Integration of Actors in HPC Ecosystems: Transdisciplinarity, Interdisciplinarity and Interaction

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ABSTRACT

Interest in High-Performance Computing (HPC) has surged, driven by the demand for skills to utilize advanced computing methods. These methods include managing vast amounts of data, implementing complex algorithms, and developing Artificial Intelligence (AI) applications. HPC ecosystems play a crucial role in tackling intricate scientific and engineering problems. However, integrating various stakeholders demands a deep understanding of collaboration and innovation within HPC settings. This proposal explores how different stakeholders—from students across diverse fields to scientists and policymakers—have been integrated at various levels. This integration is facilitated by introducing new formal courses, incorporating relevant topics into existing curricula, and other related activities.

KEYWORDS

Education, HPC, Training, Best Practices

1 INTRODUCTION

The enhancement of High Performance Computing (HPC) skills is vital for multiple professional sectors, extending beyond advanced scientific and technological domains to encompass a diverse array of fields and applications. With the ongoing expansion of artificial intelligence (AI) applications, acquiring knowledge and competencies in parallel computing across various levels and disciplines is imperative, whilst promoting interactivity among them to enhance conception, development, and utilization. Institutions and communities pursue various initiatives [1] and recommendations tailored to specialized communities and interest groups [2], involving individuals in transformative experiences focused in implementations addressed to build knowledge or innovations [1, 3].

These individuals can be categorized in several ways, primarily as participants interacting with High-Performance Computing (HPC) resources and possessing distinct requirements [12]. They may be classified into three distinct groups: HPC system engineers, who integrate, monitor, tune, optimize, and evaluate the performance of HPC hardware and software; these professionals are also referred to as DevOps professionals [2]. The second group consists of HPC software engineers, who are responsible for developing parallel programs, debugging and analyzing application performance, and optimizing HPC software cycles. The third group encompasses computer scientists, who, while classified as users, require specialized skills for HPC, such as coding, executing, and efficiently deploying parallel programs. These three groups engage in continuous interaction and are required to share common knowledge. It is pertinent to note, however, that these categories are not uniform development spaces; rather, they can vary in depth based on individual interests and levels of interaction. On the other hand, it is important to understand that the actors are not isolated but are in constant interaction and that these actors, at their base, can be part of other disciplines (and not only at the user level), which implies transdisciplinarity and interdisciplinarity [4, 7].

This proposal outlines an experience centered on integrating actors within the HPC ecosystem, considering various factors: interaction spaces, transdisciplinary and interdisciplinary approaches, competency levels, and knowledge depth. Over more than a decade, this experience has been gathered through diverse activities, including the Supercomputing and Distributed Systems Camping School (SCCAMP) [3], specialized certifications with the technology industry, mainly conducting workshops and seminars with NVIDIA under the NVIDIA Deep Learning Institute[4] and formal courses and certification training at Universidad Industrial de Santander (from the Spanish acronym UIS, Universidad Industrial de Santander) [5], facilitated by the High Performance and Scientific Computing Center (SC3UIS, from the Spanish acronym of Supercomputación y Cálculo Científico de la Universidad Industrial de Santander)[6]. This effort has led to the identification and development of effective practices in training ecosystem participants, significantly impacting the advancement of computing in both the academic sector and related communities.

2 APPLYING KEY CONCEPTS

In our proposal, we outlined two significant concepts: transdisciplinarity and interdisciplinarity. Transdisciplinarity encompasses integrating knowledge from various fields and stakeholders, underscoring the importance of collaboration in addressing complex issues. Within High-Performance Computing (HPC), this approach involves computational scientists, domain experts, and end-users.

[1]For example, the HPC Forum https://www.hpcuserforum.com/
[2]Such as the HPC Certification Forum https://www.hpc-certification.org/, and the Education Chapter on ACM Special Interest Group in HPC https://sighpceducation.hosting.acm.org/

[3]More about SCCAMP in https://www.sc-camp.org
[4]More information about NVIDIA DLI in https://www.nvidia.com/en-us/training/
[5]For more information about the UIS: https://www.uis.edu.co
[6]More information about SC3UIS in: http://www.sc3.uis.edu.co

https://doi.org/10.22369/issn.2153-4136/16/1/1

Interdisciplinarity, conversely, merges knowledge from diverse disciplines to tackle specific problems, fostering collaboration to develop innovative computational techniques and applications within HPC ecosystems. We wish to emphasize the critical significance of interactions both within and across disciplines, as previously explained, which transcends a mere multidisciplinary approach. Consequently, interactions are paramount, as this article will elaborate on.

