponding to your operating system and follow the standard installation procedure. Depending on your platform, this consists of running the Windows installer, opening the macOS application bundle, or executing the Linux AppImage. No additional compilation steps are required before you can start using TopIso3D v2026.

TopIso3D v2026 can be used either to perform new TOPOND analyses or to explore previously generated results. Although a local installation of the CRYSTAL `PROPERTIES` module is strongly recommended when you intend to run new analyses directly from the software, it is not required for importing and exploring existing outputs such as `trho.out`, `tlap.out`, or `atbp.out`.

Tip

Linux users may need to grant execution permission to the AppImage before the first launch.

2.2 The Main Window

After launching TopIso3D v2026, the main window opens with the **Workspace** module already selected (Figure 2.1). This is the starting point for every scientific investigation, since all subsequent operations are performed within the context of a selected project.

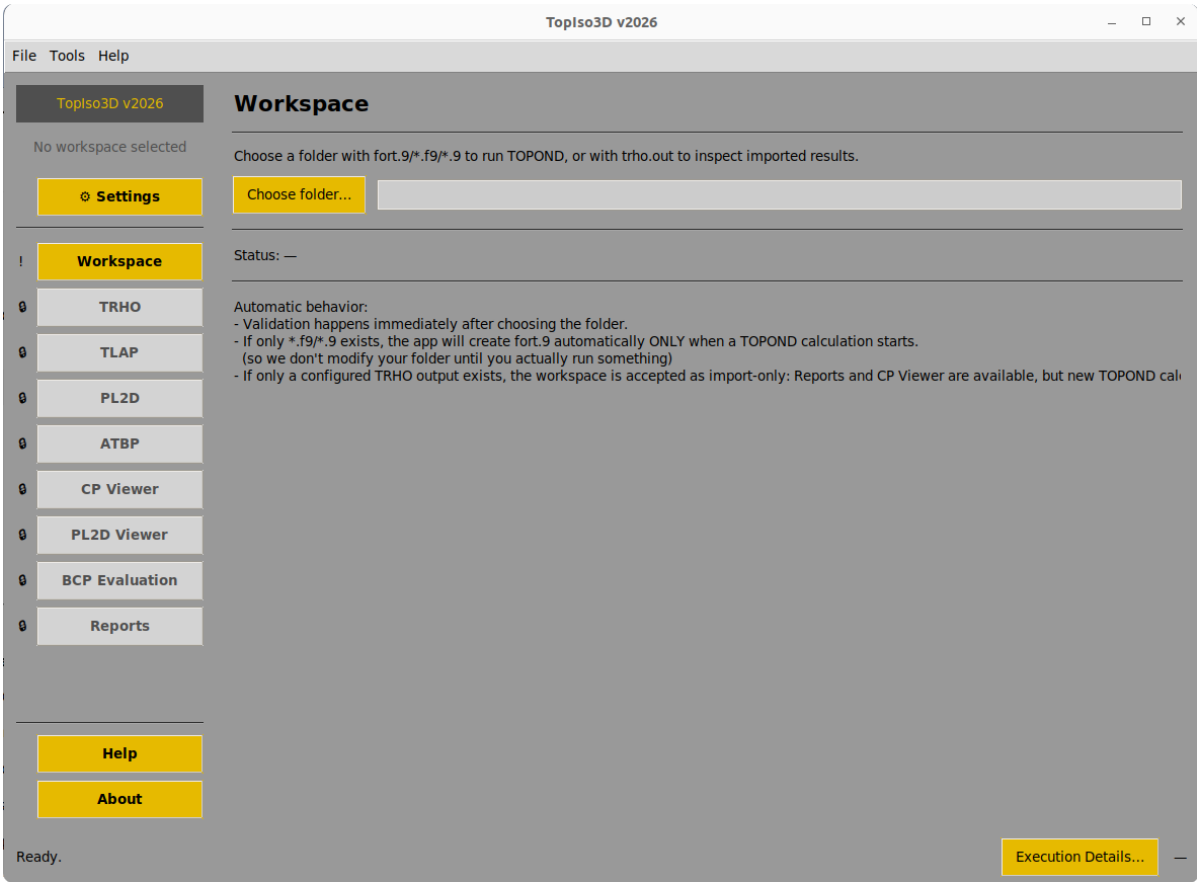

Figure 2.1: Main window of TopIso3D v2026 immediately after startup.

The main window is composed of two permanent areas: a navigation panel on the left and a central working area on the right. The navigation panel provides access to all TopIso3D v2026 modules, while the central area displays the controls and information associated with the currently selected module.

Throughout a TopIso3D v2026 session, the navigation panel remains unchanged, whereas the contents of the central area are updated according to the selected module. This provides a consistent interaction model across the entire environment.

Some operations open additional windows dedicated to specific tasks, such as software configuration, interactive visualizations, file selection, or execution details. These auxiliary windows complement the main interface without interrupting the current scientific investigation.

2.3 Settings

The **Settings** module allows you to customize the internal behavior of TopIso3D v2026 according to your computational environment and personal preferences. Although the software can be used immediately after installation, configuring the available options before starting your first project is strongly recommended. Most settings only need to be defined once and remain available for all future projects.

Figure 2.2 presents the **Settings** window, where you can configure the main operational aspects of TopIso3D v2026. After this initial configuration, you can focus on your scientific investigations without revisiting the Settings module unless your computational environment or personal preferences change.

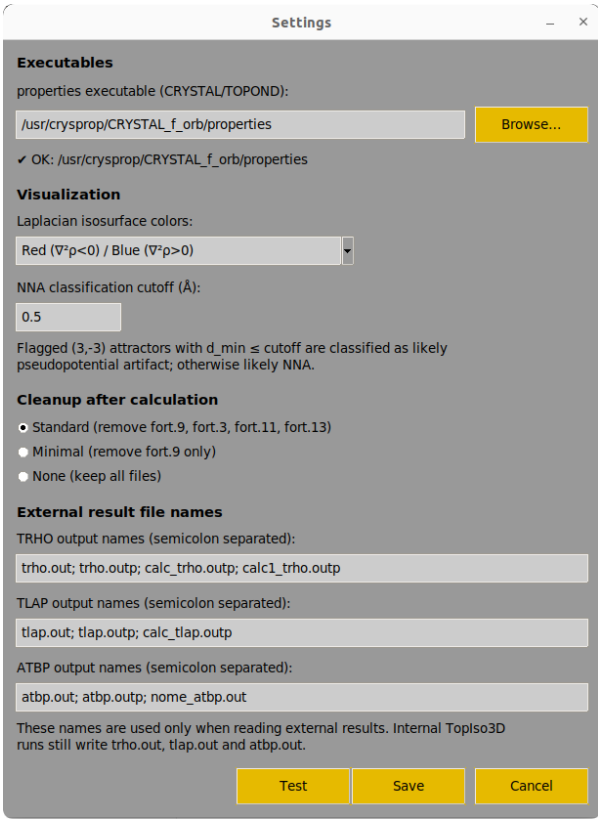

Figure 2.2: Settings window.

The following sections describe each configuration group shown in Figure 2.2 and explain how these options influence the behavior of the software.

2.3.1 Executables

Use this section to specify the location of the CRYSTAL `PROPERTIES` executable. This configuration is strongly recommended if you intend to perform new TRHO, TLAP, PL2D, or ATBP analyses directly from TopIso3D v2026. If the executable is not configured, you can still explore previously generated TOPOND outputs.

2.3.2 Visualization

Laplacian isosurface colors

Choose the color convention used to display positive and negative Laplacian isosurfaces. This option changes only the graphical representation and does not modify the calculated data.

NNA classification cutoff

Specify the cutoff distance used during the classification of Non-Nuclear Attractors (NNAs).

Important

Change the default NNA cutoff only when the scientific criteria adopted in your investigation require a different value.

2.3.3 Cleanup after calculation

Choose how TopIso3D v2026 handles temporary files generated during TOPOND calculations.

Standard Removes `fort.9`, `fort.3`, `fort.11`, and `fort.13`.

Minimal Removes only `fort.9`.

None Keeps all generated files.

2.3.4 External result file names

Enter accepted filenames for TRHO, TLAP, and ATBP outputs. Separate multiple names with semicolons.

These alternative names are used only when reading external results. Internally generated runs continue to use the default filenames `trho.out`, `tlap.out`, and `atbp.out`.

2.3.5 Buttons

Browse... Opens a file-selection dialog for locating the `PROPERTIES` executable.

Test Tests the selected configuration.

Save Saves the current settings and closes the window.

Cancel Closes the window without saving the current changes.

2.4 Creating a project

Every TopIso3D v2026 investigation is organized as a project. A project consists of a single directory that contains the files associated with one topological investigation together with all results generated by the software. This directory becomes the common workspace used by all TopIso3D v2026 modules throughout the investigation.

To create a new project, first create an empty directory with the name you want to assign to your investigation. This directory will become the project workspace used by TopIso3D v2026.

If you intend to perform new TOPOND calculations directly from TopIso3D v2026, place the optimized `fort.9` file corresponding to your system inside the project directory before opening the project.

If your TOPOND analyses were performed externally (for example, on a computing cluster), simply copy the corresponding output files into the project directory before opening the project in TopIso3D v2026. The software automatically recognizes these files, extracts their scientific information, and makes the results immediately available for exploration.

Although TopIso3D v2026 automatically detects supported output files placed in the project directory, we recommend organizing externally generated calculations using the same directory structure adopted by the software itself. For example, TRHO results may be stored inside a `trho_runs` directory, TLAP results inside `tlap_runs`, and ATBP results inside `atbp_runs`. Following this organization facilitates project management, especially when multiple calculations are associated with the same investigation.

Once the project has been opened, TopIso3D v2026 automatically creates any additional directories required by the different scientific workflows as they become necessary during the investigation.

2.5 Workspace

Important

Concept — Project Workspace
In TopIso3D v2026, a project is represented by a single directory that serves as the common workspace for an entire scientific investigation. This directory contains the input files provided by the researcher together with all results, reports, exported data, and auxiliary files generated throughout the investigation.

As shown in Figure 2.1, the Workspace module is where you define the project that will be used throughout a scientific investigation. Before using any scientific module, select the directory corresponding to your project by clicking the **Choose folder...** button.

The selected directory becomes the project workspace shared by all TopIso3D v2026 modules. It defines where the software searches for files associated with the investigation and where all calculations, imported results, reports, exported datasets, and auxiliary files generated during the investigation are organized.

To open a project, click **Choose folder...** and select the directory corresponding to your investigation. Immediately after a project directory is selected, TopIso3D v2026 validates its contents and determines which scientific workflows are available. According to the detected files, the software automatically enables the corresponding modules in the navigation panel and adapts the workspace to the current state of the project.

The presence of a valid `fort.9` file is required for enabling TOPOND-based computational workflows, but it is not, by itself, sufficient to make all scientific workflows immediately available. A valid `fort.9` allows the TRHO workflow to be executed. Once a valid TRHO result is available, either generated within TopIso3D v2026 or imported from an external calculation, the scientific information parsed from the TRHO output enables the subsequent TLAP, ATBP, and PL2D workflows.

Consequently, workflow availability reflects both the presence of the structural input required by TOPOND and the scientific dependencies of each module. Buttons are enabled only when the information required by the corresponding workflow is available.

The workspace can be changed at any time during a TopIso3D v2026 session. By selecting a different project directory, the workspace is immediately reconfigured according to the contents of the newly selected project. This allows multiple investigations to be explored sequentially without restarting the application.

3 Scientific Workflows

3.1 TRHO

Figure 3.1 presents the TRHO workflow. In this example, the selected project contains a valid `fort.9` file but no previously generated TRHO results. Consequently, the TRHO module is enabled, while the remaining scientific workflows and exploration modules remain unavailable until the required information becomes available.

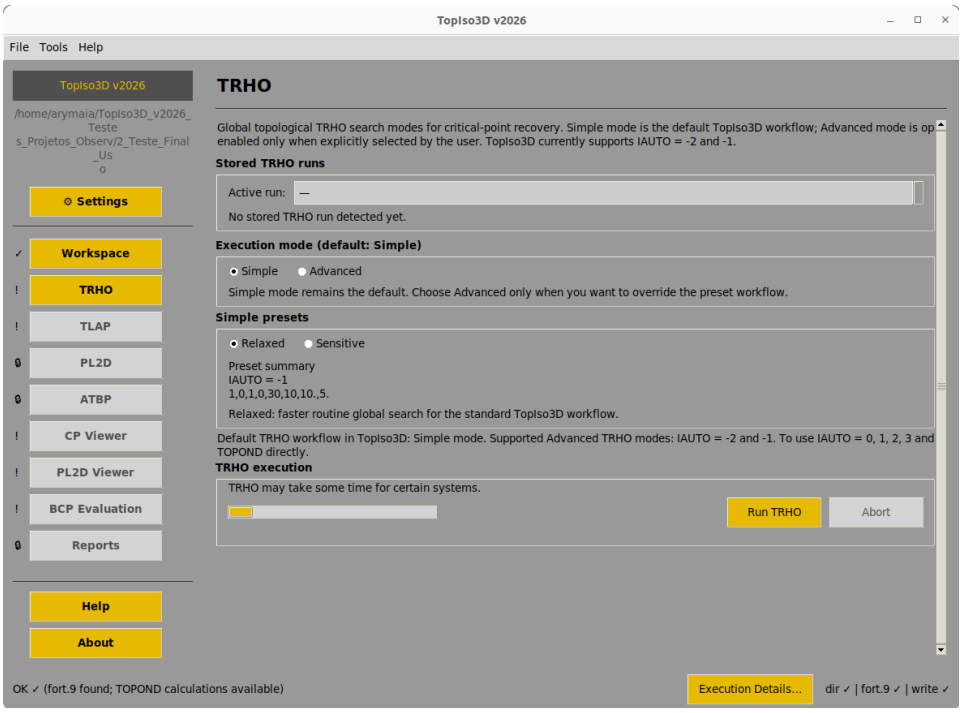

Figure 3.1: TRHO Workflow window.

The TRHO workflow constitutes the first stage of most TopIso3D v2026 investigations. Its purpose is to prepare, execute, import, and organize TOPOND electron-density analyses [3, 4], providing the structured information required by the subsequent scientific workflows and exploration modules.

The availability of the TRHO workflow depends on the validation performed by the Workspace module. When an optimized `fort.9` (or equivalent wavefunction file) is detected in the selected project, TopIso3D v2026 automatically enables the TRHO module, indicating that the project is ready for a new TOPOND electron-density analysis.

Although TRHO, TLAP, ATBP, and PL2D are independent TOPOND analyses, TopIso3D v2026 adopts the information extracted from the `trho.out` file as the canonical source for constructing the internal crystallographic representation of the project. Consequently, the TLAP, ATBP, and PL2D workflows become available only after a valid `trho.out` file is present in the current project, regardless of whether it was generated by TopIso3D v2026 or imported

from an external calculation.

After a successful TRHO calculation or after importing a previously generated `trho.out` file, TopIso3D v2026 automatically parses the textual output, extracts the available scientific information, and constructs the internal representation shared by the different exploration modules. Once this process is completed, the corresponding visualization, reporting, comparison, and export capabilities become immediately available within the environment.

3.1.1 Stored TRHO runs

The Stored TRHO runs section allows you to manage all TRHO calculations associated with the current project. During initialization, TopIso3D v2026 searches the project workspace, specifically the `trho_runs` directory, and identifies every available TRHO calculation.

TRHO calculations executed directly from TopIso3D v2026 are automatically stored using the recommended project organization. Previously generated calculations may also be recognized, provided that each `trho.out` file is stored inside its own subdirectory within `trho_runs`. This organization allows multiple TRHO calculations associated with the same scientific investigation to coexist within a single project.

By default, TopIso3D v2026 automatically generates a unique name for each TRHO run based on the execution date and time. These automatically generated identifiers facilitate the organization and retrieval of multiple calculations performed within the same scientific project. User-defined directory names are also fully supported and preserved when externally generated TRHO calculations are imported into the project.

The **Active run** field (Figure 3.2) displays the TRHO calculation currently selected as the default dataset for the project. This information is retrieved from the project metadata stored by TopIso3D v2026 in its internal configuration files, allowing the previously selected TRHO workflow to be automatically restored whenever the project is reopened.

