University of Cincinnati

Date: 7/12/2023

I, Mahmoud Junior Suleman, hereby submit this original work as part of the requirements for the degree of Master of Science in Information Technology.

It is entitled:

The Use of High-Performance Computing Services in University Settings: A Usability Case Study of the University of Cincinnati's High-Performance Computing Cluster.

Student's name: **Mahmoud Junior Suleman**

This work and its defense approved by:

Committee chair: **Jess Kropczynski, Ph.D.**

Committee member: **Shane Halse, Ph.D.**

Committee member: **Amy Latessa, Ph.D.**

UNIVERSITY OF Cincinnati

46694

The Use of High-Performance Computing Services in University Settings: A Usability Case Study of the University of Cincinnati's High-Performance Computing Cluster

A thesis submitted to the

Graduate School

of the University of Cincinnati

in partial fulfillment of the

requirements for the degree of

Master of Science

in the School of Information Technology

of the College of Education, Criminal Justice, Human Services and Information Technology

by

Mahmoud Junior Suleman

August 2023

Committee Chair: Dr. Jess N Kropczynski, Associate Professor and AD Graduate Education

Abstract

The University of Cincinnati's Advanced Research Computing Center employs effective ways through this study in order to make the High-Performance Computing Cluster accessible across all disciplines on campus and the Cincinnati Innovation District. To understand the needs of our users, we employed Norman Nielsen's Group principles of conducting a usability study which involved a survey and think-aloud activity to draw a cognitive understanding of our participants expectations while performing basic tasks and conducted a heuristic evaluation to rate the severity of issues participants identified. Our findings which gave a high-level understanding of how the HPC Cluster can be made more accessible across all disciplines regardless of the user's technical skills, involved the need to build a customized graphical user interface HPC management portal to serve users' needs.Also, investing in workforce development by introducing an academic credit-based High-Performance Computing Course for students and partnering with other faculty's to introduce special programs, e.g. Student Cluster Competitions which would draw more student interest.

Dedication

To my Parents with love and Admiration especially my Step- Mother ***Adiza Suleman Sinare*** *in whom I found peace and love when I was lost as a child.*

Secondly to my Cousin and Mentor ***Louis 'Abu ' Voegtli*** *,who has been very supportive and instrumental in my life and career not only as a brother but a Mentor and Life Coach.My Career in Information Technology was nurtured due to his generous investment and confidence in my talent.*

Also to ***Professor Emeritus Edward J. Latessa*** *of Blessed Memory ; Father of* ***Amy Latessa,PhD****, She has been very instrumental in my Research Computing career.*

Acknowledgments

First and foremost, I am deeply grateful to my advisor, Dr Jess Kropzynski, for her invaluable mentorship and expertise. Her guidance, advice and belief in my abilities have been instrumental in shaping this thesis. I am grateful for the countless hours dedicated to helping me refine my research and pushing me to achieve my best. Also, to my committee members, Dr Shane Halse and Dr Amy Latessa whom have contributed greatly with very informative feedback and ideas that shaped this research.

Secondly, I would also like to extend my Immerse appreciation to Dr Amy Latessa, Jane Combs and the team at the Advanced Research Computing Center for the opportunity they offered me as a Graduate Student Researcher Facilitator; through them is how my dreams of working with a High-Performance Computer Cluster became a reality and Also a Digital Futures Summer 2022 Fellow at the University of Cincinnati. The team's support, guidance, network and opportunities offered to me shaped this thesis and my career immensely.

To the Smart Synergies Lab, their collaboration, camaraderie, and shared knowledge have created a stimulating and inspiring environment. The insightful discussions, brainstorming sessions, and support from fellow researchers have contributed significantly to developing ideas and this thesis's overall quality.

I am forever grateful to my family especially my father Alhaji Adamu Suleman for the unwavering support, love, and understanding. Their encouragement and belief in me, even during challenging times, have given me the strength to persevere. Their sacrifices and constant presence have been the foundation of my success, and I am truly blessed to have them by my side.

I would like to express my gratitude to my friends especially Rockmans Bondam Amoako for being the friend and brother I ever needed ,Also colleagues who have provided me with encouragement and motivation throughout this journey.

Furthermore, I would like to acknowledge the Office of Research and the School of Information Technology for the funding opportunities offered to me during my Masters program.

Finally, I extend my appreciation to all those who have played a part, no matter how big or small, in supporting me during this thesis endeavour. Your belief in my abilities, words of encouragement, and understanding have been a constant source of inspiration. I am humbled and grateful for your contributions to my academic and personal growth.

Table of Contents

List of Tables

Table Page

List of Figures

Figure | Page

1 The Use of High-Performance Computing Services in University Settings: A Usability Case Study of the University of Cincinnati's High-Performance Computing Cluster

1.1 Introduction

High-performance computing (HPC) has become an essential tool to advance scientific discovery over the last two decades, and it's an area where researchers actively create larger systems to accommodate new modes of scientific discovery with complex workflows. Advocating for large-scale scientific programming and HPC have become more essential to achieving national goals considering the discoveries made by academic researchers and industry professionals who contribute greatly to national development, and further increase the importance of adequately educating the next generation [28]. National labs, academic institutions and industry have a strong need for scientists and staff that understand high-performance computing (HPC) and the complex interconnections across individual topics in HPC.However, domain science and computer science undergraduate programs need to provide more educational resources and are far from conveying the interdisciplinary and collaborative nature of the HPC environment [25].

Academic Institutions that are research (R1) based invest resources to acquire and build Centers to manage HPC Systems on campus for Scientists to improve and foster their research capabilities. Over the past years, some HPC Centers encounter challenges encouraging Scientists to use HPC Resources effectively for their research. There is an HPC expertise and knowledge gap because very few educators have the skill set to use HPC Systems made available on campus, making it difficult for non-stem students to learn and access available HPC resources[32].

HPC is adapted in a diverse area of disciplines which makes it difficult for students to understand the different domains of its uses and its applications. Moreover, launching an HPC application is not a simple matter of creating a ”hello world” program, as these applications contain multiple components that require different handling, which requires high-level skills and learning curves to be able to use them [48].

High-Performance Computing (HPC) requires users to learn materials from a broad range of topics that do not necessarily all build on one another to acquire a particular skill set to use them effectively for their research; Learning these skills does not guarantee your ability to use HPC's effective because it requires months of constant practice and use to improve their skills. These subjects, for example, are typical HPC curricula – often designed for STEM students without much background in computer science – including subjects such as Computer Literacy, Programming and algorithms, Parallel computing, Version control and Debugging etc. [49]. Student researchers from different departments who don't have computing knowledge require extra training to be able to use the system effectively in their research which creates an additional hurdle to jump in order to achieve their desired goals. To address this problem the goal of this research is to conduct a usability study to find out why students and faculty find it difficult to use the available local high-performance computing resources. Toward this goal, this paper aims to address the following overarching research question:

- *How can HPCs be made more accessible for use across disciplines in institutes of higher education?*

1.2 Background Literature

1.2.1 Evolution of High-Performance Computers

Over the years, there has been rapid growth in computing and communications technology; the past decade has witnessed a proliferation of powerful parallel and distributed systems and an ever-increasing demand for the practice of high-performance computing (HPC). HPCs have moved into the mainstream of computing. They have become a key technology in determining future research and development activities in many academic and industrial branches. They must cope with very tight timing schedules when solving large and complex problems [1].

In computing, historians often celebrate the work of Charles Babbage and his famous Difference Engine – the first complete design for an automatic calculating device. This device is mostly credited as the first computing project that received government support but set a bad precedent since it was never completed. The project was officially abandoned in 1842 after 19 years work and a government investment of £17,000 – then a very large sum of money. Despite its failure, Babbage remained resolute to his work and invented another machine, the Analytical Engine which, in contrast to the original Difference Engine, was intended to be a programmable general-purpose machine capable of solving virtually any mathematical problem [11]. The external program for the Analytical Engine, for example, was specified on punched cards, in a similar fashion to the cards used by Joseph-Marie Jacquard to control an automatic loom. It is also often said that Augusta Ada Byron, daughter of the famous poet Lord Byron, was the first programmer. Ada, in whose honour the modern programming language is named, wrote an influential article about the machine and how to program it. The Analytical Engine also had the capability to perform a "conditional jump" or "branching" and this was one of the key features that raised the capabilities of Babbage's machine beyond those of a mere calculator. The machine was never built but Babbage's design nevertheless remains as a remarkable leap of human imagination[26].

In 1985, the National Science Foundation established a partnership between five research centres: the San Diego Supercomputer Center (SDSC) at the University of California San Diego, the Pittsburgh Supercomputer Center (PSC) at the University of

Pittsburgh, the National Center for Supercomputing Applications (NCSA) at the University of Illinois Champagne-Urbana, the Cornell Theory Center at Cornell University [47].In the last decade, there has been significant advancement relating to the reliability and performance of computing elements such as processors, disks, and network devices. Computational power has increased in desktops and laptops by the availability of processors; the advent of these reliable and powerful off-the-shelf computational elements has also spurred a new generation of high-performance computing systems [15].

1.2.2 The Value of High-Performance Computing centres on University Campuses

Stewart et al [39] defined Cyberinfrastructure as “consisting of computing systems, data storage systems, advanced instruments and data repositories, visualization environments and people, all linked by high-speed networks to make possible scholarly innovation and discoveries not otherwise possible. ” Research by Amy Apon [12] showed that the presence of a Top 500 supercomputer on a campus (an input) positively impacts the institution’s overall research output. Analyzing a cross-section of data across universities, this work was the first peer-reviewed publication discussing ROI of cyberinfrastructure and serves as a foundation for most of the ROI work that has followed and for this dissertation. Apon [13] also studied the impact of HPC investment on research output at the departmental level and found that several fields (Chemistry, Physics, Civil and Environmental Engineering) are more productive in universities with local HPC resources. Apon stated that “Broadly speaking, universities combine faculty effort, physical plant, and other inputs to produce outputs such as research and education. Apon’s works show statistical analyses of cyberinfrastructure’s impact on institutional productivity.