2.1 Implementing Transdiciplinarity

In order to implement transdisciplinarity, as defined in the preceding discussion, the establishment of specialized courses tailored to distinct groups of undergraduate and graduate programs was proposed. Initially, we developed the following undergraduate courses: High Performance and Scientific Computing, which is available to all disciplines; Introduction to Parallel Computing, designed specifically for students in the Systems and Informatics Engineering program; and a high-performance computing course that was first offered to postgraduate students of the university's School of Systems Engineering and Computer Science. After a period of three years, this course was subsequently made available to all postgraduate programs at the university, including both master's and doctoral courses. The courses commence simultaneously, and while there are dedicated sessions for each course, they also incorporate shared challenges and activities to ensure interaction and foster a unified perspective on complex problems across diverse disciplines and levels.

The different activities carried out during these years have been diverse: for example, a collaborative mid-course project developed in specific sessions with students from the (3) different courses to address an evaluated challenge in distributed memory programming with MPI, or the final project of the course, developed in slightly larger teams including students of different levels.

Over time, we identified consequential aspects to implement this transdisciplinarity: inclusion of different actors (not necessarily direct actors of the programs in science and engineering of the University or the academic community), collaborative learning environments (i.e., platforms or collaborative *fun* activities) [11], vision on transformation knowledge and a systemic approach [5]. With these aspects, the courses were evolving towards popularization activities in which the students participated: for example, hackathons, activities framed within science and technology festivals with the participation of high school students or inhabitants of the neighborhoods surrounding the university, and students of human and health sciences disciplines.

Figure 1 shows the participants in different activities: on the top left, microbiology students in the data analytics course with R; on the bottom left, participants in the smart vehicle challenge based on NVIDIA Jetson; and on the right, children from the supercomputing nursery in schools and neighborhoods surrounding the university.

The transdisciplinary initiative fostered a strong interdisciplinarity. In the next section, we will outline how this prompted the creation of specialized courses for postgraduate students. These courses focus on managing large-scale data within microbiology and bioinformatics, utilizing parallel processing. Additionally, we will discuss proposed courses in physics and chemical engineering, as well as developments in digital humanities [9].

Figure 1: Participants in transdisciplinary activities

2.2 Developing Interdisciplinarity

In our approach, interdisciplinarity refers to an educational strategy that integrates insights and methods from multiple disciplines to address complex problems or questions that a single field cannot adequately solve. This approach is increasingly recognized as essential in academic research and practical applications, as it allows for a more comprehensive understanding of nuanced issues.

Clearly, in the academic university environment, there is more familiarity with interdisciplinarity, and that is why we develop it further in this section. Although there are clearly aspects that can be considered equally transdisciplinary, the focus given allows us to identify the important activities and characteristics:

- Complex Problem Solving: many challenges require interdisciplinary research and actions to synthesize knowledge from various fields. For this reason, different specific courses and seminars were created addressed to specific domains. In the case of the computer science students (undergraduate or postgraduate), their technical skills were directed towards understanding specific scientific formalisms for different areas of interest (in physics, for example, with quantum computing).
- Innovate Solutions: by merging traditional educational notions, interdisciplinary work can lead to innovative solutions that are more effective than those derived from a single discipline. This is particularly relevant in business careers and humanities. And for the creation of entrepreneurial spirits in students.
- Cognitive Development: interdisciplinary instruction enhances cognitive abilities by encouraging them to integrate concepts from different disciplines. This fosters skills such as perspective-taking, which is crucial for understanding diverse viewpoints and approaches to problem-solving. This aspect is closely related to the resolution of complex problems.

