Multi-site dynamic computational ensembles with `libEnsemble` + `funcX`

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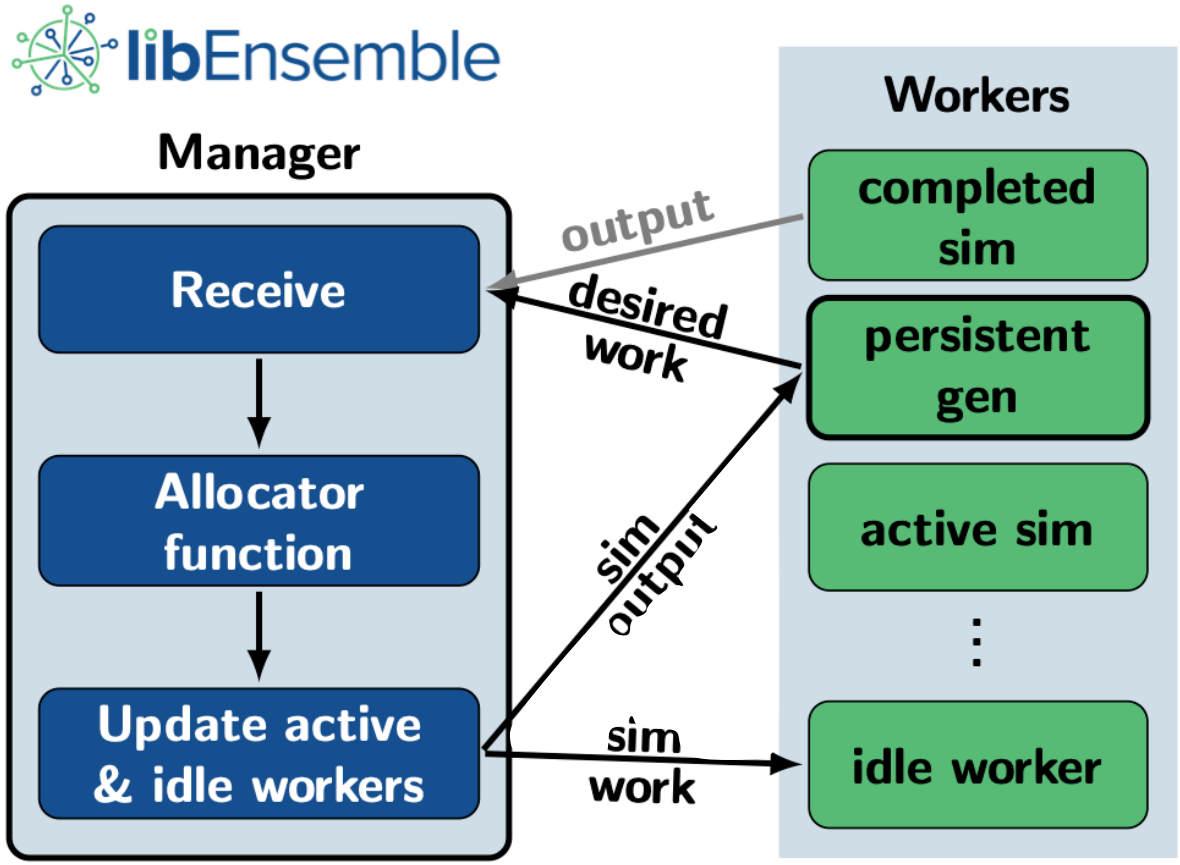
What is `libEnsemble`?