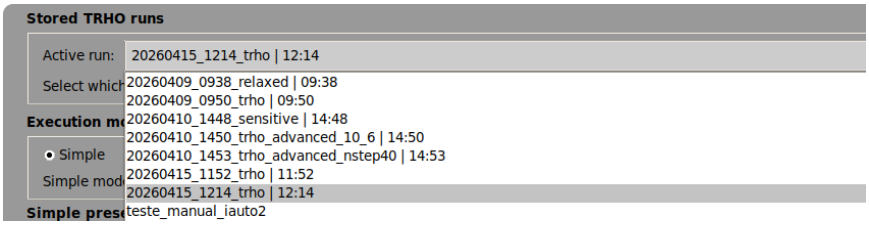

Figure 3.2: Selection of the active TRHO run. Each entry corresponds to a stored TRHO calculation available in the current project.

To activate a different TRHO calculation, click the selector located to the right of the Active run field and choose one of the available calculations from the list. The selected calculation immediately becomes the active TRHO dataset for the current session, making its results available to all workflows and exploration modules that depend on TRHO information.

3.1.2 Execution mode

The **Execution mode** determines how the parameters used to construct the TRHO input for TOPOND are defined. Two modes are available: Simple and Advanced.

In **Simple mode**, TopIso3D v2026 defines the TRHO parameters automatically according to one of two predefined parameter sets: **Relaxed** or **Sensitive**. **Simple mode** is the default TopIso3D v2026 workflow and is intended to provide reproducible parameter configurations without requiring you to specify each TRHO parameter individually.

In **Advanced mode**, the predefined parameter sets are replaced by explicit parameter controls. You can then define the supported TRHO parameters individually before the TOPOND

calculation is launched.

The distinction between **Simple** and **Advanced** therefore concerns how the TRHO input parameters are defined, rather than different types of TRHO calculation. Changing the execution mode affects the configuration of the next TRHO run and does not modify previously stored results.

Simple presets

When **Simple** execution mode is selected, you can choose between two predefined TRHO parameter sets: **Relaxed** and **Sensitive**. Both presets use the same TRHO search strategy (`IAUTO = -1`) but differ in selected parameters controlling the extent of the global search.

Relaxed is the default preset and provides the standard TopIso3D v2026 configuration for routine TRHO calculations. It uses `NNB = 10, RMAX = 10.0`, and `TH = 5.0`.

Sensitive expands the search by using `NNB = 15, RMAX = 12.0`, and `TH = 6.0`. It is intended for cases in which critical-point recovery is more difficult or when additional search coverage is desirable.

Whenever you select a preset, the Preset summary displayed immediately below the selection controls shows the actual parameter values that TopIso3D v2026 will use to construct the TRHO input. This allows the calculation settings to remain transparent even though the individual parameters are managed automatically in **Simple mode**.

Advanced TRHO

When **Advanced** execution mode is selected, TopIso3D v2026 allows you to define the parameters used to construct the TRHO input explicitly (Figure 3.3). This mode is intended for users who need direct control over the critical-point search configuration rather than one of the predefined Simple presets.

TOPOND provides four global TRHO search strategies, identified by the IAUTO parameter. TopIso3D v2026 provides direct interface support for two of them:

- IAUTO = -1 — Global automatic search around NEAs
- IAUTO = -2 — Global automatic search from a seed point

The available `IAUTO` strategies correspond to TOPOND search strategies; their formal definition and complete parameterization are described in the TOPOND23 User's Manual [2].

The selected TRHO strategy determines the structure of the parameter set presented by TopIso3D v2026. With `IAUTO = -1`, the interface exposes the general TRHO parameters. With `IAUTO = -2`, an additional **Seed point** section is displayed because this strategy requires the corresponding seed-point information.

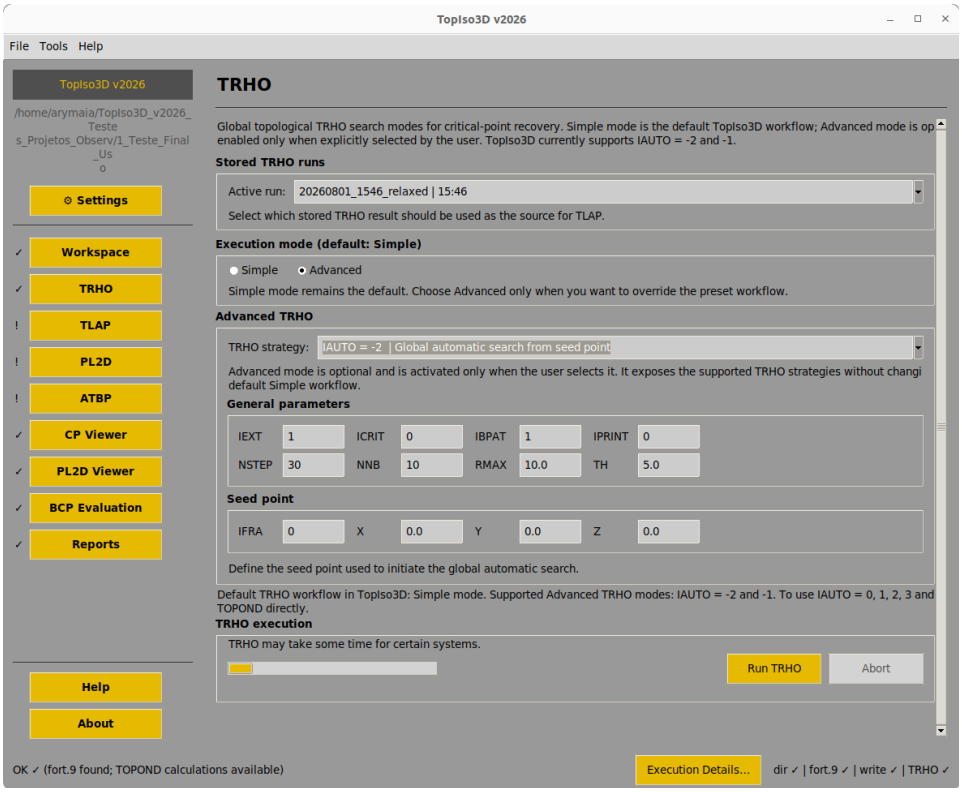

Figure 3.3: Advanced TRHO configuration with `IAUTO = -2`. In addition to the general TRHO parameters, this strategy requires the definition of a seed point.

The parameter values entered in the interface are used to construct the TRHO input passed to TOPOND. TopIso3D v2026 does not redefine the meaning of these parameters. For their definitions, valid values, and implications for the critical-point search, refer to the TOPOND documentation.

Tip

Advanced mode requires knowledge of the TOPOND TRHO parameters.
Use Advanced mode only when you understand the parameters you are defining and their effect on the critical-point search. Inappropriate values may restrict or otherwise alter the search and can lead to incomplete or misleading results, including failure to locate existing critical points. If you are unsure about the appropriate parameter values, use one of the Simple presets and consult the TOPOND documentation before configuring an Advanced calculation.

Important

Other TOPOND TRHO strategies
TOPOND also provides the global search strategies `IAUTO = 0` and `IAUTO = 3`. These strategies are not implemented in the TopIso3D v2026 execution interface. If your analysis requires either of them, run the TRHO calculation directly with TOPOND and import the resulting `trho.out` into the TopIso3D v2026 project. Imported TRHO results can then be managed and explored in the same environment as calculations launched directly from TopIso3D v2026.

3.1.3 TRHO execution

After the execution mode and the corresponding TRHO parameters have been defined, click **Run TRHO** to start the calculation.

Before launching TOPOND, TopIso3D v2026 displays a confirmation dialog (Figure 3.4a) reminding you that TRHO calculations may be computationally demanding and can require significant execution time. Select **Yes** to continue or **No** to return to the TRHO configuration without starting the calculation. The main stages of the execution workflow are illustrated in Figure 3.4.

Figure 3.4: TRHO execution sequence. (a) Confirmation before execution; (b) Definition of the run name; (c) Selection of the new result as the Active TRHO result.

If execution is confirmed, TopIso3D v2026 asks you to assign a name to the new TRHO run (Figure 3.4b). A unique name containing the current date and time is automatically suggested, but you may replace it with a more descriptive name. The run name is used to identify the calculation within the project's `trho_runs` directory.

After confirming the run name, TopIso3D v2026 launches the TRHO calculation using the selected configuration. During execution, the progress bar indicates that the calculation is active, and the **Abort** button becomes available. You may use this button to interrupt the calculation when necessary.

When the calculation finishes successfully, TopIso3D v2026 processes the resulting TRHO output and stores the run in its corresponding subdirectory under `trho_runs`. A final dialog (Figure 3.4c) reports the name under which the result was saved and asks whether the newly completed calculation should become the Active TRHO result.

If **Yes** is selected, the new run becomes the active TRHO result and is immediately available as the current source for subsequent operations that depend on TRHO data. If **No** is selected, the calculation remains stored and available for later selection, while the previously active TRHO result is preserved.

3.2 TLAP

The TLAP workflow extends the topological analysis to the Laplacian of the electron density and its associated critical-point structure [5, 6].

Figure 3.5 presents the TLAP workflow, which provides access to the TOPOND topological analysis of the Laplacian of the electron density.

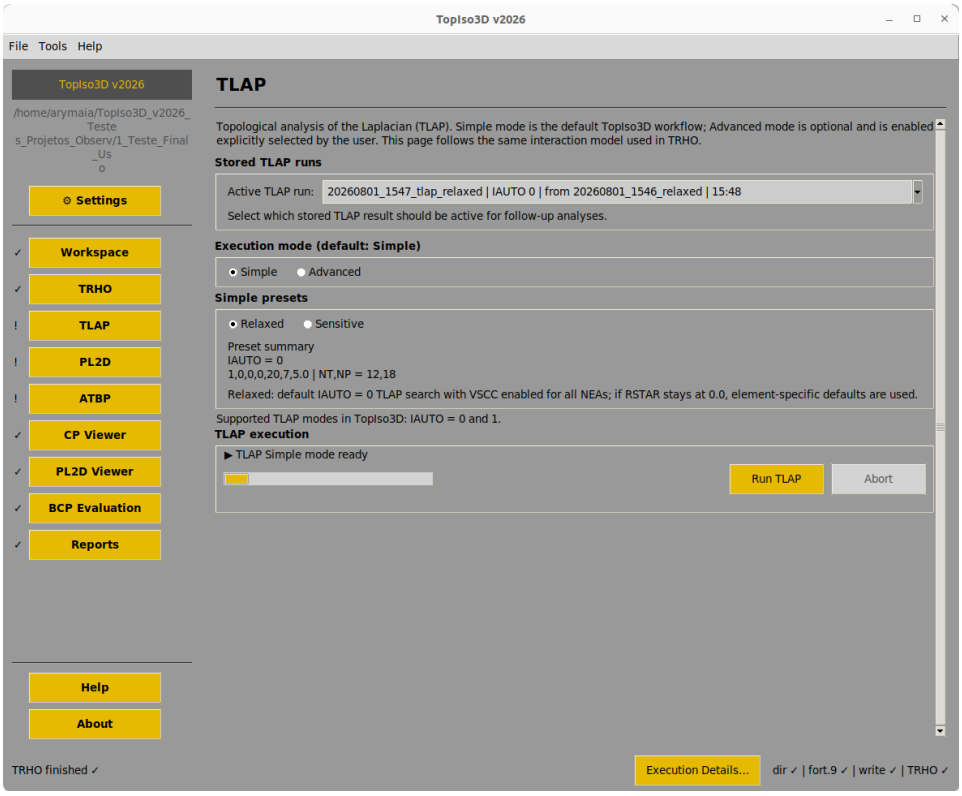

Figure 3.5: TLAP Workflow window.

Although TLAP is an independent TOPOND calculation, within TopIso3D v2026 the workflow becomes available only after a valid TRHO result has been parsed for the current project. The structured information recovered from TRHO provides the crystallographic and topological context used by TopIso3D v2026 to configure, organize, and subsequently explore the TLAP analysis.

The TLAP workflow follows the same general interaction model described for TRHO. Stored runs, active-result selection, Simple and Advanced execution modes, run naming, progress monitoring, and result management operate according to the same principles. The following sections therefore focus on the configuration and behavior specific to TLAP.

3.2.1 Stored TLAP runs

The **Stored TLAP runs** section lists the TLAP calculations available in the current project and identifies the result currently selected as the Active TLAP run. As in the TRHO workflow, you can switch between stored calculations without rerunning the analysis.

Each TLAP run also retains its association with the TRHO result from which it was launched. This provenance information is displayed together with the stored-run identification, allowing you to recognize the TRHO dataset associated with each TLAP analysis.

3.2.2 Execution mode

TLAP uses the same **Simple** and **Advanced** execution modes introduced for TRHO. In **Simple mode**, TopIso3D v2026 defines the calculation parameters through predefined presets. In **Advanced mode**, you can define the supported TOPOND TLAP parameters explicitly.

Simple mode remains the default workflow and should be preferred unless direct control over the TLAP parameters is required.

Simple presets

When Simple execution mode is selected, TLAP provides the **Relaxed** and **Sensitive** presets. Both use the `IAUTO = 0` TLAP search strategy, with VSCC enabled for all non-equivalent atoms (NEAs), but employ different predefined parameter sets controlling the search.

Relaxed is the default TopIso3D v2026 configuration for routine TLAP calculations, whereas **Sensitive** provides a broader search configuration when additional search coverage is required.

As in the TRHO workflow, the Preset summary displays the actual parameter values associated with the selected preset. These values are automatically used by TopIso3D v2026 to construct the corresponding TOPOND input.

Advanced TLAP

When **Advanced** execution mode is selected, TopIso3D v2026 provides direct interface access to two TOPOND TLAP search strategies:

- IAUTO = 0 — Automatic TLAP search
- IAUTO = 1 — TLAP search from starting points

Figure 3.6 shows the Advanced TLAP interface configured for the IAUTO = 0 automatic search strategy.

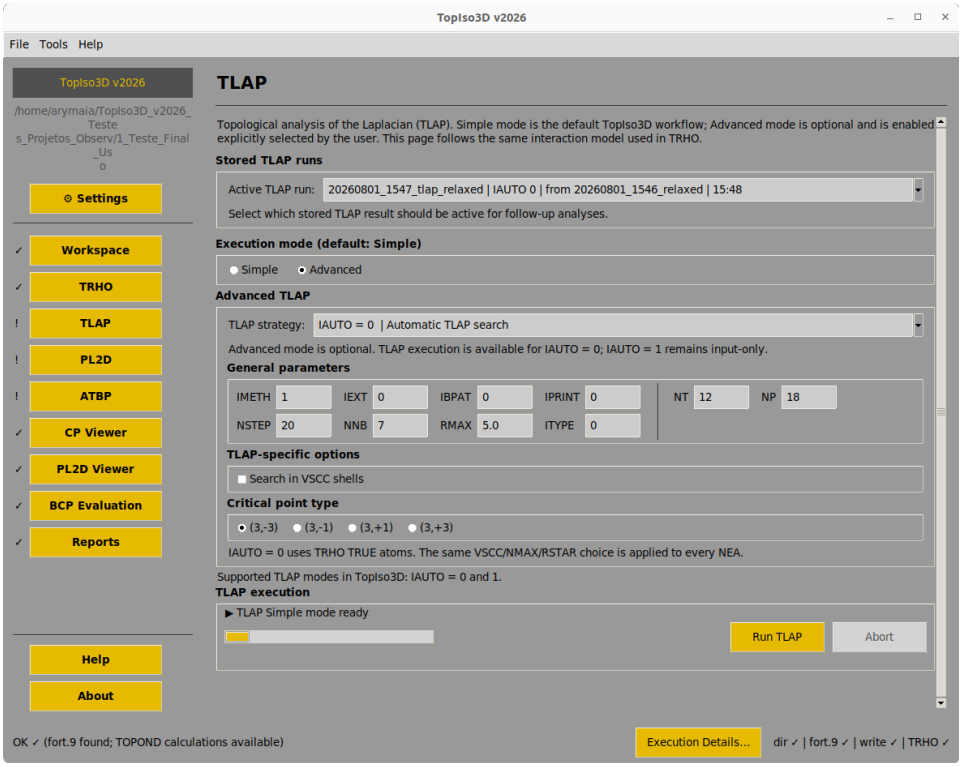

Figure 3.6: Advanced TLAP configuration for the IAUTO = 0 strategy. General parameters, TLAP-specific options, and critical-point selection are exposed for direct configuration.

`IAUTO = 0` corresponds to the global automatic TLAP search and can be configured and executed directly from TopIso3D v2026. The interface exposes the general calculation parameters together with the TLAP-specific options and the critical-point type to be searched.

