Using HPC systems for Python-based AI/ML tasks

UM Fall HPC/Cloud Workshop

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Why the talk is about Python AI/ML on HPC?

- **Everyone (almost) is using Python for AI / ML**
- **HPC has high performance hardware and software**
  - NVIDIA (and AMD) GPUs
  - High bandwidth, Low-latency Interconnect (NVidia Infiniband)
  - Scalable, parallel File Systems (VAST, CEPH, DDN Infinia) or local SSD NVMe
- **HPC community has a data centre infrastructure**
  - Power; high efficiency cooling
- **Many AI shops do use same HPC technology**
  - **SLURM, Linux, etc.**
  - Some do use Kubernetes and containerized workflows

This talk is about using our HPC infra

- HPC presents a few issues for running AI workflows:
    - How to maintain the (largely Python-based) software on HPC?
        - Need to be able to get software and AI Models running

    - Good to have some ability to interactive workflows for debugging
    - How to adapt it to the SLURM based, batch workflow
        - Need to match HPC resources with AI workflow efficiently

- SaaS competition! (Google Colab, for example).

Artificial Intelligence and Machine Learning revolution

https://static.googleusercontent.com/media/research.google.com/en//pubs/archive/35179.pdf "The Unreasonable Efficiency of Data"

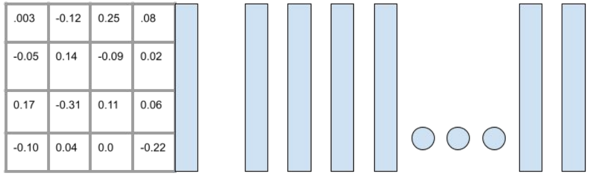
http://www.incompleteideas.net/IncIdeas/BitterLesson.html "The Bitter Lesson"

https://dl.acm.org/doi/10.5555/3295222.3295349 "Attention is all you need"

https://blogs.nvidia.com/blog/what-are-foundation-models/ NVidia on foundational models.

What are those AI and “models”

- Layers of numerical weights, and metadata about them
- Specific to the model’s software and hardware (precision)
    - (“transformers” would have attention layer, etc.)



- **Training/tuning** optimizes the weights of all or some layers
- **Inference** converts a prompt into a numerical representation , passes through model layers and generates outputs

https://poloclub.github.io/transformer-explainer/

Working with AI software and “models”

- Python packages : matrix math and optimization (*torch*, *arrow*, *JAX*, …), ML models (*transformers*, *diffusers*, …) , training (*accelerate*, *LoRa*, etc.)
  - Need to manage software dependencies (modules, pip, virtualenv)
  - Must use optimized libraries from the host (CUDA, MPI, BLAS/LAPACK, Arrow) → modules
  - Common tools like *conda* are often unwelcome in HPC
- The AI Models themselves (layers, weights) need to be obtained

- A popular community hub Huggingface : https://huggingface.co/
- https://docs.alliancecan.ca/wiki/Huggingface

Typical tasks for AI / ML on HPC

- Training new models : optimize the weights
- Tuning existing models on additional datasets (LoRA, etc., but more economical: selected layers)
- Inference: getting predictions/generalizations out of existing models
  - Tokenize the “prompt”,
  - Feed it through the layers
  - Convert the representation back to the “output”

- For this Session we will try three examples: Interactive inference for text, text to graphics and tuning/training a graphic model in a batch job.
- Using Grex (mainly) or Magic Castle: need GPUs!

Managing Python dependencies with pip

- Dependencies: Pip handles (mostly) Python dependencies, relying on OS for non-Python ones
  a. Unlike conda, uv etc, that would package all binary dependencies as well.
  b. HPC folks like to provide their own optimized binary software : load “modules”!
- Repositories: pip fetches packages from https://pypi.org/ or a local repository.
  a. On CCEnv, each and every package must be repackaged to their “wheelhouse”.
  b. On local software stack SBEnv, manylinux wheels can be used from pypi.org
- Installation destination: in particular when invoked in a Jupyter notebook cell.
  a. user’s home directory $HOME/.local/{bin,lib,share} . (Grex)
  b. Throw-away virtual environment under $SLURM_TMPDIR (Alliance HPC , MagicCastle)
  c. Explicit virtualenv (create, activate and install) : best method. Needs a Jupyter kernel added.

1. Project one: text generation using Qwen3

- We will generate text based on a prompt, with reasoning using a small LLM
- https://huggingface.co/Qwen/Qwen3-0.6B
- The code has three general stages
  1. But first, use pip to install packages in Jupyter.
     1.1. Don’t forget to load Lmod modules (Lmod tab) !
     1.2. Monitoring tab for Node and GPU resources.
  2. Import Python packages and see if they load
  3. Set up encoders for the prompt
  4. Run the inference/generation step
  5. Decode the output, print result
- Can be made into a chatbot with tools like Gradio.

2. Project two: inference using SD-1.5

- We will generate images based on a text prompt
- https://huggingface.co/stable-diffusion-v1-5/stable-diffusion-v1-5
  - (used to be **runwayml/stable-diffusion-v1-5**)
  - Will use *torch*, *transformers* and *diffusers*
  - Needs a GPU! On Grex or MagicCastle
  - Will use HuggingFace convenient "*pipe*" interface that lets us set a pretrained model and abstract the encoding, decoding steps.
- Let us use same pip environment in Jupyter as for the project 1.

