# GROMACS - Task #2893

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

## Integrate gmxapi Python package

03/14/2019 03:42 PM - Eric Irrgang

| | | |
|---|---|---|
| **Status:** | Resolved | |
| **Priority:** | Normal | |
| **Assignee:** | Eric Irrgang | |
| **Category:** | gmxapi | |
| **Target version:** | 2020 | |
| **Difficulty:** | uncategorized | |

**Description**

The Python package distributed through GitHub is to be merged with the GROMACS repository.
This issue addresses the migration to the GROMACS repository as the new canonical source of the package.

Goal: Centralize gmxapi project sources, design documentation, tests, and ongoing development in the GROMACS code management ecosystem.

Criteria for completion:
- Expressed functional goals are articulated with a mechanism for testing acceptable implementation.
- Ongoing gmxapi development can be pursued reasonably as changes staged through Gerrit for GROMACS master.
- A framework has been established to express project requirements, achieve design consensus, and propose incremental development in a clear context.

Explicitly deferred:
- testing infrastructure exercised through Jenkins
- Python packaging details
- documentation integration
- unified CMake infrastructure

To minimize the intrusiveness of early commits, a new directory `python_packaging`
holds documentation, testing tools, and Python package sources.

Design documentation describes numbered functional requirements that can be
cross-referenced as "FR#" in commit messages, tests, documentation, and other
tagging mechanisms as needed, where "#" is an integer.
Reference
https://redmine.gromacs.org/projects/gromacs/repository/revisions/master/entry/python_packaging/roadmap.rst

Comment:
First change establishes directory structure for initial commits of documentation, packaged code, and basic infrastructure to support development and testing.

Second change expresses functional goals in a roadmap.rst, with acceptance criteria as a set of Python (pytest) unit tests.

**Subtasks:**

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|---|---|
| Bug # 3144: gmxapi.mdrun does not clearly expose the output trajectory. | **New** |

**Related issues:**

| | |
|---|---|
| Related to GROMACS - Task #2912: C++ extension module for Python bindings | **Resolved** |
| Blocks GROMACS - Task #2894: Wrap importable Python code. | **Resolved** |
| Blocks GROMACS - Task #2895: gmxapi Output proxy establishes execution depend... | **Resolved** |

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## Associated revisions

**Revision fae19655 - 03/29/2019 10:39 AM - Eric Irrgang**

Plumbing for gmxapi 2019 Q1/Q2 project roadmap.

Provide infrastructure so that dependent change can focus on content
of project plan.

Ref: #2893

Change-Id: Idd72e9ede890f7fc97a680c5a5bffe97499eaaf5

**Revision 4a1d0408 - 04/09/2019 11:25 AM - Eric Irrgang**

gmxapi 2019 Q1/Q2 project roadmap.

Lay out project goals, functional requirements, and testing plans.
Provides roadmap.rst and pytest acceptance tests
expressing the required functionality of the Python package.

Ref: #2893

Change-Id: I71ec79eb5d8a6e4d61fb5d7d6e20176c9c07a6af

**Revision 476e2dc2 - 04/24/2019 03:12 PM - Eric Irrgang**

Infrastructure updates for dependent changes.

- Introduce gmxapi.exceptions.ProtocolError.
- Add some pytest configuration and helpers.
- Update some comments.

Refs: #2893

Gerrit patch set 9367/5

**Revision 4f265b31 - 04/24/2019 03:12 PM - Eric Irrgang**

Command line wrapper with data flow.

Introduce gmxapi.commandline_operation(), a fused operation that allows
data flow constraints to be mapped to input and output file arguments.

Expand gmxapi.operation tools to support the data flow constraints.

Achieves functional requirements 1, 2, and 3 as described
in the documentation submitted under #2893.

Updates some acceptance tests duplicated in a companion change.

Fixes: #2894

Gerrit patch set 9371/10

**Revision 8ef8d2bc - 05/02/2019 07:22 PM - Eric Irrgang**

Infrastructure updates for dependent changes.

- Introduce gmxapi.exceptions.ProtocolError.
- Add some pytest configuration and helpers.
- Update some comments.

Refs: #2893

Change-Id: I71030c3b552d568df7263115430631208812b9dc

**Revision d0536976 - 05/09/2019 09:11 AM - Eric Irrgang**

Expand gmxapi.operation tools to support the data flow constraints.

Achieves functional requirements 1, 2, and 3 as described
in the documentation submitted under #2893.

Updates some acceptance tests duplicated in a companion change.

Fixes: #2894

Change-Id: I26b1413c83e3ad176f2fd70f93e8b8e1033667ae

**Revision ffab5391 - 08/22/2019 04:30 PM - Eric Irrgang**

Python wrapping code for gmxapi mdrun bindings.

Expose the mdrun bindings to the Python interface. Imports workflow.py
and context.py from 0.0.7.4 tagged release of external project at

https://github.com/kassonlab/gmxapi with minimal modifications.

Refs #2893
Refs #2912
Refs #3027

Change-Id: I44a66646eceb191a2ec755169671af326f22526a

**Revision 6cb31a6b - 09/03/2019 09:52 AM - Eric Irrgang**

Python wrapping code for gmxapi mdrun bindings.

Expose the mdrun bindings to the Python interface.

Updates workflow.py and context.py from 0.0.7.4 tagged release of external project.

Refs #2893
Refs #2912
Refs #3027

Change-Id: I44a66646eceb191a2ec755169671af326f22526a

## History

**#1 - 03/14/2019 03:44 PM - Gerrit Code Review Bot**

Gerrit received a related patchset '11' for Issue #2893.
Uploader: M. Eric Irrgang (ericirrgang@gmail.com)
Change-Id: gromacs~master~Idd72e9ede890f7fc97a680c5a5bffe97499eaaf5
Gerrit URL: https://gerrit.gromacs.org/9202

**#2 - 03/14/2019 03:45 PM - Gerrit Code Review Bot**

Gerrit received a related patchset '3' for Issue #2893.
Uploader: M. Eric Irrgang (ericirrgang@gmail.com)
Change-Id: gromacs~master~I71ec79eb5d8a6e4d61fb5d7d6e20176c9c07a6af
Gerrit URL: https://gerrit.gromacs.org/9241

**#3 - 03/14/2019 03:56 PM - Eric Irrgang**

*- Tracker changed from Feature to Task*

*- Description updated*

**#4 - 03/14/2019 03:57 PM - Eric Irrgang**

*- Blocks Task #2894: Wrap importable Python code. added*

**#5 - 03/14/2019 04:03 PM - Eric Irrgang**

*- Blocks Task #2895: gmxapi Output proxy establishes execution dependency. added*

**#6 - 03/29/2019 04:46 PM - Gerrit Code Review Bot**

Gerrit received a related DRAFT patchset '1' for Issue #2893.
Uploader: M. Eric Irrgang (ericirrgang@gmail.com)
Change-Id: gromacs~master~I71030c3b552d568df7263115430631208812b9dc
Gerrit URL: https://gerrit.gromacs.org/9367

**#7 - 03/31/2019 05:26 PM - Eric Irrgang**

*- Related to Task #2912: C++ extension module for Python bindings added*

**#8 - 04/09/2019 11:27 AM - Mark Abraham**

*- Description updated*

**#9 - 04/09/2019 12:18 PM - Eric Irrgang**

*- Description updated*

**#10 - 04/09/2019 12:20 PM - Eric Irrgang**

*- Status changed from New to Resolved*

Unless there are requests for additional infrastructure or procedures, this task appears to be resolved.