Integration of High Performance Computing into Engineering Physics Education

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Professor Lemley teaches thermo-fluid engineering and works with undergraduates to perform fluid dynamics research that is mostly focused on small scale flow problems. He is currently an Assistant Dean of Mathematics and Science and a Professor of Engineering and Physics at the University of Central Oklahoma, his home institution for more than fifteen years. Previously, Professor Lemley worked as a mechanical engineer in the power industry. His bachelor’s degree is in physics from Hendrix College and his M.S.M.E. and Ph.D. were earned at the University of Arkansas.

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Adam Dorety is currently a senior at the University of Central Oklahoma (UCO). He is involved in Fluid dynamics research observing entropy loss through tee junctions for low viscosity and reynolds numbers fluids. He is also a past UCO chapter of the American Society of Mechanical Engineers chair, vice-chair and treasurer. He began his research on the Underwater Remote Operated Vehicle (ROV) as well as an Unmanned Aerial Vehicle (UAV). He hopes to graduate in 2016 and join the workforce. His experience with undergraduate research has undoubtedly strengthened his commitment to mechanical engineering.

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Abstract
Computational skills are foundational in engineering physics education. Computational exercises, labs, and projects often employ instructive small-scale problems. These small-scale problems serve to introduce content and process, and as such, serve the purpose for which they were intended. Small-scale problems do not serve to introduce students to solving problems at industrial-scale or with research-quality as required in the workplace or graduate laboratory. This paper describes the integration of industrial-scale and research-quality high-performance computing (HPC) into a senior/graduate level fluid dynamics course.

This paper focuses on a combined senior level-graduate level course (enrollment of 12) in fluid dynamics at the University of Central Oklahoma, a predominantly undergraduate institution (PUI). A HPC cluster, Buddy has been deployed recently at the UCO. The first author operates and administers the Buddy cluster and serves as instructor of the fluid dynamics course, providing an opportunity to advance the course outcomes to include a high impact project that takes advantage of distributed computing. These projects will be transformative for the students and expose them to HPC “at scale.” The projects require the use of computational fluid dynamics (CFD) on an HPC system; intentionally exposing students to a new way of doing things. The issues that students must confront include: 1) complex geometric modeling that result in very large file sizes, 2) meshing geometries that are large or require many nodes, 3) transitioning files generated on a desktop computer to a HPC environment, 4) understanding navigation and use of an HPC system, 5) understanding the use of parallelism in a distributed computing environment, 6) quantifying results, and 7) visualizing results.

The goal of this work is to impact the student’s long term ability to deal with computationally intensive problems. Although we cannot determine the impact long term yet, we are using a rubric to gauge the immediate impact and surveying the students to determine their perceptions.

Introduction
The National Science Foundation (NSF) report entitled “Cyberinfrastructure Vision for 21st Century Discovery”1 addresses how high performance computing (HPC) is necessary to science and engineering disciplines to answer the most basic research questions and to solve technical problems of national need. More recently the White House has undertaken the National Strategic Computing Initiative2 which is a call to “maximize the benefits of high performance computing (HPC) research, development, and deployment.” The increased use
of HPC clearly results in the need to train engineers how to appropriately use HPC in their work as HPC becomes more ubiquitous in industry.

The use of computational tools in engineering education is so common it is essentially codified by ABET; currently as part of Criterion 3. Student Outcomes\(^3\). Accordingly, students across undergraduate engineering programs get exposed to computer programming, modeling software, mathematical engines, spreadsheets, and simulation. Specific engineering disciplines are exposed to more focused software for computer-aided design, circuit design, machining, data acquisition; and more and more students are using microcontrollers to implement their own electro-mechanical systems. These software, and where appropriate, the attached hardware, are almost exclusively run on or controlled by either desktop or laptop computers. As a result of the availability and accessibility of HPC resources some have been able to enhance traditional engineering and computing curricula using HPC\(^4-6\).

