

GROMACS - Task #2894

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

Wrap importable Python code.

03/14/2019 03:50 PM - Eric Irrgang

Status:	Resolved	
Priority:	Normal	
Assignee:	Eric Irrgang	
Category:	gmxapi	
Target version:	2020	
Difficulty:	uncategorized	
Description		
Provide basic tools for wrapping Python code to implement gmxapi compatible tools.		
The wrappers provided in the operation module are used to build basic built-in gmxapi functionality as well as user extensions. Future updates to gmxapi data flow, checkpointing, control flow, and interoperability should be engineered to have minimal impact on code expressed with the provided tools.		
Functional requirements:		
<ul style="list-style-type: none">• FR1 requires a basic gmxapi.operation Python module• FR2 requires that Operations built with the wrappers in gmxapi.operation should behave with correct execution dependency.• FR3 requires that Operation output can be chained to the input of other Operations.		
Criteria for completion: Demonstrate with chains of <code>commandline_operation</code> .		
Related issues:		
Blocked by GROMACS - Task #2893: Integrate gmxapi Python package		Resolved
Blocks GROMACS - Task #2912: C++ extension module for Python bindings		Resolved

Associated revisions

Revision 7123128e - 04/09/2019 02:15 PM - Eric Irrgang

Introduce gmxapi operations and basic data model.

Ref: #2894

Change-Id: I4e899e63287370fd2fdde89ddc1b2ea39c3fe67d

Revision 52c830b8 - 04/24/2019 03:12 PM - Eric Irrgang

Support basic command line wrapper in gmxapi

Introduces `gmxapi.commandline` module and updates `gmxapi.operation` to support `gmxapi.commandline.cli()` operation.

Ref: #2894

Gerrit patch set 9370/6

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 09c9269d - 05/09/2019 08:11 AM - Eric Irrgang

Support basic command line wrapper in gmxapi

Introduces gmxapi.commandline module and updates gmxapi.operation to support gmxapi.commandline.cli() operation.

Ref: #2894

Change-Id: I9f6c113f21d3a1ce97184a1e48b8bd4856c5c924

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

History

#1 - 03/14/2019 03:57 PM - Eric Irrgang

- Parent task deleted (#2893)

#2 - 03/14/2019 03:57 PM - Eric Irrgang

- Blocked by Task #2893: Integrate gmxapi Python package added

#3 - 03/14/2019 04:03 PM - Eric Irrgang

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

#4 - 03/14/2019 05:41 PM - Gerrit Code Review Bot

Gerrit received a related patchset '10' for Issue [#2894](#).

Uploader: M. Eric Irrgang (ericirrgang@gmail.com)

Change-Id: gromacs~master~11b56858e8e50c1a06273f43dc69c9b812158d82

Gerrit URL: <https://gerrit.gromacs.org/9204>

#5 - 03/29/2019 05:16 PM - Eric Irrgang

- Description updated

#6 - 03/29/2019 05:23 PM - Gerrit Code Review Bot

Gerrit received a related DRAFT patchset '1' for Issue [#2894](#).

Uploader: M. Eric Irrgang (ericirrgang@gmail.com)

Change-Id: gromacs~master~14e899e63287370fd2fde89ddc1b2ea39c3fe67d

Gerrit URL: <https://gerrit.gromacs.org/9369>

#7 - 03/29/2019 05:23 PM - Gerrit Code Review Bot

Gerrit received a related DRAFT patchset '1' for Issue [#2894](#).

Uploader: M. Eric Irrgang (ericirrgang@gmail.com)

Change-Id: gromacs~master~I9f6c113f21d3a1ce97184a1e48b8bd4856c5c924

Gerrit URL: <https://gerrit.gromacs.org/9370>

#8 - 03/29/2019 05:23 PM - Gerrit Code Review Bot

Gerrit received a related DRAFT patchset '1' for Issue [#2894](#).

Uploader: M. Eric Irrgang (ericirrgang@gmail.com)

Change-Id: gromacs~master~I26b1413c83e3ad176f2fd70f93e8b8e1033667ae

Gerrit URL: <https://gerrit.gromacs.org/9371>

#9 - 04/03/2019 08:37 PM - Eric Irrgang

- Blocks Task #2912: C++ extension module for Python bindings added

#10 - 04/09/2019 11:27 AM - Mark Abraham

- Description updated

#11 - 04/09/2019 12:24 PM - Eric Irgang

- Description updated

#12 - 04/09/2019 12:25 PM - Eric Irgang

- Description updated

#13 - 04/09/2019 12:26 PM - Eric Irgang

- Blocks deleted (Task #2895: gmxapi Output proxy establishes execution dependency.)

#14 - 04/18/2019 02:44 PM - Eric Irgang

- Status changed from New to Fix uploaded

#15 - 04/18/2019 02:46 PM - Eric Irgang

- Parent task set to #2045

#16 - 04/24/2019 04:00 PM - Eric Irgang

- Status changed from Fix uploaded to Resolved

Applied in changeset [4f265b31c1a97cbef40d1be75949284985f16455](#).

#17 - 05/09/2019 11:30 AM - Eric Irgang

Applied in changeset [d0536976ee5454d8c7f2f9c823e154085b4c7121](#).