- A toolkit for coordinating workflows of concurrent *asynchronous and dynamic* computations

- Aims for:
  - Extreme scaling
  - Dynamic ensembles (concurrent evals)
  - Dynamic Resource Management
  - Monitoring/cancelling apps
  - Resilience/fault tolerance
  - Portability and flexibility
  - Exploitation of persistent data/control
  - Low start-up cost

The `libEnsemble` Paradigm

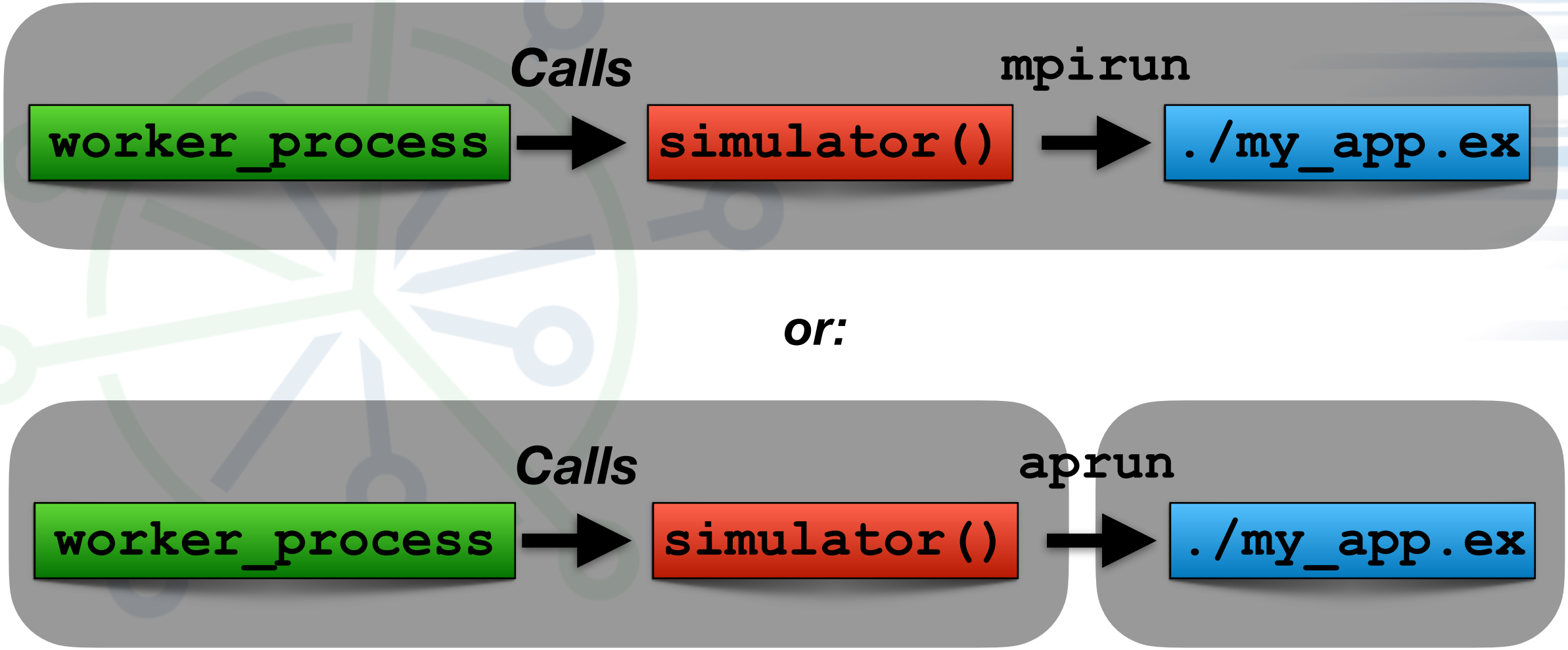
- ***Worker*** processes run either ***simulator*** or ***generator*** functions
- The ***Manager*** distributes output from a worker's *generator* function to workers to evaluate via *simulator* functions.
- How/when output is distributed is customizable via an optional ***allocation*** function



