

High-performance computing in undergraduate education at primarily undergraduate institutions in Wisconsin: Progress, challenges, and opportunities

 $\label{eq:continuous} \begin{tabular}{ll} Jordan Hebert$^3 \cdot Ryan Hratisch$^3 \cdot Rahul Gomes$^3 \cdot William Kunkel$^7 \cdot Daniel Marshall$^5 \cdot Abhimanyu Ghosh$^5 \cdot Isabella Doss$^1 \cdot Ying Ma$^1 \cdot Derek Stedman$^6 \cdot Blake Stinson$^6 \cdot Anthony Varghese$^6 \cdot Molly Mohr$^2 \cdot Pricilla Rozario$^4 \cdot Sudeep Bhattacharyya10$

Received: 3 October 2023 / Accepted: 15 February 2024 © The Author(s), under exclusive licence to Springer Science+Business Media, LLC, part of Springer Nature 2024

Abstract

High-performance computing (HPC) has become a strategic resource that drives innovation and economic growth. In addition, it is important to educate a workforce with advanced computational skills to maintain economic competitiveness. In this project, we studied 133 domestic and international university HPC centers to understand the status of HPC. Diverse operating models have been identified and analyzed. To explore the need for and challenges associated with HPC within Wisconsin, faculty and students within the University of Wisconsin System and personnel in local industries were surveyed; in addition, we engaged in conversations with university leaders and officials from government agencies. A strong need for HPC resources has been identified, as well as several serious challenges. A state-wide initiative, the Wisconsin Big Data Alliance, which requires legislative support, is recommended as the platform to foster public–private partnerships, drive scientific and technological innovations, and promote workforce development, leading to an efficient usage of computing resources.

Keywords High performance computing \cdot Curriculum development \cdot Policies \cdot Survey

1 Introduction

Published online: 09 March 2024

High-performance computing (HPC) refers to the use of large-scale computing resources involving many central processing unit (CPU) cores to deliver performance that cannot be achieved by ordinary computers. HPC and visualization offers

Derek Stedman and Blake Stinson contributed equally to this work.

Extended author information available on the last page of the article



tools for solving complex and resource-intensive problems in science, engineering, and business (Fernández et al., 2021; Lynn et al., 2020; Pyzer-Knapp et al., 2022; Raj et al., 2020). As a result, the science, technology, engineering, and mathematics (STEM) communities have experienced a significant growth in HPC activities in education and research (Chen et al., 2019; Hati & Bhattacharyya, 2016; Hunter, 2019; Mullen et al., 2017; Neelima, 2017; Ponce et al., 2019; Samuel et al., 2022; Shields, 2020; Townsend-Nicholson, 2020). A significant correlation in the growth of HPC use in undergraduate education has been observed worldwide (Chaudhury et al., 2018; Cui et al., 2016; Karsakov et al., 2015; Mullen et al., 2017; Neelima, 2017). In many cases, these developments occurred across more than one discipline giving rise to growth in multidisciplinary computational sciences (Chaudhury et al., 2018; Fernández et al., 2021; Ponce et al., 2019; Raj et al., 2020; Vavilala, 2020). HPC resources have been used worldwide to perform cutting-edge research in many fields to accelerate the rate of scientific discovery (Pyzer-Knapp et al., 2022). Private companies have been early adopters of HPC, accounting for about 30% of supercomputer customers in the U.S. as early as 1982. The use of HPC in industry is widespread and has given rise to a need for sustainable computing (Shuja et al., 2017).

The significance of HPC in propelling innovation and economic advancement has grown considerably (Ezell & Atkinson, 2016). This recognition is widespread, with major nations across the globe making significant investments in HPC technology. Some states in the United States, such as New Jersey, are at the forefront of HPC education, workforce development, and economic growth. Additionally, a handful of Midwest states including Indiana, Illinois, and Minnesota have access to HPC resources that rank among the most powerful worldwide. Due to our increasingly data-driven economy, modern industries rely heavily on HPC for data analysis and advanced modeling to improve their products and services. HPC has become "a strategic resource for economic competitiveness, scientific leadership, and national security" (Ezell & Atkinson, 2016) to the point where investments in HPC systems have become national priorities. Examples of such initiatives include: the United States (Frontier), China (Sunway TaihuLight), Germany (JUPITER), France (Leonardo HPC System), Japan (Fugaku), the United Kingdom (ARCHER2), and Russia (NDMC). The speed of an HPC system is measured by the number of floating-point operations per second (FLOPS). The TOP500 project, which ranks the most powerful supercomputers in the world, has shown that the performance of the top systems in the world have grown from from 60 GigaFLOPS to 1 ExaFLOPS in 2023, which is about a 18 million fold increase in computing power. The first exa-scale system, speeds above 10¹⁸ FLOPS and has recently become operational in the United States.

Wisconsin has several HPC systems: the Center for High Throughput Computing (CHTC) at the University of Wisconsin-Madison (UW-Madison) houses a 312-node HPC with 6,240 CPU cores, the University of Wisconsin-Milwaukee (UWM) is home to a 116-node HPC with 2,724 CPU cores, and the University of Wisconsin-Eau Claire UWEC) is the only comprehensive campus within the UW System with an HPC facility. It has a history of excellence in HPC-related undergraduate education and discovery. In 2013, a faculty-driven effort to establish a campus-wide HPC was awarded a differential tuition funding of \$145,000. This brought forth a



number of high-profile research fostering solid growth in the HPC-based research in Chemistry, Physics, Biology, and Material Science. To cope up with the increasing demand, UW-Eau Claire faculty secured a Major Research Instrumentation (MRI) grant from the National Science Foundation (NSF) in 2019, totaling \$350,000, supported with an in-kind Hewlett Packard Enterprise grant of \$363,426 to UWEC. These grants enabled the creation of the Blugold Center for High-Performance Computing (BCHPC) with a HPC cluster consisting of 3904 CPU cores. UWEC is growing into a regional HPC center in northwestern Wisconsin and attracting users from the University of Wisconsin-Stout (UWS) and the University of Wisconsin-River Falls (UWRF).

However, Wisconsin still lags behind states like Arizona and Virginia in terms of computational power. First, consider the small business sector, which produce significantly more patents than large businesses and universities. Almost 40% of American scientists and engineers are employed by small businesses. The lack of HPC resources and expertise is quite evident in the small businesses and thus providing high-quality HPC service is expected to greatly expedite technological innovations. Second, efficient utilization of HPC resources requires workforce with sophisticated computational knowledge and skills. Thus, there is a pressing need in the educational sector to bridge the gap. Educating our students, the twenty-first century teachers, scientists, engineers, lawyers, and entrepreneurs with advanced computational skills is an absolute necessity. These skills include, but not limited to computational thinking, high-throughput experimenting, database handling, discipline-specific computational technics, data processing tools, and some coding (Adenaike et al., 2023; Al-Jody et al., 2021; Hati & Bhattacharyya, 2016; Kruchten, 2020; Ponce et al., 2019; Shields, 2020). The data processing includes a number of skills including handling of large datasets, abstraction, analysis, visualization, and interpretation. All these are inseparable from active learning, yet unfortunately, HPC-related computational skills are rarely covered in an undergraduate curriculum, and research projects on HPC are mostly limited to campuses with existing HPC resources (Al-Jody et al., 2021).

