SmartSim Introduction



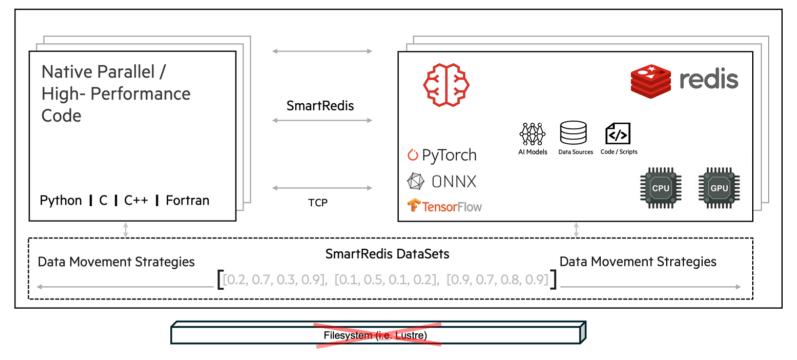
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SmartSim

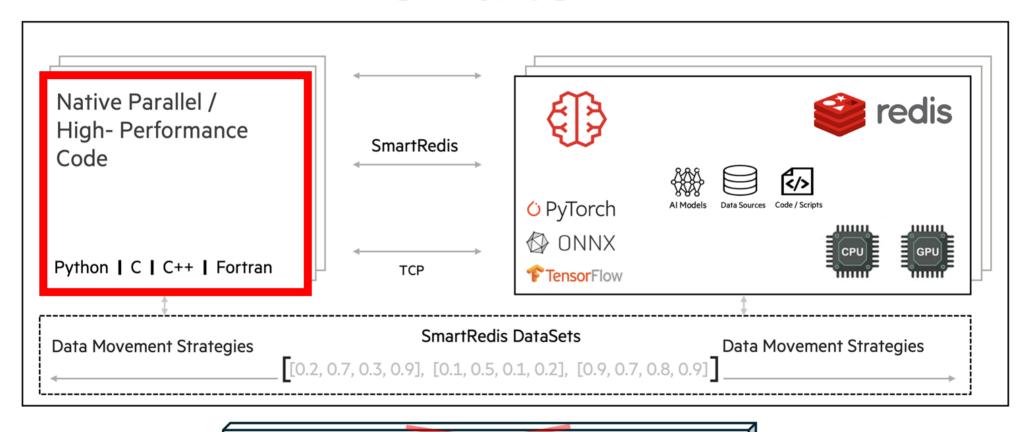
SmartSim enables scientists to utilize machine learning inside traditional HPC workloads

SmartSim provides this capability by:



- •Automating the deployment of HPC workloads and distributed, in-memory storage (Redis).
- •Making TensorFlow, Pytorch, and ONNX callable from Fortran, C, and C++ simulations.
- •Providing flexible data communication and formats for hierarchical data, enabling online analysis, visualization, and processing of simulation data.

SmartSim



Filesystem (i.e. Lustre)

SmartSim

The main goal of SmartSim is to provide scientists a flexible, easy to use method for interacting at runtime with the data generated by simulation. The type of interaction is completely up to the user:

- •Embed calls to machine learning models inside a simulation
- Create hooks to manually or programmatically steer a simulation
- •Visualize the progression of a simulation integration from a Jupyter notebook

SmartSim (Infrastructure Library)

automate process of deploying HPC workloads alongside in-memory database

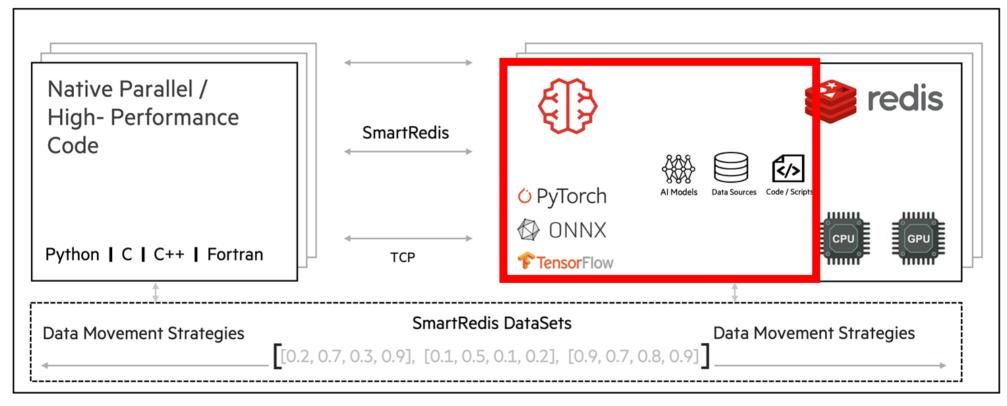
deploy **distributed**, shared-nothing, **in-memory cluster of Redis instances** across compute nodes → **Orchestrator**

Orchestrator + HPC applications

→ connect workloads (e.g. trained ML models) to other applications with SmartRedis clients

- •An API to start, monitor, and stop HPC jobs from Python or from a Jupyter notebook.
- •Automated deployment of in-memory data staging (Redis) and computational storage (RedisAI).
- •Programmatic launches of batch and in-allocation jobs on PBS, Slurm, LSF, and Cobalt systems.
- Creating and configuring ensembles of workloads with isolated communication channels.

