



## EuroCC@Türkiye

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# HIGH PERFORMANCE COMPUTING FOR CHEMISTS AND CHEMICAL ENGINEERS

## 1. Problem Identification

The research team, led by Nihan Çelebi Ölçüm at Yeditepe University, Department of Chemical Engineering, is engaged in advanced molecular modeling of organic and bioorganic phenomena using state-of-the-art computational methods. The team primarily consists of undergraduate and graduate students with varying levels of experience in chemical engineering but little to no background in high-performance computing (HPC). As the students are required to perform complex simulations on supercomputer clusters, they face significant challenges due to their lack of familiarity with essential HPC concepts and scripting. These challenges include understanding the architecture of supercomputers, effectively utilizing queuing systems, executing file operations, and mastering the command-line interface to run simulations and analyze output data

## 2. First Suggestion

The tentative project plan is as follows:

Timeline	Tasks and Milestones
November-December 2024	<b>Phase 1: Needs Assessment and Planning</b> <b>Tasks:</b> <ul style="list-style-type: none"><li>Identify key topics for the training curriculum.</li><li>Linux Shell basic commands</li><li>Linux Shell advanced commands</li><li>Writing scripts using the learned commands.</li></ul> <b>Milestones:</b> <ul style="list-style-type: none"><li>Writing scripts for For outputs generated by programs used in HPC.</li></ul>



### 3. Solution Stage

#### Training Sessions

**Command Line Basics:** Teach basic & advanced command line operations, including file management, navigating directories, and running simple scripts.

**Scripting Languages:** Introduce scripting languages commonly used in HPC, like Bash or Python. Focus on writing scripts for job submission, data processing, and automation.

### 4. Results and Achievements

Expected results and achievements for the “Linux Shell Scripting” training project are as follows:

- Successfully identified key topics for the training curriculum, ensuring a comprehensive learning experience.
- Provided in-depth training on **Linux Shell basic commands**, enabling participants to navigate and operate within a Linux environment effectively.
- Covered **Linux Shell advanced commands**, equipping learners with the necessary skills for complex system operations and task automation.
- Guided participants in **writing scripts using the learned commands**, enhancing their ability to automate repetitive tasks and improve efficiency in a high-performance computing (HPC) environment.

This structured approach has strengthened participants’ command-line proficiency and scripting capabilities, preparing them for real-world applications in HPC and beyond.

### 5. HPC Benefits

- **Optimized Workflow Efficiency:** Identified key topics for the training curriculum to ensure a targeted and effective learning path, leading to improved productivity in HPC environments.
- **Enhanced System Navigation & Management:** Provided in-depth training on **Linux Shell basic commands**, enabling users to efficiently interact with HPC systems, manage files, and execute essential operations.
- **Improved Automation & Performance:** Delivered training on **Linux Shell advanced commands**, equipping participants with skills to handle complex operations, optimize job scheduling, and improve computational efficiency.



- **Streamlined HPC Workflows through Scripting:** Enabled participants to **write scripts using learned commands**, allowing for task automation, job submission optimization, and efficient resource utilization in HPC systems.

These achievements contribute to better system performance, reduced computational overhead, and increased productivity in high-performance computing environments.

By leveraging the benefits of HPC, the project can significantly advance the team's research capabilities, ultimately leading to more impactful contributions to the field of chemical engineering and molecular modeling.

## 6. Challenges

- **Lack of Prior Knowledge:** Many participants had no prior experience with Linux systems or HPC environments, making it challenging to grasp fundamental concepts at the beginning of the training.
- **Steep Learning Curve:** The transition from basic Linux commands to advanced scripting required significant effort, especially for those unfamiliar with command-line interfaces.