SMAUG Toolbox Version 1.0

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SMAUG Toolbox: Starting Guide

***Introduction***

Welcome to the Single Molecule Analysis Unified Graphical (SMAUG) Toolbox! This software package contains the code for Segment Clustering, a hypothesis generation tool for single molecule distance/conductance breaking traces recently described in Bamberger et al. 2020 [link]. However, as the name suggests, the SMAUG toolbox contains additional graphical analysis tools for breaking trace data, all incorporated into a single unified framework. These tools range from the simple and common (e.g. 1D and 2D histograms histograms) to more advanced statistical techniques developed in the literature (e.g. conductance correlation histograms). Capabilities for other clustering approaches not described in Bamberger et al. 2020 are also included.

***Software Requirements***

The SMAUG toolbox has been fully tested using MATLAB R2019b, but will likely work with older version of MATLAB as well. Please contact us if you run into any forward- or backward-compatibility issues ([monti@email.arizona.edu](mailto:monti@email.arizona.edu)). In addition to a general download of MATLAB, the following common MATLAB packages should be downloaded and installed: Curve Fitting Toolbox, Statistics and Machine Learning Toolbox, and the Parallel Computing Toolbox (if parallelization is going to be used to speed up clustering).

***Navigating the Documentation***

Here is a high-level guide for how to explore and use this software package:

1. Before doing anything else, run the “RUN\_ME” function in the top-level SMAUG directory. This function adds all SMAUG sub-folders to your MATLAB path so that any function can be run from anywhere inside the package.
2. All SMAUG analysis functions require raw data to be stored in the same common “Trace Structure” format. Use the live script “How\_To\_Format\_Input\_Data.mlx” to learn how to put your data into this format. Once you’ve done this, you’ll be able to easily employ all SMAUG tools!
3. For a quick tutorial on how to apply Segment Clustering to a dataset, use the live script “Quick\_Introduction\_To\_Clustering.mlx”, which shows an example of clustering an example dataset included in this package.
4. For a quick tutorial on how to use the other common analysis tools in the SMAUG toolbox, use the live script “Quick\_Introduction\_To\_Other\_Analysis\_Tools.mlx”, which shows examples using the example dataset included in this package.
5. For a more complete list of the different tools available in this package and their capabilities, see “Detailed\_Function\_Guide.pdf”.
6. For detailed information on any particular function in this package, see the comments at the very start of the file, which will include a brief description of what the function does as well as each of its inputs and outputs.

***Fair Use and Making Additions***

The SMAUG toolbox is publicly available free of charge under a Creative Commons Attribution-NonCommercial 4.0 International License (to view a copy of this license, visit <http://creativecommons.org/licenses/by-nc/4.0/>). This essentially means that anyone can make use of any part of this software package for any non-commercial use, as long as that use is attributed to the SMAUG toolbox. Users are actively encouraged not only to use existing SMAUG tools for their own research, but also to add new tools and capabilities to the package. Any additions that seem generally useful to the single molecule transport community will, with the consent of the adding users, be incorporated with attribution into future releases of the SMAUG toolbox.

***Getting Help***

If you run into apparent software bugs or encounter difficulties while trying to use this package, please contact us at [monti@email.arizona.edu](mailto:monti@email.arizona.edu). We want people to use this code, so we are very motivated to fix any problems or help with any confusion!