

Development of Undergraduate High-Performance Computing Capacity with the CIMUSE Consortium

Short Title: CIMUSE Consortium

A consortium to support HPC at undergraduate institutions in Missouri

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The Computational Infusion for Missouri Undergraduate Science and Engineering (CIMUSE) consortium has been formed for integrating high-performance computing into the undergraduate curriculum at primarily undergraduate institutions (PUIs). This consortium is between Missouri Western State University, Southeast Missouri State University, Truman State University, and Webster University. The consortium has received an NSF CC* Regional Grant to purchase an HPC system to be hosted by the University of Missouri – Columbia. The plans, activities, and challenges of the consortium will be described.

CCS CONCEPTS Applied computing~Physical Science and Engineering, Applied computing~Education

Additional Keywords and Phrases: High-performance computing, Undergraduate research, Undergraduate education, Consortium

1 Introduction

With 40% of STEM bachelor's degrees coming from Primarily Undergraduate Institutions (PUIs), ensuring seamless access to essential tools for future success is critical. The surge in computational power also underscores the importance of integrating computational modeling and simulation into STEM education. During the last decade, the advancement in computational power has integrated computational modeling and simulations into nearly every aspect of scientific exploration. However, the existing university-level STEM curriculum often relegates computational modeling to a secondary role. While experimental measurement remains integral to scientific inquiry, we advocate for a more pronounced emphasis on the ever-evolving capacity to model the natural world in undergraduate STEM education. Furthermore, as graduates transition to graduate school, they will encounter an academic landscape increasingly reliant on computational work. A survey of the academic literature from SciFinder Scholar, a premier database of STEM-related publications, revealed that papers

matching the keywords “modeling” or “simulation” increased by 870% from 1990 to 2020 ([Figure 1](#)). It is increasingly clear that for students to remain competitive, they will need both a solid foundation in laboratory skills as well as simulation techniques.

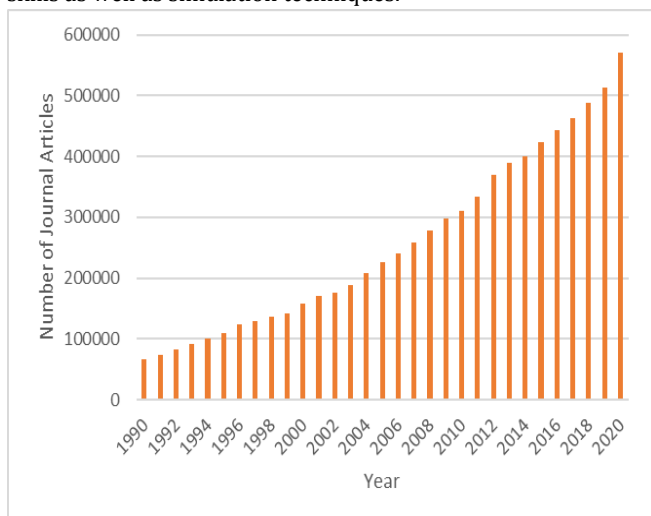


Figure 1. Bar graph of the number of SciFinder Scholar citations that match a search query for "simulation" or "modeling", from 1990 to 2020.

2 The CIMUSE Consortium

Four PUIs – Missouri Western State University (MWSU), Southeast Missouri State University (SEMO), Truman State University, and Webster University – are the leading cohort of a statewide consortium, the Computational Infusion for Missouri Undergraduate Science and Education (CIMUSE). Members of the consortium have pledged to make computational simulations a greater focus of undergraduate research and education at the consortium institutions.

The goals of this consortium are:

1. Undergraduate Research: To involve undergraduate students in novel, cutting-edge STEM research using HPC.
2. Undergraduate Education: To teach undergraduate students techniques associated with modern HPC simulations as a normal part of the undergraduate curriculum.
3. Outreach: To publicize the activities of the consortium and to expand the reach of HPC to more Missouri PUIs.
4. Professional Development: To facilitate professional development in areas of computational science for STEM faculty and students at Missouri PUIs.

3 Historical Development

In the summer and fall of 2021, Dr. Jeff Woodford, Dr. Marcus Bond, and Mr. Chip Byers collaborated to establish CIMUSE with the aim of expanding HPC access to PUIs across Missouri. With support from a Campus Cyberinfrastructure (CC*) Planning Grant [NSF 22-01505], they organized a workshop for the Summer of 2022, hosted at MOREnet in Columbia, Missouri. STEM faculty from over 40 PUI institutions were invited. The workshop covered HPC fundamentals, introduced the CIMUSE consortium concept, and featured speakers who engaged undergraduates in HPC research or teaching. Participants were invited to join a grant-writing endeavor, resulting

in a CC* Area 5 Regional Proposal submitted in February 2023. The proposal, in collaboration with the University of Missouri-Columbia, aimed to acquire and maintain an HPC system. The proposal was funded in August 2023 [NSF 23-22084], with a start date of December 1, 2023. A follow-up workshop was convened in August 2023.

