

Certificate in Computational Science and Engineering

December 2, 2008

Contents

1	Introduction	3
2	Admission to the Program	3
3	Requirements	3
4	Satisfactory progress	4
5	Course structure	5
6	Sample Courses of Study	5
7	Using credits elsewhere	5
8	Administration	6
8.1	Director and committee	6
8.2	Web page	6
8.3	Modifying the courses and requirements	6
8.4	Admissions Procedure	6
8.5	Affiliated Faculty	6
8.6	Signatures and Awarding the Certificate	7
A	Appendix: Courses	8
A.1	Chemical Engineering	8
A.1.1	Core course	8
A.1.2	Advanced courses	8
A.2	Civil and Environmental Engineering	8
A.2.1	Foundation Courses	8
A.2.2	Advanced Courses:	9
A.3	Computer and Information Sciences	9
A.4	Electrical and Computer Engineering	11
A.4.1	Foundation course	11
A.4.2	Advanced course	11
A.5	Mathematical Sciences	12
A.5.1	Core course	12
A.5.2	Foundation courses	12
A.5.3	Background courses	12
A.5.4	Advanced courses	13
A.6	Mechanical Engineering	13
A.6.1	Advanced courses	13

A.7	Physics and Astronomy	13
A.7.1	Core courses	13
A.7.2	Foundation courses	14
B	Appendix: Checklist for Certificate Completion	15

1 Introduction

The goal of this document is to outline the structure and requirements of a Certificate in Computational Science and Engineering at the University of Delaware. The philosophy of the program is that we increase the capabilities and understanding of the student in a broad range of areas utilizing floating point or symbolic computation for solving medium to large scale problems in computational mathematics, science and engineering.

This is an interdisciplinary program currently involving seven departments and two colleges (Arts & Science and Engineering). The post-baccalaureate Certificate in Computational Science and Engineering may be completed with non-degree graduate status or as part of a graduate degree program. Students in this certificate program may thus have full- or part-time status.

This program grew out of a series of meetings from faculty and students interested in Computational Science and Engineering that began in the 06F semester; these meetings were organized by P. Monk (Mathematical Sciences). The Certificate program was developed in a joint effort by the following members of an *ad hoc* committee beginning in the 08S semester: R. Braun (Mathematical Sciences), A. Beris (Chemical Engineering), J. MacDonald, (Physics and Astronomy), L. Pollock (Computer and Information Sciences), M. Shay (Physics and Astronomy), M. Taufer (Computer and Information Sciences), L-P. Wang (Mechanical Engineering), D. Weile (Electrical and Computer Engineering) and P. Monk. This program also benefitted from significant input from a number of other faculty, notably D. Saunders (Computer and Information Sciences).

2 Admission to the Program

Application to the Certificate in Computational Science and Engineering program is submitted using the on-line graduate admission application that includes a statement of purpose, two letters of recommendation and transcripts from all previous college or university study.

Students currently matriculated in a graduate degree program should complete a “Change of Classification Form” to seek approval to add the Certificate in Computation Science and Engineering Program.

3 Requirements

We propose a 15 unit requirement for the certificate and that it be a post-baccalaureate certificate. Students must have a Bachelor degree in the sciences or engineering and should have background in the following areas: (i) fluency in a programming language such as C, C++, or Fortran, etc.; (ii) linear algebra; (ii) differential equations; (iv) multidimensional calculus; (v) undergraduate-level data structures. Non mathematics students may be able to make up one of these areas via mathematics courses listed below.

Students are required to choose an appropriate advisor associated with the certificate program, or have an appropriate advisor appointed by the Director of the Certificate Program, who will be the primary contact for questions. The student will develop a plan for the certificate with the advisor before the beginning of the second course. The Director of the Certificate Program will verify that the student has completed the requirements for the certificate and will approve the application for the certificate upon successful completion of the requirements.

A total of 15 credits from the list given below are required for this post-baccalaureate certificate. The student is required to take CISC 621 and *one* of the following: MATH 607, PHYS 660 or CHEG 827. The student must complete courses in three different departments from the list in Table 1. At least one 800 level course must be taken from the certificate course list in this table; CHEG 827 does not satisfy this requirement.

