Training the next generation of computational scientists through a new undergraduate course

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\textbf{ABSTRACT}

We introduce a newly designed undergraduate-level interdisciplinary course in scientific computing that aims to prepare students as the next generation of research-oriented computational scientists and engineers. The course offers students opportunities to explore a diverse set of projects and develop the necessary programming skills to implement ideas and algorithms within high performance computing environments. The training includes how to think about, formulate, organize, and implement programs in scientific computing. The emphasis of the course is on problem solving within a wide range of applications in science and engineering.

\textbf{KEYWORDS}
Computational science and engineering; programming; problem solving; mathematics education; evaluation

1. Introduction

Computational Science and Engineering (CSE) is a rapidly growing field. Theory and experiments are supported by computational work to understand the behavior of complex systems arising in science and engineering applications. The set of knowledge and skills needed in CSE lies at the intersection of mathematics, computer science and natural sciences and engineering. Many scientific and engineering problems are described by mathematical models, the models are analyzed and solved using numerical algorithms, which in turn are implemented using programming languages. The development of efficient, accurate and robust software for the numerical simulation of complex systems is the key point in CSE research. The current trends on CSE is are captured through the following indicators:

- The U.S. Department of Energy (DOE) Advanced Scientific Computing Research (ASCR) ([https://science.energy.gov/ascr](https://science.energy.gov/ascr)) program states the importance of CSE: “It is generally accepted that computer modeling and simulation offer substantial opportunities for scientific breakthroughs that cannot otherwise—using laboratory experiments, observations, or traditional theoretical investigations—be
realized. At many of the research frontiers, computational approaches are essential to continued progress and play an integral and essential role in much of twenty-first century science and engineering."

- Officers of the Society for Industrial and Applied Mathematics (SIAM) Activity Group on Computational Science and Engineering (Rüde et al., 2018) examine the role of CSE in the 21st-century and discuss the challenges and opportunities in CSE research including mathematical methods and algorithms, high performance computing, and data science.

- The ASCR Scientific Discovery through Advanced Computing (SciDAC) program brings computational scientists, applied mathematicians, and computer scientists together with the mission to develop the scientific computing software and hardware infrastructure needed to advance scientific discovery using supercomputers. Two SciDAC institutes, (i) FASTMath – Frameworks, Algorithms, and Scalable Technologies for Mathematics and (ii) RAPIDS – SciDAC Institute for Computer Science and Data, are designed to develop scientific advances in petascale computing. The ASCR Applied Mathematics program supports research on numerical methods, optimization, multiphysics-multiscale computation and math software development for the numerical studies in computational fluid dynamics, climate modeling, nuclear reactor design, subsurface flow modeling, and many other applications.

While advanced computational efforts are growing rapidly, it is important to adapt student education to keep up with the requirements of a career in academia and industry. Therefore, there have been many undergraduate student opportunities provided at universities and national laboratories/facilities supported by National Science Foundation (NSF) Research Experience for Undergraduates (REU) programs and U.S. Department of Energy’s Science Undergraduate Laboratory Internships (SULI). Moreover professional organizations such as the American Mathematical Society (AMS), the Association for Women in Mathematics (AWM), and Society for Industrial and Applied Mathematics (SIAM) provide support for undergraduate students’ developments. The SIAM working group on CSE undergraduate education stresses the importance of CSE, the need of training in CSE fundamentals at undergraduate level and the skills needed for the training of students.

We believe that scientific computing should be an essential part of students’ education if they are to be active participants in the development of future technology. Specifically, it is important for students to be able to develop an understanding of the methods, algorithms, and computing skills that are necessary for scientific computing during their undergraduate studies. Therefore, we proposed a new course, MATH 4343 “Introduction to Scientific Computing” in the Department of Mathematical Sciences at the University of Arkansas which was taught in Spring 2021 for the first time. The learning objectives of the MATH 4343 are divided into three parts:

(i) understanding the problem with its mathematical model;
(ii) learning the algorithms needed for solving the mathematical models; and
(iii) the implementation of algorithms in the Linux environment.