- Multidisciplinary Approach: this aspect involves the integration and collaboration of knowledge, skills, and methodologies from multiple academic disciplines. In the university, it is particularly valuable to improve soft skills such as communication and the growth of deep scientific knowledge.
- Adaptative Knowledge: The adaptive knowledge management process systematically and intentionally collects and selects information and connects it to the right people at the right time to increase the likelihood that students, researchers or decision-makers see, understand, and use the knowledge [6]. This is an essential pillar for multi-level transdisciplinary activities.
- Collaborative Skills: To achieve collaboration, for example, it is necessary to establish a common language, given by good practices, aspects related to paradigms in programming languages, and, of course, modeling and simulation (as well as systemic approaches).

Several strategies may be utilized to identify these characteristics. For instance, phased integration—a structured methodology for interdisciplinary research—can encompass phases such as comparing disciplines, comprehending their methodologies, and engaging in cross-disciplinary thinking. This approach fosters the establishment of a cohesive framework for assimilating diverse insights. Consequently, it facilitated the development and design of the curriculum. The educational programs at our university ought to be structured to promote collaboration among various disciplines. This may involve the creation of modules that necessitate students to leverage knowledge from multiple fields in order to address real-world challenges. In light of this, the topics covered in formal courses within the domains of science and engineering include, but are not restricted to, the utilization of tools and techniques that incorporate high-performance computing support, thereby enriching the entire ecosystem. Such was the case in courses such as Fluid Dynamics for Mechanical Engineering, Numerical Methods in Engineering, Computer Architecture for Computer Science, and Data Analytics for Human Sciences.

The table 1 below illustrates examples of different topics and subjects in courses related to specific degrees at UIS, at both undergraduate and postgraduate levels. In the first column, example topics shared across various courses are listed in the second column, alongside their corresponding academic programs in the third column. For instance, the topic of Parallel Programming Paradigms appears in two courses with different focuses: Parallel Programming, which is available for all degrees (including both undergraduate and graduate), and Parallel Computing, offered only for the undergraduate program in Systems Engineering (Sys. Eng.). Within this topic, we explore shared memory programming (using OpenMP), distributed memory programming (with MPI), and hybrid programming with directives (such as OpenACC or CUDA). Regarding the second topic, Parallel and Distributed Computation, we find that it is taught in Numerical Analysis for the Sys. Eng. program, as well as in Numerical Methods in Chemical Engineering (Chem. Eng.) and Fluid Dynamics in Mechanical Engineering. Another intriguing topic worth noting involves GPGPUs, which is covered in both postgraduate and undergraduate courses, such as Computer Architecture and Parallel Computing for Sys. Eng., HPC for the MSc. in Computer Science (C.S.), and Advanced Computing Architecture for the MSc. in Electronic Engineering.

Table 1: Topics, Courses and Involved Programs

Topics	Course	Career
Parallel Programming Paradigms	Parallel Programming Parallel Computing	All Sys. Eng.
Parallel and Distributed Computation	Numerical Analysis Numerical Methods Fluid Dynamics	Sys. Eng. Chem. Eng. Mec. Eng.
Data Reduction and Visualization	Data Analytics Computing Tools Data Analysis	Biology Social Work Medicine
Debugging, Profiling, and Monitoring	Algorithms and HPC Parallel Computing Parallel Programming Data Analytics	Physics Sys. Eng. All Biology
GPGPUs Systems	Computer Architecture Parallel Computing HPC Advanced Computer Architecture	Sys. Eng. Sys. Eng. MSc. in C. S. MSc. in Electronic Enginnering

These courses are integrated, featuring a collaboration between professors and engineers from SC3UIS. In all instances, specific activities and sessions—both theoretical and practical—are conducted with participants from various courses, disciplines, and study levels. This approach fosters a unified language and coordinated efforts among the diverse participants[7].

However, implementing transdisciplinary and interdisciplinary approaches can be complex due to critical challenges: Coordination and Collaboration through the different programs require significant coordination among diverse professors and stakeholders, which can be time-consuming and resource-intensive. Institutional Support, acquiring buy-in from the administration, and securing funding for interdisciplinary and transdisciplinary initiatives can be complex. Skill Development can also be complex because the parties need to develop leadership and cooperation skills to navigate the collaborative nature of interdisciplinary and transdisciplinary work.

