TRAVIS - A free Analyzer and Visualizer for MC and MD Trajectories

http://www.uni-leipzig.de/~travis

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GNU GPL

Introducing TRAVIS

We present TRAVIS ("**TR**ajectory **A**nalyzer and **VIS**ualizer"), a free program package for analyzing and visualizing Monte Carlo and molecular dynamics trajectories. The aim of TRAVIS is to collect as many analyses as possible in one program, creating a powerful tool and making it unnecessary to use many different programs for evaluating simulations. This should greatly rationalize and simplify the workflow of analyzing trajectories. TRAVIS is written in C++, open-source freeware and licensed under the terms of the GNU General Public License. It is easy to install (platform independent, no external libraries) and easy to use.
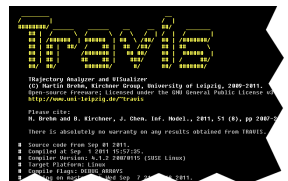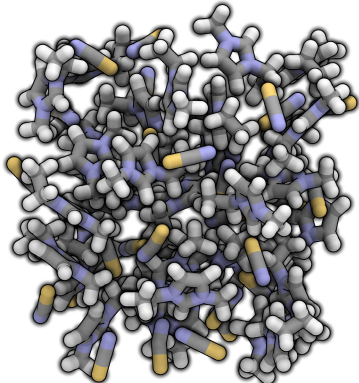

Fig. 1: Snapshot of our example AIMD Trajectory

Fig. 2: Console Interface of TRAVIS

On this poster, we present some of the algorithms that are implemented in TRAVIS - many of them widely known for a long time, but some of them also to appear in literature for the first time. All shown analyses only require a standard MD trajectory as input data.
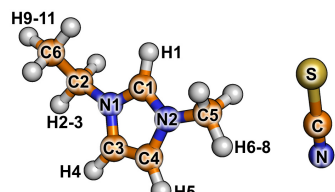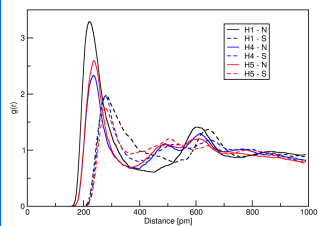

Fig. 4: Radial Distribution Function between [EMIM] and [SCN]

The direct result of any MC or MD simulation is a trajectory, containing the positions and velocities of the simulated particles at discrete time steps. If N particles have been simulated, this trajectory can be regarded as a path through the 6N-dimensional phase space of the system. Because of its high-dimensional nature, this path is not suitable for direct evaluation or interpretation. Algorithms for the reduction of dimensionality have to be applied, converting the input data into two- or three-dimensional data sets, which can be interpreted and visualized much easier.
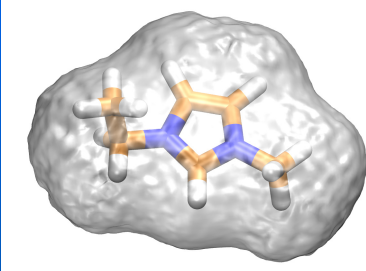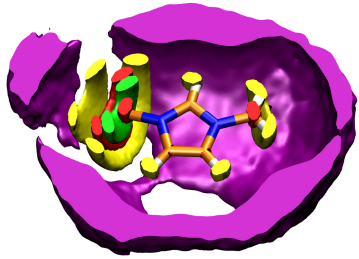

Fig. 3: Example System: Ethyl-Methyl-Imidazolium Thiocyanate ([EMIM] [SCN])

Fig. 5: Spatial Distribution of SCN (purple) around [EMIM] with a clip plane

Fig. 6: Exclusion Volume of the [EMIM] cation

Advanced Algorithms

TRAVIS reads any trajectory that results from a MC or MD simulation. The molecules in the simulation box are recognized automatically. The atoms are sorted by a topological algorithm and equivalent atoms are signified. Trajectories can be wrapped and unwrapped automatically. All kinds of histograms are created using our equitable binning approach. The calculation of autocorrelation functions is greatly accelerated by use of FFT. Smoothing of the distribution functions yields better appearance (see Fig. 7).
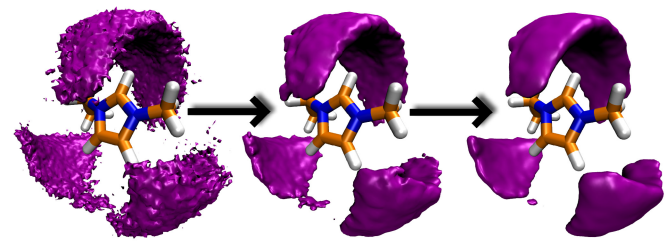

Fig. 7: Smoothing of Spatial Distribution yields an immense gain of visual appearance