To tackle these challenges, a collaborative effort is required involving all stake- holders, such as the government, industries, and universities. Policymakers worldwide are taking action to adapt to the increasingly data-driven world. In Europe, the Partnership for Advanced Computing in Europe (PRACE), (Bethune et al., 2012) consisting of 25 member countries, was established to provide HPC resources to businesses and researchers, as well as to support the development of professionals with digital skills. In the United States, the National Science Foundation created the Advanced Cyberinfrastructure Coordination Ecosystem: Services & Support (ACCESS) to aid computational and data-intensive research. At the state level, The New Jersey Big Data Alliance (NJBDA) was created in 2013 to promote competitiveness, generate a highly skilled workforce, foster innovation, and spur data-driven economic growth for New Jersey. Regrettably, a targeted, statewide initiative to build and foster collaboration among universities and local industries, to educate a workforce with advanced computational skills that meet the needs of our state, is absent in Wisconsin at this time. HPC training is integral to the long-term growth of the workforce in the state, where



a significant section of students come from farming backgrounds and are of first-generation, female and/or underrepresented communities. However, there is no protocol for sharing of computational resources across the state for these students. Thus, one of the questions we wanted to delve in:

1. How can institutional barriers be eliminated to facilitate the sharing of computational resources across UW System schools to benefit undergraduate education and discovery?

The role of HPC in healthcare research has become increasingly relevant as revealed in the recent fight against the COVID-19 pandemic (Fighting COVID-19 with HPC & Nature Comp., 2021; Gomes et al., 2022a; Heifetz, 2024). At UW-Eau Claire, during lock-down phase of the pandemic, UW-Eau Claire undergraduates continued their research studies using HPC and were able to make substantial contributions to the science (Fossum et al., 2022; Gomes et al., 2022b; Suhail et al., 2020). Furthermore, curricular initiative in course-embedded research involving HPC has been greatly successful in UW-Eau Claire campus resulting peer-review publications (Wozney et al., 2022; Zajac et al., 2020). The strong evidence of the connectivity between HPC resources and research productivity in undergraduate settings prompted us to ask about collaborative HPC resources accessible to undergraduates all parts of Wisconsin:

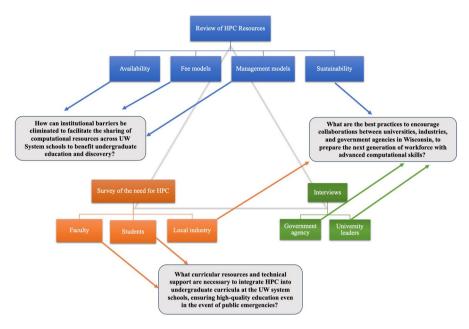
2. What curricular resources and technical support are necessary to integrate HPC into undergraduate curricula at the UW system schools, ensuring high-quality education even in the event of public emergencies?

Finally, we have stepped into the age, where machine learning and big data are continuing to pave the way for frontier discoveries in healthcare sciences, where the state-mediated industry-academia collaboration appears to play a dominant role. Thus, our last question to review is:

3. What are the best practices to encourage collaborations between universities, industries, and government agencies in Wisconsin, to prepare the next generation of workforce with advanced computational skills?

Herein, we report the findings of the study which aimed to answer these questions by examining the infrastructure, collaborative platforms, and the status of HPC education globally as well as within the UW system. Although not every US state has statewide HPC programs, there are now enough regional centers and state-level HPC projects to gather this data. Previous work has focused on some of the major supercomputing centers around the world but has neglected undergraduate education and research. Our goal is to determine the best path for a statewide HPC initiative in Wisconsin that involve primarily undergraduate Universities spread out geographically and hence can reach most of the state population. We believe this HPC initiatives will create a pathway to be followed by other regions in the US. Furthermore, HPC centers around the world would be able to collaborate to continue gathering the kind of data we have presented to mark the progress of HPC in impacting undergraduate education and research.





Scheme 1 A structured representation of the research methodology

2 Methodology

The study consisted of three parallel efforts including a review of HPC infrastructure within and beyond Wisconsin, surveying faculty and students from UW System and local industries, and interviewing government officials and university leaders. Information from each effort was analyzed and cross-compared to address one of the three questions raised earlier (Scheme 1), as shown below. The questions in survey and interviews were prepared by utilizing standardized questionnaires available at the Qualtrics (https://www.qualtrics.com) without further validation and reliability study.

2.1 Review of HPC resources

To determine the best ways to promote HPC-related education and discovery in Wisconsin and effectively share HPC resources, it is important to understand current practices both within and beyond the state and their associated implications. Therefore, we examined the status of HPC both internationally and in the U.S. to better identify our needs in Wisconsin. HPC centers were identified for all 50 states and abroad institutes using web-based searches. Once ensured that the information is up-to-date, these cluster centers were studied from the posted information on their web-pages.



2.2 Survey of the need for HPC

To comprehend the necessity of HPC in Wisconsin, we conducted surveys targeting faculty, students, and industry professionals. We utilized Qualtrics as our survey platform and all surveys were granted Institutional Review Board (IRB) approval. The overall distribution was divided into three campuses (UW-Eau Claire, UW-Stout, and UW-River Falls) to avoid the threshold set by our University's Learning and Technical Services to enable securely sending mass emails. The student surveys were sent to various UW System schools, including UW-Whitewater, UW-Eau Claire, UW-Stout, UW-Superior, UW-Madison, and UW-La Crosse. Faculty surveys were approved for UW-Eau Claire, UW-Stout, UW-Superior, UW-Madison, and UW-La Crosse. Although we attempted to contact other UW System schools, we were unable to obtain permission in time.

The objective of the student survey was to evaluate their existing knowledge and awareness of HPC. To establish a baseline, we aimed to understand whether students.

were aware of HPC and, if so, which disciplines they were mostly used in. We collectively developed these questions in consultation with our IRB. Table S1 provides an overview of the survey questions sent to students.

The faculty survey aimed to investigate the necessity of HPC in classroom education and their research objectives. Frequently, due to a lack of access to a centralized infrastructure or issues with connecting to existing infrastructure with different programming environments, faculty resort to paid services provided by Amazon or Google or purchase costly equipment, which impedes progress in pedagogy and professional development. We asked questions to investigate how the HPC environment available at UWEC could be beneficial for HPC needs. Table S2 summarizes the questions we asked.

Computational resources are essential for many fundamental activities beyond academia, such as weather monitoring and prediction, biomedical engineering, soft- ware development, artificial intelligence simulations and sales prediction for survival, growth, and expansion. With the industry survey, we aimed to determine the computational resource needs of local industries, particularly in the North-West region of Wisconsin. The survey analyzed their awareness of computational resources available at UW-Eau Claire and how they could use them in the future. Table S3 outlines the questions we asked.

2.3 Interview with government and university leaders

To investigate the existing HPC infrastructure and assess the HPC requirements across Wisconsin, we conducted virtual interviews with university administrators and government officials, with the research team consisting of two or more members present at each interview. Approval was obtained from the IRB before conducting the interviews, which lasted approximately 30 min each. Table S4 outlines the questions asked of the university administrators, which were designed to identify



their perceptions of HPC in undergraduate education, awareness of their institutions' HPC-related needs, and investigate potential barriers to implementing HPC in university systems, as well as best practices for overcoming those barriers.

