Coupling Simulations with AI

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AI4Science Series:
Advanced Topics in AI for Science
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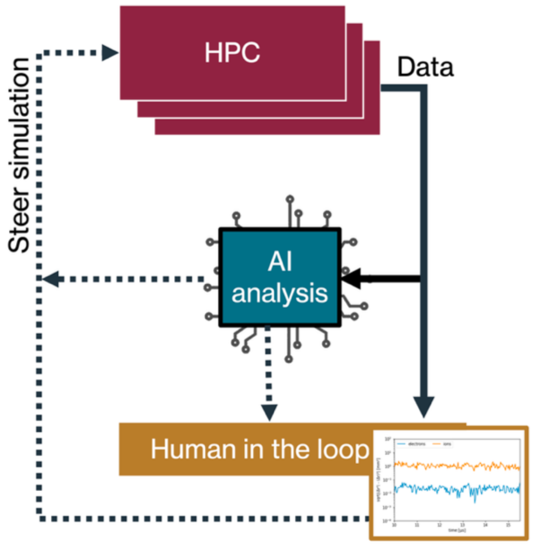
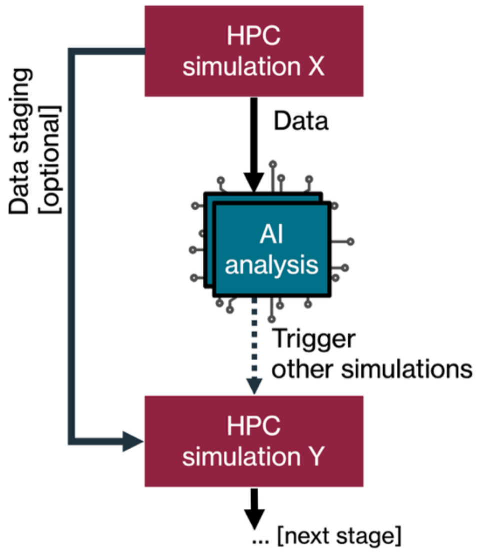
Why Couple HPC Simulations with AI/ML?

- ❑ Substitute inaccurate or expensive components of simulation with ML models
  - ➢ E.g.: Closure or surrogate modeling
- ❑ Optimize simulation parameters on-the-fly
  - ➢ E.g.: Select solver parameters at runtime based on AI inference
- ❑ Avoid IO bottleneck and disk storage issues during offline training
  - ➢ E.g.: In situ/online training through data streaming or in-memory staging
- ❑ Active learning and model fine-tuning
  - ➢ E.g.: Continuous fine-tuning and deployment of model
  - ➢ E.g.: Access training data not available during offline pre-training
- ❑ Steering of simulation ensembles
  - ➢ E.g.: Design space exploration or parameter optimization guided by AI

How to Couple HPC Simulations and AI/ML?