A team from Indiana University [38] calculated the ROI of 3 cyberinfrastructures: IU’s Big Red 2, the Jetstream Cloud, and XSEDE. Similar to Carlyle et al. (2010), Stewart's methods explored acquisition costs, not evaluating costs of data movement and storage. Even without data costs, Stewart found that Indiana's campus cluster yielded a cost savings of 2.5-3.7x vs an alternative on the Amazon commercial cloud. Scrivner[35] described XDMOD-VA, a visualization plug-in to the XDMOD [36] metric tool widely used in US academic HPC centers to easily present value proposition metrics. This clearly showed how the use of super computers is cost effective for most educational institutions.

At many Universities, high-performance computing is critical to attracting research grants, recruiting, and retaining top faculty, and teaching students' cutting-edge data-intensive research methods. The NSF's CI2030: Future Advanced Cyberinfrastructure report examines the need and future of cyberinfrastructure (CI) in the US and argues that: "An integrated CI that reaches from university and college campuses to the national centres is needed; this will require coordinated investments by all of the stakeholders." and that ". the vast majority of capacity-class computing activities will be carried out on campuses.", it continues, "communication and collaboration across research silos offer the possibility of building and deploying an integrated cyberinfrastructure that effectively and efficiently supports a broad range of scientific and engineering research" [4] .

Most Universities and research facilities employ the services or integrate high-performance computing to process large data that requires high computational resources. HPC service centers are a vital part of the academic infrastructure of higher education organizations, as they serve as a bridge between the university community and the high-performance computing system. HPC centres house and manages the HPC clusters of the organization, they provide large research project computational resources, computing-related data storage and network transfers within and beyond the campus to facilitate data movement among researchers [45]. HPC centres provide consultation and assistance to college researchers with advanced computational software and/or hardware needs, as well as support, configuration, and guidance to users porting and optimizing applications to make the most of HPC capabilities.

1.2.3 Usability of High-Performance Computing in STEM and other disciplines

The use of high-performance computing is becoming increasingly prominent in higher education. The introduction of super computers in education is a challenge that provides a broader range of opportunities. In this sense, the possibility of managing high volumes of data and information has prompted educators and researchers to take a different teaching approach to promote the use of these infrastructures in teaching. Computing Education (CE), as a popular research field, faces new challenges that require students' motivation, which is the foundation in systems as the SAIL—a System for Adaptive Interest-based Learning [24]. New tasks and challenges arise for the Higher Education System (HIES) which require extensive and complete training.

This training has to face the limitations of the integration of technologies in teaching and at the same time be included in the standard curriculum as a constraint related with the use of super computers. Currently, the use of Supercomputers is becoming critical to the improvement of study in STEM and other disciplines of higher education, despite the lack of experience and basic skills in this field and low availability of Supercomputing facilities due to the high costs [22]. Supercomputing education has become very important for innovation, modernization, and technological development, contributing to the creation of a new generation of professionals, companies and organizations from STEM and other disciplines.

This area is also in charge of specific training, mainly for students of computational science and engineering, and also for students of various fields of knowledge, that use computational, mathematical, and engineering tools for problem solving [23]. Currently, many educational institutions worldwide are seriously introducing computer science concepts into the basic training of students, which raises the question of how important the training in Supercomputing for the professional future of students is. The introduction of new information and communication technologies (ICT) in the training sessions of students of all levels has been considered one of the main tools in the modernization of all educational systems. It has contributed to evolution from the “society of the information” to the “society of knowledge”, allowing forming students, in an appropriate way, for the exercise of a great variety of professions. This consideration means that the use of super computers will be important to STEM and non-STEM disciplines and will be essential for solving complex data problems[22].

Over the years, traditional HPCs have been widely used by researchers in Computing and Engineering fields and other closely related fields. Using HPCs require users to have strong coding and Unix backgrounds in order to achieve their research goals which is a big barrier for researchers in non-STEM fields, Most non-STEM researchers and other researchers in STEM who do not have experience using Unix (Linux) have to take a crash course or hire a Unix experience researcher on the team which makes it difficult for researchers without these means to find other ways of analyzing their data instead of going through the dark paths mentioned above. In previous years HPCs have been strictly made available for Computing and Engineering fields and this sounds like a myth to non-STEM researchers when HPC is mentioned. In this modern age of technology, Big Data and Artificial Intelligence have a significant impact on Academic Research, Education, Business, Governance, and Social Intervention. Big Data and AI hold significant potential for creating value and transforming Human life and its potential can be realized only through the use of appropriate technological implementations. Specifically, more powerful computing to scale up data processing, networking, and storage capabilities is required to harness the Vast promise of Technology and Large amounts of data [34].

For students in non-STEM disciplines, supercomputing training represents a specific learning activity. It provides an integrated and experimental approach in the use of technologies for higher education students in advanced contents. These contents are designed to provide experiences in the analysis of real cases to be used as pedagogical resources. At the same time, it increases learner engagement, making students feel involved in the course content, improving the level of technical expertise and expectations regarding technology. The level of training provided in these courses covers a wide range of areas that depend on the target category of the trainees. They are supported by specialists in many fields of knowledge that help students in solving complex computation-intensive applied problems. Supercomputer education is based on a wide variety of courses and tools, under different forms of educational programs that permit the development of these skills. In general, courses linked to Supercomputing differ from those in STEM programs and other disciplines.

Supercomputing training for STEM Programs can be divided into three main areas: system architecture, applications in computing science/computing education, and specific-domain courses. For higher education students in other disciplines, supercomputing training offers several advantages. First, students can explore real problems through hands-on experience, learning the most advanced functionalities of computers and linking theory with practical problem solving. Second, supercomputing training helps students use mathematical models to describe problems in a specific research field and extract conclusions. Third, simulations and data design in a supercomputer prepare students for the role of leaders in research using very large database systems. Finally, supercomputing contributes to inventing new tools and new philosophies of work, which enhances the learning about computing.

1.2.4 Demystifying High performance computing for non-Linux users:The introduction of Remote computing desktops.

The introduction of web-based portals for managing and using HPCs by end users has been a remarkable achievement. It has improved users' time navigating their way around HPCs to complete a task. This is not only limited to the time involved by HPC centres to train new users, especially non-Linux users, to adapt to the Command Line Interface (CLI) to complete their tasks. Not only have end users been relieved, but System admins and Research Computing facilitators; these portals give them a one-stop shop to manage these clusters and easily support end users. In this era of computing, more emphasis on graphical and intuitive interfaces is essential to clear barriers away from researchers from all respective fields to use computing resources with ease and not deal with rigid legacy system designs. Mastering the CLI is an essential skill, but it becomes intimidating for researchers who want to use the High-Performance computing resources of a university [5]. According [43]Over 75 percent of users say that the desktop services are either moderately or extremely important for their ability to use HPC resources. During training sessions at Indiana University, they observed that researchers who were constant Linux users who didn't know about HPC were enthusiastic about learning and trying out the HPC system and wanted to know more about its capabilities and features. However, they mostly complained about the Job Schedulers, e.g. SLURM and longer wait times for their jobs would be in the queue. Non-Linux researchers/users have more reservations towards using HPC systems; most had no choice but to learn the command-line and how to eventually use the Job schedulers due to the nature of their research and the size of their data sets. In Summary, most HPC Users were demotivated to use the HPC system for their research. This concluded that the command line and the batch job scheduling are significant barriers for potential HPC users [43].

1.2.4.1 Web-based Portals for Managing High Performance Computing Clusters

Web-based portals for HPCs were introduced in the 1990s with Java applets, making it easy to access HPC resources using a variety of use cases remotely. This identified the key features and functional and non-functional requirements of these portals [16]. Web-based management portals aid in reducing barriers that limit the adoption of high-performance computing (HPC), which addresses an important challenge affecting the STEM community. Through the Cyber-Infrastructure grant, the NSF has supported Higher Education institutions and National Supercomputing Labs to develop web-based HPC management portals to help researchers with little computer science skills adapt and foster the use of HPCs in their research [8].Some benefits of having Web-based portals include but are not limited to

1. Increasing the use of HPC resources among disciplines not well represented in the community but desiring need for HPC resources.

2. It is also beneficial to HPC stakeholders because it is easier to adopt advanced features to monitor and visualise system needs and upgrades.

3. This creates a working model for training and workforce development to expand the cyberinfrastructure space for computer science. In 2016, the first version of Open on-demand launched, the Open On-demand project, funded through the NSF Cyberinfrastructure grant ([7]) with the goal of making accessing HPC resources easier. The Open on Demand Project was an Open source software project hosted by the Ohio Super Computing Center that enables HPC centres to install and deploy advanced web and graphical interfaces for their users [9].

Open On-Demand is a one-stop shop with an intuitive Dashboard upon logging in. The dashboard provides navigational aid to the user with a unified experience while allowing them to access the various tools and resources provided by the HPC Center [10].

