

GROMACS - Feature #2985

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

Task # 2698 (In Progress): gmxapi documentation integration

Python package documentation

06/19/2019 12:24 PM - Eric Irrgang

Status:	Closed
Priority:	Normal
Assignee:	
Category:	documentation
Target version:	2020.1
Difficulty:	uncategorized
Description	
<p>Some infrastructure and organizational details need to be worked out to build and publish documentation related to the gmxapi Python package.</p> <p>For gmxapi <= 0.0.7, the Python package is in a separate repository on GitHub that is automatically downloaded and built by readthedocs. This is a little more complicated to do with the Python package in a subdirectory of the primary GROMACS repository, but we also probably want to integrate the Python package documentation with the rest of the GROMACS documentation.</p> <p>The Python gmxapi package needs to be built and importable in order for Sphinx to automatically extract docstrings from the C++ bindings module.</p> <p>This Redmine Issue is currently a stub to catch details of infrastructure, layout, contents, integration, publishing, and automation.</p>	

Associated revisions

Revision f29a1758 - 10/03/2019 11:57 AM - Eric Irrgang

Build gmxapi documentation in main GROMACS documentation.

- Update gmxapi Python package installation instructions and remove quickstart.rst
- Minor updates to main installation guide document.

Refs #2698

Refs #2985

Change-Id: I6f1d6e6fe59e618144e4f14c0d2fe9f9b8c2c901

Revision 9124029b - 10/31/2019 09:42 AM - Eric Irrgang

Deduplicate gmxapi documentation.

`docs/gmxapi` seems to have settled down and does not have substantial layout changes from the documentation in python_packaging/documentation. Compartmentalized doc builds, e.g. with docs.dockerfile, still warrant a separate simple conf.py, so that much is retained. Otherwise, it looks like documentation for the standalone gmxapi package or development can be maintained in a unified way with the GROMACS project documentation, so this change removes the transitionally duplicated content.

- Remove most of python_packaging/documentation
- Update python_packaging/docker/docs.dockerfile

Refs #2698

Refs #2985

Change-Id: I0c23f6526894ec1eec4e910463c8c9d08a7315f6

Revision 37c5c0ae - 11/17/2019 04:01 PM - Eric Irrgang

Add transitional links for online gmxapi Python package reference.

- Update and clarify pythonreference stub for when Python package was not available.

- Note related Redmine reference.
- Remove `python-procedural` label, which had lost meaning and which could cause awkward repositioning for the pythonreference stub with no section heading to follow the label.

Refs #2985

Change-Id: If81ba6500ce078fe4fc94bf37285324ec5702b1b

Revision fea93810 - 01/03/2020 02:38 PM - Eric Irrgang

Remove transitional links for online gmxapi Python package reference.

Provide link to current GROMACS gmxapi documentation, built by GitLab Runner.

Fixes #2985

Change-Id: I1e56828aba4cc2568bbc9e6617863ca10197058d

History

#1 - 11/08/2019 08:55 PM - Eric Irrgang

I believe this is blocked on deployment of GitLab Runner, but it appears that Python package documentation will ultimately live at <http://manual.gromacs.org/current/gmxapi/>

In the mean time, a single version is manually updated at <http://gmxapi.org/> and at <https://hub.docker.com/r/gmxapi/docs>

#2 - 12/11/2019 11:36 AM - Eric Irrgang

If there is a tracked issue for the GitLab Runner infrastructure, we could make this issue dependent on it and update the target version to match. Otherwise, I need to defer to Paul on reasonable target version.

#3 - 12/27/2019 04:05 PM - Paul Bauer

- Target version changed from 2020 to 2020.1

I created [#3272](#) to act as an umbrella task

#4 - 01/03/2020 11:02 AM - Eric Irrgang

Paul Bauer wrote:

I created [#3272](#) to act as an umbrella task

I see that the 2020 release docs include the full Python package docs, but I don't know if the automation is fully set up. Should we consider this issue complete?

#5 - 01/03/2020 02:45 PM - Eric Irrgang

- Status changed from New to Resolved

Applied in changeset <fea93810335c01acca5ed53fd1d98b85b9a8351e>.

#6 - 01/10/2020 11:29 AM - Paul Bauer

- Status changed from Resolved to Closed