MATH 4343 provides students with a theoretical and practical background sought after in the industry by introducing a diverse set of real world problems in science and engineering such as the Nelder-Mead downhill simplex, the heat equation, the
porous medium equation, and the Finite Elements Method (Rostamian 2014a). The emphasis of MATH 4343 is on problem solving, and offers multiple projects based on the students’ backgrounds. This course was originally designed for the students of Applied Mathematics in the Department of Mathematical Sciences to help them quickly acquire mathematical and programming skills to solve a diverse set of problems from a variety of engineering areas. Meanwhile, it has gained popularity among other science and engineering students at the University of Arkansas.

MATH 4343’s main goal is to motivate and prepare undergraduate students for their role as future computational scientists and engineers. The course is designed to support programs with computational concentration, which recommend or require certain level of programming expertise to students. To take advantage of the current computational resources provided at the university, the students become familiar with C programming language in the Linux environment and auxiliary software packages and libraries needed for visualizing. The prerequisite for this course is only linear algebra which is the highest level mathematics course taken by most of the natural sciences and engineering students; however no previous programming experience in C is required. The time required to teach C programming from basics to a moderately advanced level is built into the course design, and meshes well with the additional activities through lecture series on programming (see section 2.3).

In section 2 we describe the course’s details, including the content (section 2.1) and performance assessments (section 2.2) which are designed based on the enrolled students’ needs and backgrounds. In section 2.3 we present a list of activities designed to achieve the course’s main goal and address the importance of additional learning activities in the form of seminars and workshops to train and prepare students for their future careers. In section 3 we present the opportunities specifically presented to students who complete the course and wish to conduct research. Student evaluation of the course and instructor are presented in section 4. Finally, we present the concluding remarks and future plans in section 5.

2. Course Details

In this section, we present the three primary components of the course, which consist of i) the learning objectives, ii) assessments, and iii) instructional strategies. The learning objectives component is designed with the purpose of guiding the student on how to interpret and analyze a diverse set of problems derived from science and engineering, and then devise and implement algorithms to produce quantitative information about them. The skills learned here provide a foundation upon which other courses within the scientific computing domain can build.

We examine the relative efficiency of various algorithms applied to a given problem, such as explicit, implicit, hybrid finite difference schemes (Isaacson and Keller 1994) for solving initial/boundary problems associated with the classical heat equation. The understanding gained here paves the way to handling more complex problems such as the porous medium equation (Vázquez 2007) which arises in the study of diffusion of gasses, and also in population dynamics (Gurtin and MacCamy 1977).

In our experience, a solid knowledge of undergraduate multivariable calculus and linear algebra provides sufficient mathematical background for this course. We have had success with setting MATH 3093 (Abstract Linear Algebra) for mathematics students, or MATH 3083 (Linear Algebra) for engineering students as the prerequisite for this course.
Most of the undergraduate students who enroll in this course have had prior exposure to elements of programming through Python and/or MATLAB, or perhaps lower level procedural languages such as C and Java. Students who lack experience with C or a C-like procedural programming language, can still succeed through self-study and some extra help from the instructor and their classmates.

On the first day of the class we administer a survey to learn about the students’ backgrounds. The survey questions are based on two of the Mathematics Attitudes and Perceptions Survey (MAPS) (Code et al., 2016) categories: interest and expertise. The feedback from the survey helps the instructor to design the project-based course content including a two-week crash course on the C programming language, and the programming environment on the university’s high performance computing system, Pinnacle. It’s safe to say that upon completion of this course, the students will have been exposed to about 90% of the C programming language features.

There were ten students enrolled in Spring 2021 when MATH 4343 was offered for the first time. Twenty-five percent of the students who enroll in this course are juniors who have earned between 60 and 90 credit hours. The rest are seniors who have earned 90 or more credit hours. Figure 1 displays these ten students’ major areas of study. On the first day of class, a survey was given to learn more about the students’ interests and learning preferences. See a summary of survey responses for each question in Table 1.