The critical features of the Open On-demand dashboard are e.g. in figure 1.1;

- *File access allows users to access and commit files from their local workstations and the cluster to the home directories.*

- *Job creation and monitoring is a critical part of running projects on HPC systems because this process is where sessions are created and also monitor the status of jobs in the queue; this portal makes it easier for end users to monitor the status of their jobs, also edit and update them.*

- *Though the goal is to eliminate the command line interface from users, it is imperative for users to have access to the CLI, which makes it diverse for users who enjoy the CLI to use it without difficulties. As at March 2023, Open On-Demand has been widely adopted in the HPC eco-system and has surpassed more than 400 active installations [30]*

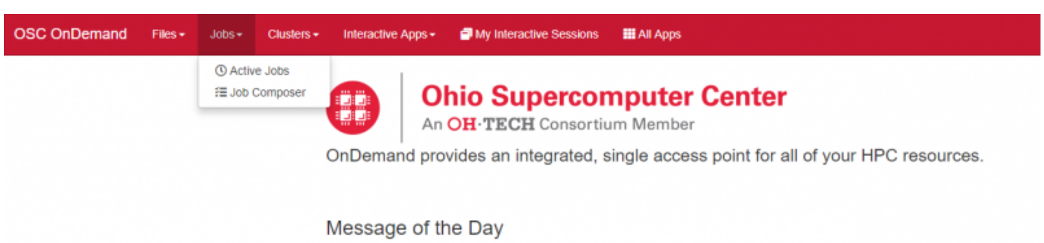

Figure 1.1: Dashboard of Open on-demand, a Web-based portal for managing HPCs.

1.2.5 Next Generation of HPC Workforce Development: Making HPC Systems Usable through Workforce Development

Attaining the goal of having a long term and competent computing infrastructure depends on the severity of the skills and expertise of domain scientists and committed and well-trained advanced computing professionals. In contrast to computing hardware, the human infrastructure of technical skills and expertise in operating, maintaining, and evolving advanced computing systems and technology has a limited lifeline. To ensure optimal operation of High-Performance Computing systems, specialized and advanced training is required. This identifies that there is a huge gap for individuals with skillset on High Performance Computing, and the intense global competition for computing talent. There is a perpetual and critical need for innovative approaches to help limit or close the gap and create a well-prepared, next generation High Performance Computing workforce. While HPCs have become a long-standing and essential tool to advance scientific discovery and achieve national goals and are an area of active and advancing research, there exists a gap between the technical skillsets needed, particularly at the entry-level, and the exposure and skillsets provided in current undergraduate (and even graduate level) academic programs. Recognizing this gap and the resulting unrelenting organizational strain due to an inadequately prepared entry-level pipeline, Los Alamos National Labs (LANL) set out just over a decade ago to actively engage to bridge this gap for a specific pipeline need, establishing the Computer System, Cluster, and Networking Summer Institute (CSCNSI) in 2007 [20].

A division at Los Alamos National Laboratory (LANL) i.e., The High-Performance Computing Division supervises world-class supercomputing centers in support of the Laboratory's national security science mission. The scope of work encompasses specifying, operating, and assisting in the use of open and secure high-performance computing (HPC), storage, and emerging data intensive information science production systems for multiple programs. Also, the LANL, and national laboratories, require and are always looking for scientists and staff who understand and could operate, use, and help advance HPC systems and technology. With a proven program with nearly five highly successful years under its belt and an expanded goal to broaden CSCNSI outreach and impact, LANL collaborated with the newly established New Mexico Consortium (NMC) on a joint proposal to the National Science Foundation (NSF) with the result that the CSCNSI received five years of NSF support (2011-2015) as an educational component of PRObE, the Parallel Reconfigurable Observational Environment[21] .

PRObE is an NSF-funded low-level, large-scale computer systems research facility located in Los Alamos, NM and housed by the NMC at the Los Alamos Research Park. The primary mission of PRObE is to provide the national systems research community resources in the form of several largescale testbeds (of 1000+ computing nodes) built from repurposed supercomputers from LANL and dedicated to computer systems research [29]. As such, PRObE is the only facility of its kind in the world. The CSCNSI has had two successful outreach programs that share some important attributes with each other and with the CSCNSI while addressing different but related aspects of the HPC education gap:

1. The New Mexico Supercomputing Challenge which started in 1990

2. Student Cluster Competition developed and debuted in 2007.

These two successful programs and the CSCNSI have differences. The Supercomputing Challenge is engaging elementary, middle school, and high school students in how real-world problems are modeled mathematically, translated into computer code, and analyzed with a larger goal of attracting students to continue their education and pursue STEM fields [20]. The Student Cluster Competition is engaging undergraduate students directly in an intense 48-hour challenge to broaden their HPC exposure, while it simultaneously seeks to affect undergraduate curricula. Further, size of student engagement also varies. The CSCNSI is a relatively small and non-competitive (in terms of competition between student teams) program that seeks to leverage (not necessarily affect) typical undergraduate computer science and computer engineering programs with the goal of systematically growing a targeted HPC skillset to provide a strong student intern and early-career staff pipeline [25]. All three provide useful and important approaches to bridging various aspects and levels of the HPC skillset gap.

1.2.6 Case Study: Advanced Research Computing centre at the University of Cincinnati

The University of Cincinnati's Advanced Research Computing (ARC) centre offers a readily accessible hybrid CPU/GPU computing cluster, supporting computational and data science researchers while developing a highly competitive workforce amongst the university community.

[14]. ARC partners with researchers to utilize the core suite of HPC services and resources. With the resources ARC has available researchers advance theoretical knowledge and expand the realm of discovery, generating leading-edge research and applications suitable for innovation and commercialization in line with the University of Cincinnati's "Next Lives Here" strategic direction. The centre has a sustainable high-performance computing (HPC) infrastructure with technical support that leverages HPC services to accelerate the time to discovery and enables sophisticated and increasingly realistic modelling, simulation, and data analysis and which helps to bridge users to the local, regional, and national HPC ecosystem [14].

ARC provides a wide range of services that support and promote the research community on the university campus to use the services and resources of the high-performance computing cluster for their research to achieve desirable results.

The Advanced Research Computing Centre (ARC) at the University of Cincinnati provides consultation services to discuss research data analysis, data transfer, and data storage needs for the research community. They offer grant support by providing quotations for computing/storage and grant language to support data security compliance. High-performance computing is the core business of ARC, but due to the growing demand for resources by the University's research community, ARC has partnered with Ohio Supercomputing Center (OSC) [17] and Jetstream2 by Indiana University [6] to provide more computing resources to researchers. They also provide secure data transfer and management through a web-based platform called "Globus." ARC invests in training and education for students to use high-performance computing efficiently, organizing periodic training sessions for the general student body, and providing external training opportunities.

1.3 Methods

In this methods section, to understand user needs of the High-Performance Computing Center, we employed the combination of methods used by [31] to get a better understanding and feedback from users. We used three complementary data collection methods, which were rolling out an online survey, using qualitative methods to collect user feedback through a think-aloud activity which is a one-on-one interview to have a more profound cognitive understanding of users' needs and what they think about the design by voicing out their misconceptions and converting actionable steps into design recommendations. Also, we conducted a heuristic evaluation which used key evaluators to measure the severity of the current design not adhering to usability principles.The methods were approved the Institutional review Board (IRB) and certified the actions to be taken above in order to achieve our needed results for this research.

1.3.1 Research Participants

According to [41], selecting our participants for this research depended on the nature of the study and the results we expected. This information went further to provide some essential demographics of the recruitment and user patterns, e.g. how participants of the survey were selected to satisfy the interest of the research outcome, who selected the participants, the number of participants, and how the study was presented to the participants, including the entire recruitment plan for both the survey, think aloud activity and heuristic Evaluation. Our target population for the survey were students and faculty members of the University of Cincinnati, especially current and future non-Linux researchers who intend to use or use the resources of the High-Performance Computing cluster.

For the survey audience, aimed at Science, Technology, Engineering, and Mathematics (STEM) students and faculty members, and also we chose not to limit our audience not only to a particular group but open to all potential users that had an interest in using the cluster regardless of their technical skills or background. This diversified our participants, which gave us more information to feed into our future design.

Participants will be recruited in two stages or categories:

- **Current University Researchers** Active and Non-active users of the HPC cluster: Researchers eg (Postdocs , Research Assistants etc) at the University of Cincinnati who currently use the HPC Cluster or potential future users.

- **Students (Undergraduate, Masters,PhD)** Students from all STEM Departments e.g., Engineering, School of Information Technology, College of Medicine, Department of Art and Planning.Also expanded recruitment to students from Non-STEM departments.

- **Faculty** These are Faculty who teach courses that require access to cloud or High Powered computing resources and Principal Investigators that lead research labs in various departments at the University of Cincinnati.

- **Staff** Individual staff members of the University that use or potential users that use the resources of the HPC centre for their departmental work or other, e.g. UC Medical Center, Business and Data Analytics.

1.3.2 Recruitment

Given the demographics of our survey participants, our goal and the recommendation of the University of Cincinnati's High-Performance Computing Center; we conducted an online survey, and our audience were STEM students, researchers and Faculty members at the University of Cincinnati. The survey was hosted on a secure cloud platform provided by the University named ”Qualtrics”; our potential participants were identified and recruited through a list of active and non-active users of the HPC Center. We cast a wide net by sending emails to all users of the HPC Center in order to draw their interest and fill out the survey; The survey had 27 questions with topics that ranged from understanding their experiences with High-Performance Computers and recommendations.

1.3.3 Data Collection

Our purpose conducting a qualitative analysis was to interpret the collected data and the resulting themes, and facilitate understanding of the phenomenon the study. The study aimed to collect cognitive and constructive feedback from selected research participants. We designed a survey with questions that focused on getting users' feedback to understand the design issues' needs and severity.A one on one think aloud activity are recorded, which will then be transcribed to create text for qualitative coding and analysis. By Considering these Qualitative data collection methods (e.g., focus groups, one-to-one interviews, online surveys), the process will involve the generation of large amounts of data [40].