A student with sufficient background may waive up to six credits of the required courses.

Department	Courses		
	500 level**	600 level	800 level
Chemical Engineering (CHEG)			827*, 831, 841
Civil and Environmental Engineering (CIEG)		601, 605	801
Computer and Information Sciences (CISC)		601, 603, 604, 621*, 636, 637, 649, 675, 681, 683	841, 849, 879 [‡] , 886, 887, 889
Electrical and Computer Engineering (ELEG/CPEG)		CPEG 655	ELEG 841
Mathematical Sciences (MATH)	503, 529, 535	607*, [†] , 611, 612, 694	838
Mechanical Engineering (MEEG)			867 [‡]
Physics and Astronomy (PHYS)		650, 660*	

Table 1: The courses for the Certificate in Computational Science and Engineering program. * indicates the courses from which the required courses must be selected. **Credit for one of these 500 level background courses can be applied to the certificate requirements for students not in a degree program in the Department of Mathematical Sciences. [†]These courses are to be created by the respective departments. [‡]These topics courses may have multiple descriptions and subjects.

Students may earn up to three credits as 866 Special Problems if approved by the advisor instead of one of the nine credits after the required core courses above. The advisor will grade the 866 course if the work is done as part of employment outside the university.

4 Satisfactory progress

Students in the Computational Science and Engineering certificate program must achieve a grade of B- or better to obtain credit for a course from the list. Students must obtain at least a 3.0 cumulative grade point average in the courses from the list to obtain the certificate.

5 Course structure

We propose that the student take two of the following core courses. The required course list is

- CISC621 Algorithms

and *one* of the following

- MATH 607 Survey of Scientific Computation.
- PHYS 660 Computational Methods in Physics.
- CHEG 827 Chemical Engineering Problems.

The student must take courses from three different departments. One course must be at the 800 level (CHEG 827 does not satisfy this requirement).

Student with sufficient background may waive up to 6 credits to replace one or both of the required courses from the required course list above with the approval of the advisor. No credits may be transferred from another University or degree program toward this certificate.

6 Sample Courses of Study

The following sample courses of study are examples, and in no way exhaust the many possibilities of combining courses to obtain this Certificate.

General Emphasis	Courses
Mathematics	CISC 621, MATH 607, 612, 838, and CHEG 831
Bioinformatics	CISC 621, 637, 849, CHEG 827, CPEG 655
Chemical Engineering	CISC 621, CHEG 827, CPEG 655 and CHEG 831, 841
Finite Element Analysis	CISC 621, PHYS 660, CIEG 601, 801, MATH 838 or MEEG 867 or CHEG 831 or ELEG 841
Fluid Dynamics	CISC 621, CHEG 827, CPEG 655 and MEEG 867 (both flavors)

7 Using credits elsewhere

Credits may be applied to a degree program at the discretion of the Department housing the degree program. We expect that, at a minimum, the majority of credits may be applied to a graduate degree program. This also applies to dual Bachelor/Master degrees.

8 Administration

8.1 Director and committee

We propose that the Director of the Certificate in Computational Science and Engineering program be a rotating position, and that the Director be the chairperson of a committee consisting of one representative from each department offering courses for the certificate. The total number on the committee should be the number of departments involved plus one. There will be one vote per department; the Director and departmental representative will decide between them the method for casting that single vote. The Director will be a rotating position among departments interested in hosting the position; this will be subset of the departments offering courses for the certificate. Because of a significant amount of time and effort spent in starting up the program, we propose that the Director be located in Mathematical Sciences for the first two years to get things started. Then, the position will rotate annually.

8.2 Web page

A web page needs to be developed for the program as well. We propose that this begin in Mathematical Sciences for the first two years, and that the web page be placed on the university server. The annual change of director will move responsibility for maintaining the web page to that same department.

8.3 Modifying the courses and requirements

Proposed changes to the course list for the certificate program may originate in participating departments, from the Director, or from the committee. We propose that the committee vote on proposed changes, with a 2/3 majority required for passage. Votes may be via email or meeting. It is the responsibility of the Director to implement, or to delegate to the appropriate Director of Graduate Studies, the changes in the catalog, the web page and any other location required. These will need to be submitted through the Faculty Senate and its Graduate Studies Committee; program changes and course changes in Arts and Science need to go through the CAS Educational Affairs committee.

