Integrating AI and Simulations

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Why Couple AI and Simulation?

Choose best simulations to launch

- Active learning: ones that improve ML model
- Or “experiment design”
- Diverse set?
- Ones likely to improve quantity of interest?
- If ML model degrading, collect more data?
- Sample space more effectively

Example:
“Machine Learning Inter-Atomic Potentials Generation Driven by Active Learning” Sivaraman, et al.
https://arxiv.org/abs/1910.10254
https://github.com/argonne-lcf/active-learning-md

Surrogate modeling

Replace *part* of simulation with ML surrogate model

- Expensive part?
- Inaccurate part?

ML model output fed back into rest of simulation

Example:
“A turbulent eddy-viscosity surrogate modeling framework for RANS simulations”
By Maulik, et al.
https://doi.org/10.1016/j.compfluid.2020.104777
https://github.com/argonne-lcf/TensorFlowFoam

Reduce I/O

- Apply ML model to save compressed simulation results
- Train online during simulation (skip I/O bottleneck)
- *In situ* analysis giving feedback on simulations before completed
  - Need to adjust something?

Example:
"In Situ Compression Artifact Removal in Scientific Data Using DeepTransfer Learning and Experience Replay" by Madireddy, et al.
https://doi.org/10.1088/2632-2153/abc326

Control Simulation with ML

- Select simulation parameters
- Select numerical scheme

Example:
“Distributed Deep Reinforcement Learning for Simulation Control”
By Pawar & Maulik
https://arxiv.org/pdf/2009.10306.pdf
https://github.com/Romit-Maulik/RLLib_Theta/

Other Use Cases

- Data assimilation
- Augmenting simulation with ML closure/discrepancy model
- Solver as part of ML loss function

Ways to Couple AI & Simulation

How Close is the Coupling?

Proximity

- On node
- Off node, same computing resource
- Distinct computing resource

Data Access

- Direct: share same logical memory space
- Indirect: distinct logical memory
- Either way: need to synchronize data

May or may not require copy

"A terminology for in situ visualization and analysis systems" by Childs et al. 2020