1.3.3.1 Think-Aloud Activity

The method of collecting think-aloud data involves participants spontaneously verbalising words that come to mind as they complete an activity [46].This makes it very essential to conduct usability testing, it allows users to verbalise their thinking as they use a new system. This allows evaluators to infiltrate the mind of users and acknowledge individual differences.

To further understand users' needs in-depth, we selected some users by their responses to the survey and participants who voluntarily signed up for a Think Out activity.We reached out to survey respondents across the sample for a 1-on-1 interview, if they opt-in to choosing to be interviewed. We selected five users out of the respondents of the Survey,3 of whom were super users and two were non-superusers. We opened the conversation for users to have cognitive thinking, which would have them expand their thoughts when using the portal; we further asked questions regarding in two folds ,for Superusers and Non-Superusers :

- **Superusers** were asked what connection methods to the cluster they preferred and whether they needed an intuitive Graphical User Interface portal. Also, what were their current needs for the graphical user interface portal? Furthermore, what can be done to improve the usability of the portal?
- **Non-Superusers** who are mostly Non-Linux users were asked about their concerns with the HPC portal and what they expected from the HPC cluster in order not to use the CLI.

Common questions we asking during the think aloud activity were? What feature did they want to see change on the portal? What feature they wanted to be maintained on the portal? How the portal would make their use of the cluster easy eg. job submission and job status monitoring ?.

In order not to influence users thinking and have their ideal participation whiles offering their honest thoughts spontaneously ,we did not prompt users during the conversation; however, to avoid too much silence or stiltedness, we had signs with important information, e.g. keep talking, Go on, that is interesting etc. For pre-orientation and housekeeping, we dedicated the first fifteen minutes of the session to explain how the think-aloud activity would be facilitated and an overview of the 'think-aloud' method was provided in a pre-interview facilitator script [46].

Considering the schedule of participants of the interview since they offered to join voluntarily, The interviews were conducted virtually, over Microsoft Teams, in order to make it easy to record and transcribe the audio, which would aid in the qualitative coding of the statement. However, participants that did not have access to Microsoft Teams were also given the option to chose another secured video conferencing platform of their choice [18].

We conducted construed and semi-construed one on one interviews with the selected participants of the survey. Participants were categorized into Super and Non-Super Users; Super users had extensive experience using Linux and all other methods connecting and using the HPC Cluster, while non-superusers had minimal to zero experience using the HPC Cluster.

During the interviews, we focused more on how to use the HPC Cluster, from connection methods to Job submissions using Slurm, Job monitoring and exporting results using Secure Shell Host (SSH) and tools like Putty, MobaXTerm and via Open

On-Demand. Also, we had to consider what it takes when users wanted to modify their already submitted job scripts.

Our participants were users allowed to reflect more on the best options that worked for them when using the cluster and why they prefer them. After that, we focused on the feature of each connection method to understand their perceptions and whether they had HPC experience from their previous organisations or personal use. We also Observed and noted their behaviours in real-time,Which was also feed into feedback we drew from the session of each participant.

The participants were motivated to share more about the positives of the current HPC System and how they would like to improve it. Also, to be inclusive, we asked participants to reflect on and recommend which features of the current system ”they would not like to be changed” and which feature ”they would like to be changed /modified immediately ”.Furthermore, we asked users, especially non-Linux, to recommend their ideas for the best intuitive Graphical user Interface Dashboard.

After interviewing all participants and collecting data, we performed a Qualitative Thematic analysis by manually reviewing all transcribed audios ; we linked related patterns and keywords based on other participants. The thematic analysis aimed to identify themes, i.e., patterns in the data that are important or interesting, and use these themes to address or say something about the research. This is much more than simply summarising the data; an excellent thematic analysis interprets and makes sense of it. According to [19], the best-practised method is to use the main interview questions as the themes.

1.3.3.2 Heuristic Evaluation

In 1990, a published article by web usability pioneers Jakob Nielsen and Rolf Molich defined Heuristic Evaluation as a set of principles used in ” Improving a Human-Computer Dialogue ”.Heuristics evaluation is a process to determine or certify a design or product's usability systematically; researchers review the product's interface and compare it with other usability principles, and the results are accompanied with recommendations to improve the current system [2].

- *Heuristic evaluation is a usability engineering method for finding usability problems in a user interface design, thereby making them addressable and solvable as part of an iterative design process. It involves a small set of expert evaluators who examine the interface and assess its compliance with "heuristics," or recognized usability principles. Such processes help prevent product failure post-release [44] .*

When conducting a usability study, the easiest, most cost-effective and most accessible method to improve a product is a Heuristic evaluation. The Ideal reason is to invest some time and resources in conducting this test which helps researchers identify key usability issues with products/systems [33].We based our Heuristic evaluation on the ten most fundamental principles that were given by the Nielsen Norman Group , which are listed below in 1.2

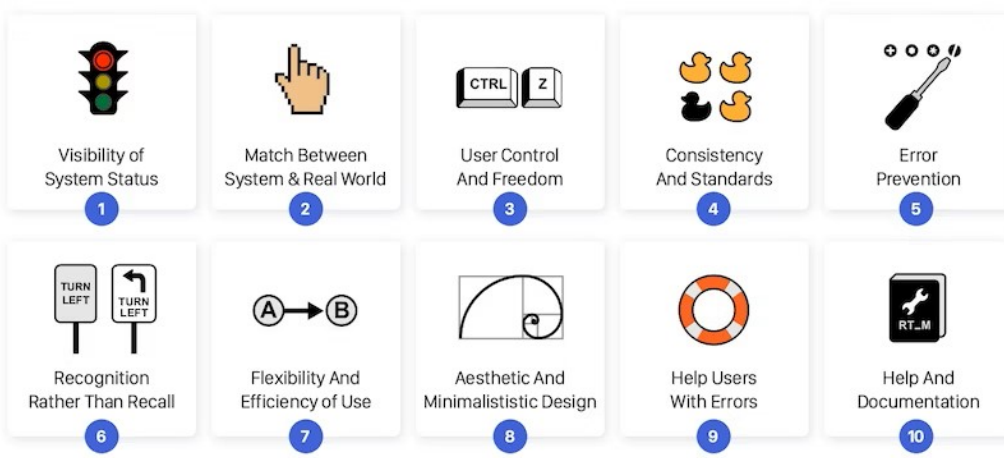

Figure 1.2: Nielsen and Molich's 10 User Interface Design Heuristics.

Conducting the heuristic evaluation, a group of examiners evaluated the user interface of the University of Cincinnati's High-performance Computing cluster interface according to a set of heuristics rules based on 1.2.

We observed and interpreted the user's actions to give us an insight into how these actions were in connection with the usability challenges of the current design whiles our users analyzed issues identified with the portal. We recorded the results of the evaluations independently as they examined the portal. In contrast, the evaluator was responsible for analyzing the user interface, and it allowed the observer to record the evaluator's comments about the interface. However, there was no need to interpret the evaluator's actions[3].We provided a severity rate scale of 5 for each violation to measure the severity of design problems; at the end of the heuristic evaluation, we rated these design problems accurately to reflect the responses and evaluation of our participants.The schema for the severity ratings is listed below :

- **0** - don't agree that this is a usability problem
- **1** - cosmetic problem
- **2** - minor usability problem
- **3** - major usability problem; important to fix
- **3** - usability catastrophe; imperative to fix

1.3.3.3 Data Analysis

Due to the nature of our study , We employed a mixed methods approach to collecting data in this study, which involved both qualitative (survey) and quantitative (Think -aloud activity) methods.According to [42] mixed methods offer confirmation and complementarity that "enables the researcher to simultaneously answer confirmatory and exploratory questions, and therefore verify and generate theory at the same time.we found similarities between topics discussed by the participants which was be generated as themes by performing a Qualitative Thematic analysis. Because we employed a mixed methods approach to collecting data , we focused more on participants engagements that influenced our research which are ; positive and negative feedback, participants describing experiences with using the HPC Cluster during our conducted Think aloud activity and ideas to design an intuitive customized graphical user Interface.

After manually reviewing collected data which includes surveys, transcribed audio and videos, the data in order to be analyzed were categorised into codes and potential themes.For thematic data analysis [27] grouped themes into broad and sub themes in relation to the research questions and analyzed data with regard to how identified themes related to the research questions.

1.4 Results

This chapter highlights our findings from collected and analyzed data, Also to give in-depth insights into recommendations from our participants.

1.4.1 Description of Users and Results from Survey

The survey had 21 responses, and we voided two after review due to incomplete filling, 11 respondents representing (57%) out of the 19 were superusers, and the remaining 8 (43%) were novice or non-superusers. To give more details about the demographics of our participants, the majority of the HPC Cluster users were Graduate students (15) being (75%), 11 (73%) students out of the (75%) were PhD or Doctoral students, four students representing (27%) were pursuing a Masters Degree. Furthermore, Faculty members (Postdoctoral Fellows / Principal Investigators) represented (20%) of the respondents being a number of 4, We had one staff member at the Office of Research that used the resources of the HPC for their heavy data analytics and complex reporting, which represented (5%) of the respondents.

However, to understand the demographics of our respondents, we dived deeper by asking questions about their experience using UNIX /Linux and HPC Clusters in general, the number of years they used an HPC Cluster, the usage frequency of the current cluster, and the Reason for using the cluster; Superusers (57%) had from 3- 10 years experience using HPC Clusters in general either at the University of Cincinnati or a previous university.Non-Superusers (43%) had zero and 1-3 years of experience using a cluster but were not heavy or regular users, and most were first-time users of an HPC cluster. For frequency of use (50%), they used the cluster once or twice a week for their projects, about (27%) used the cluster every day for their research, and (23%) used the cluster either once or twice a month. Most of the respondents, to our understanding, were seasonal users; thus, using the HPC cluster when they had ongoing research projects.

