Hewlett Packard Enterprise

LUMI AI Course:

Coupling machine learning with HPC simulation

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Agenda

- Where might machine learning play a role in simulation?
- Workflows for coupling HPC simulation with AI
- Challenges and approaches
- SmartSim
- SmartSim Examples (+ some non-SmartSim ones)

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Where might machine learning play a role with Simulation

Completely replace a simulation

- AI model learns to produce output by observing simulation inputs/outputs

Use simulation as one input to a machine learning model

- For example, use an ML model to account for location-specific history (weather)

Replace modeling of physical processes or parameterised models with machine learning, Examples..

- Reduce search space for Drug discovery
- a turbulence model in an ocean simulation
- Particle physics: particle tracks
- Atomic potentials (computational chemistry)

- We will concentrate on the case where AI is coupled with simulation

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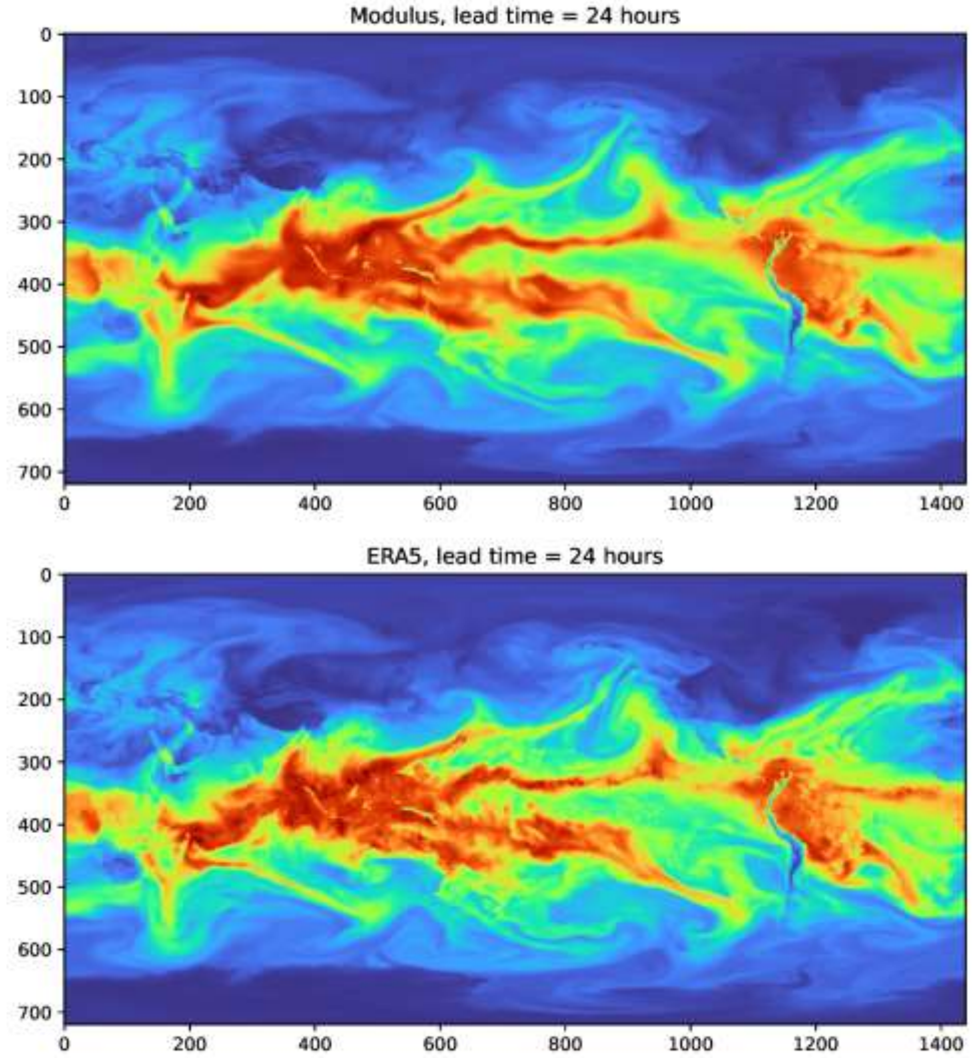
Why HPC and AI instead of HPC vs. AI?

- Can AI replace numerical-based approaches?
  - Short answer: no, still limited by data
- Benefits of AI models
  - Can be run more quickly than traditional numerical models
  - Simpler to run, does not need complicated software infrastructure and HPC resources
  - Skillful models can be considered lower-order representations of 'true' simulation
    - Useful for exploring parameter space/uncertainties
- Downsides of AI models
  - How do you add process complexity?
  - Can they extrapolate beyond the data they have been trained on?
- Challenges to combining HPC&AI
  - Numerical: How can you characterize the stability and accuracy of an ML model in that context
  - Technical:
    - How do you connect Fortran/C/C++ codebases to ML packages?
    - How do you appropriately balance high-value/cost GPU resources in predominantly CPU-based code?



https://docs.nvidia.com/deeplearning/modulus/modulus-sym/user_guide/neural_operators/fourcastnet.html#introduction

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HPC Applications combined with AI software drive innovation