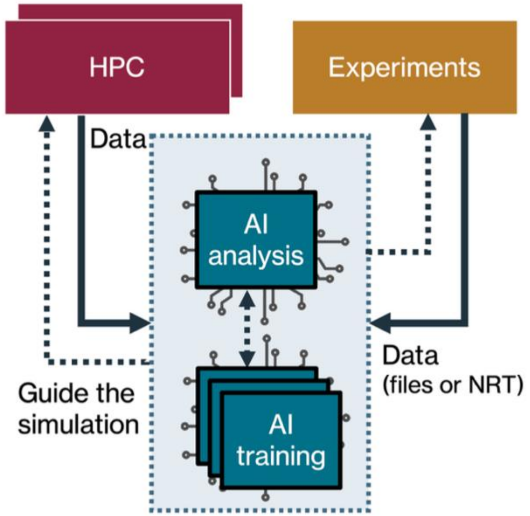
Steering of Ensembles

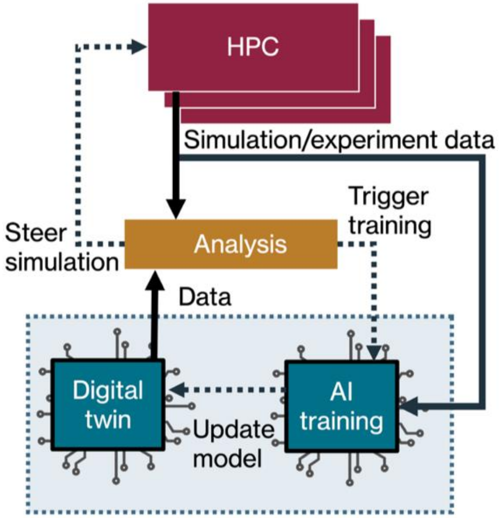




Optimize Simulation Parameters

Active Learning/
Online Fine-Tuning





Digital Twin

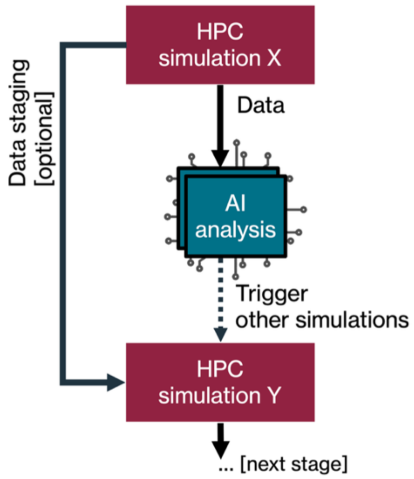
Brewer et al. "AI-coupled HPC workflow applications, middleware and performance." *arXiv:2406.14315* (2024)

How to Couple HPC Simulations and AI/ML?

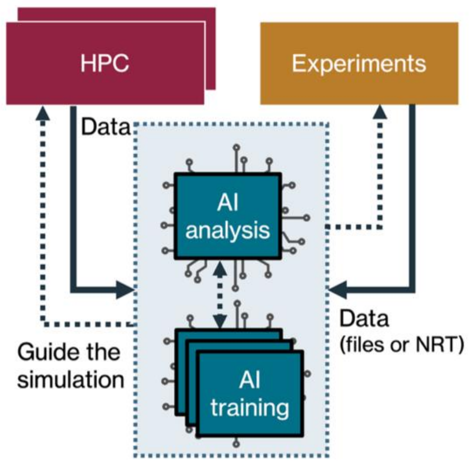
Type of Coupling

- ❑ ML inference only
- ❑ ML training only
- ❑ Both training and inference

Inference Only



Training and Inference



Programming Languages and Programming Models

- ❑ Simulation and ML components often written in different languages
- ❑ AI/ML relies heavily on vendor libraries (stuck with vendor language or programming model)
- ❑ Separate or shared parallelism strategies
  - ➢ Shared vs. separate MPI communicators
  - ➢ Domain decomposition vs. batch or model parallelism

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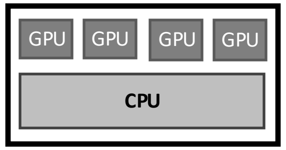
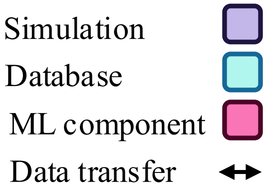
How to Couple HPC Simulations and AI/ML?

