Testing Framework for Ensemblemd

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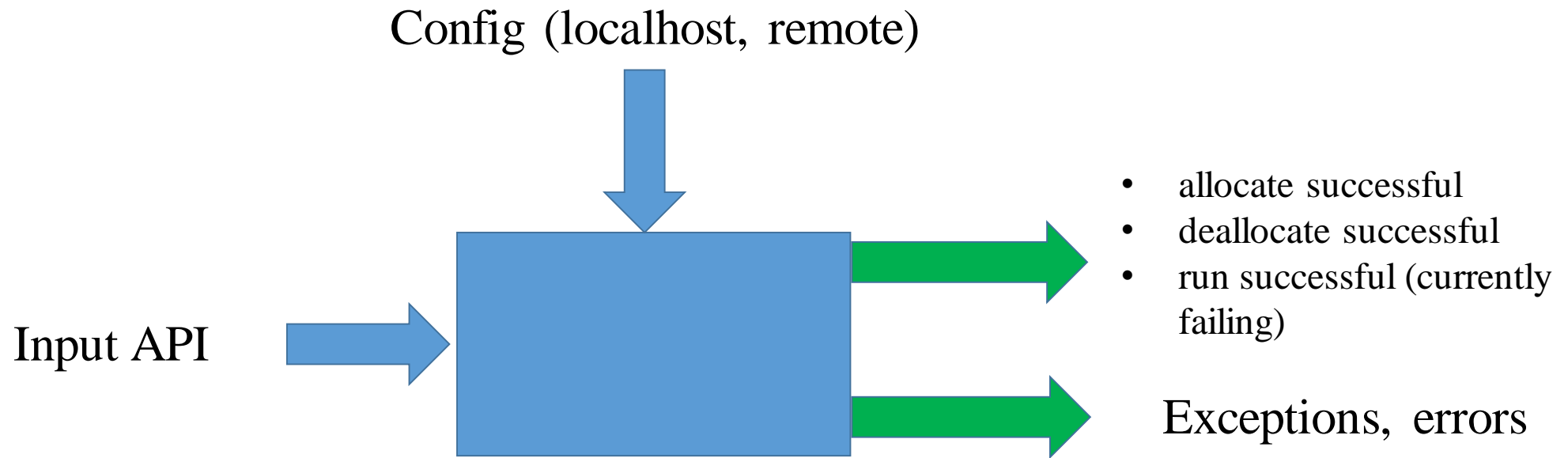
- Blackbox Testing
- EnsembleMD API Testing
- End-to-End Testing

EnsembleMD API Testing

- Building Block API Test cases
- Pattern API Test cases

Building Block API Test

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

Config (localhost, remote)

Input API

- allocate successful
- deallocate successful
- run successful (currently failing)

