Graduate Program in Computational Science (GPCS)

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Computational Science is a thriving field of study at the interface of computer science, mathematics and statistics, the natural sciences, engineering, and financial engineering. Practitioners of the art develop mathematical models, construct and optimize numerical algorithms, then deploy them on increasingly powerful computers to address real-life problems in fields where quantitative/compute-intensive modeling and simulation are essential to optimal design, predictive analytics, and inference.

The Graduate Program in Computational Science (GPCS) at AUB is open to students with a background in computer science, applied mathematics and statistics, the natural sciences, engineering, economics, or business who wish to further their undergraduate experience with computers and computing via intensive, hands-on study, development, and application of state-of-the-art numerical algorithms.

Having completed core courses in the program, a student will then follow a sequence of elective courses, then formulate and tackle problems in computationally-intensive fields currently explored at AUB (e.g., data analytics, computational theory, bioinformatics, biostatistics, computational biosciences, physics, astrophysics, hydrogeology, continuum mechanics, optimization, operations research, and risk analysis).

The program prepares its students for an academic adventure in applied mathematics, computational sciences and related fields, as well as a career in industries or research centers where numerical modeling, simulation, design, and/or optimization are key.

Admission Requirements

Admission to the master’s program in computational science follows basic AUB regulations, and will be ultimately based on interview. To be considered, applicants to the program should either: 1) be holders of a bachelor’s degree in the natural sciences, business, computer science, economics, engineering, or mathematics; have successfully completed the equivalent of CMPS 200, MATH 201, MATH 202, MATH 218 or 219; and have acquired proficiency in discrete mathematics, numerical analysis and statistics, at a level equivalent to MATH/CMPS 211, MATH/CMPS 251, and STAT 230 (233), respectively; or 2) be holders of a bachelor’s degree, and have completed the equivalent of MATH 202, STAT 230 and of the FAS core course requirements for a minor in computational science. Some candidates may be admitted as prospective students until full completion of the required undergraduate courses.

Graduate assistantships (GFAP) are available for some applicants to the program based on qualifications.

Graduation Requirements

- 9 credits consisting of three core courses in advanced numerical methods, optimization and data science, to be selected from the following three baskets respectively:

1. Advanced Numerical Methods (3 credits)
   A. General
   - MATH/CMPS 350 Discrete Models for Differential Equations
   - MATH/STAT 348 Monte Carlo Methods

   B. Discipline Specific
   - BIOL 370 Bioinformatics
   - PHYS 310A Computational Physics
   - MECH 663 Computational fluid dynamics

2. Optimization (3 credits)
   - MATH/CMPS 351 Optimization and Nonlinear Problems
   - ENMG 616 Advanced Optimization Techniques

3. Data Science (3 credits)
   - CMPS 392 Machine Learning
   - EECE 633 Data Mining
   - EECE 664M/ Introduction to Machine Learning
   - EECE 667 Pattern Recognition
   - EECE 693 Neural Networks

- 12 credits of electives which the student would typically select within one of the program's approved tracks: Data Analytics, Computational Theory, Bioinformatics, Biostatistics, Computational Biosciences, Computational (Astro)-Physics, Hydrogeology, Continuum Mechanics , Optimization, Operations Research, or Risk Analysis. Alternatively, students can, in coordination with their advisor, and with the approval of the GPCS committee, define a 12-credit track that best suits their background and research interests.
- a 9-credit thesis (CMTS 399) in which qualified students demonstrate the ability of constructing, implementing and/or proficiently using computational tools to address problems in their chosen track.

Courses that count towards credit in Computational Science:

MATH/CMPS 350 Discrete Models for Differential Equations 3.1; 3 cr.
A detailed study of methods and tools used in deriving discrete algebraic systems of equations for ordinary and partial differential equations: finite difference and finite element discretization procedures; generation and decomposition of sparse matrices, finite-precision arithmetic, ill-conditioning and pre-conditioning, Scalar, vector and parallelized versions of the algorithms. The course includes tutorial "immersion" sessions in which students become acquainted with state-of-the-art scientific software tools on standard computational platforms. *Prerequisites: Linear algebra and the equivalent of MATH/CMPS 251 (which can be taken concurrently) or consent of the instructor. Occasionally.*

PHYS 310 Special Topics 3.0; 3cr. (each)
May be repeated for credit.