Heterogeneous HPC node

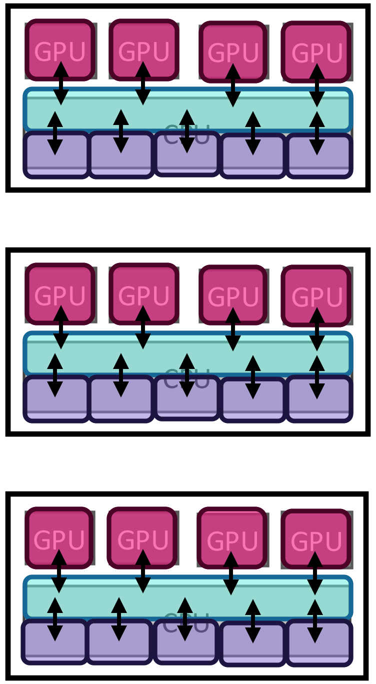




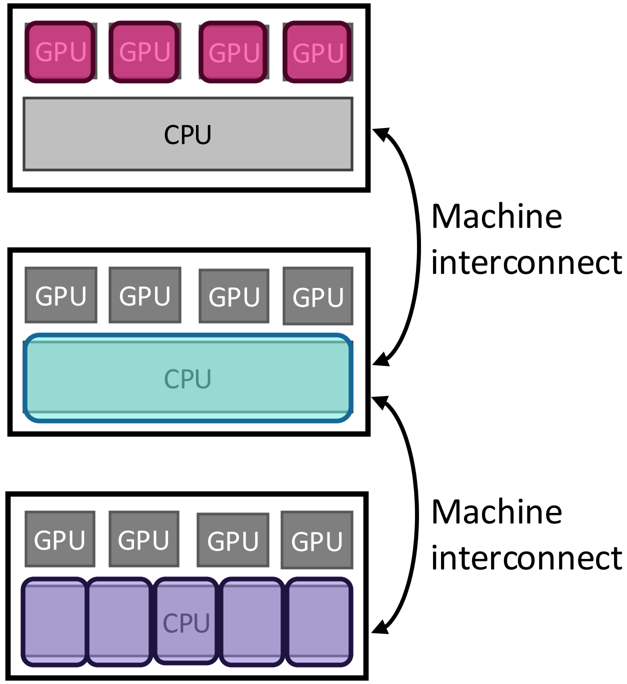
<u>Physical Proximity</u>

- ❑ Colocation: components share the same nodes
- ❑ Node-level clustering: components use different nodes on the same system
- ❑ Multi-system: components are run on separate specialized systems

Colocated Deployment



Node Clustered Deployment



System Clustered Deployment

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How to Couple HPC Simulations and AI/ML?

Data Access

- Coupling simulation and ML requires frequent data sharing/transfer between components
- Direct: components share same memory space (may allow for zero-copy data transfer)
- Indirect: components use distinct logical memory (requires data copy and may require data transfer)

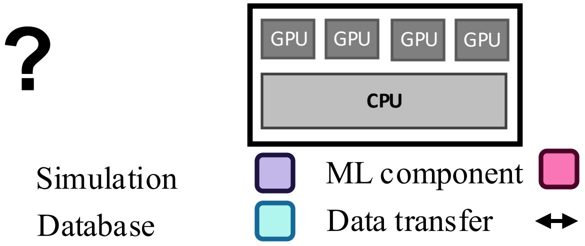
Data Staging or Streaming

- Staging: data is staged in memory or on disk (can reduce idle time but increases number of transfers)
- Streaming: data is streamed directly between components (can increase idle time due to synchronization)

Childs et al., "A terminology for in situ visualization and analysis systems", Intl. Journal of High Performance Computing Applications, 2020

How to Couple HPC Simulations and AI/ML?