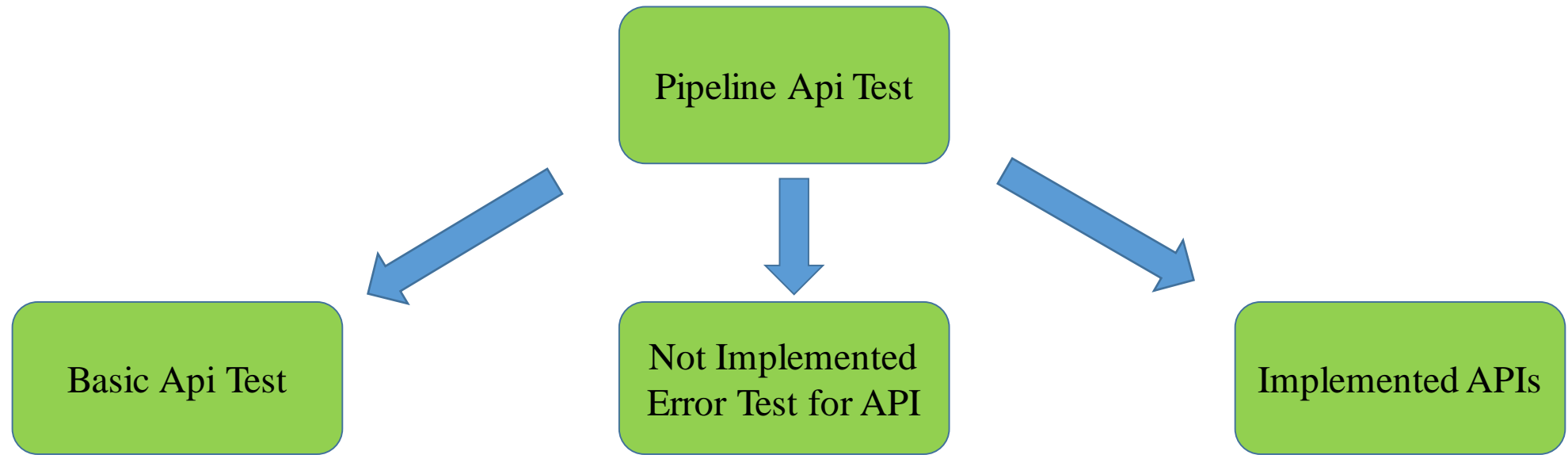Exceptions, errors

- 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()
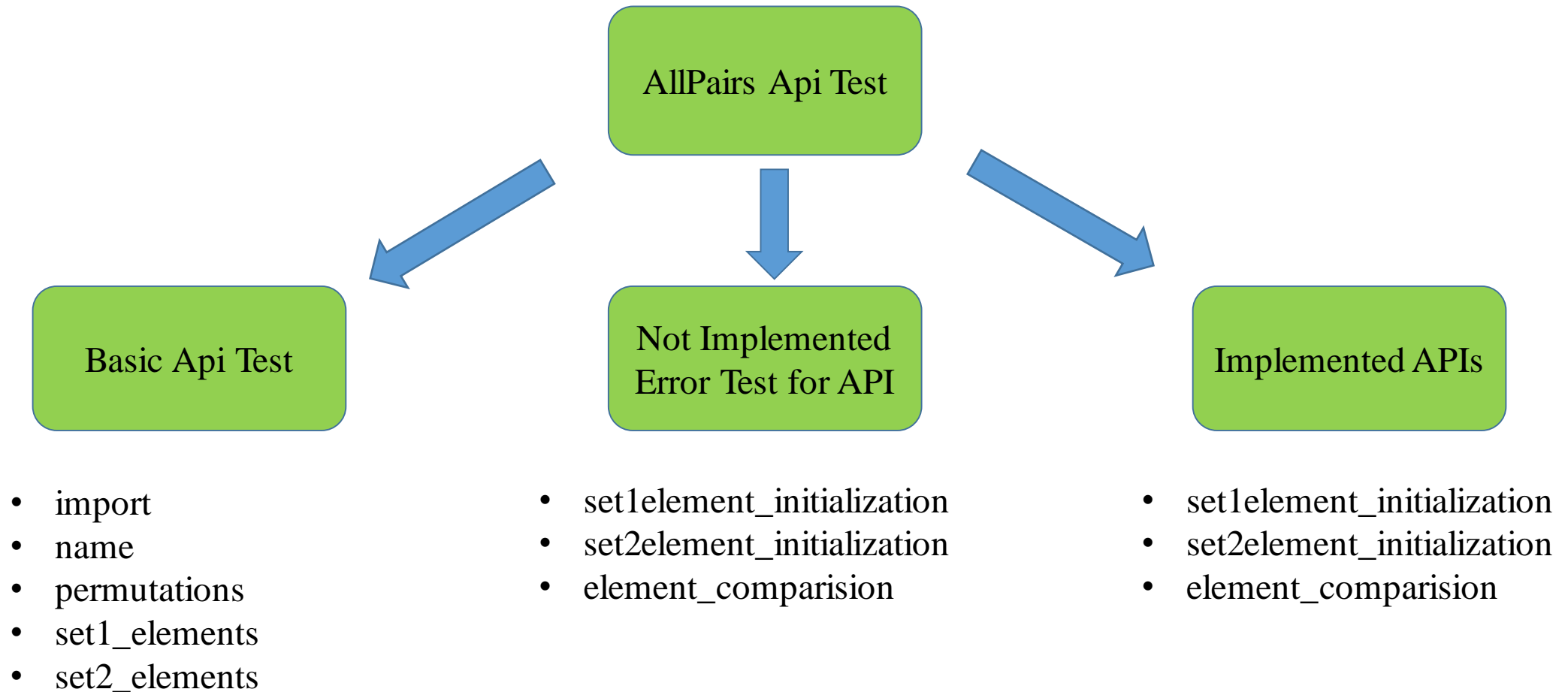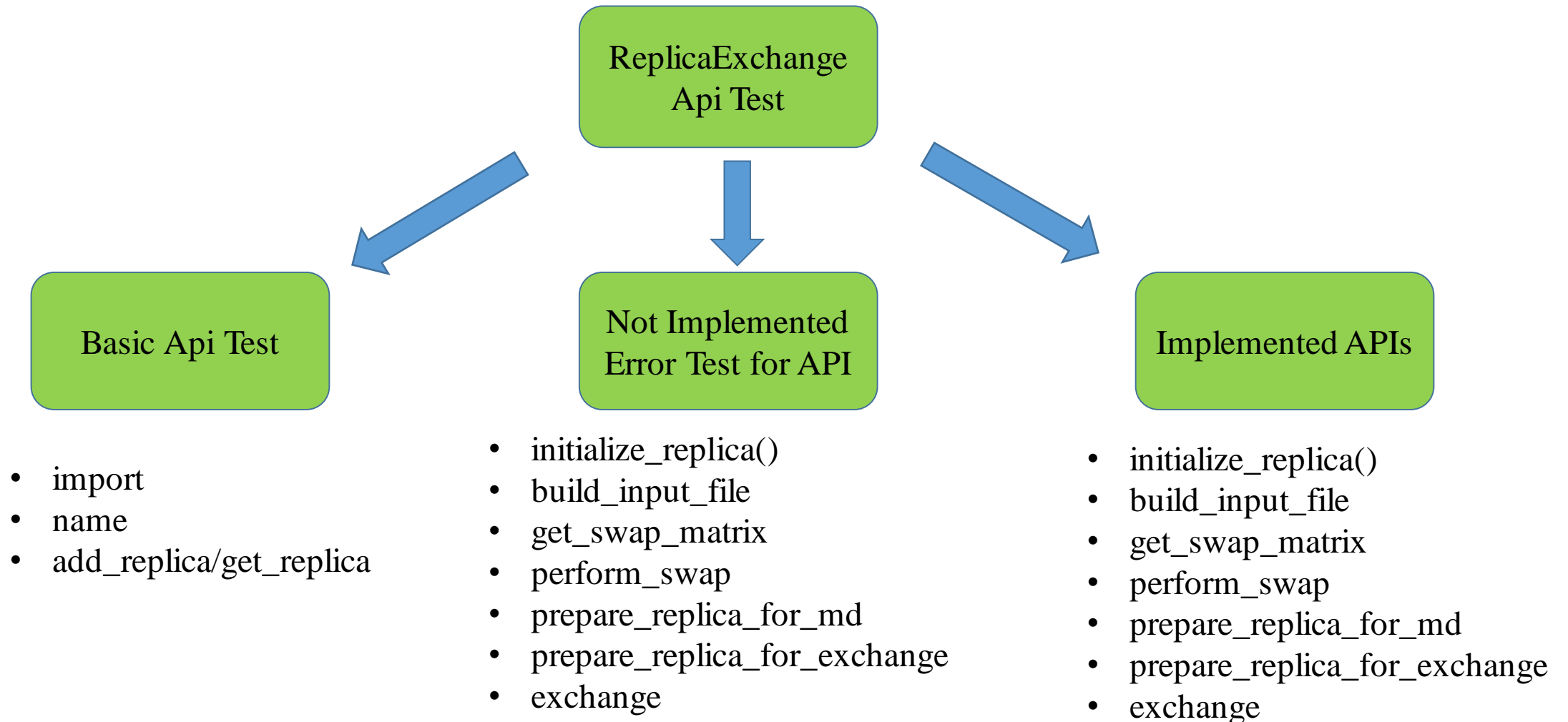 - link_input_data()

Pattern API

Pipeline API

AllPairs API

ReplicaExchange API

ReplicaExchange Api Test

Basic Api Test

- import
- name
- add_replica/get_replica

Not Implemented Error Test for API

- initialize_replica()
- build_input_file
- get_swap_matrix
- perform_swap
- prepare_replica_for_md
- prepare_replica_for_exchange
- exchange