For reasons why respondents used the HPC Cluster, 37% used the cluster for research projects that were Research or Departmental Lab affiliated on Campus, 21% used the cluster for their personal research projects, i.e. conference papers, 16% used the HPC Cluster for External grant Funded Research, because some grant application especially the NSF required HPC resource allocation as part of their grant application requirements, Another 16% used the HPC Cluster for their Thesis and Dissertation and 10% used the HPC Cluster for Class projects. This further explains why 75% of our survey respondents/users of the HPC Cluster were Graduate students (Masters and PhD). Below is a more representation in Table 1.1

About 80% of the users chose the HPC Cluster on campus because it was readily accessible, convenient and they were confident their confidential data was safe and protected by the University Infrastructure; also, they emphasized that it was cost-effective considering the rates charged by other cloud providers and the ARCC technical team is readily available to support if users had any challenges.47% of our respondents did not need UNIX /LINUX training before they started using the cluster, These explains why Majority of the respondents were superusers; They, therefore, had prior HPC experience before using the University of Cincinnati's HPC Cluster.

38% of users required Linux training, therefore, utilizing the training sources made available by the Advanced Research computing Center[14] or other training methods to catch up with their LINUX skills whiles 15% were not sure either they need training or not. To understand how users transferred data to the cluster for their projects, 42% percent of our respondents used the File Transfer Protocol (FTP), 25% used an Application Programming Interface (API) for data transfer, whiles 16.5% used Globus, and others did not transfer any data.

Most respondents selected that the software they needed was installed on the cluster. About 15% had to reach out directly to the ARCC Technical team to have their needed software installed. 20% of our respondents installed their soft wares personally on the cluster without the help of the ARCC technical team.

70% of respondents preferred both methods of connecting to the cluster which per the data are superusers, this is justified because though there is an Interactive GUI some task need the Command Line Interface (CLI) to troubleshoot or debug. Also, a disaster recovery measure. Overall the participants rated the HPC Cluster as Efficient, Engaging, Error tolerant and Easy to use. See Figure 1.3

Table 1.1: Participant Demographics and Descriptive Reported by Expertise

Descriptor	All Participants	Super Users	Novice Participants
N	19	11	8
No. of Years at University			
1 – 3	9	2	5
3 – 5	4	3	3
5 – 10	6	6	0
Role at University	*n* (%)	*n* (%)	*n* (%)
Faculty Researcher or PI	3 (1.5)	3 (10.0)	0(0)
Masters Student	4 (2.2)	1 (2.5)	3(7.5)
PhD Student	11 (5.78)	7 (6.3)	5(3.7)
Staff	1 (0.52)	1 (10.0)	0(0)
Previous Use of HPC	*n* (%)	*n* (%)	*n* (%)
Never Used	0(0)	0 (0)	0(0)
Seasonal User (several uses total)	1 (0.54)	1 (10.0)	0(0)
Once per Month	3 (1.59)	2 (6.3)	1(3.7)
Two or Three Times per Week	10 (5.26)	5 (5.0)	5(5.0)
Everyday	5 (2.6)	3 (6.0)	2(4.0)
Type of Project			
Personal Project	4	3	1
Class Project	1	0	1
Thesis or Dissertation	4	3	1
Internally Funded Research	7	3	4
Externally Funded Research	3	2	1

1.4.2 Identified Codes and Themes from the Think-Aloud activity

For our Thematic Coding analysis, as suggested by [31], We analysed data from the Think aloud activity and created a thematic coding scheme to identify common patterns in the experiences of our participants using the HPC Cluster; after identifying key themes and concepts mentioned by our participants via the interview , we searched for patterns to in these codes after reaching saturation point. We identified key themes/codes from our participants, which we explained in the subsections below. The interviewees for the Think aloud activity were five, and to be more specific in identifying them, we reference participants as P1, P2, P3 etc. Three superusers and two non-supers users participated in the Think aloud activity. However, to incorporate qualitative responses from our survey participants, we referenced them as S1, S2, S3 etc.

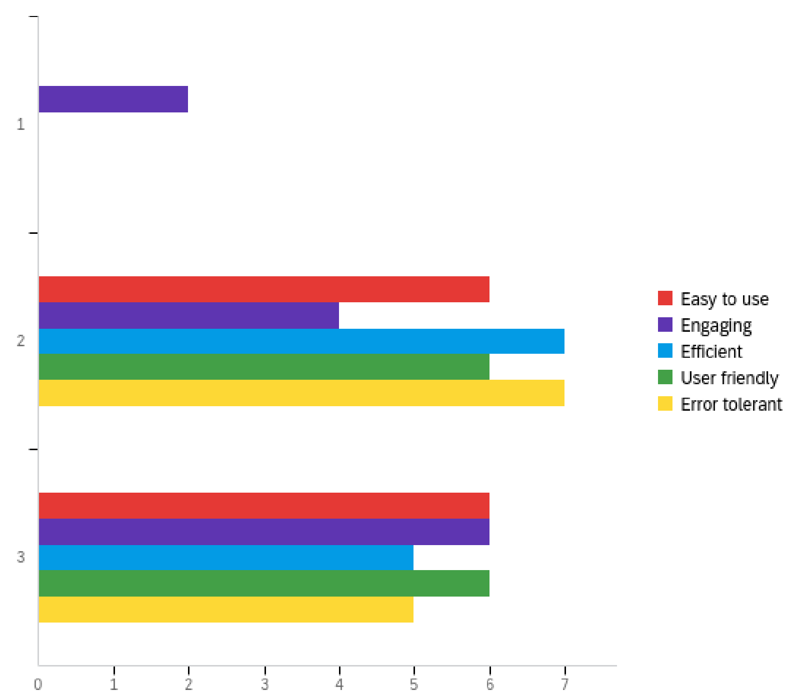

Figure 1.3: A Visualized report of respondents ratings of the current HPC Web Portal

1.4.2.1 Theme 1 : Connection methods to the HPC Cluster

For theme (1) we focused on understanding which connection methods (eg. CLI ,SSH ,Open On-Demand) users preferred when connecting to the HPC Cluster:

Generally all users were interested in the instructions made available by the Advanced Researched Computing Center [14] either on their website or shared by the Research Computing Facilitator who serves as the point of contact when users had challenges or needed first hand information regarding the cluster eg. Specific soft wares , GPU/CPU Allocations, Job Queues Etc.

All users mentioned that enough instructions were on the Advanced Research Computing Center's website, which gave detailed information on all the methods for connecting to the cluster. Users did not have many problems connecting to the cluster on campus since they used the network resource made available by the University; participants P1, P2, and P3 did not appreciate connecting to the cluster via VPN when they were off campus network, though it was a measure to secure confidential information, they believe it hindered collaboration with other non-University of Cincinnati collaborators, They preferred that users could connect to the HPC Cluster without having to go through the cluster, P1 and P2 believed they are other methods to secure the information on the cluster without connecting through the VPN.

All Users preferred to connect via the Current user interface made available, which is Open on-demand; P3 and P4 were non-superusers; they used open on-demand entirely because they did not have UNIX/LINUX skills to connect to the HPC Cluster via the Command Line Interface (CLI) or Secure Shell Host (SSH). Furthermore, Open on-demand saved them the stress of transferring their job files from their local workstations to the cluster since uploading a Python file on the web portal and submitting a job was more accessible than using FTP via a secure shell host(SSH) or an Application

Programming Interface (API). Also, all the other software they needed, especially P1, was a heavy Matlab user, available for her to use without any stress.

P1 and P2 were Superusers but preferred connecting to the HPC Cluster via Open on-demand; P1 did not like using UNIX/Linux, and therefore Open-on-demand served his needs fully. It was easy to access the software he used most for Data analysis and reporting, which is Wolfram Mathematica. P2, also a superuser, preferred connecting to the cluster via Open on-demand due to his experience; P2 is a heavy cloud system user, especially AWS for building docker and Kubernetes containers, he was not too of a fan using the Job scheduler SLURM, Open on-demand had his preferred software available for use which is Jupyter notebooks, it was accessible and easy to submit jobs whiles monitoring their progress.

Participants, both Superuser and Non-superusers users, preferred connecting to the cluster via Open on-demand because it was an intuitive graphical user interface and was accessible and easy to use, especially for first-time users of the cluster or non-superusers. Also, users mentioned heavily how important the quarterly *Introduction to HPC* training organized by the Advanced Research Computing Cluster was and helped them navigate the cluster. Non-superusers used the opportunity to learn basic commands and how to use the cluster effectively, whiles Superusers used the opportunity during these training sessions as an on-boarding opportunity; However, though they did have experience using UNIX/Linux or clusters in general, and it gave them an understanding of how to navigate through the University of Cincinnati Cluster.

Below are quotes to support theme one (1)

"P1: It was OK because I think I was following some of the instructions.You see, IT had some instructions on that. About like first users. So it was. I had thought that that was pretty smooth."

