L1: Software Engineering for HPC and AI – Introduction & Development Environment

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Master Calcul Haute Performance et Simulation - GLHPC | UVSQ

- 1. Introduction to Software Engineering for HPC and Al
- 2. HPC Architectures
- 3. Shell Basics and Scripting
- 4. Package Management
- 5. Version Control Systems

Introduction to Software Engineering for HPC and Al

Syllabus

- Lecture 1: Introduction & Development Environment
- Lecture 2: Performance Aware C Computing
- Lecture 3: Building, Testing and Debugging Scientific Software
- Lecture 4: Experimental Design, Profiling and Performance/Energy Optimization
- Lecture 5: HPC for AI & Environmental Impact of Computation

Project: Inference Engine for a Deep Network

Introduction & Development Environment

- Principles of software engineering applied to HPC and Al.
- Introduction to computing architectures.
- **Development tools**: shell scripts, package management, Git, IDEs, etc.

Analytical solution to the 2-Body Problem

Consider two particles with masses m_1 and m_2 at positions x_1 and x_2 under gravitational interaction.

$$m_1.a_1 = -\frac{G.m_1.m_2}{\|x_1 - x_2\|^3}(x_2 - x_1)$$

$$m_2.a_2 = -\frac{G.m_1.m_2}{\|x_1 - x_2\|^3}(x_1 - x_2)$$

Solved by Bernoulli in 1734, x_1 and x_2 can be expressed as simple equations that depend on time, masses, and initial conditions.

Why Simulate the n-Body Problem?

- For n=3 or more, no practical analytical solution exists.
- Even advanced mathematical solutions (e.g., Sundman, 1909) are too slow for real use.
- Computer simulations allow us to study the motion of many interacting particles.
 - Efficient algorithms (e.g., Barnes-Hut, Fast Multipole) make large-scale simulations possible.
- HPC is essential to simulate realistic systems in physics, astronomy, and Al.
 - Simulation + HPC = understanding complex systems!

```
// Compute accelerations based on gravitational forces
for (int i = 0; i < num_particles; i++) {</pre>
  double ax = 0.0, ay = 0.0, az = 0.0;
  for (int j = 0; j < num_particles; j++) {</pre>
    if (i == j) continue;
    double dx = p[j].x - p[i].x;
    double dy = p[j].y - p[i].y;
    double dz = p[j].z - p[i].z;
    double d_sq = dx * dx + dy * dy + dz * dz;
    double d = sqrt(d_sq);
    double f = G * p[i].m * p[j].m / (d_sq * d);
    ax += f * dx / p[i].m;
    ay += f * dy / p[i].m;
    az += f * dz / p[i].m;
 p[i].ax = ax;
  p[i].ay = ay;
 p[i].az = az;
```

Naive n-Body Simulation in C

Introduce a time step at and update positions based on gravitational forces.

```
// Update positions based on computed accelerations
for (int i = 0; i < num_particles; i++) {
  p[i].x += p[i].ax * dt * dt;
  p[i].y += p[i].ay * dt * dt;
  p[i].z += p[i].az * dt * dt;
}</pre>
```

High Performance Computing

Fugaku (2020, 442 petaflops, 7.3 million cores)

• n-body: integrates 1.45 trillion particules per second.

How to achieve such performance?

- Algorithmic improvements:
 - Use tree-based methods (Barnes-Hut) to reduce complexity from $O(n^2)$ to $O(n\log n)$ or better.
- Parallelization: distribute computation accross many cores.
- Vectorization: use SIMD instructions to process multiple data points in parallel.
- Data locality: optimize data access patterns to minimize memory latency and maximize cache usage.

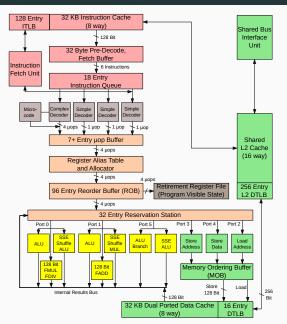
Compiler optimizations, performance tuning, hardware acceleration are also crucial.

HPC Architectures

CPU & Instruction Set (ISA) — quick review

- CPU core executes instructions; machine state = registers, program counter and flags.
- Assembly encodes the instructions; compilers translate high-level code into the ISA.
 - types: arithmetic/logical, load/store (memory), control flow (branches, calls), system calls
- Registers are the fastest storage; register pressure influence performance.