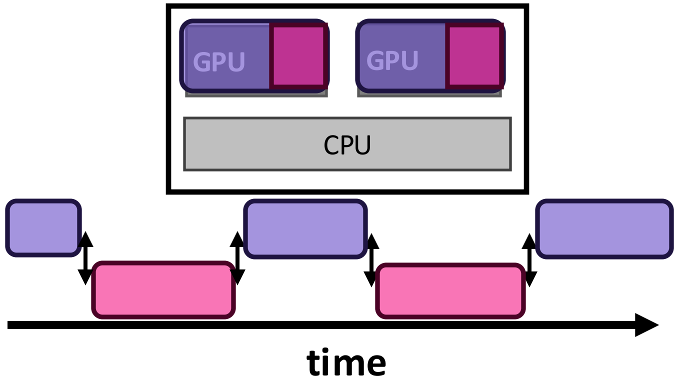
Heterogeneous HPC node



Execution Management

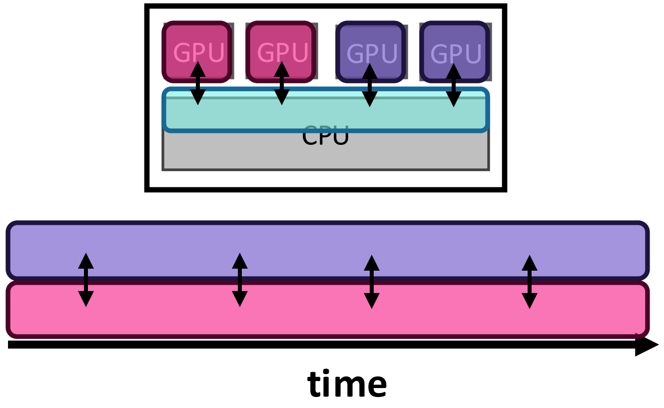
- ❑ Time division (tight coupling)
  - ➢ Components run on same compute resources (may even use same processes)
  - ➢ Staggered in time, execution of one component halts the other
  - ➢ May allow for direct memory access and no data copy/transfer
  - ➢ Idle time of individual components may be significant

Time Division: Same Compute Hardware



- ❑ Space division (loose coupling)
  - ➢ Components run on separate compute resources
  - ➢ Concurrent in time, components run simultaneously
  - ➢ Minimal idle time of components for fast data copy/transfer
  - ➢ Usually requires indirect memory access with data copy/transfer

Space Division: Separate Compute Hardware



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How to Couple HPC Simulations and AI/ML?

- ❑ Coupling simulation and AI/ML can be a complex space to navigate
- ❑ Implementation choices can vary significantly depending on ML task and application needs
- ❑ This session will cover some common tools and approaches supported at ALCF

Exercise 1: ML-in-the-Loop for Molecular Design

Science Problem: identify high value molecules (i.e. molecules with high ionization energy) among a large search space of potential candidates

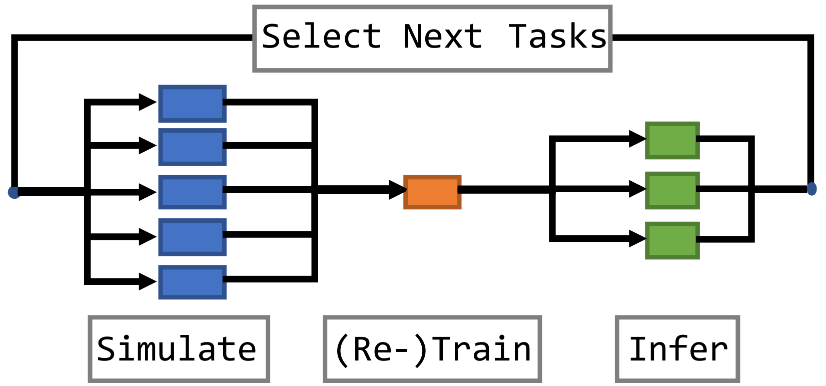
Challenge: The simulation is too computationally expensive to run for every candidate molecule