MECH 663 Computational Fluid Dynamics 3.0; 3 cr.
A course that deals with the discretization process in fluid dynamics; numerical approaches and applications; iterative and direct matrix methods; numerical implementation of turbulence models. *Prerequisites: MECH 314 and MECH 412.*

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MATH/CMPS 351 Optimization and Nonlinear Problems 3.1; 3 cr.
A study of practical methods for formulating and solving numerical optimization problems that arise in science, engineering and business applications. Newton's method for nonlinear equations and unconstrained optimization. Simplex and interior-point methods for linear programming. Equality and inequality-constrained optimization. Sequential quadratic programming. Emphasis is on algorithmic description and analysis. The course includes an implementation component where students develop software and use state-of-the-art numerical libraries. *Same as MATH 351. Annually.*

ENMG 616 Advanced Optimization Techniques 3.0; 3 cr.
The course is divided into four parts covering integer programming, nonlinear programming, stochastic programming and heuristic methods. Students will develop skills in modeling complex systems using mathematical programming, analyzing the structure of mathematical programs, and developing and applying the correct solution techniques. Students will also have hands-on experience in using software packages for solving optimization problems.

Data Analytics

CMPS 392 Machine Learning 3.0; 3 cr.
This course covers the theory, algorithms and applications of machine learning. The course focuses mainly on supervised learning approaches and balances theory and practice. Topics include the theory of generalization; bias-variance tradeoff; overfitting and regularization; the linear models including linear regression, logistic regression and support vector machines, and neural networks including deep ones such as convolutional neural networks and recurrent neural networks. The course provides hands-on training with the trendiest machine learning libraries such as Scikit-learn and Tensor Flow. Students are expected to build a real-world machine learning application as a course project. *Prerequisite: Consent of advisor. Annually.*

EECE 633 Data Mining 3.0; 3 cr.
This course is an introduction to data mining. Data mining refers to knowledge discovery, using huge amounts of data to arrive at non-trivial conclusions. Topics will range from statistics to machine learning to database, with a focus on analysis of large data sets. The course will target at least one new data mining problem involving real data, for which the students will have to find a solution. *Prerequisite: EECE 330 or consent of instructor.*

EECE 664M **Introduction to Machine Learning** **3 cr.**
The course provides an overview of machine learning theory and algorithms that learn from experience to predict or control yet to be seen instances. The course discusses the intuition and the theory of some selected modern machine learning concepts as well as practical know-how to successfully apply them to new problems. It covers topics in supervised learning such as parametric/ non-parametric, generative/ discriminative algorithms for classification and regression and in unsupervised learning for clustering, dimensionality reduction and reinforcement learning. The course also includes case studies and applications so that students can gain practice on regularization, model selection, parameter estimation, Bayesian networks, hidden Markov models, support vector machines, reinforcement learning, neural networks and deep learning. *Students cannot receive credit for both EECE 664M and EECE 633 and 667. Prerequisites: EECE 330, and MATH 218 or MATH 219, and STAT 230 or STAT 233 or consent of instructor.*

EECE 667 **Pattern Recognition** **3 cr.**
The course provides an overview of the algorithms used in machine learning. The course discusses modern concepts for model selection and parameter estimation, decision-making and statistical learning. Special emphasis will be given to regression and classification for supervised modes of learning. Students will be assigned typical machine learning problems to investigate as projects.

EECE 693 **Neural Networks** **3 cr.**
The course provides a comprehensive foundation to artificial neural networks and machine learning with applications to pattern recognition and data mining; learning processes: supervised and unsupervised, deterministic and statistical; clustering; single layer and multilayer perceptrons; least-mean-square, back propagation, deep learning; Al-Alaoui pattern recognition algorithms; radial basis function networks; committee machines; principal component analysis; self-organizing maps; current topics of interest.