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A Proposal for a Certificate Program in Simulation-Based Engineering and Science (SBE&S)

I. Introduction

Over the past fifteen years, in response to the increasingly important role of high-performance computing in scientific and engineering research, graduate and undergraduate educational programs in computational science and engineering have blossomed throughout the US. A good starting point for the discussion of such programs is the Society for Industrial and Applied Mathematics' (SIAM) report available at www.siam.org/students/resources/report.php, which also has a link to a number of CSE programs worldwide, as well as the synopsis of the panel discussion of such programs which took place at the last SIAM Conference on Computational Science and Engineering (see the May 2009 issue of SIAM News). Given SMU's emphasis on scientific computing, ongoing efforts to strengthen graduate programs in the sciences and engineering, and opportunities to serve local industry, we believe that such a program should be developed here.

Nationally, two distinct program structures can be found - full-fledged degree programs and minors and/or certificates. We believe the latter is more appropriate at SMU.

The purpose of the proposed SBE&S certificate program is, first of all, to provide students in Engineering, Science and Mathematics the opportunity to complete a structured educational program in applied high-performance computing, while still satisfying all requirements of a traditional degree program, and, second, to allow people who have already completed their degree program to further their professional development. The key points in the design of the program are:

- a.** Development of a coherent and meaningful set of courses whose completion will prepare students to use high-performance computing within their disciplines. This should benefit not only the students but also research programs within the departments.
- b.** Facilitate the broad participation of departments in Science and Engineering as well as industry by keeping the requirements as streamlined as possible. In particular, SBE&S students should be able to fully satisfy departmental degree requirements without significantly delaying graduation.
- c.** Encourage collaboration among faculty and students interested in the application of high-performance computing in their disciplines.

II. Details

Requirements: Requirements for completing the certificate would include:

1. Completion of a two-course core sequence. Proposed content is discussed below.
2. Completion of a third elective - individual departments, with the approval of the program, will determine which courses will satisfy the requirement for their majors. For example, mathematics would require an outside course emphasizing computation in some application discipline, while other departments may require courses which focus on discipline-specific software packages. A general list of electives for certificate-only students will be maintained.
3. Two semesters of participation in the SBE&S seminar. (One credit per semester.) We feel this additional requirement is important both to develop a sense of camaraderie between the participating students and to foster collaborative research. Speakers will include participating faculty and students from SMU, as well as outside speakers. (We expect the University to provide some funding for the latter.)

Administration: The Center for Scientific Computing (CSC) will provide a home for the program. A committee consisting of the director of the Center and participating faculty from throughout the university (as well as an industry representative if possible) will be responsible for monitoring the program (courses, seminar, etc). The committee will be appointed by the director of the CSC with the approval of the chairs of the participating departments. The director will be provided administrative assistance by the mathematics department to keep track of students (handling applications, checking graduation requirements, etc).

Core Courses and Admission Requirements : A list of core material for SBE&S education typically includes some combination of numerical and statistical methods as well as computing languages and operating systems. Our proposed design of these courses will allow broad participation, including biological, chemical, and earth scientists as well as students from engineering and physics. Therefore, we would like to have the minimal prerequisites needed to run meaningful courses - linear algebra, calculus, and some computing experience (e.g. with Matlab, Maple, or Mathematica). Proposed topics for the core sequence are:

Course 1: Introduction to Computational Science i. Compiled language programming in the Unix environment - (e.g. C, C++, F90).

ii. Direct and iterative linear solvers with an introduction to relevant software (LAPACK).

iii. Nonlinear solvers (Newton's method and variants, optimization).

iv. Quadrature and differential equations with an introduction to relevant software.

v. Monte Carlo methods.

Course 2: Introduction to Parallel Scientific Computing i. Shared- and distributed-memory parallel programming and performance evaluation (e.g. OpenMP, MPI).

ii. Parallel solver libraries (e.g. PETSc, ScaLAPACK, TriLin, FFTW).

iii. Applications to solving partial differential equations and/or large scale optimization and data analysis problems.

The expertise for teaching such classes resides not only within mathematics, so the courses may be cross-listed with other departments as appropriate.

Funding: We expect the administrative costs associated with the program will be minimal, and will be handled by the staff assigned to the CSC. (At its current level of activity this is provided by the mathematics department.) Some small budget will be needed to support the SBE&S seminar, particularly to support one outside speaker per semester. In addition it would be desirable if the program were able to offer a small number of TAs. This would encourage participating departments to recruit graduate students interested in scientific computing. The TAs could assist in the teaching of the required courses and also be given tasks at the University's high-performance computing facility (e.g. user support, software installation etc). The CSC will also seek outside funding for students in the certificate program.