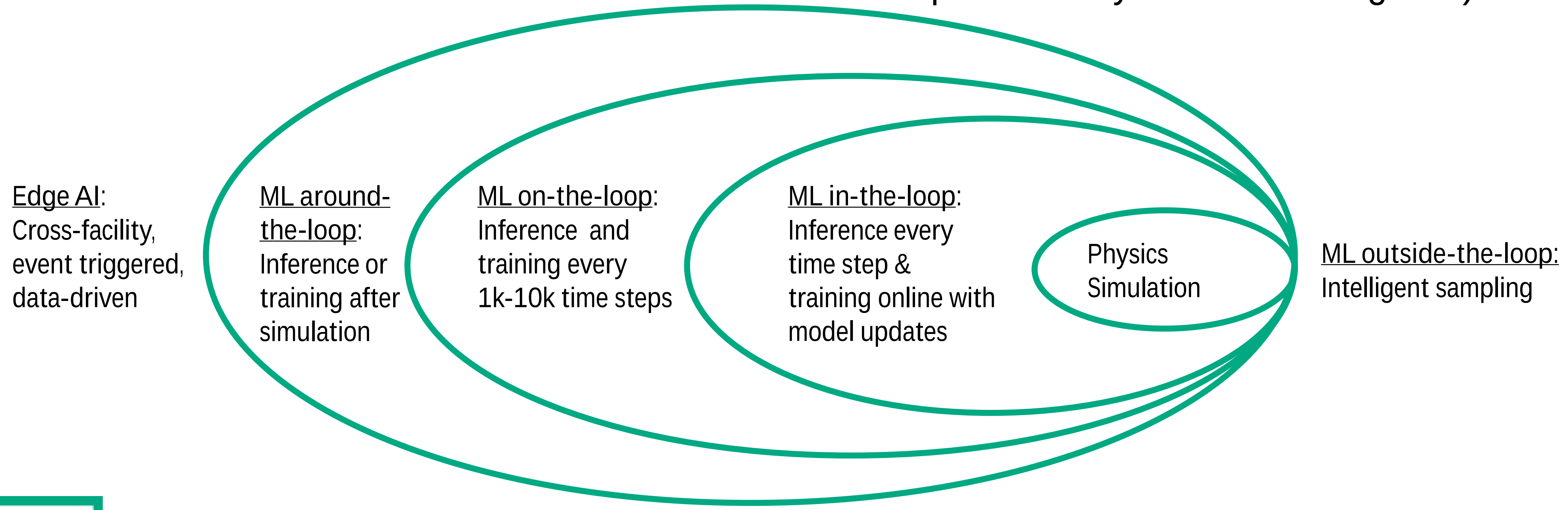
Combining AI software and traditional HPC applications at different levels of a workflow unlocks innovative solutions

ML around-the-loop

- Automatic parameter tuning
- New data assimilation techniques

ML in-the-loop

- Embedding machine-learning predictions within numerical solvers
- On-the-fly analysis and visualization (e.g. principal component analysis via streaming SVD)



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Challenges and approaches

- Machine learning frameworks are invariably accessed via Python
- HPC simulation is most likely written in C/C++/Fortran
- We could implement ML in our simulation language but…
  - A lot of work for something likely already done and likely more efficiently than we will
  - We don’t get access to tools to train models
  - Hard to integrate a model externally developed

Some approaches:

- Use language-interoperability to interface between simulation and Machine Learning
- Couple ML components to our simulation (sockets, messaging transports, files)
- Use a framework designed to provide such interoperability (via network transport or APIs)
  - Fortran Keras Bridge
  - SmartSim (originally from Cray)

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Language Interoperability

Interoperability by calling conventions

- Fortran and Python
  - f2py and fmodpy or forpy can help build wrappers to call Fortran from Python
  - ISO C bindings on the Fortran side interfaced to ctypes/Cython on the python side
  - Really helpful if what you are interfacing to has direct support for the Numpy C API
- C++/C and Python
  - Cython, pybind11, SWIG

Interoperability at Framework Level (Fortran)

- Directly call Tensorflow or Torch APIs from Fortran using ISO C interoperability

  In both cases you may have to save model in a special format

Alternatively

- Communicate workflow components via filesystem or network

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About SmartSim

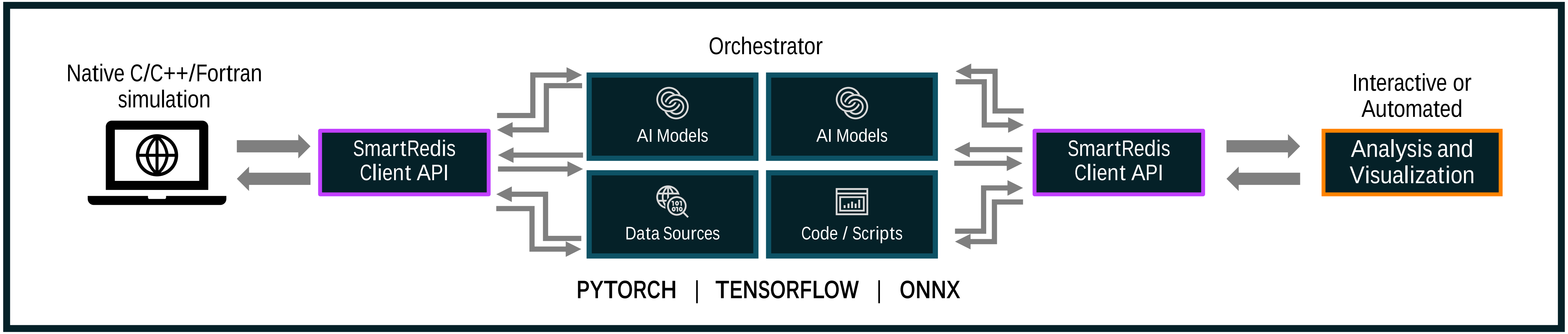
The SmartSim open-source library bridges the divide between traditional numerical simulation and data science

- Provides a loose-coupling philosophy for combining HPC & AI

SmartSim enables simulations to be used as engines within a system, producing data, consumed by other services to create new applications

- Use Machine Learning (ML) models in existing Fortran/C/C++ simulations
- Communicate data between C, C++, Fortran, and Python applications
- Train ML models and make predictions using TensorFlow, PyTorch, and ONNX
- Analyze data streamed from HPC applications while they are running