2.1. Course content

The course content and its pace are adjusted to what typical undergraduate students can handle. In the following subsections we list the typical course content.

\[^{1}\text{C is a particularly compact programming language and the bulk of it may be learned rather quickly.}\]
Table 1. Student interests and learning survey summary

| Questions                                      | Answers         | Responses (%) |
|------------------------------------------------|-----------------|---------------|
| When I am learning something new, I prefer to | have someone show me | 70%           |
|                                                | have someone tell me | 20%           |
|                                                | figure it out myself | 10%           |
| I prefer to work                               | individually with a group | 50%           |
| What is your level of programming?            | beginner        | 30%           |
|                                                | intermediate    | 70%           |
|                                                | advanced        | 0%            |
| How experienced are you in C programming?     | novice          | 50%           |
|                                                | advanced beginner | 40%           |
|                                                | competent        | 10%           |
|                                                | proficient       | 0%            |
|                                                | expert           | 0%            |
| How experienced are you in Linux environment? | novice          | 40%           |
|                                                | advanced beginner | 40%           |
|                                                | competent        | 0%            |
|                                                | proficient       | 0%            |
|                                                | expert           | 0%            |
| How many programming based courses have you taken? | 1                | 20%           |
|                                                | 2               | 40%           |
|                                                | 3               | 10%           |
|                                                | 4               | 20%           |
|                                                | 5+more          | 10%           |
| Have you been involved in undergraduate research? | yes             | 30%           |
|                                                | no              | 70%           |
| If not, are you interested in acquiring research experience? | yes             | 0%            |
|                                                | no              | 100%          |

2.1.1. A two-week crash course on programming and computing environments

The B.S. degree in Natural Sciences with Computational Concentration programs requires core courses that include Calculus I–II, Elementary Differential Equations, Linear Algebra, as well as computer science courses such as Programming Foundations I–II and Programming Paradigms.

Some other engineering and science programs recommend, but do not require, courses in programming as degree requirements. To reach as wide an audience as possible, and to establish a common background for all enrolled students in MATH 4343 course, we begin with the basics concepts of C programming (data representation, conditional and iterative statements, functions, arrays, strings), and then continue with more advanced topics of C (pointers, structures, dynamic allocations, recursion, linked lists, binary trees, unions and function pointers). The bare minimum of the C programming language introduced this way is mostly adequate for the average student. To the more ambitious students, who desire further reading and a comprehensive reference, we recommend the book by Kochan (Kochan, 2014) which integrates well with this course’s objectives.

We introduce the Arkansas High Performance Computing Center (AHPCC) computing environment which is used throughout this course. AHPCC provides high performance computing hardware, storage, support services, and training to enable computationally-intensive and data-intensive research. The AHPCC is available to faculty, staff and students at all of the Arkansas public universities, and supports educational allocations which are used in teaching this course. The undergraduate students first get familiar with the Linux system and the command-line based terminal. This was a new experience for all but one of the students who had used the system previously in another research project.

A benefit of using the AHPCC is the creation of a uniform computing environment for all students, as they don’t need to download and install compilers and third-party tools.
software packages in order to work on their programming projects. The students can
easily switch between different compilers such as the GNU and Intel C compilers and
experiment with different software tools for debugging, performance analysis, etc. In
addition, third-party software packages such as Geomview, Triangle, and Umfpack are
readily available for their use.

After the two-week crash course on programming and computing environments, we
closely follow the textbook “Programming Projects in C for Students of Engineering,
Science and Mathematics” (Rostamian, 2014a) throughout the semester. This book is
designed for early graduate students and advanced undergraduate students. The text-
book consists of two parts. The six chapters of Part I (A Common Background) are
prerequisites for Part II (Projects) which we now describe.