`IAUTO = 1` corresponds to a specific search initiated from user-defined starting points. TopIso3D v2026 provides input configuration support for this strategy, but does not execute

it directly. Calculations requiring this strategy must therefore be performed directly with TOPOND.

TOPOND also provides the `IAUTO = 2` specific-search strategy. This option is not implemented in the TopIso3D v2026 interface and should be used directly through TOPOND when required.

TLAP execution

TLAP calculations follow the same execution sequence described for the TRHO workflow. After configuring the calculation, click **Run TLAP** to start the analysis. TopIso3D v2026 requests confirmation, assigns a suggested name to the new run, monitors the calculation while it is running, and allows you to interrupt it using the **Abort** button.

After successful completion, the result is stored automatically in the project's `tlap_runs` directory, and you can choose whether the newly generated result should become the Active TLAP run.

The stored run retains its association with the Active TRHO result used to launch the TLAP calculation, preserving the provenance between the two workflows.

3.3 PL2D

Figure 3.7 presents the PL2D workflow, which provides an integrated environment for defining, executing, and organizing sequences of two-dimensional TOPOND calculations over a user-defined spatial region.

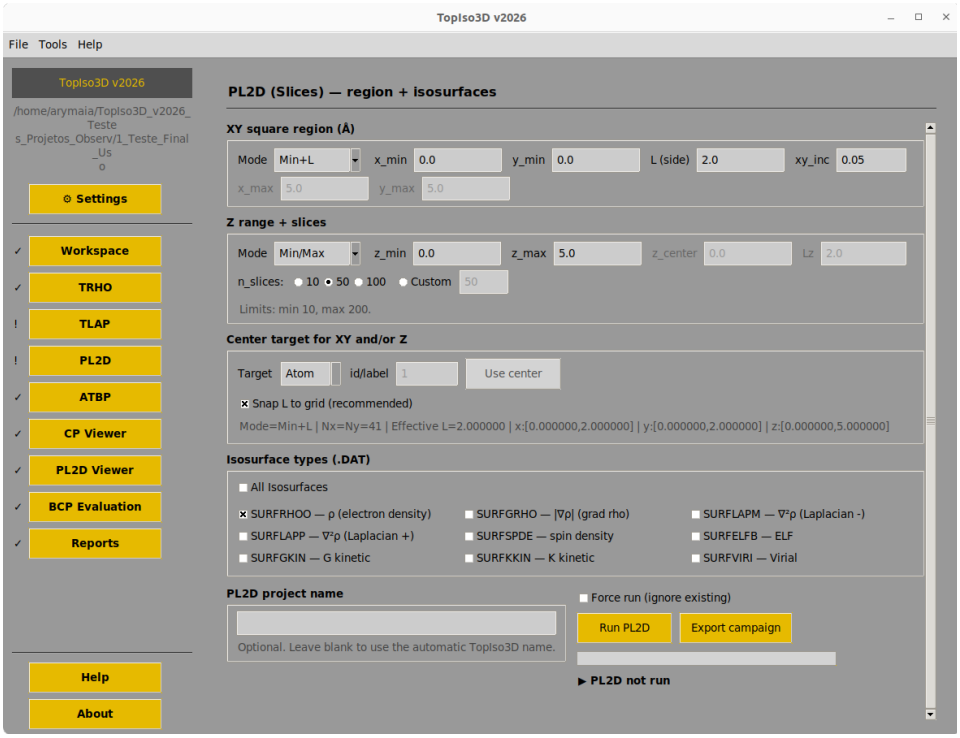

Figure 3.7: PL2D Workflow window.

Unlike the TRHO and TLAP workflows, PL2D operates on a spatial region defined by the user. A single TOPOND PL2D calculation evaluates selected scalar properties on a two-dimensional plane. TopIso3D v2026 extends this procedure by automatically constructing a sequence of parallel xy planes distributed along the z direction.

Each plane corresponds to an independent PL2D calculation. The complete set of calculations forms a **PL2D campaign**, in which the number of planes is controlled by the selected number of slices. The resulting two-dimensional property maps can subsequently be combined by TopIso3D v2026 to provide a three-dimensional sampling of the selected scalar field.

This strategy also provides a computationally efficient alternative to the direct three-dimensional evaluation available through the TOPOND PL3D functionality. Rather than evaluating the selected property over an entire three-dimensional grid, TopIso3D v2026 constructs the sampled volume from a controlled number of independent PL2D slices. This can substantially reduce the computational cost, while allowing the user to adjust the sampling density along the z direction according to the resolution required for the resulting three-dimensional representation.

The slice-based approach adopted by TopIso3D v2026 is therefore not intended to replace PL3D, but to provide a more flexible and computationally economical route for the three-dimensional exploration supported by this workflow.

Within TopIso3D v2026, PL2D calculations are organized as spatial sampling campaigns rather than as isolated planes. The sampling region can be defined directly in Cartesian space or relative to scientific entities already identified in the workspace, including atoms and critical points (bond critical point (BCP), ring critical point (RCP), cage critical point (CCP), or non-nuclear attractor (NNA)). This entity-oriented formulation allows the user to explore the spatial behavior of scalar fields around chemically or topologically meaningful references while preserving direct correspondence with the underlying TOPOND calculations.

3.3.1 Defining the spatial region

XY square region

The **XY square region** defines the lateral extent of each PL2D slice, while its spatial resolution is controlled by the xy grid increment described below. Depending on the selected mode, the region can be specified directly from its limits or constructed around a reference position or scientific entity.

The available modes are:

- **Min+L** — defines the region from minimum x and y coordinates and a side length L;
- **Min/Max** — defines the region directly from minimum and maximum x and y coordinates;
- **Center+L** — constructs a square of side L around a user-defined center;
- **Atom+L**, **BCP+L**, **RCP+L**, **CCP+L**, and **NNA+L** — construct the square around the coordinates of the selected scientific entity.

Z range and slices

The **n_slices** parameter defines the number of intervals used to divide the selected z range. Because both limits of the interval are included, a campaign with n slices is represented by $n+1$ parallel PL2D planes. For example, selecting 10 slices generates 11 PL2D planes distributed from zmin to zmax, including both boundary planes.

TopIso3D v2026 provides three predefined values:

- **10 slices** — 10 intervals and 11 calculated planes, suitable for rapid preliminary visualization;
- **50 slices** — 50 intervals and 51 calculated planes, the default configuration providing a balance between computational cost and three-dimensional resolution;
- **100 slices** — 100 intervals and 101 calculated planes, providing finer sampling along z at a higher computational cost.

A custom number of slices can also be specified within the limits accepted by the interface.

Tip

Start with fewer slices. When exploring a new region, a 10-slice campaign can be useful for quickly checking the spatial extent and selected properties before launching a more demanding calculation. Increasing the number of slices improves the resolution along z, but also increases the number of independent PL2D calculations that must be performed.

Center target

When a reference-based mode is selected for the xy region or the z range, TopIso3D v2026 automatically updates the **Target** selector to the corresponding entity type.

Enter the identifier of the desired atom, BCP, RCP, CCP, or NNA in the **id/label** field and click **Use center**. TopIso3D v2026 retrieves the coordinates of the selected entity and uses them to construct the corresponding spatial limits according to the selected side or range length. If reference-based modes are used, verify the selected **Target** before clicking **Use center**, particularly when the xy and z modes have been changed independently.

XY grid resolution

Each PL2D slice is defined over a square xy region. The **xy_inc** parameter controls the spatial increment of the grid along both the x and y directions and therefore determines the in-plane resolution of each calculated map.

Because the PL2D slices used by this workflow must preserve a square grid, TopIso3D v2026 automatically adjusts the effective side length to the selected **xy_inc** value so that the x and y directions contain the same number of regularly spaced grid points. The resulting grid dimensions and adjusted side length are reported in the interface as **Nx=Ny** and **Effective L**, respectively.

When the requested side length is already compatible with the selected grid increment, **Effective L** is identical to the specified L. Otherwise, TopIso3D v2026 adjusts it to the nearest compatible grid length.

Smaller values of **xy_inc** produce a finer sampling within each slice, increasing the spatial resolution of the resulting map at the cost of a larger number of grid points and greater computational demand.

3.3.2 Selecting isosurface types

The **Isosurface types (.DAT)** section defines which scalar properties will be evaluated by TOPOND for each PL2D slice of the campaign. At least one property must be selected for the campaign to be executed; by default, **SURFRHOO** is already selected when the PL2D workflow is opened.

Each selected option corresponds to a TOPOND PL2D scalar function and to the associated `SURF*.DAT` output generated for every calculated plane. When multiple properties are selected, the same set of PL2D slices is evaluated for each of them, providing a common three-dimensional sampling region for the selected scalar fields.

TopIso3D v2026 provides the following property selections, as defined by the corresponding TOPOND property-map keywords [2].:

- **SURFRHOO** — electron density, ρ;
- **SURFGRHO** — magnitude of the gradient of the electron density, $|\nabla\rho|$;

- **SURFLAPP** — Laplacian of the electron density, $\nabla^2\rho$;
- **SURFLAPM** — negative of the Laplacian of the electron density, $-\nabla^2\rho$;
- **SURFSPDE** — spin density;
- **SURFELFB** — ELF (Becke electron localization function);
- **SURFGKIN** — Lagrangian kinetic energy density, G;
- **SURFKKIN** — Hamiltonian kinetic energy density, K;
- **SURFVIRI** — virial field density, V.

The selected properties are evaluated over the same spatial region and using the same xy grid and z sampling defined for the campaign. This common spatial discretization facilitates the subsequent comparison and three-dimensional visualization of different scalar fields.

3.3.3 PL2D campaign organization and execution

A PL2D calculation in TopIso3D v2026 is organized as a *campaign*, comprising the complete set of individual plane calculations required to sample the selected spatial region. Each campaign is stored in a dedicated subdirectory of the project's `pl2d_runs` directory.

You may optionally assign a name to the campaign using the **PL2D project name** field. If this field is left blank, TopIso3D v2026 automatically generates a unique name for the campaign. If a user-defined name is already present in `pl2d_runs`, TopIso3D v2026 preserves the existing campaign and creates the new one using a numerical suffix, such as `_2`, `_3`, and so forth.

Within the campaign directory, TopIso3D v2026 creates one subdirectory for each calculated plane, sequentially named `slice000`, `slice001`, `slice002`, and so forth. Each slice directory contains the corresponding PL2D input and output files, together with the `.DAT` files generated for the scalar properties selected in **Isosurface types**. A `manifest.json` file stored at the campaign level records the configuration and status of the campaign.

After the spatial region, the `n_slices` value, and the scalar properties have been defined, click **Run PL2D** to start the campaign. TopIso3D v2026 then launches the individual PL2D calculations sequentially and automatically manages their corresponding directories and files.

Unlike the progress indicators used for TRHO, TLAP, and ATBP, the PL2D progress bar represents the actual advancement of the campaign. Because the total number of planes is known before execution begins, TopIso3D v2026 can report the current plane and the total number of planes throughout the calculation. The **Abort** button can be used to interrupt an active campaign when necessary.

When all planes have been successfully processed, the complete campaign remains stored under `pl2d_runs` and is available for subsequent visualization and analysis with the PL2D Viewer.

3.3.4 Exporting a PL2D campaign

PL2D campaigns can also be prepared in TopIso3D v2026 and executed outside the local TopIso3D v2026 environment. This option is particularly useful for large systems containing many atoms, for which the computational cost of the individual PL2D calculations may make execution on a computing cluster more appropriate. The number of slices also contributes to the overall cost of a campaign, but even campaigns containing a large number of slices may remain computationally inexpensive for systems of moderate size.

After configuring the spatial region, the `n_slices` value, and the scalar properties, click **Export campaign**. TopIso3D v2026 creates the complete campaign structure without executing the individual PL2D calculations. The exported campaign contains the `manifest.json` file,

the wavefunction file `fort.9`, and one `sliceXXX` directory for each plane. Each slice directory contains the corresponding `pl2d.inp` file required to perform that calculation.

TopIso3D v2026 also generates auxiliary shell scripts for executing the campaign outside the graphical interface. The exported files support sequential execution (`run_all.sh`), parallel execution (`run_parallel.sh`), and submission to a Slurm-based computing cluster (`submit_slurm.sh`). A `README_RUN.txt` file provides basic instructions for using and adapting these scripts.

The supplied scripts assume that the CRYSTAL/TOPOND properties executable is available in the execution environment. Paths, module loading commands, parallelization settings, and Slurm directives may therefore need to be adapted to the configuration of the target computer or cluster.

During execution, the `fort.9` file stored at the campaign level is temporarily copied to each slice directory. The corresponding PL2D calculation is then performed using its `pl2d.inp` file, and the resulting output and selected `.DAT` property files are stored within that slice directory.

After external execution, the auxiliary `cleanup_for_return.sh` script can be used to remove temporary execution files before transferring the campaign back to the local environment. The scientifically relevant PL2D input, output, error, and `.DAT` files are preserved, allowing the externally calculated campaign to be subsequently used for visualization and analysis.

3.4 ATBP

Figure 3.8 presents the ATBP workflow, which provides access to the TOPOND atomic basin analysis and integrates calculation execution, result management, automatic parsing, and data export within the TopIso3D v2026 environment. Unlike the TRHO and TLAP workflows, the ATBP interface combines calculation controls and the resulting atomic properties in the same workspace.

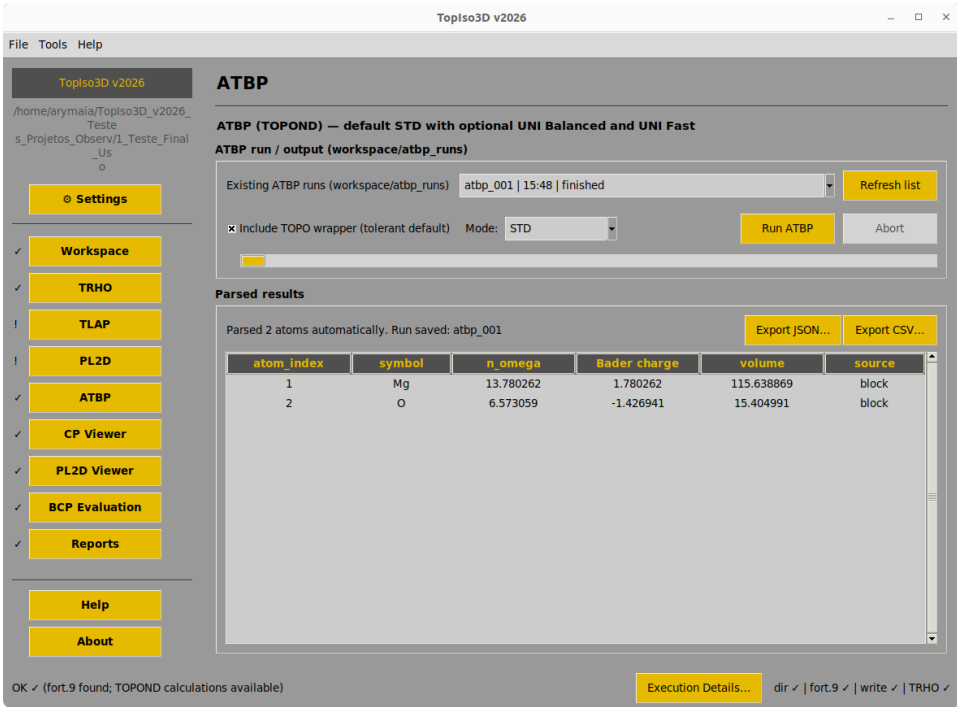

Figure 3.8: ATBP workflow window.

3.4.1 Existing ATBP runs

TopIso3D v2026 automatically organizes completed ATBP calculations in the `atbp_runs` directory of the current project. The **Existing ATBP runs** list provides access to these stored calculations without requiring them to be executed again.

When you select a stored ATBP run, TopIso3D v2026 automatically loads and parses the corresponding result. The **Parsed results** table is immediately updated to display the atomic-basin properties associated with the selected calculation. In this way, you can move between different ATBP results within the same project and inspect their data directly from the interface.

The **Refresh list** button updates the list whenever new ATBP runs become available in the project.

3.4.2 ATBP calculation modes

TopIso3D v2026 provides three predefined modes for ATBP calculations: **STD**, **UNI Balanced**, and **UNI Fast**. These modes determine how the ATBP input is constructed before the calculation is submitted to TOPOND. The three calculation modes exposed by TopIso3D v2026 correspond to the `UNI` strategies defined by TOPOND [2].