During the interviews with university administrators, five questions were asked, with the first sought to identify administrators' perceptions of HPC in undergraduate education and question, and the second focused on helping establish administrators' awareness of their institutions' current HPC-related needs. Questions three and four dealt with the barriers and best practices to overcome those barriers. Question five asked about the role of industry in popularizing the use of HPC in undergraduate education.

Each interview involved a standardized set of six questions, with questions 1 through 5 (see Table S4) used in the analysis discussed in this report. Question 6 was an open-ended opportunity for administrators to ask any questions they may have had about the project, but the responses to this question were not analyzed for this study. The interviewees were asked the same set of questions one at a time and were allowed to respond freely without interruption. Throughout the interview process, researchers took notes on what was said and compiled them after each interview.

To assess the level of HPC awareness among government agencies, we followed a similar approach as with the university administrators by conducting interviews with government officials. However, the questions asked were tailored to focus on the role of HPC in workforce development within the state of Wisconsin and how the state can assist universities in achieving this objective. The questions asked during these interviews are listed in Table S5, which shows the list of the questions associated with.

these interviews. The sixth question, not shown in the table, was again an opportunity for the interviewees to ask questions about the project or HPC in general.

Table S6 includes the institution and departments that participated in the interview process. This list comprises a diverse group of individuals, including representatives from Academic Affairs, the Office of Research and Sponsored Programs, Learning and Technology Services at various UW campuses, and faculty members from UW institutions.

3 Results and discussion

3.1 HPC infrastructure

We found a substantial number of HPC centers, including 21 foreign centers from Canada, Germany, France, Switzerland, Netherlands, Australia, Hong Kong, China, New Zealand, India, Morocco, South Africa, and Chile. While the most powerful HPC clusters are typically located at national labs in the United States or their foreign counterparts, their funding and resource-sharing policies vary significantly from those of university HPC centers. Our project focused on university HPC centers since they are comparable to the existing resources in Wisconsin. We studied a total of 133 university HPC centers, with a focus on aspects such as availability, fee models, management models, and sustainability. Information was obtained from



publicly accessible official websites of these centers. We compared and analyzed the differences in these aspects, which informed our recommendations for HPC policies that best meet the needs of our state. Typically, HPC resources are measured by the number of nodes, which are standalone computer servers with dedicated CPU, memory, and disk space, or by the number of core hours, which are the number of processor units used to run a simulation multiplied by the duration of the job. Generally, a CPU node has 1–4 CPUs, each containing a few tens of cores. Graphics processing units (GPU) have become increasingly popular in scientific computing, and an increasing number of HPC clusters now include GPU nodes for performing calculations. Some centers also offer a data storage service, measured in gigabytes (GB) of disk storage space.

3.2 Availability

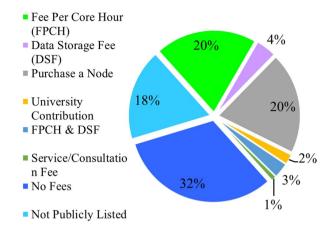
Among the 133 HPC centers, 46% restrict access to their resources to internal users from the same institution as the center, such as the University of the Witwatersrand in Africa, the Chinese University of Hong Kong, and the City University of Hong Kong. Similarly, the HPC resource provided by UWM in Wisconsin is mainly restricted to UWM users and a limited number of users from within the UW System. This is understandable as the demand for HPC resources is very high, and the internal users' requests alone often exceed the total core hours offered by the center. However, 32% of HPC centers are open to both internal and external users. For instance, the CHTC at UW-Madison offers HPC resources to researchers from UW-Madison and UW System, as well as external collaborators with an on-campus sponsor. The **Blugold Center for High-performance Computing** (BCHPC) at UWEC welcomes external users without an on-campus sponsor, subject to a service fee. This availability model of BCHPC could potentially benefit local industries and promote public—private partnerships. Moreover, information about the availability of HPC resources is not shared publicly by 22% of the centers investigated.

3.3 Fee models

Apart from the initial investment in hardware and software, running an HPC center comes with significant operating costs that include power, cooling, maintenance, and staffing. Although some centers (32%) provide HPC services for free, many (50%) charge a service fee to cover a portion of the operating costs. More detailed discussions on sustainability can be found elsewhere. However, it is worth noting that 18% of HPC centers don't disclose information about service fees. Figure 1 illustrates the diverse fee models identified, totaling 7. Out of the 50% of centers that charge a fee, the most common fee models are either charging the user per core hour or requiring them to purchase a node. Other less common fee models used by 1%-4% of HPC centers include universities requiring an annual departmental contribution, charging only for data storage, charging for both per core hour and data storage fee, and charging a service or consultation fee. When resources are available to both internal and external users, a higher fee is often charged for external users.



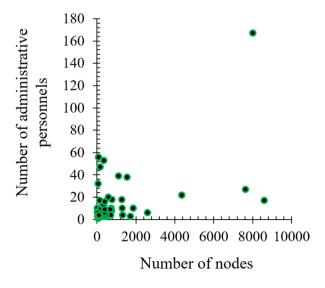
Fig. 1 Fee models of the 133 HPC centers examined in the study



3.4 Management models

Operating an HPC center requires specialized expertise in system administration, hardware deployment, software installation, and profiling. Each center employs a dedicated team of part-time and full-time staff members with different responsibilities. Out of the 133 HPC centers that were studied, 63 provided information regarding the number of staff members and nodes in their cluster, and Fig. 2 shows that there is a positive correlation between the number of nodes and the number of staff members. However, there are significant variations in the number of staff members needed due to the different services offered at different centers. Some centers provide only the hardware and software required for computing, which requires relatively few staff members whose responsibility is solely system administration. In contrast, other centers employ many staff members to provide a range of services,

Fig. 2 The system administrative features in various highperformance computing centers surveyed in the study





such as the Texas Advanced Computing Center which employs 167 full-time staff members with responsibilities ranging from system administration, user services, research and development, education, com- munity outreach, and industrial partnerships in the year of 2022. While such services may not be essential to the operation of an HPC center, they add significant value to existing resources. Dedicated staff members for user service enhance user experiences and expedite the scientific discovery, while a point of contact for industries promotes public–private partnerships and increases economic competitiveness. Interestingly, there are several universities nationally and internationally that share an HPC cluster, such as the Center for Computationally Assisted Science and Technology (CCAST) at North Dakota State University (NDSU), (Ponce et al., 2019) which provides HPC services to researchers from NDSU, undergraduate and master's institutions within the North Dakota University System (NDUS), and tribal colleges and universities in the state of North Dakota. Considering the cost of hardware, software, and staffing, a shared HPC center may be the most feasible option in many cases.

3.5 Sustainability

Although Moore's Law no longer strictly applies, the continued growth of computing power in HPC clusters means that it remains relevant in today's world. However, as scientific and societal challenges become more complex and require increasing computing power, HPC hardware quickly becomes outdated. As a result, sustaining an HPC center requires periodic hardware updates, possible expansions, and regular maintenance and staffing. Typically, an HPC cluster needs replacement every five years, coinciding with the maximum warranty period offered by hardware manufacturers. Running an HPC cluster beyond its warranty period poses a significant risk of malfunction leading to service disruption.