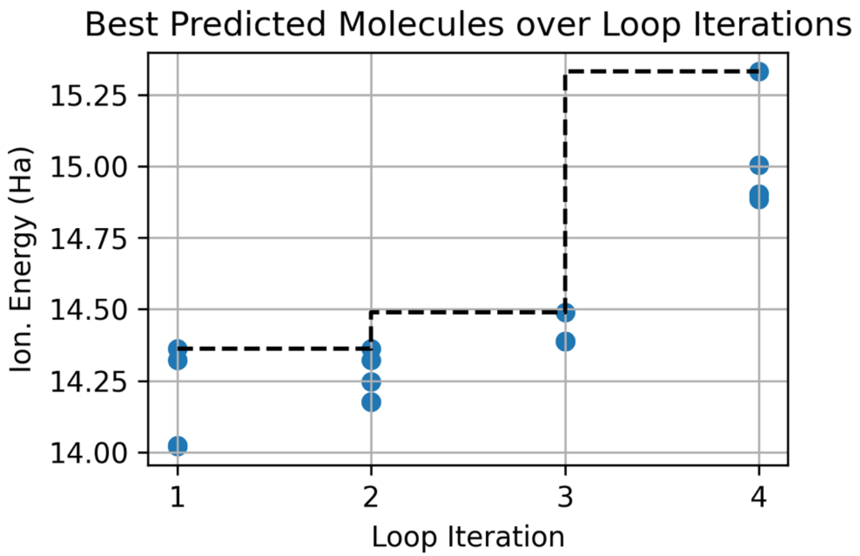
Approach: Create an active learning workflow that couples simulation with machine learning to simulate only high value candidates

Tools:

- ❑ **Parsl** is used for task launching and integration
- ❑ Use RDkit and scikit-learn to train a k-nearest neighbor (knn) model
- ❑ Simulations done with MD package xTB

Workflow Pattern: ML Components steer Simulations





ML-in-the-Loop Workflow for Molecular Design

Hands-On Time

Observations from ML-in-the-Loop Exercise

- AI/ML methods can significantly speed up traditional compute-heavy simulation tasks
  - From `2_training_and_inference.py`, screening through ~130,000 compounds with knn model is significantly faster than simulating even just a few compounds

```
Submitted 16 simulations to start training ...
...
Training data collected in 9.65 seconds!

...

Starting training and inference ...
Training and inference completed in 5.13 seconds!

...
```

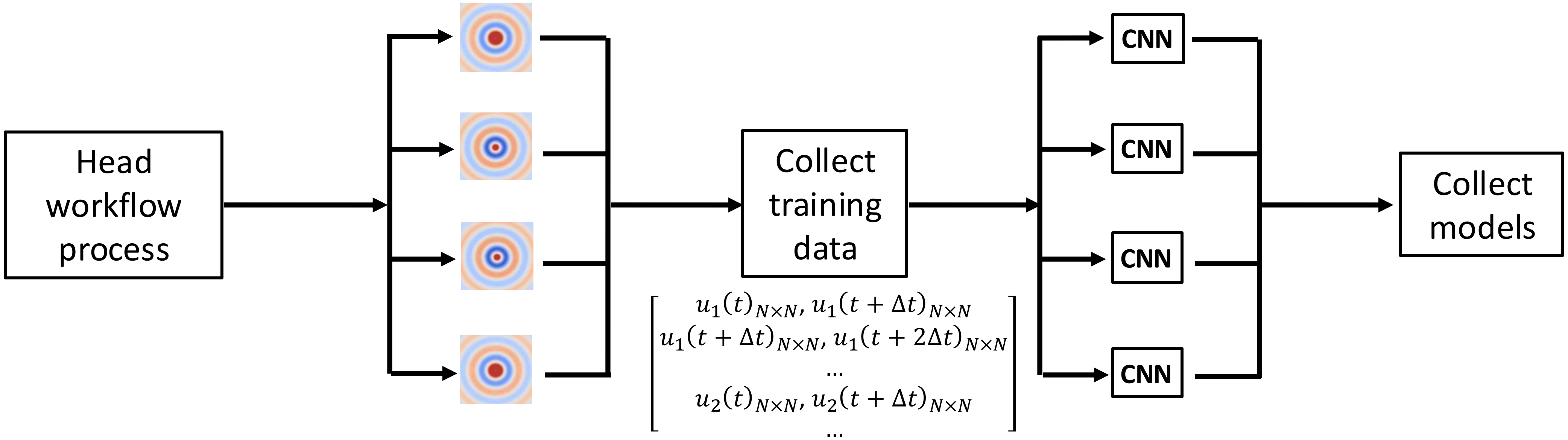
- Active learning can help refine AI/ML models by intelligently selecting training data and fine-tune models towards a specific task
- Parsl allows us to seamlessly automate and scale sim+AI workflows by deploying tasks in parallel on multiple Polaris nodes and handling required data dependencies