All of these can be done *without touching the filesystem*



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Creating a SmartSim experiment

Integration steps

1. Embed SmartRedis calls (C/C++/Fortran) into the application (~10 lines of code)
2. Write a driver script using the SmartSim Python library to describe and launch the workflow

   Driver script can check status of components

1. Added simulation code

```fortran
client = smartredis_CS%client

...

sr_return_code = client%put_tensor("features"//CS%key_suffix, CS%features_array, shape(CS%features_array))
model_out(1) = "EKE"//CS%key_suffix
model_in(1) = "features"//CS%key_suffix
sr_return_code = smartredis_CS%client%run_model(CS%model_key, model_in, model_out)

sr_return_code = client%unpack_tensor( model_out(1), CS%MEKE_vec, shape(CS%MEKE_vec) )

...
```

2. SmartSim Driver Script

```python
# Create experiment

experiment = Experiment("AI-EKE-MOM6", launcher="auto")

# Create ensemble

ensemble_batch_settings = experiment.create_batch_settings(
    nodes      = ensemble_size*nodes_per_member,
    time       = walltime,
    batch_args = mom6_batch_args
)

mom6_run_settings = experiment.create_run_settings(mom6_exe_path)
mom6_run_settings.set_tasks_per_node(tasks_per_node)
mom6_run_settings.set_tasks(nodes_per_member*tasks_per_node)

mom_ensemble = experiment.create_ensemble(
    "MOM",
    batch_settings = ensemble_batch_settings,
    run_settings   = mom6_run_settings,
    replicas       = ensemble_size
)

mom_ensemble.attach_generator_files(
    to_configure=glob("../MOM6_config/configurable_files/*"),
    to_copy="../MOM6_config/OM4_025",
    to_symlink="../MOM6_config/INPUT"
)
```

```python
# Configure ensembles

MOM6_config_options = {
    "SIM_DAYS": 15, # length of simulations
    "EKE_MODEL": eke_model_name,
    "EKE_BACKEND": eke_backend,
    "DOMAIN_LAYOUT": domain_layout,
    "MASKTABLE": mask_table
}

MOM6_config_options.update( {
    "SMARTREDIS_COLOCATED":"False",
    "SMARTREDIS_COLOCATED_STRIDE":0,
    "SMARTREDIS_CLUSTER": "False"
})


MOM6_config_options.update( {'SMARTREDIS_CLUSTER':'True'} )

for model in ensemble:
    model.params = MOM6_config_options
    model.register_incoming_entity(model)


# Create in-memory database

orchestrator = exp.create_database(
    port = orchestrator_port,
    interface = orchestrator_interface,
    db_nodes = orchestrator_nodes,
    time=walltime,
    threads_per_queue=2,
    batch=True)

orchestrator.set_cpus(18)
orchestrator.set_batch_arg("constraint", orchestrator_node_features)
orchestrator.set_batch_arg("exclusive",None)

experiment.generate( mom_ensemble, orchestrator, overwrite=True )

experiment.start(mom_ensemble, orchestrator, block=True, summary=True)
```

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Added client simulation code

Reference to initialized client

Put data into database (Orchestrator) naming it

Execute ML models output to database

```
client = smartredis_CS%client

...

sr_return_code = client%put_tensor("features"//CS%key_suffix, CS%features_array, shape(CS%features_array))
model_out(1) = "EKE"//CS%key_suffix
model_in(1) = "features"//CS%key_suffix
sr_return_code = smartredis_CS%client%run_model(CS%model_key, model_in, model_out)

sr_return_code = client%unpack_tensor( model_out(1), CS%MEKE_vec, shape(CS%MEKE_vec) )

...
```

Retrieve previously named data

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SmartSim driver script (create ensemble)

Driver Script
- Describes, launches and manages workflow with applications and ML infrastructure

Experiment
- Top level object that provides factory methods to create workflow objects

Batch Settings
- Can be used if application is to be launched non-interactively, including as ensembles

RunSettings object
- Describes system-specific resources (nodes, accelerators, cpus etc.

Model object
- Holds information on user application

Application file handling
- Can be parameterized (also args)

```python
# Create experiment

experiment = Experiment("AI-EKE-MOM6", launcher="auto")


# Create ensemble

ensemble_batch_settings = experiment.create_batch_settings(
    nodes      = ensemble_size*nodes_per_member,
    time       = walltime,
    batch_args = mom6_batch_args
)

mom6_run_settings = experiment.create_run_settings(mom6_exe_path)
mom6_run_settings.set_tasks_per_node(tasks_per_node)
mom6_run_settings.set_tasks(nodes_per_member*tasks_per_node)

mom_ensemble = experiment.create_ensemble(
    "MOM",
    batch_settings = ensemble_batch_settings,
    run_settings   = mom6_run_settings,
    replicas       = ensemble_size
)

mom_ensemble.attach_generator_files(
    to_configure=glob("../MOM6_config/configurable_files/*"),
    to_copy="../MOM6_config/OM4_025",
    to_symlink="../MOM6_config/INPUT"
)
```

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SmartSim **driver script… (configure ensemble members)**

```
# Configure ensembles

MOM6_config_options = {
    "SIM_DAYS": 15, # length of simlations
    "EKE_MODEL": eke_model_name,
    "EKE_BACKEND": eke_backend,
    "DOMAIN_LAYOUT": domain_layout,
    "MASKTABLE": mask_table
}

MOM6_config_options.update( {
    "SMARTREDIS_COLOCATED":"False",
    "SMARTREDIS_COLOCATED_STRIDE":0,
    "SMARTREDIS_CLUSTER": "False"
})


MOM6_config_options.update( {'SMARTREDIS_CLUSTER':'True'} )

for model in ensemble:
    model.params = MOM6_config_options
    model.register_incoming_entity(model)
```

