Nanopore Conductance Analysis GUI — User Guide

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1) What this app does

A desktop GUI for analyzing I–V data from nanochannels/nanopores. It lets you: - Load I–V curves (multiple files). - Convert units consistently (original → target) and re-scale plots/data in place. - Compute conductance (global and user-selected voltage ranges). - Detect the zero-current crossing (E_{total} : left/mid/right) and annotate plots. - Switch between **IV** and **G–V** views with one click. - Compare experimental vs theoretical conductance/ conductivity (σ–C). - Calculate drift–diffusion quantities, redox/Em, and ion mobilities (μ^{+}/μ^{-}, μ^{+}, μ^{-}) for monovalent and general salts. - Compute enclosed area of a looped I–V curve and log frequency-normalized metrics. - Manage an **Electrolyte details** table (e.g., KCl/LiCl conductivity vs concentration) for quick reference in calculations. - Export figures and data to PNG/CSV.

> **Non-blocking plotting:** Live plotting (if enabled) runs decoupled from acquisition in a separate module/process. Interacting with the plot window (drag/resize/zoom) will **not** affect measurement timing.

> **Communication latency note:** Due to VISA/SCPI round-trip and instrument measurement time, even with *dwell per step* = 0, the effective time spacing between points is typically **~25 ms**.

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2) Requirements

- **Python** 3.9+
- **Libraries:** `tkinter`, `numpy`, `pandas`, `matplotlib`, `mplcursors`
- Optional (not required for analysis): `pyvisa` (for instrument discovery in other tooling)

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3) Launching the app

Run the main analysis script (e.g., `python analysis_gui.py`). The window has: - **Left panel:** file controls, unit conversion, analysis actions, export buttons. - **Right panel:** active plot **or** results table (context-dependent).

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4) Supported data formats

- **Excel (`.xlsx`)**: first two columns are **Voltage (V)** and **Current (A)**.
- **CSV (`.csv`)**: header row is skipped; column 2 → **Voltage**, column 3 → **Current**.

- **Text (`.txt`)**: two numeric columns → **Voltage**, **Current** (whitespace-separated).

Files are cleaned for `NaN` rows before use. If a file has fewer than two numeric columns, you'll be asked to fix the input.

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5) Quick start (typical workflow)

1. **Load files** → multiple I–V curves can be added/removed at any time.
2. **Set units** → choose the **original units** of your data (e.g., V, mV, A, nA) and your **target units**. Click **Rescale** to convert in place. (This respects the chosen *original* unit as the baseline—no hidden resets.)
3. **Inspect IV plot** → the app automatically:
4. Fits a global linear conductance (shows slope on the figure).
5. Finds zero-current crossings and labels **Etotal (left, mid, right)**.
6. Displays hover readouts via `mplcursors`.
7. **Switch mode** → use the top-right buttons **IV** / **G–V**.
8. **IV mode:** current vs voltage, colored by sweep direction; legends auto-update.
9. **G–V mode:** conductance envelopes vs voltage; y-axis is **Conductance (S)**.
10. **Selected-range conductance** → click **Calculate Conductance in Selected Region**.
11. A small window opens (separate from the main UI). Enter your voltage range.
12. The app computes the local linear conductance and shows a zoomed plot.
13. Results are written into an editable table and can be exported.
14. **Enclosed area** (optional) → **Calculate Enclosed Area** opens a plot and an editable table for polygon area of looped I–V curves. You can append the corresponding frequency for normalization.
15. **Export** → save current figure as PNG and data as CSV. "Save all" writes every active series/table.

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6) Zero-current crossings (Etotal) and table behavior

- The midpoint crossing is auto-filled in the table after loading a curve.
- Selecting **Etotal (left/mid/right)** from the dropdown updates the **currently selected row** in the drift–diffusion table (it does **not** add a new row).
- These values can be edited later and are used directly in mobility and Em workflows.

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7) Drift–diffusion & mobility module

This module computes Em, mobilities, and ratios based on your inputs.

Inputs - Concentrations on each side (C_H , C_L) and, if needed, activity coefficients γ . - Temperature T . - Valences z^+ , z^- (monovalent or general salts). - Either **Em directly** *or* a **redox potential** (from which Em is derived).

Outputs - μ^+/μ^- , μ^+ , μ^- and conductivity σ , using the Henderson form (monovalent) or the general-salt formulation.

Usage tips - For KCl/LiCl, you can enter **activity coefficients (γ)** per side if required. - All results are placed into an editable table. Use **Update** to recompute for a row after editing inputs.

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8) Electrolyte details (conductivity table)

Click **Enter Electrolyte Details** to open a side table with prefilled KCl/LiCl conductivity (S/m) at common concentrations. You can: - Edit values and add new salts/concentrations. - Save the table for later runs. - Use these values directly in theoretical conductance/σ computations.

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9) Reference window

Open the **References** window for a concise explanation of the underlying formulas and clickable links to source papers/handbooks. This is a separate window you can open anytime; reading it will not interrupt ongoing analysis.

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10) Unit conversion

Use **Attach Unit Conversion UI** to pick both **original units** and **target units**. Press **Rescale** to convert all loaded data and any dependent tables/plots. This applies to IV plots, G–V, and σ–C figures.

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11) Exports & data management

- **Save Figure** → PNG of the current plot.
- **Export Data** → CSV for the visible table or the active curves.
- **Save All** → batch export of all displayed curves/tables.
- Tables are editable: double-click to change a cell; use **Save** to persist.

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12) Performance & timing

- **Non-blocking UI:** Live plots run in a separate module/process; UI actions won't block acquisition.
- **25 ms floor:** Even with dwell per step = 0, communication + measurement overhead limits the effective point interval to ≈25 ms.

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13) Troubleshooting

“File must contain at least two numeric columns.” Check the file format and column order (V first, I second). For CSV, ensure the first line is a header (it will be skipped).

“Plot shows wrong units.” Confirm you set **original** units correctly before clicking **Rescale**.

“Selected-range conductance not saved.” Ensure the sub-window says “Result written to table.” If you closed it before saving, re-run the calculation.

“G–V looks empty.” If you switched from IV after hiding data, click **IV** then **G–V** again to refresh envelopes.

Performance feels slow. Close unused figures; avoid extremely large CSV/Excel files; confirm you aren’t plotting millions of points at once.

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14) Tips

- Use hover (mouse over points) to see precise coordinates.
- Keep a consistent naming scheme for files so exported CSVs map back to raw data easily.
- For batch comparisons, load files together, rescale once, then export “All.”

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15) Known limits

- CSV dialects with irregular delimiters may fail auto-sniffing; open and save as standard CSV if needed.
- Extremely noisy I–V data may degrade linear fits. Use **Selected-range conductance** to focus on regions with good linearity.

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16) Change log (highlights)

- Live plot moved to its own module/process (non-blocking).
- Etotal selection updates the current table row (no extra rows created).
- Added **Selected-range conductance** window and zoomed preview.
- Added **Electrolyte details** table and σ–C integration.
- Unified unit-conversion UI across IV, G–V, and σ–C.

Questions or requests? Feel free to annotate this guide with your notes; we’ll keep it updated as the app evolves.