Even though 50% of the HPC centers we studied require a service fee, the fee collected is not sufficient to cover maintenance, and staffing, let alone purchasing an entire HPC cluster. Many centers, such as the Vermont Advanced Computing Center (VACC), offer free or paid services in tiers, and some, including the CHTC at UW- Madison and BCHPC at UWEC, offer a "buy-in" option or "condominium" model, where researchers or university community members can purchase nodes for priority access. However, all HPC centers studied rely on funding from central and/ or local governments, as federal funding through research or instrumentation grants and state appropriations and endowment funds often provide significant hardware and operating cost support. Unfortunately, federal grants are highly competitive, and funding is limited, which raises questions about the long-term sustainability of HPC centers.

One successful model is the New Jersey Big Data Alliance (NJBDA), which was established in 2013 and recognized as "New Jersey's Advanced Cyberinfrastructure Consortium" in 2014 by the state legislature. The alliance includes 18 higher education institutions, government agencies, and industry members, and its support from state legislation enables sustainable access to state-of-the-art HPC resources for both university and industry users. This collaboration promotes the development



of a skilled workforce and drives innovation and accelerates data-driven economic growth for New Jersey.

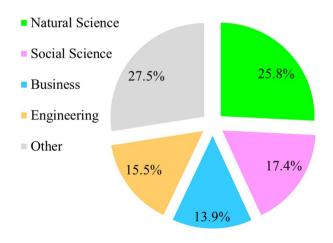
In summary, the present study surveyed 133 domestic and international university HPC centers and found that there are various models, fee schedules, management styles, and sustainability methods available. One popular model is the "condominium" model where users fund the hardware. Over 50% of HPC centers charge a service fee to help cover maintenance costs. A successful model involving a partnership between universities, industries, and government has also been identified: the New Jersey Big Data Alliance.

3.6 Results of student survey

A total of 79,268 email invitations were sent with 2,598 responses. Excluding incomplete and non-consent responses, a total of 1,370 valid responses were collected and analyzed (raw data in Table S7). A field-based analysis was conducted and presented in Fig. 3, which displays the student participants in the survey and the fields of their study. We inquired about the students' exposure to HPC, whether it be through research or as part of their coursework. White the data showed most students (63.5%) had no prior experience with HPC and a significant percentage of students (33.1%) had utilized HPC in some capacity, which is a promising figure considering the importance of HPC. Interestingly, a notable variation was observed among different fields of study. While 57.7% of natural science students and 52.4% of engineering students lacked HPC experience, the corresponding figures for social sciences, business, and other disciplines were 67.2%, 74.7%, and 67.5%, respectively. It is worth mentioning that the "Other" category encompasses subjects such as formal sciences, law, and medical sciences.

The subsequent inquiry aimed to assess their inclination toward enrolling in a course related to HPC. Among the respondents, 25.9% expressed an interest in HPC. coursework or had already taken such a course. However, 46.7% of the participants had no plans or were uncertain about pursuing HPC coursework. A notable 18.1% of respondents identified facing obstacles that impeded their pursuit of

Fig. 3 Pie chart showing the fields of study and the percentage of those who responded to the student survey





HPC coursework. Finally, we asked about the student's experience and interest in HPC-related research. Although a significant portion (46.7%) responded that they do not plan to participate in HPC-related research (Table S7), a notable percentage of students expressed a strong interest in such opportunities. About 8.4% and 8.2% of students are either interested in or already conducting HPC-related research, and 10.1% of students show interest, despite the unavailability of such projects.

The data presented in Table S7 regarding 'Interest and Experience in HPC-Related Coursework' and 'HPC-Related Research Experience' was analyzed further to deter- mine the level of interest in HPC among student respondents. Figure 4 displays the percentages of students who are either interested or potentially interested in HPC- related coursework or research projects, categorized by field of study. Those who selected 1 or 2 in'Interest and Experience in HPC-Related Coursework' or 1, 2, or 5 in 'HPC-Related Research Experience' were considered 'interested', while those who chose 4 in both subsections were labeled as 'potentially interested'. A significant level of interest was observed among engineering students, followed by those in natural science. Even in social science, 18.1% of students expressed interest (Fig. 4), indicating a notable level of interest across disciplines. The percentage of 'potentially interested' or 'not sure' responses across fields of study was around 30%-40%, mostly due to a lack of familiarity with HPC. However, we anticipate that introducing an HPC curriculum would convert many of these 'potentially interested' students into 'interested' students. Overall, the study revealed a strong interest in HPC among the student respondents. Figure 5 highlights significant barriers faced by interested students. For instance, among engineering students, 28.9% expressed interest in taking HPCrelated courses that were not offered to them. The percentage was 18.4%, 9.7%, 21.6%, and 15.2% for natural science, social science, business, and other fields of study, respectively. Similarly, 9.1%, 10.1%, 15.3%, 8.5%, and 9.3% of students in natural science, social science, business, engineering, and other fields of study (Fig. 5), respectively, showed interest in HPC-related research projects, but no such opportunities were available to them.

Fig. 4 Interests in HPC-related courses and research projects among students from different fields of study

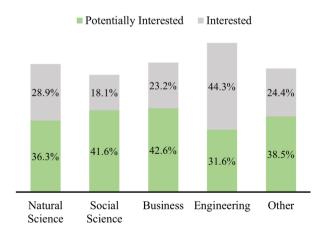
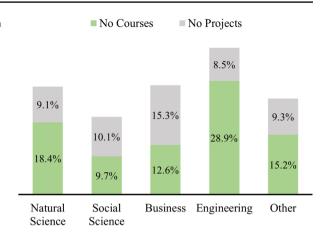




Fig. 5 Student percentages from different fields of study, who faced significant barriers in taking HPC courses or finding HPC-related research projects



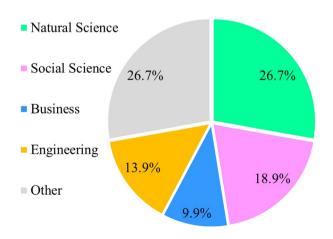
3.7 Faculty survey

Surveys were sent to faculty members at UW-Madison, UW-Stout, UW-Superior, and UW-La Crosse. A total of 4,415 email invitations were sent with 426 responses (Table S8). Excluding incomplete and non-consent responses, a total of 382 valid responses were collected and analyzed. Figure 6 shows the fields of study of faculty members who participated in the survey.

In the question of experience, a large number of faculty (69.0%) responded that they have had no experience with HPC, which is consistent to the result of the student survey (Table S7). For the interest levels of the faculty survey respondents in integrating HPC into their curricula, most respondents (60.3%) don't have a need to integrate HPC. Notably, many respondents are interested in teaching HPC, however, resource barriers, including the lack of HPC hardware (11.2%) and having no curricular materials (21.3%), prevent them from doing so.

For the interest and experience that faculty survey respondents have in HPC-related research, over half of the respondents (52.3%) don't need to utilize HPC

Fig. 6 Pie chart showing the fields of study and the percentage of those who responded to the faculty survey





in their research. Again, a significant portion of respondents is interested in HPC-related research, although 12.5% of respondents have no HPC resources and 10.3% have no support to set up their calculations.