**Background**
This paper documents activities of integrating HPC at the University of ___ (U__), which is a metropolitan university with an enrollment of over 17,000 students and a predominantly undergraduate institution (PUI). At UCO, undergraduate research has been supported and nurtured across campus; and recognized by the Council on Undergraduate Research (CUR) as a national model for implementing programs in undergraduate research\(^7\). Campuswide grant programs for faculty grants and student grants are in place. The student grants program is of particular note; in Research, Creative, and Scholarly Activities (RCSA) Grants encourage students to collaborate with a faculty member to write a grant proposal. If funded the student receives up to $500 for supplies and equipment, works five hours per week as a research assistant, and receives a partial tuition waiver. This program has grown considerably in the last several years and now funds over 130 students each year. Within the College of Mathematics and Science (CMS) additional programs are in place to cultivate undergraduate research. Center for Undergraduate Research and Education in Science, Technology, Engineering, and Mathematics (CURE-STEM) Scholars (approx. one-third of CMS faculty) receive funding for reassignment time, travel, student research assistants, and supplies. The CURE-STEM Scholars are required to submit one national-level (e.g. National Science Foundation - NSF) grant per year. This program has been in place for eight years and has shown a tremendous return on investment of over $10 brought in for every $1 invested.

Co-author Lemley has been a CURE-STEM Scholar and also serves as the director of a computational center within CMS called CREIC (Center for Research and Education in Interdisciplinary Computation), whose goal is to stimulate and enable faculty and their students to embed computation into their research and classes. CREIC has been focused on establishing a HPC resource on campus for several years, and was successful in obtaining an NSF Major Research Instrumentation (MRI) grant, with co-author Lemley as the Principal Investigator (PI), in early 2015. The NSF-MRI has funded the first HPC cluster
supercomputer (Buddy) on campus and now co-author Lemley is helping researchers at UCO use Buddy to perform their work.

This study described in this paper was conducted, in part, during a 3-semester hour fluid dynamics course, ENGR 4533/5443, in Fall 2015 at UCO. This course is a follow-on course to a junior level engineering fluid mechanics course and was made up of six undergraduates and five graduates. This course covers continuum viscous fluid dynamics; the first portion of the course is focused on understanding and applying the Navier-Stokes equations (NSE), which are a set of partial differential equations describing fluid flow. The latter part of the course is focused on using computational fluid dynamics (CFD) to solve the NSE. Individual CFD projects were completed by the students. In these projects, students were required to develop a problem that needed significant computational resources - such that it was not reasonable to run the simulations on a single computer workstation.

The goals for implementing the CFD project in this way was to make an impact on the student’s long term ability to use HPC when they graduate, which is becoming a necessary engineering technical skill.

**Methodology**

The CFD projects in ENGR 4533/5443 were started in late September 2015. The students were asked to develop a problem that was either of research interest or industrial-scale, meaning, not only would CFD be required, but HPC using the Buddy supercomputer cluster would also be required. The project was carried out as shown in Table 1.

**Table 1.** Details of CFD Project in ENGR 4533/5443.

<table>
<thead>
<tr>
<th>Assignment</th>
<th>Description</th>
<th>When</th>
<th>Credit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Project Proposal</td>
<td>Up to two page proposal with citations.</td>
<td>Late September</td>
<td>10% Homework / 2.5% Course</td>
</tr>
<tr>
<td>Project Description</td>
<td>Five Minute Proposal to Class</td>
<td>Early October</td>
<td>10% Homework / 2.5% Course</td>
</tr>
<tr>
<td>Computer-Aided Design Model</td>
<td>Email to Instructor</td>
<td>Mid-October</td>
<td>10% Homework / 2.5% Course</td>
</tr>
<tr>
<td>Meshed Geometry</td>
<td>Email to instructor</td>
<td>Late October</td>
<td>10% Homework / 2.5% Course</td>
</tr>
<tr>
<td>Project Poster Session</td>
<td>Large Format Poster - Interviews by faculty on oral presentation and appearance (rubric).</td>
<td>Early December</td>
<td>50% Project / 12.5% Course</td>
</tr>
</tbody>
</table>
The Project Proposal was a two-page proposal with citations that described the problem on which the student wanted to work. The requirements were the motivation for working on a given problem, the geometry that would be considered, and as much detail about boundary conditions as possible. This proposal was emailed to the instructor, who then either spoke with the student in class or emailed them about tweaking their proposal so that it was appropriate for the class and truly needed a cluster supercomputer for solution.