8.4 Admissions Procedure

Committee of the Director plus departmental representatives shall meet during the last month of the semester to review applicants for the certificate program. We propose application deadlines of November 15 and April 1st for this program for students seeking graduate non-degree status. Students entering degree programs who have expressed interest in the Certificate in Computational Science and Engineering will have the admission decision made by the department with the degree program; the student may subsequently use a change of classification form to enter the certificate program.

8.5 Affiliated Faculty

We propose that the affiliated faculty be any faculty who helped draft this document listed above, the Graduate Program Directors of participating departments (those with courses listed here) and

any faculty who have taught the courses listed below, or are interested in teaching them, and express interest in being affiliated with the program.

8.6 Signatures and Awarding the Certificate

Upon successful completion of the certificate requirements, each student will receive a printed certificate. The certificate itself is printed by the Office of the Assistant Provost for Graduate and Professional Education. It will be signed by the Office of Graduate and Professional Education, the Provost and the Director of the Certificate in Computational Science and Engineering Program at the time of completion. The certificate will be noted on the student's transcript.

A Appendix: Courses

Potential contributions from Departments (in alphabetical order) are given below.

A.1 Chemical Engineering

A.1.1 Core course

CHEG 827 Chemical Engineering Problems. (3) *Description:* The application of numerical methods for the solution of chemical engineering problems. Linear and nonlinear analysis. Numerical methods applied to the solution of ODEs, PDEs and optimization problems with applications to fluid flow, heat and mass transfer reaction engineering. Monte-Carlo and molecular dynamics. PREREQ: Undergraduate linear algebra and differential equations.

A.1.2 Advanced courses

CHEG 831 Chemical Engineering Principles I. (3) *Description:* Equips incoming graduate students with necessary applied mathematical background emerging from a discussion of Chemical Engineering Principles in Kinetics, Thermodynamics, and Transport phenomena. Linear algebra, ordinary differential equations, and stochastic differential equations are typical topics covered. PREREQ: n/a.

CHEG 841 Chemical Engineering Principles II. (3) *Description:* Second of two required courses (first one CHEG831) to equip graduate students with applied mathematical and statistical background emerging from a discussion of Chemical Engineering Principles in Kinetics, Thermodynamics and Transport Phenomena. Topics include vector and tensor analysis, partial differential equations, statistical analysis of experiments, design of experiments and molecular dynamics, and stochastic simulations. PREREQ: n/a.

A.2 Civil and Environmental Engineering

A.2.1 Foundation Courses

CIEG 601 Introduction to the Finite Element Methods (3). *Description:* Discusses the following approximate solution techniques: finite difference method, weighted residual and variational methods, and the finite element method. Develops finite element solutions for various one- and two-dimensional problems in applied mechanics. Detailed discussions of various aspects associated with the finite element method (e.g., interpolation functions, element mapping, programming techniques). PREREQ: CIEG 381.

CIEG 605 Intermediate Topics in Finite Element Analyses (3). *Description:* Topics include finite element analyses of linear steady-state scalar field problems, linear elastostatics, analysis techniques for linear transient and dynamic analyses of solids, overview of elements commonly used in matrix structural analyses. In each case, element formulations and solution algorithms are assessed, limitations and possible improvements are presented and numerical methods examined. PREREQ: CIEG 601.

A.2.2 Advanced Courses:

CIEG 801 Advanced Finite Element Methods (3). *Description:* Discusses sources of nonlinearities in finite element analyses. Applies the finite element method to nonlinear one-, two-, and three-dimensional problems in solid mechanics. Discusses basic and advanced numerical methods and computer programming techniques appropriate to nonlinear finite element analyses. PREREQ: CIEG 401.

A.3 Computer and Information Sciences

Core Course

CISC 621 Algorithms (3). *Description:* Emphasis on developing expertise in the design and analysis of algorithms. Equal importance given to techniques and specific algorithms. Particular topics include advanced data structures, graph algorithms, disjoint set manipulation, sorting and selection, amortized analysis, NP-completeness, and matrix and polynomial multiplication. PREREQ: Undergraduate algorithms and discrete math courses.