Example: Intel Core2 Architecture



Pipeline, Memory Hierarchy & Interrupts

- Pipeline increases instruction throughput, classic 5-stages:
 Fetch → Decode → Execute → Memory → Write-back
- Hazards: data hazards (dependencies), control hazards (branch prediction), resource conflicts.
- Memory hierarchy: registers → L1/L2/L3 caches → DRAM → persistent storage; spatial and temporal locality drive cache effectiveness.
- Buses, coherence and NUMA: cross-socket memory access has higher latency; cache coherence and memory bandwidth limit scalability.
- Interrupts and exceptions: asynchronous interrupts signal external events; exceptions/traps handle synchronous faults; the OS performs context switching and servicing.

Multicore memory hierarchy (more in next lecture ...)

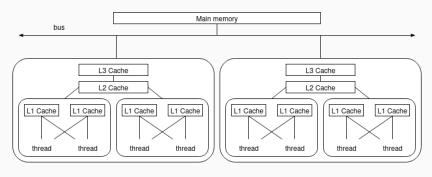


Figure 2: Memory hierarchy

System hierarchy (physical view)

- Rack → chassis → node → socket → core → hardware thread: a multi-level physical organization.
- Nodes often include accelerators (GPUs, TPUs, FPGAs) and have their own memory (DRAM, sometimes HBM).
- Heterogeneous hardware and multi-level parallelism are the norm in modern HPC systems.

Interconnects and I/O

Interconnects

- Two key metrics: latency (small-message cost) and bandwidth (sustained transfer rate).
- Fabrics: Ethernet, InfiniBand, Omni-Path; features to note: RDMA, kernel bypass, hardware offloads.
- Network topology affects routing, contention and scalability.

Storage and I/O

- Parallel file systems provide shared high-throughput storage for HPC jobs.
- Design I/O to avoid bottlenecks and to fit checkpoint/analysis cadence (collective I/O, buffer in NVMe).

Levels of parallelism & mapping

- Inter-node (distributed memory) via MPI; intra-node threading via OpenMP/pthreads; SIMD/vector units for data-level parallelism.
- Accelerator offload (CUDA/HIP/OpenCL) creates hybrid MPI+X application patterns.
- Choose mapping to match algorithm characteristics (communication-heavy vs compute-dense).

Software stack, operations & current trends

- Typical stack: compilers, MPI/libfabric, math libraries, system libs
- Job schedulers (Slurm/PBS) handle resource allocation, queues and batch workflows

Shell Basics and Scripting

What is the Shell?

- **Definition**: A shell is a command-line interface to interact with the operating system.
- Purpose: Execute commands, run programs, and automate tasks.
- · Common Shells: bash, zsh, fish, sh.
- · Why Learn It?
 - Essential for HPC environments.
 - Enables automation and efficient system interaction.

Basic Shell Commands

- File and Directory Management:
 - 1s: List files and directories.
 - cd <directory>: Change directory.
 - pwd: Print current working directory.
 - mkdir <directory>: Create a new directory.
 - rm <file>: Remove a file.
- · File Viewing:
 - cat <file>: Display file contents.
 - less <file>: View file contents interactively.
 - head <file>: Show the first 10 lines.
 - tail <file>: Show the last 10 lines.

Redirections

- Standard Input/Output:
 - <: Redirect input from a file.
 - >: Redirect output to a file (overwrite).
 - >>: Append output to a file.
- Examples:
 - cat file.txt > output.txt: Save contents of file.txt to output.txt.
 - grep "error" log.txt >> errors.txt: Append lines containing "error" to errors.txt.

Pipes

- **Definition**: Pipes (I) connect the output of one command to the input of another.
- Examples:
 - 1s | grep ".txt": List .txt files.
 - cat file.txt | wc -1: Count the number of lines in file.txt.
- Why Use Pipes?
 - · Combine simple commands to perform complex tasks.
 - Avoid creating intermediate files.

Variables and Environment

- Variables:
 - VAR=value: Define a variable.
 - \$VAR: Access the variable's value.
- Environment Variables:
 - echo \$HOME: Display the home directory.
 - export PATH=\$PATH:/new/path: Add a directory to the PATH.
- Example:

```
NODES=4
PROGRAM="my_hpc_program"
echo "Running $PROGRAM on $NODES MPI nodes..."
mpirun -np $NODES ./$PROGRAM
```

Writing a Simple Script

- What is a Script?
 - A file containing a sequence of shell commands.
- · Creating a Script:
 - 1. Create a file: vim script.sh.
 - 2. Add commands:

```
#!/bin/bash
echo "Hello, World!"
```

- 3. Make it executable: chmod +x script.sh.
- 4. Run it: ./script.sh.

