GROMACS - Feature #2710

Separate dvdl for each molecule (of couple-moltype) when running FEP

10/25/2018 01:56 PM - Magnus Lundborg

Status:	New	
Priority:	Normal	
Assignee:		
Category:	mdrun	
Target version:	2020	
Difficulty:	uncategorized	

Description

I think it would be good to be able to decouple multiple molecules and get their dvdl reported separately (in the energy file on the separate output file). Would there be any major problems with this?

History

#1 - 10/25/2018 04:01 PM - Berk Hess

This adds another dimension to the already complex lambda infrastructure. The current infrastructure should be cleaned up first.
It would also need charge interpolation instead of Hamiltonian interpolation to make it tractable with PME, but we would want that option anyhow.

#2 - 10/25/2018 08:50 PM - Mark Abraham

What's the advantage over simulations with only single-group decoupling? This kind of complexity approaches having a built-in scripting language, which is the opposite of the way we should go. I'm kind of hoping that gmxapi will mean that some of the existing complexity can go live as python.

And I agree with Berk that we need to do some cleanup - at least basic classes with std::vector and being able to write output to TNG.

#3 - 10/25/2018 10:47 PM - Magnus Lundborg

I guess you're right that selection groups might be taking it a bit too far. I guess it would be good enough to get reports for each copy of a molecule instead of the total dvdl. So, just keeping it more like it is, but making it possible to split the output. Does that sound more reasonable? (If so, I could update the subject above.) The advantage would be that you could speed up FEP simulations by decoupling more than one instance of a molecule, e.g. in multiple independent binding sites or if you grow in more than one copy of a molecule into a system (far enough apart).

#4 - 10/26/2018 10:24 AM - Magnus Lundborg

- Subject changed from Separate dvdl for selection groups when running FEP to Separate dvdl for each molecule (of couple-moltype) when running FEP

I've now updated the subject, changing from separate output per energy group to separate output for each molecule (of couple-moltype).