2.1.2. Projects

The identification and formulation of engineering problems via mathematical modeling,
the solution of problems using numerical methods, and the design of computer programs,
are the fundamental blocks of training for students who plan to pursue a career as
computational scientists and engineers. We therefore begin with identifying a list of
projects that are relevant to the students’ backgrounds.

The projects presented in the textbook are interesting, intriguing, inviting, challenging,
and illuminating on their own, apart from their programming aspects. Some of the
favorite projects in the textbook are:

(1) The Nelder–Mead simplex algorithm (Nelder and Mead, 1965; Press et al., 1992)
for minimizing functions, with application to computing finite deformations of
trusses under large loads via minimizing the energy, as well as training neural
networks;

(2) The Haar wavelet transform, with application to image analysis and image com-
pression (Nievergelt, 2013; Stollnitz et al., 1995, 1996);

(3) The evolution of species and the effect of the environment on the emergence of
genetically distinct species (Barski, 2011; Dewdney, 1989);

(4) Finite difference (FD) algorithms for solving the time-dependent linear heat equa-
tion and extending the algorithms to solve the porous medium equation (Isaacson
and Keller, 1994; Rostamian, 2014a);

(5) Finite element methods (FEM) for solving second order elliptic partial differential
equations on arbitrary two-dimensional domains through unstructured triangular
meshes and linear elements (Gockenbach, 2006; Szabó and Babuška, 2021);

(6) Neural networks (NN) applied to solving ordinary and partial differential equa-
tions (Lagaris et al., 1998; Sirignano and Spiliopoulos, 2018).

In Spring 2021, based on the students’ backgrounds and interests, we selected the
topics 1, 4, and 5 from the above list. In view of the interdependencies of the contents
of the various chapters as seen in Figure 2, we included several prerequisite chapters,
which led to the following complete course syllabus:

Chapter 7: Memory allocation.

Dynamic allocation of memory lies at the core of practically every scientific com-
puting program in C. This chapter sets up a safe “wrapper” around the C Standard
To find the prerequisites of a chapter, find the chapter title along the left edge, go across horizontally to the bullet marks, and then go vertically to the prerequisite chapters. For instance, Chapter 23: Triangulation depends on Chapter 7: Xmalloc, and Chapter 8: array.h. Chapters prior to Chapter 7 are not listed; these provide a general background for the entire book and should be considered prerequisites for everything.
Library’s `malloc()` function to verify the success of the calls to `malloc()` and to take appropriate action in case of failure.

Chapter 8: Vectors and matrices. Almost all of the book’s projects call for allocating and freeing of memory for vectors and matrices of dynamically determined dimensions. This chapter puts the C preprocessor to good use by producing generic macros that perform the arduous task of constructing and freeing vectors and matrices of arbitrary dimensions.

Chapter 18: The Nelder–Mead simplex method. The Nelder–Mead algorithm is a robust method for locating the minima of functions of the type $f : \mathbb{R}^n \to \mathbb{R}$. The great appeal of the Nelder–Mead algorithm lies in the fact that it requires neither the differentiability of $f$, nor a knowledge of its gradient. That should be contrasted against the conjugate gradient algorithm and its variants, which do call for the knowledge of the often mathematically and computationally expensive calculation of the gradient.

Chapter 20: Finite difference methods. This chapter introduces several finite difference algorithms for solving the one dimensional time dependence heat equation $\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$. The methods include the well-known explicit and implicit Euler and the Crank–Nicolson algorithms, as well as the lesser known but very versatile Seidman scheme.

Chapter 11: Sparse matrices. As a first step toward the implementation of the finite element methods of chapters 25 and 26, this chapter introduces the concept of Compressed Column Storage (CCS) form for memory-efficient storage of large sparse matrices. The ideas discussed here form the foundation for understanding and appreciating the details of the next chapter’s Umfpack library.