STD uses the standard ATBP procedure provided by TOPOND. In this mode, TopIso3D v2026 writes the `STD` keyword without exposing additional integration parameters. This mode delegates the integration parameters to the standard configuration defined by TOPOND.

The **UNI Balanced** and **UNI Fast** modes use the `UNI` procedure of TOPOND with parameter sets predefined by TopIso3D v2026. Unlike STD, these modes operate on the TRUE atoms identified from the TRHO results. TopIso3D v2026 automatically retrieves their nuclear effective atomic numbers (NEAs) and constructs the corresponding ATBP input blocks.

For each TRUE atom, TopIso3D v2026 also assigns the element-specific default `TOL` value used by TOPOND. When the element is not available in the internal table, the software asks you to provide a positive `TOL` value manually before the input can be generated.

The two UNI presets differ in the numerical parameters used to construct the integration grid:

Mode	NVI	IPHI	ITH	IBETP	IMUL	IEXT	NOSE	ACC
UNI Balanced	6	48	32	96	1	0	0	0.005
UNI Fast	6	32	24	64	0	0	0	0.01

Table 3.1: Predefined parameter sets used by the TopIso3D v2026 UNI calculation modes.

Important

Keep the TOPO wrapper enabled
The **Include TOPO wrapper** option must remain enabled when running ATBP calculations from TopIso3D v2026. The `TOPO` keyword is required to access the TOPOND module through the CRYSTAL `PROPERTIES` executable.
Do not disable this option during the standard TopIso3D v2026 ATBP workflow.

Use **UNI Balanced** when you prefer the more demanding of the two predefined UNI configurations. **UNI Fast** provides a less demanding preset, using reduced angular/grid parameters and a less restrictive accuracy value.

Note

TopIso3D v2026 UNI presets
UNI Balanced and **UNI Fast** are TopIso3D v2026 presets for the `UNI` procedure; they are not TOPOND keywords. ATBP procedures or parameterizations not exposed by TopIso3D v2026 should be configured directly according to the TOPOND documentation.

3.4.3 ATBP execution

After selecting the ATBP calculation mode, click **Run ATBP** to start the calculation. TopIso3D v2026 first displays a confirmation dialog reminding you that ATBP calculations can be computationally demanding and may require significant execution time.

Once confirmed, the calculation starts and its execution status is shown by the progress bar. During this period, the **Abort** button becomes available and can be used to interrupt the calculation when necessary.

After successful completion, TopIso3D v2026 automatically stores the new run in the project's `atbp_runs` directory, parses the resulting ATBP output, and updates the **Parsed results** table with the atomic-basin properties obtained from the calculation. The new run also becomes available in the **Existing ATBP runs** list.

3.4.4 Parsed results

After an ATBP calculation is completed or an existing run is selected, TopIso3D v2026 automatically parses the corresponding TOPOND output and displays a compact set of atomic-basin properties in the **Parsed results** table.

Each row represents an atomic basin identified in the ATBP output. The displayed quantities are extracted from the corresponding atomic-basin integration block and organized into the following columns:

- **atom_index** — index of the atom associated with the atomic basin, as reported by TOPOND;
- **symbol** — chemical symbol of the corresponding atom;
- **n_omega** — electronic population of the atomic basin, $N(\Omega)$, obtained from the `N` value reported under `ATOMIC POPULATIONS`;
- **Bader charge** — net charge of the atomic basin, obtained from the `Q` value reported under `ATOMIC POPULATIONS`;
- **volume** — volume of the atomic basin, obtained from the `VTOT` value reported under `ATOMIC VOLUMES AND RELATED POPULATIONS`;
- **source** — identifies the parsing route used by TopIso3D v2026 to recover the displayed ATBP data. The value `block` indicates that the quantities were extracted from the detailed atomic-basin blocks of the TOPOND output, whereas `table` indicates recovery from a compact atom/charge table when available.

The **source** column is an internal provenance indicator of the TopIso3D v2026 parser and does not represent an atomic property calculated by TOPOND.

The table is updated automatically whenever a new ATBP calculation finishes or a different calculation is selected from the **Existing ATBP runs** list. This allows you to inspect and compare the principal atomic-basin properties from different calculations without manually searching the corresponding TOPOND output files.

TOPOND reports additional atomic properties that are not currently included in the **Parsed results** table. The table therefore provides a structured summary of selected ATBP quantities rather than a replacement for the complete `atbp.out` file.

3.4.5 Exporting parsed results

The structured ATBP data displayed in the **Parsed results** table can be exported directly in CSV or JSON format using the **Export CSV...** and **Export JSON...** buttons.

Both export formats contain the parsed dataset associated with the currently selected ATBP run, including the atom identification, $N(\Omega)$, Bader charge, atomic-basin volume, and parsing-source information.

When either export option is selected, TopIso3D v2026 opens a file-selection dialog that allows you to choose the destination and filename. The directory of the currently selected ATBP run is used as the initial location.

The CSV format provides a conventional tabular representation suitable for spreadsheets and subsequent data analysis. The JSON format stores the same information as a sequence of structured records, facilitating reuse in scripts, databases, and other computational workflows.

The preceding sections described the **calculation workflows** through which TopIso3D v2026 prepares, executes, and organizes TOPOND calculations. The following modules operate primarily on scientific information already available in the project, providing complementary capabilities for interactive visualization, quantitative evaluation, and structured exploration of the calculated results. Together, these modules extend the workflow from calculation execution to **scientific exploration and interpretation**.

3.5 CP Viewer

The **CP Viewer** provides an interactive three-dimensional environment for exploring the critical-point topology recovered from the active TRHO and, when available, TLAP results. Rather than performing additional TOPOND calculations, the module operates directly on the structured scientific information already available in the project, integrating atomic positions, critical points, bond paths, and associated topological descriptors into a single interactive representation.

Figure 3.9 presents the main **CP Viewer** interface, where you can select the active topological data sources, choose the critical-point classes to be displayed, and configure the parameters used to generate the interactive visualization.

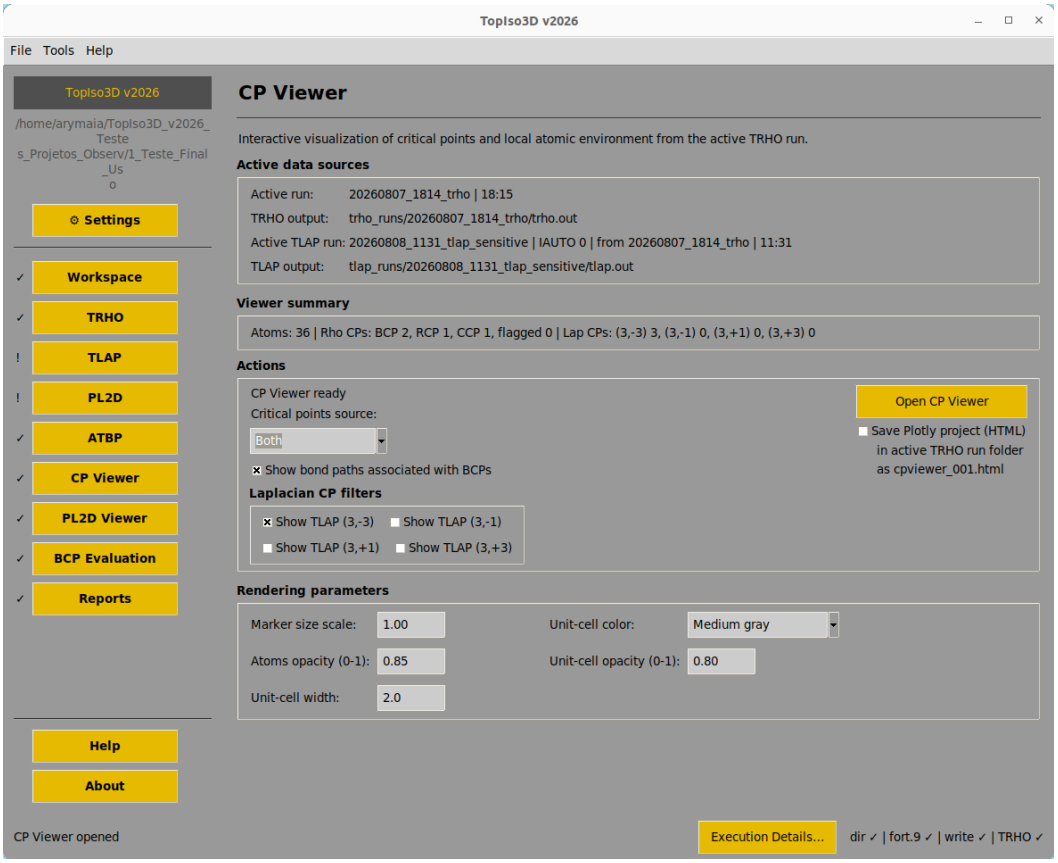

Figure 3.9: Main CP Viewer interface.

3.5.1 Active data sources

The CP Viewer uses the active TRHO result as its primary data source. The corresponding TRHO output provides the structural and topological information required to construct the visualization, including the critical points of the electron-density topology and their associated atomic environments.

When an active TLAP result is available, its critical-point data can also be included in the visualization. The **Active data sources** panel identifies the TRHO and TLAP runs currently available to the Viewer together with their corresponding output files.

The **Viewer summary** provides a compact description of the data available for visualization, including the number of atoms represented, the numbers of electron-density critical points, and the available Laplacian critical points.

The number of atoms reported by the Viewer does not necessarily correspond to the number of TRUE atoms in the primitive cell. Because critical points obtained from periodic TOPOND calculations may involve atoms located in neighboring cells, TopIso3D v2026 automatically extends the structural representation as required to include the atoms needed to display the critical points and their associated atomic environments.

3.5.2 Critical-point selection

The **Critical points source** selector determines which topological data are included in the visualization. Three options are available: **Rho**, **Laplacian**, and **Both**.

Select **Rho** to visualize critical points obtained from the active TRHO result. Depending on the critical points identified in the calculation, the visualization may include BCPs, RCPs, and CCPs together with the corresponding atomic environment.

Select **Laplacian** to visualize critical points obtained from the active TLAP result. The **Laplacian CP filters** allow the individual selection of the $(3,-3)$, $(3,-1)$, $(3,+1)$, and $(3,+3)$ critical-point classes. Only critical-point classes available in the active TLAP result can be represented; therefore, the available visualization reflects the types previously calculated in the TLAP workflow.

Select **Both** to combine the electron-density and Laplacian topologies in the same interactive visualization. The Laplacian CP filters remain available, allowing selected TLAP critical-point classes to be displayed together with the TRHO critical points.

The **Show bond paths associated with BCPs** option adds the connections between each BCP and its two associated atoms to the visualization. These connections provide a direct spatial representation of the atomic pair associated with each BCP and can be disabled when a less crowded visualization is preferred.

3.5.3 Rendering parameters

The **Rendering parameters** control the appearance of the interactive visualization without modifying the underlying topological data.

The **Marker size scale** adjusts the overall size of the markers used in the visualization, while **Atoms opacity** controls the transparency of the displayed atoms. These parameters can be useful for improving the visibility of critical points in structurally crowded regions.

The appearance of the unit cell can be adjusted independently using **Unit-cell color**, **Unit-cell opacity**, and **Unit-cell width**. These settings control, respectively, the color, transparency, and line width of the unit-cell representation.

3.5.4 Interactive visualization

After defining the critical-point source, filters, and rendering parameters, click **Open CP Viewer**. TopIso3D v2026 constructs the selected representation using the Plotly open-source graphing library for Python [7] and automatically opens the resulting interactive visualization in the default web browser. Figure 3.10 shows an example containing the atomic structure, critical points, bond-path representations, and the unit cell.

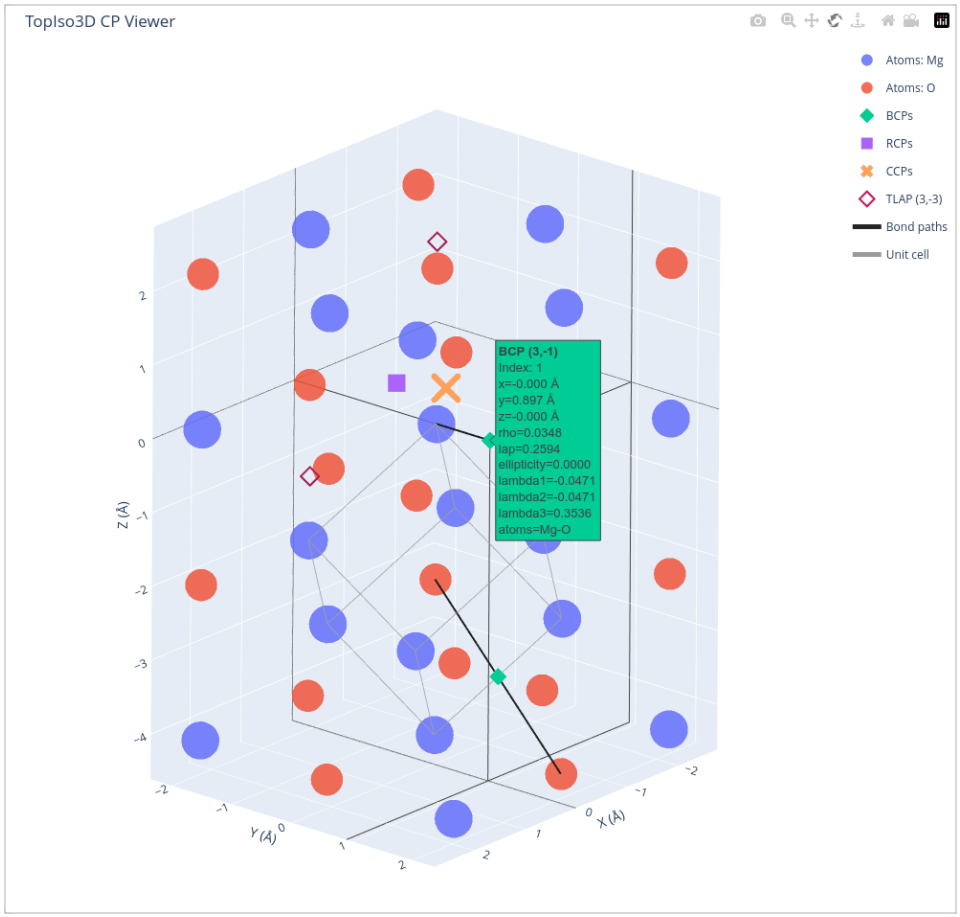

Figure 3.10: Interactive CP Viewer visualization generated with Plotly for the MgO system. The hover information shown for a BCP provides direct access to its available topological descriptors.

The Plotly environment allows the three-dimensional representation to be explored interactively. You can rotate and translate the structure, zoom into regions of interest, and adjust the viewpoint directly in the browser using the toolbar shown in the upper-right corner of Figure 3.10. The interactive legend can also be used to show or hide individual components of the representation, such as atomic species, critical-point classes, bond paths, and the unit cell. This is particularly useful for reducing visual complexity when several topological features are displayed simultaneously.

Moving the pointer over an atom or critical point displays information associated with that object. For atoms, the hover information includes their identity, periodic-cell reference, and spatial coordinates. For critical points, the information displayed depends on the critical-point type and on the data available in the corresponding active analysis.

BCPs from the electron-density topology provide a more extensive set of topological descriptors, including their coordinates, electron density, Laplacian, ellipticity, Hessian eigenvalues, and the associated atomic pair. Laplacian $(3, -3)$ critical points similarly provide an extended set of available descriptors. Other critical-point classes display the information available in their corresponding parsed records.

The hover functionality therefore provides more than object identification: it allows selected topological information to be inspected directly within its three-dimensional structural context, without requiring the user to return to the original TOPOND output.

If you want to preserve the interactive visualization, enable **Save Plotly project (HTML)** before opening the Viewer. TopIso3D v2026 saves the visualization in the active TRHO run directory using sequential names such as `cpviewer_001.html`, `cpviewer_002.html`, and so

forth.

The saved HTML file can subsequently be opened directly in a web browser without reopening the CP Viewer in TopIso3D v2026. The interactive features of the Plotly visualization, including rotation, zoom, legend-based visibility control, and hover information, are preserved.