Exercise 2: Scaling a Producer-Consumer Workflow

- ML-in-the-loop exercise relied on small amounts of data to train the model and perform inference
- What happens when we scale up the size of the data?
- Let's consider a simple producer-consumer workflow to perform online training of an ML surrogate

<u>Data Producer</u>
Ensemble of toy simulations to advance 2D wave equation on $N \times N$ grid and produce training data $(u(t)_{N\times N}, u(t+\Delta t)_{N\times N})$

<u>Data Consumer</u>
Ensemble of simple CNNs to train auto-regressive model, $u(t+\Delta t) = \mathrm{CNN}(u(t))$, spanning various hyperparameters



Exercise 2: Scaling a Producer-Consumer Workflow

- As workflow and data scale up, Parsl implementation runs into transfer speed and memory bottlenecks
  - Collecting all training data on a single node can lead to out-of-memory issues
  - Multi-node concurrent future implementation relies on TCP transfer (inefficient for large data)

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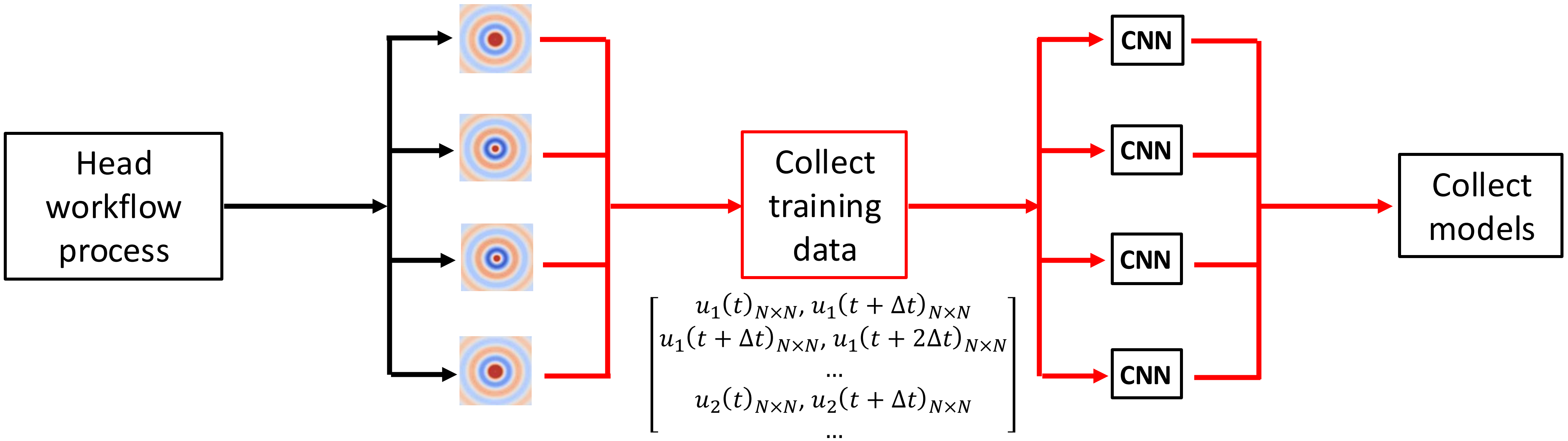

Exercise 2: Scaling a Producer-Consumer Workflow

- Immediate solution would be to store data on the parallel file system (PFS)
  - Each simulation writes its own data to the file system (1 file per simulation, total of N_{sim} files)
  - Each training instance reads all data from simulations (N_{CNN} processes read N_{sim} files)

