

## Capability profile

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Capability profile is defined as capacity to perform tasks in a given role. It consists of 2 components.

- i) Core function – main function of a given role
- ii) Competency – related competencies of a profile

There are 5 levels of each discipline as follows.

1. **Apprentice**      Have limited set of skills. Able to work on guided projects or narrow specific tasks. Supervision is needed for brand-new or complex tasks.
2. **Practitioner**      Have basic set of skills covering the majority of aspects. Able to work on specific tasks. Recommendation is needed for complex tasks.
3. **Competent**      Able to apply set of skill to solve real-world problem. Able to solve common problems independently.
4. **Proficient**      Able to lead a project for solving real-world problems. Able to solve unseen problems with some advice.
5. **Expert**      Able to lead a team to conduct a research or development project. Able to solve unseen problems and create new research protocols.

### Disclaimer

This competency and capability profile framework does not cover the diversity of background knowledge in research domain. They are packed in *D1 Scientific background knowledge, methodology, process, and tools*. The diversities are in *A high performance computing* and *B computing competency*. The competency of *E Soft skills* is not covered in this version.

Competency/Role	HPC AI specialist			HPC computational chemistry specialist		
	Apprentice	Practitioner	Competent	Apprentice	Practitioner	Competent
A1 Estimate benefit of HPC on specific use case	remember	understand	apply	remember	understand	apply
A2 Running specific software/tool/workflow on HPC environments	remember	apply	analyze	remember	apply	analyze
A3 Performance optimization on HPC		understand	apply		understand	apply
A4 Debugging software/workflow on HPC						
A5 Operating HPC system						
B1 Working remotely in Linux environment via command line interface	apply	apply	evaluate	apply	apply	evaluate
B2 Managing programming languages and their packages via package manager	understand	apply	analyze			apply
B3 Installing and managing scientific software and preparing a related environment	remember	understand	understand	remember	understand	apply
B4 Using specific tools, software, or IDEs as each individual or together	apply	apply	analyze	understand	apply	analyze
B5 Estimating computing resource requirement	remember	apply	analyze		apply	analyze
B6 Distribute software, data, or trained model						
C1 Compliance with license, policy, and ethics	understand	understand	apply	remember	understand	apply
D1 Scientific background knowledge, Methodology, process, and tools	understand	understand	apply	understand	understand	apply
D2 Literature Review	remember	understand	apply	remember	understand	apply
D3 Scientific Data management and analysis	apply	apply	apply	apply	apply	apply

**Roles**

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## HPC AI specialist apprentice

### Computational core function

- Able to utilize a node of HPC for running AI workload
- Able to prepare a Python environment by following a guideline
- Able to work in batch and offline mode which is a common HPC environment

### Research core function

- Basic knowledge of related topics
- Communicate finding results

### Competency

- A1 remember
- A2 remember
- B1 apply
- B2 understand
- B3 remember
- B4 apply
- B5 remember
- C1 understand
- D1 understand
- D2 remember
- D3 apply

## HPC AI specialist practitioner

### Computational core function

- Able to utilize HPC for running AI workload using multinode
- Able to prepare a Python environment by adapting from a guideline
- Able to set relevant environment variables efficiently by following guidelines
- Able to work in batch and offline mode which is a common HPC environment

### Research core function

- Basic knowledge of related topics
- Able to find relevant articles, publications, or repositories
- Communicate finding results

### Competency

- A1 understand
- A2 apply
- A3 understand
- B1 apply
- B2 apply
- B3 understand
- B4 apply
- B5 apply
- C1 understand
- D1 understand
- D2 understand
- D3 apply

## HPC AI specialist competent

### Computational core function

- Able to utilize HPC for running AI workload using multinode efficiently
- Able to write guidelines to prepare a Python environment for specific environment
- Able to set relevant environment variables efficiently by applying knowledge from guidelines
- Able to work in batch and offline mode which is a common HPC environment

### Research core function

- Basic knowledge of related topics
- Able to find and describe relevant articles, publications, or repositories
- Share ideas and efficiently communicate finding results

### Competency

- A1 apply
- A2 analyze
- A3 apply
- B1 evaluate
- B2 analyze
- B3 understand
- B4 analyze
- B5 analyze
- C1 apply
- D1 apply
- D2 apply
- D3 apply

## HPC computational chemistry specialist apprentice

### Computational core function

- Able to utilize HPC for performing given tasks according to the instructions strictly
- Able to work in batch and offline mode which is a common HPC environment

### Research core function

- Basic knowledge of related topics
- Communicate finding results

### Competency

- A1 remember
- A2 remember
- B1 apply
- B3 remember
- B4 understand
- C1 remember
- D1 understand
- D2 remember
- D3 apply

## HPC computational chemistry specialist practitioner

### Computational core function

- Able to utilize HPC for performing given tasks by applying knowledge from guidelines
- Able to set relevant environment variables efficiently by following guidelines
- Able to work in batch and offline mode which is a common HPC environment

### Research core function

- Basic knowledge of related topics
- Able to find and describe relevant articles, publications, or repositories
- Communicate finding results

### Competency

- A1 understand
- A2 apply
- A3 understand
- B1 apply
- B3 understand
- B4 apply
- B5 apply
- C1 understand
- D1 understand
- D2 understand
- D3 apply



## HPC computational chemistry specialist competent

### Computational core function

- Able to utilize HPC for performing a given task from a guideline efficiently
- Able to set relevant environment variables efficiently by applying knowledge from guidelines
- Able to prepare software and related environments by following guidelines
- Able to work in batch and offline mode which is a common HPC environment

### Research core function

- Basic knowledge of related topics
- Able to find and describe relevant articles, publications, or repositories
- Share ideas and efficiently communicate finding results

### Competency

- A1 apply
- A2 analyze
- A3 apply
- B1 evaluate
- B2 apply
- B3 apply
- B4 analyze
- B5 analyze
- C1 apply
- D1 apply
- D2 apply
- D3 apply