3.6 PL2D Viewer

The PL2D Viewer provides interactive three-dimensional visualization of scalar fields generated from PL2D campaigns. Rather than displaying the individual two-dimensional maps produced by TOPOND separately, TopIso3D v2026 combines the sequence of calculated planes to reconstruct the sampled three-dimensional scalar field and generate isosurfaces of the selected property.

The PL2D Viewer does not perform additional TOPOND calculations; it operates on PL2D results already available in the project.

The workflow integrates the PL2D results stored in the current project with visualization controls for isosurface construction, structural and topological overlays, and interactive rendering. The reconstructed field can be explored directly through a Plotly-based three-dimensional view or exported for subsequent visualization and analysis.

Figure 3.11 shows the main PL2D Viewer window. The workflow is organized around the selection of an existing PL2D campaign and scalar property, followed by the definition of the isosurface and overlay parameters used to construct the three-dimensional representation.

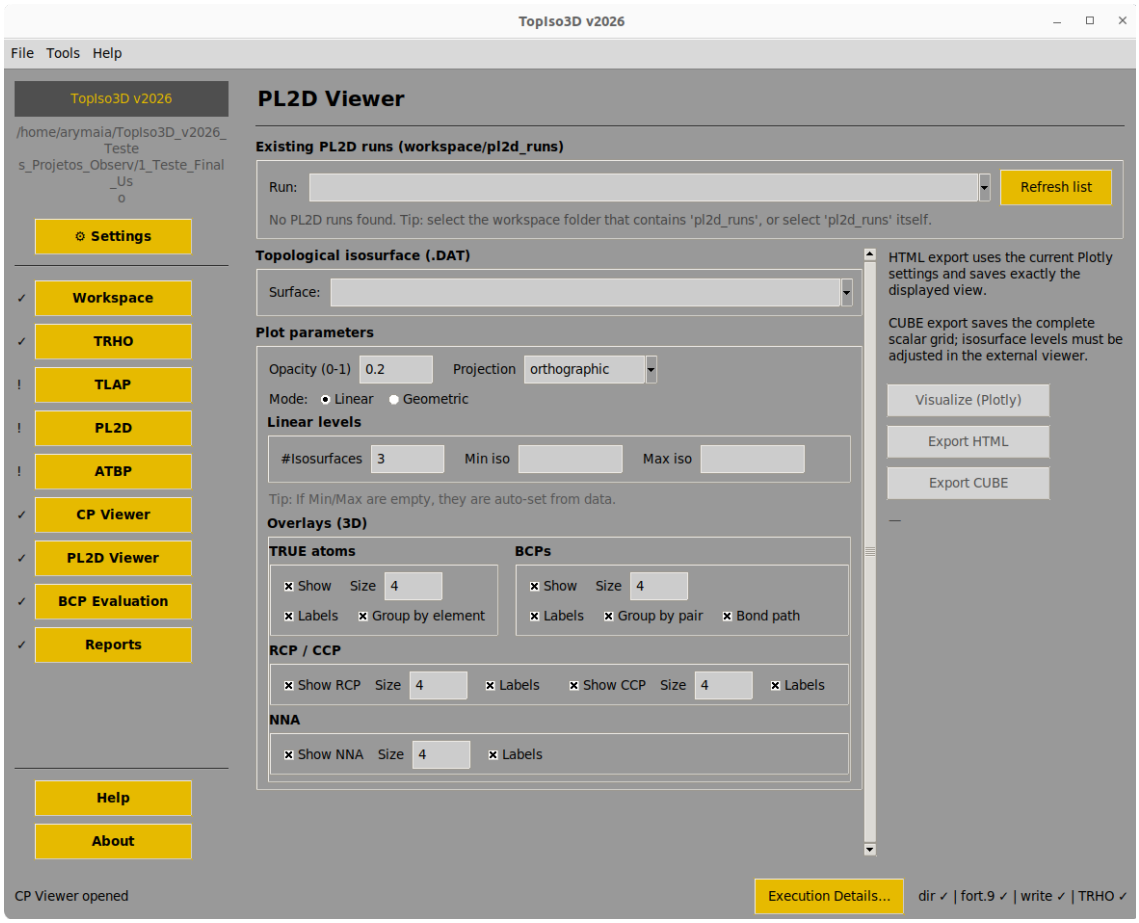

Figure 3.11: PL2D Viewer main window.

Existing PL2D runs

The PL2D Viewer operates on previously calculated PL2D campaigns stored in the `pl2d_runs` directory of the current project. Click **Refresh list** to scan the directory and update the **Run** selector with the available campaigns.

When a campaign is selected, TopIso3D v2026 inspects its `sliceXXX` directories and reports the number of available planes. This information reflects the campaign contents currently detected by the software and does not, by itself, verify that the original campaign is complete.

A campaign can therefore appear in the **Run** selector even when some of its expected results are not yet available. Visualization depends on the presence of the required scalar-field data in the detected `sliceXXX` directories.

Topological isosurface (.DAT)

After a PL2D campaign has been selected, the **Topological isosurface (.DAT)** section lists the scalar fields associated with the calculated PL2D campaign. The contents of the **Surface** selector therefore depend on the properties requested when the campaign was created and on the corresponding `.DAT` files generated by TOPOND.

Select the desired property from the **Surface** list. For example, `SURFRHOO` selects the electron-density data generated for the PL2D planes. Other properties become available when their corresponding `.DAT` datasets are present in the campaign.

Before constructing the three-dimensional scalar field, TopIso3D v2026 checks the consistency of the selected dataset across the required PL2D planes. If a corresponding `.DAT` file is missing from any required slice, the visualization is interrupted and the missing file is identified in an error message.

Plot parameters

The **Plot parameters** control the construction and graphical representation of the three-dimensional isosurfaces generated from the reconstructed scalar field.

The **Opacity** parameter controls the opacity of the displayed isosurfaces and accepts values between 0 and 1. The default value is 0.2, corresponding to 20% opacity. The use of partially transparent surfaces is particularly useful when several nested isosurfaces are displayed simultaneously, since inner regions remain visible through the outer surfaces.

The **Projection** selector controls the camera projection used for the three-dimensional representation. You can choose between **orthographic** and **perspective** projection. This setting affects only the visual representation and does not modify the scalar field or the generated isosurfaces.

Two modes are available for defining the isosurface levels: **Linear** and **Geometric**.

Linear levels In **Linear** mode, specify the number of isosurfaces together with the lower and upper values of the interval using **#Isosurfaces**, **Min iso**, and **Max iso**. The requested number of levels is distributed linearly between the selected limits.

If **Min iso** or **Max iso** is left empty, TopIso3D v2026 automatically uses the minimum or maximum value, respectively, found in the reconstructed dataset.

Tip

Automatic limits should be used with care. Extreme values of a scalar field may not represent the range in which most of the scientifically relevant data are concentrated. In such cases, a linear distribution over the complete dataset range may generate isosurfaces that poorly represent, or do not intersect, the region of interest. Defining appropriate minimum and maximum values allows you to focus the visualization on the relevant

range of the selected property.

Geometric levels In **Geometric** mode, the isosurface values are generated as a geometric progression. This mode is useful when the relevant values of a scalar field span different orders of magnitude and a linear spacing would provide an inadequate sampling of the field.

By default, the **Geometric** mode uses an **Ascending** sequence. In this mode, **Base iso (Min)** defines the first level and each subsequent value is obtained by multiplying the previous one by the selected **Factor**:

$$v_{n+1} = v_n f.$$

For a descending sequence, enable **Descending**. The interface then uses **Base iso (Max)** as the starting value and successive levels are generated by division:

$$v_{n+1} = \frac{v_n}{f}.$$

The progression continues until the specified **Limit** is reached or the number defined by **Max levels** has been generated, whichever occurs first.

Note

Geometric levels are generated only from positive values. Both the base level and the limiting value must be greater than zero and must lie within the range of the selected dataset. Use Linear mode when the desired visualization requires levels that include zero or negative values.

Overlays (3D)

The **Overlays (3D)** controls allow you to superimpose topological objects obtained from a TRHO analysis onto the three-dimensional PL2D representation. This provides a direct spatial connection between the scalar-field visualization and the topological information previously identified in the system.

You can independently display **TRUE atoms**, **BCPs**, **RCPs**, **CCPs**, and **NNAs** within the region represented by the current PL2D dataset. The displayed objects correspond to those available from the TRHO analysis whose coordinates fall within the spatial limits of the visualized region.

For **TRUE atoms**, the **Group by element** option separates the displayed atoms according to their chemical element. Each element is represented as an independent group in the three-dimensional visualization, facilitating the identification and selective inspection of different atomic species.

For **BCPs**, the **Group by pair** option organizes the displayed bond critical points according to their associated atomic pair. Each pair is represented as an independent group, making it easier to distinguish different types of interactions within the visualized region.

The **Labels** options control whether the identifiers associated with the corresponding objects are displayed in the rendered visualization. Marker sizes can be adjusted independently for **TRUE atoms**, **BCPs**, **RCPs**, **CCPs**, and **NNAs** using their respective **Size** fields.

For BCPs, the **Bond path** option adds the corresponding atom–BCP–atom connections to the visualization. These connections represent the association between each BCP and its two associated atoms as identified in the TRHO data.

Together, these overlays allow the reconstructed scalar field to be examined in the context of the relevant topological objects, helping you relate features of the three-dimensional isosurfaces to the local topological environment of the selected region.

Visualization and export

After selecting the PL2D campaign, scalar field, isosurface parameters, and optional overlays, you can visualize the reconstructed field interactively or export it for subsequent use.

Visualize (Plotly): Click **Visualize (Plotly)** to generate the three-dimensional representation using the current visualization settings. TopIso3D v2026 reconstructs the scalar field from the PL2D planes, generates the requested isosurfaces, adds the selected structural and topological overlays, and automatically opens the resulting Plotly visualization in the default web browser.

The visualization provides the same interactive navigation capabilities described for the CP Viewer, including rotation, translation, zoom, viewpoint adjustment, and interactive control of the displayed groups through the Plotly legend.

An example of an interactive representation generated by the PL2D Viewer is shown in Figure 3.12. In this example, the visualized region is centered on a selected BCP of MgO and the electron-density isosurfaces are generated using the geometric mode.

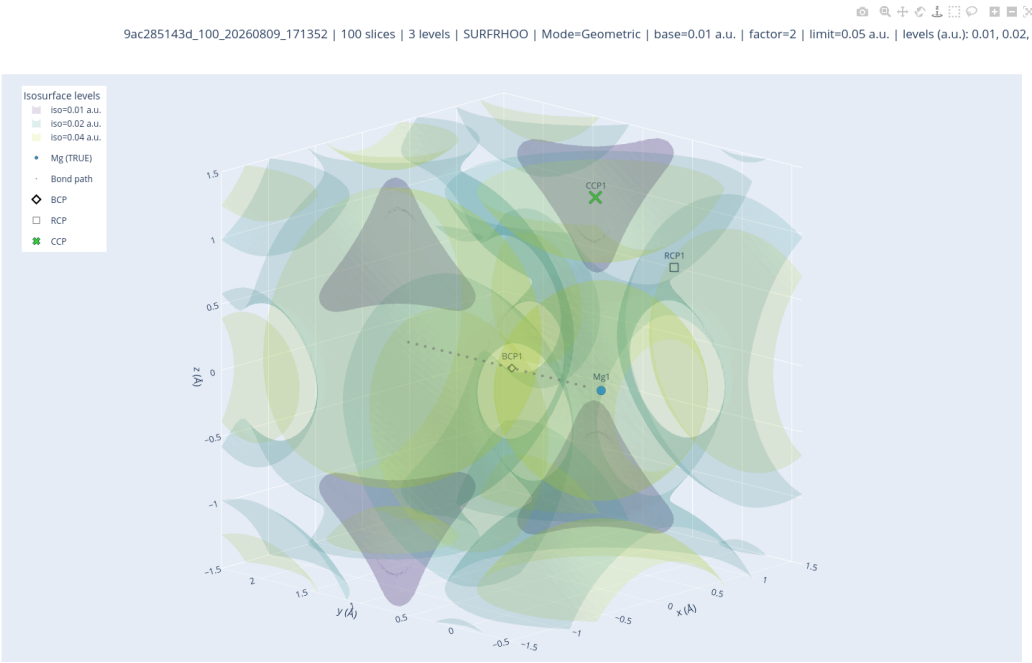

Figure 3.12: Interactive three-dimensional visualization generated by the PL2D Viewer for the electron density (`SURFRHOO`) in a region centered on a selected BCP of MgO. Three isosurfaces were generated using the geometric mode with a base value of 0.01 a.u. and a factor of 2, resulting in levels of 0.01, 0.02, and 0.04 a.u. TRUE atoms, BCPs, RCPs, CCPs, and bond-path information are included as structural and topological overlays.

The simultaneous representation of the scalar field and its topological objects also provides an intuitive spatial view of critical points such as RCPs and CCPs, whose positions and relationships with the surrounding electronic structure may be difficult to appreciate from numerical data alone.

Export HTML: Click **Export HTML** to save the current Plotly visualization as an interactive HTML file in the directory of the selected PL2D campaign within `pl2d_runs`.

The HTML file preserves the current visualization settings, including the selected isosurfaces and overlays, and can subsequently be opened directly in a web browser while retaining the

interactive capabilities of the Plotly representation.

Export CUBE: Click **Export CUBE** to save the reconstructed three-dimensional scalar field in CUBE format. The file is stored in the directory of the selected PL2D campaign within `pl2d_runs`.

Unlike the HTML export, the CUBE file is not restricted to the isosurface levels currently selected in the PL2D Viewer. It contains the complete reconstructed scalar grid, including the full range of values available for the selected property. Isosurface levels can therefore be defined independently when the CUBE file is subsequently opened in an external visualization program.

3.7 BCP Evaluation

The module combines three descriptors commonly employed in the characterization of chemical interactions within the QTAIM framework: the Laplacian of the electron density ($\nabla^2\rho$), the bond degree (H/ρ), and the ratio between the potential and kinetic energy densities ($|V|/G$) [3, 5].

Rather than examining these descriptors independently, BCP Evaluation projects them pairwise into three two-dimensional property spaces:

- $\nabla^2\rho$ versus H/ρ;
- $|V|/G$ versus H/ρ;
- $|V|/G$ versus $\nabla^2\rho$.

This integrated representation facilitates the comparative examination of BCP populations by allowing each critical point to be evaluated simultaneously with respect to two complementary descriptors.

By combining these descriptors graphically, BCP Evaluation provides a complementary perspective to conventional tabular analysis. Instead of considering one BCP at a time, you can examine the distribution of all BCPs simultaneously and identify groups of interactions occupying similar regions of the corresponding property spaces. Each point remains associated with its original BCP and can be individually inspected through the interactive Plotly visualization.

Reference lines associated with characteristic values of the plotted descriptors are included directly in the graphs, providing visual guides for the interpretation of the BCP distribution. These guides are intended to support scientific analysis rather than to impose an automatic classification: the interpretation of the observed populations and individual BCPs remains with the researcher.

Figure 3.13 shows the main BCP Evaluation interface. From this panel, you can open each of the three interactive plots or save the corresponding Plotly project as an HTML file for later exploration.

3.7.1 The three BCP evaluation plots

BCP Evaluation provides three complementary plots that combine the electronic properties available for each Bond Critical Point. The same set of BCPs is represented in each plot, allowing the interaction landscape to be examined from different, but related, QTAIM perspectives.

$\nabla^2\rho$ versus H/ρ

The first plot combines the Laplacian of the electron density, $\nabla^2\rho$, with the total energy density normalized by the electron density, H/ρ. Dashed reference lines at $\nabla^2\rho = 0$ and $H/\rho = 0$ divide the plot into regions defined by the signs of the two descriptors.

