

2023 - 2024

CSE Graduate Student Handbook





Computational Science and Engineering M.S. and Ph.D. Programs

WELCOME!

Fall 2023

TO: New Graduate Students

FROM: Elizabeth M. Cherry

Director of the CSE Graduate Programs

This handbook is your guide to the Computational Science and Engineering (CSE) Graduate Programs at Georgia Tech. The CSE Programs include the Master of Science degree program (CSE M.S.) and the Doctor of Philosophy degree program (CSE Ph.D.).

We have prepared this handbook for currently enrolled students, but prospective students should also find it helpful.

If you have questions about any of the material in this handbook, please email cse-advisor@cc.gatech.edu or consult the Home Unit Coordinators section of this handbook to find the right person for your questions or comments.

On behalf of the entire CSE Graduate Programs faculty, staff, and students, we are pleased that you have joined the CSE family and wish you success in your graduate studies.

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2 PROGRAM DESCRIPTION AND OBJECTIVES

Computational science and engineering (CSE) is the systematic study of computer-based models of natural phenomena and engineered systems. Students, researchers, and practitioners of CSE master domain-independent ideas that cut across computer science, applied mathematics, statistical data analysis and data mining, and the science and engineering disciplines. They use these ideas to solve problems having great societal impact, such as how to grow cities sustainably; how to design power-efficient buildings and aircraft; how to discover new materials with specific properties; or how to create novel biomedical devices, effective drugs, and efficient health care delivery systems; to name just a few.

The goal of the CSE Graduate Programs ("CSE Programs") at Georgia Tech is to help you master the unique body of knowledge and professional practices that constitute CSE by working in multidisciplinary teams of faculty and students who have a deep common interest in computational and data-driven models.

More specifically, the CSE programs aim to help you

- master and advance the state of knowledge and/or practice in the computational science and engineering discipline;
- integrate and apply principles from mathematics, science, engineering, and computing to innovate, create computational models, and apply them to solve real-world problems;
- work in multidisciplinary teams of individuals whose primary background is in computing, mathematics, and/or particular science or engineering domain; and
- become leaders in industry, government (e.g., national laboratories), and academia, both in terms of knowledge and computational (e.g., software development) skills.

Toward this end, the CSE programs curriculum engages you in a variety of activities designed to achieve the following educational goals. You will

- develop a solid understanding of fundamental principles across a range of core areas in the computational science and engineering discipline;
- develop a deep understanding and set of skills and expertise in a specific computational specialization of the computational science and engineering discipline;
- be able to apply and integrate the knowledge and skills you have developed and demonstrate your expertise and proficiency in an application area of practical importance; and
- be able to engage in multidisciplinary activities by being able to communicate complex ideas in their area of expertise to individuals in other fields. You will also be able to understand complex ideas and concepts from other disciplines and incorporate these concepts into your own work.

3 DESIRED QUALIFICATION OF STUDENTS

Students admitted to the program must be able to demonstrate the following competencies:

- An undergraduate level understanding of concepts from computer science, applied mathematics, statistics, a physical science (e.g., physics, chemistry, or biology), and/or engineering. Typically, a student demonstrates such understanding by a bachelor's degree in one of these subject areas. However, a student with a different background may also apply. The admissions process examines all aspects of the applicant's background, including all work and other academic experience.
- Computing skills in algorithms, data structures, and programming in a language such as C or FORTRAN
 is required. At a minimum, this requirement is an introductory computer science course or equivalent
 experience. However, at least two semester courses are strongly recommended, and the more
 algorithms and programming experience, the better.
- Undergraduate mathematics in calculus is required. Undergraduate course work in areas such as
 mathematical analysis, numerical differential equations, linear algebra, discrete mathematics, and
 probability and statistics are also highly recommended, and may be required for certain programs of
 study selected by the student.
- Students missing one or more of these competencies may still apply. However, they will be expected to fill any gaps in their background by, for instance, completing preparatory coursework upon joining the program.

4 HOME UNITS AND HOME UNIT REQUIREMENTS

As a student in a CSE Program, you must choose a *home unit*. A home unit is an academic unit (Department, Division, or School) at Georgia Tech that has agreed to formally participate in the CSE programs. Each home unit designates a *Home Unit Coordinator and a Program Coordinator*. The home unit coordinator is a faculty member with overall responsibilities for CSE programs activities as they pertain to that home unit. The program coordinator represents that home unit in administrative activities that pertain to the program as a whole.

You and the home unit must mutually agree to your home unit affiliation. An initial home unit is determined either during the admissions process or in the process of transferring to a CSE program from another academic program at Georgia Tech. Once admitted, you may change to a new home unit if that unit agrees.

Each academic unit determines the rules for allocation of space and financial assistance (e.g., teaching and research assistantships) for students homed in that unit. If you are a Ph.D. student, your dissertation advisor should have an appointment in your home unit, in addition to being a member of the CSE programs faculty.

Of course, you are welcome to explore research opportunities with faculty in other units beyond your home unit. If a faculty member in another home unit becomes your advisor, you would normally change your home unit accordingly.

Regardless of your home unit, you must fulfill the degree requirements specified in this document to complete your program. Some home units have additional degree requirements, as summarized below. Be sure that you understand and satisfy these requirements as well. Requirements apply to both M.S. and Ph.D. program unless noted otherwise.

- School of Aerospace Engineering.
 - No additional degree requirements are specified.
- School of Biological Sciences.
 - No additional degree requirements are specified.
- Coulter Department of Biomedical Engineering (BME).
 - Students must take application specialization courses from the BME department, as approved by the BME home unit coordinator.
 - At least three of the five of the Ph.D. dissertation committee members must be CSE Program faculty or faculty members from the home unit.
 - Ph.D. students must participate in the BME teaching practicum program, serve as a teaching assistant in BME courses for two semesters, and participate in the BME seminar course for their first two academic years in residence.
- School of Chemistry and Biochemistry.
 - Students must take application specialization courses from the School of Chemistry and Biochemistry as approved by the school's home unit coordinator. Students should enroll in at least one course offered by the school during each semester when the student serves as a teaching assistant for the school.
 - At least three of the five of the Ph.D. dissertation committee members must be CSE Program
 faculty or faculty members from the home unit.
 - Beyond the second semester, the student's principal research advisor must be a member of the School of Chemistry and Biochemistry faculty to be eligible to serve as a teaching assistant in that school.

- School of Civil and Environmental Engineering (CEE).
 - Students must complete a 12-hr specialization in CEE.
- School of Computational Science and Engineering.
 - Ph.D. students must fulfill a two-semester teaching apprenticeship.
- School of Electrical and Computer Engineering (ECE).
 - Students must take application specialization courses from the School of ECE, as approved by the school's home unit coordinator.
 - At least three of the five of the Ph.D. dissertation committee members must be CSE Program faculty or faculty members from the home unit.
- School of Industrial and Systems Engineering.
 - o No additional degree requirements are specified.
- School of Materials Science and Engineering (MSE).
 - Students must take application specialization courses from the School of MSE, as approved by the school's home unit coordinator.
 - At least three of the five of the Ph.D. dissertation committee members must be CSE Program faculty or faculty members from the home unit.
- School of Mathematics.
 - Ph.D. students must take at least 9 hours having the MATH course designations which are not cross-listed with another department.
 - For Ph.D. minor requirement, (in addition to CSE 9.6 Minor Requirement) these classes should be 6000-level or higher, but not including 8900. These classes should be a cohesive group that best complements the students research and career goal and must be passed with a grade of B or better.
 - o Ph.D. student's Oral exam format is different (see section on CSE Qualifying Examination).
 - At least one individual of the Ph.D. dissertation committee must be faculty member from the school of Mathematics.
- The George W. Woodruff School of Mechanical Engineering (ME).
 - Students must take application specialization courses from the Woodruff School of ME as approved by the ME home unit coordinator.
 - At least three of the five of the Ph.D. dissertation committee members must be CSE Program faculty or faculty members from the home unit.
 - Ph.D. students must complete the ME teaching practicum (see section on Teaching Requirements) and fulfill the seminar requirement (see http://www.me.gatech.edu/graduate/phd/seminars).
- School of Physics.
 - Students must take application specialization courses from the School of Physics, as approved by the school's home unit coordinator.
 - At least three of the five of the Ph.D. dissertation committee members must be CSE Program faculty or faculty members from the home unit.