RedisAI (Client Library)



Filesystem (i.e. Lustre)

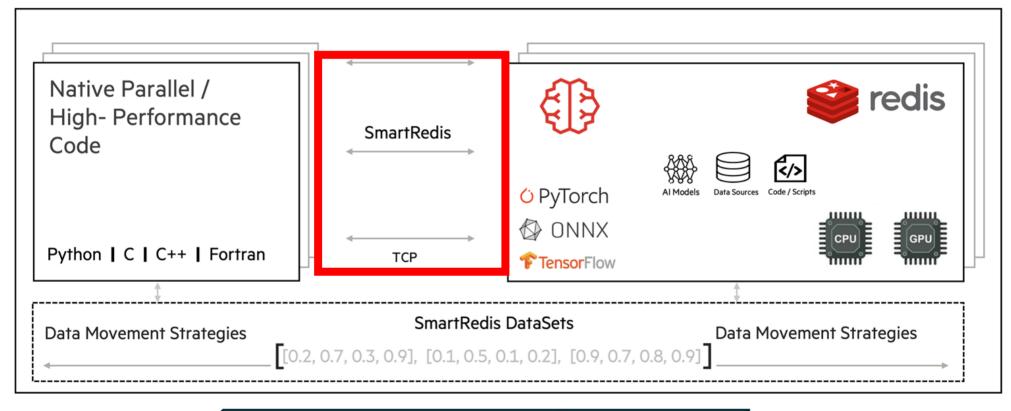
RedisAl (Client Library)

Redis module for executing Deep Learning/Machine Learning models and managing their data.

Key features of RedisAl supported by SmartRedis

- A tensor data type in Redis
- TensorFlow, TensorFlow Lite, Torch, and ONNXRuntime backends for model evaluations
- TorchScript storage and evaluation
- Data locality

SmartRedis (Client Library)



Filesystem (i.e. Lustre)

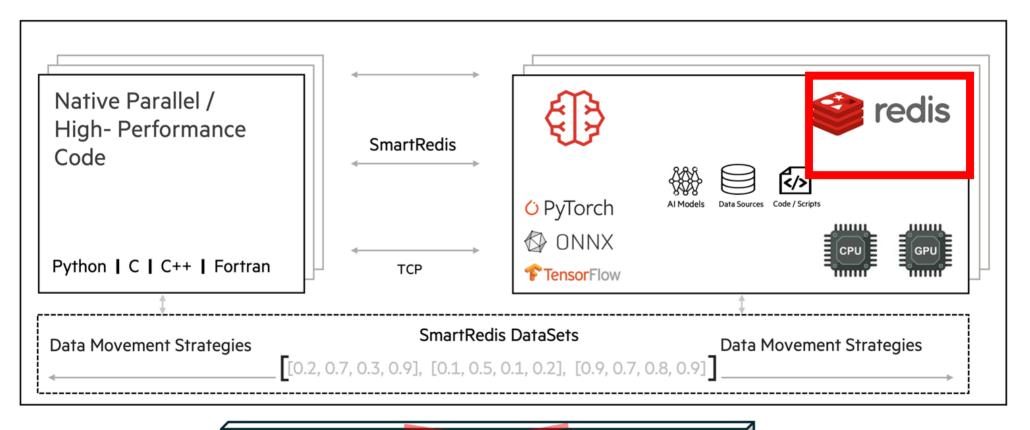
SmartRedis (Client Library)

collection of Redis clients supporting RedisAl capabilities and include additional features for HPC applications

Key features of SmartRedis developed for large, distributed HPC architectures

- Redis cluster support for RedisAl data types (tensors, models, and scripts).
- Distributed model and script placement for parallel evaluation that maximizes hardware utilisation and throughput
- A **DataSet storage format** to **aggregate multiple tensors** and metadata into a **single Redis cluster** hash slot to **prevent data scatter** on Redis clusters and maintain contextual relationships between tensors. Useful when clients produce tensors and metadata that are referenced or utilised together.
- . An **API for efficiently aggregating DataSet objects** distributed on one or more database nodes.
- Compatibility with SmartSim ensemble capabilities to prevent key collisions with tensors, DataSet, models, and scripts when clients are part of an ensemble of applications.

Redis



Filesystem (i.e. Lustre)

Redis

open source, **in-memory** data store.

Can be used as:

- Database
- Cache
- Message broker

Provides data structures (like strings, hashes, lists, sets, sorted sets with range queries, bitmaps, hyperloglogs, geospatial indexes, and streams).

Built-in replication, Lua scripting, LRU eviction, transactions, and different levels of on-disk persistence.

Atomic operations

Asynchronous replication, with fast non-blocking synchronization and auto-reconnection with partial resynchronization on net split.