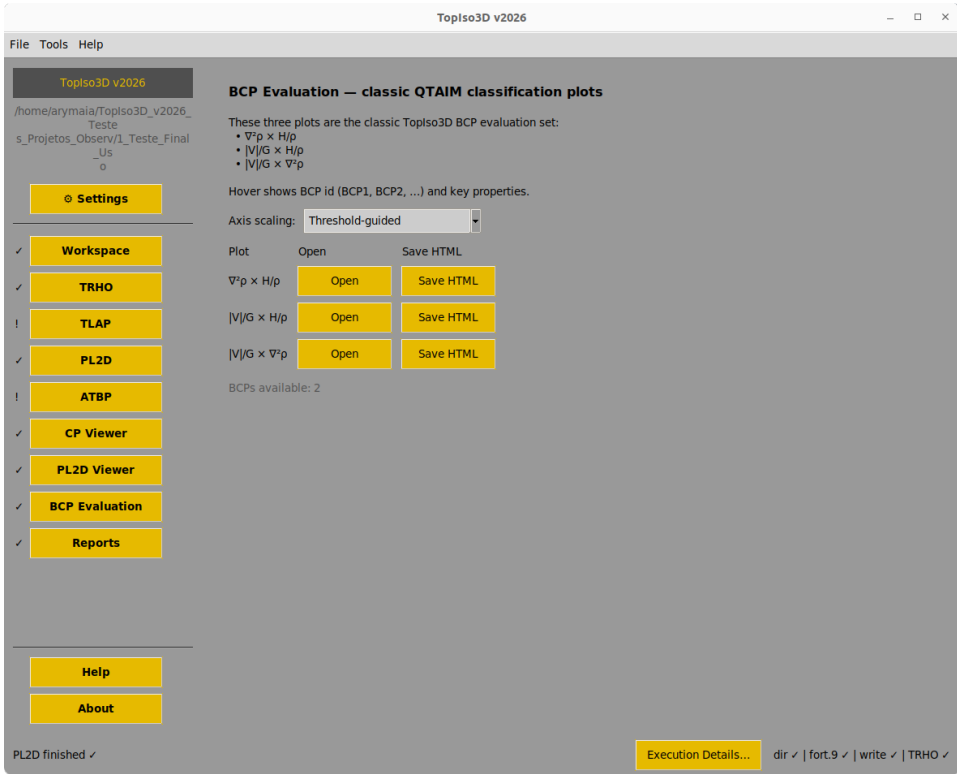

Figure 3.13: Main BCP Evaluation interface.

This representation allows the distribution of the BCP population to be inspected simultaneously with respect to electron-density concentration or depletion and the local energetic balance represented by H/ρ. An example of the resulting interactive representation is shown in Figure 3.14.

Because all available BCPs are displayed simultaneously, this plot is particularly useful for recognizing groups of interactions with similar energetic characteristics and for identifying BCPs located near, between, or far from the reference boundaries.

$|V|/G$ versus H/ρ

The second plot combines the ratio between the magnitude of the potential energy density and the kinetic energy density, $|V|/G$, with H/ρ. Reference lines at $|V|/G = 1$, $|V|/G = 2$, and $H/\rho = 0$ provide characteristic boundaries directly in the visualization.

$|V|/G$ versus $\nabla^2\rho$

The third plot combines $|V|/G$ with $\nabla^2\rho$, bringing together the energetic ratio and the spatial behavior of the electron density at the BCP. The corresponding reference lines are displayed directly in the interactive plot.

Taken together, the three representations provide complementary views of the same BCP dataset. In addition to indicating the position of each BCP relative to conventional reference thresholds, the plots preserve the continuous variation of the descriptors. This allows interactions to be compared in terms of greater or lesser character, similarities, trends, and transitions within the BCP population, rather than reducing the analysis to discrete interaction classes.

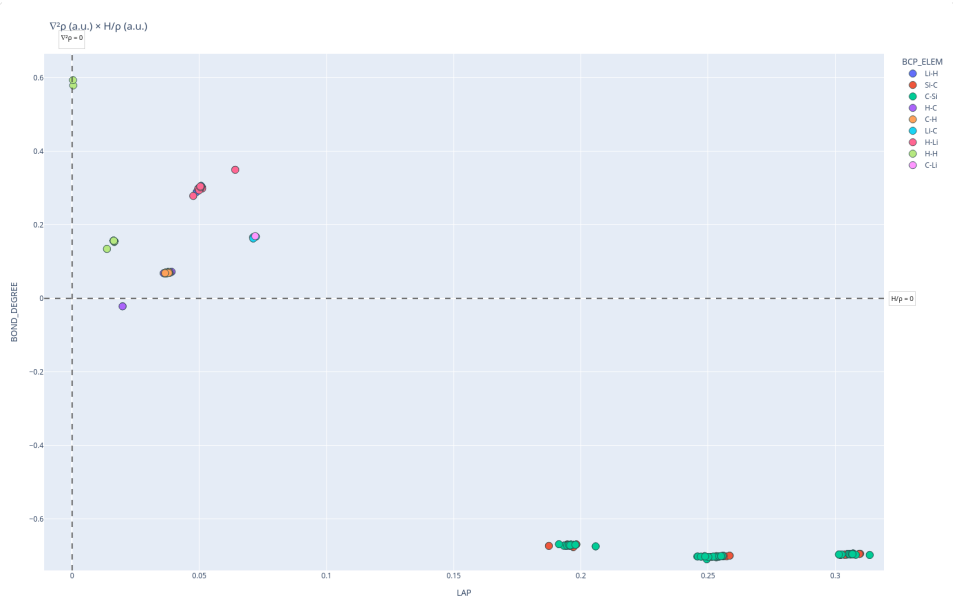

Figure 3.14: Interactive BCP Evaluation plot showing the relationship between the Laplacian of the electron density and the bond degree (H/ρ) for the BCPs recovered from the selected calculation. The computational system used in this example was previously investigated in Ref. [8]. The visualization shown here was generated with TopIso3D v2026 from the corresponding computational data.

3.7.2 Axis scaling

The **Axis scaling** selector controls how the plotting ranges and the characteristic reference thresholds are represented in the three BCP evaluation diagrams. Changing the scaling mode does not modify the BCP data or the reference thresholds; it changes only how the property space is organized and emphasized in the visualization.

Three scaling modes are available: **Auto**, **Auto + thresholds**, and **Threshold-guided**.

Auto

In **Auto** mode, the plotting ranges are determined from the distribution of the BCP data themselves, and the characteristic reference thresholds are not displayed. The visualization therefore focuses exclusively on the range effectively occupied by the analyzed BCP population.

This mode is particularly useful when the objective is to compare BCPs relative to one another, inspect the internal structure of a population, or identify trends, groups, and atypical points without using the conventional reference thresholds as part of the visualization.

Auto + thresholds

The **Auto + thresholds** mode retains the data-driven automatic scaling used in **Auto**, while additionally displaying the characteristic reference thresholds relevant to the selected descriptors. The thresholds are represented at their corresponding positions within the resulting property space, without being used to center the visualization.

This provides a compromise between data-oriented visualization and threshold-based inspection: the distribution of the BCP population remains the primary determinant of the displayed range, while its position relative to the conventional reference values can be examined directly.

Threshold-guided

In **Threshold-guided** mode, the characteristic reference thresholds actively guide the organization of the property space. The thresholds are positioned centrally in the visualization, and the axis ranges are adjusted accordingly so that the BCP population can be examined relative to these reference values.

This mode is particularly useful when the objective is to evaluate how individual BCPs or populations are distributed around the characteristic regions defined by the QTAIM descriptors. The thresholds should nevertheless be regarded as reference guides rather than absolute boundaries between fundamentally discrete types of chemical interaction.

3.7.3 Interactive visualization and export

After selecting the desired BCP evaluation plot and axis-scaling mode, click **Open** to generate the corresponding interactive Plotly visualization. TopIso3D v2026 automatically opens the plot in the default web browser.

Each point in the diagram represents an individual BCP. Moving the pointer over a point displays its associated information, allowing individual BCPs to be examined without losing the context provided by the complete BCP population.

The hover information is particularly useful in this module because it connects population-level exploration with the inspection of individual interactions. Once a group, trend, transition, or atypical point is recognized in the property space, the corresponding BCP and its descriptors can be immediately identified without leaving the interactive plot.

The BCPs are grouped according to their associated atomic pairs. These groups can be independently shown or hidden through the Plotly legend, making it possible to isolate particular families of interactions or compare them with the remaining BCP population.

Click **Save HTML** to save the selected interactive plot as an HTML file. The exported file preserves the Plotly interactivity and can subsequently be opened directly in a web browser without requiring a new TopIso3D v2026 session.

The HTML files are stored in the `bcp_evaluation` directory created inside the current project folder.

3.8 Reports

The **Reports** module provides direct access to the structured topological information recovered and processed by TopIso3D v2026. Rather than requiring you to inspect the original sequential TOPOND output or to export the processed data before examining them, the module allows the results to be inspected directly within the TopIso3D v2026 environment. Reports can also be exported for subsequent analysis using external software.

The main Reports interface is shown in Fig. 3.15. At the top of the window, TopIso3D v2026 summarizes the critical-point information recovered from the selected calculation, including the numbers of TRUE atoms, BCPs, RCPs, and CCPs.

3.8.1 Report source

The **Report source** panel determines which topological calculation is used to construct the report. Select the desired method and the corresponding available run. When **TRHO** is selected, the report contains information recovered from the selected TRHO run. When **TLAP** is selected, the corresponding TLAP results become available instead.

This run-based selection allows results from different calculations stored in the same project to be inspected independently by selecting the corresponding run.

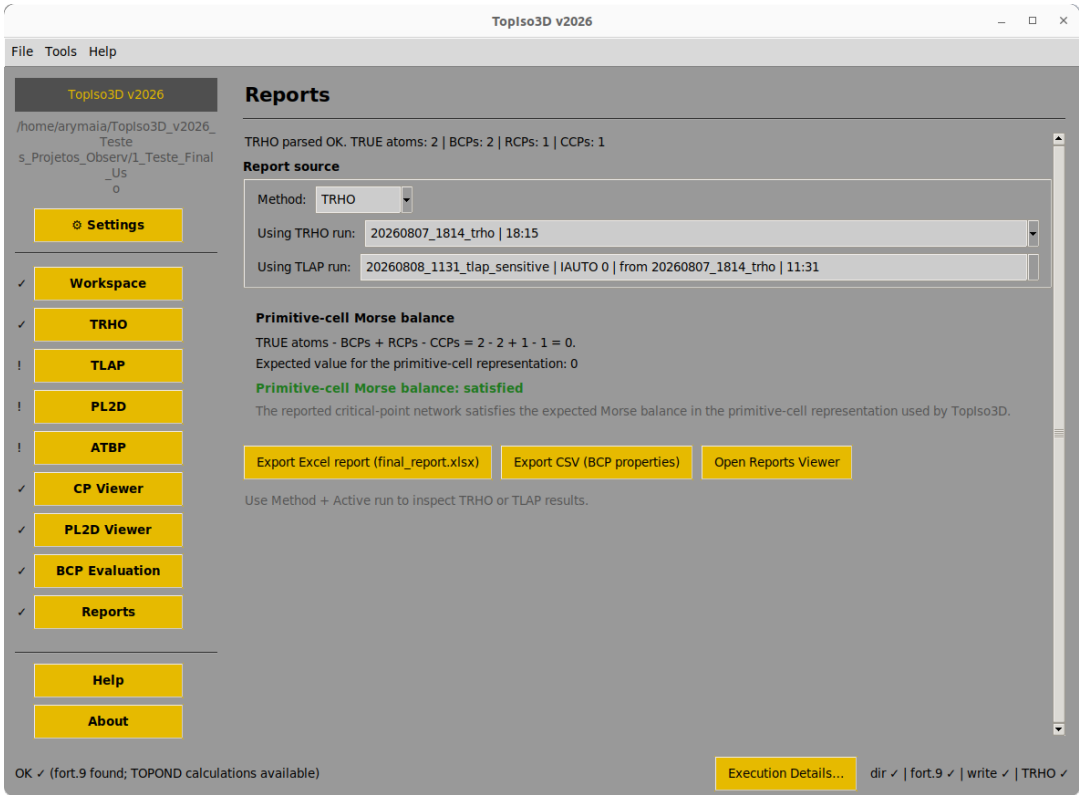

Figure 3.15: Main interface of the Reports module.

3.8.2 Primitive-cell Morse balance

For TRHO results, the Reports module displays the primitive-cell Morse balance calculated from the numbers of TRUE atoms and critical points:

$$N_{\mathrm{TRUE}} - N_{\mathrm{BCP}} + N_{\mathrm{RCP}} - N_{\mathrm{CCP}}.$$

The expected value for the primitive-cell representation used by TopIso3D v2026 is zero. When this condition is fulfilled, the interface reports that the **Primitive-cell Morse balance** is satisfied.

This provides a convenient consistency check of the critical-point network recovered from the selected TRHO calculation.

3.8.3 Exporting report data

The processed results can be exported directly from the Reports interface. The **Export Excel report (final_report.xlsx)** command generates an Excel workbook containing the structured topological information associated with the selected run. The **Export CSV (BCP properties)** command exports the BCP property table as a CSV file.

Both files are written to the directory of the corresponding run. For **TRHO** reports, they are stored with the selected calculation inside the project's `trho_runs` directory; for **TLAP** reports, they are stored with the corresponding calculation inside `tlap_runs`. This keeps the exported reports associated with the calculation from which they were generated.

Exporting the data is not required for inspecting the results. Click **Open Reports Viewer** to explore the processed information directly within TopIso3D v2026.

3.8.4 Reports Viewer

The **Reports Viewer** provides an interactive interface to the structured data associated with the selected topological calculation (Figure 3.16). It opens initially in the **Summary** tab and organizes the available information into separate tabs for **TRUE atoms**, **NNA**, **BCP**, **RCP**, and **CCP**. The number shown in parentheses in each tab indicates the number of corresponding entries recovered from the selected calculation.

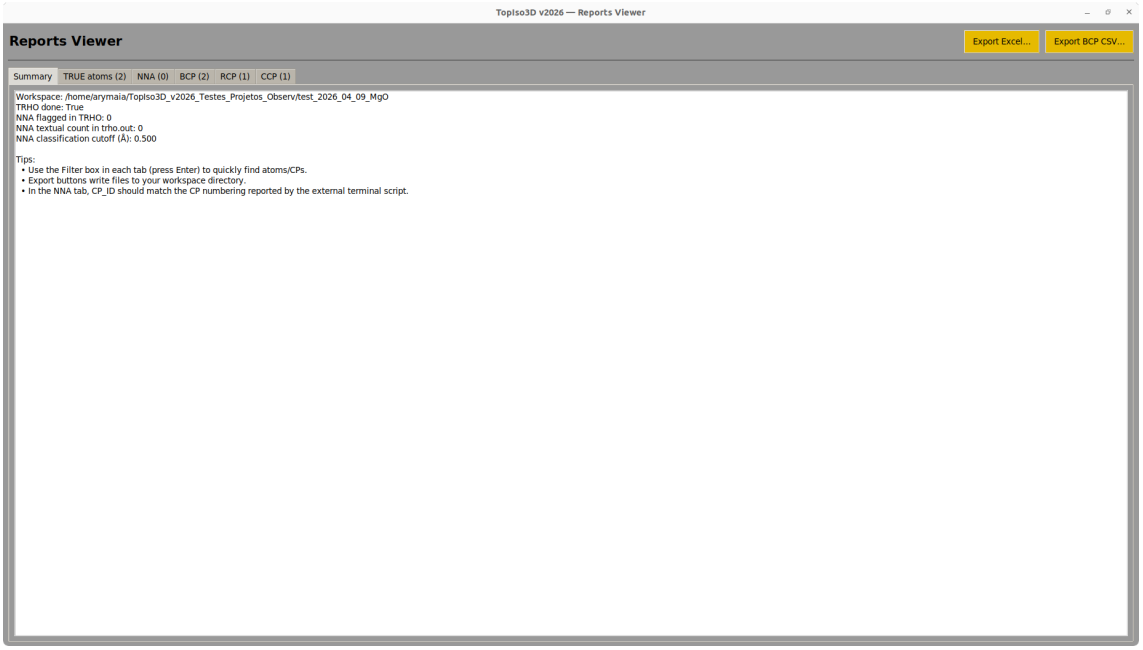

Figure 3.16: Reports Viewer providing interactive access to the structured topological data recovered by TopIso3D v2026.

The **Summary** tab provides general information about the selected run and the data available for inspection. The remaining tabs expose the corresponding atomic or critical-point tables together with the properties recovered or derived by TopIso3D v2026.

The **TRUE atoms** tab lists the atoms identified in the selected topological calculation. The **NNA** tab contains the detected non-nuclear attractors, when present. The **BCP**, **RCP**, and **CCP** tabs provide the corresponding bond, ring, and cage critical-point data, respectively. When no entries of a particular type are available, the corresponding tab remains accessible and indicates that no data are present.

