

Testing Framework for Ensemblemd

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Testing Framework

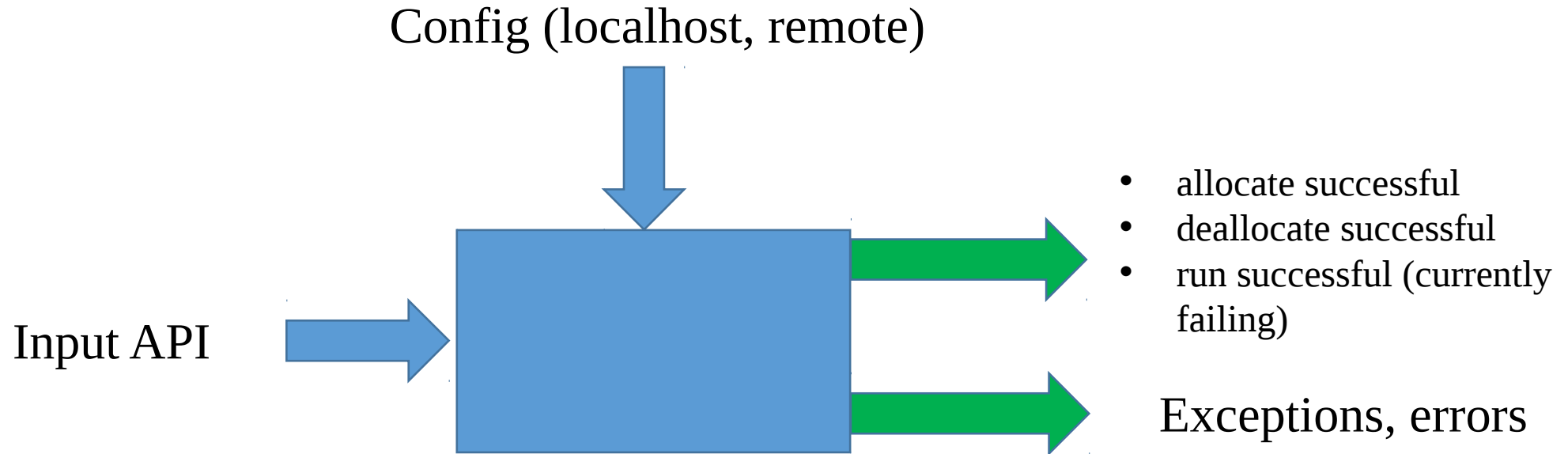
- Blackbox Testing
- EnsembleMD API Testing
- End-to-End Testing