5 PROGRAMS ADMINISTRATION AND POINTS OF CONTACT

The CSE Graduate Programs Office administers the programs, in conjunction with administrative personnel from each of the participating units. It coordinates the various program activities and provides a single "interface" to the programs both from outside Georgia Tech as well as within Tech (e.g., the registrar's office). The CSE programs director is a faculty member who has overall responsibility for management and administration.

In addition, each participating unit designates a *Home Unit Coordinator and a Program Coordinator*. The home unit coordinator is a faculty member with overall responsibilities for CSE programs activities as they pertain to that home unit. The program coordinator represents that home unit in administrative activities that pertain to the program as a whole.

You should first consult with your home unit coordinator for advice and recommendations concerning your program, and consult with the CSE programs director as needed.

CSE Programs Director

Elizabeth M. Cherry Associate Professor

School of Computational Science and Engineering

Website: http://cc.gatech.edu/~echerry

Office: Coda E1346B Phone: (404) 894-3889 Email: elizabeth.cherry@gatech.edu



CSE Programs Coordinator

Iris Hamilton

CSE Academic Program Coordinator Office: Coda E1344A

Phone: (404) 385-5662 Email: ihamilton9@gatech.edu



6 CSE Home Unit Coordinators and Program Coordinators

Home Un	it Coordinators	Program Coordinators
Aerospace I Dr. Dimitri M Website: Office: Phone: Email:	Engineering Mavris, Professor https://www.ae.gatech.edu/people/dimitri-mavris Weber 301A (404) 894-1557 dimitri.mavris@aerospace.gatech.edu	Ryan Sanders, Academic Program Manager Office: Montgomery Knight 301C Phone: (404) 894-3433 rsanders72@gatech.edu
Biological S Dr. King Jor Website: Office: Phone: Email:	cciences rdan, Professor http://biosci.gatech.edu/people/king-jordan EBB - 2109 (404) 385-2224 king.jordan@biology.gatech.edu	Lisa D. Redding, Academic Program Coordinator II lisa.redding@biosci.gatech.edu
	Engineering Wang, Professor http://miblab.bme.gatech.edu/ 4106 U.A. Whitaker Biomedical Engineering Building (404) 385–2954 maywang@gatech.edu	Mitchell Everett, PhD Program Manager mitchell.everett@bme.gatech.edu
	Ind Biochemistry I Sherrill, Professor https://chemistry.gatech.edu/people/david-sherrill 2100N Molecular Science and Engineering (404) 894-4037 sherrill@gatech.edu	Dr. Kenyetta Johnson, Director, Graduate Studies kenyetta.johnson@chemistry.gatech.edu
	vironmental Engineering Stewart, Associate Professor https://ce.gatech.edu/directory/person/lauren-stewart Mason 3141A (404) 385-1919 lauren.stewart@ce.gatech.edu	Danielle Ramirez, Graduate Programs Manager danielle.ramirez@ce.gatech.edu
	h M. Cherry, Associate Professor http://cc.gatech.edu/~echerry Coda S1319 (404) 894-3889 elizabeth.cherry@gatech.edu	Iris Hamilton, CSE Academic Program Coordinator ihamilton9@gatech.edu
	nd Computer Engineering oder, Associate Professor http://yoder.ece.gatech.edu/ Bunger-Henry 219 (404) 385-2652 doug.yoder@gatech.edu	
	nd Systems Engineering s Alexopoulos, Professor (PhD + MS) https://www.isye.gatech.edu/users/christos-alexopoulos 429 Groseclose Building (404) 894-2361 christos@isye.gatech.edu	Amanda Ford, Graduate Programs Manager amanda.ford@isye.gatech.edu

Materials Science and Engineering Dr. Seung Soon Jang, Professor website: https://cnbt.mse.gatech.edu/ Office: Love 351 Phone: (404) 385-3356 Email: SeungSoon@mse.gatech.edu	Laura Alger, Academic Advising Manager laura.alger@mse.gatech.edu Teresa Nelson, Academic Program Coordinator teresa.nelson@mse.gatech.edu
Mathematics Dr. Sung Ha Kang, Professor website: http://people.math.gatech.edu/~kang/ Office: Skiles 247 Phone: (404) 385-7678 Email: kang@math.gatech.edu	Dr. Chris Jankowski, Director of Graduate Advising and Assessment cjankowski3@gatech.edu
Mechanical Engineering Dr. Surya Kalidindi, Professor website: http://me.gatech.edu/faculty/kalidindi Office: Bunger Henry Room 192 Phone: (404) 385–2810 Email: surya.kalidindi@me.gatech.edu	Glenda Johnson, Academic Advisor Manager Phone: (404) 385-0586 Email: glenda.johnson@me.gatech.edu
Physics Dr. Edwin Greco, Senior Academic Professional website: http://physics.gatech.edu/academics/graduate Office: Howey W206 Phone: (404) 385-5628 Email: ed.greco@gatech.edu	Gary Longstreet, Academic Program Manager Phone: (404) 894-7073 Email: longstreet@gatech.edu

7 CSE PROGRAMS FACULTY

7.1 Aerospace Engineering

Karen Feigh, Eric Feron, Sathya Hanagud, Graeme Kennedy, Dimitri Mavris, Suresh Menon, Joseph Oefelein, Elizabeth Qian, Stephen Ruffin, Massimo Ruzzene, Lakshmi Sankar, Marilyn J. Smith, Evangelos Theodorou, Vigor Yang, PK Yeung

7.2 Biological Sciences

Yuhong Fan, King Jordan, Matthew Torres

7.3 Biomedical Engineering

Mark Borodovsky, Melissa Kemp, Cassie S. Mitchell, Peng Qiu, Saurabh Sinha, Eberhard Voit, May Dongmei Wang, Ajit Yoganathan

7.4 Chemistry and Biochemistry

Marcus Cicerone, Joshua Kretchmer, Jesse McDaniel, David Sherrill

7.5 Civil and Environmental Engineering

Chloé Arson, Sheng Dai, James David Frost, Aris Georgakakos, Angshuman Guin, Emily Grubert, Michael Hunter, Laurence Jacobs, Aditya Kumar, Jorge Laval, Jian Luo, Jorge Macedo, Eric Marks, Patricia Mokhtarian, Rafi Muhanna, James Mulholland, Glaucio Paulino, Srinivas Peeta, Ameet Pinto, Armistead G. Russell, Phanish Suryanarayana, Yi-Chang James Tsai, John Taylor, Jingfeng Wang, Donald White, Sotira Yiacoumi

7.6 Computational Science and Engineering

Srinivas Aluru, Mark Borodovsky, Spencer Bryngelson, Ümit V. Çatalyürek, Nisha Chandramoorthy, Polo Chau, Peng Chen, Elizabeth Cherry, Edmond Chow, Bo Dai, Victor Fung, Felix Herrmann, Nabil Imam, Surya Kalidindi, Srijan Kumar, Yunan Luo, Haesun Park (Chair), Raphaël Pestourie, B. Aditya Prakash, Elizabeth Qian, Florian Schäfer, David Sherrill, Rich Vuduc, Kai Wang, Angi Wu, Helen Xu, Chao Zhang, Xiuwei Zhang

7.7 Electrical and Computer Engineering

Ali Adibi, Ghassan AlRegib, David Anderson, Vince Calhoun, Faramarz Ferki, Santiago Grijalva, Pan Li, Douglas Yoder

7.8 Industrial and System Engineering

Christos Alexopoulos, Dave Goldsman, Seong-Hee Kim, Sigrun Andradottir, Martin Savelsbergh, Craig Tovey, George Nemhauser, Arkadi Nemirovski, Brani Vidakovic, Yao Xie, Tuo Zhao

7.9 Materials Science and Engineering

Hamid Garmestani, Karl Jacob, Seung Soon Jang, Mo Li, David McDowell, Chris Muhlstein, Rampi Ramprasad, Naresh Thadhani, Aaron Stebner, Donggang Yao

7.10 Mathematics

Greg Blekherman, Leonid Bunimovich, Hannah Choi, Luca Dieci, Guillermo Goldsztein, Christine Heitsch, Christian Houdre, Sung Ha Kang, Vladimir Koltchinskii, Rachel Kuske, Lew Lefton, Anton Leykin, Wing Li, Wenjing Liao, Yingjie Liu, Galyna Livshyts, Rafael De La Llave, Doron Lubinsky, Cheng Mao, John McCuan, Dmitrii Ostrovskii, Martin Short, Molei Tao, Mayya Zhilova, Haomin Zhou

7.11 Mechanical Engineering

Alexander Alexeev, Seung-Kyum Choi, Nazanin Bassiri-Gharb, Chaitanya Deo, Itzhak Green, Jianxin Jiao, Surya Kalidindi, Satish Kumar, David McDowell, Julien Meaud, Tianye Niu, Christopher Saldana, Emily Sanders, Yan Wang, Shuman Xia, Ye Zhao

7.12 Physics

Tamara Bogdanovic, Laura Cadonati, Flavio Fenton, Daniel Goldman, Roman Grigoriev, Harold Kim, Sabetta Matsumoto, Kurt Wiesenfeld, John Wise

8 MASTER OF SCIENCE DEGREE PROGRAM (M.S. CSE) REQUIREMENTS

The Master of Science degree in CSE is designed to provide you with (1) a base of knowledge and skills in core CSE areas; (2) in-depth knowledge of advanced computational methods; and (3) experience in applying computational methods to relevant and important problems within the context of at least one specific application domain. The program is also designed for you to flexibly tailor the program to your individual career objectives.