Each data tab includes interactive tools for exploring the table. Enter text in the **Filter** field and click **Apply** to search across the displayed information. Click **Clear** to restore the complete table. In addition, clicking a column header sorts the table according to that property in ascending or descending order. These operations are particularly useful for calculations containing large numbers of critical points, since they allow specific atoms, critical points, chemical environments, or ranges of properties to be located without exporting and manually searching the complete dataset.

Tip

For large topological datasets, use filtering and column sorting before exporting the data. This allows you to explore the critical-point network directly in TopIso3D v2026 and rapidly identify features of interest for subsequent analysis or visualization.

The **N** column provides the selection index used by TopIso3D v2026 when an atom or critical point is referenced in subsequent workflows. This is particularly useful when identifying

centers for PL2D calculations: after locating an atom or critical point of interest in the Reports Viewer, its selection index can be used when defining the corresponding PL2D-centered project.

The **BCP** tab contains both the properties recovered from the TOPOND calculation and descriptors subsequently derived by TopIso3D v2026. The table therefore provides a compact environment for inspecting and comparing the electronic and geometrical characteristics of the available bond critical points.

A direct connection with the **BCP Evaluation** module is also provided. Click **Open BCP evaluation plots (Plotly)** to generate the three BCP evaluation plots described in the previous section. When opened from the Reports Viewer, these plots use the **Auto** axis-scaling mode. This provides a convenient shortcut from inspection of the tabulated BCP properties to their graphical comparison.

The export commands remain available in the Reports Viewer. Therefore, you can first inspect, filter, sort, and compare the results and then export the corresponding Excel report or BCP CSV file without returning to the main Reports window.

3.9 Help, About, and Execution Details

Additional interface resources provide quick access to workflow guidance, software information, and technical details associated with calculation execution.

3.9.1 Help

The **Help** button provides quick access to basic information about the TopIso3D v2026 workflow. The dialog summarizes the main sequence of operations: selecting a workspace, allowing TopIso3D v2026 to validate it, and running TRHO or another TOPOND module.

The dialog also reminds you that for macOS installations, additional information about the runtime environment can be collected through **Help > System Diagnostics**.

3.9.2 About

The **About** button displays general information about the installed TopIso3D v2026 version, including its purpose, authorship, institutional affiliation, and supported operating systems. The dialog also provides the address of the TopIso3D v2026 project website.

3.9.3 Execution Details

The **Execution Details** window provides real-time access to technical information associated with the current calculation. It can remain open while a TOPOND calculation is running, allowing the execution output to be followed as it is produced. In addition to the command and working directory associated with the active run, the **Log** area displays information generated during the execution.

When the calculation finishes, the same window records the final execution messages and the subsequent processing performed by TopIso3D v2026, including output parsing and recovery of the calculated topological information. The **Execution Details** window therefore provides a direct way to follow the computational process without leaving the TopIso3D v2026 environment (Figure 3.17).

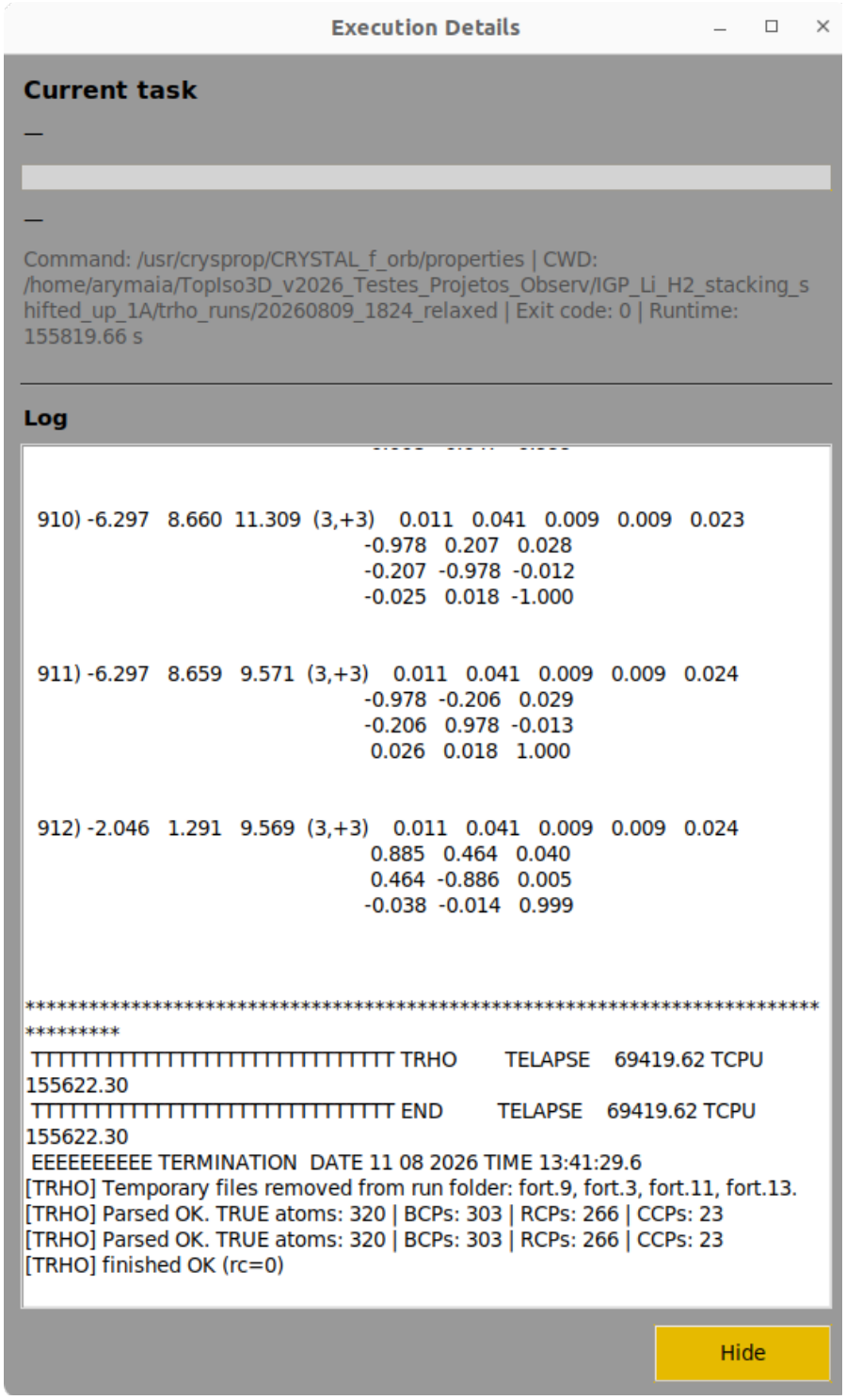

Figure 3.17: Execution Details window displayed at the completion of a TRHO calculation. The window provides access to the execution output and is updated while the calculation is running, including the final processing and parsing messages generated by TopIso3D v2026. The computational system used in this example was previously investigated in Ref. [8]. The execution shown here was performed with TopIso3D v2026 from the corresponding computational data.

4 Project Organization and Data Management

TopIso3D v2026 organizes calculations, parsed data, and generated scientific products around a project directory. Rather than requiring the user to manually assemble a predefined directory tree, the environment creates and manages module-specific directories as they become necessary during the scientific workflow.

A new project may therefore begin with little more than the CRYSTAL wavefunction file, typically `fort.9`. As calculations and analysis modules are used, TopIso3D v2026 progressively creates the directories required to store their corresponding runs and generated products.

This organization keeps the original computational data, TOPOND calculations, parsed information, and subsequent analysis products associated with the same scientific project while preserving the individual history of each calculation.

4.1 Project directory

The project directory is the central workspace used by TopIso3D v2026. A minimal project can initially contain only the `fort.9` file associated with the electronic-structure calculation to be analyzed.

For example, a newly created project may initially have the simple structure

```
TopIso3D_Project/
‘-- fort.9
```

The remaining project structure is created progressively. When a module that performs a TOPOND calculation is used for the first time, TopIso3D v2026 creates the corresponding module-managed directory.

After TRHO, TLAP, ATBP, and PL2D calculations have been performed, and BCP Evaluation products have been saved, a project may contain, for example,

```
TopIso3D_Project/
|-- fort.9
|-- trho_runs/
|-- tlap_runs/
|-- atbp_runs/
|-- pl2d_runs/
|-- bcp_evaluation/
|-- topiso3d.log
‘-- topiso3d_state.json
```

The exact contents of a project therefore reflect the workflows that have actually been performed. Directories associated with modules that have not yet been used do not need to exist.

4.2 Module-managed directories

TopIso3D v2026 separates calculations according to their scientific responsibility. TRHO, TLAP, ATBP, and PL2D calculations are stored in the corresponding `trho_runs`, `tlap_runs`, `atbp_runs`, and `pl2d_runs` directories.

These directories are containers for individual calculations or campaigns; the calculation files themselves are not normally placed directly in the project root.

For TRHO and TLAP, each execution creates an individual run directory. A typical organization is

```
trho_runs/
|-- <TRHO_run_1>/
`-- <TRHO_run_2>/

tlap_runs/
|-- <TLAP_run_1>/
`-- <TLAP_run_2>/
```

The run names may contain information such as the execution date, execution time, workflow type, or selected preset, depending on how the run was created.

ATBP follows the same general principle, with individual calculations stored under `atbp_runs`. For example,

```
atbp_runs/
|-- atbp_001/
|-- atbp_002/
|-- atbp_003/
`-- atbp_004/
```

The `bcp_evaluation` directory has a different role. It stores BCP Evaluation products explicitly saved by the user, such as interactive HTML plots. It is therefore an analysis-product directory rather than a TOPOND calculation directory.

Files associated with other analysis or visualization modules may also be stored within the run from which their underlying data were obtained. For example, HTML projects created with CP Viewer and exported BCP-property tables can be stored in the corresponding TRHO run directory.

4.3 Calculation runs and generated files

Each run directory preserves the files associated with an individual TOPOND calculation. This provides a direct correspondence between a calculation, its input, its output, and the metadata or scientific products subsequently derived from it.

A TRHO run may contain, for example,

```
<TRHO_run>/
|-- trho.inp
|-- trho.out
|-- run.json
|-- bcp_properties.csv
`-- cpviewer_001.html
```

The essential computational output is `trho.out`. Additional files may be generated during execution or subsequently saved by other TopIso3D v2026 modules. In the example above,

the CSV table and CP Viewer HTML project were produced after the TRHO calculation but remain associated with the same run from which their data originated.

A TLAP run may contain

```
<TLAP_run>/
|-- tlap.inp
|-- tlap.out
|-- run.json
‘-- tlap_generation_summary.txt
```

whereas an ATBP run may contain files such as

```
<ATBP_run>/
|-- atbp.inp
|-- atbp.out
|-- fort.96
|-- run.json
|-- atbp_parse.json
|-- atbp_snippet.txt
‘-- source_output_path.txt
```

The precise set of auxiliary files may vary according to the workflow and the products generated during subsequent analysis. The run directory should therefore be understood as the persistent record of a calculation and its associated TopIso3D v2026 products rather than as a directory with a rigidly fixed list of files.

4.4 PL2D campaign organization

PL2D requires a more structured organization because a three-dimensional sampling campaign is constructed from a sequence of independent two-dimensional TOPOND calculations. Consequently, an entry inside `pl2d_runs` represents an entire PL2D campaign rather than a single calculation.

A project may contain several independent campaigns:

```
pl2d_runs/
|-- <campaign_1>/
|-- <campaign_2>/
|-- <campaign_3>/
‘-- <campaign_4>/
```

Within each campaign, the individual planes are stored in ordered `sliceNNN` directories. A campaign containing eleven slices, for example, may have the structure

```
<campaign>/
|-- slice000/
|-- slice001/
|-- slice002/
|   ...
|-- slice009/
|-- slice010/
|-- manifest.json
‘-- <generated campaign products>
```

For a locally executed campaign, each slice directory contains the input and output files associated with that PL2D calculation together with the data files generated for the selected property. For a SURFRHOO campaign, for example, a slice may contain

```
slice000/
|-- pl2d.inp
|-- pl2d.out
|-- pl2d.err
|-- P2DCRYIN.DAT
`-- SURFRHOO.DAT
```

The campaign directory also provides the organizational context needed to combine the individual slices into the volumetric representation used by PL2D Viewer. Generated campaign products, including saved HTML visualizations and spreadsheet files, remain associated with the corresponding campaign.

This organization is particularly important because the scientific object handled by PL2D Viewer is not an isolated plane, but the ordered set of planes defining the sampled three-dimensional region.

4.5 Externally executed TOPOND calculations

TopIso3D v2026 does not require TRHO, TLAP, or ATBP calculations to have been executed from within the environment. Calculations performed externally, for example on a computing cluster, can be incorporated into an existing TopIso3D v2026 project by placing their directories inside the corresponding `trho_runs`, `tlap_runs`, or `atbp_runs` directory.

For an externally generated run to be recognized, its directory must contain the corresponding TOPOND output file with a filename recognized by TopIso3D v2026. The filenames used to identify external results are configured under **Settings**, in the **External result file names** fields, with separate lists for TRHO, TLAP, and ATBP outputs.

By default, these lists include the standard filenames

- `trho.out` for a TRHO run;
- `tlap.out` for a TLAP run;
- `atbp.out` for an ATBP run.

External results may, however, use different filenames. A user-defined filename can be added to the corresponding list in **Settings**, allowing TopIso3D v2026 to recognize and parse that file without requiring it to be renamed.

This configuration applies only to externally generated results. Calculations executed directly by TopIso3D v2026 continue to use the standard internal filenames `trho.out`, `tlap.out`, and `atbp.out`. The name of the directory containing an imported run does not need to reproduce the naming scheme used by TopIso3D v2026 itself.

This makes it possible to combine GUI-based analysis with conventional TOPOND workflows. A calculation may, for example, be prepared and executed independently on a remote computing system and subsequently introduced into the TopIso3D v2026 project for parsing, visualization, and scientific analysis.

PL2D calculations require a different approach. A PL2D campaign is composed of an ordered set of slices, and subsequent reconstruction and visualization depend on the expected campaign directory architecture. For this reason, TopIso3D v2026 provides an export mechanism that generates the complete campaign structure before external execution.

An exported campaign contains the individual slice directories with the corresponding `pl2d.inp` files together with the files needed to preserve and execute the campaign. Depending on the exported configuration, the campaign may also contain files such as

```
fort.9
manifest.json
README_RUN.txt
run_all.sh
run_parallel.sh
submit_slurm.sh
cleanup_for_return.sh
```

This mechanism allows the campaign to be transferred to a computing cluster or another execution environment while preserving the directory organization required by TopIso3D v2026. The launcher scripts can be used or adapted to automate execution of the individual PL2D calculations on the target computing infrastructure.

The export mechanism is therefore particularly useful for PL2D campaigns involving computationally demanding calculations: TopIso3D v2026 defines and organizes the scientific campaign, whereas its computational execution can be performed in the environment most appropriate to the available resources.

4.6 Opening and reusing an existing project

A TopIso3D v2026 project is intended to remain reusable after the original calculations have been completed. When an existing project is opened, the environment can recover the calculations and scientific products stored in its module-managed directories and make them available to the corresponding workflows.

This organization allows a project to evolve incrementally. New TRHO, TLAP, ATBP, or PL2D calculations can coexist with previous runs without requiring the earlier results to be replaced. Likewise, visualization and analysis products can remain associated with the calculations from which they were derived.

The project directory consequently acts as the persistent connection between the original electronic-structure data, TOPOND calculations, structured information recovered by TopIso3D v2026, and the scientific analysis products generated during subsequent exploration.

5 Troubleshooting

This chapter summarizes common situations that may prevent a workflow from being executed as expected. In many cases, the messages displayed by TopIso3D v2026 indicate a missing configuration, an incomplete project, or an unavailable input rather than a software failure.

5.1 The CRYSTAL PROPERTIES executable is not configured

TopIso3D v2026 requires access to a functional CRYSTAL/TOPOND `properties` executable when new TOPOND calculations are to be launched directly from the environment. The executable path is configured under **Settings**.

After selecting the executable, use the **Test** button to verify that it can be launched by TopIso3D v2026. A successful test confirms that the selected executable is accessible and operational.

A licensed CRYSTAL installation is not necessarily required for this purpose. The DEMO distribution of CRYSTAL23 includes a functional `properties` executable and may therefore be used with TopIso3D v2026, subject to the limitations of the DEMO version itself.

The absence of a configured `properties` executable does not prevent the analysis of previously calculated TOPOND results. External TRHO, TLAP, and ATBP calculations may be incorporated into the corresponding module-managed directories, provided that the expected output files are available, as described in Chapter 4.