3. Project 3: using LoRa to train SD-1.5

- The SD-1.5 model is unaware of certain things. I want to add some knowledge to it: an ElderScrolls game character, Scamp
  - https://en.uesp.net/wiki/Lore:Scamp
  - Will use a handful of images from the fandom wiki (dataset 2)
  - Will use a handful of auto generated images from ChatGPT 4o. (dataset 1)
  -
- Low Rank Adaptation of Large Language Models (LoRa) technique
  - Only adding a few layers, freezing the rest of the model
  - https://huggingface.co/docs/diffusers/en/training/lora

```
unet_lora_config = LoraConfig(
    r=args.rank,
    lora_alpha=args.rank,
    init_lora_weights="gaussian",
    target_modules=["to_k", "to_q", "to_v",
"to_out.0"],
)

unet.add_adapter(unet_lora_config)
lora_layers = filter(lambda p:
p.requires_grad, unet.parameters())
```

3. Project 3: using LoRa to train SD-1.5

- Using Huggingface “*accelerate*” training script from “*diffusers*” repo
  - Get an interactive job on a GPU node
  - Git clone the repo TBD
  - Create a virtualenv (SBEnv on Grex, CCEnv on Jupyter)
  - Install pip packages, including current versions of *diffusers* from git
  - Download / copy the training data
    - Dataset 1 and dataset 2 with “Scamps”.
  - Run a salloc training job, obtaining new LoRa weights.
  - Validate the model, repeat etc.

3. Project 3: using LoRa to train SD-1.5

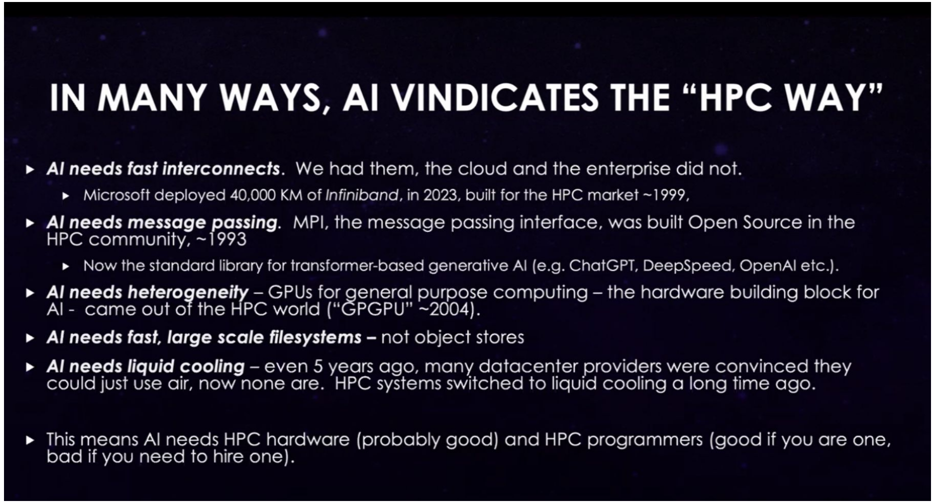
- Using Jupyter, repeat the exercise 2 but use generation with new layers added.
  - Will use HuggingFace convenient "*pipe*" interface that lets us set a pretrained model and abstract the encoding, decoding steps.
  - Let us use same pip environment in Jupyter as for the project 2.
  - The only change is to add our new extra layers to the model.
  - Try to generate an image about a "Scamp".

Strategies for larger AI Model training

- Large datasets, take a lot of time on a single GPU
- Large models would not fit into memory of a single GPU
- Distributed parallel training frameworks: .
  - Huggingface *accelerate* ,
  - Microsoft *DeepSpeed* ,
  - etc,
- Data parallelism (split the data across GPUs)
- Pipeline parallelism (distribute model layers)
- Tensor parallelism (domain decomposition)

May rely on collective MPI operations (AllReduce, AllGather etc,)

DRI (Digital Research Infrastructure) for AI



A slide by Dan Stazione, Director of TACC

***tamIA**, a real AI supercomputer of LavalU*

Which system for which workload?

Digital Research Alliance of Canada

System, kind (2025)	# GPU nodes	GPUs per node layout	Interconnect	Storage, PB
TamIA , HPC (Laval)	42 (H100)	**4 x** NVIDIA HGX H100 SXM	**4 x** HDR200 Infiniband, **non-blocking**	?
Vulcan, HPC (UofA)	205 (L40s)	4 x NVIDIA L40s	1x100Gbps Ethernet	5PB
Killarney, HPC (UofT)	168 (L40s) 10(H100)	4 x NVIDIA L40s, 8 x NVIDIA H100 SXM	1x HDR100, 2x HDR200	1.5 PB
HPC systems ?				
Fir, HPC	160	4 x NVidia H100 SXM	1x HDR200 Infiniband, blocking	51PB
Nibi, HPC	36	8 x Nvidia H100 SXM	1x Nokia 200/400G Ethernet	25PB
Trillium, HPC	60	4 x NVidia H100 SXM	1x NDR200/ NDR400 Infiniband	29PB

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