Cordouan - An Interactive GUI for Nelly

Uriel T. Tayvah

Jacob A. Spies

Jens Neu

Charles A. Schmuttenmaer

Department of Chemistry

Yale University

Version 1.0

26 June 2021

Abstract

This documents provides an introduction and "quick start" guide to *Cordouan*, a graphical user interface (GUI) for the terahertz spectroscopy data analysis software *Nelly*. The following describes how to import data, define sample geometries, run the data analysis, and export data in the GUI.

Contents

1 Introduction

Cordouan is an interactive graphical user interface (GUI) for the *Nelly* terahertz (THz) spectroscopy data analysis package in MATLAB.

Cordouan was developed in MATLAB R2020b, but is backwards compatible with MATLAB versions dating back to R2018b. *Cordouan* is also available as a standalone executable using the freely available MATLAB runtime.

Cordouan is separated into three panels. In the first, the user enters the input file names, and plots the time-domain data and Fourier transformed spectra for inspection. In the next panel, the user enters the geometry of the sample and starts the data processing routine. Once this has completed, the user can view the results in the final panel and export the processed data.

! → The latest version of *Cordouan* and *Nelly* can be found online in the following GitHub repository: https://github.com/YaleTHz/nelly

2 Quick Start Tutorial

2.1 Data Input and Output

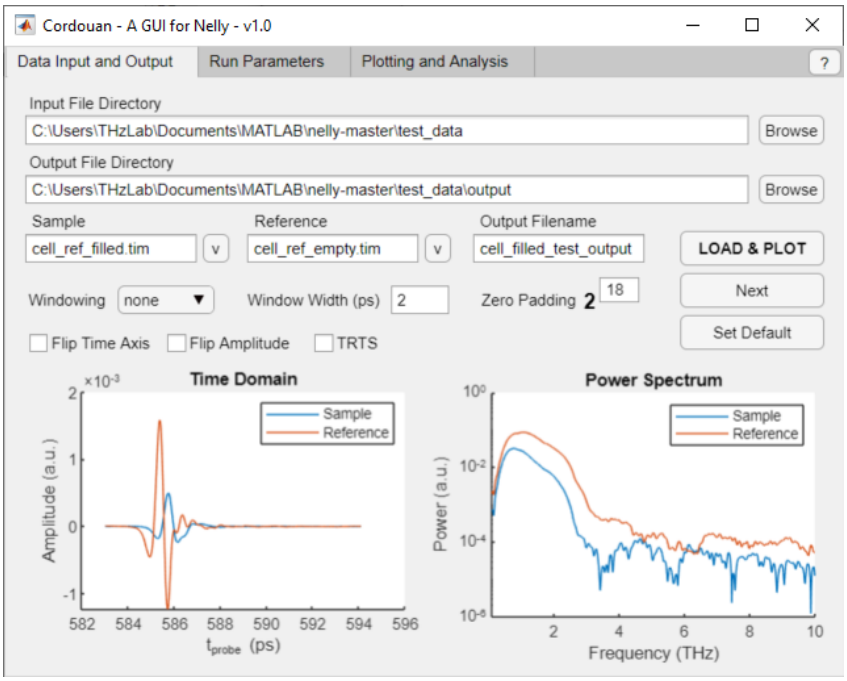

Figure 1: Data Input and Output in *Cordouan*.

2.1.1 Setting input and output directories and filenames.

Using either the Browse buttons or by manually typing the path, set the directories for input and output file. The input file directory must be the directory containing your sample and reference time-domain traces. The output file directory sets where output files will be saved, but does not have any restrictions.

Select "Sample" and "Reference" files using the drop down buttons (v), which browse for files within the Input File Directory denoted. Then, enter a meaningful Output Filename to be the default filename for exported data, though this is not essential as a filename can be specified later during the export process.

2.1.2 FFT and data pre-processing settings.

Time-domain traces loaded into *Nelly* can be processed as is without windowing for etalon suppression (recommended) by choosing "Windowing"

→ "none". Windowing of the time-domain trace can also be performed choosing "Gaussian" or "Square" and a window width of the preferred window type (in picoseconds), which multiplies the specified function center on the peak of the time-domain trace with the input data. This windowing can be used to suppress reflections in the time-domain or to minimize noise from regions not containing important signal information. Zero padding is also be applied by specifying the desired power. The applied FFT algorithm uses multiples of two and the data is automatically extended with zeros to the next power of two. Higher padding will create a smoother signal. If you are unsure what to use, just leave the parameters at their default values.

Nelly requires that time moves in the positive direction, so if it is reversed in your data, you can flip it using the "Flip Time Axis" check box. If your data amplitudes are 180° out of phase, you can flip them using the "Flip Amplitude" check box, though this will not affect the data processing.