Foundation (6xx) and Advanced (8xx) courses

CISC 601 Theory of Computation (3). *Description:* General models of computation, formal languages and automata theory, and algorithmic unsolvability. PREREQ: A course in which the student was required to prove theorems.

CISC 604 Logic (3). *Description:* Formal introduction to first-order logic with emphasis on its relevance to computer science. Syntax, semantics, models, formal proofs and results on soundness, consistency, completeness, compactness and undecidability. Automated theorem proving also covered. PREREQ: CISC304 equivalent.

Building Reliable Software Systems

CISC 603 Program Validation (3). *Description:* Specification and verification of programs. Testing through the use of formal and informal verification techniques, program design is made more effective and product quality (meeting specifications) is enhanced. PREREQ: CISC304 equivalent.

CISC 675 Software Engineering (3). *Description:* Introduction to software engineering concepts, methodologies and tools. Requirement analysis, specification, design and implementation of object oriented software development process. Students will be presented with several real life examples and homework projects to cover all aspects of object oriented lifecycle, from the requirements to coding in C++. RESTRICTIONS: Requires C/C++ and permission of instructor. Credit cannot be received for both CISC675 and CISC475. PREREQ: n/a.

CISC 879 Software Testing and Maintenance (3). *Description:* This course is a study of software testing and maintenance methodologies for object-oriented, component-based, concurrent, distributed, and web software. Topics include approaches to automatic test case

generation, test oracles, coverage analysis, prioritized testing, construction of tools, regression testing and impact analysis. A primary focus will be program-based software testing and maintenance approaches. PREREQ: n/a.

CISC 879 Software Support for Multicore Architectures (3). *Description:* Introduction on how to properly design applications to utilize multicore parallelism. The course will address the problem of optimizing multicore software spanning multiple levels of the software stack. Students will participate in discussions about current multicore architectures and parallel programming models. PREREQ: n/a.

Bioinformatics

CISC 636 Intro to Bioinformatics (3). *Description:* Introduction to concepts, methodologies, and tools in bioinformatics. Abstraction of biological problems for computational solutions. Genome sequencing and assembly, bio-sequence comparison and database search, dynamics programming, hidden Markov models, and phylogenetic trees. PREREQ: CISC220 or permission of instructor. RESTRICTIONS: Credit can not be earned for both CISC636 and CISC436.

CISC 841 Bioinformatics (3). *Description:* Advanced topics in current bioinformatics research, such as hidden Markov models, kernel based methods, and bayesian based analysis with applications to functional annotation, structural prediction, and biological networks inferences. PREREQ: CISC436 or CISC636 or permission of instructor.

CISC 849 Performance Parallel Algorithms for Computational Science (3). *Description:* This course presents Molecular Dynamics and Monte Carlo algorithms for computational science applications, parallelization of these algorithms on high performance computing systems using MPI and OpenMP, and performance analysis and optimization of the parallel applications. PREREQ: C programming skills required.

Application-specific Computation Techniques

CISC 637 Databases (3). *Description:* Physical and logical organization of databases. Data retrieval languages, relational database languages, security and integrity, concurrency, distributed databases. PREREQ: CISC220 and CISC304 or equivalent. RESTRICTIONS: Credit cannot be received for both CISC637 and CISC437.

CISC 683 Introduction to Data Mining (3). *Description:* Data Mining attempts to identify interesting structural patterns in large data sets that can be used to make future predictions. This course will introduce fundamental strategies and methodologies for data mining along with the concepts underlying them, and will provide hands-on experience with a variety of different techniques. Students will learn to use the Weka workbench, a set of data mining tools. PREREQ: n/a.

CISC 889 Machine Learning (3). *Description:* Machine Learning is the study of computing systems that improve their "performance" with "experience". The primary focus is to provide an understanding of the underlying algorithms used in various widely-studied learning

methods and show how they are used in practice. PREREQ: Requires permission of instructor.

CISC 886 Multi-agent systems (3). *Description:* Introduction to the field of Multi-Agent Systems, examining issues that arise when groups of self-interested or cooperating autonomous agents interact to solve shared problems. Issues include reasoning about the knowledge and beliefs of other agents, communication and negotiation, computational organization, coordination and control. PREREQ: CISC681 or equivalent.