5.2 The project is opened in import-only mode

The availability of the scientific modules therefore reflects the data that can actually be recovered from the project. For example, if a valid `trho.out` is available in a run contained in `trho_runs/`, modules that operate on parsed TRHO information, such as **Reports**, **CP Viewer**, and **BCP Evaluation**, may remain available.

The **TRHO** module itself also remains accessible because an existing TRHO run can be selected and inspected. This should not be interpreted as indicating that a new TRHO calculation can be executed. When no wavefunction file is available, the **Run TRHO** button remains disabled. The Workspace status identifies the project as **IMPORT-ONLY** and indicates that new TOPOND calculations require a `fort.9` (or compatible `*.f9`/`*.9`) file.

Thus, TopIso3D v2026 distinguishes between *module availability* and *calculation availability*: a module may remain accessible because compatible results are already present in the project, while its execution controls remain disabled when the computational inputs required for a new TOPOND calculation are unavailable.

This behavior is intentional and allows externally calculated TOPOND results to be explored without requiring the original CRYSTAL wavefunction to be present in the project.

To enable new TOPOND calculations, place the corresponding `fort.9` (or compatible `*.f9`/`*.9`) wavefunction file in the project directory and reopen or reload the project as appropriate.

5.3 An external TOPOND result is not recognized

If an externally calculated TRHO, TLAP, or ATBP result is present in the project structure but the corresponding modules are not enabled, verify that the output filename is recognized by TopIso3D v2026.

The filenames used to identify external results are configured under **Settings**, in the **External result file names** fields. Separate lists are provided for TRHO, TLAP, and ATBP outputs. If the filename of an imported result is not included in the corresponding list, TopIso3D v2026 will not identify that file as a compatible result and modules that depend on its parsed information may remain unavailable.

Add the required filename to the appropriate list in **Settings**, save the configuration, and reload the project so that the available results can be detected again. Alternatively, rename the imported output file to one of the filenames already configured for the corresponding calculation type in **Settings**.

This configuration applies only to externally generated results. Calculations executed directly by TopIso3D v2026 continue to use the standard internal filenames `trho.out`, `tlap.out`, and `atbp.out`.

5.4 A TRHO result is detected, but cannot be parsed

The presence of a recognized TRHO output file does not necessarily mean that the file contains a complete and usable TRHO result. TopIso3D v2026 first detects stored runs from the expected project structure and recognized output filenames, and then evaluates whether the information required by individual modules can actually be recovered from the selected result.

Consequently, an incomplete or invalid `trho.out` may be detected as a stored TRHO run while modules that require successfully parsed topological data, such as **CP Viewer** and **BCP Evaluation**, remain unavailable. Module availability therefore depends on the data that can be recovered from the result, rather than simply on the presence of the output file.

In this situation, **Reports** may remain available and can provide diagnostic information about the parsing failure. For example, TopIso3D v2026 may report that the TRHO output was found but that no TRUE atoms or critical points could be recovered. This usually indicates that the TOPOND calculation stopped before completing the TRHO search or that the selected file is not a valid or complete TRHO result.

Inspect the corresponding output file to identify the underlying TOPOND error. One possible cause, explicitly recognized by TopIso3D v2026, is the presence of f-functions in the basis set, for which TOPOND may terminate with a message such as:

```
NO F-FUNCTIONS IN TOPOND
```

After correcting the underlying problem, rerun the TOPOND/TRHO calculation and replace or reimport the incomplete result. Once a valid result containing the required topological information is available, TopIso3D v2026 will enable the corresponding analysis modules.

5.5 A PL2D visualization is incomplete or cannot be generated

The PL2D Viewer reconstructs a three-dimensional scalar field from the slice directories available in a PL2D campaign. Problems with the completeness of the campaign may therefore affect the resulting visualization in different ways, depending on whether an entire slice directory or only a required data file is missing.

Because the current campaign structure does not store an independent record of the expected number of slice directories, the PL2D Viewer reconstructs the campaign from the slices that are actually available.

If one or more `sliceXXX` directories are absent, the PL2D Viewer may still recognize and visualize the campaign using the slices that are actually available. In this case, the resulting three-dimensional representation may be incomplete or discontinuous without preventing the visualization from being generated. The number of slices detected for the selected campaign is displayed in the PL2D Viewer interface and is also reported in the generated Plotly visualization. If the displayed number is smaller than expected, inspect the campaign directory and verify that all expected slice directories are present.

A different behavior occurs when a slice directory exists but the data file required for the selected topological surface is missing. For example, if `SURFRHOO` is selected and one of the detected slices does not contain `SURFRHOO.DAT`, TopIso3D v2026 interrupts the visualization and identifies the missing file and corresponding slice, with a message such as:

```
Failed to plot: Missing SURFRHOO.DAT in slice008
```

In this situation, inspect the affected slice and determine whether its TOPOND calculation was completed successfully and whether the expected descriptor file was generated or correctly transferred back to the campaign directory.

For campaigns executed externally, verify that the complete directory structure and all generated slice results have been returned to the corresponding campaign folder before using the PL2D Viewer.

5.6 ATBP does not run after disabling the TOPO wrapper

The current ATBP workflow in TopIso3D v2026 expects the generated ATBP input to be enclosed within the corresponding TOPOND `TOPO` block. In the present version, the **Include TOPO wrapper** option should therefore remain enabled.

If this option is disabled, the generated input may not follow the structure required by the ATBP workflow used by TopIso3D v2026, and the calculation may fail to start or may terminate without producing the expected ATBP result.

If an ATBP execution fails after this option has been changed, return to the ATBP configuration, enable **Include TOPO wrapper**, generate the input again, and rerun the calculation.

This control is retained in TopIso3D v2026 for compatibility with the current interface, but disabling it is not recommended for the standard TopIso3D v2026 ATBP workflow.

5.7 The PL2D Effective L differs from the requested L

When defining a PL2D sampling region, the value of `L` specifies the requested side length of the square xy region. The effective sampling region, however, must also be compatible with the selected spatial discretization.

For this reason, TopIso3D v2026 applies a snapping procedure that adjusts the requested region to the discrete sampling grid. The resulting **Effective L** may therefore differ slightly from the value originally entered by the user. The corresponding **Nx** and **Ny** values indicate the number of sampling points used along the two in-plane directions.

This behavior is intentional and does not indicate an error in the PL2D campaign. The displayed **Effective L**, rather than the original requested value of `L`, represents the side length actually used to construct the sampled region.

Because PL2D sampling planes are constructed as square xy regions, the snapping procedure also preserves the geometric requirements of the campaign. When the exact spatial extent of the sampled region is important, verify the reported **Effective L**, **Nx**, and **Ny** values before launching the calculation.

5.8 A PL2D campaign is created with a modified name

TopIso3D v2026 does not overwrite an existing PL2D campaign when a new campaign is created with the same requested name. Because a campaign may contain multiple slice calculations together with visualization and exported data products, preserving an existing campaign prevents previous scientific results from being replaced unintentionally.

If the requested campaign name is already present in `pl2d_runs`, TopIso3D v2026 automatically generates a unique directory name by adding a numerical suffix, such as `_2`, `_3`, and so forth.

For example, if

```
pl2d_runs/my_campaign/
```

already exists, a subsequent campaign requested with the same name may be stored as

```
pl2d_runs/my_campaign_2/
```

This behavior is intentional and does not indicate that the campaign name was entered incorrectly. If an existing campaign is no longer required, it should be reviewed and managed explicitly rather than replaced automatically during creation of a new campaign.

5.9 Laplacian critical points are not available in CP Viewer

The visualization of Laplacian critical points in the CP Viewer requires an active and successfully parsed TLAP result. A valid TRHO result alone provides the electron-density critical-point information, but it does not provide the Laplacian critical points required by the **Laplacian** and **Both** visualization modes.

When no active TLAP result is available, the CP Viewer indicates this condition in the **Active data sources** and **Viewer summary** sections. If **Laplacian** or **Both** is selected as the critical-point source, TopIso3D v2026 prevents the visualization from being generated: the **Open CP Viewer** button and the option to save the Plotly project as an HTML file remain disabled.

This behavior does not indicate a failure of the CP Viewer. To enable these visualization modes, a valid TLAP calculation must first be available, parsed, and selected as the active TLAP run. Alternatively, select the electron-density critical-point source when only TRHO data are available.

A Supported File Formats

The following files and formats are directly used, recognized, generated, or exported by TopIso3D v2026 as part of its scientific workflows.

File or format	Role in TopIso3D v2026
`fort.9`	CRYSTAL wavefunction file used as the electronic-structure input for TOPOND calculations.
`trho.out`	TOPOND TRHO output recognized and parsed by TopIso3D v2026.
`tlap.out`	TOPOND TLAP output recognized and parsed by TopIso3D v2026.
`atbp.out`	TOPOND ATBP output recognized and parsed by TopIso3D v2026.
`.DAT`	Plane-resolved scalar-field data generated by TOPOND PL2D calculations and used by TopIso3D v2026 for three-dimensional field reconstruction and isosurface visualization.
`.json`	Structured metadata used by TopIso3D v2026 to preserve information associated with projects, runs, or exported computational campaigns.
`.html`	Self-contained interactive Plotly visualization that can be reopened in a web browser independently of TopIso3D v2026.
`.csv`	Structured tabular-data export for subsequent analysis with external software.
`.xlsx`	Spreadsheet export containing structured topological information.
`.cube`	Volumetric scalar-field export for visualization or analysis with compatible external software.

B Quick Reference

This appendix provides a compact overview of the principal TopIso3D v2026 modules, their scientific roles, required data, and main products. For configuration details and complete workflows, refer to the corresponding sections of Chapter 3.

Module	**Purpose**	**Required data/result**	**Main product**
TRHO	Topological analysis of the electron density	`fort.9` for new calculations, or a recognized TRHO output for imported results	Critical points, bond paths, and structured topological information
TLAP	Topological analysis of the Laplacian of the electron density	`fort.9` and an available TRHO result	Laplacian critical-point information
PL2D	Generation of parallel two-dimensional scalar-field maps	`fort.9` and PL2D campaign configuration	Ordered PL2D slices and scalar-field datasets
ATBP	Calculation of atomic-basin properties	`fort.9`	Atomic-basin properties and structured results
CP Viewer	Interactive exploration of critical points and their structural environment	Parsed TRHO result; parsed TLAP result for Laplacian critical points	Interactive 3D visualization and HTML project
PL2D Viewer	Three-dimensional reconstruction and exploration of PL2D scalar fields	Completed PL2D campaign with the required slice datasets	Interactive 3D isosurfaces, HTML project, and CUBE export
BCP Evaluation	Comparative analysis of bond critical-point descriptors	Parsed TRHO result	Interactive descriptor-correlation plots and HTML project
Reports	Inspection and export of structured topological results	Parsed TRHO or TLAP result	Interactive tables, XLSX, and CSV data

External calculations

TRHO, TLAP, and ATBP results generated outside TopIso3D v2026 can be incorporated into a project when their output filenames correspond to names configured in **Settings**. PL2D calculations require the campaign directory structure expected by TopIso3D v2026; for external execution, the recommended procedure is therefore to generate and export the campaign from TopIso3D v2026 before running it on the external computing system.

C Glossary

Active run The stored result currently selected as the data source for a TopIso3D v2026 workflow or analysis module.

ATBP TOPOND calculation used to evaluate properties associated with atomic basins.

BCP Bond Critical Point, a critical point of rank 3 and signature -1, denoted $(3, -1)$ in QTAIM terminology.

BCP Evaluation TopIso3D v2026 module for comparative exploration of descriptors associated with bond critical points.

Bond path Topological path of maximum electron density connecting two attractors through a bond critical point.

Campaign An organized set of related PL2D calculations consisting of multiple parallel slices generated from a common spatial and scalar-field configuration.

CCP Cage Critical Point, a critical point of rank 3 and signature $+3$, denoted $(3, +3)$.

CP Critical Point. In TopIso3D v2026, the term may refer to electron-density or Laplacian critical points depending on the selected data source.

CP Viewer Interactive TopIso3D v2026 module for three-dimensional exploration of critical points, atoms, bond paths, and their local structural environment.

Effective L The effective side length of a PL2D square sampling region after the requested geometry has been adjusted to the discrete sampling grid.

Geometric mode Isosurface-level selection mode in PL2D Viewer in which successive levels follow a geometric progression.

Linear mode Isosurface-level selection mode in PL2D Viewer in which successive levels are equally spaced between the selected minimum and maximum values.

NNA Non-Nuclear Attractor, an electron-density attractor not associated with a nuclear position.

PL2D TOPOND procedure used to evaluate a selected scalar field on a two-dimensional plane.

PL2D campaign See *Campaign*.

PL2D Viewer TopIso3D v2026 module that reconstructs and interactively visualizes three-dimensional scalar fields from an ordered set of PL2D slices.

RCP Ring Critical Point, a critical point of rank 3 and signature $+1$, denoted $(3, +1)$.

Run A stored computational result managed within the corresponding TopIso3D v2026 run directory.

Slice One two-dimensional sampling plane belonging to a PL2D campaign. An ordered sequence of slices provides the data used for three-dimensional scalar-field reconstruction.

Snapping Adjustment of a requested PL2D sampling region to the discrete grid accepted by the underlying calculation, producing the corresponding effective dimensions and grid-point counts.

TLAP TOPOND topological analysis of the Laplacian of the electron density.

TOPOND Topological-analysis component of the CRYSTAL program suite used to perform the underlying electron-density, Laplacian, atomic-basin, and scalar-field calculations accessed and managed by TopIso3D v2026.

TRHO TOPOND topological analysis of the electron density used to recover critical points and associated topological information.

TRUE atom Atomic position explicitly identified by TOPOND as belonging to the reference unit cell, as opposed to symmetry- or periodicity-related atomic images used to represent the surrounding environment.

Workspace The project directory recognized by TopIso3D v2026 and used to organize electronic-structure input, computational runs, parsed results, visualization products, and exported data.

Acknowledgments

The author gratefully acknowledges Prof. Julio Ricardo Sambrano and Dr. Nicolas Ferreira Martins for kindly providing the computational data used to construct one of the topological-analysis examples presented in this manual.

The author gratefully acknowledges Prof. Silvia Maria Casassa for her scientific supervision and for the collaborative research environment in which the development of TopIso3D v2026 was carried out. This manual was prepared in the context of the scientific collaboration between the Universidade Federal da Paraíba (UFPB), Brazil, and the Università degli Studi di Torino (UNITO), Italy, during the author's postdoctoral research period at UNITO under her supervision.

The author gratefully acknowledges the Brazilian National Council for Scientific and Technological Development (CNPq) for financial support through a Postdoctoral Fellowship Abroad (PDE), grant No. 201714/2025-6. The author also acknowledges the Universidade Federal da Paraíba (UFPB) for granting the institutional leave required for the postdoctoral research period, and the Università degli Studi di Torino (UNITO), particularly the CRYSTAL group, for the hospitality and scientific environment provided during the author's research stay in Turin, Italy.

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Support and Citation

Support

For questions related to the use of TopIso3D v2026, bug reports, feature requests, or problems encountered while reproducing a workflow described in this manual, users are encouraged to consult the official TopIso3D v2026 repository and the documentation distributed with the software.

When reporting a problem, include whenever possible the TopIso3D v2026 version, operating system, relevant project structure, and the message displayed by the software. For execution-related problems, the information available in the **Execution Details** window may also help identify the source of the issue.

Official resources

The source code, software releases, documentation, and additional information about TopIso3D v2026 are available through the official project website and the TopIso3D v2026 GitHub repository:

https://www.topiso3d.ufpb.br
https://github.com/arymaia/TopIso3D_v2026

Software archival record

Archived releases, supplementary material, and persistent identifiers associated with TopIso3D v2026 may be made available through Zenodo or another long-term scientific repository.

How to cite TopIso3D v2026

When TopIso3D v2026 contributes to a scientific investigation, users are encouraged to cite the corresponding software publication and, when appropriate, the specific software release used in the study.

The recommended citation for the TopIso3D v2026 environment will be provided with the official release and associated scientific publication.

How to cite this manual

The recommended citation for this manual is:

> Ary da Silva Maia. *From Topological Data to Scientific Exploration: TopIso3D v2026 User Manual*. 1st ed., 2026. ISBN: 978-65-02-29867-1. DOI: 10.5281/zenodo.21945798.