*"**P1**: And so again,my process would just be to upload. I usually edited these scripts on my like computer separately and then uploaded."*

*"**P1**: The semester is it's been a while since I had done that, and so there there's those instructions that are pretty clear and I think I might have also been a part of a workshop with the beginning of, like, the very it was maybe like 2021 or something. I think, I was getting confused and I was asking someone else how to use it, but then when I started using it, it was through this workshop and they actually had."*

*"**P3**: I think Open On-demand is great idea because it opens the door for people to start like me. I'm not sophisticated with Linux, I'm not you know , it's a good tool for me because it got me.*

***P3** New users don't get frustrated so that they can just get in that the help is close on hand and that all the resources they need are like a few clicks away is probably the if they're trying to attract new users.*

***P3** For most things you do on campus, the two-factor work, so it would be easier if it were just too far."*

*"**P4**: But I would say I'm familiar with multiple different computing platforms, so it's made it fairly easy for me to use because I'm pretty well situated with cloud computing, virtualized computing of many different sorts of cell.So I guess in terms of supercomputing, the only other platform that I really done any type of like intense computing would be on a AWS which is a cloud platform, I would say compared to a AWS.*

***P4** So I guess my use cases for each will be different. It's kind of like if I do stuff in the cloud. If I want quick access or to be able to quickly manage and launch things, I'll use the dashboard. Or in this case open on demand for the HPC. But if I have something where it might be a tedious job where I want to script it, the command line is better for it in that regard because I can just SSH, I can write the script, let it do its thing. I don't need to click through a bunch of things, I can just run a Stacy simple batch script so.In that* *regard, I would say that's why I would use one versus the other. Typically I use on demand because I'm not really doing anything administrative, at least not right now on the ARCC cluster.*

*"**P1**: Maybe if you had certain blocked or suspicious IP like there's a list, you can go to likehoneypot.org and you can find suspicious IP from IP or malicious actors and you can implement security that way where certain IP ranges you're not allowed to pool from. Or you might even like since they have root level security."*

1.4.2.2 Theme 2 : Jobs Management (Job Scheduling, Queue Management and Execution of Jobs)

Job submission and Queue management is an essential step when using the HPC Cluster; All jobs on the cluster would achieve the desired results based on the accuracy and correctness of your Job submission file. The Primary tool for Job Scheduling, queue management and execution of Jobs on the HPC Cluster is called 'The Slurm Workload Manager".SLURM takes some information about the requirements of resources and sends these calculations to the compute nodes that run the jobs to satisfy the criteria or requirements. It ensures resources are allocated to all users fairly and based on priority.

Two ways to submit jobs on the HPC Cluster currently are using SLURM via the Command Line Interface "CLI" or ARCC Desktop on Open On-Demand.

Our participants (P1-P4) appreciated using the ARC Desktop through Open on-Demand (Interactive Desktop) portal, which made it easy and accessible to submit their jobs by quickly uploading your Python file. This also allows users to select their preferred resources, e.g. (Number of hours, Number of nodes and partitions) it also has an email notifications option for when your session starts if selected. Open On-demand has a File Transfer button, Job Management, shell access and the ARCC Desktop.

SLURM is an excellent tool for Job scheduling, queuing and submission; However, our participants, both superusers and non-superusers, appreciated working with an interactive graphical user interface desktop.

Below are quotes to support theme Two (2)

P4 *"I think using the SLURM platform is a little bit challenging for me as a beginner. The Open On-Demand is more helpful and straight forward."*

P4 *"I think the On-Demand platform helped me a lot when I used the advanced research computing for my dissertation."*

P3 *"To difficult to or like I can still run things and get an output, so it's so that so I put it in the middle.Helpful, but it was still usable, so it wasn't too difficult to use. I think it was.Sometimes it does seem that something more interactive could be.*

Well, like, I feel like I'd be in the middle. Like it wasn't too difficult, but I feel like there are some aspects about like, troubleshooting that could be easier. I with the way that I've been studying up. So I kind of just like send a job and then."

P2 *"I haven't used that cause I don't really use it like I I think I mentioned before. I don't really use SDK's and I don't like programming, so I haven't used it. I've looked at it, I've read about it and I understand how it works, but I haven't personally like submitted any jobs through it."*

P1 *"I'm able to understand multi-threading and multiprocessing and do it in a way where it I don't feel intimidated and then it got me confident to where I could. I was able to branch out and start doing some other things with Linux and with SLURM and so I think that's all good and but I don't like using SLURM."*

1.4.2.3 Theme 3: Navigating the HPC Web portal

The core reason users choose the web portal to access the cluster other than other preferred methods is the ease of access, efficiency and optimized performance. From our results from the Think aloud activity, Our participants, Super and Non-superusers, preferred to use the interactive graphical user interface portal since it came with a File Transfer, Job Management, shell access and the ARCC Desktop features. This makes it very accessible for users to interact with the portal for their activities.

Though it was evident users preferred the Interactive Desktop, the current Graphical user interface had some cosmetic issues our participants identified and recommended to make the portal more accessible and usable.

Below are quotes to support theme three (3)

P1 *"I do feel like the ability to edit on stuff like these scripts on on-Demand. I was thinking one of the things that had been helpful with on demand is just the ability to edit the scripts right here.*

P1 *If there was an issue. I think when I had been using other programs because I'm using a windows.So by being able to edit the files within on-demand, that was helpful, especially since a lot of the problems would just be like a typo or something that I just go in to change very quickly. So I thought that was very useful with.*

P1 *Like, I guess, ranking priorities of things that was useful with using on demand that the ability, the ability to go into a file and edit was would be the first priority and then the second would be being able to see what her job is there are."*

P4 *"Probably just go back to the containers like you could honestly just teach people how to use containers and in that you have like a tiny little bit of Linux that you teach them how to use and that would be enough to get them through like they really only need a handful of commands to do a lot of the jobs that they're going to learn how to do. And I don't think.*

P4 *Pull the container, run the container and then just get their data to it, and that's that's three commands right there, and if you talk about the Linux commands, they only have what's not even technically a Linux. It's the HPC. Just make checking the modules* *and then enabling the module so you you can get it down to 5 commands there and people would be able to run their jobs. "*

P4 *" You know, Welcome to the arc ?, you know follow these steps one upload your data too you know and then this is how to use open on demand. I think just having that on this front page there's other things I think would make it better but. "*

P3 *" I'm using about the same amount of cores every time, so I'm typically it's like I'm. I'm running the same setup every time, so it seems like going in and then having to type in the stuff I usually have.*

P3 *Visual Studio code or Mathematica through a portal on open on demand I there's a I'd say there's a decent likelihood I would use it."*

Figure 1.4: A Text Analysis of Keywords from the Quantitative Data

1.4.3 Results from Heuristic Evaluation

After the Think-aloud activity, we conducted a Conducting heuristic evaluation to measure the severity of errors concerning the current Interactive web-based Graphical User Desktop for managing the HPC Cluster. We reviewed to identify violations that led to usability problems during usability testing and the results summaries using a 5 rating scale. To be more specific and conscience, The heuristic violations statements were classified into two groups: Group one consisted of specific violations that were directly actual usability problems, and Also these problems affected the functionality of the web portal, which could affect users' ability to use the system, and the second consisting of general violations that suggested, but did not directly affect the functionality of the website but where usability problems users desired to be reviewed [37].

Specific heuristic violations we identified were design features, such as buttons and menu items, that could be directly tied to the failure or difficulty to complete a task. General heuristic violations, on the other hand, tended to highlight visual and functional designs that could have resulted in a number of usability problems.Violations and severity ratings were tabulated below Table 1.2

In total, 18 Problems were identified with a severity greater or equal to 0, of which 8 were Problems greater than or equal 2. The primary usability problems were related to complex methods of connecting to the cluster. Also, with the Web-based HPC Cluster, there are some User interface design problems, e.g. pages with large blank spaces in which some information could be displayed to inform users. Also, other users mentioned that after submitting jobs using the ARC Desktop, they want to see an intuitive button that gives them the status of their Jobs and allows them to edit their job scripts.The rest of the issues identified by users were cosmetics problems that could easily be fixed.

Table 1.2: Results of Heuristic Evaluation.

Violations by Task	**Heuristic**	**Severity**
Task 1 Going through long procedures to get an account set up	User Control and Freedom	2 -minor usability problem
Task 2 Users reported difficulty knowing the status of a job and whether an error occurred after submission	Visibility of System Status	4 -usability catastrophe; imperative to fix
Task 3 No violations	none	N/A
Task 4 we found violations with page alignments, consistency in terms of alignments and fonts	Atheistic and Minimalist Design	1- Cosmetic problem
Task 5 we found violations were users didn't know either if their submitted jobs were running or an estimated completion time	Flexibility and efficiency of use	4 - usability catastrophe; imperative to fix
Task 6 Users could not edit their already submitted jobs	User Control and Freedom	2 - minor usability problem
Task 7 Landing page underutilized, could contain tips or documentation section	Help and Documentation	1- cosmetic problem
Task 8 Users not able to use other software installed on the Cluster on the web portal	Consistency and Standards	4- usability catastrophe; imperative to fix
Task 9 Users wanted a more intuitive and interactive web portal	Aesthetic and minimalist design	3 - major usability problem; important to fix

1.5 Recommendation and Discussion

Our results show that users of the HPC Cluster managed by the Advanced Research Computing Center are satisfied with the services provided by ARCC, as shown in Figure 1.3. This further proves that HPC plays a significant role in fostering the research capabilities of researchers at the University of Cincinnati. Although there were many ways for users to connect to the clusters, Open on-Demand was the preferred connection method for job submission, file transfer, and managing job queues.

To address our research question of how HPCs can be made more accessible across disciplines in institutes of higher education, specifically at the University of Cincinnati as our case study and also providing standardize HPC tools; we recommend taken the following actions:

- **Develop a customized graphical user interface (GUI) web HPC management portal** This would tailor to the needs of users at the University of Cincinnati, taking into account the research and user environment. Open On-Demand is an excellent HPC portal, but it is a generic system that's used by other HPC centers to manage their clusters. However, designing an accessible and customized GUI portal for the University of Cincinnati would improve users' needs and make their use of the High-Performance Computing cluster more accessible.

- **Allow the HPC to be internet facing** This would allow users to connect to the cluster from off-campus, which would be beneficial for researchers who need to access the cluster from home or other locations. Also this goes further to enable researchers especially industry companies that need the services of the cluster to integrate third-party systems eg APIs to improve their research needs. The clusters can be made more secure by implementing 2-factor authentication methods eg. The current DUO system is used University-wide which would serve the security needs as needed.

