GROMACS - Feature #1658

Feature # 1332 (In Progress): Supporting multiple end states instead of just A and B

Electrostatics treatment for multiple lambda sites

12/11/2014 07:43 PM - Michael Shirts

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

Description

Bookkeeping and timing are likely to be challenging when dealing with the electrostatics of many alternate sites. This feature post is for discussion of how to best implement this.

History

#1 - 07/11/2016 08:05 PM - Mark Abraham

- Target version deleted (5.x)

- Private changed from Yes to No