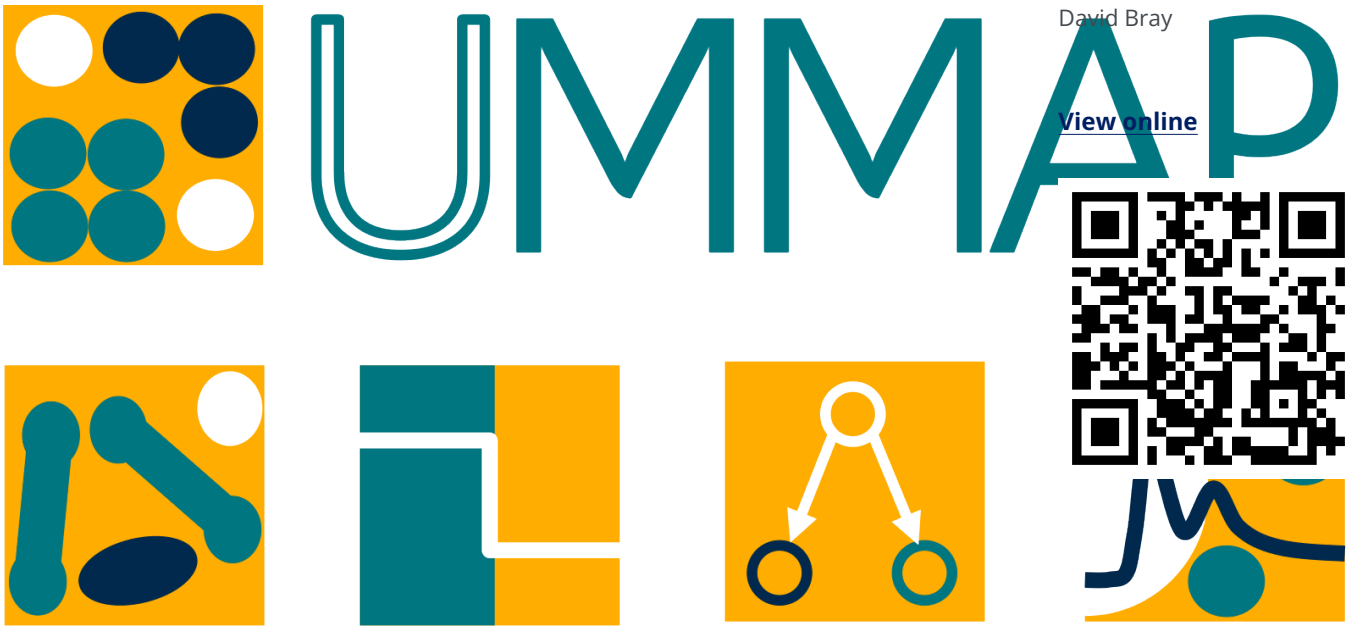
UMMAP

Analysis package for MD, CG and DPD simulation trajectories.



Category

Software/UMMAP

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UMMAP stands for the Universal Molecular Analysis Package. On the surface it is yet another software program for the analysis trajectory files produced by particle dynamics simulations, this time specialising in soft matter liquids, however deeper it is much more than that as you shall see.

It is universal because it is designed to read a number of common trajectory and topology formats produced by the leading molecular dynamic (e.g LAMMPS, NAMD, GROMACS) and mesoscale Dissipative Particle dynamics (DL_MESO) simulation engines.

UMMAP is a fully integrated program that can simultaneously run a series trajectory analysis tools for molecular/particulate simulations accessed through a common terminal interface. Doing so allows the UMMAP tools to takes advantage of common statistical methods and allows the user to specify complex group and frame selections for the analysis.

What UMMAP can do:

- Analyse large simulations from multiple trajectory files
- Select parts of the trajectory file to read
- Make complex group selections
- Provide Information on the trajectory and topology file
- Produce graphics and snapshots images
- Results in a portable organised output directory which can be added to and is protected against mixing of simulations and redefinition of groups
- Produces log records and searchable manifest giving key information on what has been done
- Provides an in-program manual

Current version is UMMAP 2.24.X

Operating system

UMMAP will run on Linux or OS Mac based system.
It is a terminal based code.

References

1. David J. Bray, Annalaura Del Regno, Richard L. Anderson(16/12/2019) , https://www.tandfonline.com/doi/abs/10.1080/08927022.2019.1699656, https://www.tandfonline.com/journals/gmos20, 46, 308-322