Why HPC?

High-Performance Computing: CCMAR's CETA & National Infrastructure

January 2026, David Palecek

Laptop to HPC

High-Performance Computing (HPC) is not about “faster computers”
It’s about making certain problems possible at all

- HPC removes artificial constraints on ideas
- Modern research & data workflows exceed laptop limits

Laptops break down when:

- Datasets exceed RAM
- Analyses take days or week
- You need reproducibility at scale

HPC is about possibility, not luxury

Memory vs Compute

If your data doesn't fit in memory, computation fails, not just slows

- Large matrices, graphs, genomes, images
- In-memory analytics (pandas, numpy, R)
- Slow disk swapping and crashes
- Genome assembly

More CPU doesn't just make things faster:

- Enables higher resolution models
- Parameter space sampling
- Batch processing of many samples at once
- Makes "load once, analyze many times" possible

Understand your bottleneck = smarter HPC use

Warning: most programs are single-threaded

- Many standard tools use only 1 CPU core
- More cores ≠ faster by default
- HPC does not magically parallelize your code

Common examples:

- Many bioinformatics tools
- Default Python / R scripts
- Legacy scientific software

You must choose parallel tools or parallelize workflows

Common patterns

1. Many independent jobs
    - Run 1,000 single-core jobs at once
    - BLAST
2. Multithreaded programs
    - One job using many cores
3. Distributed workflows
    - Pipelines, task schedulers, workflow engines
    - Nextflow, Snakemake, CWL

Applications

AI
- Generative
- scientific

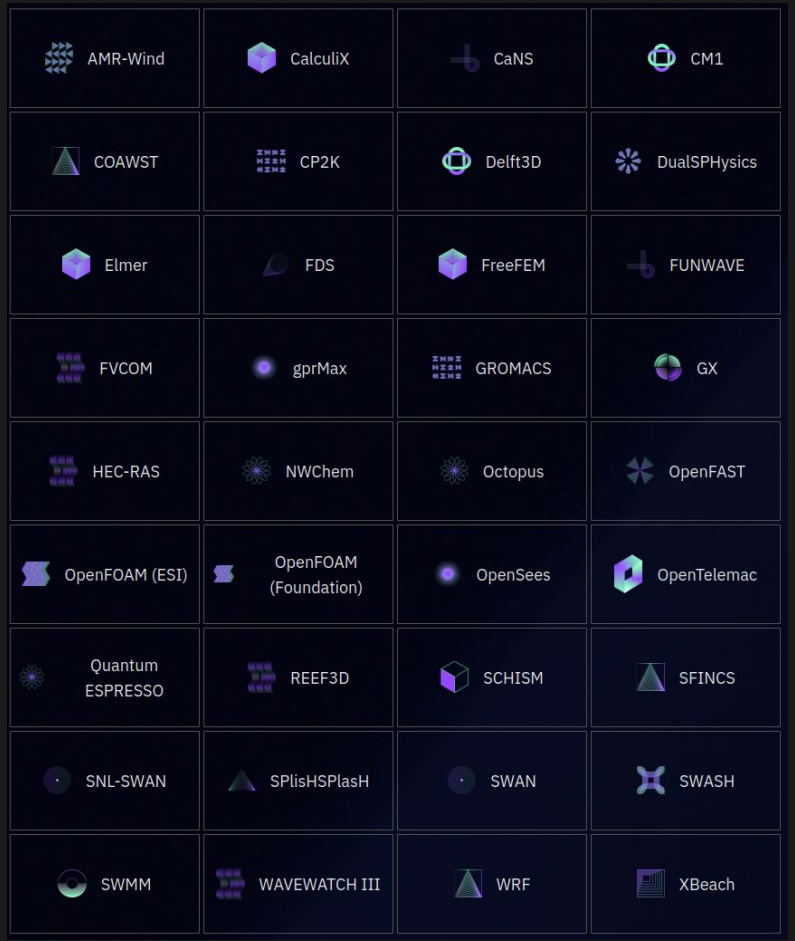
Bioinformatics, molecular dynamics
- Drug discovery
- Protein folding
- Genomics
- Quantum simulations

Weather forecast

Climate modeling

Engineering
- Fluid dynamics
- Fusion
- Electronics and manufacturing

Finance
- Trading
- Fraud detection



Taken from https://inductiva.ai/simulators

CETA

Only ssh login, only from the UAlg network, use VPN from your home.

5 nodes
- 128 GB
- 54 CPUs

1 large memory node
- 900 GB
- 54 CPUs

Submission via job queue system, SLURM. Any other compute from the login node is FORBIDDEN.

The more resources you ask for, the longer you will wait to get your job started (on commercial Cloud or EU/national infrastructure), you get billed by what you allocated, not by what you used).

Ask for help, whenever unsure.