Ensemble members have identical parameters in this example

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SmartSim **driver script… (configure and start ensemble members)**

```
# Create in-memory database

orchestrator = exp.create_database(
    port = orchestrator_port,
    interface = orchestrator_interface,
    db_nodes = orchestrator_nodes,
    time=walltime,
    threads_per_queue=2,
    batch=True)

orchestrator.set_cpus(18)
orchestrator.set_batch_arg("constraint", orchestrator_node_features)
orchestrator.set_batch_arg("exclusive",None)

experiment.generate( mom_ensemble, orchestrator, overwrite=True )

experiment.start(mom_ensemble, orchestrator, block=True, summary=True)
```

Setup Orchestrator (stores ML models/tensors and executes models

Write all files needed for workflow entities

GO

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Online Inference, multiple languages

Fortran

```fortran
call client%put_tensor(in_key, array, shape(array))

inputs(1) = in_key
outputs(1) = out_key
call client%run_model(model_name, inputs, outputs)
result(:,:) = 0.
call client%unpack_tensor(out_key, result, shape(result))
```

C++

```cpp
// Put the image tensor on the database
client.put_tensor(in_key, img.data(), {1,1,28,28},
                  SmartRedis::TensorType::flt,
                  SmartRedis::MemoryLayout::contiguous);

// Run model already in the database
client.run_model(model_name, {in_key}, {out_key});

// Get the result of the model
std::vector<float> result(1*10);
client.unpack_tensor(out_key, result.data(), {10},
                     SmartRedis::TensorType::flt,
                     SmartRedis::MemoryLayout::contiguous);
```

Python

```python
client.put_tensor("input", torch.rand(20, 1, 28, 28).numpy())

# put the PyTorch CNN in the database in GPU memory
client.set_model("cnn", net, "TORCH", device="GPU")

# execute the model, supports a variable number of inputs and outputs
client.run_model("cnn", inputs=["input"], outputs=["output"])

# get the output
output = client.get_tensor("output")
print(f"Prediction: {output}")
```

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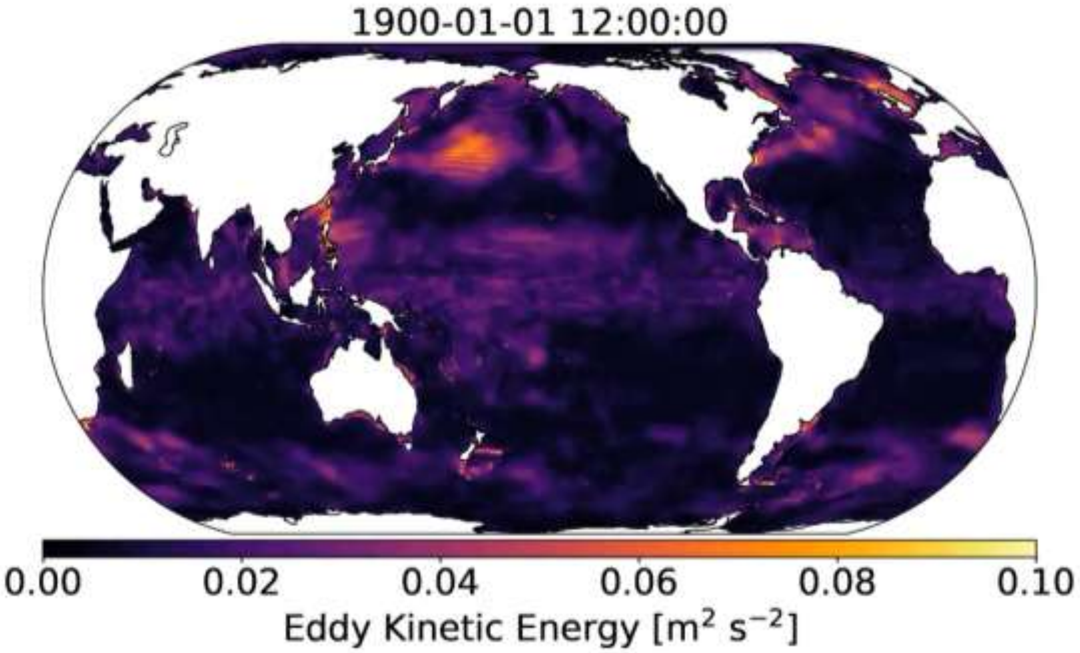
EXAMPLES OF USING AI IN-THE-LOOP IN THE MOM6 OCEAN MODEL