Implemented APIs

- initialize_replica()
- build_input_file
- get_swap_matrix
- perform_swap
- prepare_replica_for_md
- prepare_replica_for_exchange
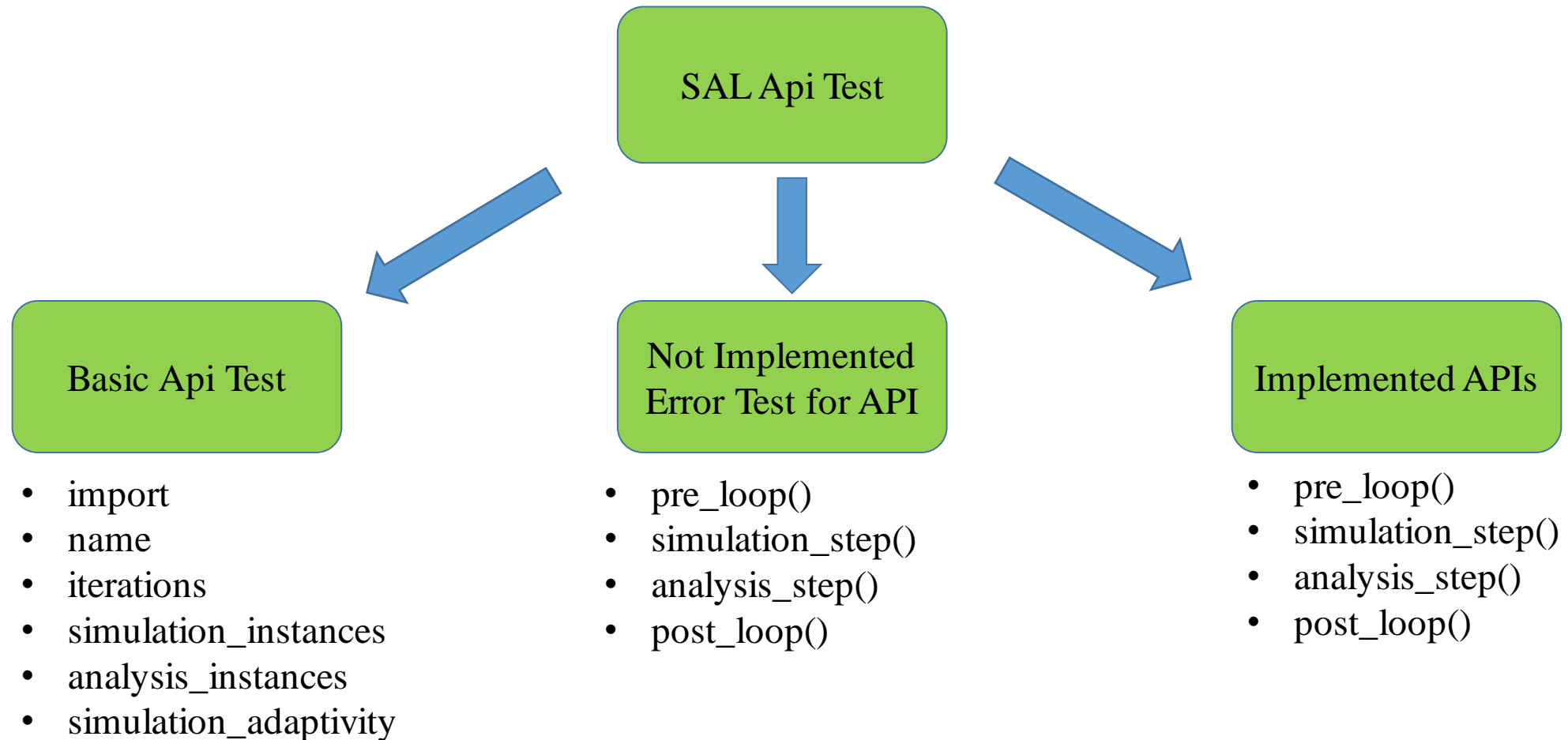- exchange

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 2/6/2016

- E2E Testing: To be completed by 2/10/2016

- Blackbox testing: To be completed by 2/20/2016, simultaneously start writing

Suggestions/ Improvements