

GROMACS - Feature #3177

Task # 2045 (New): API design and language bindings

Feature # 2896 (Feedback wanted): Python packaging

Spack package management support

10/24/2019 02:36 PM - Eric Irrgang

Status:	New	
Priority:	Normal	
Assignee:		
Category:	build system	
Target version:		
Difficulty:	uncategorized	
Description		
<p>The Spack package management system is increasingly used by HPC administrators, and specifically addresses some of the issues that users encounter when building software that links against GROMACS. It provides good awareness of multiple compilers, system-provided MPI libraries, and cross-compiling in Cray environments. It can direct CMake driven software builds in concert with the Python build/packaging system, so it can easily manage mutually compatible MPI-enabled GROMACS, gmxapi, mpi4py, and other libraries that will be dynamically loaded in the same Python interpreter.</p> <p>A Spack package.py has been maintained outside of the GROMACS project for a while, but users and HPC administrators could be better served if one were maintained and tested within the GROMACS project, either as an alternate or upstream source. Moreover, we may find that users of gmxapi or other GROMACS extension code would be better or more easily served by the addition of a Spack-based installation option.</p>		
Related issues:		
Related to GROMACS - Feature #2961: How should Python package find GROMACS re...		New
Related to GROMACS - Feature #3395: Consider scripted composition of Dockerfiles		Feedback wanted

History

#1 - 10/24/2019 02:36 PM - Eric Irrgang

- Related to Feature #2961: How should Python package find GROMACS resources under various circumstances? added

#2 - 11/06/2019 06:25 PM - Erik Lindahl

As long as we have a volunteer maintainer it sounds great. But we do need someone who will check it regularly to avoid this too ending up on Paul's list ;-)

#3 - 11/06/2019 06:37 PM - Christoph Junghans

I bumped the version of said package in past a couple of times and added features as requested, seems pretty low overhead.

#4 - 02/27/2020 04:39 PM - Eric Irrgang

- Related to Feature #3395: Consider scripted composition of Dockerfiles added