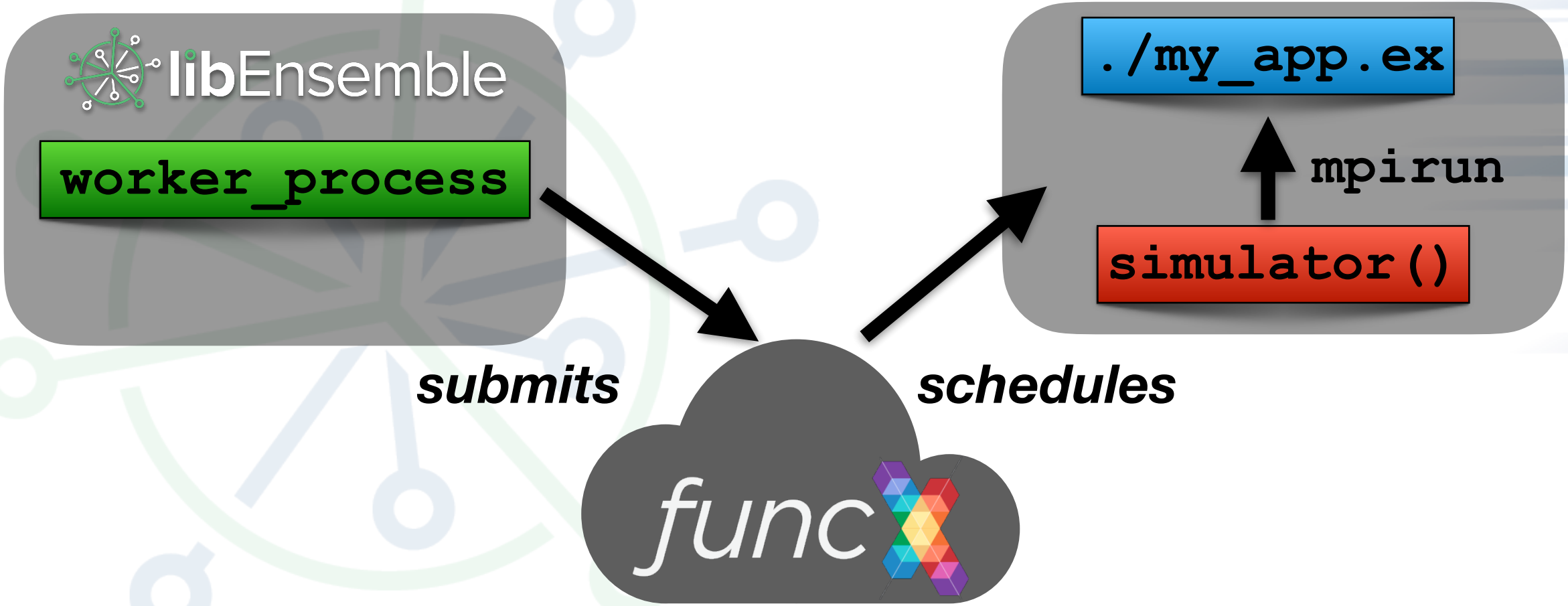
Example functions

- **Generators:**
  - Asynchronously Parallel Optimizer for Solving Multiple Minima (`APOSMM`, included with `libEnsemble`)
  - Surrogate model calibration/ inference (via `Surmise`)
  - Sparse Grids sampling (via `Tasmanian`)
- **Simulators:**
  - Accelerator structure and beam line analysis (via `OPAL`)
  - Particle-in-cell evaluations (via `WarpX`)
  - Ice sheet modeling
  - RNN-training