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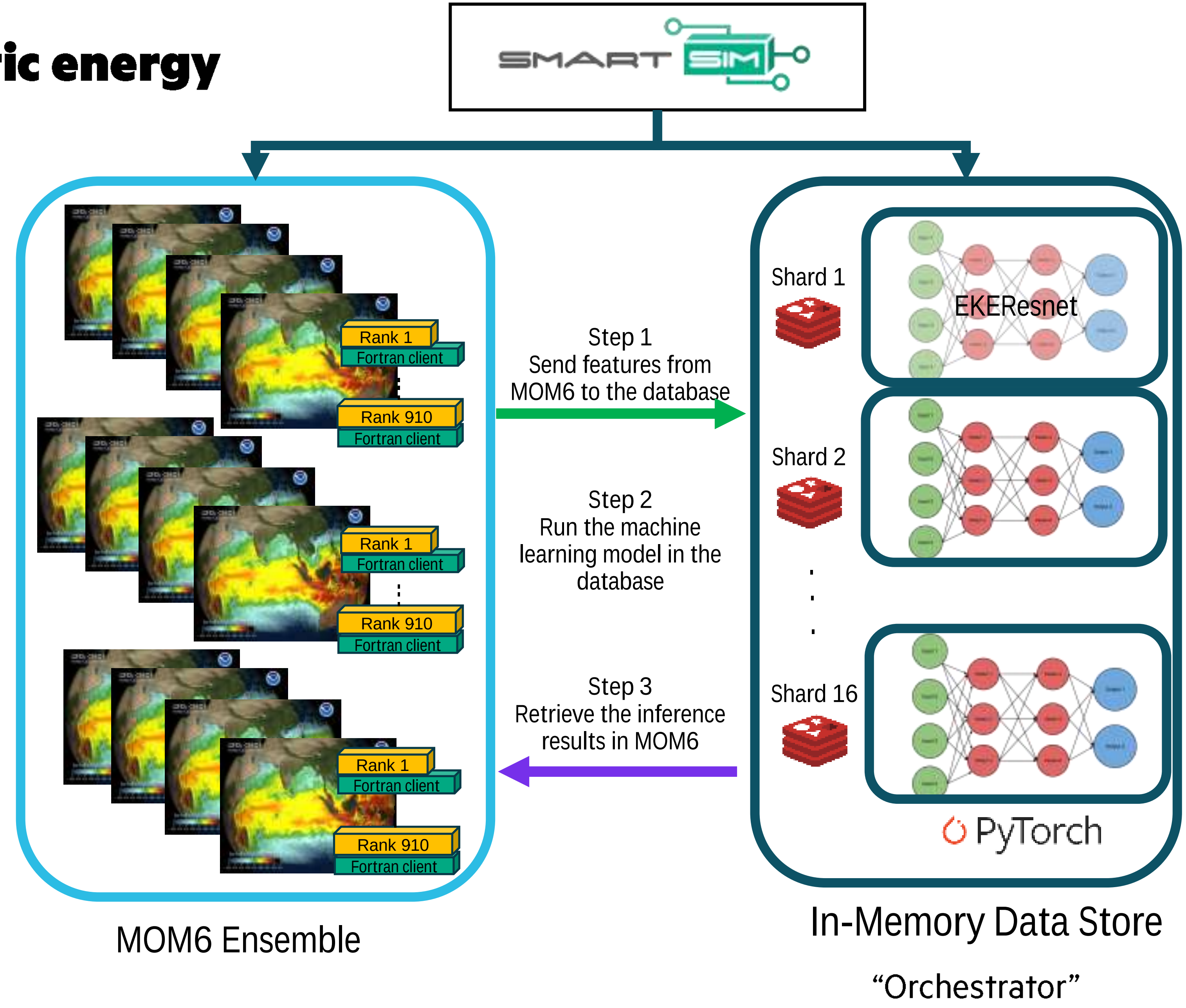
Improving MOM6’s eddy kinetic energy

Original MEKE Scheme (Jansen et al. [2015]):
- Integrate a prognostic eddy kinetic energy equation with parameterized sources/sinks
- Use length-scale relations to convert EKE to Gent-McWilliams, Redi, and viscosity coefficients

Known shortcomings
- EKE equation has terms which are tunable and/or have errors which may be first-order

Propose ML-based solution
- Use an eddy-resolving simulation to train a neural network to learn the relationship between large-scale quantities and eddy kinetic energy
- Embed neural network predictions in eddy-permitting simulations



SmartSim IL launching MOM6 and Orchestrator

MOM6 retrieves input features

EKEResNet predicts and returns turbulent kinetic energy values

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Using SmartSim in mom6 for turbulence modelling [NCAR+HPE]

- Experiment setup
  - 12 ensemble members
  - 10,920 CPUs (~200 nodes) and 16 P100s (16 nodes)
  - Inference embedded at the tracer timestep (3hr)
    – 970 billion inferences over 10 simulation years
    – 1.6 million inferences per second

- Key results:
  - Offloading ML inference to dedicated nodes improves GPU utilization while incurring small communication cost
  - With SmartSim, the accuracy over the current state of the art improved by over 20%
  - Neural network more accurately predicts (20% RMSE improvement) rather than the prognostic approach
  - Overall performance only decreased by 10% while only minimally increasing hardware footprint of the model

Partee et al. [2022]: Using Machine Learning at scale in numerical simulations with SmartSim: An application to ocean climate modeling

