Proposal Overview and Table of Contents

1. Project Description

A. Project Request: Capital University on behalf of the Undergraduate Computational Science Educational Consortium, respectfully submits this request for $487,451 from the W. M. Keck Foundation to establish the **Keck Undergraduate Computational Science Educational Consortium** (**KUCSEC**) for the development and implementation of educational materials that contribute to an undergraduate Computational Science curriculum. This project addresses the current lack of integration of mathematics and computer science with other sciences at the undergraduate level. The 25-month project will span from June 2002 to June 2004.

B. Institutional Computational Science History: Capital University has demonstrated leadership in undergraduate Computational Science – recognizing that this emerging and rapidly growing interdisciplinary field integrates computing, mathematical modeling, and visualization to solve problems in the physical, natural and behavioral sciences, finance and engineering. Computational Science is one of the top priorities of Capital University, as demonstrated by the October 2000 visit by Capital's former President to the W. M. Keck Foundation and by the continuing support by Capital's current President and Board of Trustees (Administrative Letters of Support are in **Appendix E**). Computational Science fits with Capital University's mission and vision to earn national recognition for excellence in academics. The proposed project is a natural extension of the current leadership of Capital University in the development of Computational Science at the undergraduate level.

Over the last 5 years, we have successfully piloted some course materials in chemistry, physics, and Computational Science I. However, student appetite for Computational Science has been only partially satisfied. Recently, eleven Capital faculty from nine disciplines were awarded an NSF CCLI grant (DUE 9952806, June 2000 - July 2003) and a grant from Battelle Memorial Institute (2000) to create educational materials for a Computational Science curriculum that culminates in an undergraduate interdisciplinary minor. The KUCSEC represents an evolution of these efforts and will afford greater national impact through collaboration with other institutions nationwide.

In the Spring 2001 semester, Capital offered the first course within the Computational Science curriculum. The response was very positive. Assessment data were collected and reflect a significant positive increase in students' attitudes toward and comfort with Computational Science and its various components. Enrollment for the Fall 2001 offering of Computational Science I is over four times the enrollment of the previous Spring offering.

Co-PIs from the NSF CCLI grant have presented curricular materials at seven discipline specific and interdisciplinary science conferences (such as the Project Kaleidoscope Summer Institute, 2001) and have attracted national attention from educators who would like to develop additional Computational Science educational materials. It is evident that, in order to have a larger national impact in this area, many institutions with faculty having vested interests must be involved in the collaborative creation of such materials. To this end, eight institutions have come together, with Capital University as the host institution. This collaborative alliance developed from the efforts of the PI, Dr. Ignatios Vakalis, in order to cultivate highly qualified and motivated scientists who are interested in and have experience with promoting Computational Science at the undergraduate level. The goal of the consortium is to alleviate the paucity of course materials at the undergraduate level and to extend the national repository of undergraduate Computational Science resources at Capital University. This repository will work closely with other national libraries such as the San Diego Supercomputer Center National Laboratory for Computational Science and Engineering, the Digital Library for Earth Science Education (DLESE), and the Partnership for Advanced Computational Infrastructure (EOT-PACI) to make these materials available to all institutions.

Members of the consortium include nine faculty from Capital University, three faculty from Ohio State University, three faculty from Pomona College, two faculty from San Diego State University, two faculty from Wofford College, and one faculty from each of the following: the San Diego Supercomputer Center, Harvey Mudd College, and College of the Holy Cross. This team of experts and educators is dedicated to undergraduate Computational Science and promoting this emerging field at the national level.

C. Need: Computational Science is a field at the intersection of mathematics, computer science, and science (hereafter, broadly defined to include biology, chemistry, engineering, environmental science, finance, geology, medical science, neuroscience, physics, and psychology). Computational Science offers an interdisciplinary approach to scientific research and provides an important tool, alongside theory and experimentation, in the development of scientific knowledge. In recent years, Computational Science has resulted in enormous advances in almost all fields of scientific inquiry such as DNA sequencing, behavioral modeling, global climatic predictions, drug design, and medical visualization.

Many traditional undergraduate curricula have yet to effectively integrate the fields of mathematics and computer science with the sciences. The intersection of these disciplines is where many of the important recent breakthroughs in science are occurring and will continue to occur. According to Dr. Rita Colwell, Director of the National Science Foundation, "Interdisciplinary connections are absolutely fundamental. They are synapses in this new capability to look over and beyond the horizon. Interfaces of the sciences and math are where the excitement will be most intense." The lack of integration of mathematics, computer science, and science in the undergraduate liberal arts setting can be attributed to the following:

- a widely shared perception in science and engineering that mastery of a single programming language suffices as a knowledge base for Computational Science;

- the standard expectation that students need to take a large number of traditional mathematics and computer science courses to build a background in Computational Science; and
- the lack of textbooks and materials to teach undergraduate Computational Science.