Workers *call* Simulator and Generator functions

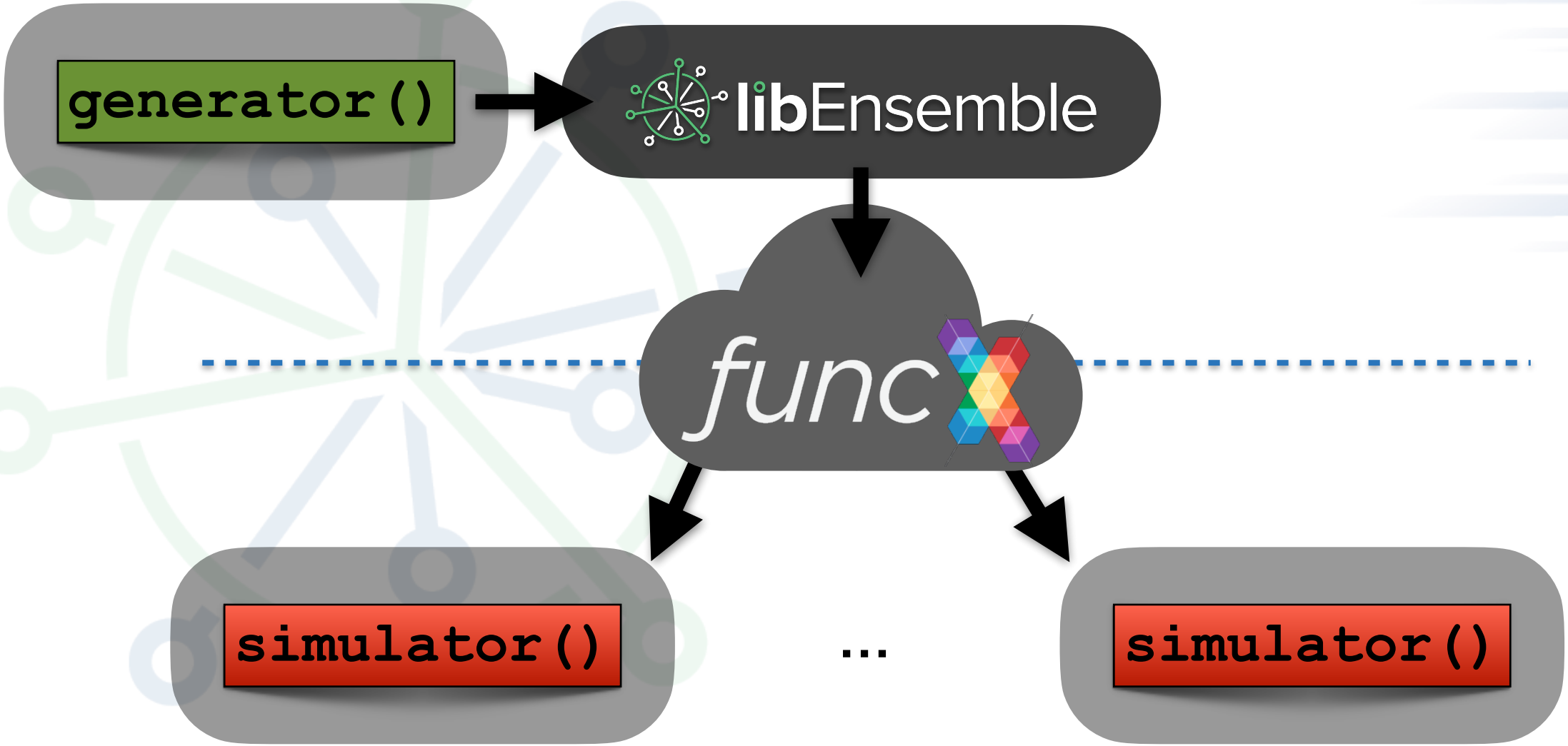


libEnsemble and funcX integrate nicely!



Easy cross-system, heterogenous ensembles!

Multi-site dynamic ensembles



Configuring a libEnsemble function for submission to funcX

```
from simulation_module import my_sim_func
. . .
sim_specs = {
          'sim_f': my_sim_func,
          'in': ['input1, 'input2],
          'out': [('output1', float)],
          'funcx_endpoint': '3af6dc24-3f27-4c49-8d11-e301ade15353'
}
```

Configuration script

Function

```
def my_sim_func(Input, persis_info, sim_specs, _):

    # All imports need to be within function
    from libensemble.executors import MPIExecutor

    # Instantiate an MPI Executor instance
    exctr = MPIExecutor()

    # Register our app
    exctr.register_app(full_path='/local/path/forces.ex', app_name='forces')

    # Submit our app using the autodetected MPI runner
    task = exctr.submit(app_name='forces')

    # Simply wait for the app to complete
    flag = exctr.polling_loop(task)
    . . .
```

Future Work

- Launch *persistent* functions to remote machines?
  - How to send intermediate results back to Manager?
- How to send/receive manager-kill signals for running apps?
- Experiment with dynamically choosing endpoints?
- …Find interested users!

Questions?

libEnsemble

- https://libensemble.readthedocs.io
- https://github.com/Libensemble/libensemble

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- **Thank you very much!**