Note: The requirements described below form the general framework of the degree program; within this framework, each home unit may have specific custom rules. Examples appear in the text, but **be sure to check for requirements specific to your home unit**.

The CSE M.S. requires a minimum of 30 semester hours. (A typical course is 3 semester hours.) Table 1 summarizes these requirements.

Curriculum Component	Semester Hours
CSE core courses	12
Computation and application specialization – home unit minor	12
Additional computation and application electives (non-thesis option)	6
CSE Thesis (thesis option)	6
Total	30

Table 1. Curriculum Overview (30 hours)

- The core courses define a core body of knowledge in CSE. You must take 12 hours of core courses.
- The computation and application specialization is a set of technical elective courses that focus on developing more in-depth knowledge of both computational techniques and the application of computational methods in an application domain. A minimum of one application course must be included in this area.* This set of courses will typically form a body of material in close alignment with your home unit. It also forms a minor course of study aligned with your home unit. You must take 12 hours of courses to fulfill this requirement.

*As a guideline, your "Computation Specialization" is supposed to give you more depth in computational techniques; your "Application Specialization" is supposed to give you exposure to one or more application domains in which you could apply those techniques. For example, you might take a course in HPC or machine learning to study general mathematical and algorithmic methods, and then take a course in, say, biology, materials engineering, or finance to learn more about an area in which you might apply such methods. (The course does not have to be about applying the methods; the idea is that you learn enough about some area *outside* computation.) This is just an example; in evaluating your program of study, we will consider reasonable arguments. That's why we ask you to choose your application specialization course(s) *and* explain how they fit this notion of an application specialization.

- Finally, you must complete an additional 6 hours by completing either the thesis option or additional technical electives.
- You must maintain a grade point average (GPA) of at least 3.0 for all courses listed on your degree
 program. All courses listed in the degree program must be taken on the A-F grading basis if the A-F
 grading basis is offered.
- A M.S. degree must be completed within six years from the date of the first coursework on the degree program, including any transfer credits.

8.1 CSE Core (12 Semester Hours)

To fulfill the core courses requirement, you must complete four courses of the five listed in Table 2. If, prior to entering the program, you have completed a core course or its equivalent course at another institution (subject to approval), you may substitute an additional specialty course for the core course, consistent with your intended specialization.

Five courses comprise the CSE core. These courses have several objectives:

- Provide you with knowledge of a variety of areas within the CSE discipline.
- Ensure you have strong software development skills, so that you can develop substantial computational artifacts.
- Train you to integrate and synthesize concepts from mathematics, computing, science, and engineering to solve computational problems.
- Develop your ability and skills to perform multidisciplinary research involving complex concepts from computing, mathematics, science, and engineering.

Core Course Number and Title	Credit Hours
CSE/Math 6643 Numerical Linear Algebra	3
CSE 6140 Computational Science and Engineering Algorithms	3
CSE 6730 Modeling and Simulation: Fundamentals & Implementation	3
CSE/ISYE 6740 Computational Data Analysis	3
CSE 6220 High Performance Computing	3

Table 2. CSE Core (12 hours; pick any four courses)

8.2 Computation and Application Specialization - Home Unit Minor (12 Semester Hours)

The Computation and Application Specialization requirement is a set of technical electives that forms a focused area of specialization in CSE in conjunction with your declared home unit. The aims of this specialization are to (1) increase your depth of knowledge and skills in CSE computational techniques, (2) equip you with knowledge of a particular application domain to enable you to attack problems within that domain by applying advanced computational techniques, (3) provide sufficient flexibility for you to tailor course selections to your individual needs and long-term career objectives, and (4) ensure you complete a well-structured, coherent program of study. The specialization requirement is designed to help you develop multidisciplinary skills in at least two areas among computation, science, and engineering.

To fulfill this requirement, you must take an additional 12 hours of courses that meet the following criteria:

- The set of courses must clearly support graduate work in the computational science and engineering discipline.
- The courses must include at least one application domain, in addition to providing advanced knowledge of computational techniques. At least one course applying CSE techniques to a specific domain is necessary to fulfill this requirement.
- The set must include at least 6 hours of coursework offered outside computing (i.e., not carrying a CS or CSE course designation).
- During the first semester of study in the program, you must propose the technical specialization to be applied to your CSE degree. Both the home unit coordinator and CSE programs director must

approve it.

There are numerous courses offered at Georgia Tech that are appropriate for "graduate work in the computational science and engineering discipline." You should consult with your home unit coordinator and/or the CSE programs director for guidance in constructing an appropriate course of study.

8.3 Program of Study Approval

You must obtain approval of your proposed program of study in your first semester of enrollment in the CSE program. Both your home unit coordinator and the CSE programs director must approve it. This approval process is designed to ensure that you have a good plan for meeting the degree requirements, and that your overall program of study is consistent with your intended career objectives.

8.4 CSE Master's Thesis

If you wish to carry out graduate-level research on a topic in the CSE discipline, consider the Master's thesis option. This option is a great way to "go deep" on a topic, interact closely with faculty, and build an impactful body of work over multiple semesters.

To complete a M.S. thesis, you must show that you can perform independent research, in collaboration with a faculty advisor, and you must defend this work to a committee of faculty. More specifically, you must:

- Define a suitable research problem and approach in consultation with a thesis advisor. Your thesis
 advisor must be a CSE program faculty member from your home unit.
- Complete 6 semester hours of the course CSE 7000 (Master's Thesis).
- Document this work in a Master's thesis. Typically, this document describes the research problem, summarizes relevant related work, explains the approach used to attack the problem, presents the results of using this approach, and concludes by speculating on areas of additional follow-on work that merit investigation.
- Defend the research and results of the work to a thesis committee. This committee must include at least three individuals.

Your thesis committee must include at least one faculty member with an appointment in the College of Computing and one with a faculty appointment in the College of Science or the College of Engineering. The home unit coordinator and CSE programs director must approve your research problem statement and your list of members of your thesis committee prior to starting the thesis option.

Lastly, note that the campus provides general guidelines relevant to all M.S. thesis degrees. This material includes suggestions about how to register if you are, for instance, a Graduate Research Assistant (GRA) and how to sign up for additional semester hours of independent study, thesis work, or GRA section, as your thesis work may require.

Please see: http://www.gradadmiss.gatech.edu/theses-dissertations.

8.5 Obtaining a CSE Master's Degree while Pursuing a Ph.D. Degree

If you are pursuing a Ph.D. degree, you may obtain a CSE Master's degree if the CSE Master's degree program requirements are fulfilled. See the CSE graduate programs advisor for details.

8.6 Transfer of Credits

You must request any transfer of credit during your first semester in residence at Georgia Tech. Per campus rules, you may receive up to six semester hours of transfer credit toward the CSE M.S. degree for graduate-level courses taken at an institution accredited by a Canadian or U.S. regional accrediting board or at a foreign school or university that has a signed partner agreement with Georgia Tech. You may not apply transferred credits toward another degree unless otherwise specified.

You must ask the CSE programs director whether the courses to be transferred are a logical part of the graduate program at Georgia Tech. You will then need to give the CSE programs advisor a copy of your current transcript, which should display the course(s), and also provide some descriptive course materials, such as a catalog description, syllabi, exams, assignments, and textbooks — the more information you can provide, the better. The CSE programs director will consult with Georgia Tech faculty in the appropriate area to determine the equivalent Georgia Tech course and the number of credit hours to be accepted. Once the CSE programs director approves the course(s) for transfer credit, the Non-Resident Credit Report is prepared and sent directly to the Georgia Tech Registrar with the supporting documentation.