If you are using a difference signal for the sample (as in a time-resolved THz spectroscopy, or TRTS, measurement), select the "TRTS" check box to automatically calculate the photoexcited sample and dark reference time-domain traces required to run Nelly.

2.1.3 Plotting imported data to check for errors.

Click **LOAD & PLOT** to import and plot the sample and reference data. This calculates the FFT and applies the selected settings to plot the time-domain traces and Fourier-transformed power spectra. This is a good time to look over the imported data and make sure that there are no importing errors and that the correct data was imported. If these directories and settings will be standard for your data processing, you can click on Set Default to change the default start-up settings (the default settings are stored in `initGUI.json`).

To continue you can either click Next to advance to the "Run Parameters" tab or you can manually select the tab. It is worth noting that you do not have to load and plot your data to continue and run the data analysis (but it never hurts to check your work).

2.2 Run Parameters

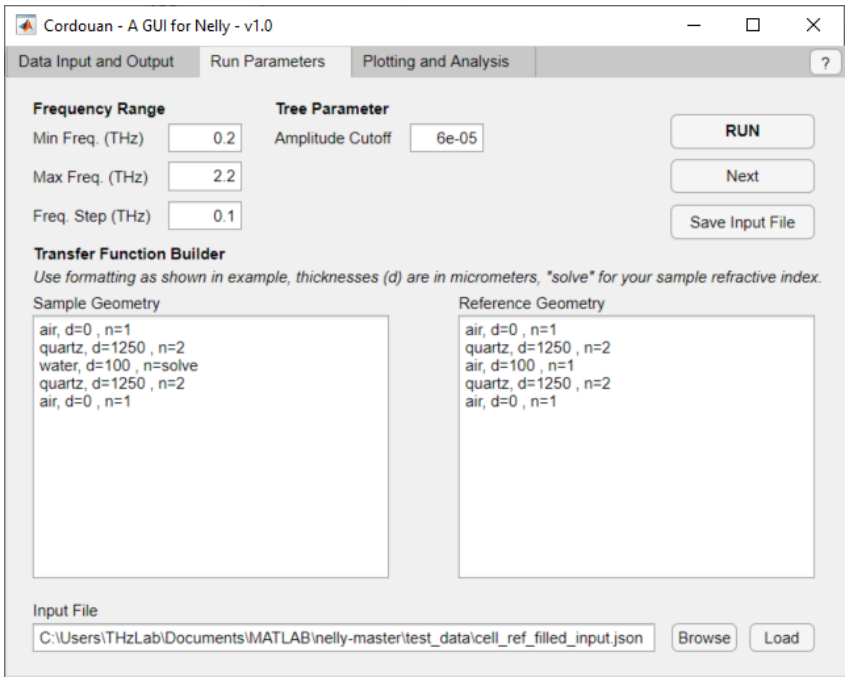

Figure 2: Run Parameters tab in *Cordouan* showing the interface for setting up the frequency range, tree amplitude cutoff, transfer function builder, and running *Nelly*.

2.2.1 Set frequency range and amplitude cutoff for tree method.

Enter the desired frequency range and step width for the data analysis run. *Nelly* ignores all reflections with amplitude less than the amplitude cutoff. The value is given as a fraction relative to the amplitude of the incident pulse. If you are unsure what to put here, you can leave it as the default value or input a value corresponding to the noise floor of the measurement, which will exclude any reflections that are indistinguishable from noise (i.e., that have an amplitude less than the noise floor).

2.2.2 Setting up the sample geometry.

The sample geometry can be specified in one of two ways as detailed in the next two subsections: either manually in the text-entry box or by importing a separate file.

1. Manual entry of the sample geometry. Using the example format provided you can manually input the sample and reference geom-

etry. Layers are ordered from top to bottom corresponding to the propagation direction of the THz pulse (i.e., first material listed is the first material that the THz pulse passes through). The medium surrounding the sample (e.g., air) must be specified as well (typically as a layer with thickness d = 0).

The thickness, denoted as `d=` is expressed in micrometers (µm).

The refractive index, denoted as `n=`, allows you to set the reference refractive index or indicate which layer should be calculated by *Nelly*. To indicate which layer *Nelly* should calculate the refractive index for, use the keyword `solve`. You can also use complex-valued reference data by including the filename of the reference refractive index spectrum, i.e. `n='file.csv'`. If the reference spectrum is in the same path as the input files, only the filename is needed. Otherwise, the full path must be specified.

2. Loading an input file that contains the transfer function parameters You can also load an input file that was written in an external editor. This input file is a JSON-formatted file that is interpreted by MATLAB and contains information on the FFT parameters, frequency range parameters, tree parameters, and sample/reference geometries. The file `sample_input.json` found in the folder `sample_files` provides an example of this format with annotations explaining each field.

