

# HPC Computational science competency

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There are 5 groups:

- A. High performance computing
  - B. Computing
  - C. Law and compliance
  - D. Research
  - E. Soft skills
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## **A. High performance computing**

1. Estimate benefit of HPC on specific use case
2. Running specific software/tool/workflow on HPC environments
3. Performance optimization on HPC
4. Debugging software/workflow on HPC
5. Operating HPC system

## **B. Computing**

1. Working remotely in Linux environment via command line interface
2. Managing programming languages and their packages via package manager
3. Installing and managing scientific software and preparing a related environment
4. Using specific tools, software, or IDEs as each individual or together
5. Estimating computing resource requirement
6. Distribute software, data, or trained model

## **C. Law and compliance**

1. Compliance with license, policy, and ethics

## **D. Research**

1. Scientific background knowledge, Methodology, process, and tools
2. Literature Review
3. Scientific Data management and analysis

## **E. Soft skills**

1. Teamwork
2. Communication
3. Human-driven service provision and support

**Reference:**

<https://competency.ebi.ac.uk/framework/bioexcel/3.0/competencies> and

<https://journals.plos.org/ploscompbiol/article?id=10.1371/journal.pcbi.1005772>

Red – AI generated content [using local LLM] (will be refined later)

Blue – fast thinking and subjected to be edited later

Black – may has minor change layer

### **A.1. Estimate benefit of HPC on specific use case**

#### **Description**

The ability to assess the potential benefits of using HPC to solve a specific problem or improve a process.

#### **Remember**

Recalling relevant benefits of HPC on common use cases

#### **Understand**

Understanding the basic capabilities and limitations of HPC systems for common use cases.

#### **Apply**

Applying knowledge to evaluate the benefit of HPC for specific use cases

#### **Analyze**

Identifying trade-offs and considering alternative solutions to determine the best approach for a specific use case.

#### **Evaluate**

Assessing the overall impact of using HPC on the problem or process, including its benefits and costs.

#### **Create**

Developing new methods or approaches to predict the accurate benefit of HPC in a specific case.

## **A.2. Running specific software/tool/workflow on HPC environments**

### **Description**

The ability to deploy and execute specific software or tools on HPC systems, such as running a simulation, analyzing data, or optimizing an algorithm.

### **Remember**

Deploying and executing specific software or tools on HPC systems by using template script with only minor change in input filename and without manually setting an environment.

### **Understand**

Describing the meaning of each line of job submission script and understanding how job schedule works

### **Apply**

Modifying scripts based on given guidelines and configuring the environment to meet specified requirements.

### **Analyze**

Analyzing the implications of changes in job submission scripts and describing the relationship between parameter values and HPC hardware.

### **Evaluate**

Evaluating the quality of job submission scripts in multiple perspectives, including performance, usability, and reproducibility.

### **Create**

Creating the job submission scripts from scratch for deploying and executing unseen software or tools

### **A.3. Performance optimization on HPC**

#### **Description**

The ability to optimize the use of HPC resources by improving performance.

#### **Remember**

Recalling related theory, methods, and tools.

#### **Understand**

Describing the relation between theory, methods, and tools.

#### **Apply**

Designing methods and applying tools to perform profiling or benchmarking.

#### **Analyze**

Identifying potential issues or bottlenecks that may arise during execution and proposing solutions to optimize performance and improve accuracy.

#### **Evaluate**

Assessing the overall effectiveness of the optimization process on the HPC system, including any improvements in performance and results.

#### **Create**

Developing new methods or approaches to improve the performance of parallel programs on HPC systems.

#### **A.4. Debugging software/workflow on HPC**

##### **Description**

The ability to debugging software/workflow using HPC resources.

##### **Remember**

Recalling the principles and techniques of debugging, including how to identify errors, locate their sources, and correct them.

##### **Understand**

Understanding the relationship between common errors and sources.

##### **Apply**

Running the software or workflow on an HPC system with debugging tools to identify and correct errors.

##### **Analyze**

Identifying potential issues or bottlenecks that may arise during execution and proposing solutions to optimize performance and improve accuracy.

##### **Evaluate**

Assessing the overall effectiveness of the debugging process on the HPC system, including any improvements in performance and results.

##### **Create**

Developing new methods or approaches to optimize the use of HPC resources, including improving performance, reducing costs, and achieving better results.

### **A.5. Operating HPC system**

The ability to operate high-performance computing (HPC) system, such as supercomputers or clusters, for a given purpose.

#### **Remember**

Recalling HPC glossary, recent specifications of HPC components, performance matrixes and related technologies including cooling technology and engineering technologies.

#### **Understand**

Understanding the relation between specifications of HPC components and the application performance.

#### **Apply**

Applying related knowledge and technique to operate a HPC for a narrow specific purpose

#### **Analyze**

Analyzing the advantages and disadvantages of various HPC technologies for a given task.