For more information on transfer of graduate credits, see: http://catalog.gatech.edu/academics/graduate/policies-and-regulations/.

8.7 Sample Programs

Non-Thesis Option

Semester 1 (Fall)	Semester 2 (Spring)	Semester 3 (Fall)
CSE-core (3)	CSE-core (3)	Specialization (3)
CSE-core (3)	CSE-core (3)	Specialization (3)
Specialization (3)	Specialization (3)	Specialization (3)
Specialization (3)		

Thesis Option

Note: This table represents a three–semester program; however, most students take four semesters to build up enough background knowledge to successfully complete their thesis research.

Semester 1 (Fall)	Semester 2 (Spring)	Semester 3 (Fall)
CSE-core (3)	CSE-core (3)	Specialization (3)
CSE-core (3)	CSE-core (3)	Specialization (3)
Specialization (3)	CSE 7000 (MS Thesis) (3)	CSE 7000 (MS Thesis) (3)
Specialization (3)		

9 DOCTOR OF PHILOSOPHY (PH.D.) DEGREE PROGRAM REQUIREMENTS

The CSE Ph.D. program is designed to provide you with the flexibility to tailor your program of study to your individual career objectives. You define the program of study with the approval of the dissertation advisor, home unit coordinator, and CSE programs director. However, your program of study must also satisfy the minimum course requirements below.

Note: The following discussion describes the general framework of the CSE Ph.D. program requirements; **be sure to check for variations specific to your home unit.**

The Ph.D. degree in CSE requires a minimum of 31 semester hours of coursework. (A typical course is 3 semester hours.) Table 3 summarizes these requirements. These requirements are designed give you breadth of knowledge in CSE, depth in specific computational methods and techniques, and knowledge to apply these techniques to problems within the context of a specific application domain. The required coursework for CSE Ph.D. program includes:

- CSE core. You must take twelve semester hours of CSE core courses. These courses give you breadth
 of knowledge in the major areas of CSE. These courses provide a base of knowledge and skills
 spanning several core areas of computational modeling.
 - In addition, you must take a one-hour introductory course that focuses on an introduction to the CSE discipline and multidisciplinary communication. You should take this course in your first year.
- Computation specialization. You must take nine semester hours in a set of courses that help you develop in-depth knowledge of advanced computational methods and techniques.
- Application specialization. You must take nine semester hours of courses in an application domain. The
 purpose of this requirement is for you to acquire sufficient knowledge and experience to apply
 computational methods to relevant and important problems within the context of such a domain.

Curriculum Component	Semester Hours
CSE 6001 Intro to CSE	1
CSE core courses	12
Computation specialization (may include special problems)	9
Application specialization (may include special problems)	9
Total	31

Table 3. Curriculum Overview (31 hours)

In parallel to requirements listed above:

Special problems. You must complete one special problems course with a minimum of three semester
hours. A special problems course is an independent study course taken under a CSE Programs faculty
member. You may apply special problems course hours toward either your computation or application
specialization requirements. See below for details.

These requirements constitute the minimum amount of coursework to fulfill degree requirements. Your dissertation advisor and <u>your home unit may impose additional course requirements</u> in accordance with the home unit's rules and with your specific research activities and long-term professional objectives.

You must maintain a GPA of at least 3.3 for all courses listed on your program of study. You must take these courses on an A-F grading basis if offered.

You must complete your Ph.D. degree within ten years from the date of the first coursework on the degree program, including any transfer credits.

You may complete a CSE M.S. degree along the way; see Section 8.5 and related topics.

Lastly, the campus provides general guidelines relevant to all Ph.D. degrees. This material explains, for instance, how to register if you are a Graduate Research Assistant (GRA) or Graduate Teaching Assistant (GTA) in a given semester.

Please see: http://www.policylibrary.gatech.edu/student-affairs/policy-hour-loads-graduate-students.

9.1 Computation Specialization (9 Semester Hours)

You must complete nine hours of technical electives focusing on advanced computational methods. This specialization increases your depth of knowledge and skills in computation. The set of computation specialization courses that you take must clearly support graduate work in the CSE discipline. (You must justify your chosen courses by arguing how they advance your knowledge of computational techniques and methods relevant to your research.)

Georgia Tech currently offers many courses that involve computational methods. A recommended list of suitable courses and concentrations is included in handbook. You should consult with your research advisor to select a suitable set of courses.

In general, simply using computer software in the course does not qualify the course for the computation specialization. Rather, the course must include intellectual content in computational methods or techniques, ideally in the context of some domain or class of applications. Courses listed under "CSE core" (Table 2) that are not used to satisfy the core course requirement may be used to partially fulfill the computation specialization requirement.

9.2 Application Specialization (9 Semester Hours)

You must complete an additional nine hours of technical electives focusing on an application domain where advanced computational techniques may be applied. Courses fulfilling this requirement need not necessarily have a computation focus. For instance, a course may provide essential background knowledge of an application area (e.g., a science or an engineering field) that enables you to apply computational techniques in that domain. See application courses section for examples.

Note that the computation and application specialization courses, when taken together, must constitute a coherent program of study. "Coherent" means that there is a strong argument the courses will enable you to develop and apply advanced computational techniques and methods to relevant problems in a specific field of study. Your advisor and the CSE programs director can provide more detailed guidance and feedback.

Additional requirements or restrictions may apply, depending on the home unit. Here is a general quideline for the Application Specialization:

*As a guideline, your "Computation Specialization" is supposed to give you more depth in computational techniques; your "Application Specialization" is supposed to give you exposure to one or more application domains in which you could apply those techniques. For example, you might take a course in HPC or machine learning to study general mathematical and algorithmic methods, and then take a course in, say, biology, materials engineering, or finance to learn more about an area in which you might apply such methods. (The course does not have to be about applying the methods; the idea is that you learn enough about some area *outside* your computation specialization.) This is just an example; in evaluating your program of study, we will consider reasonable arguments. That's why we ask you to choose your application specialization course *and* explain how it fits this notion of an application specialization.

9.3 Special Problems Requirement (3 to 6 Semester Hours)

The aim of this requirement is for you to conduct preliminary research with a CSE program faculty member early in the Ph.D. program. As such, we highly recommend you take it in your first semester. You and the supervising faculty member define the work to be done and the terms for successful completion. You must take at least 3 semester hours in one special problems course. You may apply special problems course hours toward your specialization requirements. However, you may only apply a

maximum of 6 semesters hours toward such requirements. (Moreover, you may apply each special problems course toward either your computation specialization or toward your application specialization, but not both.) You must declare your intent in your program of study.

The special problems course number and rules for signing up vary by home unit; for instance, the course is CSE 8903 for students homed in CSE and requires the CSE permit form (available at http://www.cse.gatech.edu/academics/current-students/forms) approved by the supervising faculty member.

9.4 Program of Study Approval

You must file an approved program of study located on the CSE website indicating which courses will be used to fulfill the degree requirements. You must do so after successfully passing the Qualifying Exam. Your dissertation advisor, the home unit coordinator, and the CSE programs director must approve your proposed program of study.

9.5 Minor Requirement

You must complete a focused program of study including at least 9 semester hours of courses outside the computational science and engineering field. These courses should not carry the CSE course designation and, for students with a home unit of CSE, they also should not carry the CS course designation. Courses that are used to fulfill the computation or application specialization requirements and that do not carry the CSE designation (CS/CSE designation, for students with CSE home unit) may also be used to fulfill the minor requirement.

9.6 Sample Program

The following is a sample program that you might follow to complete your Ph.D. course requirements in two years:

Semester 1 (Fall)	Semester 2 (Spring)	Semester 3 (Fall)	Semester 4 (Spring)
Intro to CSE: CSE 6001 (1)	CSE core (3)	Specialization (3)	Specialization (3)
CSE core (3)	CSE core (3)	Specialization (3)	Specialization (3)
CSE core (3)	Specialization (3)		
Special problems (3)			

9.7 Ph.D. Annual Review

Ph.D. students homed in CSE will be reviewed on an annual basis to determine progress and performance in the Ph.D. program. Other home units also may review students' progress and performance in the Ph.D. program; details of this review process vary by the home unit. For example, if you are homed in the School of CSE, you complete a self-evaluation of your performance. Your faculty advisor then reviews your self-evaluation, and submits a recommendation of your status. A Ph.D. Review Committee considers these materials and then assigns you one of five possible status designations: satisfactory, minor concern, concern, warning, and probation. If you do not receive a satisfactory designation, the committee will reevaluate your case in the Spring semester. If you receive a probation status, you are in jeopardy of losing financial support. Furthermore, any student placed on academic probation by the institute, e.g., due to a low GPA, shall automatically be placed on probation status. You should receive the result of the review in writing prior to the end of the Fall semester.

