

GROMACS - Feature #3038

Improvements to MD plugin development environment

07/17/2019 02:14 PM - Eric Irrgang

Status:	New	
Priority:	Normal	
Assignee:	Eric Irrgang	
Category:	gmxapi	
Target version:	2021-infrastructure-stable	
Difficulty:	uncategorized	
Description		
<p>This issue is a parent for several improvements to the MD plugin development environment laid out in <code>sample_restraint</code></p> <p>https://github.com/kassonlab/sample_restraint is a project that can be forked as the starting point for developing GROMACS 2019 compatible MD plugins for use with gmxapi 0.0.7. For GROMACS 2020 and beyond, the primary source code will be managed under the GROMACS repository. Several improvements are necessary for ongoing GROMACS compatibility and to improve the experience of plugin developers.</p> <ul style="list-style-type: none">• Create a new skeleton repository that researchers can clone to get the <code>python_packaging/sample_restraint</code> subtree, plus additional project helpers.• Improve documentation and set-up of the new project, such as with CookieCutter wrapping.• Add more call signatures and use cases for restraint calculation.• Update various internals to use modern GROMACS facilities and features.• Extract boiler plate to template headers.• Modernize expression of inputs, outputs, and factory functions, as enabled in core GROMACS.• Prepare template headers to be moved to the GROMACS installed headers (to be moved in GROMACS 2021)• Improve documentation and documentation integration with GROMACS manuals.		
Related issues:		
Related to GROMACS - Feature #2896: Python packaging		Feedback wanted
Related to GROMACS - Task #3027: Move <code>sample_restraint</code> development from GitHub...		Closed
Related to GROMACS - Task #3040: Refactor Restraint module		New

Associated revisions

Revision 75dd2560 - 08/27/2019 07:39 PM - Eric Irrgang

More templating in `sample_restraint`.

Start moving towards a template header library to replace the boiler plate in the `sample_restraint` code. Separate out the most important bits of a Potential implementation. Use templates to wrap the Restraint aspect and input/output resources.

Refs #3038

Change-Id: `Ice946eb0e6722eafbe75aeae6a45fe872ea602eb`

History

#1 - 07/17/2019 02:15 PM - Eric Irrgang

- Description updated

#2 - 07/17/2019 02:15 PM - Eric Irrgang

- Related to Feature #2896: Python packaging added

#3 - 07/17/2019 02:15 PM - Eric Irrgang

- Related to Task #3027: Move `sample_restraint` development from GitHub to Gerrit added

#4 - 07/17/2019 02:15 PM - Eric Irrgang

- Description updated

#5 - 07/18/2019 03:59 PM - Eric Irrgang

- *Related to Task #3040: Refactor Restraint module added*

#6 - 12/10/2019 01:58 PM - Eric Irrgang

- *Target version changed from 2020 to 2021-infrastructure-stable*