High-Performance Computing for Scientific Applications (P.S.M.)

About The Program:

Computation, in tandem with theory and experiment, is highly regarded in the advance of scientific knowledge and engineering practice. In recognition of a growing need for experts cross-trained in relevant computational sciences, applied mathematics, statistics, and traditional scientific fields such as chemistry and physics, the Professional Science Master's (P.S.M.) program in High-Performance Computing for Scientific Applications is targeted toward STEM graduates seeking to use high-performance computation as their primary research instrument in the physical sciences, life sciences, and engineering. The core curriculum introduces students to the architecture of high-performance computing systems, mathematical techniques employed in high-performance computing, the software tools used in parallel calculations, and computational methods used in the sciences and engineering. A distinguishing feature of the program is its paired emphasis on the algorithms and technology of high-performance computing in applications to problems in science and engineering. Cross-disciplinary techniques are emphasized, and learning through applications and individually designed projects are prioritized over theory.

Career Options: Students in the program are connected to internships in industry and government laboratories by the P.S.M. Scientific Advisory Committee. Graduates are then well prepared to compete for high-quality positions in industry, government laboratories, and academia.

Prerequisites for Admission: The P.S.M. program has been designed for recent graduates and professionals who have a bachelor's degree or equivalent in a STEM field.

Requirements of Programs:

- **Total Credit Hours**: 30
- **Culminating Events**:
  Capstone Research Project:
  The Capstone Research Project provides students with the opportunity to develop, apply, and demonstrate their skills in a professional high-performance computing environment. The project must be approved in advance by the P.S.M. Steering Committee and requires a supervisor from either the Temple faculty or the P.S.M. Scientific Advisory Committee. Students can undertake their research projects in whole or in part during student internships.

Core Courses

Fundamentals of Computer Programming for Scientists and Engineers – Scientists and engineers use computers for a multitude of purposes. Even with ready-to-use applications, some amount of computer programming is commonly required to adapt to changing technology while attaining the rigorous standards of each specific discipline. This course focuses on fundamental computer programming constructs, introducing the languages Python, C++ and Fortran. Through lectures and intensive exercises students will learn to implement fundamental mathematical constructs and solve basic programming problems relevant to scientific applications. The course briefly reviews also the Linux environment, its software development tools and language interoperability. For each programming language, the course focuses on constructs and syntax designed for performance and numerical accuracy, in connection with methods from applied science, mathematics and engineering. The students taking the course are expected to have sufficient mathematical maturity, as evidenced, for example, by having completed an undergraduate Calculus sequence. The majority of the grade is determined by a mid-term and a final exam, both including a combination of questionnaires and supervised programming assignments.

Introduction to High-Performance Computing Technology for Scientists – This course is an introduction to the technology used in Linux clusters and supercomputers dedicated to calculations in applied science and engineering. The basic architecture of modern computers (processing units, memory, storage, operating system) is briefly reviewed, emphasizing the role and performance impact of each element in numerical computation. The core of the course focuses on setup and management of computer hardware specialized for scientific computing, and on its impact on commonly used strategies and methods for scientific computation. The material is organized in a combination of lectures and hands-on exercises, using computer hardware hosted at local facilities as well as virtualized resources. The majority of the grade is determined by a mid-term and a final exam, both including a combination of questionnaires and identification of the most efficient solution to common numerical problems.

Two High-Performance Computing Courses (6 credits)

Ethics Course (2 credits)

Professional Development Course (1 credit)

Electives

Select three courses from the following:

Structural Bioinformatics I – This course will cover the basic concepts of protein structure analysis, with focus on database searching and molecular modeling techniques. A broad qualitative overview of macromolecular structure and protein folding will be provided before addressing the issues of sequence alignment, secondary structure calculation, and tertiary structure prediction. The course will also cover few selected advanced topics such as prediction of quaternary structure, Hidden Markov Models, and other approaches for building probabilistic models of sequence ensembles. Computer-based activities will allow students to develop a strong familiarity with molecular visualization software and web-based tools.

Quantum Chemistry – Introduction to quantum mechanics and its application to chemical systems.

Statistical Thermodynamics – The basic concept of statistical mechanical ensembles and their application.

Analysis and Modeling of Social and Information Networks – Scope and limitations of modern synthetic methods, including silicon reagents, organometallic and radical chemistry.

Neural Computation – Neural networks provide powerful techniques to model and control nonlinear and complex systems. The course is designed to provide an introduction to this interdisciplinary topic. The course is structured such that students from computer science, engineering, physics, mathematics, statistics, cognitive sciences, and other disciplines learn the main principles of this area as well as have an opportunity to explore promising research topics through hands-on experience with neural network simulators applied to classification and prediction problems ranging from biomedical sciences to finance and business.