4 The CC* Regional Grant

As mentioned above, the CIMUSE consortium was awarded a CC* Area 5 Regional Grant. In this grant proposal, we outlined several projects we would undertake to further the goals of the consortium, presented in [Table 1](#).

Table 1. Goals and Associated Projects for the CIMUSE Consortium

| Goal(s) | Projects |
|---------------------------------------|---|
| Undergraduate Research | <ul style="list-style-type: none"> • Dr. Colin DeGraf (Truman, Physics) will pursue simulations pertaining to the collisions of black holes. • Dr. Jeff Woodford (MWSU, Chemistry) will pursue simulations on the Pseudo-Jahn-Teller Effect on saturated cyclic organic molecules. • Dr. Marcus Bond (SEMO, Chemistry) will pursue simulations on novel inorganic perovskite materials with innovative magnetic and thermochromic properties. • Dr. Baoqiang Yan (MWSU, Computer Science) will pursue rapid analysis of large security log files for intrusion detection. |
| Undergraduate Education | <ul style="list-style-type: none"> • Dr. Xiaoyuan Suo (Webster, Computer Science) will pursue the creation of a Virtual Data Science Lab for use in the classroom to teach concepts pertaining to data science and analytics. • Dr. Colin DeGraf (Truman, Physics) will pursue the implementation of galaxy simulations in advanced upper-division astronomy classes. • Dr. Baoqiang Yan (MWSU, Computer Science) will pursue the development of a cybersecurity curriculum utilizing the CyberRange platform |
| Outreach and Professional Development | <ul style="list-style-type: none"> • Dr. Jeff Woodford and Mr. Chip Byers will work to publicize the events of the consortium and to expand the consortium's activities to more faculty at each campus and to other PUIs. • Faculty at each consortium institution will identify outstanding undergraduate students to receive a scholarship to attend the Introductory Workshop from the Linux Cluster Institute (LCI). |

To implement these goals, the consortium will purchase twenty Dell PowerEdge C6525 Servers. Each server contains the following equipment:

- 2xAMD EPYC 7713 ("Milan" Processors (64C/128T))
- Direct Liquid Cooling Loop
- Broadcom Dual Port 10GbE BASE-T Adapter
- iDRAC9 Enterprise Controller
- 16x32GB RDIMMs (512GB), 3200MT/s
- 1.6TB Enterprise NVMe

Each node will be connected via Mellanox ConnectX-6 VPI with NVIDIA Passive Copper Splitter Cables for Infiniband.

A key barrier to implementing HPC at PUIs is that, in general, PUIs tend to be poorly resourced [1], and hence tend to be unable to justify financially the cost associated with maintaining specialized computational hardware such as an HPC system. Therefore, our consortium decided to form a partnership with Research Support Solutions at the University of Missouri-Columbia, which houses and maintains the Hellbender HPC cluster[2] for the university community. MU has agreed to house and maintain the CIMUSE HPC cluster; in exchange, the consortium pays a maintenance fee, as well as permitting the MU community access to the CIMUSE HPC cluster while CIMUSE users retain priority access. Furthermore, the hardware that is to be purchased for the CIMUSE HPC cluster is virtually identical to the existing Hellbender cluster at MU, reducing the maintenance burden on MU staff. We believe such partnership arrangements between PUIs and R1 institutions can be a viable means to expand access to HPC to all segments of higher education.

5 Project Timeline

The project timeline is composed of the implementation of four milestones.

- Milestone 1: Assemble and configure an HPC cluster for PUI use. Implementation of this milestone is currently in progress.
- Milestone 2: Manage the cluster for effective utilization. Our team holds weekly virtual meetings for discussion on how to manage the cluster. We held one formal meeting in February and will hold another formal in-person meeting in August, to coincide with the workshop, in Columbia, MO.
- Milestone 3: Provide applied learning opportunities for high-performance computing to undergraduates. To implement these milestones, we shall award LCI scholarships to outstanding undergraduate students.
- Milestone 4: Disseminate results and expand the consortium. We are planning to consult with interested faculty at our own institutions as well as at other prospective institutions in the state, as well as to publicize our work to demonstrate how HPC may be utilized for undergraduates.

6 Summary

Our presentation provides an overview of the project's vision, highlights both its successes and challenges during implementation, and extends an invitation for collaboration to interested parties. Moving forward, we encourage open dialogue and welcome constructive feedback to optimize our approach and effectively achieve our objectives.

Acknowledgments

We acknowledge the support of a National Science Foundation CC* Planning Grant [NSF 22-01505] and a National Science Foundation CC* Regional Grant [NSF 23-22084].-

¹ Final Report: Study on Higher Education Performance Funding and Efficiency/Reform. National Center for Higher Education Management Systems (NCHEMS), July 3, 2023, p. 20. Retrieved June 18, 2024 from <https://dhewd.mo.gov/about/legislative/documents/MissouriSecondReport.pdf>

² Computing Resources. University of Missouri Division of Information Technology. Retrieved June 18, 2024 from <https://doit.missouri.edu/services/research/computing-resources/>.