Finally, for opinions of faculty survey respondents about utilizing the UWEC HPC cluster, 47.5% of them express interest in utilizing the UWEC HPC cluster, including 8.4% who are willing to pay a service fee.

Further field-based analysis demonstrated that a significant disciplinary difference exists observed. Combining data from 'Levels of Interest in HPC-Related Curricula' and 'Interest and Experience in HPC-Related Research' in Table S8, we see significant interest in HPC among faculty respondents. Figure 7 shows the percentages of faculty respondents from various fields of study who are interested in teaching HPC (choices 2 and 4), or HPC-related research (choices 2 and 3). Note that a faculty member may be interested in using HPC in only teaching, only research, or both. Engineering is again the field with the highest percentage, followed by natural science. However, interested faculty members faced serious hurdles in educating students about HPC skills, as shown in Fig. 8. The percentages of faculty

Fig. 7 Interests among faculty respondents from different fields of study in teaching HPC and HPC- related research

- Teaching- No Curricular Materials
- Teaching- No Resources

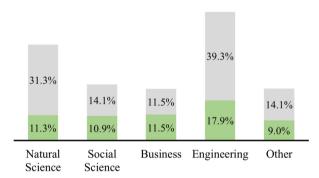
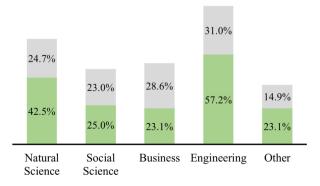


Fig. 8 Obstacles in incorporating HPC in teaching for faculty members from different fields of study

- Interested in HPC use in Research
- Interested in HPC Use in Teaching





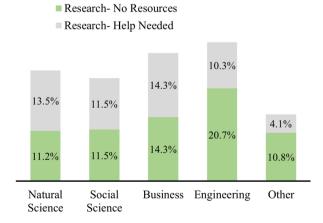
members who were interested in incorporating HPC in their teaching but had no HPC resources are 11.3%, 10.9%, 11.5%, 17.9%, and 9.0% for natural science, social science, business, engineering, and others, respectively. Understandably, teaching materials in HPC including textbooks and lab manuals, especially those targeting undergraduate students, are not well-established because it is a relatively new field of technology. Consequently, an even higher percentage of faculty respondents complained that they were interested in teaching HPC but with no curricular materials. As shown in Fig. 7, the percentages are 31.3%, 14.1%, 11.5%, 39.3%, and 14.1% for natural science, social science, business, engineering, and others, respectively.

The primary obstacle faced by faculty respondents in conducting their scholarly activities was the lack of HPC resources, as evidenced in Figs. 8 and 9. There exists significant interest in using HPC in teaching and research across disciplines including natural, social science, business, engineering (Fig. 8). However, various obstacles are also evident. In natural science, social science, business, engineering, and other fields of study, 11.2%, 11.5%, 14.3%, 20.7%, and 10.8% of faculty respondents, respectively, expressed interest in utilizing HPC in their research but reported that no resources were available to them (Fig. 9). Additionally, to use HPC resources effectively, a significant amount of training, profiling, and testing is required, which often falls outside the faculty member's area of expertise. However, such support is unavailable, preventing them from utilizing HPC for their research, as reported by 13.5%, 11.5%, 14.3%, 10.3%, and 4.1% of faculty respondents (Fig. 9) from natural science, social science, business, engineering, and other fields of study, respectively.

3.8 Industry survey

During our survey of local industries, we encountered difficulties in obtaining proper contact information for local companies. Despite sending out 10,914 emails, we received only 145 responses, of which 88 were valid (excluding those who did not consent to participate). The valid responses represented a variety of industries, including manufacturing (9.1%), healthcare/medical/biomedical (12.7%), agriculture (3.6%), electronics (3.6%), pharmaceutical (1.8%), and others (69.1%). The "other"

Fig. 9 Obstacles in conducting HPC-related research for faculty members from different fields of study





category included industries such as law, real estate, recreation, public administration, hospitality, tourism, retail, and non-profit services. Unfortunately, we did not receive any valid data from the energy, mining, and metallurgical/materials engineering industries.

The participants were asked to rate the importance of specific tasks to their organizations, such as modeling and simulation using finite element analysis (FEA) or computational fluid dynamics (CFD), smart manufacturing and automation, Internet of Things (IoT), AI tools for enterprise resource planning (ERP), and contingency analysis, all of which could benefit from HPC. As demonstrated in Table S9, while more than half of the responses for all tasks indicated no current need, a significant percentage of local industries (ranging from 5.5% to 25.4%) were already engaged in these activities. Furthermore, a comparable percentage of organizations (7.3% to 20%) planned to undertake these tasks in the future, indicating a growing demand for HPC among local industries.

In terms of HPC utilization, the responses were almost evenly divided among participants. 51% of respondents indicated that their organizations currently utilize or plan to do so in the future, while the remaining 49% did not. Those who indicated current or future HPC utilization in their organizations were further surveyed regarding the benefits, access to, and cost of HPC. Figure 10 summarizes their views on the benefits of HPC utilization, with 96.8% of respondents indicating that their organization has benefited from HPC. The most common benefit reported was the optimization of business processes, followed by improving the quality of products and services, improving business results, and increasing competitiveness. A variety of HPC service providers were identified, including organizations with their own HPC clusters, access to HPC centers outside Wisconsin, access to HPC centers in Wisconsin, cloud-based HPC resources, and outsourcing to third-party providers. Additionally, most respondents (63.2%) pay a service fee, with an average of \$675,000 per year. Interestingly, only a small percentage (5.7%) of local industries utilize resources from Wisconsin HPC centers. The second group of respondents, who do not and have no plan to use HPC, was asked about HPC utilization in their industry and the obstacles (Fig. 11) preventing their organizations from using HPC. Half of these participants responded that other organizations in their industry

Fig. 10 The benefits of HPC to local industries

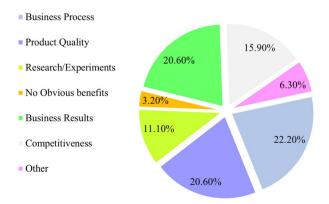
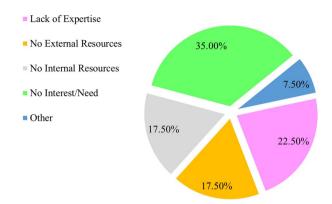




Fig. 11 Obstacles preventing HPC utilization among local industries



utilized HPC resources, indicating higher utilization than suggested by the survey. Most of this group (65%) faced some form of an obstacle, such as a lack of expertise (22.5%), lack of resources (35%), or other obstacles (7.5%). Overall, it is reasonable to conclude that these organizations could benefit from HPC if resources and expertise were made available to them.

Finally, participants were asked about their opinion on collaborating with universities. Many respondents (79.6%) agreed that partnering with universities could benefit their organization, and almost half (47.7%) reported having already partnered with a university and found it to be advantageous. However, only 15.9% of participants confirmed that they were knowledgeable about the process for gaining access to a university's HPC center.

3.9 University administrators interview

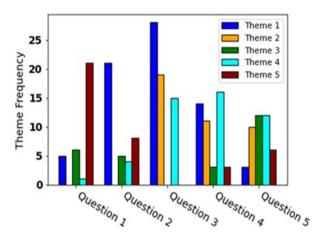
Administrators from various universities and organizations within the UW System were asked five questions designed to address the overarching research questions this study sought to answer:

- 1. What the barriers are and how can they be overcome?
- 2. How collaborations between universities and industry can be formed to equip undergraduate students with industry-needed computational skills?