EnsembleMD API Testing

- Building Block API Test cases
- Pattern API Test cases

Building Block API Test

- Execution Context API
 - `allocate()`, `deallocate()`, `run()`

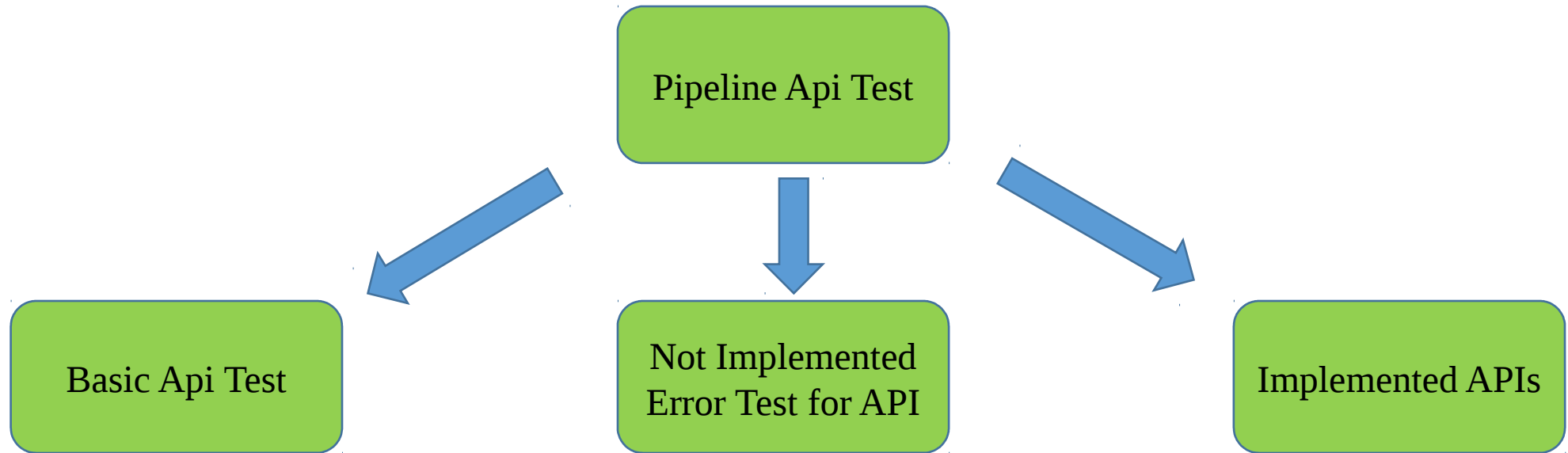


- Application Kernel API

- copy_input_data
- copy_output_data
- cores
- download_input_data
- download_output_data
- upload_input_data
- get_arg()
- get_instance_type
- get_raw_args()
- link_input_data()

