Simulating 2D Conductance-Displacement Histograms

Simulating 2D conductance-displacement histograms uses the molstat-simulator, image charge gap renormalization, and random number distributions to calculate the statistics of many single molecule break junction experiments. The procedure for simulating 2D conductance-displacement histograms first involves simulating a number of break junction traces using a python script and the molstat-simulator. The inputs into the python script specify

1. The number of break junction traces to be simulated, n_t
2. The number of distance points per trace, n_d
3. The trace length (distance at which molecular junction is broken), t_l

Two molstat-simulator input files are required. The input files both run a single trial and use a static conductance observable. The first input file specifies the molecular regime. In this regime, the transport models must have ε, the site energy, as an input parameter. It is assumed that ε represents the transport level of the relaxed molecule in the junction, not the transport level with respect to vacuum. Distances less than the trace length fall into this regime. The second input file specifies the tunneling regime and must use the rectangular barrier transport model. Distances greater than the trace length fall into this regime.

The python script then simulates a single trace as follows. The script

1. Calculates the distance dependent image charge renormalization of the site energy, ε, relative to the relaxed configuration.
2. Edits the appropriate input file for each distance point
    a. If the distance point is in the molecular regime, ε is updated
    b. If the distance point is the tunneling regime, the distance is updated
3. Runs the molstat-simulator with the appropriate input file for each distance point to generate a conductance distance pair.
4. Save all conductance distance pairs to a single file to form a simulated trace
5. Repeat steps 1-4 to simulate the desired number of traces

The output of the python script is n_t molecular traces and n_t tunneling traces. These traces can then be imported into MATLAB and a 2D conductance-displacement histogram can be generated. Sample python scripts for simulation and MATLAB scripts for histogram generation can be found under Molstat/src/tests and sample molecular and tunneling input files can be found under Molstat/src.