CISC 887 Internet Information (3). *Description:* Approaches to information gathering, filtering, and integration including work in the heterogeneous database, information retrieval and agent-oriented communities. Text indexing, vector-based and probabilistic retrieval, semantic web technologies, wrappers and mediators, query planning and optimization, collaborative filtering, information agents, applications. PREREQ: CISC681 or equivalent.

CISC 649 Computer Vision (3). *Description:* Introduction to the analysis of images and video to recognize, reconstruct, model, infer static, and dynamic properties of objects in the 3D world. Study geometry of image formation; basic concepts in image processing; segmentation; techniques for 3D reconstruction, and image registration methods. PREREQ: n/a. RESTRICTIONS: Credit cannot be received for both CISC649 and CISC449.

CISC640 Computer Graphics (3). *Description:* Computer graphics technology, two- and three-dimensional systems, graphics software systems, modeling and object hierarchy, and animation. PREREQ: CISC220 or equivalent. COREQ: CISC320 recommended. RESTRICTIONS: Credit cannot be received for both CISC640 and CISC440.

CISC 681 Artificial Intelligence (3). *Description:* Programming techniques for problems not amenable to algorithmic solutions. Problem formulation, search strategies, state spaces, applications of logic, knowledge representation, planning and application areas. PREREQ: CISC220 and CISC304 or equivalent. RESTRICTIONS: Credit cannot be received for both CISC681 and CISC481.

A.4 Electrical and Computer Engineering

A.4.1 Foundation course

CPEG 655 High-Performance Computing w/Commodity Hardware (3). *Description:* New commodity parallel computing devices, including Graphics processing units (GPUs) and IBM Cell processor, bring the originally elite high performance computing into the reach of general public. To program and accelerate applications on the new high performance computing devices, we must understand both the computational architecture and the principles of program optimization. This course discusses GPU and IBM Cell hardware, as well as concepts and techniques for optimizing general purpose computing on the new architectures. PREREQ: None.

A.4.2 Advanced course

ELEG 841 Advanced Computational Electromagnetics II (3). *Description:* Introduces the major modern computational methods for the analysis of frequency domain electromagnetics

problems. The finite element method and the method of moments are covered. Students will apply these techniques to radiation and scattering problems involving metal and dielectrics. PREREQ: ELEG 648.

A.5 Mathematical Sciences

A.5.1 Core course

MATH 607 SURVEY OF SCIENTIFIC COMPUTING (3). *Description:* Numerical solution of linear systems; interpolation; differentiation and quadrature; transforms/FFT; non-linear equations; initial value problems; boundary value problems; monte carlo methods; finite difference methods for partial differential equations. Additional topics at the discretion of the instructor. PREREQ: Linear algebra, differential equations, multivariable calculus. RESTRICTION: Cannot be applied toward a degree program in the Department of Mathematical Sciences.

A.5.2 Foundation courses

MATH 611 INTRO TO NUMERICAL ANALYSIS AND SCIENTIFIC COMPUTING (3). *Description:* Introduction to numerical computing, analysis and solution of systems of linear equations, linear least-squares, eigenvalue problems, methods for unconstrained optimization, solution of systems of nonlinear equations. Experience with standard computer packages, code development and simulations of applied problems. PREREQ: Linear algebra and multivariate calculus.

MATH 612 INTRO TO NUMERICAL METHODS FOR PDEs (3). *Description:* Basic finite difference schemes for standard model problems. Schemes for integrating time dependent problems (including ordinary differential equations). Curved boundaries. Dispersion and Von Neumann analysis. Lax equivalence theorem and the CFL condition. PREREQ: linear algebra, multivariate calculus and differential equations.

MATH 694 METHODS OF OPTIMIZATION (3). *Description:* Methods of solving optimization problems in finitely many variables, with or without constraints. Steepest descent, quasi-Newton methods (e.g. BFGS and conjugate gradient). Quadratic programming and complementarity. Interior point methods. Sequential quadratic programming. Cutting planes and non-smooth optimization. Max-flow/min-cut for network optimization. PREREQ: Multivariate calculus and linear algebra.