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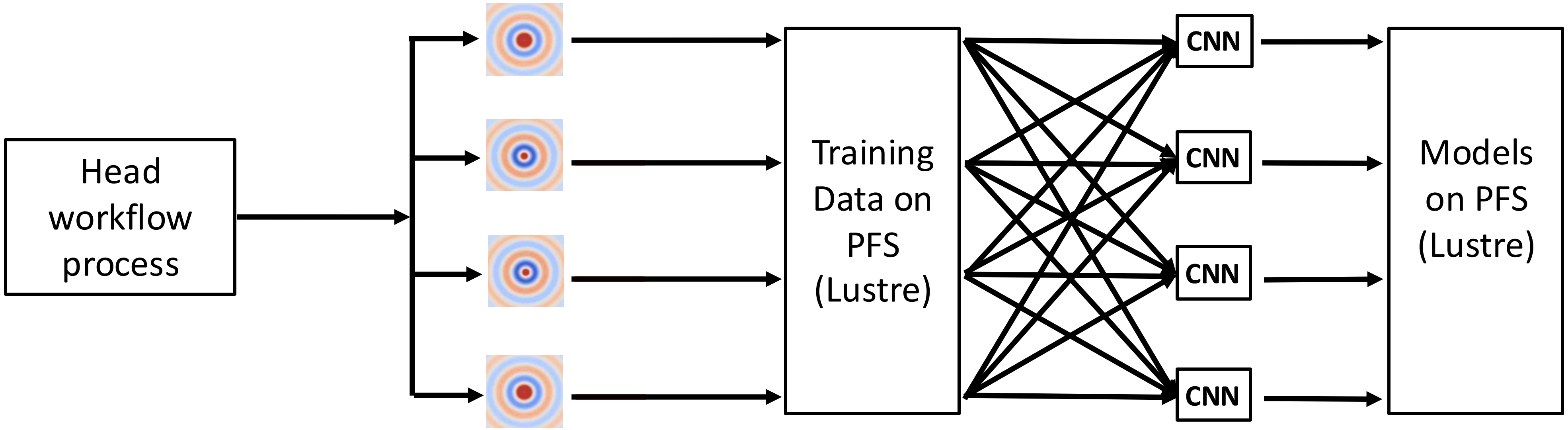

Exercise 2: Scaling a Producer-Consumer Workflow

- At large scale, the file system can become a bottleneck too
  - Metadata server contention from too many concurrent file open/close operations
  - Limited parallel IO bandwidth (~650 GB/s for Eagle on Polaris)

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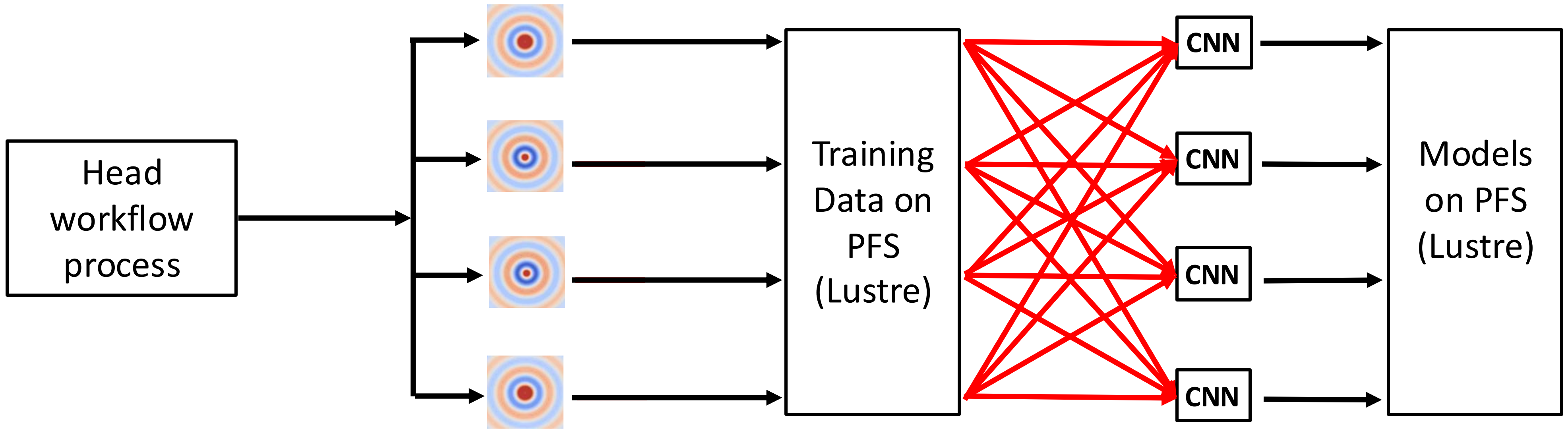

