

NSA Cube

Interactive 3D Viewer for Kintecus
Normalized Sensitivity Analysis

User Guide & Reference

nsa_cube.py • *command-line tool and self-contained HTML viewer*

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1. Overview

NSA Cube turns a folder of Kintecus Normalized Sensitivity Analysis output files (SENSIT001.TXT, SENSIT002.TXT, ...) into a single interactive 3D heat-map cube that you can rotate, zoom, slice, and crop in any modern web browser.

The tool is a single Python script, `nsa_cube.py`. It reads the SENSIT files, assembles a three-dimensional grid of sensitivity values, and writes one self-contained HTML file. That HTML file is the viewer — there is no server to run and, when built in offline mode, no internet connection is required to view it.

1.1 The cube model

Each sensitivity value occupies one cell in a 3D grid. The three axes are:

- **X — Species / column labels:** the species (and any trailing columns such as Temperature or Volume) read from the header row of each SENSIT file.
- **Y — Rate constants (reactions):** the “Rate Constant n” rows in each file. This is the reaction axis.
- **Z — Time:** one slice per SENSIT file, in file-number order, labelled with each file’s analysis time.

A cell’s colour and opacity encode the sensitivity value at that species / reaction / time point. Small magnitudes are nearly transparent; large magnitudes are nearly opaque. Cells closer to the camera are rendered slightly more transparent so you can see into the volume.

1.2 Why a logarithmic scale

Normalized sensitivity values routinely span many orders of magnitude, because the normalization can divide by a species concentration that approaches zero. A linear colour scale keyed to the largest value would make almost every cell invisible. NSA Cube therefore maps magnitude logarithmically, with a “Dynamic range (decades)” control that lets you choose how many decades below the peak remain visible. This is central to reading the data and is described under the viewer controls.

2. What’s in the Package

The distribution ZIP contains a ready-to-run kit. The most important items are:

Item	Purpose
<code>nsa_cube.py</code>	The tool. Reads SENSIT files and writes the HTML viewer. Run it from Python, or build it into an <code>.exe</code> .
<code>Run NSA Cube.bat</code>	Windows launcher. Double-click to open a folder picker and build an offline viewer that opens in your browser.
<code>Install requirements.bat</code>	Run once to install the only dependency, <code>numpy</code> .
<code>build_exe.ps1</code>	PowerShell script that builds a standalone <code>nsa_cube.exe</code> (no Python needed to run it afterwards).
<code>build_exe.bat</code>	Batch equivalent of the PowerShell build script.

Item	Purpose
sample_data\...	60 example SENSIT files for the O2/H2 mechanism, for testing.
sample_viewer (offline demo).html	A pre-built viewer made from the sample data; double-click to see the result with no setup.
README.txt	Condensed quick-start and flag reference.

3. Requirements

- **To run the Python tool:** Python 3.9 or newer, plus numpy. Nothing else.
- **To build the .exe:** a Windows PC with Python 3 installed (PyInstaller and numpy are installed automatically by the build script). The resulting .exe then needs no Python at all.
- **To view the output:** a modern browser with WebGL (Chrome or Edge recommended). In offline mode no internet is required.

4. Installation and Quick Start

4.1 Easiest path (Windows, no command line)

1. Install Python 3 from python.org and tick “Add Python to PATH” during setup.
2. Double-click Install requirements.bat once.
3. Double-click Run NSA Cube.bat.
4. In the folder picker, choose a folder of SENSIT files (try sample_data\O2_H2_sensitivity_analysis to test).
5. The viewer is built and opens in your default browser.

To simply view a finished result with no setup, double-click “sample_viewer (offline demo).html”.

4.2 Command line

Run the tool with Python. If you omit -f, a folder-picker dialog opens.

```
python nsa_cube.py -f "C:\path\to\SENSIT_files"
python nsa_cube.py                (no -f -> folder picker opens)
python nsa_cube.py -h              (show all options)
python nsa_cube.py -f data --three-inline (fully offline output)
```

5. Building a Standalone Executable

If you want a single double-click program that needs no Python on the machines that use it, build an .exe once on any Windows PC that has Python 3 installed.

5.1 PowerShell (recommended)

6. Place `build_exe.ps1` in the same folder as `nsa_cube.py` (this is already the layout in the package).
7. Right-click `build_exe.ps1` and choose “Run with PowerShell”. If Windows blocks it, open PowerShell in that folder and run:

```
powershell -ExecutionPolicy Bypass -File .\build_exe.ps1
```

8. The script locates Python, installs PyInstaller and numpy, builds `nsa_cube.exe` into the folder, and cleans up the build leftovers.