A.5.3 Background courses

These courses could count toward the certificate for students who are not in a degree program in the Department of Mathematical Sciences. The 500 level courses count as graduate courses in other departments; up to one 500 level course from this list may be applied to the certificate requirements.

MATH 503 ADVANCED CALCULUS FOR APPLICATIONS (3). *Description:* Change of variables, surface integrals, Stokes Theorem, Divergence Theorem, Calculus of Variations, Eulers Equation, Brachistochrone and isoperimetric problems. Introduction to the qualitative theory of ordinary differential equations, including linear systems, phase space analysis,

Lyapunovs Methods, and elements of the analysis of nonlinear systems. PREREQ: 300 level or above courses in ordinary differential equations and linear algebra.

MATH 529 FUNDAMENTALS OF OPTIMIZATION (3). *Description:* Maximization and minimization of functions of finitely many variables subject to constraints. Basic problem types and examples of applications; linear, convex, smooth, and non-smooth programming. Optimality conditions. Saddle points and dual problems. Penalties and decomposition. Overview of computational approaches. PREREQ: Linear algebra (MATH349) and vector calculus (MATH243).

MATH 535 PARTIAL DIFFERENTIAL EQUATIONS (3). *Description:* Theory and applications of parabolic, elliptic and hyperbolic partial differential equations originating from various mathematical physics problems. (includes classification, separation of variables, series and transform solutions, simple nonlinear problems. The prerequisites should have "or equivalent" added here.) PREREQ: MATH302 or MATH342 or MATH352.

A.5.4 Advanced courses

MATH 838 TOPICS IN NUMERICAL ANALYSIS (3). *Description:* Topics in numerical analysis at the discretion of the instructor. PREREQ: MATH612 or equivalent.

A.6 Mechanical Engineering

A.6.1 Advanced courses

MEEG 867 Mesoscopic CFD method (3). *Description:* Introduction to lattice Boltzmann equation and its applications as a numerical approach to single and multiple-phase flows. Relationships between microscopic operation rules and macroscopic differential equations. Treatment of complex boundary conditions and multiscale fluid-fluid and fluid-particle interfaces. Examples of lattice-Boltzmann computer simulations. PREREQ: n/a.

MEEG 867 Computational Multiphase Flows (3). *Description:* Overview of different numerical methods for multiphase flows involving moving boundaries and fluid-fluid interfaces. Students will work with example codes to understand physical and numerical issues such as variations with key governing parameters, numerical convergence, accuracy, and stability. PREREQ: MEEG 630 or permission of instructor.

A.7 Physics and Astronomy

A.7.1 Core courses

PHYS 660: Computational Methods in Physics (3). *Description:* Introduction to basic computational techniques in science with application to a number of disciplines of current research interest, such as quantum physics, biophysics, statistical mechanics and chaos. PREREQ: n/a.

A.7.2 Foundation courses

PHYS 650 Quantum computation (3). *Description:* Introduction to quantum computation and quantum information. Quantum logic gates and quantum circuits. Efficient quantum algorithms: quantum Fourier transform and its applications and quantum search algorithms. Physical implementations of quantum computation. Quantum error-correction and fault-tolerant quantum computation. Quantum cryptography. **PREREQ:** Prior knowledge of quantum mechanics recommended and familiarity with linear algebra.

B Appendix: Checklist for Certificate Completion

Checklist for the Computational Science and Engineering Certificate
University of Delaware

Name of Student: _____ Begin Date: _____

Status: Non-degree _____ Degree _____ Department: _____

Advisor: _____

Requirements:

CISC 621 _____ or waived _____ (3 cr)

MATH 607 or PHYS 660 or CHEG 827 _____ or waived _____ (3 cr)

Courses from the list and from at least three participating depts _____

At least one 800 level course from the list above (excluding CHEG 827) _____

A total of 9 credits from allowed course list _____

All grades B- or better in the 15 credits from the Certificate courses _____

Cumulative GPA of 3.0 or better for the Certificate courses _____

I hereby certify that the above student has completed the requirements for the Computational Science Certificate.

Director, Certificate in Computational Science and Engineering Date

Upon approval, please route this form to the Office of Graduate and Professional Education.