Pattern *API*

Pipeline API

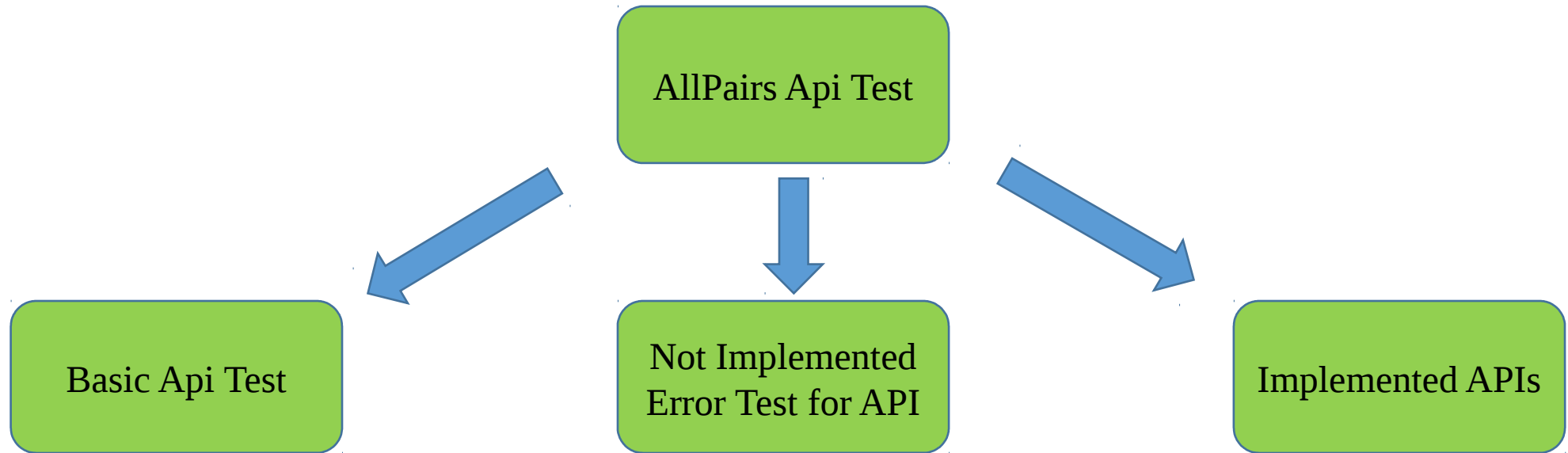


- import
- name
- instances
- steps

- step_n

- step_n

AllPairs API

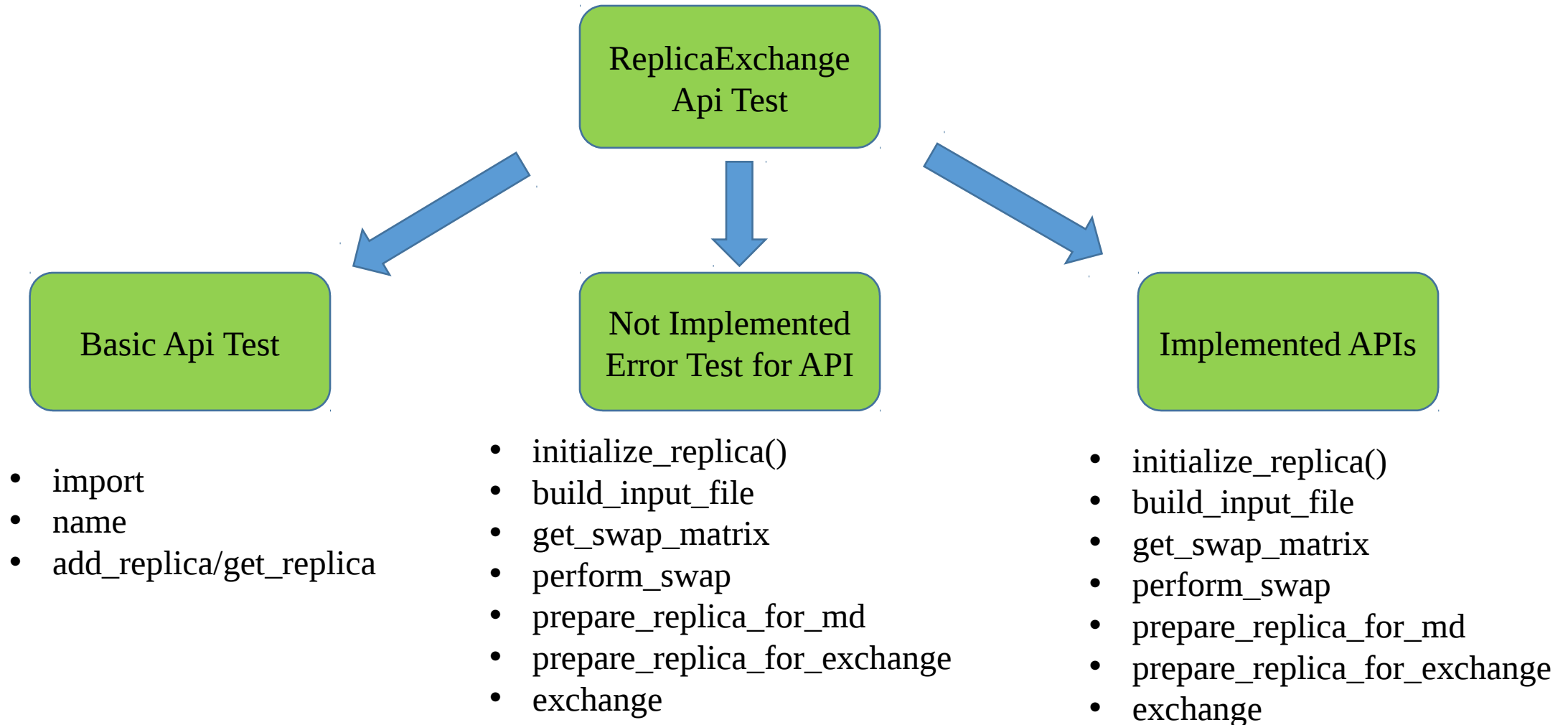


- import
- name
- permutations
- set1_elements
- set2_elements

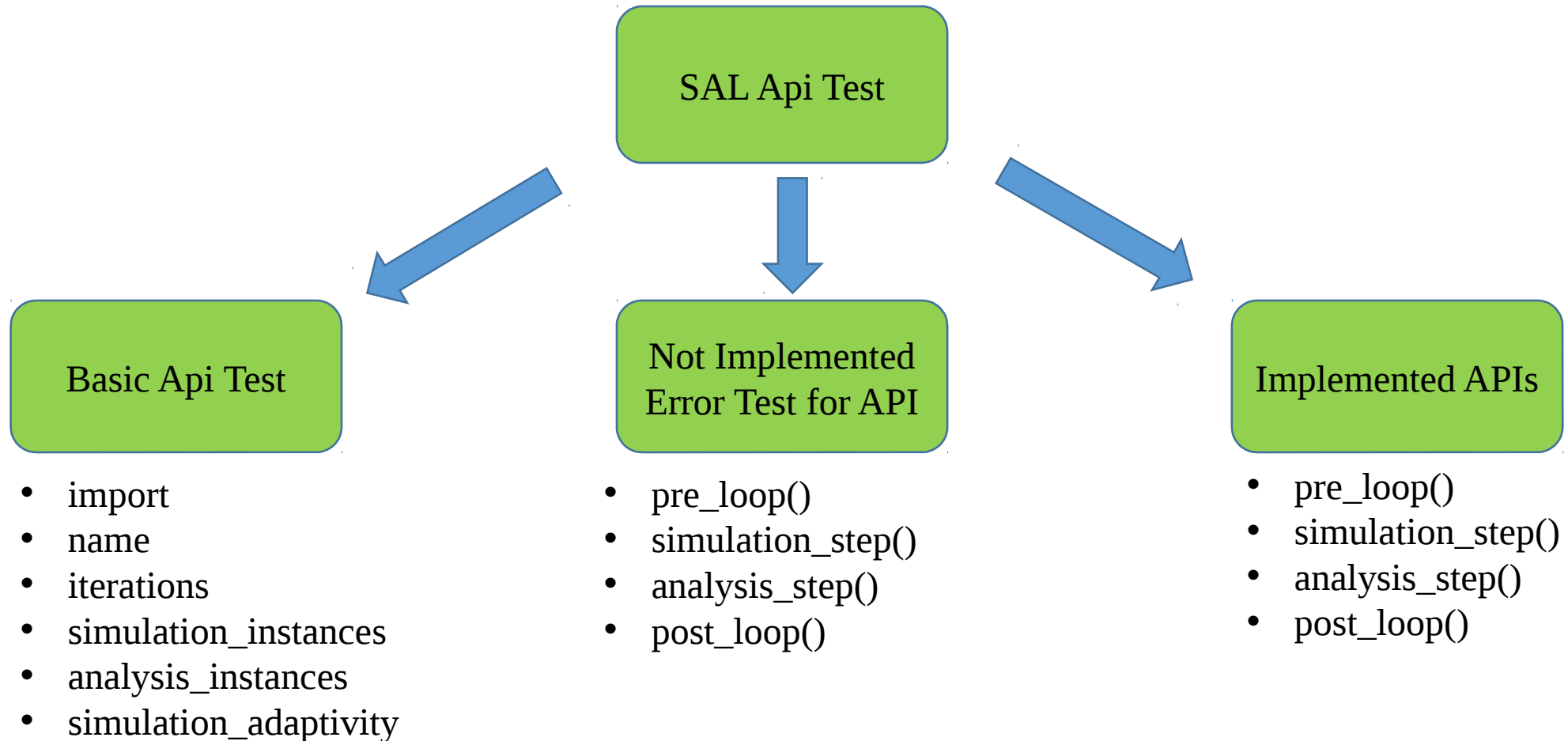
- set1element_initialization
- set2element_initialization
- element_comparision

- set1element_initialization
- set2element_initialization
- element_comparision

ReplicaExchange API



Simulation Analysis Loop API



E2E Testing

- Execute each pair with basic kernel on:
 - local host
 - remote host
- Suggestions:
 - Any better idea to execute E2E

Blackbox Testing

- Tried running coco example but failing on stampede
- Suggestion:
 - How to start?
 - What is expected?

Issues

- Resolved:
 - allocate() did not return, giving I/O operation fail error
 - failing deallocate()
- Open:
 - run()- successfully executes but does not return anything
 - coco example: execution failed
 - No files are generated when Test cases are executes unlike a normal code

Road Map

- EnsembleMD APIs:
 - Pattern APIs - Completed
 - Execution API - To be completed by 1/6/2016
- E2E Testing: To be completed by 1/10/2016
- Blackbox testing: To be completed by 1/20/2016, simultaneously start writing

Suggestions/ Improvements