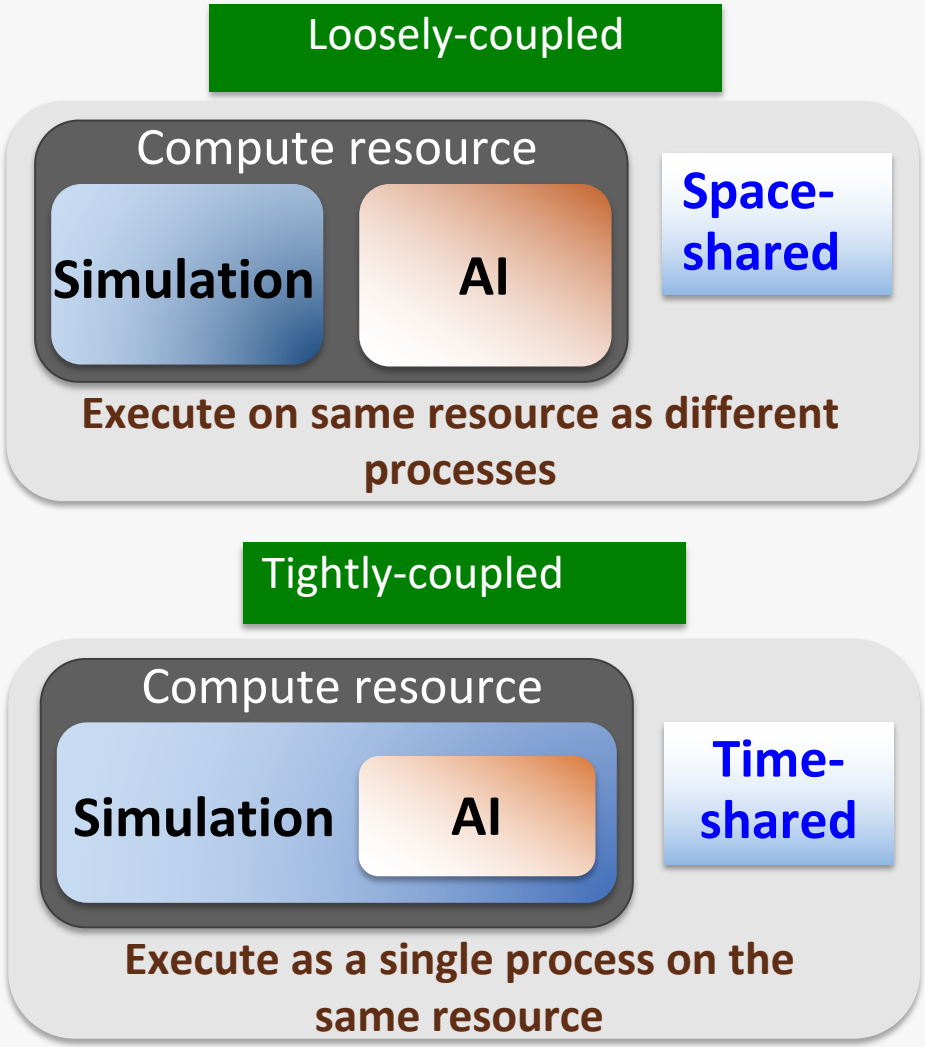
Division of Execution

- Space Division (Different physical compute resources)
  - Can allocate appropriate resource to each
  - But need to keep both utilized & transfer data

- Time Division (Some compute resources alternate simulation vs. AI)
  - Less or no synchronization & data transfer
  - But always blocking one or the other

"A terminology for in situ visualization and analysis systems" by Childs et al. 2020

Example Modes



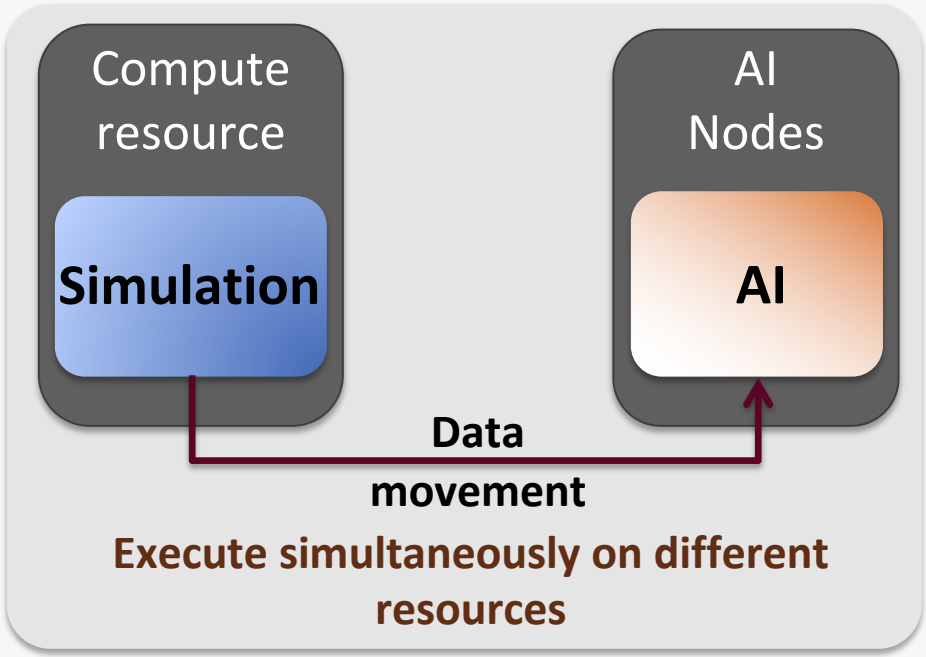


Figure adapted from Venkat Vishwanath

"A terminology for in situ visualization and analysis systems" by Childs et al. 2020