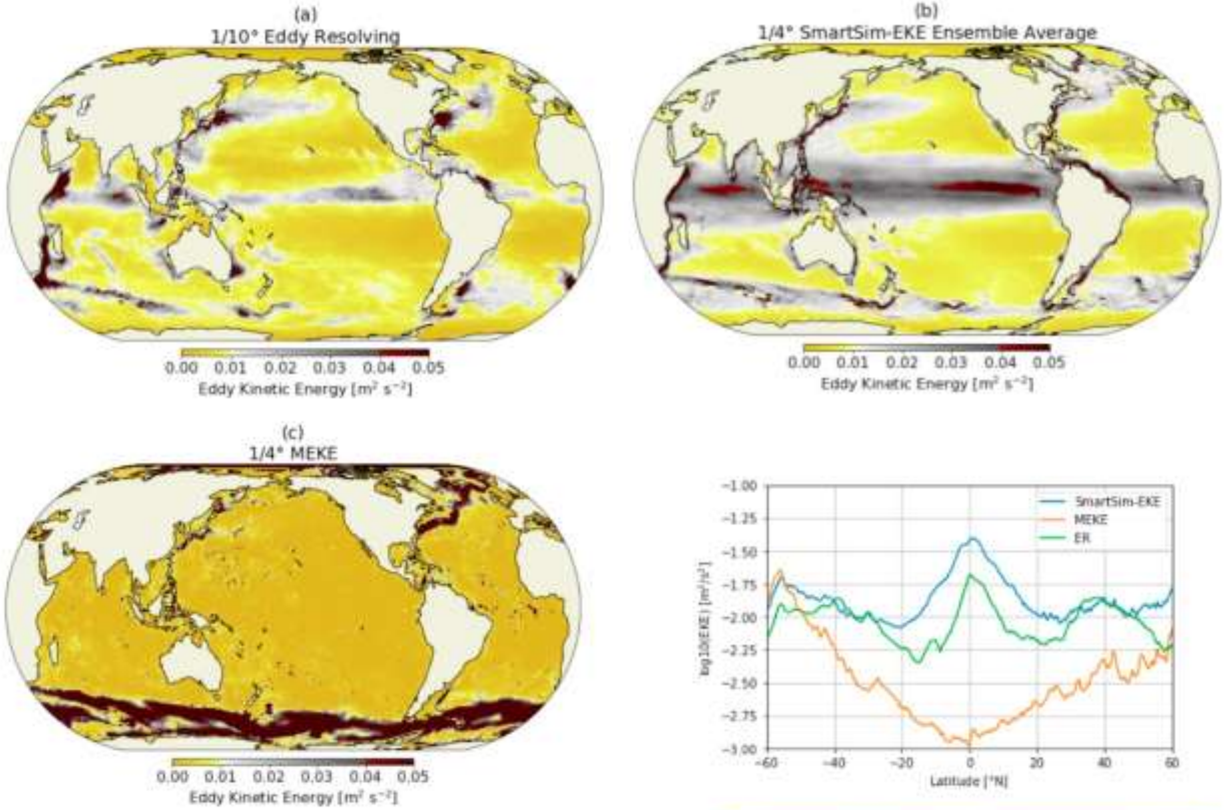

Fig. 7. Zonally averaged EKE (on a log10 scale) as a function of latitude from the ER, SmartSim-EKE, and MEKE.

EXAMPLES OF USING AI AROUND-THE-LOOP

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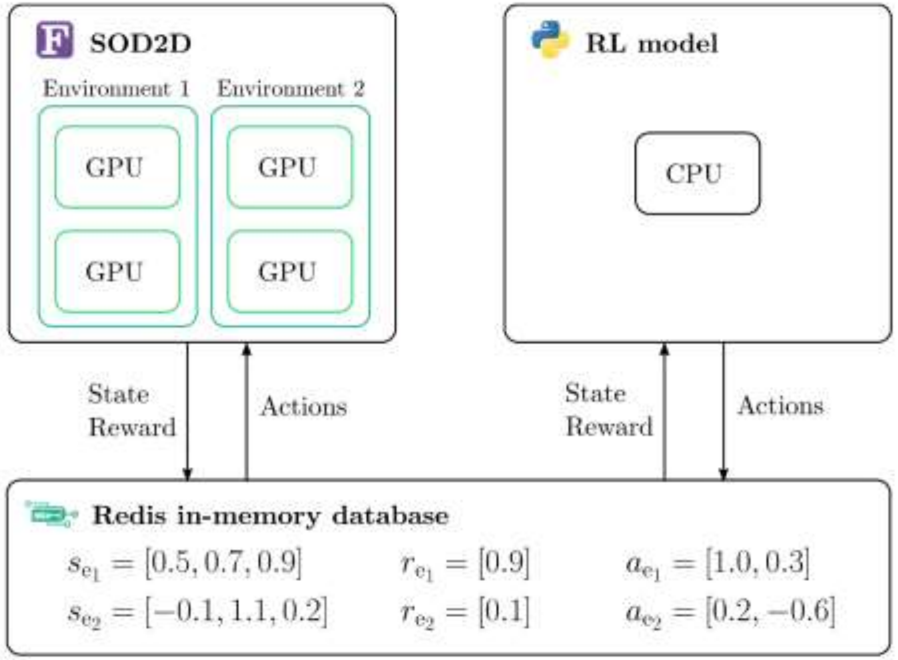
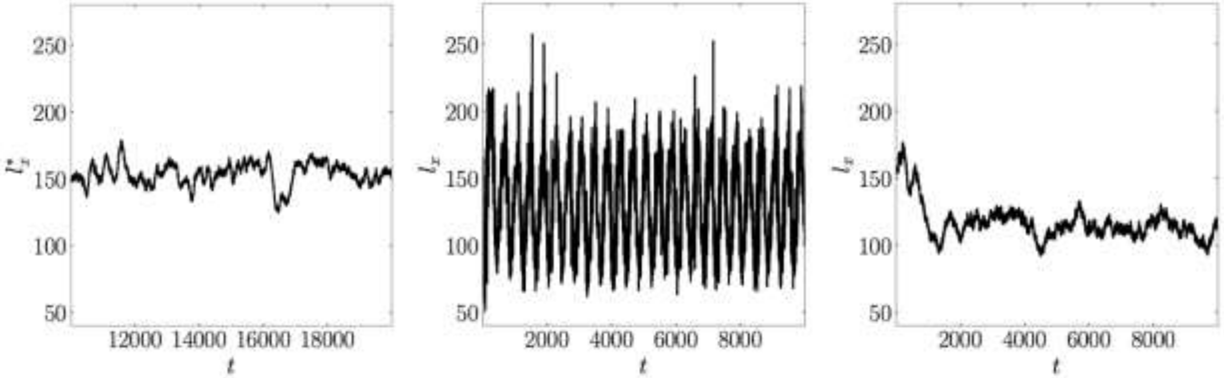
Active flow control through deep Reinforcement learning