Exercise 2: Scaling a Producer-Consumer Workflow

- ❑ File system bottlenecks can be alleviated by leveraging distributed in-memory key-value data stores
  - ➢ E.g., DragonHPC Distributed Dictionary or sharded databases, such as Redis
  - ➢ Enable fast IO storing data on nodes' DRAM memory in distributed fashion
  - ➢ Data transfer across system interconnect (TCP or more efficient RDMA/MPI)
  - ➢ In some cases, enable full colocation of data and compute avoiding any inter-node transfer (VERY fast and scalable!)

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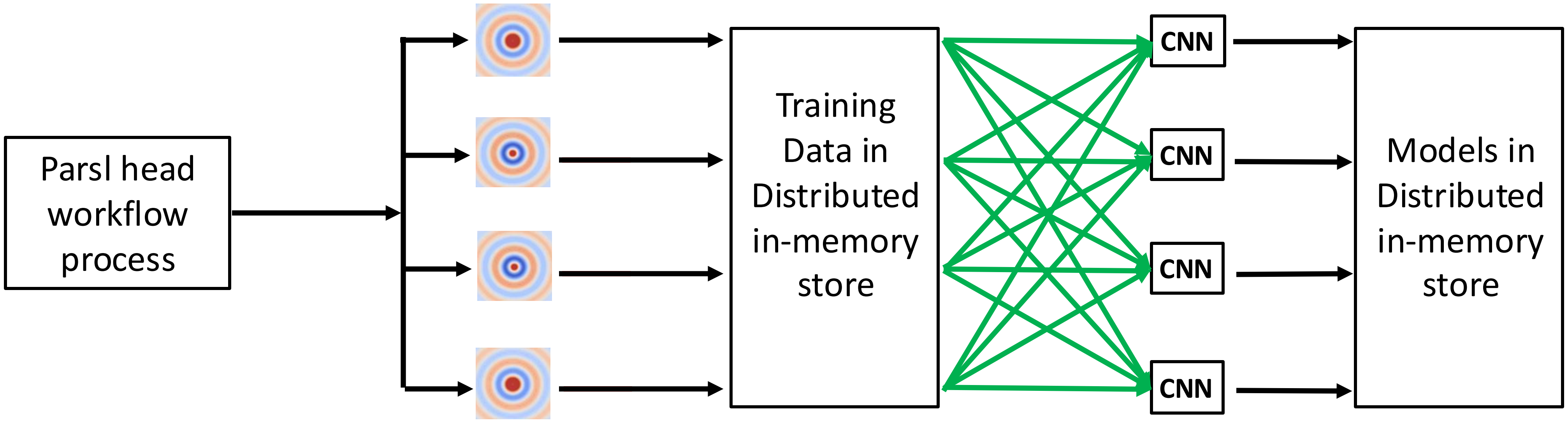

Scaling a Producer-Consumer Workflow

Hands-On Time

Observations from Producer-Consumer Hands On

- ❑ On a single node, the parallel file system offers the best performance
- ❑ What happens as the workflow scales up in size, both data size and number of nodes? The homework will help you explore this question.

In-depth webinar available:

Methods, Tools, and Best Practices for Coupling Simulation and AI on ALCF Systems

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