Interview questions aimed at answering the research questions were then derived and can be found in Table S5. Five themes emerged from a thematic analysis of the interview responses, as listed in Table S10. Figure 12 shows the frequency of responses by question, contained in each theme. Theme 1 comes up most frequently in responses to questions 2 and 3, dealing with the status of HPC at their institutions and the difficulties of sharing resources. Themes 2 and 4 appear most often in responses to questions 3, 4, and 5, asking about difficulties and best practices for better sharing of HPC resources and the role of industry-academia partnerships. Theme 3 is most prevalent in responses to question 5, as can be expected, but is also present often in responses to questions 1 and 2. Theme 5, identifying how benefits



Fig. 12 A display of the frequency of themes represented in each question. From left to right Theme 1, Theme 2, Theme 3, Theme 4, and Theme 5 are represented on the chart, for each question

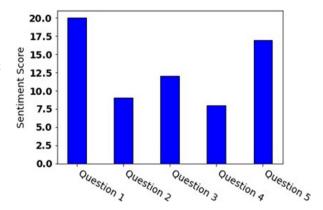


vary between different groups of users, is most commonly present in responses to question 1.

The sentiment analysis conducted on all responses to each question revealed that the interviewees generally had a positive outlook. This can be observed in Figs. 13 and 14, which group sentiments by interview questions and themes, respectively. Questions 1 and 5 garnered the most positive sentiment, while questions 2, 3, and 4 received a slightly positive score, almost neutral. The overall sentiment of the question was also reflected in the sentiment of the corresponding theme. While some questions and themes were expected to elicit more positive or negative responses, the semi-structured interview format allowed interviewees to control their perspectives when answering questions. Some interviewees approached the questions with a possibilities mindset, resulting in more positive responses, while others adopted a problem-identification approach, leading to more negative responses. Examples of these two approaches separated by question are provided below.

A detailed understanding of the meanings of the themes and sentiments arising out of the interviews, along with excerpts from the responses, can be found

Fig. 13 A display of sentiment scores by questions shows the overall sentiment score of each question. There is only a positive axis on this graph indicating a net positive sentiment of all questions. To give context to the scores, questions 1 through 5 had 33, 31, 53, 43, and 36 codes derived from them, respectively





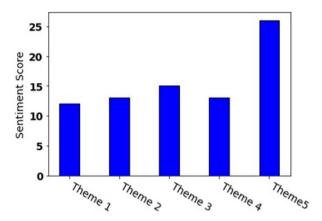


Fig. 14 A display of sentiment scores by themes shows the overall sentiment score of each theme. There is only a positive axis on this graph indicating a net positive sentiment of all questions. To give context to the scores, the questions had the following total number of codes derived from them themes 1 through 5 had 71, 40, 27, 48, and 38 codes derived from them, respectively. Note that the number of codes in this figure is slightly higher than Fig. 13, as some codes were placed in multiple themes

in our recently published study (Ghosh et al., 2023). As discussed in detail in this study (Ghosh et al., 2023), different financial capabilities of anticipated users, lack of awareness of resources, and intra and inter-institutional barriers are the biggest roadblocks toward an efficient resource-sharing framework. Equitable cost-sharing models, policies and procedures toward generating awareness, and incentivizing the breakdown of intra and inter-institutional barriers are the key to overcoming them. Emphasized repeatedly in the interviews was the importance of students acting as ambassadors to improve collaborations between universities and industry. Better integration of high performance computing in undergraduate curriculum should go a long way in enabling that.

3.10 Government officials' interview

We intended to interview government officials from multiple agencies including the Department of Workforce Development (DWD) and the Wisconsin Economic Development Corporation (WEDC). These agencies work with statewide business and education partners, and their view on HPC could have a profound impact on eco-nomic growth and workforce development in HPC-related fields. Unfortunately, only one response was obtained from multiple requests for an interview. Some of the key points raised when answering the five questions listed in Table S6 include:

1. Importance of HPC for economic growth in WI: HPC is a new area where the WI government needs a sector strategy. Wisconsin is moving from a heritage of manufacturing to the knowledge industry and needs to attract new businesses like Hewlett Packard Enterprise (HPE) in Eau Claire that will be able to use the talents of technical graduates around the state.



- 2. Addressing the growing need for HPC: We need to draw attention to HPC for future growth in Wisconsin.
- 3. Partnerships for innovations in HPC: Just as the Big Data Alliance in New Jersey fosters a national leadership role for New Jersey in big data. A partnership that includes the Wisconsin industry and institutes of higher learning needs to be on the radar for future job growth.
- 4. Promoting HPC in undergraduate education: The industry will be able to tell the UW system how to design programs and research experiences for its undergraduates.
- 5. The growth of businesses like Epic in Verona, HPE in Eau Claire, and Rockwell Automation in Milwaukee indicate a demand for technically prepared graduates in the field of HPC within the state.

4 Conclusions

Use of surveys across UW campuses demonstrated that there is a strong interest in HPC-related courses and research projects among students from various disciplines, particularly engineering and natural sciences. Faculty members may have limited experience with HPC but are interested in incorporating it into their teaching and research, especially those in engineering and natural sciences. Based on the survey results, we recommend that a local consortium be formed to include UW-Eau Claire, UW-Stout, and UW-River Falls as a pilot project to investigate the feasibility of forming a larger group of UW-System campuses. We will explore the issues involved in setting up such a consortium so that a larger group serving students and faculty across the state can be achieved. Local industries expressed strong interest in HPC and belief that it would benefit their business, but many are not aware of the resources available in the UW System and instead pay service fees averaging \$675,000 annually for HPC services. University leaders widely recognize the importance of HPC in education, research, workforce development, and economic growth, but also acknowledge the challenges in maintaining and sharing HPC resources. Although awareness of HPC among government officials is low, the significance of a partnership between the Wisconsin industry and institutes of higher education has been recognized.

However, various obstacles exist that prevent some organizations from utilizing HPC resources. This study revealed that Wisconsin lags behind other states in terms of available HPC resources and HPC-based education, discovery, and economic growth. While the support and interest from various stakeholders are encouraging, significant challenges must be addressed before Wisconsin can fully benefit from HPC in this data-intensive era. These challenges include:

- a) Limited awareness and access to existing HPC resources.
- b) Curricular materials and technical support in HPC are not readily available.
- c) Current HPC resources are close to their capacity and cannot accommodate the needs of faculty, students, and the industry identified in this project. In addition,



- no clearly defined policy exists in terms of resources and cost-sharing among multiple campuses.
- d) The ability of these HPC centers to provide sustainable services is questionable, which is highly contingent on funding for hardware, maintenance, and staffing.
- e) Although local industries value partnerships with universities, conversations regarding collaboration in HPC are needed. It is unclear how the industry can benefit from HPC resources.
- f) The role of government agencies in promoting partnerships among various stakeholders within the state in HPC and related fields is unclear or undefined, which could be a serious competitive disadvantage.

