

GROMACS - Task #909

Task # 665 (New): Port existing trajectory analysis tools to use the new framework

Reimplement displacement calculation module

03/27/2012 08:27 PM - Teemu Murtola

Status:	New
Priority:	Normal
Assignee:	
Category:	analysis tools
Target version:	future
Difficulty:	uncategorized
Description	
<p>The code currently in <code>src/gromacs/analysisdata/modules/displacement.*</code> is an incomplete port of <code>src/gromacs/gmxlib/trajana/displacement.c</code> (and the related header in <code>legacyheaders</code>) to the new analysis framework. This is more of a proof-of-concept implementation than a real one, and there is currently nothing that uses the new module.</p> <p>This task should include the following:</p> <ul style="list-style-type: none">• Improve/rewrite the <code>AnalysisDataDisplacementModule</code> class such that it provides more flexibility.• Change the handling of the MSD histogram module such that it is created and managed internally within the displacement module, and only gives out an <code>AbstractAverageHistogram</code> handle (this gives more freedom in writing the module as well).• Use storage facilities provided by the data object to which the module is attached instead of storing old values internally. If/when support for trestart-type of functionality from <code>g_msd</code> is needed, the storage facilities in <code>AbstractAnalysisData/AnalysisDataStorage</code> also need to be extended.• Add unit tests for the module.• Add a real analysis module under <code>src/gromacs/trajectoryanalysis/modules</code> that uses the displacement module to find out what are the requirements for the module. For example, port <code>g_msd</code> to the new framework.	

History

#1 - 07/14/2014 11:30 AM - Teemu Murtola

- *Category set to analysis tools*

- *Target version set to future*