Ph.D. students homed in Math will follow the same review process as Ph.D. in Math students yearly.

9.8 Teaching Requirements

If your home unit is the School of CSE, you must complete a two-semester teaching apprenticeship. Through this requirement, you will develop general skills in pedagogy, communication, curriculum develop, and organization. This type of practical experience should help you become an effective communicator, regardless of whether you intend to pursue an academic or industrial career. During each semester you are serving as a teaching apprentice, you must also take an additional seminar course. Please see the Graduate Programs Advisor for additional details.

If your home unit is the Woodruff School of Mechanical Engineering, you must complete three semester hours of Teaching Practicum (ME/NRE 7757) during the course of their doctoral studies. See http://www.me.gatech.edu/graduate/phd/practicum for details.

9.9 CSE Qualifying Examination

The Ph.D. qualifying examination is designed to ensure that you have achieved sufficient knowledge in core areas of CSE as well as in your chosen specialization area, as preparation for advanced research.

9.9.1 Declaration of Intent

If you plan to take the qualifying exam, you must submit the CSE Written Qualifying Exam Form at least 6 weeks prior to the date of the written portion of the exam. On this form, you will specify the core areas in which you choose to take the written exam (Numerical Methods, Discrete Algorithms, Modeling and Simulation, Computational Data Analysis, High Performance Computing).

Once you have passed the CSE Written Qualifying Exam, you must submit the CSE Oral Specialization Exam and Artifact Defense Form within 2 weeks. You will use this form to request Ph.D. Oral Qualifying Exam Committee members.

9.9.2 CSE Ph.D. Qualifying Exam Format

The CSE Ph.D. Qualifying Exam consists of two independent parts.

- Written qualifying exams: The written exams cover core areas of CSE. You select two areas among the following five: numerical methods, discrete algorithms, modeling and simulation, computational data analysis, and high-performance computing. These areas correspond with the five CSE core courses. The written exams include the topics from these courses, possibly augmented with a reading list provided to the student as preparation for the examination. The format is a day-long written examination.
- Oral specialization exam and artifact defense: This portion of the exam has two purposes: (1) to
 assess your knowledge in your specialization area and your preparation for advanced research in
 a computing, engineering, or science discipline; and (2) to check that you can integrate knowledge
 in mathematical foundations, computational methods, and knowledge in a specific engineering or
 science discipline to synthesize a concrete "computational artifact," e.g., a significant computer
 program. The student will create and document the computational artifact prior to the
 examination and share it with the committee members. The student must answer questions
 regarding the artifact itself and the accompanying written document following an oral
 presentation to the committee.

Student must pass two written qualifying exams to continue to the oral exam. The written exams are common to all home units. In contrast, each home unit typically has specific requirements for the specialization exam and artifact, as discussed below. If no specific requirements for a particular home unit are listed, the requirements for that home unit default to the requirements for the Computational Science and Engineering home unit.

9.9.3 Written Qualifying Exam

The written qualifying exams cover the five core areas, of which you select two: numerical methods, discrete algorithms, modeling and simulation, computational data analysis, and high-performance

computing. Each of these core areas provides a reading list composed of books and articles, and its scope covers the general topics taught in the corresponding core courses plus more advanced materials and application-oriented special topics (see Appendix A).

Each written exam contains four questions from one of the above core areas. Of these, you are expected to answer three questions during the written exam.

Grading and Results

You are expected to answer exactly three questions in each area. If you answer more than three questions in any area, then only the lowest scored three answers will be counted in that area.

There are two possible outcomes for each written exam: "pass" or "fail". Any student who passes their written exams in both areas may continue with the oral specialization exam and artifact defense. Students who do not pass a written exam will need to retake it (see Section 9.9.6), but if the student has passed one exam, only one exam will need to be retaken. It is not necessary to retake the written exam(s) in the same area(s) not passed previously. The CSE Written Exam Committee is responsible for developing and grading the written exams and determines the results.

9.9.4 Ph.D. Oral Qualifying Exam Committee

Your Ph.D. Oral Qualifying Exam Committee consists of your advisor (and co-advisor, if any) and three additional CSE program faculty members. One of the three committee members is assigned by the CSE programs director. The CSE programs director must approve your proposed committee.

The qualifying exam committee shall be present for the oral portion of the qualifying exam, which will take place after the written examination has been completed. The qualifying exam committee determines the outcome of the oral portion of the qualifying examination. To pass, a majority of your committee members, including at least three individuals, must vote "pass."

9.9.5 Oral specialization exam and artifact defense

Only students who passed written exams in two areas can take the oral exam. Each home unit typically has specific requirements for the specialization exam and artifact, as discussed below.

9.9.5.1 School of Biological Sciences

The second portion of the qualifying exam will cover both the computational artifact and the student's specialization area of Biological Sciences. This exam will consist of a formal written grant proposal following National Institutes of Health (NIH) or National Science Foundation (NSF) guidelines that will normally outline the student's thesis research proposal. The grant proposal is expected to describe, as part of the preliminary results, the student's prior research and development of a computational artifact that is related to the student's proposed thesis research. It will also include an oral presentation to the student's thesis committee of the student's prior research accomplishments working under the direction of his or her principal research advisor, with the biological research aspects of the work highlighted. The student will then defend the artifact and the thesis proposal, answering questions orally from the committee.

Frequently, the computational artifact will have been developed or will be under development as part of the student's research project. In such cases, the student must be sure to explain the biological relevance of this work and how it has or will be applied to biological problems. Students will be expected to demonstrate an understanding of basic biological concepts as they relate to their research project. The grant proposal should be submitted to the committee at least two weeks prior to the oral exam.

Finally, completion of the second portion of the qualifying exam fulfills the CSE program requirement for a dissertation proposal defense. Therefore, students homed in the School of Biological Sciences are not required to complete a separate thesis proposal defense in addition to the qualifying examination.

9.9.5.2 School of Chemistry and Biochemistry

The specialization and artifact defense is an exam that will cover both the computational artifact and the student's specialization area of Chemistry in a single oral examination session. The computational artifact

defense is an oral defense of the artifact (typically a software program developed by the student). The specialization part of the exam will consist of an oral presentation of the student's prior research accomplishments working under the direction of his or her principal research advisor, with the chemical aspects of the work highlighted. The student should also explain the relevance of this research and discuss their current and future research plans. Frequently, the computational artifact will have been developed as part of the student's research project. In such cases, the student must be sure to explain the chemical relevance of this work and how it has or will be applied to chemical problems. Students will be expected to demonstrate an understanding of basic chemical concepts as they relate to their research project. A written description of both the computational artifact and a summary of prior and current research (no more than 10 pages) should be submitted to the committee at least two weeks prior to the oral exam.

9.9.5.3 School of Civil and Environmental Engineering

The specialization exam and artifact defense will cover both the computational artifact and the student's specialization area within Civil and Environmental Engineering in a single oral examination session. The computational artifact defense is an oral defense of the artifact (typically a software program developed by the student). The specialization part of the exam will consist of an oral presentation of the student's prior research accomplishments working under the direction of his or her principal research advisor, with the CEE specialization aspects of the work highlighted. The student should also explain the relevance of this research and discuss their current and future research plans. Frequently, the computational artifact will have been developed as part of the student's research project. In such cases, the student must be sure to explain the civil and environmental engineering relevance of this work and how it has been or will be applied to CEE problems. Students will be expected to demonstrate an understanding of basic CEE concepts as they relate to their research project. A written description of both the computational artifact and a summary of prior and current research (no more than 10 pages) should be submitted to the committee at least two weeks prior to the oral exam.

9.9.5.4 School of Computational Science and Engineering

The oral exam consists of a student presentation of (a) prior and current research accomplishments of the student carried out under the direction of his/her principal research advisor; and (b) a computational artifact created by the student based on the above-mentioned research accomplishments. The student should explain the relevance of this research and discuss his/her current and future research plan.