This is the first ever study to investigate the status of HPC in Wisconsin. By investigating the source of these challenges, the study also identified some opportunities and targeted reforms possible within UW system giving forth new public policies. First, to establish the Wisconsin Big Data Alliance (WBDA) involving the UW System, industries across Wisconsin, other public/private institutions of higher education in Wisconsin, and government agencies including DWD and WEDC. Such an alliance would enable all interested parties to work collectively to address challenges in HPC education, innovation, and economic growth. Second, we recommend an interdisciplinary approach to curriculum development across the three campuses (Eau Claire, Stout, and River Falls) in such a way as to allow students in Biochemistry, Biomedical Engineering, Engineering, and Computer Science to take courses offered on all three campuses. Potential partners in this curriculum development project may include UW-Extended Campus, which has an established history of developing distance education to students around the state and the nation. Third, it would be meaningful to create a central repository of curricular materials that could be maintained by a team of faculty and students from academia and perhaps with from some inputs from the industry. These materials should be available for free to all public institutions in Wisconsin and can be further optimized to meet specific needs such as during public emergencies. Fourth, to create an education committee within WBDA, whose members include representatives from faculty, students, and industry, to oversee the creation and sharing of educational resources and programs that are responsive to local needs, foster collaboration among universities, communities, and industries, and build a strong workforce pipeline in HPC and related fields. Fifth, to find a dedicated funding source at the state level to support the long-term growth and stability of the existing HPC centers within the UW System. Finally, to make the HPC resources freely available to faculty and students from public institutions across Wisconsin. This could be done by developing a reasonable fee structure for industrial versus not-for-profit users and creating FTE positions in system administration, user service, K-12 education, and industrial outreach.

Supplementary Information The online version contains supplementary material available at https://doi.org/10.1007/s10639-024-12582-6.

Acknowledgements This work was supported in part by in part by Tommy G. Thompson Center on Public Leadership Grant, Madison, WI (project entitled "Exploring Policies to Promote High-Performance



Computing in Post-Pandemic Undergraduate Education in Wisconsin") and by the National Institutes of Health (Grant Number 2R15GM117510-02 to SB).

Date:12/20/2023

Data availability The authors declare that the data supporting the findings of this study are available within the paper and its Supplementary Information files.

Declarations

Conflict of interest None

References

- Adenaike, O., Olabanjo, O. E., & Adedeji, A. A. (2023) Integrating computational skills in undergraduate microbiology curricula in developing countries. *Biology Methods and Protocols*, 8. https://doi.org/10.1093/biomethods/bpad008
- Al-Jody, T., Aagela, H., & Holmes, V. (2021). Inspiring the next generation of hpc engineers with reconfigurable, multi-tenant resources for teaching and research. *Sustainability (switzerland)*,13, 11782. https://doi.org/10.3390/su132111782
- Bethune, I., Carter, A., Guo, X., & Korosoglou, P. (2012). Million atom KS-DFT with CP2K partnership for advanced computing in Europe. https://era.ed.ac.uk/handle/1842/6543
- Chaudhury, B., Varma, A., Keswani, Y., Bhatnagar, Y., & Parikh, S. (2018). Let's HPC: A web-based platform to aid parallel, distributed and high performance computing education. *Journal of Parallel Distributed Computing*, 118, 213–232. https://doi.org/10.1016/j.jpdc.2018.03.001
- Chen, S., He, Z., Han, X., He, X., Li, R., Zhu, H., Zhao, D., Dai, C., Zhang, Y., Lu, Z., Chi, X., & Niu, B. (2019). How big data and high-performance computing drive brain science. *Genomics, Proteomics & Bioinformatics*, 17, 381–392. https://doi.org/10.1016/j.gpb.2019.09.003
- Cui, S., Wang, Y., Li, L., Peng, X., & Yalvac, B. (2016). Introducing high performance computing to undergraduate students. Computers in Education Journal, 16. https://doi.org/10.18260/p.25453.
- Ezell, S. J., & Atkinson, R. D. (2016). The vital importance of high- performance computing to US competitiveness (pp. 1–58). ITIF. https://itif.org/publications/2016/04/28/vital-importance-high-performance-computing-us-competitiveness/
- Fernández, Á., Fernández, C., Miguel-Dávila, J. Á., & Conde, M. (2021). Integrating supercomputing clusters into education: A case study in biotechnology. *J. Supercomp.*,77, 240–253. https://doi.org/10.1007/s11227-020-03360-5
- Fossum, C., Laatsch, B., Lowater, H., Narkiewicz-Jodko, A., Lonzarich, L., Hati, S., & Bhattacharyya, S. (2022). Pre-Existing oxidative stress creates a docking-ready conformation of the SARS-CoV-2 receptor-binding domain. ACS Bio & Med Chem Au, 2, 84–93. https://doi.org/10.1021/acsbiomedchemau.1c00040
- Ghosh, A., Kunkel, W., Varghese, A., Ma, Y., Gomes, R., Bhattacharyya, S., Mohr, M., Doss, I., Hebert, J. (2023). Inter-institutional Resource Sharing in Undergraduate HPC Education: Interviews with University Administrators. In SIGCSE 2023 - Proceedings of the 54th ACM Technical Symposium on Computer Science Education. https://doi.org/10.1145/3545945.3569784
- Gomes, R., Kamrowski, C., Langlois, J., Rozario, P., Dircks, I., Grottodden, K., Martinez, M., Tee, W. Z., Sargeant, K., LaFleur, C., & Haley, M. (2022a). A comprehensive review of machine learning used to combat COVID-19. *Diagnostics*, 12, 1853. https://doi.org/10.3390/diagnostics12081853
- Gomes, R., Kamrowski, C., Mohan, P. D., Senor, C., Langlois, J., & Wildenberg, J. (2022b). Application of deep learning to IVC filter detection from CT Scans. *Diagnostics*, 12, 2475. https://doi.org/10.3390/diagnostics12102475
- Hati, S., & Bhattacharyya, S. (2016). Incorporating modeling and simulations in undergraduate biophysical chemistry course to promote understanding of structure-dynamics-function relationships in proteins. *Biochemistry and Molecular Biology Education*, 44, 140–159. https://doi.org/ 10.1002/bmb.20942



