GROMACS - Feature #1162

Implement gb_saltconc

02/26/2013 04:09 PM - Justin Lemkul

Status:	New	
Priority:	Normal	
Assignee:	Berk Hess	
Category:	mdrun	
Target version:	future	
Difficulty:	uncategorized	

Description

This would be a useful feature. There have been hints that someone will work on it in time, but it seems to have been lost in the crowd of other to-do's.

History

#1 - 02/26/2013 05:33 PM - Matthew Zwier

- File gromacs-4.5.3-gbsalt.patch added

Joe Kaus (joekaus@gmail.com, all credit to him) implemented this for GROMACS 4.5.3 while in our group at U. Pittsburgh, and sent this patch to Per Larsson. It at least works in single-precision, and seems to permit stability with 1 - 1.5 nm cutoffs and scaling far beyond the 1-2 core limit Justin has mentioned several times in the mailing list. It also compares favorably in both absolute energies and energy conservation compared to AMBER 11 (though I'm not sure where that data wound up, so I can't offer any hard data to back up that claim.) We don't have the time to update the patch to the latest version, or even to test it properly, but the patch is attached if it is at all useful.

The salt term is activated by specifying userint1=1, with concentration set with userreal1.

Files

gromacs-4.5.3-gbsalt.patch	20.4 KB	02/26/2013	Matthew Zwier