#### **Evaluate**

Evaluating the bottleneck of current HPC system design and suggesting for improvement/

#### **Create**

Designing a HPC system for specific purposes or general purpose.

## **B.1. Working remotely in Linux environment via command line interface**

### **Description**

Ability to work remotely with Linux system using text-based command.

### **Remember**

Remember common Linux command line. Being able to understand the basic concepts and commands of a Linux operating system and their usage.

### **Understand**

Understanding how each of common Linux command including its common options works.

### **Apply**

Able to use command line interface in remote environment to complete tasks.

### **Analyze**

Analyzing the advantages and disadvantages of Linux commands in different situations.

### **Evaluate**

Being able to critically evaluate the efficiency and effectiveness of different Linux tools and commands in a remote environment and make informed decisions about which ones to use for specific tasks.

### **Create**

Developing new strategies and approaches for working remotely in a Linux environment and sharing knowledge and best practices with others.



## **B.2. Managing programming languages and their packages via package manager**

The ability to install, update, and remove programming languages and its packages using a package manager

### **Remember**

Recalling related tools and command of package manager.

### **Understand**

Understand how each command works. Knowing how to use a package manager to install, update, and remove packages, and being able to explain the advantages and disadvantages of different package managers.

### **Apply**

Able to manage dependencies for a project, including installation, configuration, and troubleshooting.

### **Analyze**

Analyzing the complexity of dependencies and being able to explain to others

### **Evaluate**

Evaluating different package manager tools in terms of their features, performance, and compatibility with specific project requirements.

### **Create**

Developing new strategies for managing packages, such as creating custom package repositories or developing new approaches.

### **B.3. Installing and managing scientific software and preparing a related environment**

#### **Description**

The ability to install, configure, and manage scientific software packages and their dependencies in a Linux environment.

#### **Remember**

Recalling related Linux environment variables, compiler, and tools.

#### **Understand**

Understand how related Linux environment variables play a role in the installation process.

#### **Apply**

Applying knowledge of scientific software management to manage dependencies for a scientific project, including installation and configuration.

Analyze

Troubleshooting issues in the software installation or management processes.

#### **Evaluate**

Evaluating different software installation or management approaches and suggesting the solution for a specific task.

#### **Create**

Developing new strategies or tools to simplify the complexity of software installation and management.

#### **B.4. Using specific tools, software, or IDEs as each individual or together**

##### **Description**

The ability to use various tools, software, or integrated development environments (IDEs) to simulate, develop, test, and deploy software applications.

##### **Remember**

Recall related command and able to follow the tutorial.

##### **Understand**

Understanding why using a specific command for a specific purpose.

##### **Apply**

Using tools, software, or IDE to do a specific task.

##### **Analyze**

Analyzing advantages and disadvantages of tools, software, or IDE for performing a specific task.

##### **Evaluate**

Evaluating the effectiveness of tools, software, or IDE for performing a specific task or project and suggesting an improvement.

##### **Create**

Developing new strategies for using tools, software, or IDE efficiently.

## **B.5. Estimating computing resource requirement**

### **Description**

The ability to accurately estimate the amount of computational resources required for a given task, such as memory, CPU/GPU time, and storage.

### **Remember**

Recalling suggested computational resources from the guideline.

### **Understand**

Understanding the basics of computational resource requirements and being able to explain the differences between various types of resources.

### **Apply**

Applying estimation techniques to estimate the required computational resources for a given task.

### **Analyze**

Analyzing the underlying principles of computational resource requirements and being able to apply this understanding to solve complex computational resource estimation problems.

### **Evaluate**

Evaluating different estimation techniques in terms of their features, performance, and compatibility with specific project requirements.

### **Create**

Developing new strategies for estimating computational resource requirements, such as creating custom resource estimation tools or developing new resource management techniques.

## **B.6. Distribute software, data, or trained model**

### **Description**

The ability to accurately distribute software, data, or trained models.

### **Remember**

Recalling of standard tools or platforms and their usage for distributing software, data, or trained model

### **Understand**

Understanding the basic concepts of related tool or platforms.

### **Apply**

Applying distributing approaches and knowledge to distribute software, data, or trained model in respect with compliance, policy, and law.

### **Analyze**

Analyzing advantages and disadvantages of different distributing approaches.

### **Evaluate**

Evaluating the quality of distributing approaches and suggesting improvement.

### **Create**

Developing new approaches, techniques, or tools for distributing software, data, or trained model.

## **C.1. Compliance with laws, policies, and ethics**

### **Description**

The ability to conduct duties in accordance with laws, regulations, organizational policies, and ethical standards.

### **Remember**

Able to recall relevant laws, policies, and ethical standards.

### **Understand**

Able to explain the importance of compliance and ethical behavior in the operation/research duties.

Understand consequences of non-compliance with policies and ethical guidelines.

### **Apply**

Applying compliance and safety protocols and ethical guidelines in a practical setting. Follow rules, regulations, and policies in daily tasks.