Variety of Analyses

TRAVIS incorporates a variety of different analyses, including very common ones as well as new evaluations that have not appeared in literature before.
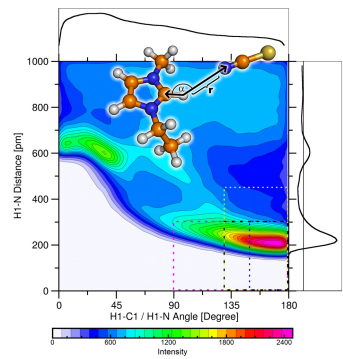

Fig. 8: Combined Radial/Angular Distribution Function indicating the Hydrogen Bond

With TRAVIS, all kinds of two-dimensional analyses can be combined to result in three-dimensional CDFs (Combined Distribution Functions). To give two examples, see Fig. 8, in which a Radial and an Angular Distribution are combined, and Fig. 9., where two Radial Distributions are joined. The latter plot involves three different molecules at a time, like shown in the sketch. CDFs are a powerful tool and offer thousands of different combinations.
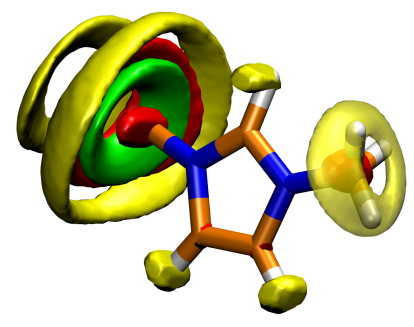

Fig. 11: Lifetime of Anion-Cation pairs in dependence of Neighborhood

Fig. 12: Dimer Existence Autocorrelation Functions showing the Lifetime of the Hydrogen Bond

Fig. 13: Temporal Development Overlay Plot

Fig. 7: Spatial Distribution of the atoms in the [EMIM] cation
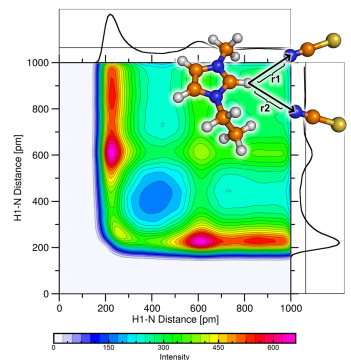
Fig. 9: Combined Radial/Radial Distribution Function

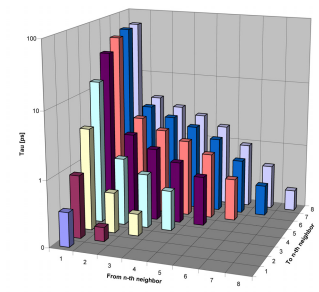## Investigating Neighborhood

TRAVIS offers many analyses related to the neighborhood of particles. As an example, the decomposition of a Radial Distribution Function into its contributions from 1st, 2nd, ..., neighbor is shown in Fig. 10. Broad areas indicate that this neighbor position is distributed over a wide distance range.
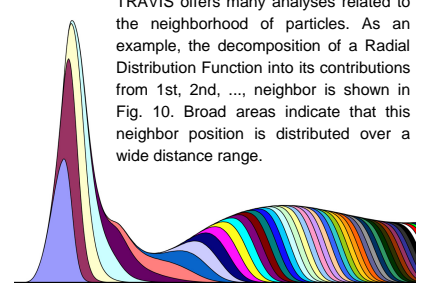

Fig. 10: Decomposition of Radial Distribution Function into Contributions from next Neighbors

Analyzing Dynamics

Many of the most important properties that can be gained from MD simulations are of a dynamic nature. TRAVIS offers ways to calculate those properties, ranging from Dimer Autocorrelation Functions (Fig. 12) to Power Spectra (Fig. 14).
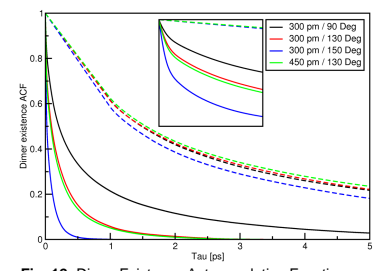
The curves from Fig. 12 can be automatically created for a matrix of different criteria, fitted by poly-exponential functions and integrated, directly yielding lifetimes like presented in Fig. 11.
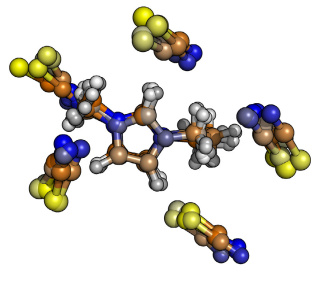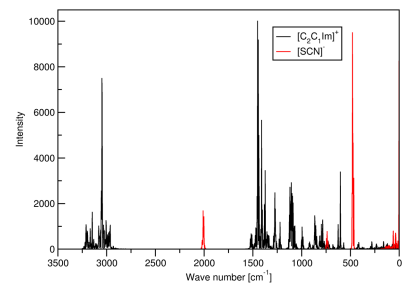

Fig. 14: Power Spectra of [EMIM] and [SCN]