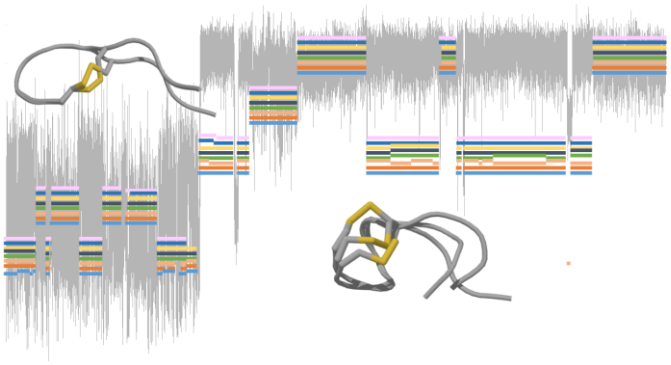
DASH: Analysis of microsecond-scale molecular-dynamics trajectories

Elke Haensele[1,2], David Whitley[1], Lee Banting[1,2], Timothy Clark[1,3]

[1]Centre for Molecular Design, University of Portsmouth, UK
[2]School of Pharmacy and Biomedical Sciences, University of Portsmouth, UK
[3]Computer-Chemie-Centrum and Interdisciplinary Center for Molecular Materials, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany



Natural time-scales for conformational changes may last milliseconds to seconds, *e.g.* protein-folding. Although current molecular-dynamics simulations (MD) typically cover time scales of 10 to 100 nanoseconds, the computational power has become readily available to run simulations on a microsecond scale.

However, such long simulations create the technical problem of how to analyse the increased volume of output within a reasonable time without being forced to reduce the number of considered data points drastically. This is where common clustering methods reach their limits.

DASH (Dynamic Analysis by Salt and Hudson) [1] provides an alternative solution by using a time series of torsion angles instead of similarity matrices of Cartesian coordinates (clustering) to find representative conformations (states). Time-series analysis is very fast, making ***DASH*** capable of analysing considerable large datasets.

The principles of ***DASH*** will be explained and ***AmberDASH***, an interface for the user-friendly application of ***DASH*** to ***AMBER*** trajectories, will be introduced.

The performance of ***DASH*** and the consistency of its results will be demonstrated using a 5 microsecond MD trajectory of 8Arg-Vasopressin as an example.

DASH 1.0	Program for extracting states from molecular-dynamics simulations; distributed under the terms of the GNU General Public License; download via www.port.ac.uk/research/cmd/software
AmberDASH	*DASH* interface for *AMBER* trajectories (unpublished); currently provided via email (please contact Dr David Whitley david.whitley@port.ac.uk)

[1] D.W. Salt, B.D. Hudson, L. Banting, M.J. Ellis, M.G. Ford, *J Med Chem*, **2005**, *48*, 3214-3220