Script options:

- `-KeepBuildFiles` keep the `build\`, `dist\`, and `nsa_cube.spec` leftovers instead of deleting them.
- `-NoConsole` build a windowed `.exe` with no console window.

5.2 Batch alternative

Double-click `build_exe.bat` to do the same thing without PowerShell.

5.3 Important note on platforms

PyInstaller cannot cross-compile. An `.exe` must be built on Windows to run on Windows. Build it on any Windows PC with Python; the resulting `.exe` then runs anywhere with no Python installed. Once built, double-click `nsa_cube.exe` to open the folder picker, or run it from a command prompt exactly like the Python script (for example, `nsa_cube.exe -f "C:\path\to\SENSIT_files"`).

6. Input Data and Validation

6.1 File naming

Input files must be named `SENSIT001.TXT` through `SENSITnnn.TXT` (three digits, 001–999). The match is case-insensitive, so `.TXT` and `.txt` both work. The files must be numbered consecutively starting at 001 with no gaps.

The tool validates the chosen folder and exits with a clear message (not a crash) if something is wrong:

Situation	Message
Folder does not exist	ERROR: folder not found: ...
No SENSIT files present	ERROR: no SENSITnnn.TXT files found ...
Numbering does not start at 001	ERROR: numbering must start at SENSIT001.TXT ...
A file is missing in the sequence	ERROR: SENSIT files are not consecutive ... missing: SENSIT003.TXT

6.2 File contents

Each SENSIT file is expected to contain:

- **Line 1:** an analysis time, given after a colon (used to label the time axis).

- **Line 2:** column headers (tab- or comma-delimited); the first field is the row-label column, followed by species names and any trailing columns such as Temperature(K) or Volume.
- **Lines 3+:** rows beginning “Rate Constant n” followed by the sensitivity values.

The parser handles Windows line endings, tab or comma delimiters, and Fortran-style scientific notation (leading-dot mantissas, three-digit exponents, and D-exponents).

6.3 Consistency requirement

All SENSIT files within one folder must share the same species and reaction counts; the number of files becomes the length of the time axis. Different folders (different datasets) may have completely different dimensions — the viewer sizes itself to whatever it is given.

7. Using the Viewer

The viewer opens with the cube centered on screen and a control panel on the side. The following controls are available.

7.1 Navigation

Action	How
Rotate	Left-click and drag
Zoom	Mouse wheel
Pan	Right-click drag, or Shift + drag
Inspect a cell	Hover the pointer over it to see species · reaction · time · value

7.2 Appearance controls

Control	What it does
Opacity	Overall transparency of the cells.
Dynamic range (decades)	How many orders of magnitude below the peak remain visible. This is the primary control for revealing small values on the logarithmic scale.
Contrast (γ)	Gamma applied to the magnitude mapping, to emphasize high or low values.
Threshold	Hides cells below a chosen magnitude.
Depth fade	How much nearer-to-camera cells are faded so you can see into the volume.
Cell gap	Shrinks each cell box to leave gaps between cells.
Species / Reaction / Time scale	Three independent sliders that stretch or shrink the cube along one axis (and widen the cells to match), so you can make the box longer in the species, reaction, or time direction. Found just above the buttons.
Colour mode	Signed diverging (blue–grey–orange), magma magnitude, or mono.

Control	What it does
Bounding box / Axis labels / Auto-rotate	Toggles for the cube outline, the axis tick labels, and slow automatic rotation.

7.3 Slicing: Species, Reaction, and Time

Three slice sections — Species slice (X), Reaction slice (Y), and Time slice (Z) — each provide a “Show from” and “Show to” slider. Dragging them hides every cell outside the selected range and trims the axis labels to match, while the cube keeps its full extent (the hidden cells simply leave gaps). The three slices combine, so you can isolate, for example, a few species across a band of reactions over a window of time.

7.4 Adjust view

The Adjust view button (next to Reset view and Stats) commits the current Species, Reaction, and Time ranges as a new drawn extent. The cube is rebuilt so that only the selected block is shown, re-centered and rescaled to fill the view; the bounding box shrinks to the selection; the camera refits to the new size while keeping your current viewing angle; and the X, Y, and Z axes are relabeled to just the selected species, reactions, and time points. After adjusting, the sliders rebind to the new window, so you can slice further within it and press Adjust view again to drill in.

