GROMACS - Task #3306

Document gmx dos tool more clearly

01/20/2020 02:31 PM - Christian Blau

Status:	New
Priority:	Normal
Assignee:	Christian Blau
Category:	analysis tools
Target version:	future
Difficulty:	simple

Description

#request

Users on the mailing list stumble regularly over the dos tool and do not know what the output means, specifically if the heat capacity is the c_v or c_p.

In the code the output quantity is named cP, but from reading through the source code it is likely c_v.

More details about the implementation are found in https://pubs.acs.org/doi/10.1021/ct200731v

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- I'm trying to calculate the specific heat of my system (specifically, c_p) using gmx dos, and I
was curious about how exactly gmx dos calculates c_p. I can't seem to find any documentation anywh
ere about what formulas are used; all I can ascertain from the gmx dos source code is that it invo
lves integrating the diffusion and solid components of the density of states (each multiplied by s
ome weighting factor). Any help would be greatly appreciated.

- I have found density of states (Dos) of a protein ligand system from gmx dos command of gromacs.
 I would like to know if it employs the same principle component analysis as used in g_covar. If n
ot what are the differences.

- Also the Dos obtained from gmx dos has solid and diffusive components, please can anyone shed li
ght on what are they exactly?
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