- Heifetz, A. (2024). Accelerating COVID-19 drug discovery with high-performance computing. *Methods in Molecular Biology*, 2716. https://doi.org/10.1007/978-1-0716-3449-3_19
- Hunter, J. (2019). Pedagogy, leading from the middle and digital technologies: Potent forces for STEM education in Australian primary schools. *Australian Educational Leader*, 41, 6–28.
- Karsakov, A., Bilyatdinova, A., & Bezgodov, A. (2015). Improving visualization courses in russian higher education in computational science and high performance computing. *Procedia Computer Science*. https://doi.org/10.1016/j.procs.2015.11.083
- Kruchten, A. E. (2020). A curricular bioinformatics approach to teaching undergraduates to analyze metagenomic datasets using R. Frontiers in Microbiology, 11, 578600. https://doi.org/10.3389/ fmicb.2020.578600
- Lynn, T., Fox, G., Gourinovitch, A., & Rosati, P. (2020). Understanding the determinants and future challenges of cloud computing adoption for high performance computing. *Future Internet.*,12, 135. https://doi.org/10.3390/FI12080135
- Mullen, J., Byun, C., Gadepally, V., Samsi, S., Reuther, A., & Kepner, J. (2017). Learning by doing, high performance computing education in the MOOC era. *Journal of Parallel and Distributed Computing*, 105, 105–117. https://doi.org/10.1016/j.jpdc.2017.01.015
- Neelima, B. (2017). High performance computing education in an Indian Engineering Institute. *J. Parallel Distrib Comput.*, 105, 73–82. https://doi.org/10.1016/j.jpdc.2017.01.019
- No Author. (2021). Fighting COVID-19 with HPC. *Nature Computational Science*, 1, 769–770. https://doi.org/10.1038/s43588-021-00180-2
- Ponce, M., Spence, E., van Zon, R., & Gruner, D. (2019). Scientific computing, high-performance computing and data science in higher education. *Journal of Educational Computing Research*, 10, 24–31. https://doi.org/10.22369/issn.2153-4136/10/1/5
- Pyzer-Knapp, E. O., Pitera, J. W., Staar, P. W. J., Takeda, S., Laino, T., Sanders, D. P., Sexton, J., Smith, J. R., & Curioni, A. (2022). Accelerating materials discovery using artificial intelligence, high performance computing and robotics. NPJ Computational Materials, 8, 84. https://doi.org/10.1038/s41524-022-00765-z
- Raj, R. K., Romanowski, C. J., Impagliazzo, J., Aly, S. G., Becker, B. A., Chen, J., Ghafoor, S., Giacaman, N., Gordon, S. I., Izu, C., Rahimi, S., Robson, M. P., Thota, N. (2020). High performance computing education: Current challenges and future directions. In *ITiCSE-WGR'20*, pp. 51–74. https://doi.org/10.1145/3437800.3439203
- Samuel, J., Brennan-Tonetta, M., Samuel, Y., Subedi, P., & Smith, J. (2022). Strategies for democratization of supercomputing: Availability, accessibility and usability of high performance computing for education and practice of big data analytics. *Journal of Big Data Theoretical Practice*, 1, 51–65. https://doi.org/10.54116/jbdtp.v1i1.16
- Shields, G. C. (2020). Twenty years of exceptional success: The molecular education and research consortium in undergraduate computational chemistry (MERCURY). *International Journal of Quantum Chemistry*, 120, e26274. https://doi.org/10.1002/qua.26274
- Shuja, J., Ahmad, R. W., Gani, A., Abdalla Ahmed, A. I., Siddiqa, A., Nisar, K., Khan, S. U., & Zomaya, A. Y. (2017). Greening emerging IT technologies: Techniques and practices. *Journal of Internet Services and Applications*, 8, 9. https://doi.org/10.1186/s13174-017-0060-5
- Suhail, S., Zajac, J., Fossum, C., Lowater, H., McCracken, C., Severson, N., Laatsch, B., Narkiewicz-Jodko, A., Johnson, B., Liebau, J., Bhattacharyya, S., & Hati, S. (2020). Role of Oxidative Stress on SARS-CoV (SARS) and SARS-CoV-2 (COVID-19) Infection: A review. *Protein Journal.*,39, 644–656. https://doi.org/10.1007/s10930-020-09935-8
- Townsend-Nicholson, A. (2020). Educating and engaging new communities of practice with high performance computing through the integration of teaching and research: Using technology to transform learning. *Interface Focus*, 10, 20200003. https://doi.org/10.1098/rsfs.2020.0003
- Vavilala, V. S. (2020). Combining high-performance hardware, cloud computing, and deep learning frameworks to accelerate physical simulations: Probing the Hopfield network. *European Journal* of Physics, 41, 035802. https://doi.org/10.1088/1361-6404/ab7027
- Wozney, A. J., Smith, M. A., Abdrabbo, M., Birch, C. M., Cicigoi, K. A., Dolan, C. C., Gerzema, A. E. L., Hansen, A., Henseler, E. J., LaBerge, B., Leavens, C. M., Le, C. N., Lindquist, A. C., Ludwig, R. K., O'Reilly, M. G., Reynolds, J. H., Sherman, B. A., Sillman, H. W., Smith, M. A., ... Bhattacharyya, S. (2022). Evolution of stronger SARS-CoV-2 variants as revealed



through the lens of molecular dynamics simulations. *Protein Journal*.https://doi.org/10.1007/s10930-022-10065-6

Zajac, J., Anderson, H., Adams, L., Wangmo, D., Suhail, S., Almen, A., Berns, L., Coerber, B., Dawson, L., Hunger, A., Jehn, J., Johnson, J., Plack, N., Strasser, S., Williams, M., Bhattacharyya, S., & Hati, S. (2020). Effects of Distal Mutations on Prolyl-Adenylate Formation of Escherichia coli Prolyl-tRNA Synthetase. *Protein Journal.*, 39, 542. https://doi.org/10.1007/s10930-020-09910-3

Publisher's Note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

Springer Nature or its licensor (e.g. a society or other partner) holds exclusive rights to this article under a publishing agreement with the author(s) or other rightsholder(s); author self-archiving of the accepted manuscript version of this article is solely governed by the terms of such publishing agreement and applicable law.

Authors and Affiliations

Jordan Hebert³ · Ryan Hratisch³ · Rahul Gomes³ · William Kunkel⁷ · Daniel Marshall⁵ · Abhimanyu Ghosh⁵ · Isabella Doss¹ · Ying Ma¹ · Derek Stedman⁶ · Blake Stinson⁶ · Anthony Varghese⁶ · Molly Mohr² · Pricilla Rozario⁴ · Sudeep Bhattacharyya² ©

- Rahul Gomes gomesr@uwec.edu
- Abhimanyu Ghosh ghosha@uwstout.edu
- Anthony Varghese anthony.varghese@uwrf.edu
- Sudeep Bhattacharyya bhattas@uwec.edu

Jordan Hebert hebertj4194@uwec.edu

Ryan Hratisch hrastirt9447@uwec.edu

William Kunkel kunkelw2898@my.uwstout.edu

Daniel Marshall marshalld0237@my.uwstout.edu

Isabella Doss dossic2069@uwec.edu

Derek Stedman derek.stedman@my.uwrf.edu



Blake Stinson blake.a.stinson@gmail.com

Molly Mohr mohrml5732@uwec.edu

Pricilla Rozario rozaripp5369@uwec.edu

- Materials Science and Biomedical Engineering, University of Wisconsin-Eau Claire, 105 Garfield Avenue, Eau Claire, WI 54702, USA
- Chemistry and Biochemistry, University of Wisconsin-Eau Claire, 105 Garfield Avenue, Eau Claire, WI 54702, USA
- Omputer Science, University of Wisconsin-Eau Claire, 105 Garfield Avenue, Eau Claire, WI 54702, USA
- ⁴ Psychology, University of Wisconsin-Eau Claire, 105 Garfield Avenue, Eau Claire, WI 54702, USA
- ⁵ Engineering and Technology, University of Wisconsin-Stout, 1712 South Broadway Street, Menomonie, WI 54751, USA
- ⁶ Computer, Information, and Data Sciences, University of Wisconsin, River Falls, 410 S. 3 Street, River Falls, WI 54022, USA
- Mechanical Engineering, University of Wisconsin, Madison, 1513 University Ave, Madison, WI 53706, USA

