

GROMACS - Bug #2978

Some suggestions about the gmx current tool

06/13/2019 12:41 PM - Mahsa Ebadi

Status: New	
Priority: Normal	
Assignee:	
Category:	
Target version:	
Affected version - extra info:	Difficulty: uncategorized
Affected version: 2018.3	

Description

Hi gmx-developers,

I use gmx current tool to calculate static conductivity by version 2018:

```
gmx current -f md.xtc -o -dsp -md -mj -temp 423 -nojump -n index.ndx -s topol.tpr
```

Indeed the tool is useful, but I think some parts in the output are confusing and need to be improved.

I think the generated dsp.xvg file which reports the MSD of translational dipole moments vs time has the wrong unit in the plot. The unit should be (S/m) ps according to equation 9 in this paper:

<https://aip.scitation.org/doi/10.1063/1.2868752>

and the pre-factor fit reported in the output of dsp.xvg in my case is:

$$1 / 6 * V * K_B * T = 7.20677e-12$$

but $[(1.6 * 10^{-19})^2 * (10^{-18})] / [6 * V * K_B * T]$ is equal to 7.20677e-12 considering the conversion of MSD of dipole moments from (enm)² to (em)²

so it would be really helpful to add a hint in the documentation or the code about that.

Finally, as far as I understood the reported sigma value in the output of dsp.xvg should be multiplied by 10⁻¹² manually.

It took sometime for me to understand what is going on in the output :-)

Please correct me if I'm wrong or missed something in these comments.

Best regards,

Mahsa

Files

Screen Shot 2019-06-12 at 14.35.45.png

18 KB

06/13/2019

Mahsa Ebadi