Install SmartSim:

https://www.craylabs.org/docs/installation_instructions/basic.html

Or Use our installed version:

- Login to Cirrus
- Activate the Miniconda environment and load the modules
- Bout++ and SmartSim are installed in:
 - /work/tc045/tc045/shared/bpp_5_0_0_ss_0_4_2/BOUT-dev
 - /work/tc045/tc045/shared/bpp 5 0 0 ss 0 4 2/SmartSim

from smartsim import Experiment

Import **Experiment** from smartsim

```
# Init Experiment and specify to launch locally exp = Experiment(name="getting-started", launcher="local")
```

from smartsim import Experiment

```
# Init Experiment and specify to launch locally exp = Experiment(name="getting-started", launcher="local")
```

Initialise the Experiment; called **exp**.

Provide a name.

For simplicity, we will start on a single host and only launch single-host jobs.

```
# Init Experiment and specify to launch locally
exp = Experiment(name="getting-started", launcher="local")

# settings to execute the command "echo hello!"
settings = exp.create_run_settings(exe="echo", exe_args="hello!", run_command=None)

# create the simple model instance so we can run it.

M1 = exp.create model(name="tutorial-model", run_settings=settings)
```

from smartsim import Experiment

```
# Init Experiment and specify to launch locally
exp = Experiment(name="getting-started", launcher="local")

# settings to execute the command "echo hello!"
settings = exp.create_run_settings(exe="echo", exe_args="hello!", run_command=None)

# create the simple model instance so we can run it.

M1 = exp.create_model(name="tutorial-model", run_settings=settings)
```

Experiment.create_run_settings is used to create a **RunSettings** instance for our **Model**. **RunSettings** describe how a **Model** should be executed provided the system and available computational resources.

Our first Model will simply print **hello** using the shell command **echo**.

```
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exp = Experiment(name="getting-started", launcher="local")

# settings to execute the command "echo hello!"
settings = exp.create_run_settings(exe="echo", exe_args="hello!", run_command=None)

# create the simple model instance so we can run it.
M1 = exp.create_model(name="tutorial-model", run_settings=settings)

exp.start(M1, block=True, summary=True)
```

from smartsim import Experiment

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# Init Experiment and specify to launch locally
exp = Experiment(name="getting-started", launcher="local")

# settings to execute the command "echo hello!"
settings = exp.create_run_settings(exe="echo", exe_args="hello!", run_command=None)

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M1 = exp.create_model(name="tutorial-model", run_settings=settings)

exp.start(M1, block=True, summary=True)
```

Once the **Model** has been created by the **Experiment**, it can be **started**.

By setting **summary=True**, we can see a summary of the experiment printed before it is launched.

We also explicitly set **block=True** (even though it is the default), so that Experiment.start waits until the last **Model** has finished before returning.

from smartsim import Experiment

```
# Init Experiment and specify to launch locally
exp = Experiment(name="getting-started", launcher="local")

# settings to execute the command "echo hello!"
settings = exp.create_run_settings(exe="echo", exe_args="hello!", run_command=None)

# create the simple model instance so we can run it.
M1 = exp.create_model(name="tutorial-model", run_settings=settings)

exp.start(M1, block=True, summary=True)
```

print("Content of tutorial-model.out:")
with open(outputfile, 'r') as fin:
 print(fin.read())
print("Content of tutorial-model.err:")
with open(errorfile, 'r') as fin:
 print(fin.read())

outputfile = './tutorial-model.out' errorfile = './tutorial-model.err'

The model has completed and two output files have been created.

Normal output in **tutorial-model.out**Error output in **tutorial-model.err**

```
# Init Experiment and specify to launch locally
exp = Experiment(name="getting-started", launcher="local")
# settings to execute the command "mpirun -np 2 echo hello world!"
openmpi settings = exp.create run settings(exe="echo",
                          exe args="hello world!",
                          run command="mpirun")
openmpi settings.set tasks(2)
# create and start the MPI model
ompi model = exp.create model("tutorial-model-mpirun", openmpi settings)
exp.start(ompi model, summary=True)
exp.start(ompi model, block=True, summary=True)
outputfile = './ tutorial-model-mpirun.out'
print("Content of tutorial-model-mpirun.out:")
with open(outputfile, 'r') as fin:
  print(fin.read())
```

Use **mpirun**

```
# Init Experiment and specify to launch locally
exp = Experiment(name="getting-started", launcher="local")
# settings to execute the command "mpirun -np 2 echo hello world!"
openmpi settings = exp.create run settings(exe="echo",
                          exe args="hello world!",
                          run command="mpirun")
openmpi settings.set tasks(2)
# create and start the MPI model
ompi model = exp.create model("tutorial-model-mpirun", openmpi settings)
exp.start(ompi model, summary=True)
exp.start(ompi model, block=True, summary=True)
outputfile = './ tutorial-model-mpirun.out'
print("Content of tutorial-model-mpirun.out:")
with open(outputfile, 'r') as fin:
  print(fin.read())
```