GROMACS - Feature #1654

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

How to carry out movement between chemical end states in a multiple end state framework?

12/05/2014 05:02 AM - Michael Shirts

Status:	New
Priority:	Normal
Assignee:	Michael Shirts
Category:	mdrun
Target version:	
Difficulty:	uncategorized

Description

Note: this subtopic is being kept private since there are some open research questions.

One of the biggest issues is how to visit back and forth between the multiple states of interest. There are a number of methods for moving between two end states, and all are fairly similar in performance: but this becomes much more complicated for multiple states. There is a large multidimensional space of methods, and we should coordinate closely to ensure that we arrive at a solution is both sufficiently efficient, maximally robust and flexible, and maximally simple and maintainable. It will likely involve a combination of the different ideas that different people are exploring.

History

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

- Target version deleted (5.x)

- Private changed from Yes to No