

## GROMACS - Task #1515

### improve g\_bar output

06/02/2014 08:17 PM - Szilárd Páll

<b>Status:</b>	New
<b>Priority:</b>	Normal
<b>Assignee:</b>	Szilárd Páll
<b>Category:</b>	analysis tools
<b>Target version:</b>	
<b>Difficulty:</b>	uncategorized

#### Description

The original [Bennett paper](#) never mentions standard deviation, but instead calls the overlap measure the "variance of the two-ensemble estimate" expressed in form of an overlap integral. Therefore, the BAR output "stdev" column should probably be corrected to sigma.

Alternatively, we could entirely switch to calculating variance, i.e.  $\sigma^2$  rather than sigma.

Not naming-related, but it would also be useful if g\_bar respected the -prec argument for printing the lambda values not only the rest of the floating point values in the results table.

#### History

##### #1 - 06/02/2014 08:19 PM - Szilárd Páll

Comments on the former would be welcome, the latter is an easy fix.

##### #2 - 07/11/2016 08:10 PM - Mark Abraham

- Target version deleted (5.x)