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THzTools: data analysis software for terahertz time-domain spectroscopy

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Software

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Summary

Terahertz time-domain spectroscopy (THz-TDS) uses short electromagnetic pulses to probe the electromagnetic response of matter over frequencies from about 0.1 THz to about 10 THz, where 1 THz $= 10^{12}$ Hz (Neu & Schmuttenmaer, 2018). A typical measurement compares two electromagnetic pulses, one of which has interacted with a material and another which has not. The pulses are measured as a function of time, but the electromagnetic properties of matter are most naturally described as a function of frequency, so statistical signal processing techniques must be used to relate the time-domain measurements to the frequency-domain properties of interest. The `THzTools` package provides an interface for implementing maximum-likelihood methods for THz-TDS analysis, described previously (Mohtashemi et al., 2021).

Statement of need

In the conventional approach to THz-TDS analysis (Neu & Schmuttenmaer, 2018), one transforms the time-domain measurements into the frequency domain for further analysis. This approach has well-known problems, however, which can be resolved by using a maximum-likelihood estimation procedure in the time domain (Mohtashemi et al., 2021). To support this mode of analysis, the `THzTools` package provides functionality and documentation that are unavailable in existing THz-TDS analysis software (Lee et al., 2023; Peretti et al., 2019; Tayvah et al., 2021). It provides functions to simulate THz-TDS measurements, apply a frequency response function to a THz-TDS waveform, characterize the noise of a THz-TDS system, and fit a parameterized frequency response function to a pair of input and output waveforms.

We developed some of the functionality of `THzTools` in an earlier MATLAB implementation, which remains undocumented (Dodge et al., 2021). After translating this codebase to Python, we introduced new functionality, optimized the code for speed and efficiency, and revised the user interface to make it easier to use.

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