The student will have created and documented the computational artifact prior to the examination and must answer questions regarding the artifact itself. For example, the student may be required to describe the purpose of the artifact and assess its strengths, weaknesses, and aspects of its design, such as the choice of computational algorithms or data structures. The student must also submit a written description of both the computational artifact and a summary of prior and current research (no more than 30 pages). The student must send this description to the committee members and the School of CSE's Programs Coordinator at least two weeks prior to the oral exam. Committee members may also ask to evaluate the source code comprising the computational artifact, which must also be available two weeks prior to the oral exam.

9.9.5.5 School of Mathematics

The written qualifying exam portion will be the same as for all CSE students. The oral part of the Qualifying exam can be combined with the Oral Comprehensive exam with approval of the CSE Math home unit coordinator after passing two written exams.

There will be one Oral Comprehensive exam for Ph.D. students homed in Math. This covers both a computational artifact and the student's specialization area of Applied and Computational Mathematics. The goal of the exam is for the students to present the chosen topic of their eventual dissertation to a core group of faculty who will likely become part of the Dissertation Committee.

The specialization part of the exam will consist of a report from the student on the research papers read and research accomplishments to date, highlighting the components related to applied and computational mathematics. It is expected that students will demonstrate an understanding of basic concepts in applied

and computational mathematics as they relate to their research project. The students will also be asked to explain the relevance of their specialization in the broad context of the CSE focus. This part of the exam follows the Oral Comprehensive Exam format of the Math Ph.D. program (http://www.math.gatech.edu/oral-comprehensive-exam). This is considered to be the thesis proposal in the school of Math, and the students will follow the same timeline as for the Math Ph.D.

In addition, a part of the oral presentation should have a section on the computational artifact. The computational artifact part will follow the same format as for all CSE Ph.D. students.

It is expected that the computational artifact will have been developed as part of the student's coursework and directed study under the direction of their advisors. The students will need to explain the relevance of this work in the context of applied and computational mathematics. The students will also need to explain how the computational artifact will be used as a platform for future computational methodology, theory and code developments.

A short description of the computational artifact and a list of selected readings, coursework, and relevant references (not to exceed 5 pages in total) will need to be submitted before the oral exam. After the exam, the students are required to submit the same paperwork as Ph.D. in Math (the Oral Comp Form and Oral Comp Survey form) to the Math home unit coordinator, in addition to filing all CSE program paperwork with CSE department.

9.9.5.6 Other Home Units

Other home units will follow the procedures outlined above for the CSE home unit. For additional information about the qualifying examination for other home units, please contact the home unit coordinator or CSE programs director.

9.9.6 CSE Qualifying Exam Administration and Final Exam Outcome

The written qualifying exam is usually offered in the Fall and Spring semesters. For Fall semester it is usually on the last Friday before the week of semester classes starts, and for Spring it is usually on Friday in the second week of the semester.

Students can declare intent, and attempt to pass written exams, at most three times. You must attempt the qualifying exam by the end of the second year of your enrollment in the CSE Ph.D. program. In each attempt, a student can take as many exams as needed to satisfy the remaining requirement. That is, in the first attempt, or if a student had failed both written exam areas in the previous attempt, the student can take two exams. Otherwise, if a student passed one exam and failed one exam, the student can take only one exam. If you do not pass the exam, you should retake it in the next semester when the exam is offered. Each student must pass two different areas to complete the written exams and can choose a different area in the second or third attempt.

Students may attempt to pass the oral exam at most two times. You should not schedule the oral portion during the first four weeks of classes, during which time the written exam is graded. If you do not pass the oral portion, you may attempt it a second time.

If you are homed in the School of CSE, some additional rules apply. You must take the oral portion of the exam in the same semester you complete the last written exam. You must pass the qualifying exam as a whole (both written and oral portions) by the end of the second year of enrollment in the CSE Ph.D. program.

To successfully complete the CSE Ph.D. qualifying exam, you need to pass both the written exams and the oral specialization and artifact exam. If you cannot, you should seek a Master's degree, as you will not be able to continue in the CSE Ph.D. program.

9.10 CSE Doctoral Dissertation

Your doctoral dissertation forms a central component of your CSE Ph.D. Through it, you show your ability to perform independent research, in collaboration with a faculty advisor, which you can defend to a committee of faculty. To complete your dissertation, you must complete three principal milestones:

• Ph.D. proposal defense. The aim of the proposal defense is for you to show that you are

prepared to carry out a high-quality doctoral dissertation. The proposal defense has two components. First, you must submit a written proposal documenting the research problem being addressed, discussion of related work, discussion of the research approach used to attack the problem, preliminary research results, and plans to complete the doctoral dissertation research. Second, you must defend this proposal to the doctoral dissertation committee in an oral defense. The proposal defense should be completed after some preliminary research has been conducted.

For students homed in the School of Biological Sciences, note that this requirement is combined with the second part of the qualifying examination.

- Ph.D. dissertation. You must document the body of your research work and your results in a
 formal dissertation document. Your research advisor (and co-advisor, if applicable) and
 doctoral dissertation committee must approve the final document. For campus guidelines on
 formatting, filing, and other logistics of your dissertation, please see
 http://www.gradadmiss.gatech.edu/theses-dissertations.
- *Ph. D. dissertation defense*. You must present an oral defense of the body of work included in the doctoral dissertation to the doctoral dissertation committee.

9.11 Applying to Ph.D. Candidacy

After you successfully present your research proposal (i.e., pass your Ph.D. proposal defense), you must petition for admission to Ph.D. candidacy by submitting the Georgia Tech Request for Admission to Ph.D. Candidacy form. To qualify for Ph.D. Candidacy, you must complete all coursework requirements, achieve a satisfactory scholastic record (3.3 GPA), pass the CSE Qualifying Examination, and submit an approved program of study and an approved thesis committee member form to the CSE programs advisor.

9.12 Doctoral Dissertation Committee

The doctoral dissertation committee includes at least five individuals and must include a balance of faculty spanning multiple disciplines. Typically, you would satisfy this latter requirement by having at least two members of the committee with an appointment in the College of Computing and at least two with an appointment in the College of Engineering or the College of Science. Your main Ph.D. advisor should be a member of your home unit and also a member of the CSE programs faculty. At least one of the five committee members must be a member of the faculty of another academic unit at Georgia Tech.

If you declared the Coulter Department of Biomedical Engineering, School of Chemistry and Biochemistry, School of Electrical and Computer Engineering, School of Materials Science and Engineering, Woodruff School of Mechanical Engineering, or School of Physics, as your home unit, at least three of the five Ph.D. dissertation committee members must be CSE Program faculty or faculty members from the home unit.

9.13 Obtaining a CSE Master's Degree while Pursuing a Ph.D. Degree

You have the option of obtaining a CSE Master's degree along the way to your Ph.D. once you have fulfilled the CSE M.S. requirements. You simply need to complete the CHANGE OF MAJOR/LEVEL FOR GRADUATE STUDENTS form, located through https://registrar.gatech.edu/info/change-majorlevel-form-graduate-students, and submit it to the CSE programs advisor, who will check that you may be awarded the CSE M.S.

10 SAMPLE COMPUTATION SPECIALIZATION COURSES

The following is a list of sample computational specialization courses. The courses are primarily grouped based on the five CSE core areas. (Courses marked with a '+' after the course number are the CSE core courses.) Courses marked '*' are offered through the distance learning program at the time of this writing.