3 INTEGRATING ACTORS IN HPC ECOSYSTEMS

Dynamic exchanges exist between different actors within the HPC ecosystem. Effective interaction fosters communication, knowledge sharing, and collaborative problem-solving. It is essential for building trust and understanding among stakeholders, which is crucial for successfully integrating and implementing HPC solutions. By uniting diverse perspectives through transdisciplinary and interdisciplinary approaches, HPC ecosystems can tackle complex

[7]The courses developed, and the associated material can be consulted (mainly in Spanish originally) at: https://wiki.sc3.uis.edu.co/

problems more effectively. This integration allows for exploring innovative solutions that may not emerge within isolated disciplines and enhanced problem-solving. Figure 2 shows the different elements impacted by each one of the roles in the HPC environment in levels, from infrastructure to applications.

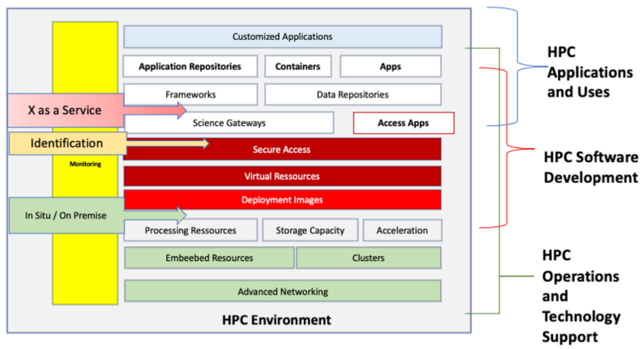

Figure 2: HPC Roles in the HPC Environment.

Figure 2 presents three primary actors in advanced computing projects: HPC technology and operations engineers, HPC software developers, and HPC scientists. These groups continually interact to meet their objectives and ensure the effective deployment and performance of applications in these initiatives. Additionally, specific skills are necessary for engaging with various components of an HPC system. For example, the scientific end user, who relies on the HPC environment for research support, customizes application usage and ensures accurate execution and deployment. In contrast, the developer establishes development and image deployment environments for scientists while facilitating communication with both users and DevOps actors. Furthermore, the administrator (DevOps), as depicted in the figure, offers operational support directly from the architecture figure 2, the integrating element is monitoring and performance evaluation.

Collaborative actions can lead to a more efficient use of resources, including computational power, funding, and human expertise. By pooling resources and knowledge, actors can achieve more significant outcomes than they could individually. This pooling can be considered resource optimization. Furthermore, collaboration among various stakeholders can stimulate innovation and transfer technology from research to practical applications. This is particularly important in HPC, where advancements in computational methods can significantly impact various industries.

Integrating actors from diverse backgrounds helps build capacity within the HPC ecosystem. It enhances participants' skills and competencies, preparing them to address future challenges collaboratively. Transdisciplinary approaches ensure that HPC research effectively addresses societal needs and challenges. By involving community stakeholders, researchers can align their work with real-world issues, enhancing the relevance and impact of their findings.

For example, in courses developed for undergraduate and graduate students in areas other than computer science, emphasis is placed on the proper use of resources and appropriate interaction with developers and administrators [5]. In computer science courses that involve implementing development and execution environments and/or supporting platforms aimed at end users, the need for interaction is raised to understand requirements and ensure customization and good performance, for example, by following good practices for monitoring and analyzing the performance of HPC environments.

Monitoring and observing the status of both high-level code and low-level processes allows, for example, identifying faults, efficient execution environments, load balancing, and time management without affecting accuracy. On the other hand, from this interaction, new common areas of research have been developed, thinking about sustainability: observing, for example, software quality, useful lifetime, energy efficiency, learning curves, and even, very recently, frugality[10].

On the other hand, training courses have been created that can be considered as specific modules of the different formal courses, for example, using the training given by NVIDIA within the academic programs of the NVIDIA DLI (or now via academy NVIDIA Academy programs. Likewise, activities within Summer schools we have hosted on campus or co-organized with our university in different years or even in specific tutorials.

The interaction between different courses, students, and levels has allowed the recognition of various actors and their roles and competencies and the development of shared spaces around good practices, as will be discussed in the following section. This generates challenges and allows the implementation of diverse strategies according to the interests and skills sought, searching integration.