Conditional Statements

```
if [ -f "config.json" ]; then
  echo "config.json exists. Running the HPC program..."
    ./my_hpc_program --config=config.json
else
  echo "Error: config.json does not exist."
fi
```

Loops

```
for i in {1..5}; do
  echo "Running simulation with parameter set $i..."
   ./my_hpc_program --config=config_$i.json
done
```

Functions in Shell Scripts

```
run_simulation() {
  echo "Starting with config file: $1 and $2 nodes..."
  mpirun -np $2 ./simulation_program --config=$1
  echo "Simulation completed."
}
run_simulation "simulation_config.json" 8
```

Debugging and Best Practices

- · Debugging:
 - Run with bash -x script.sh to trace execution.
 - Use set -e to exit on errors as the first command.
- Best Practices:
 - Use comments (#) to explain code.
 - Write reusable functions.
 - Check for errors (if [\$? -ne 0]; then).
 - Test scripts on small inputs before scaling up.

Package Management

Package Management: Overview

- Problem Solved: Simplifies software installation, updates, and dependency management.
- Ensures compatibility between libraries and applications.
- Tracks installed software versions for easy upgrades or rollbacks.
- Examples: dnf (Fedora/RHEL), apt (Debian/Ubuntu).

Package Managers for HPC

- Cluster-Specific Tools: spack, guix enable software installation without root privileges.
- Useful in HPC environments where users lack admin rights.
- Manage multiple versions of libraries and tools for reproducibility.
- Facilitate deployment of complex scientific software stacks.

Language-Specific & Containers

- Language-Specific Managers: pip (Python), cargo (Rust) simplify language ecosystem management.
- Containers: Tools like Docker/Singularity encapsulate software and dependencies.
- Enable portability across systems and reproducible environments.
- Virtualization/containerization is becoming popular in modern HPC workflows.

Version Control Systems

What is Version Control?

Version control involves **tracking and managing** the **changes** made to project files.

Each version is associated with a date, an author, and a message. Developers can work on a copy corresponding to a specific version.

Objectives

- Enhance communication among developers (track code evolution, messages).
- Isolate experimental developments (work branches).
- Ensure code stability (stable version on the main branch, ability to revert to a stable version).
- Manage releases (tags for specific versions).

Vocabulary for Versions

- Version a recorded state or revision in the project's history.
- Commit a snapshot of the project at a given version with metadata.
- Branch an independent line of development (use one branch per feature/experiment).
- Tag a stable label pointing to a specific commit (e.g., releases).
- Diff / Patch textual representation of changes between versions.
- Conflict incompatible concurrent edits that must be resolved manually.

Vocabulary for Storage

- Repository storage of the project's history (local .git and metadata).
- Clone a full local copy of the repository including history.
- Working copy editable files checked out from a repository.
- Index / Staging area area to stage selected changes for the next commit.
- Remote hosted repository (e.g., origin on GitHub/GitLab) for collaboration.

Distributed VCS

Distributed Version Control System (DVCS)

Advantages

- Multiple repositories can exist.
- Version control can be performed locally.
- No need for network connectivity.

Examples

- Mercurial (2005) (Mozilla, Python, OpenOffice.org)
- Bazaar (2005) (Ubuntu, MySQL)
- Git (2005) (Linux Kernel, Debian, VLC, Android, Gnome, Qt)

Introduction to DVCS: Git

History

- Git was created in 2005 to version the development of the Linux kernel.
- Designed as a distributed version control system (replacing BitKeeper).

Context

- Widely used by projects: Linux Kernel, Debian, VLC, Android, Gnome, Qt, etc.
- Accessible via command-line interface.
- Graphical tools available: gitk, qgit.

Core Principles of Git

- Git does not store differences between commits (unlike SVN).
- Instead, Git stores snapshots of the project's file hierarchy at each commit.
- These snapshots are based on hierarchical structures of objects.
- Git operations revolve around manipulating these objects.

Hash

- Each object has a unique hash (SHA1).
- Git identifies identical objects by comparing their hashes.
- The same content stored in different repositories will always have the same hash.

Git Objects

Object types include:

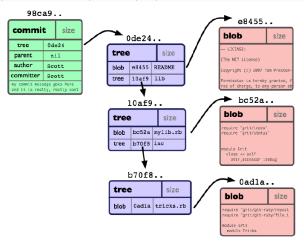
- Blob: Stores file data.
- Tree: References a list of other trees or blobs.
- Commit: Points to a single tree, representing a project snapshot. Includes metadata like timestamp, author, and parent commits.
- Tag: Labels a specific commit for easy reference.

