Software for Building Markov State Models

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11.1 MSMBuilder

MSMBuilder is an open source software package for constructing Markov state models. The software is primarily written in python to facilitate rapid integration of new methods and readable implementations of existing methods. Time-sensitive routines are implemented in C with python wrappers to enhance the performance of the software. At the time of this writing, stable public releases of MSMBuilder are available via the SimTk software repository (https://simtk.org/home/msmbuilder; http://msmbuilder.org). The current development build is also available via GitHub (https://github.com/SimTk/msmbuilder).

11.2 EMMA

EMMA is a software library and set of command-line tools for constructing, validating and analyzing Markov state models. The library is written in Java, thus being fast and platform-independent without requiring local compilation or installation. At the time of this writing, stable public releases of EMMA are available via the SimTk software repository (https://simtk.org/home/emma). The Java source code is available on request. As soon as publicly available, it will be linked on the simtk.org website.

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