The Project Description took place roughly two weeks after the Project Proposal and involved a five-minute presentation in a regular class meeting. By this point the students were expected to have a sketch or initial computer-aided design (CAD) of the geometry and detailed boundary conditions. There was a small amount of time for questions by the audience.

Over the next several weeks the instructor spent several class periods covering the topics in Table 2, with the goal of taking student through a complete project starting with a CAD drawing all the way to visualizing and calculating results. The goal was to ensure that students had seen the many issues that arise in what is often a tedious process. In addition, by having some sessions where the students worked on their projects using the Buddy Cluster, the instructor could see from the student perspective and see what did and did not work well for them. Also he could observe how well the documentation for the project and using Buddy had been written.

### Table 2. Learning Modules in the CFD Project.

<table>
<thead>
<tr>
<th>Learning Module</th>
<th>Approximate Time Used in Class</th>
</tr>
</thead>
<tbody>
<tr>
<td>Importing CAD files into Meshing Software</td>
<td>10 minutes</td>
</tr>
<tr>
<td>Meshing a Geometry and Preparation for CFD</td>
<td>30 minutes</td>
</tr>
<tr>
<td>Logging into a remote Linux system with Secure Shell</td>
<td>10 minutes</td>
</tr>
<tr>
<td>Basics of Linux Command Line Navigation and File Editing</td>
<td>30 minutes</td>
</tr>
<tr>
<td>Moving Files to/from a Remote System</td>
<td>10 minutes</td>
</tr>
<tr>
<td>Using the Web Portal for the Buddy Cluster</td>
<td>15 minutes</td>
</tr>
</tbody>
</table>
In total over 350 minutes of class-time were devoted to the project. That means almost one-third of time in class was devoted in some way to this project. As the sessions described in Table 2 were ongoing, students worked on their projects with the instructor asking them for frequent updates. About 2.5 weeks before the end of the semester the students worked in class on their projects. Finally students designed and printed large format posters describing their project results.

A Project Poster Session was held in early December in which three faculty with fluid dynamics backgrounds from the UCO Engineering and Physics Department (excluding the instructor) were invited to judge posters. Also, students judged each other’s posters. This was a formal session and judges used the a poster evaluation rubric\(^8\) to evaluate the posters. Note this rubric is focused on the appearance, format, and to a lesser degree the content.

After the poster session the instructor evaluated the posters for their technical content and quality of the work using another poster evaluation rubric\(^9\).

**Results**
The first four assignments were treated as homework assignments and their results are grouped here in Figure 1.
Figure One. Performance of graduate and undergraduates on homework-equivalent assignments for the CFD HPC Project.

Graduate students performed better overall than undergraduates earning an average over the four assignments of 90% while undergraduates averaged 78%. Of particular note is that only half of the undergraduates submitted a mesh for approval. This does not mean that the instructor did not see the meshed geometry prior to the end of the project, but it was not submitted correctly. There was some confusion about this by the students and future projects will try to make more clear what to send and when.

From the instructor’s perspective the Poster Presentation Session was as important as any one piece of the project as it required students to work on written, graphical, and oral communication skills. These were formal presentations where students were expected to dress and behave professionally at this session. The instructor also provided food for this session and invited a wide range of faculty to attend. It was held in a large open Atrium where students study, and students not in the class wandered up to have a look at posters as well. Three faculty members that have a background in fluid dynamics served as expert poster judges and other students in the class served as additional judges. The students and faculty judges were weighted equally. The results are shown in Figure 2 for each category of the rubric. Note the vertical axis starts at 84% on this chart.
The averages for graduates and undergraduates were slightly different, 95.6% for graduates and 92.6% for undergraduates. Comparing graduates to undergraduates, it appears that the graduates were better in the areas of Research Objectives, Research Methods, and Results. This trend did jibe with comments made by the faculty judges. Nearly all judges rated the text sizes on the poster to be adequate. Despite attempts to ensure text size was not an issue on the larger posters, students had been counseled on this by the instructor. It appears that recommended minimum text sizes will need to given in the future.