7.5 Reset view

Reset view restores the full dataset as the drawn extent — all three slices return to their full range and their labels are rescaled — and resets the camera to its starting position and zoom.

7.6 Legend and stats

A colour legend shows the value scale for the current colour mode. The Stats button toggles a panel summarizing the dataset (cube dimensions, active cell count, and maximum magnitude).

8. Command-Line Reference

All options below apply equally to the Python script and the built executable.

Option	Default	Description
-f, --folder DIR	(picker)	Folder of consecutive SENSIT files. If omitted, a folder-picker dialog opens.
-o, --out FILE	nsa_cube_viewer.html	Output HTML file name.
--title TEXT	(auto)	Title shown in the viewer.
--max-rows N	160	Cap the rate-constant (reaction) axis; larger axes are block-aggregated to N.
--max-cols N	0	Cap the species/column axis (0 = keep all).
--max-files N	0	Cap the number of files / time points (0 = all; otherwise evenly sampled).

Option	Default	Description
<code>--agg maxabs mean</code>	maxabs	Aggregation when downsampling reactions: keep the largest-magnitude value, or average.
<code>--cull-rel R</code>	0.0	Drop cells with $ v < R \times \max v $ (0 = keep all nonzero).
<code>--cull-abs A</code>	0.0	Drop cells with $ v $ below A (0 = drop only exact zeros).
<code>--three-inline</code>	off	Bake three.js into the HTML for a fully offline, self-contained viewer.
<code>--three-cdn</code>	off	Force the small CDN-linked viewer even when launched via the folder picker.
<code>--three-js PATH</code>	(bundled)	Inline a specific three.js build (implies <code>--three-inline</code>).
<code>--three-url URL</code>	cdnjs r128	URL or local path for the three.js build when not inlining.
<code>--no-open</code>	off	Do not open a browser after building.
<code>--template FILE</code>	(built-in)	Use a custom HTML template.
<code>-h, --help</code>	—	Show the help message and exit.

9. Large Files and Performance

The tool is designed for large inputs. Files are streamed one at a time — each is read once and released — so memory stays bounded even for very large SENSIT files. The reaction axis is block-aggregated down to `--max-rows` (default 160); increase it for more detail or decrease it for speed. Use `--max-files` to evenly sample time points and `--max-cols` to cap species. Exact-zero cells are dropped automatically; `--cull-rel` and `--cull-abs` drop additional small-magnitude cells if a dataset produces more active cells than the browser handles smoothly.

10. Offline vs. Online Output

By default the command line produces a small HTML file that loads three.js from a public CDN (it needs internet to view). Pass `--three-inline` to bake three.js into the file for a fully offline, self-contained viewer (larger file, no internet needed). When the tool is launched via the folder picker — for example by double-clicking the `.exe` or `Run NSA Cube.bat` — it produces the offline version by default and saves it next to your data; pass `--three-cdn` to force the small online version instead.

Note: the viewer also references Google Fonts for two typefaces. If those are unavailable offline, the viewer falls back to system fonts with no effect on the cube.

11. Troubleshooting

Symptom	Likely cause and fix
“Python was not found”	Install Python 3 from python.org and tick “Add Python to PATH”, then retry.

Symptom	Likely cause and fix
A numpy error on run	Run Install requirements.bat once (or: python -m pip install numpy).
Folder-picker doesn't appear	On a system without a GUI, the tool exits asking you to use -f. Pass the folder explicitly.
Blank cube / nothing renders	The browser/GPU may have WebGL disabled, or you opened it inside a restricted preview pane. Open the HTML in Chrome or Edge.
An "ERROR" about SENSIT files	Check the files are numbered consecutively from 001 with no gaps; see Section 6.
Too slow / sluggish	Lower --max-rows, sample with --max-files, or raise --cull-rel to reduce active cells.

12. Notes and Limitations

- All SENSIT files in one folder must share the same species and reaction counts.
- Files must be numbered consecutively from 001.
- The viewer requires WebGL; it is best viewed in Chrome or Edge.
- The Stats panel reports the full dataset dimensions, not the cropped Adjust-view window.
- A standalone .exe must be built on Windows (PyInstaller cannot cross-compile).