### **Analyze**

Identifying areas where policies and ethical guidelines can be improved or strengthened and proposing solutions to address these issues.

### **Evaluate**

Making judgments about the effectiveness of policies or ethical guidelines, and providing feedback on how they can be improved or applied more effectively.

Assess the impact of decisions on ethical and legal standards.

### **Create**

Lead initiatives that foster a culture of integrity and accountability.

## **D.1. Scientific background knowledge, Methodology, process, and tools**

### **Description**

Familiarity with scientific background knowledge, methodologies, processes, and tools, and the ability to select the most appropriate approach for a given research project.

### **Remember**

Recalling background knowledge, methodologies, processes, and tools used in scientific research.

### **Understand**

Understanding the advantages, disadvantages, and limitations of different methodologies, and being able to explain how they can be benefit to a particular project.

### **Apply**

Selecting the most appropriate methodologies or tools for solving research questions or problems.

### **Analyze**

Profiling the performance of various methodologies or tools in achieving a research goal and identifying areas where improvements can be made.

### **Evaluate**

Evaluating the effectiveness of various methodologies or tools in achieving a research goal.

### **Create**

Developing new methods or tools that advance current research capabilities or resolve particular scientific problems.

## **D.2. Literature Review**

### **Description**

Demonstrating the ability to conduct a comprehensive review of literature on a given topic and synthesize insights to support the development of one's own research.

### **Remember**

Recalling relevant keywords or literature related to a particular research question or topic.

### **Understand**

Understanding the key findings and contributions of literature.

### **Apply**

Applying literature reviews to inform the development of research questions, hypotheses, or study designs.

### **Analyze**

Analyzing the strengths-weaknesses and limitations of literature.

Identifying the knowledge gap of an existing knowledge base.

### **Evaluate**

Evaluating the overall quality or some parts of literature.

### **Create**

Creating new research approaches based on a comprehensive review of the literature and explaining how they add to existing knowledge.



### **D.3. Scientific Data management and analysis**

#### **Description**

Efficiently organizing and managing data to facilitate result analysis, inform research insights, support artificial intelligence development, and enhance decision-making.

#### **Remember**

Recalling standard practice use for organizing and managing data.

Recalling relevant data types and sources.

#### **Understand**

Explain the role of data organization in supporting AI and research insights.

#### **Apply**

Apply appropriate approaches, tools or techniques to manage or analyze datasets for analysis or AI development.

#### **Analyze**

Analyzing the performance of tools and techniques used in research or development.

#### **Evaluate**

Evaluating the efficiency of tools, techniques, or frameworks and identifying areas of improvement.

#### **Create**

Design and implement a data management framework tailored to specific research or AI development context.

## **E.1. Teamwork**

### **Description**

Ability to collaborate effectively with others towards a common goal, sharing knowledge, resources, and responsibilities.

### **Remember**

Recall teamwork principles, roles, and responsibilities within a team.

### **Understand**

Understanding different perspectives and needs within a team and adapting communication and collaboration strategies accordingly.

### **Apply**

Participating actively in team activities, contribute ideas, and work collaboratively on tasks.

### **Analyze**

Analyzing team dynamics. Identifying potential conflicts or inefficiencies and proposing solutions for improvement.

### **Evaluate**

Evaluate the effectiveness of teamwork strategies and make recommendations for optimization.

### **Create**

Ability to develop new strategies, tools, or processes that enhance collaboration and productivity.

## **E.2. Communication**

### **Description**

Communication is the exchange of information, ideas, or emotions through verbal, written, or non-verbal means.

### **Remember**

Recalling basic communication principles, such as encoding, decoding, and feedback.

### **Understand**

Understanding different communication styles.

### **Apply**

Ability to convey ideas effectively through written or verbal means, adjusting communication style to suit the audience and situation. Adapting communication strategies to various contexts and recognizing cultural differences in communication practices.

### **Analyze**

Analyzing messages to identify underlying assumptions, detect subtle cues, and interpret hidden meanings in communication.

### **Evaluate**

Evaluating communication effectiveness and suggesting recommendations for improvement.

### **Create**

Developing new communication strategies or techniques that improve clarity, engagement, and understanding.

### **E.3. Human-driven service provision and support**

#### **Description**

Providing assistance or resources to individuals or groups in need, guided by empathy, compassion, and a willingness to help.

#### **Remember**

Recalling a practical protocol for supporting individuals or groups in need

#### **Understand**

Understanding of the importance of human-driven provision and support in various contexts.

#### **Apply**

Providing direct or indirect assistance in a manner that is respectful, caring, and non-judgmental.

#### **Analyze**

Assessing individual or group needs, including hidden needs, and considering multifactor such as cultural background, personal history, and situational context.

#### **Evaluate**

Evaluating the effectiveness of provision and support strategies, making adjustments or improvements as needed.

#### **Create**

Developing new approaches to human-centered services and initiatives that promote a supportive and inclusive society.