- Goal: Reduce Turbulent Separation Bubble formation
- Method: Deep Reinforcement Learning with small NN
  - Reward based on recirculation length of turbulent bubble
    - Aim: minimize recirculation area
  - Environment: 72 points for the NN to “observe”
  - Action: NN can control actuators upwind of bubble





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Dynamic turbine wake steering in wind farms

- Reference: Project is work in progress, Andrew Moat, Imperial College London
- Turbine wakes can reduce efficiency of downstream turbines
- We can steer the wake by adjusting angle (yaw) of turbines
- In general, the system is very complex, changing wind direction/speed, multiple turbines, interaction of wakes etc.
- Use reinforcement learning to find some optimal set of angles to optimize power output
- Direct coupling with SmartSim an improvement over file-based coupling

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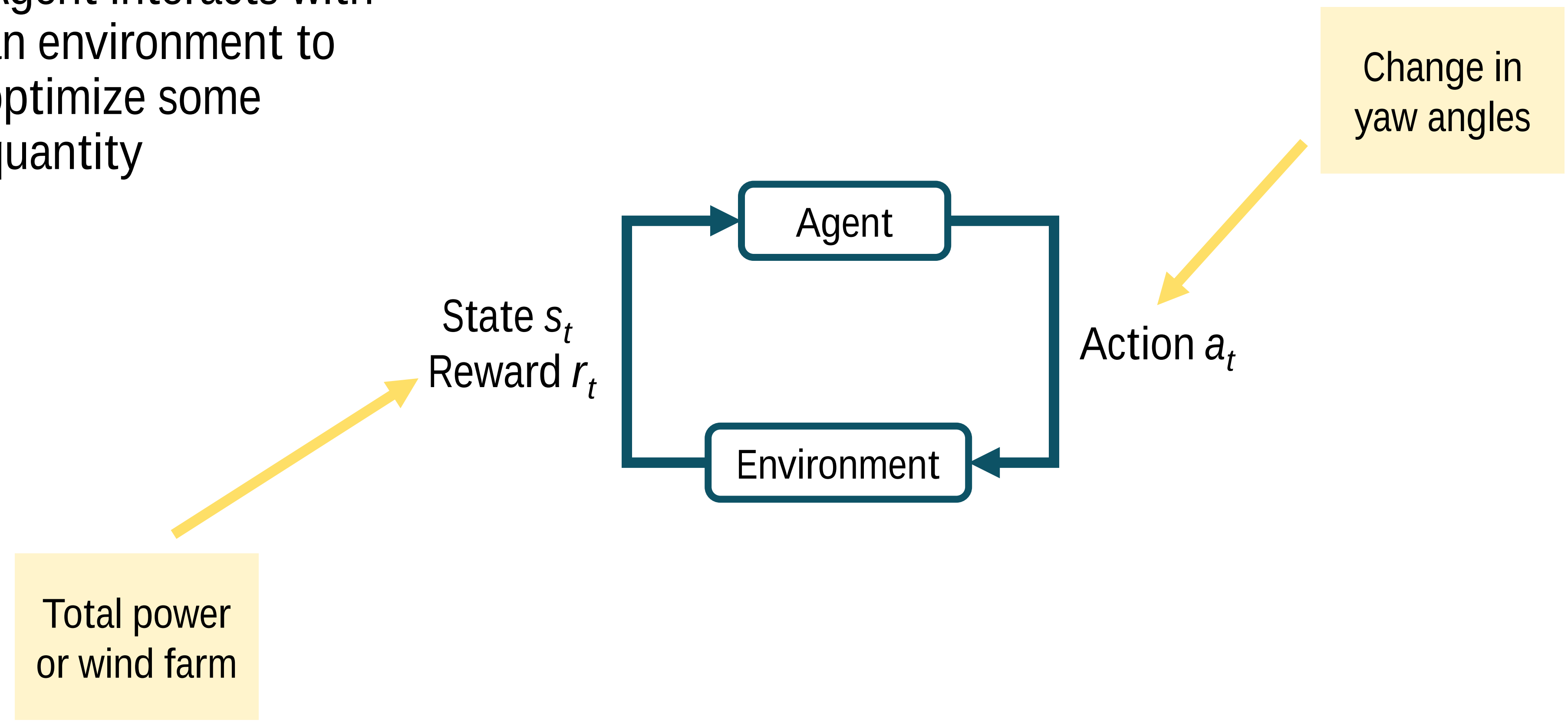
Reinforcement learning

- Agent interacts with an environment to optimize some quantity



Implementation

- Initial approach was to couple the Large Eddy simulation of the windfarm with pytorch reinforcement learning model
- Used file storage to communicate (a_t s_t r_t)
- Issues:
  - Large files often written was costly
  - Was not going to be practical when simulating larger wind farms
  - Made it difficult to train multiple environments at a time
- Moved to SmartSim
  - Now using Smart Redis database
- Modifications needed
  - XCompact3D Replace file ops with calls to send and retrieve data to smart-redis
  - Configured SmartSim to start XCompact3D environments/simulations (32 at a time for example)

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Experiment

- Setup
  - 32 Environments each with
  - 10 turbines
  - 128 cores per environment (a node)
  - 50 simulation timesteps per RL step
  - Batched into 512 frames for training