4 CHALLENGES AND STRATEGIES

Academic disciplines are characterized by distinct cultures, terminologies, and methodologies, which impede effective communication and collaboration. Surmounting these differences necessitates deliberate efforts to cultivate mutual understanding. To transcend traditional barriers, incentives for cooperation must be aligned with interdisciplinary objectives.

Managing interactions among diverse actors can be complex and is a significant challenge. It requires effective coordination and leadership. Establishing clear communication channels and collaborative frameworks is essential for successful integration and credibility. For better or worse, the academic community is hierarchical and intellectually elitist, where authority in knowledge is necessary. Inclusion is another crucial challenge, as the technology community continues to be very uninclusive, not only in terms of gender but also in terms of culture and nationality.

Ultimately, we recognize the significance of sustainability within collaborative initiatives is duly acknowledged. The challenge of ensuring the resilience of collaborative efforts can be substantial. Continuous engagement and steadfast commitment from all stakeholders are imperative for sustaining momentum and realizing long-term objectives. This notion of sustainability encompasses not only ecological aims but also the advancement and well-being of humanity. Effective collaboration necessitates equity, integration of policies, and partnerships with industry players across various strata, including large corporations and local communities, as well as an array of expertise and resources. While collaboration presents considerable advantages, it also introduces certain challenges, including coordinating diverse stakeholders, managing conflicts, and securing enduring commitments. Collaborative initiatives remain one of the most efficacious approaches to addressing the intertwined challenges of sustainability (In contexts of emerging economies, where culture, production and technological development are involved, collaborative practices strengthen sustainability [8].

Given these challenges and the nature of the training activity, the student is placed in an environment tailored to their interests, needs, and motivations. Figure 3 shows the developmental spaces.

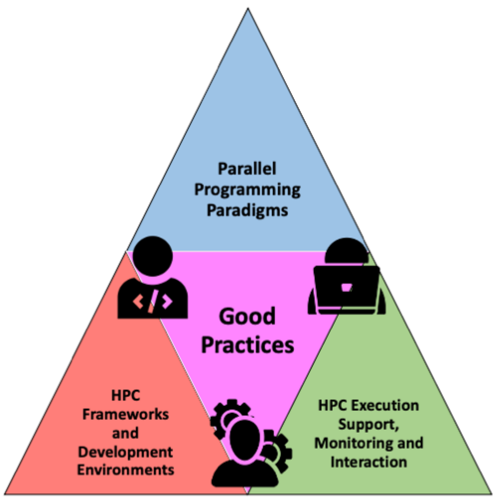

Figure 3: Skills Development Spaces. The three main actors are represented by icons clockwise from the top left: HPCRSE, HPCUSE, and HPCTOE.

The designated spaces are systematically structured around specific competencies, as shown in Figure 3, incorporating a shared lexicon and methodologies that foster enhanced communication and collaboration among all participants, irrespective of their experience levels, while cultivating trust in the instructors. Depending on the activities undertaken, various technical proficiencies and teamwork capabilities can be advanced within this ecosystem, whether through formal educational courses or specialized university programs. For individuals engaged in scientific disciplines or students from fields beyond computer science, we recommend courses concentrating on parallel programming paradigms and tools for task execution. For software developers, the curriculum underscores the utilization of frameworks, development environments, debugging techniques, and profiling methodologies. In DevOps, the courses provide an in-depth exploration of system architecture, support for high-performance computing execution, monitoring practices, and collaborative interactions.

5 CONCLUSION

Integrating a diverse range of participants within High-Performance Computing (HPC) ecosystems is crucial, fostering the synthesis of varied motivations through the principles of transdisciplinarity, interdisciplinarity, and collaboration. This integration is vital for effectively addressing complex challenges. HPC initiatives have the potential to enhance problem-solving capabilities, optimize resource utilization, and stimulate innovation by encouraging collaboration among a diverse group of stakeholders. Similarly, HPC—and generally any computational or technological training—requires establishing positions around sustainability and its impact on individuals and society. However, to realize the full potential of such collaborative efforts, it is essential to overcome cultural, institutional, and coordination challenges. A more cohesive and impactful HPC ecosystem can be created by underscoring the importance of collaboration and shared objectives.

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