- **Workforce Development** To increase workforce development, ARCC should increase the frequency of training sessions and introduce Advanced Level and specialty training for users. Users want to acquire academic credits when these courses are taken, which we believe will encourage novice and frequent users to attend the training sessions. Training can be made mandatory regardless of your experience especially new users as an on-boarding method for new users of the cluster, this would help to ensure that all users, regardless of their experience level, have the skills they need to use the HPC cluster effectively.

- **Student Cluster Competition** ARCC should introduce the student cluster competition on campus especially partnering with the School of Information Technology (SoIT) and Engineering Faculty during the annual expo,this would be a means of encouraging users to draw more interest to use the High Performance Computing Cluster.

This is because feedback from our survey respondents gave a general picture of the current usage of the HPC Cluster. especially graduate students from departmental or research labs using the Cluster for their dissertations and funded research. This proves how important it is to design a customized HPC web portal for the University of Cincinnati to make the cluster more accessible for researchers across all disciplines. This would make on-boarding and usage of the cluster very easy and direct. Training plays a pivotal role in on-boarding users with no experience and users with some experience with Linux/UNIX. However, though some users have experience with Unix; using a cluster requires some special skills, which was beneficial for all users.Frequent training and introducing special programs like the ”Student Cluster Competition ” will be a great initiative for ARCC to solidify its name across the University of Cincinnati eco-system.

1.6 Limitations and Future Work

Our Major limitations were the mobilisation of participants for the survey and especially the think-aloud activity; most super users were unavailable for various reasons, and Non-superusers were not confident about being recorded on video while doing some basic asks. There needed to be more incentives to encourage users to participate in the data collection.

We would expand our research criteria and the participant by focusing more on not only the state of Ohio but the HPC Community as a whole; this would allow us to achieve our goal of making HPCs accessible for researchers across all disciplines.We would conduct a systematic literature review on current HPC Accessibility research in the industry,Also build a customised Intuitive HPC Web management portal for the Advanced Research Computing Center at the University of Cincinnati.

1.7 Conclusion

In this research, we conducted a usability study on how to make HPCs accessible to users across all disciplines, and our Case study was the user of the Advanced Research Computing Center at the University of Cincinnati. Our results highlight several factors that back the need for the Advanced research computing cluster to build a customised, intuitive HPC management web portal. Overall, our results indicate that both super and non-superusers preferred using the Web-based HPC Management portal for job submission and queue management, and implementing our recommendation and future work would improve the ease of access to the cluster and increase the confidence of our non-superusers since the portal would make it easy for them to manage the cluster and implement several technologies through a web-based portal. A critical contribution from this study for workforce development is to expand the training sessions conducted by ArCC, which has been very instrumental to many users; this training is a resource to a lot of first-time users, especially non-superusers and a few of our respondents, were on-boarded through the training and have been using the cluster which has made them superusers. This is a suitable means to encourage the use of HPCs across all disciplines, which addresses the challenge in our research question.

References

[1] 2021. HPCC 2021 - Home. http://www.ieee-hpcc.org/2021 [Online; accessed 26. May 2023].

[2] 2021. What is Heuristic Evaluation? https://www.interaction-design.org/literature/topics/heuristic-evaluation [Online; accessed 21. May 2023].

[3] 2021. What is Heuristic Evaluation? https://www.interaction-design.org/literature/topics/heuristic-evaluation [Online; accessed 21. May 2023].

[4] 2022. OAC Vision | NSF - National Science Foundation. https://www.nsf.gov/cise/oac/vision/blueprint-2019 [Online; accessed 2. Dec. 2022].

[5] 2023. HPC everywhere: A quick-access web portal for all things HPC-related at IU. https://itnews.iu.edu/articles/2019/HPC%20everywhere%20A%20quick-access%20web%20portal%20for%20all%20things%20HPC-related%20at%20IU.php [Online; accessed 12. May 2023].

[6] 2023. Jetstream2. https://jetstream-cloud.org [Online; accessed 27. May 2023].

[7] 2023. NSF Award Search: Award # 1534949 - SI2-SSE: Open OnDemand: Transforming Computational Science through Omnidisciplinary Software Cyberinfrastructure. https://www.nsf.gov/awardsearch/showAward?AWD_ID=1534949 [Online; accessed 13. May 2023].

[8] 2023. NSF Award Search: Award # 1835725 - Frameworks: Software NSCI-Open OnDemand 2.0: Advancing Accessibility and Scalability for Computational Science through Leveraged Software Cyberinfrastructure. https://www.nsf.gov/awardsearch/showAward?AWD_ID=1835725 [Online; accessed 13. May 2023].

[9] 2023. Open OnDemand | Proceedings of the XSEDE16 Conference on Diversity, Big Data, and Science at Scale. https://dl-acm-org.uc.idm.oclc.org/doi/10.1145/2949550.2949644 [Online; accessed 13. May 2023].

[10] 2023. OSC OnDemand | Proceedings of the Conference on Extreme Science and Engineering Discovery Environment: Gateway to Discovery. https://dl-acm-org.uc.idm.oclc.org/doi/10.1145/2484762.2484780 [Online; accessed 13. May 2023].

[11] 2023. The Engines | Babbage Engine | Computer History Museum. https://www.computerhistory.org/babbage/engines [Online; accessed 26. May 2023].

[12] Amy Apon, Linh Ngo, Michael Payne, and Paul Wilson. 2014. Assessing the effect of high performance computing capabilities on academic research output. *Empirical Economics* 48 (02 2014). https://doi.org/10.1007/s00181-014-0833-7

[13] Amy W. Apon, Linh B. Ngo, Michael E. Payne, and Paul W. Wilson. 2015. Assessing the effect of high performance computing capabilities on academic research output. *Empir. Econ.* 48, 1 (Feb. 2015), 283–312. https://doi.org/10.1007/s00181-014-0833-7

[14] Advanced Research Computing at UC. 2019. Advanced Research Computing at UC. https://arc.uc.edu/citing-the-arc/

[15] Michael A. Bauer. 2007. High Performance Computing: The Software Challenges. In *Proceedings of the 2007 International Workshop on Parallel Symbolic Computation* (London, Ontario, Canada) *(PASCO '07)*. Association for Computing Machinery, New York, NY, USA, 11–12. https://doi.org/10.1145/1278177.1278180

[16] Patrice Calegari, Marc Levrier, and Paweł Balczyński. 2019. Web Portals for High-performance Computing: A Survey. *ACM Trans. Web* 13, 1 (Feb. 2019), 1–36. https://doi.org/10.1145/3197385

[17] Ohio Supercomputer Center. 1987. Ohio Supercomputer Center. http://osc.edu/ark:/19495/f5s1ph73

[18] Prateek Muneesh Chellani. 2022. Remote Device Sharing in Smart-Homes: Explained by Cultural Differences. https://etd.ohiolink.edu/apexprod/rws_olink/r/1501/10?clear=10&p10_accession_num=ucin1649927874254683 [Online; accessed 16. May 2023].

[19] Victoria Clarke and Virginia Braun. 2013. Teaching thematic analysis: Overcoming challenges and developing strategies for effective learning. *Psychologist* 26, 2 (Feb. 2013), 120–123. https://www.researchgate.net/publication/269928387_Teaching_thematic_analysis_Overcoming_challenges_and_developing_strategies_for_effective_learning

[20] Carolyn Connor, Amanda Bonnie, Gary Grider, and Andree Jacobson. 2016. Next generation HPC workforce development: the computer system, cluster, and networking summer institute. In *EduHPC '16: Proceedings of the Workshop on Education for High Performance Computing*. IEEE Press, 32–39. https://doi.org/10.5555/3018088.3018094

[21] Carolyn Connor, Andree Jacobson, Amanda Bonnie, and Gary Grider. Submitted. An Innovative Approach to Bridge a Skill Gap and Grow a Workforce Pipeline: The

Computer System, Cluster, and Networking Summer Institute. *USENIX Journal of Election Technology and Systems (JETS)* 1, 1 (Submitted). https://www.usenix.org/jesa/0201/connor

[22] Álvaro Fernández, Camino Fernández, José-Ángel Miguel-Dávila, and Miguel Á. Conde. 2021. Integrating supercomputing clusters into education: a case study in biotechnology. *J. Supercomput.* 77, 3 (March 2021), 2302–2325. https://doi.org/10.1007/s11227-020-03360-5

[23] Michail N. Giannakos. 2014. Exploring Students Intentions to Study Computer Science and Identifying the Differences among ICT and Programming Based Courses. *Turkish Online Journal of Educational Technology - TOJET* 13, 4 (Oct. 2014), 36–46. https://eric.ed.gov/?id=EJ1043181

[24] Abid Haleem, Mohd Javaid, Mohd Asim Qadri, and Rajiv Suman. 2022. Understanding the role of digital technologies in education: A review. *Sustainable Operations and Computers* 3 (Jan. 2022), 275–285. https://doi.org/10.1016/j.susoc.2022.05.004

[25] Stephen Harrell, Hai Nam, Verónica Larrea, Kurt Keville, and Dan Kamalic. 2015. Student Cluster Competition: A Multi-disciplinary Undergraduate HPC Educational Tool. https://doi.org/10.1145/2831425.2831428

[26] Anthony. J. G. Hey. 1997. High Performance Computing - Past, Present and Future. https://eprints.soton.ac.uk/251752 [Online; accessed 26. May 2023].