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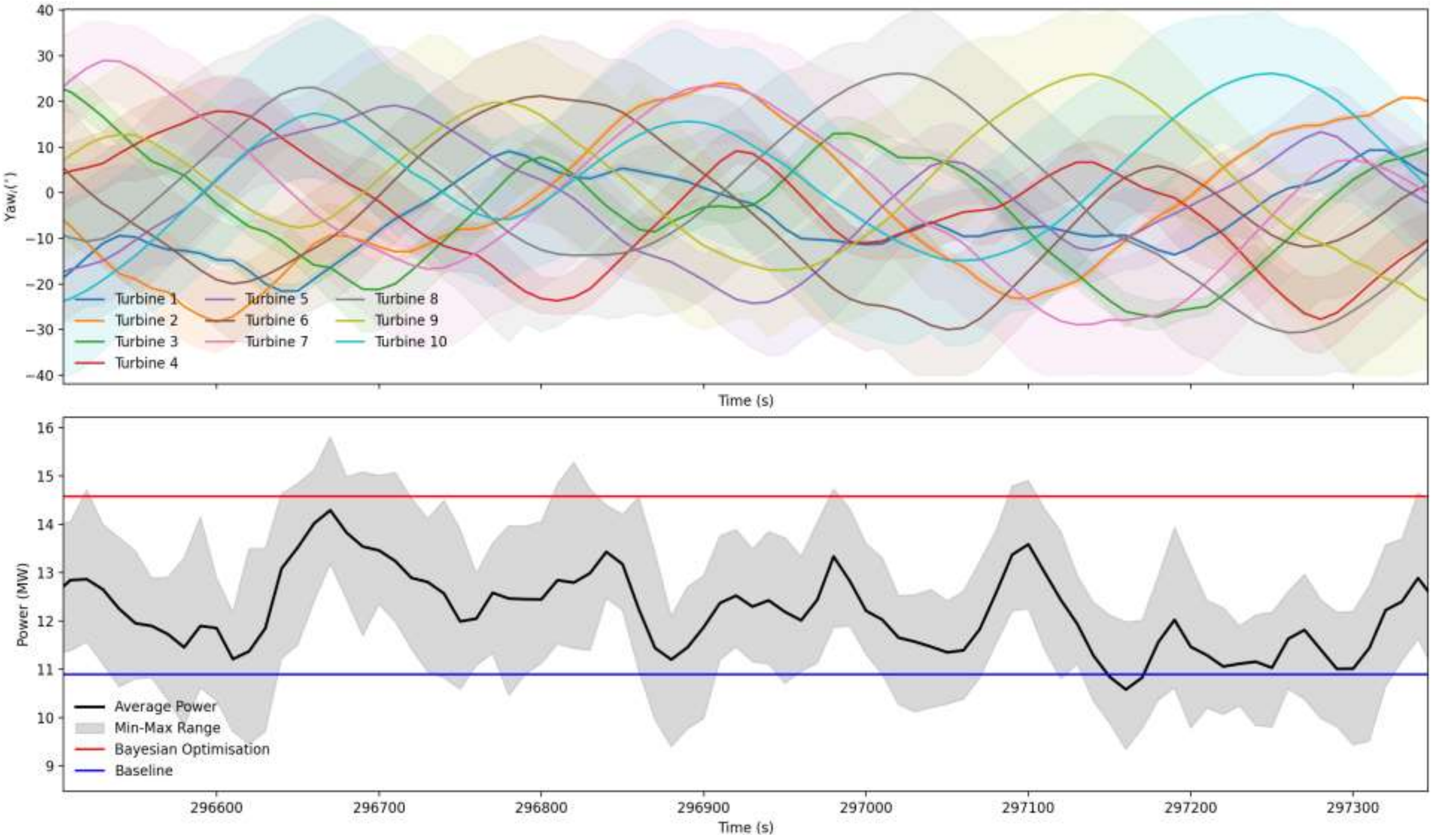
Initial Results

- After initial training the turbines settle down into being driven in sinusoidal pattern
- Better power output than without steering.



Other Examples of SmartSim use

Computational Fluid Dynamics

- OpenFOAM, FLEXI, PHASTA, libCEED, NekRS (in progress)

Climate and Weather

- MOM6, NEMO, CESM

Molecular Dynamics

- LAMMPS, OPENMM

In-situ Visualization workflow

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ML in Computational Chemistry: examples

- Examples encompass molecular dynamics, quantum simulation and macromolecules

- Density Functional Theory
  - Approximates solution to QM formulation of electron positions by parameterised basis functions
  - ML can be used to find those basis functions
  - References: Pure non-local machine-learned density functional theory for electron correlation, Large-Scale Materials Modeling at Quantum Accuracy:...
- DeepDriveMD example of selecting 'promising' protein folding solutions from an ensemble
  - Complex workflow
  - A SmartSim-based re-implementation of this workflow is available on GitHub as smartsim-openmm
  - Paper: DeepDriveMD: Deep-Learning Driven Adaptive Molecular Simulations for Protein Folding
- Nobel Prize in Chemistry 2024 for protein folding:
  Amino Acids combine to create proteins.
  Computational approaches: Rosetta -> Alphafold (NN) -> Alphafold2
  References: Nobel Press Release (includes reference to technical descriptions PDF PDF)

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References

- Language Interoperability
  - F2py and fmodpy intro https://www.matecdev.com/posts/fortran-in-python.html
  - forpy (https://github.com/ylikx/forpy)
  - pybind11 (https://github.com/pybind/pybind11)
  - Talk: Reducing the overhead of coupling machine learning models between Python and Fortran, https://www.youtube.com/watch?v=Ei6H_BoQ7g4 https://jackatkinson.net/slides/RSECon23/RSECon23.html#/title-slide

- Interoperability at framework level:
  - Fortran Keras Bridge, tensorflow but not very active
    - https://github.com/scientific-computing/FKB
    - https://arxiv.org/abs/2004.10652

- SmartSim
  - https://github.com/CrayLabs/SmartSim
  - https://github.com/CrayLabs/SmartSim-Zoo
  - ARCHER2 Webinar: Exploring new computational frontiers with SmartSim

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Questions?

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