Chapter 12: The UMFPACK library. The Umfpack is an open source library that incorporates state-of-the-art algorithms for solving algebraic linear systems of equations $Ax = b$, where $A$ is an $n \times n$ matrix and $b$ is an $n$-vector. Umfpack is particularly efficient when solving large sparse linear systems. That is exactly the type of system that arises when solving partial differential equations through the finite element method.

Chapter 23: Triangulation of polygons. Meshing or triangulation is a critical step in solving partial differential equations by a finite element method on polygonal domains. It involves partitioning of the domain into a union of non-overlapping triangles. It can be shown that the finite elements discretization error is the smallest when the triangulation involves no triangles with sharp angles. The award-winning and open-source Triangle library produces quality triangulations that come close to the best that can be achieved within the limitations of the domain’s constraints.

Appendix A: Barycentric coordinates. The geometry of the individual triangles in a domain’s triangulation is best expressed in barycentric coordinates. This appendix provides a quick overview of the barycentric coordinates. The material here is essential for understanding the developments in chapters 24 through 26.

Chapter 24: Integration on triangles. The entries of the matrix $A$ and vector $b$ noted in the earlier paragraph on Umfpack are produced through integration over individual triangles of a triangulated domain. This chapter presents a relatively recent accurate and efficient method for numerical integration on triangles (Taylor et al., 2007a,b).

Chapter 25: Finite elements (part 1). This chapter introduces a basic finite element scheme with linear basis elements for solving the Poisson problem $\frac{\partial^2 u}{\partial x^2} +$
Chapter 22: Gaussian quadrature. This chapter develops tools for integrating functions of a single variable through Gaussian quadrature. The material here can be useful on its own—see [Atkinson 1989; Kincaid and Cheney 2002] for in-depth coverage—but our main objective is directed toward Chapter 26 where we will be solving partial differential equations with prescribed boundary fluxes.

Chapter 26: Finite elements (part 2). This chapter extends Chapter 25’s elementary treatment of finite elements to the elliptic equation

\[ \nabla \cdot (\eta(x,y)\nabla u) + f(x,y) = 0, \]

where \( \nabla \) is the gradient operator and \( \eta(x,y) \) is a prescribed, and generally variable, diffusion coefficient. Arbitrary Dirichlet and Neumann data may be specified on the boundary. The finite elements formulation then calls for the integration of the Neumann data on the domain’s boundary. The integration is performed through Gaussian quadrature introduced in Chapter 22.

Chapter 26 is only briefly introduced at the end of the semester. Students are encouraged to take MATH 4373/5373: Finite Element Methods (FEM) in scientific computing, a new course developed for University of Arkansas students. This course is under continuous development to provide a broad range of support to the students in science and engineering departments. Bangerth (Zarestky and Bangerth 2014) describes a practitioner’s approach to using the principles of reflective writing and journaling to connect the material of the video lectures to student projects in a project-based course on FEM, MATH 676, offered at Texas A&M University.

2.2. Performance Assessments

Performance assessments are based on 60% assignments and 40% final project. Assignments are designed to focus on solving specific problems through the projects listed in section 2.1.2. Each project’s mathematical background and the complex aspects of
the required programming are explained in class. The students are asked to complete
the missing parts of the project. To receive full credit, the resulting programs need to
compile without warnings and errors, and run successfully.

The final projects are designed to utilize visual, verbal, and written presentation
skills—all essential ingredients for practical and successful research. For students who
are involved in research outside of this course, effort is made to pick projects that
utilize algorithms that may be applicable to their research. For others, specific projects
are offered and assigned by the instructor.

The objectives of this course are achieved by completing the final projects. Consid-
ering the students’ backgrounds, the final projects are chosen from a wide range of
applications from variable stars to self-driving cars. The student with a mathematics
major (see Figure 1) chose his final project on the graph isomorphism problem which is
a computational problem in graph theory consisting of understanding and implement-
ing an efficient algorithm to determine whether two graphs are isomorphic. The student
with a double major in Computer Science and Computer Engineering and Mathematics
completed a final project on reinforcement learning for self-driving cars which rely on
sensor inputs to perceive the environment and move safely without human interaction.