Numerical Computing and Geometric Computing

- CSE/MATH 6643*+ Numerical Linear Algebra
- CSE/MATH 6644* Iterative Methods for Systems of Equations
- MATH 6640* Introduction to Numerical Methods for Partial Differential Equations
- MATH 6641 Advanced Numerical Methods for Partial Differential Equations
- MATH 6645 Numerical Approximation Theory
- MATH 6646 Numerical Methods for Ordinary Differential Equations
- MATH 6647* Numerical Methods for Dynamical Systems
- ISYE 6669* Deterministic Optimization
- ISYE 6679* Computational Methods
- CEE 6507 Nonlinear Finite Element Analysis
- ME 6104* Computer Aided Design
- ME 6758* Numerical Methods in ME
- ME/MSE/PTFE 6795 Mathematical, Statistical, and Computational Techniques in Materials Science
- ME 6124 Finite-Element Method: Theory and Practice
- CEE 6507 Nonlinear Finite Element Analysis
- · CS 6764 Geometric Modeling
- PHYS 6260 Computational Physics

Computational Data Analysis and Visualization Modeling and Simulation

- CSE/ISvE 6740*+ Computational Data Analysis
- CSE 6240 Web Search and Text Mining
- CSE 6241 Pattern Matching
- CS 6480 Computer Visualization Techniques
- CS 6485 Visualization Methods for Science and Engineering
- ISYE 6402* Time Series Analysis
- ISYE 6404 Nonparametric Data Analysis
- ISYE 6414* Statistical Modeling and Regression Analysis
- ISYE 6416 Computational Statistics
- ISYE 6783* Financial Data Analysis
- ISYE 7406 Data Mining and Statistical Learning

Modeling and Simulation

- CSE 6730*+ Modeling and Simulation: Fundamentals and Implementation
- CSE/INTA 6742 Modeling, Simulation, and Military Gaming
- CSE/CS 6236 Parallel and Distributed Simulation
- ISYE 6644* Simulation
- ISYE 6650* Probabilistic Models
- ISYE 6645 Monte Carlo Methods
- MATH 4255* Monte Carlo Methods
- ISYE 7210 Real-Time Interactive Simulation
- ME 6105 Modeling and Simulation in Design
- AE/ISYE 6779 Dynamic System Simulation and Modeling
- INTA 6004 Modeling, Forecasting and Decision Making

CSE Algorithms

- CSE 6140*+ CSE Algorithms
- CSE 6301* Algorithms for Bioinformatics and Computational Biology
- CS 6505* Computability, Algorithms, and Complexity
- CS 6550 Design and Analysis of Algorithms
- CS 7510 Graph Algorithms

High Performance Computing

- CSE 6220*+ High Performance Computing
- CSE 6221* Multicore Computing: Concurrency and Parallelism on the Desktop
- CSE/CS 6230* High Performance Parallel Computing: Tools and Applications
- CSE/CS 6236* Parallel and Distributed Simulation
- CS 6290 High Performance Computer Architecture
- CS 7110 Parallel Computer Architecture
- CS 7210 Distributed Computing
- ECE 6101 Parallel and Distributed Computer Architecture

Optimization

- ISYE 6644* Simulation
- ISYE 6661 Linear Optimization
- ISYE 6662 Discrete Optimization
- ISYE 6663 Nonlinear Optimization
- ISYE 6669* Deterministic Optimization
- ISYE 6679* Computational Methods in Operations Research
- MATH 4580* Linear Programming
- CSE/MATH 6643*+ Numerical Linear Algebra
- CSE/MATH 6644* Iterative Methods for Systems of Equations
- MATH 6640* Introduction to Numerical Methods for Partial Differential Equations
- MATH 6641 Advanced Numerical Methods for Partial Differential Equations
- MATH 6645 Numerical Approximation Theory
- MATH 6646 Numerical Methods for Ordinary Differential Equations
- MATH 6647* Numerical Methods for Dynamical Systems
- ISYE 6669* Deterministic Optimization
- ISYE 6679* Computational Methods
- CEE 6507 Nonlinear Finite Element Analysis
- ME/MSE/PTFE 6795 Mathematical, Statistical, and Computational Techniques in Material Sci.
- ME 6124 Finite-Element Method: Theory and Practice
- CEE 6507 Nonlinear Finite Element Analysis
- · CS 6764 Geometric Modeling

11 SAMPLE APPLICATION SPECIALIZATION COURSES

The number and type of CSE-related courses in application areas at Georgia Tech is large and varied. You should work with your advisor(s) to formulate sequences of coherent application specialization elective courses that best meet your research topics, objectives, and other goals. The following is a sample list of application specialization courses. The list is by no means exhaustive but is provided to give you some guidance. Courses marked '* are offered through the distance learning program at the time of this writing.

Fluid Dynamics and Turbulence

- AE 6009 Viscous Fluid Flow
- AE 6012* Turbulent Flows
- AE 6042* Computational Fluid Dynamics
- AE 6412* Turbulent Combustion

Structural Analysis

CEE 6551 Advanced Strength of Materials

Computational Chemistry

- CHEM 6472 Quantum Chemistry and Molecular Spectroscopy
- CHEM 6491 Quantum Mechanics
- CHEM 6485 Computational Chemistry
- CHBE/CHEM/MSE/PTFE 6751 Physical Chemistry of Polymer Solutions
- CHBE/CHEM/MSE/PTFE 6755 Theoretical Chemistry of Polymers
- CHEM 6481 Statistical Mechanics

Theoretical Ecology and Evolutionary Modeling

- MATH 4755 Mathematical Biology
- BIOL 6422 Theoretical Ecology
- BIOL 6600 Evolution
- BIOL 7101 Advanced Sensory Ecology

Bioinformatics

- BIOL 6150 Genomics and Applied Bioinformatics
- BIOL 7023 Bioinformatics
- BIOL 7111 Molecular Evolution
- BIOL 7110 Macromolecular Modeling
- CSE 6301 Algorithms for Bioinformatics and Computational Biology

Transportation Systems

- CEE 6601 Linear Statistical Models in Transportation
- CEE 6602 Urban Transportation Planning
- CEE 6603 Traffic Engineering

Gaming and Defense Modeling and Simulation

CS 7497 Virtual Environments

- INTA 6004 Modeling, Forecasting and Decision Making
- AE/ISYE 6779 Dynamic System Simulation and Modeling

Computational Electromagnetics

- ECE 6350 Applied Electromagnetics
- ECE 6380* Introduction to Computational Electromagnetics
- ECE 7380 Topics in Computational Electromagnetics

Manufacturing and Logistics

- ISYE 6201* Manufacturing Systems
- ISYE 6202* Warehousing Systems
- ISYE 6203* Transportation and Supply Chain Systems

Environmental Engineering

- CEE 6310 Physical Principles in Environmental Engineering
- · CEE 6311 Biological Principles in Environmental Engineering
- CEE 6312 Chemical Principles in Environmental Engineering

Materials Science and Engineering

- MSE6140 Computational Materials Science
- MSE 8803M Atomistic-Molecular Dynamics Simulation for MSE
- MSE8803D Density Functional Theory

12 APPENDIX A - Reading List for Written Qualifying Exam

12.1 NUMERICAL METHODS

Faculty

Nisha Chandramoorthy

Peng Chen

Edmond Chow, Lead

Felix Herrmann

Sung Ha Kang

Haesun Park

Florian Schäfer

Rich Vuduc

Haomin Zhou

The Numerical Methods exam is a closed-book exam and will focus on numerical linear algebra.

Suggested readings

- Matrix Computations by Golub and van Loan
- Numerical Linear Algebra by Trefethen and Bau

Other references

- Scientific Computing: An Introductory Survey by Michael T. Heath
- Applied Numerical Linear Algebra by J. W. Demmel

Required Core Course

CSE/MATH 6643 Numerical Linear Algebra

Additional Suggested Background Courses

- CX/MATH 4640 Undergrad Numerical Analysis
- CSE/MATH 6644 Iterative Methods for Systems of Equations

Main Topics

- · Problem conditioning, perturbation theory
- Stability, error analysis
- Floating point computation, parallel computation
- Computational complexity of algorithms
- SVD, QR, and other orthogonal factorizations
- Solving linear least squares problems, including rank deficient problems
- Gaussian elimination
- Iterative methods and their convergence for solving linear systems (Jacobi, Gauss-Seidel, etc.)
- Eigenvalue problems and their solution (symmetric and nonsymmetric)
- Krylov subspace methods for eigenvalues and linear systems (Lanczos, Arnoldi, CG, GMRES)

Notes

Most of the topics are covered at an elementary but graduate level in the course CSE/MATH 6643. Additional personal study from the suggested readings (Golub and van Loan; Trefethen and Bau) is required to succeed on the qualifying examination. The other references provide additional broad numerical methods background at an undergraduate level (Heath) and provide practical details at an advanced level (Demmel).

Topics involving iterative methods, including Krylov subspace methods are covered in the course CSE/MATH 6644. The course CX/MATH 4640 covers numerical methods broadly and is useful as a first course for anyone pursing research involving numerical methods.

12.2 DISCRETE ALGORITHMS

Faculty

Srinivas Aluru Ümit Çatalyürek Nabil Imam **Xiuwei Zhang, Lead**

The Discrete Algorithms exam is a closed-book exam.

Scope

Algorithm design (divide and conquer, dynamic programming, greedy), complexity analysis (running time, space requirements), NP-completeness proof, and optimization (branch and bound, local search, approximation algorithms).

