libEnsemble

Argonne NATIONAL LABORATORY

A Python library to coordinate the evaluation of dynamic ensembles of calculations. Use massively parallel resources to accelerate the solution of design, decision, and inference problems.

libEnsemble aims for:

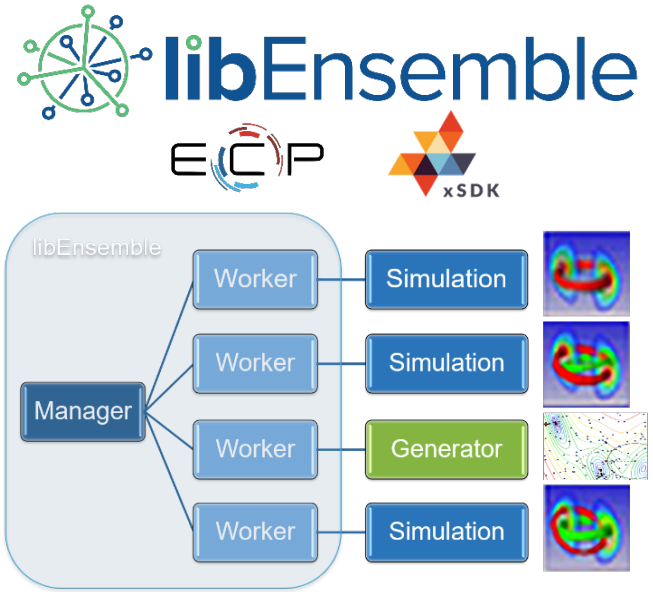
- Extreme scaling
- Resilience and fault tolerance
- Monitoring and killing tasks and recovering resources
- Portability and flexibility

libEnsemble features:

- Communications using MPI, multiprocessing, or TCP
- Support for calculations using parallel resources, including user-provided executables
- Executor auto-detects system resources and launches user executables
- Support on Summit (ORNL), Theta (ALCF), Cori (NERSC), Bridges (PSC)

Dynamic ensembles:

- Workers are allocated simulations or generate input for simulations
- One use case: an optimization method generates parameters to be evaluated by a computationally expensive simulation
- Example interfaces with PETSc, SciPy, and NLopt solvers are available



https://libensemble.readthedocs.io