The instructor meets the students twice to assign a project related to their interests
and follow-up on progress made before the final presentations. At the beginning of the
semester, each student gives a short presentation to outline his/her research interest.
At the middle of the semester, the student gives a short presentation to show his/her
progress on the project. The students write a two page final project report using the
sample LaTeX template provided by the instructor. This report includes sections on
the problem description, the algorithm to solve the problem, and the implementation
details of the algorithm outlining the results that they have achieved. In addition to
this written report, the students give a 15–20 minute presentations at the end of the
semester.

Each student’s opinion matters, therefore the students are asked to fill out and submit
the peer evaluation and feedback form that includes 10 questions. Students judge and
evaluate the presentations of each peer based on the presenter’s explanation of the topic.
The presentation is rated on a five point scale range from poor = 1, fair = 2, good = 3,
very good = 4, and excellent = 5. The poor-to-excellent rating scale provides a measure
of the student’s performance.

(1) The presenter delivered the material in a clear and structured manner.
(2) The presenter was knowledgeable about the topic.
(3) The presenter maintained my interest during the presentation.
(4) The presenter answered questions effectively.
(5) The presenter was enthusiastic about the topic.
(6) The presenter was well organized and prepared.
(7) The presentation was concise and informative.
(8) The presentation contained practical examples and useful techniques that applied
to current work.
(9) The visual aids were effective.
(10) Overall, I would rate this presentation as.

The instructor collects the evaluation forms and reviews them to assign the final grade
according to the percentage scale $A \geq 90, B \geq 80, C \geq 70, D \geq 60, F < 60.$
2.3. Educational activities

For the benefit of the graduate and undergraduate students, the SIAM student chapter at the University of Arkansas holds seminars and lecture series to provide a learning environment outside of the existing classes specifically to develop and improve the students’ mathematical and programming skills. The SIAM seminars help students to connect with faculty and learn more about the ongoing projects in various sciences and engineering departments. The lecture series are designed to provide extra help to students who have had no or very little experience in programming in C and using high performance computing systems.

We begin the semester with a lecture series that introduces programming in C in the Linux environment. We explain fundamental UNIX/Linux commands and how to use text editors such as *vim*, *nano*, and *pico*. Working on a command-line in a terminal emulator, and reading and editing programs in a text editor is a new experience for most of the students. With theory and hands-on exercises as a part of the computational activities, the students learn the basics in three 50-minute lectures. The lecture series are used to complement the weekly course activities and serve as an infrastructure for the course.

A vital pedagogical need is the monitoring of students to verify that they follow every step of the process to fully comprehend the material. We have hands-on sessions after the lectures. Students work in groups on the computer-based solution of mathematical problems that range from simple to complex. Whenever possible, we pair an undergraduate student with a graduate student to provide mentorship and facilitate solving the problems.

3. Undergraduate Opportunities

In this section, we present the undergraduate research opportunities made available annually in the *Computational and Applied Mathematics* (CAM) research group at the University of Arkansas, to help and encourage undergraduate students to engage in computational research. The positions are created under the auspices of Shodor (http://www.shodor.org/), a non-profit foundation and a national resource for computational science education, with a mission to improve mathematics and science education through the effective use of modeling and simulation technologies—“computational science”.

Under Shodor, the National Computational Science Institute (NCSI) (http://computationalscience.org) provides workshops on computational science for educators at all levels to give them ideas and resources to use in their classrooms. The NCSI is responsible running undergraduate student programs such as the *Blue Waters internship* (https://bluewaters.ncsa.illinois.edu/internships) and XSEDE–EMPOWER (Extreme Science and Engineering Discovery Environment–Expert Mentoring Producing Opportunities for Work, Education, and Research) to increase the number of students interested in developing computational skills (http://computationalscience.org/xsede-empower).