Given the rather high starting value of the vertical axis, overall performance was strong on this part of the project. The areas of improvement are really in the description of the project, methodology and results. In particular, the instructor was clear that there should be quantifiable results (not just pictures of velocity vectors, streamlines, and pressure fields) that related directly to project goals. Graduate students seemed to achieve this objective, but undergraduates struggled to fulfill this requirement. More instruction on how to move from purely graphical results to quantitative results needs to be done.

The instructor performed rubric scoring more focused on poster content, methods, and results: The Project Poster Technical Review. The results are shown in Figure 3.
Figure Three. Average performance by undergraduates by rubric category for the Project Poster Technical Review.

It should be noted that the instructor’s ratings of undergraduates and graduates were different in terms of the standards for graduate students. Those earning graduate credit for the course were held to a higher standard in most aspects of the class. Probably the most surprising category in Figure 3 is the Methods category, which resulted in a perfect score for both graduates and undergraduates. Both undergraduates and graduates did a very good job describing their methodology. The specific expectations for Methods had been laid out for the students in class and they took note and responded on their posters. The Results category was second lowest with undergraduates actually under 60%. Finally Conclusions had the lowest overall average at 68%. This may be attributable to not enough instruction time spent on this issue. Most students re-stated their results as conclusions and did not attempt to synthesize the overall results and connect back to their original objectives.

A survey has also been created to determine student perceptions of the project. It should highlight the initial impact of this type of HPC project. Ideally, a longer term survey of these students could be carried out to actually determine the long term impact of HPC projects in the workplace. As soon as written consent is received from all students, the survey will be conducted and this paper updated. It is anticipated that survey results will be presented at the 2016 ASEE Annual Conference and Exposition.

Conclusions
Although the sample size was low in this project some conclusions can be made regarding the effectiveness of embedding an HPC project into a traditional engineering course:

1. **Overall the graduate students outperformed the undergraduates**, even when accounting for the instructor holding the graduate students to higher standards on the Project Poster Technical Review. Speculatively, this is probably attributable to multiple factors such as more academic experience and interest in solving open-ended problems.

2. **More training is needed to ensure both undergraduates and graduates can produce and interpret quantitative results.** Despite discussing the need to get quantitative results not just visual results, there was generally a lack of quantitative results. It appears that detailed demonstrations of calculating quantities on surfaces and volumes are required.

3. **The students were all exposed to HPC and were able to navigate accessing and using a remote HPC system.** However, it was not their first choice. From observations in this course and of other students by co-author Lemley, the first tendency of students is to try to do modeling and simulations using a local machine. Using the local machine with a familiar operating system and software is preferred by the students. Only when students see the requirement to use a more robust HPC system such as the Buddy Cluster, are they convinced to move their work away from desktop computing.

4. **There will be some impact long term in the student’s ability to deal with computational modeling problems using HPC.** The survey will hopefully reveal the student’s current interest and perception about what the long term (3-5 years) impact will be, but the only way to know if the project will have a lasting impact on the student’s ability to understand and use HPC appropriately in the workplace, can only be measured via a long term study. It is possible that the consent to report on this longer term data collection will be sought.

The future plans for this project and new projects include:

1. Obtaining and disseminating data from a survey of the students mentioned in this paper.
2. Determining current workforce needs in HPC. The UCO is closely connected to many stakeholders in the metropolitan Oklahoma City area. A survey that details their HPC needs and future plans will be developed and administered.
3. We will design a comprehensive study to address measuring the impacts of the project described here and additional projects three-five years after graduation.

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References