   Once you have an input file prepared, you can find it using the Browse button and load the input file by clicking the Load button. It is important to note that the input file is not loaded until you press Load in the GUI. This will automatically update the geometries in the Transfer Function Builder box and relevant FFT, Frequency Range, and Tree parameters.

   You can also save an input file from the parameters you set in the GUI by clicking Save Input File. *Cordouan* will automatically interpret back and forth between the user-friendly format shown in the text boxes and the code that is interpreted by *Nelly*.

2.2.3 Running *Nelly*

When you are satisfied with the parameters set above, you can run `nelly_main.m` by clicking on the **RUN** button. Depending on your frequency spacing, sample geometry complexity, and computer speed, this can take anywhere from a few seconds to several minutes. You can view the progress in the Command Window in MATLAB, which shows in real time the progress of the frequency step-wise calculation. In the standalone application, the progress is displayed as a loading bar.

When `nelly_main.m` has finished, you can either click Next to advance to the Plotting and Analysis tab or you can manually select the tab.

2.3 Plotting and Analysis

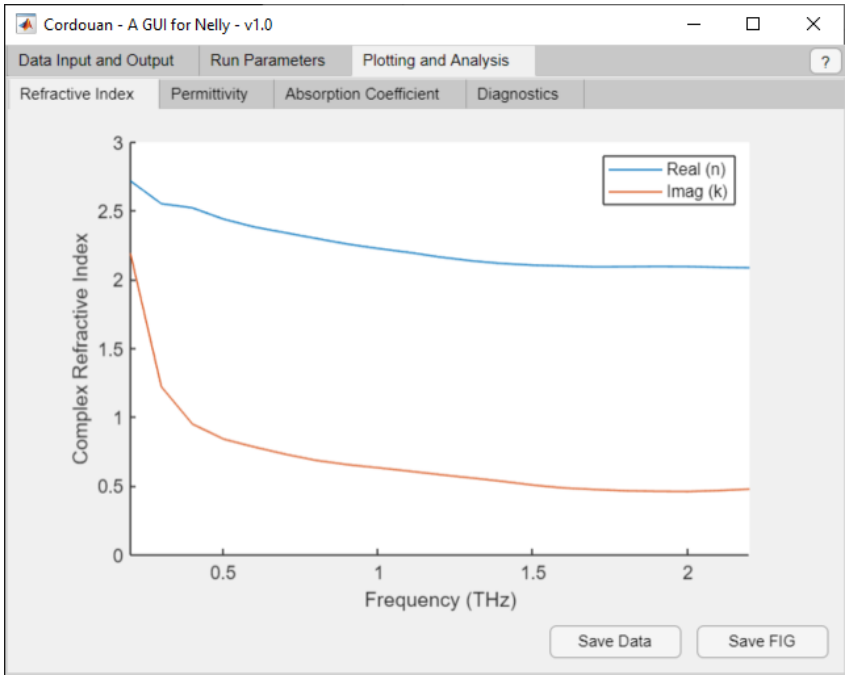

Figure 3: Plotting and Analysis tab in *Cordouan* showing the calculated complex refractive index plotted and options for other data types and export options.

2.3.1 Viewing the refractive index, permittivity, and absorption coefficient.

After *Nelly* successfully finishes, *Cordouan* will plot the complex refractive index, complex permittivity (i.e., dielectric spectrum), and absorption coefficient in the first three tabs of the Plotting and Analysis tab.

There are three ways that you can save the data. If you are using a newer version of MATLAB, you can save an image of the plot as a `.png`, `.jpg`, `.tif`, or `.pdf` using the built-in tools that show up in the upper right corner of the plot when you mouse over them. You can also save the data as a FIG file that is openable in MATLAB by clicking Save FIG in the bottom left. If you prefer to use third-party plotting software, you can export the data as a tab-delimited `.txt` file using the Save Data button.

2.3.2 Viewing diagnostics.

This tab contains some relevant diagnostic data that may be useful to help you troubleshoot or verify the accuracy of your *Nelly* run.

On the left are the magnitude and relative phase of the "experimental" and "predicted" transfer function. These should match as closely as possible, which indicates that *Nelly* was able to extract a reliable refractive index. Spikes or mismatch between the experimental and predicted transfer functions suggest that *Nelly* is having a hard time extracting reliable refractive indices, potentially due to low signal-to-noise ratio, processing outside of the spectrometer bandwidth, incorrect sample/reference geometries, etc.

On the right are the magnitude and relative phase of the Fourier transformed spectra of the sample and reference. This is similar to what is plotted in the Data Input and Output tab, but is linearly scaled, only plots in the range that *Nelly* used, and includes the phase in addition to the magnitude.

Like the preceding plotting tabs, you can save images of the plots using the built-in functionality in newer versions of MATLAB or export tab-delimited `.txt` files using the Save Transfer Functions and Save Spectra buttons to export the complex transfer function and sample/reference spectra, respectively.