A faculty member at an U.S. academic institution who would like to mentor an undergraduate student submits a research proposal to the NCSI program to create a position in his/her research group. The program provides a stipend for students per quarter, semester, summer or longer, depending on the expected level of effort. Undergraduate

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students from any U.S. degree-granting institutions are matched with a mentor who has a project that contributes to the work of XSEDE ([Towns et al.](#)) [2014]. There are three tiers of participation for students, depending on their skill levels: learner, apprentice, and intern [http://computationalscience.org/xsede-empower](http://computationalscience.org/xsede-empower). The learner level is for a student who has no experience in scientific computing. The student spends time developing necessary skills to contribute to the work through online tutorials, workshops, and self learning in programming. At the apprentice level, the student begins to transform the knowledge into skills, and has the opportunity to apply the new skills with some additional training in debugging and performance tools to perform the assigned tasks. After completing these two levels in two semesters, the students are accepted as interns in the program.

The CAM group leader has created several projects for the undergraduate students who wish to gain research experience during their studies. The goal of these projects is to engage the students in petascale/exascale computing research in the areas of modeling and simulations; numerical methods and performance optimization. As part of the Blue Waters [https://bluewaters.ncsa.illinois.edu/](https://bluewaters.ncsa.illinois.edu/) efforts to motivate and train the next generation of supercomputing researchers, two University of Arkansas undergraduate students, Edwards (major in Mathematics, minor in Physics/Computer Science) and McGarigal (major in Mechanical Engineering, minor in Mathematics) were elected as the 2018–2019 Blue Waters Student Interns. The mentor of two undergraduate students in this year-long internship was responsible for teaching and introducing the use of HPC for the numerical simulations of flow problems in the area of computational fluid dynamics. To be able to work on the proposed project, the students had to develop skills in programming languages; parallel programming models (MPI on distributed memory, OpenMP on shared memory); scientific visualization (VisIt); performance analysis tools (TAU, CPMAT); and usage of the Blue Waters systems environment. The usage of HPC systems requires familiarity with compilers on Linux systems, submitting batch scripts, and running and debugging programs. The visualization of simulation results was done through the open source, interactive, scalable, tool VisIt [https://visit.llnl.gov/](https://visit.llnl.gov/). The performance analysis of the software written during the internship was done using several different profiling tools, such as GNU profiling tool (gprof), the Cray Performance Measurement and Analysis Tools (CPMAT), and Tuning and Utility Analysis (TAU). With the help of these profiling tools, the students were able to identify performance bottlenecks in the application code, visualize the data, and achieve performance improvements through hybrid (MPI+OpenMP) programming. This modified hyper-threading version of the code was set up in a way that multiple message passing interface (MPI) processes handle the interface propagation, whereas multiple OpenMP threads handle the higher order weighted essentially non-oscillatory numerical scheme. This undergraduate research project was selected for publication in the Journal of Computational Science Education ([Kaman et al.](#)) [2021].

The directed reading course–MATH 400V–, designed to help the students who have no or very little experience in programming, is used as the building blocks for the two-week crash course of MATH 4343 on the C programming language, and the programming environment on the university’s high performance computing system. Students who complete MATH 4343 with grades of “A” are accepted to the CAM group to perform more independent work and to become more fully engaged in research.

After the research experience in the CAM group, almost all students choose to pursue graduate studies and continue to work on CSE research projects. For instance; Edwards (Blue Waters Intern) was one of ten students accepted to the Oak Ridge National Laboratory’s Pathways to Computing Internship Program to learn and develop
the next-generation explicit methods for radiation transport in astrophysics and explore programming models for GPU supported on the fastest supercomputer in the world, Summit \cite{TOP500.org,2021}. In Fall 2021, she started her graduate studies in the Computational and Mathematical Sciences at the Florida State University. Drinh (XSEDE 2019 learner) was accepted to the University of Missouri-Kansas City. De-La Cruz (XSEDE 2021 apprentice and intern) intends to pursue a Ph.D. in CSE after graduating from University of Ozarks in 2021.