[27] Barikisu Issaka. 2021. *Alienating: how the portrayal of Muslim women in US media affects Muslim women's social identities*. Ph. D. Dissertation. https://krex.k-state.edu/handle/2097/41509

[28] Peter Kogge, S. Borkar, Dan Campbell, William Carlson, William Dally, Monty Denneau, Paul Franzon, William Harrod, Jon Hiller, Stephen Keckler, Dean Klein, and Robert Lucas. 2008. ExaScale Computing Study: Technology Challenges in Achieving Exascale Systems. *Defense Advanced Research Projects Agency Information Processing Techniques Office (DARPA IPTO), Techinal Representative* 15 (01 2008).

[29] Heinz Kredel, Hans Gunther Kruse, and Sabine Richling. 2015. A hierarchical model for the analysis of efficiency and speed-up of multi-core cluster-computers. In *2015 10th International Conference on P2P, Parallel, Grid, Cloud and Internet Computing (3PGCIC)* (Krakow). IEEE.

[30] Ncsa Megan Johnson. 2023. Open OnDemand Makes Using Supercomputers Super Simple - Access. *Access* (March 2023). https://access-ci.org/open-ondemand-makes-using-supercomputers-super-simple

[31] Svati Murthy, Jess Kropczynski, and Shane Halse. 2022. Understanding Decision-Making Needs of Open Government Data Users. https://doi.org/10.24251/HICSS.2022.331

[32] Rajendra K. Raj, Carol J. Romanowski, John Impagliazzo, Sherif G. Aly, Brett A. Becker, Juan Chen, Sheikh Ghafoor, Nasser Giacaman, Steven I. Gordon, Cruz Izu, Shahram Rahimi, Michael P. Robson, and Neena Thota. 2020. High Performance Computing Education: Current Challenges and Future Directions. In *Proceedings of the Working Group Reports on Innovation and Technology in Computer Science Education* (Trondheim, Norway) *(ITiCSE-WGR '20)*. Association for Computing Machinery, New York, NY, USA, 51–74. https://doi.org/10.1145/3437800.3439203

[33] Robert Roos. 2021. *Usability Evaluation of Information Systems in Complex Domains, a Case-Study on a pension application processing system*. Ph. D. Dissertation. https://aaltodoc.aalto.fi/handle/123456789/102515

[34] Jim Samuel, Margaret Brennan-Tonetta, Yana Samuel, Pradeep Subedi, and Jack Smith. 2021. Strategies for Democratization of Supercomputing: Availability, Accessibility and Usability of High Performance Computing for Education and Practice of Big Data Analytics. *arXiv* (April 2021). https://doi.org/10.48550/arXiv.2104.09091 arXiv:2104.09091

[35] Olga Scrivner, Gagandeep Singh, Sara Bouchard, Scott Hutcheson, Ben Fulton, Matthew Link, and Katy Borner. 2018. XD Metrics on Demand Value Analytics: Visualizing the Impact of Internal Information Technology Investments on External Funding, Publications, and Collaboration Networks. *Frontiers in Research Metrics and Analytics* 2 (01 2018). https://doi.org/10.3389/frma.2017.00010

[36] Preston M Smith. 2022. The Value Proposition of Campus High-Performance Computing Facilities to Institutional Productivity - A Production Function Model. (7 2022). https://doi.org/10.25394/PGS.20341338.v1

[37] Samuel Ssemugabi and Ruth Villiers. 2010. Effectiveness of heuristic evaluation in usability evaluation of elearning applications in higher educ. *South African Computer Journal* 45 (08 2010). https://doi.org/10.18489/sacj.v45i0.37

[38] Craig A. Stewart, David Y. Hancock, Wernert Julie, Matthew R. Link, Nancy Wilkins-Diehr, Therese Miller, Kelly Gaither, and Winona Snapp-Childs. 2018. Return on Investment for three Cyberinfrastructure facilities: a local campus supercomputer; the NSF-funded Jetstream cloud system; and XSEDE (the eXtreme Science and Engineering Discovery Environment). https://scholarworks.iu.edu/dspace/handle/2022/22590 [Online; accessed 26. May 2023].

[39] Craig A. Stewart, Stephen Simms, Beth Plale, Matthew R. Link, David Y. Hancock, and Geoffrey C. Fox. 2010. What is Cyberinfrastructure? *ACM* (Oct. 2010). https://scholarworks.iu.edu/dspace/handle/2022/12967

[40] Anna Sutton. 2016. Heasuring the Effects of Self-Awareness: Construction of the Self-Awareness Outcomes Questionnaire - PMC. Europe's journal of psychology. https://doi.org/10.5964/ejop.v12i4.1178

[41] Jane Sutton, AnnaSutton and Zubin Austin. 2015. Qualitative Research: Data Collection, Analysis, and Management. In *The Canadian journal of hospital pharmacy (vol. 68,3)*. The Canadian journal of hospital pharmacy, Article , numpages = 68,3,.

[42] Tasbakkori Teddlie, C. 2023. *A. (2003). Major Issue and Controversies in the Use of Mixed Methods in Social and Behavioral Sciences. In C. Teddlie, & A. Tasbakkori (Eds.), Handbook of Mixed Methods in Social and Behavioral Sciences (pp. 3-50). Thousand Oaks, CA SAGE. - References - Scientific Research Publishing*. Ph. D. Dissertation. https://www.scirp.org/(S(lz5mqp453edsnp55rrgjct55))/reference/referencespapers.aspx?referenceid=2220642

[43] Abhinav Thota, Le Mai Weakley, Ben Fulton, H. E. Cicada Brokaw Dennis, Laura Huber, Scott Michael, Winona Snapp-Childs, Stephen Lien Harrell, Alexander Younts, Daniel T. Dietz, Christopher Phillips, and Xiao Zhu. 2019. Research Computing Desktops: Demystifying Research Computing for Non-Linux Users. In *Proceedings of the Practice and Experience in Advanced Research Computing on Rise of the Machines (Learning)* (Chicago, IL, USA) *(PEARC '19)*. Association for Computing Machinery, New York, NY, USA, Article 54, 8 pages. https://doi.org/10.1145/3332186.3332206

[44] Huy Truong. 2021. Efficient Ways to Conduct Heuristic Evaluation for Your Agile Product. https://uxplanet.org/efficient-ways-to-conduct-heuristic-evaluation-for-your-agile-product-137a4ae4f52d

[45] Texas Tech University. 2022. *High Performance Computing Center — High Performance Computing Center — TTU*. Retrieved 03/08/2022) from https://www.depts.ttu.edu/hpcc/

[46] Maaike J. Van den Haak, Menno D. T. de Jong, and Peter Jan Schellens. 2003. Retrospective vs. concurrent think-aloud protocols: Testing the usability of an online library catalogue. *Behaviour & IT* 22, 5 (Sept. 2003), 339–351. https://doi.org/10.1080/0044929031000

[47] XSEDE. 2022. *A Brief History of High-Performance Computing (HPC) - XSEDE Home - XSEDE Wiki*. Retrieved 04/08/2022) from https://confluence.xsede.org/pages/viewpage.action?pageId=1677620

[48] Il-Chul Yoon, Alan Sussman, and Adam Porter. 2005. And Away We Go: Understanding the Complexity of Launching Complex HPC Applications. In *Proceedings of the Second International Workshop on Software Engineering for High Performance Computing System Applications* (St. Louis, Missouri) *(SE-HPCS '05)*. Association for Computing Machinery, New York, NY, USA, 45–49. https://doi.org/10.1145/1145319.1145333

[49] Jill Zarestky and Wolfgang Bangerth. 2014. Teaching High Performance Computing: Lessons from a Flipped Classroom, Project-Based Course on Finite Element Methods. 34–41. https://doi.org/10.1109/EduHPC.2014.10

Appendix: Survey Questions and Materials

A.1 Consent Statement

CONSENT STATEMENT

STUDY TITLE: Leveraging the Use of High-Performance Computing Services To Improve Education: A Usability Study on University of Cincinnati's High Performance Computing Cluster

PRINCIPLE INVESTIGATOR NAME: Mahmoud Junior, Suleman

PHONE NUMBER: 513-442-6285

DEPARTMENT: School of Information Technology

INTRODUCTION: You are being asked to take part in a research study. Please read this paper carefully and ask questions about anything that you do not understand.This research is funded by the University of Cincinnati's Advanced Research Computing Center.

WHO IS DOING THIS RESEARCH STUDY? The person in charge of this research study is Mahmoud Junior Suleman, a master's student at the University of Cincinnati (UC) School of Information Technology and a Graduate Student Research facilitator at the Advanced Research Computing Center. If you sign up to complete a follow-up interview after this survey, there may be other people on the research team helping at different times during the study.

Mahmoud Junior, Suleman is Graduate Student Researcher with the Advanced Research Computing (ARC) center. As a requirement for my thesis I am conducting a usability research project with a focus on the users of the High-Performance Computing Cluster at UC to learn about users' experiences over the years and how ARC can improve the service delivery and encourage potential users to utilize the services of the HPC system at the University of Cincinnati.

Background: The University of Cincinnati's Advanced Research Computing (ARC) center offers a readily accessible hybrid CPU/GPU computing cluster, supporting the next generation of computational and data science researchers while developing a highly competitive workforce. ARC partner's with researchers to utilize the core suite of HPC services and resources. With the ARC resources, researchers can advance theoretical knowledge and expand the realm of discovery, generating leading edge research and applications suitable for innovation and commercialization in line with UC's Next Lives Here strategic direction.

Eligibility: To be eligible you need to assume one the roles below at the University of Cincinnati: - Faculty Member, Researcher, PI, Graduate student, Undergraduate student, Current User of UC's HPC.

Privacy Notice: The responses received will be compiled and stored for the sole purpose of this research, to improve the services of UC's Advanced Research Computing center and to accommodate the needs of its esteemed users. It will not be shared with third parties.