

GROMACS - Feature #2426

Trajectory analysis tool for functional mode analysis by partial least squares fitting (PLS-FMA)

02/27/2018 05:03 PM - Carsten Kutzner

Status:	In Progress
Priority:	Normal
Assignee:	
Category:	analysis tools
Target version:	future
Difficulty:	uncategorized
Description	
What is functional mode analysis?	
Functional mode analysis (FMA) is a technique to identify collective atomic motions related to a specific protein function. Given a large set to structures of one protein, for example from a molecular dynamics trajectory, the method detects a collective motion (or collective mode), that is maximally correlated to an arbitrary quantity of interest. In other words, the method aims to explain alterations in a quantity in terms of internal collective motions of the protein.	
What kind of questions can be addressed with FMA?	
Let us assume you are interested in a some 'functional' quantity that is important for the function of your protein, such as, e.g.,	
<ul style="list-style-type: none">• the volume of a binding site,• the radius of gyration of the protein,• the distance between two important functional residues,• the number of H-bonds between two groups,• the electrostatic potential at some site in the protein	
You may wonder how the protein accomplishes alterations of that quantity. FMA will detect the collective motion that is maximally correlated to your quantity and, hence, provide the link between protein function and collective motion. For instance, FMA was used to demonstrate that substrate binding and release of T4 lysozyme are triggered by a hinge bending mode, whereas a twisting mode is required for the catalytic activity.	
References:	
<ol style="list-style-type: none">1. Hub, Jochen S., and Bert L. de Groot. "Detection of Functional Modes in Protein Dynamics." PLoS Comput Biol 5, no. 8 (2009): e1000480. doi:10.1371/journal.pcbi.1000480.2. Krivobokova, Tatyana, Rodolfo Briones, Jochen S. Hub, Axel Munk, and Bert L. de Groot. "Partial Least-Squares Functional Mode Analysis: Application to the Membrane Proteins AQP1, Aqy1, and CLC-ec1." Biophys. J. 103 (4) (2012): 786–96. doi:10.1016/j.bpj.2012.07.022.	

History

#1 - 02/28/2018 03:30 PM - Gerrit Code Review Bot

Gerrit received a related DRAFT patchset '59' for Issue [#2426](#).

Uploader: berenger bramas (berenger.eu@gmail.com)

Change-Id: gromacs~master~10207bf6932078d948f185fd875ab37c3642af3a5

Gerrit URL: <https://gerrit.gromacs.org/4015>

#2 - 03/21/2018 12:17 PM - Gerrit Code Review Bot

Gerrit received a related DRAFT patchset '42' for Issue [#2426](#).

Uploader: berenger bramas (berenger.eu@gmail.com)

Change-Id: gromacs~master~107eba875fa1456bb90063dddae730cd019cd654a

Gerrit URL: <https://gerrit.gromacs.org/3277>

#3 - 10/03/2018 11:31 PM - Mark Abraham

- Target version changed from 2019 to future