

## GROMACS - Task #3139

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

Feature # 2994 (New): Data flow topology in gmxapi 2020

### gmxapi Futures should be subscribable

10/14/2019 02:17 PM - Eric Irrgang

<b>Status:</b>	New	
<b>Priority:</b>	Normal	
<b>Assignee:</b>	Eric Irrgang	
<b>Category:</b>	gmxapi	
<b>Target version:</b>		
<b>Difficulty:</b>	uncategorized	
<b>Description</b>		
In order to dispatch work between Context instances, and to better implement functionality like looping, we should move to an observer pattern for data flow implementation details. This means that a Context will maintain knowledge of subscribers to the Futures it manages so that it can notify of data availability. Additionally, if a subscriber can consume multiple iterations of a Future (subgraph nodes in a while loop), it will be much easier to update the graph state and metadata (such as input figure prints).		
<b>Related issues:</b>		
Related to GROMACS - Feature #3149: Python user interface for obtaining simul...		<b>New</b>
Related to GROMACS - Feature #3179: Clarify access to parallel data outputs		<b>New</b>
Blocks GROMACS - Feature #3138: Improve ensemble support in Context specifica...		<b>New</b>

### History

#### #1 - 10/14/2019 02:19 PM - Eric Irrgang

- Blocks Feature #3138: Improve ensemble support in Context specification. added

#### #2 - 10/15/2019 03:56 PM - Eric Irrgang

- Private changed from Yes to No

#### #3 - 10/15/2019 06:17 PM - Eric Irrgang

- Related to Feature #3149: Python user interface for obtaining simulation artifacts as files. added

#### #4 - 10/26/2019 12:21 PM - Eric Irrgang

- Related to Feature #3179: Clarify access to parallel data outputs added