Machine Learning – The goal of the field of machine learning is to build computer systems that learn from experience and are able to adapt to their environments. This introductory machine learning course will present modern machine learning algorithms for supervised and unsupervised learning. It will provide the basic intuition behind the algorithms as well as a more formal understanding of how and why they work. Students will learn how to apply machine learning algorithms on a range of real-life problems and how to evaluate their performance.

Distributed and Parallel Computer Systems – Intended for students interested in the advances of scalable parallel computing systems. The main goal is to apply distributed and parallel computing theories to practical scalable parallel application development and new parallel programming tool construction.

Numerical Linear Algebra I – The syllabus includes iterative methods, classical methods, nonnegative matrices. Semi-iterative methods. Multigrid methods. Conjugate gradient methods. Preconditioning. Domain decomposition. Direct Methods. Sparse Matrix techniques. Graph theory. Eigenvalue Problems.

Numerical Differential Equations II – Analysis and numerical solution of ordinary and partial differential equations. Elliptic, parabolic and hyperbolic systems. Constant and variable coefficients. Finite difference methods. Finite element methods. Convergence analysis. Practical applications.

Mathematical Modeling for Science, Engineering, and Industry – In this course, students work in groups on projects that arise in industry, engineering, or in other disciplines of science. In addition to being advised by the course instructors, in all projects an external partner is present. The problems are formulated in non-mathematical language, and the final results need to be formulated in a language accessible to the external partner. This means in particular that the mathematical and computational methods must be selected or created by the students themselves. Students disseminate their progress and achievements in weekly presentations, a mid-term and a final project report, and a final presentation. Group work with and without the instructors' involvement is a crucial component in this course.

Topics Computer Program

Topics in Numerical Analysis – These courses cover some basic, as well as advanced topics in numerical analysis. The topics can be changed from time to time. The usual topics include: scientific computing, numerical methods for differential equations, computational fluid dynamics, Monte Carlo simulation, Optimization, Spare matrices, Fast Fourier transform and applications, etc.

Introduction to Quantum Computing – This course will give an elementary introduction to some basics of quantum information and quantum computing that are accessible to not only physicists but also people with a variety of backgrounds. It will introduce the students to the latest scientific and technological advancement, and prepare for further study and/or initiating research if one wishes to pursue in this field.

Statistical Mechanics – Review of thermodynamics; kinetic theory; statistical definition of entropy; microcanonical, canonical, and grand canonical ensembles; applications to gases, diatomic molecules, magnetic systems, phase transitions; quantum statistics; ideal boson and fermion systems; Bose-Einstein condensation; black body radiation; models of solids; properties of liquid helium.

Capstone Course (4 credits)

Courses:

Click HERE for more information on the courses below.

- Special Topics in Math
- Linear Algebra
- Concepts of Analysis I
- Concepts of Analysis II
- Introduction to Numerical Analysis
- Introduction to Numerical Analysis II
- Ordinary Differential Equations
- Fundamentals of Computer Programming for Scientists and Engineers
- Introduction to High-Performance Computing Technology for Scientists
- Candidates Seminar
- Number Theory
- Introduction to Methods in Applied Mathematics I
- Introduction to Methods in Applied Mathematics II
- Abstract Algebra I
- Abstract Algebra II
- Numerical Linear Algebra I
- Numerical Linear Algebra II
- Numerical Differential Equations I
- Numerical Differential Equations II
- Probability Theory
- Stochastic Processes
- Real Analysis I
- Real Analysis II
- Functions of a Complex Variable I
- Functions of a Complex Variable II
- Differential Geometry and Topology I
- Differential Geometry and Topology II
- Mathematical Modeling for Science, Engineering, and Industry
- Partial Differential Equations I
- Partial Differential Equations II
- Topology
- Topics in Applied Mathematics
- Topics in Applied Mathematics II
- Topics Computer Program
- Teaching in Higher Education
- Topics in Number Theory I
- Modular Functions
- Combinatorial Mathematics
- Topics in Number Theory II
- Homological Algebra
- Representation Theory I
- Representation Theory II
- Commutative Algebra and Algebraic Geometry I
- Commutative Algebra and Algebraic Geometry II
- Riemannian Geometry
- Knot Theory and Low-Dimensional Topology I

- Knot Theory and Low-Dimensional Topology II
- Advanced Probability Theory
- Functional Analysis I
- Functional Analysis II
- Calculus of Variations
- Harmonic Analysis
- Several Complex Variables I
- Several Complex Variables II
- Lie Groups
- Riemann Surfaces
- Differential Topology
- Geometric Group Theory
- Independent Study
- Topics in Algebra
- Seminar in Algebra
- Topics in Numerical Analysis
- Seminar in Probability
- Topics in Analysis
- Topics in Functional Analysis
- Topics in Differential Equations II
- Master's Research Projects
- Preliminary Examination Preparation
- Capstone Project
- Master's Thesis Research