Suggested readings

- (KT) J. Kleinberg and E. Tardos, Algorithm Design, Addison Wesley, 1st ed., 2005 (main reference, key chapters 4,6,7,8,11)
- (CLRS) T. Cormen, C. Leiserson, R. Rivest, and C. Stein. Introduction to Algorithms, MIT Press, 2010.
- (DPV) S. Dasgupta, C. Papadimitriou, and U. Vazirani, Algorithms, McGraw Hill, 2006

Other relevant material:

- · Guy Blelloch, Algorithms in the Real World, Lecture Notes
- D.S. Johnson, A Theoretician's Guide to the Experimental Analysis of Algorithms, in Proceedings of the 5th and 6th DIMACS Implementation Challenges, M. Goldwasser, D. S. Johnson, and C. C. McGeoch, Editors, American Mathematical Society, Providence, 2002.
- Hoos, Holger H., and Thomas Stützle. Stochastic local search: Foundations and applications.
 Elsevier, 2004. (local search, and experimentation)

Required Core Course

CSE 6140 Computational Science and Engineering Algorithms

12.3 MODELING AND SIMULATION

Faculty

Spencer Bryngelson Nisha Chandramoorthy Peng Chen Elizabeth Cherry Raphaël Pestourie **Richard Vuduc, Lead**

The Modeling and Simulation exam is a closed-book exam.

Scope

- Discrete event simulation methodology
 - o Conceptual models (e.g., queueing networks, petri nets, cellular automata), formalisms
 - DES world views and paradigms (e.g., event-oriented, process-oriented, agent-based simulation)
 - o Implementation issues (e.g., event list data structures, threads)
 - o Random number and random variate generation
 - o Input and output analysis
 - o Verification and validation
- · Parallel discrete event simulation
 - conservative synchronization: Chandy/Misra/Bryant, deadlock detection and recovery, synchronous execution, lookahead
 - optimistic synchronization: Time Warp, GVT algorithms, memory management, limiting optimism
 - hybrid approaches
 - Time parallel simulation
 - o Simulation interoperability, High Level Architecture
- · Complex systems
 - o cellular automata
 - o emergence
 - linear analysis
 - o bifurcations and chaos
 - o power laws, scaling
- Continuous simulation
 - o Boundary value problems for ODEs
 - o Elliptic and parabolic PDEs
 - o Finite difference methods
 - o Finite element methods
 - o Consistency, convergence, stability

Suggested readings Books

- L. G. Birta and G. Arbez, <u>Modeling and Simulation: Exploring Dynamic System Behavior</u>, Springer, 2007
- R. M. Fujimoto, Parallel and Distributed Simulation Systems, Wiley, 2000.
- H. Sayama, <u>Introduction to the Modeling and Analysis of Complex Systems</u>, Open SUNY Textbooks, 2015 (http://bingweb.binghamton.edu/~sayama/textbook/).

Articles

- S. Robinson, "Conceptual Modeling for Simulation," Winter Simulation Conference, December 2013.
- P. L'Ecuyer, "Random Number Generation with Multiple Streams for Sequential and Parallel Computing," Winter Simulation Conference, December 2015.
- R. Sargent, "Verifying and Validating Simulation Models," *Winter Simulation Conference*, December 2014.
- D. Jones, "An Empirical Comparison of Priority-Queue and Event Set Implementations", *Communications of the ACM*, 29, 4 (April 1986), 300-311.
- W. T. Tang, R.S.M. Goh, L-J. Thng, "Ladder Queue: An O(1) Priority Queue Structure for Large-Scale Discrete Event Simulation," ACM Transactions on Modeling and Computer Simulation, 15, 3 (July 2005), 175-204.
- R. M. Fujimoto, "Research Challenges in Parallel and Distributed Simulation," ACM Transactions on Modeling and Computer Simulation, Vol. 24, No. 4, March 2016.
- R. M. Fujimoto, "Time Management in the High Level Architecture," Simulation, Vol. 71, No. 6, pp. 388-400, December 1998.

Book chapters on continuous simulations

- Chapters 1, 2, 5, 6, *An Introduction to Computer Simulation*, by M. M. Woolfson and G. J. Pert, Oxford, 1999.
- Chapters 1-3,5 Numerical Solution of Partial Differential Equations, by K. W. Morton and F. Mayers, Second edition, Cambridge, 2005.

Required Core Course

CSE 6730 Modeling and Simulation: Fundamentals and Implementation

Other related courses include:

- CSE 6236/CS4230 Parallel & Distributed Simulation Systems
- AE/CS/ISYE 6778 Simulation Systems: Product and Process Life Cycles
- AE/ISYE 6779 Dynamic System Simulation and Modeling
- MATH 6640 Introduction to Numerical Methods for Partial Differential Equations

12.4 HIGH PERFORMANCE COMPUTING

Faculty

Srinivas Aluru, Lead Ümit Çatalyürek Edmond Chow Richard Vuduc

The High Performance Computing exam is a closed-book exam.

Scope

- Parallel algorithms: including prefix sums, sorting, matrix algorithms, FFT, embeddings.
- · Parallel architectures and interconnection networks
- · Programming models and communication primitives
- Performance metrics and bounds
- Load balancing and scheduling

Suggested readings

Books

Introduction to Parallel Computing, by Ananth Grama, Anshul Gupta, George Karypis, and Vipin Kumar, Addison Weslesy, 2003.

Articles

Gustafson, "Reevaluating Amdahl's Law," Communications of the ACM, May 1988

Twelve Ways to Fool the Masses When Giving Performance Results on Parallel Computers; by David H. Bailey; *Supercomputing Review*, Aug. 1991, pg. 54–55.

Required Core Course:

CSE 6220 High-Performance Computing

Other related courses include:

- CSE 6230 / CS 6230 High-Performance Computing: Tools and Applications
- CS 6290 High-Performance Computer Architecture

12.5 DATA ANALYSIS

Faculty

Mark Borodovsky

Polo Chau

Bo Dai

Victor Fung

Srijan Kumar

Yunan Luo

Haesun Park

Aditya Prakash

Florian Schäfer

Anqi Wu

Chao Zhang, Lead

The Data Analysis exam is a closed-book exam.

Scope

- Supervised Learning
 - o Linear Regression (Ordinary Least Squares, Ridge, and Lasso Regression)
 - o Linear Classification (Logistic Regression, Perceptron, discriminant analysis)
 - Support Vector Machines (SVM) and Kernel Methods
 - o K-Nearest Neighbors (KNN)
 - Decision Trees and Ensemble Methods (Random Forest, Boosting, Bagging)
 - o Neural Networks (Feedforward, Convolutional, Recurrent)
- Unsupervised Learning
 - Clustering (K-means, DBSCAN, Agglomerative Hierarchical)
 - o Gaussian Mixture Models (GMM) and Expectation-Maximization (EM) Algorithm
 - o Principal Component Analysis (PCA) and Independent Component Analysis (ICA)
 - Non-negative Matrix Factorization (NMF) and Singular Value Decomposition (SVD)
- Optimization and Inference Techniques
 - Gradient Descent (Batch, Stochastic, Mini-Batch, Backpropagation)
 - o Newton's Method and Quasi-Newton Methods (BFGS, L-BFGS)
 - Conjugate Gradient
 - Maximum Likelihood Estimation (MLE) and Maximum A Posteriori (MAP) Estimation
 - Variational Inference
 - Monte Carlo Methods (MCMC, Gibbs Sampling, Metropolis-Hastings)
 - KKT condition and Lagrangian
- Basic Learning Theory and Evaluation
 - Bias-Variance Tradeoff
 - Overfitting and Regularization
 - Cross-Validation and Model Selection
 - o Probably Approximately Correct (PAC) Learning Theory
 - o Generalization Bounds and VC Dimension

Suggested readings

Books

- C. Bishop. Pattern Recognition and Machine Learning, Springer, 2006.
- Wasserman. All of Statistics, Springer, 2006.
- Hastie et al. The Elements of Statistical Learning, Springer, 2001.

- Kevin Murphy, Machine Learning: A Probabilistic Perspective, 2012.
- lan et al., Deep Learning, 2016.
- Mohri et al., Foundations of Machine Learning, 2018.

Required Core Course:

CSE/ISYE 6740 Computational Data Analysis

Other related courses include

- ISYE 6650 Probabilistic Models
- ISYE 6663 Nonlinear Optimization
- ISYE 6404 Nonparametric Data Analysis
- CSE 6240 Web Search and Text Mining
- CSE 6242 Data and Visual Analytics