4. Evaluation of the Course

The course is evaluated based on the six questions listed in Table 2. It shows the percentage of students who responded to the questions with SA, A, U, D, SD, which stand for strongly agree, agree, undecided, disagree and strongly disagree respectively. The instructor performance is evaluated based on the three questions listed in Table 3. The students rate this course and the instructor as excellent (50%) and good (50%). See Table 4.

| Questions                                                                 | Responses(%) |
|--------------------------------------------------------------------------|--------------|
| Q1. Assignments are related to goals of this course.                     | 25% 75% 0 0 0 |
| Q2. The teaching methods used in this course enable me to learn.         | 50% 50% 0 0 0 |
| Q3. The stated goals of this course are consistently pursued.             | 50% 50% 0 0 0 |
| Q4. I actively participate in class activities and discussions.          | 25% 50% 25% 0 0 |
| Q5. I put much effort into this course.                                  | 50% 25% 25% 0 0 |
| Q6. My problem-solving abilities improved because of this course.       | 25% 75% 0 0 0 |

| Questions                                                                 | Responses(%) |
|--------------------------------------------------------------------------|--------------|
| Q1. My instructor displays a clear understanding of the topic.            | 75% 25% 0 0 0 |
| Q2. My instructor is readily available for consultation.                 | 75% 25% 0 0 0 |
| Q3. My instructor explains difficult material clearly.                   | 50% 50% 0 0 0 |

| Questions                                                                 | Responses(%) |
|--------------------------------------------------------------------------|--------------|
| Overall, I would rate this course as:                                    | 50% 50% 0 0 0 |
| Overall, I would rate this instructor as:                                | 50% 50% 0 0 0 |

5. Concluding Remarks and Future Plans

In this paper, we have introduced the MATH 4343 “Introduction to Scientific Computing”, a course designed and first taught in Spring 2021 at the University of Arkansas, to
engage undergraduate students in research and to train them as future computational scientists and engineers. The focus of this interdisciplinary undergraduate course is on formulating a diverse set of challenging interdisciplinary problems into mathematical algorithms, and implementing these algorithms on high performance computing systems. This helps develop the students’ skill in mathematics, programming, computational modeling, simulation, visualization, and eventually prepares them for graduate studies and future careers in research and industry.

In Spring 2022, the number of students enrolled increased by 70% relative to that of the Spring 2021 semester. In addition, four graduate students (one geosciences and three mathematics) have sought permission to enroll in this undergraduate course. We are considering offering the equivalent of this course in the future at the graduate level, and begin to target graduate students not only in applied mathematics but also in other science and engineering programs.

We envision that the contents of the course will evolve in response to the shifting interests of the students, as well as those of the instructors. In view of the recent developments on the applications of neural network models to machine learning and “big data”, we intend to introduce projects on neural networks in MATH 4343 course in the immediate future. As it was briefly noted in section 2.1.2, two new chapters on neural networks have been added to the course’s textbook, and therefore we have ready-made material to work with. The two chapters highlight the application of neural networks to solving boundary value problems for nonlinear ordinary and partial differential equations. The mesh-free approach developed there enables students to solve significantly complex problems which minimal effort. Here, for instance, is a boundary value problem for a nonlinear PDE on a non-trivial two-dimensional domain:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{4}{1+u^2} = 0 \quad \text{in } \Omega,$$

$$u = 0 \quad \text{on } \partial \Omega.$$

Figure 4 shows the domain $\Omega$ and the graph of the solution $u(x, y)$ produced by our neural network. Implementing the neural network can be done fairly quickly since, as can be seen in Figure 2, there are only four prerequisite chapters to apply neural networks for solving ordinary and partial differential equations. The construction of the domain $\Omega$ and the enforcing of the boundary conditions, is made possible through Rvachev’s R-functions (Rvachev and Sheiko 1995; Shapiro 2007) which are introduced in the course’s textbook’s Chapter 28.
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