Commit Representation

(Git Community Book, ρ13)

Commit Structure

(Git Community Book, ρ14)



Git Repository

- .git directory:
 - Stores the project's history.
 - Contains metadata for version control.
 - Located at the root of the project.

```
$>tree -L 1
.
I-- HEAD  # pointeur vers votre branche courante
I-- config  # configuration de vos préférences
I-- description  # description de votre projet
I-- hooks/  # pre/post action hooks
I-- index  # fichier d'index (voir prochaine section)
I-- logs/  # un historique de votre branche
I-- objects/  # vos objets (commits, trees, blobs, tags)
`-- refs/  # pointeurs vers vos branches
```

Figure 3: Git Repository Contents

Working Directory

- Current version of project files.
- Files are replaced or removed by Git during branch or version changes.

Index / Staging Area

- Bridge between the working directory and the repository.
- Used to group changes for a single commit.
- Only the index content is committed, not the working directory.

Basic Commands

- git init: Initialize a Git repository.
- git clone <repository>: Clone a repository.
- git status: Check the status of the working directory and staging area.
- git add <file>: Stage changes for commit.
- git commit: Commit staged changes.

Basic Commands (Continued)

- git pull: Update local repository from remote.
- git push: Push local commits to remote repository.
- git log: View commit history.
- git checkout <hash>: Switch to a specific commit using its SHA1 hash.
- git branch <branchName>: Create a new branch.

Branches: Purpose

- Work on changes that diverge from the main branch or another branch.
- Isolate experimental developments.
- Avoid disrupting shared development efforts.
- Version parallel developments with the option to merge later.

Branches: Commands

- git branch Or git checkout -b <branchName>: Create a new branch.
- git checkout <branchName>: Switch to an existing branch.
- git merge <branchName>: Merge a branch into the current branch.
- git branch -d <branchName>: Delete a branch.
- git branch: List all branches and show the current branch.

Conflict Management

- Conflict: Occurs during branch merging when two changes affect the same lines.
- Resolution Steps:
 - 1. Merge is paused.
 - 2. Conflict zones are marked in the file.
 - Edit the file to resolve conflicts by choosing one version or combining changes.
 - 4. Verify and validate the resolution.
 - 5. Commit the resolved conflict.

Correction Methods

- Undo Changes: Use git reset to discard modifications.
- Amend Last Commit: Use git commit --amend to modify the previous commit.
- Branch-Based Correction: Create a new branch from a specific version and work from there.
- Rewrite History: Use git rebase to edit commits and history.

Warning

 Rewriting History: Interactive rebasing is risky. Only rewrite commits that haven't been pushed to a remote repository.
 Prefer branch-based corrections for safer handling.

Centralized Collaboration

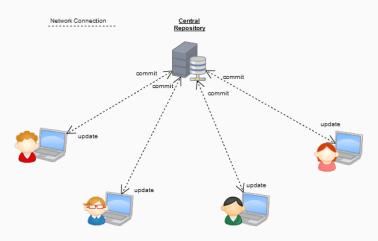


Figure 4: Interactions with a centralized system

(image from Joomla's documentation)

Decentralized with Central Repository

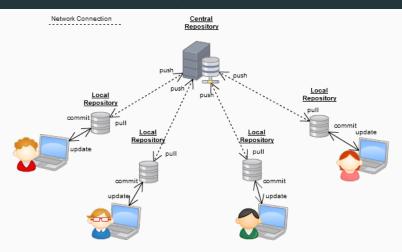


Figure 5: Constrained interactions with a decentralized system

(image from Joomla's documentation)

Fully Decentralized Collaboration

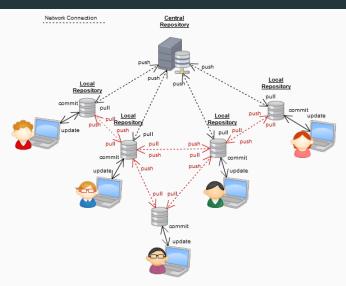


Figure 6: Interactions with a decentralized system

Best Practices for Collaborative Development

Before Development

- Define a developer charter:
 - Naming conventions for files, functions, variables.
 - Standards for technical documentation and comments.
 - Indentation rules (tabs vs spaces).
- Establish a version control strategy.

During Development

- Create isolated commits (one commit = one coherent change).
- Write concise commit messages (max 60 characters summarizing the change).
- · Add detailed commit descriptions if necessary.
- Regularly update your working copy.
- Share updates with team members.

References

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- What Every Programmer Should Know About Memory by Ulrich Drepper
- The Git Community Book
- Tech Talk: Linus Torvalds on Git (YouTube)
- TOP500 Supercomputers
- Modern Operating Systems by Andrew S. Tanenbaum
- GIT Lecture Notes by Thomas Dufaud (IUT Vélizy UVSQ)