A few liberal arts institutions have attempted to remedy this problem by offering courses in Computational Science, e.g., Macalester College and the University of Wisconsin campuses at La Crosse and Eau Claire (Swanson, 1996; see also Bromley & Gallopoulos, 1994; Johnson & Alfeld, 1994; Marchioro et al., 1995; Marchioro & Landau, 1997; Rice, 1994). Other institutions have proposed courses as part of an emphasis in Computational Science but have not yet fully implemented those curricula (e.g., Salve Regina University and Wofford College). However, to date, there has been no coordinated effort to integrate Computational Science into the undergraduate curriculum. The KUCSEC brings together a team of individuals who will be the vanguard for undergraduate training in Computational Science. This proposal is unique for two reasons: First, it develops course materials for a ***comprehensive*** Computational Science curriculum to be disseminated nationally. Second, it demonstrates the integration of a ***comprehensive*** curriculum across mathematics and science by providing opportunities for majors within many varied disciplines to enhance their mathematics and computing skills. Descriptions of courses into which the proposed materials can be incorporated are available in **Appendix A**. These courses include:

Math/ Computer Science Courses	(*Course Abbreviation*)	Discipline Specific Courses	(*Course Abbreviation*)
Computational Science I	(*Comp Sci I*)	Computational Biology	(*Comp Bio*)
Computational Science II	(*Comp Sci II*)	Computational Chemistry	(*Comp Chem*)
Computational & Applied Math	(*C & A Math*)	Computational Finance	(*Comp Fin*)
Scientific Visualization	(*Sci Vis*)	Computational Physics	(*Comp Phys*)
Parallel and High Performance Computing	(*Par & HP*)	Computational Neuroscience and Psychology	(*Comp N & P*)
		Computational Environmental Science and Geology	(*Comp EnvGeo*)

Several factors have converged which justify the need for these educational materials:

- Currently, few institutions offer undergraduate courses in Computational Science. It is imperative, therefore, that we develop educational materials in Computational Science that faculty can use to demonstrate to students the many facets of such study, using an integrated approach to problem solving. This need was expressed repeatedly by many leading scientists in *Promising Directions*, published by W. M. Keck. We see a clear and acute demand for well-developed materials in all areas of undergraduate Computational Science. Our materials will help to fill the void.
- Undergraduate mathematics and science education is the foundation for professional development of the next generation of students. Undergraduate faculty prepare the future K-12 teachers, graduate students, and workforce. Thus, the impact of reform for undergraduate mathematics and science education will be felt at all levels of the educational pipeline.
- As has been well documented (see for example NSF Science and Engineering Indicators, 1998), a majority of adults within the United States are unable to interpret data or to compare sources of information in the formation of knowledge. The use of modeling and Computational Science facilitates an investigative, interactive process where a number of “what-if” questions can be posed – this provides the types of experiences needed to learn how to interpret data and shape a body of knowledge. Many of these “what-if” questions cannot be performed in a wet-laboratory in the typical undergraduate laboratory facility.
- The degree to which faculty are willing and able to integrate educational reform into their programs is directly related to the degree to which faculty have access to appropriate curricular materials. Therefore, our plethora of class-tested, fully developed, and reviewed materials will act as a catalyst for such reform.

<u>D. Project Description</u>: The emerging field of Computational Science offers an interdisciplinary approach to scientific research that is used in both industry and academic settings. In order to be prepared for graduate studies and the workplace, students need to have experience in Computational Science. The *problem*, as previously stated, at the undergraduate level is a lack of educational materials for Computational Science. The *objective* of this project is to develop course materials (in a modular format) that culminate in a comprehensive, interdisciplinary curriculum for Computational Science at the undergraduate level. The 22 consortium faculty from research and small liberal arts institutions will develop, evaluate, class-test, and disseminate materials for computational courses in biology, chemistry, computer science, environmental science, finance, geology, mathematics, neuroscience, physics, and psychology. These materials will also be appropriate for adoption into non-Computational Science courses as a way to improve the quantitative analysis component of such courses. The proposed materials will be applicable in a variety of institutional settings, for and by students with diverse backgrounds and science career aspirations. **Appendix B** contains a detailed description of the content of the materials to be developed. A sample module for Environmental Science appears in **Appendix F** and illustrates the prototype of modules generated for the NSF CCLI grant (DUE 9952806).

The developed course materials will emphasize critical thinking and problem solving skills. These materials include core courses in Computational Science to provide the necessary mathematical and broad computational background as well as discipline-specific courses providing direct application of Computational Science skills appropriate to that discipline. Modules within specific courses are designed for a variety of abilities within the undergraduate curriculum and often follow a logical progression in difficulty and depth. However, each module is freestanding so that it can be used independent of the other modules within the discipline. The curricular materials will be site-tested (see **Section 7**) at various institutions to enhance their evaluation and adoption. Dissemination (see **Section 6**) of the proposed materials will include publication via the Web and commercial publishers, discipline-specific conference presentations, and hosting Computational Science workshops.

E. Goals and Objectives: The proposed project targets national needs to enhance students' knowledge base in Computational Science, and to improve student attitudes and appreciation of mathematics and science as creative, collaborative, and interdisciplinary fields of inquiry. The goals and objectives for this 25-month project are:

Goals and Objectives of the Keck Undergraduate Computational Science Education Consortium
Primary Goal: • To develop materials that constitute an interdisciplinary Computational Science curriculum
Secondary Goals: • To emphasize an interdisciplinary, team-based approach to science problem solving • To cultivate undergraduates' understanding of the creative nature of Computational Science • To improve written and oral communication related to scientific and technical projects • To facilitate student use of current and emerging computing technologies • To increase the number of students who pursue graduate degrees in science and mathematics

To develop a set of materials that constitutes an interdisciplinary Computational Science curriculum. The theme throughout the proposed course material development is a modular, problem-oriented approach centering on applications from various scientific disciplines. This approach was chosen because: a) without applications from various disciplines Computational Science remains abstract; b) pragmatically, students can become adept in advanced subjects without having to master large amounts of more elementary materials; c) students with less mathematical and computing experience will still be able to take those courses that best complement their educational goals; and d) the most valuable knowledge in Computational Science consists of the general concepts and the techniques for solving real-world problems, rather than knowing all the details of one software package's commands or the intricacies of a hardware system (Marchioro & Landau, 1997).

The problem-solving paradigm familiarizes students with the solution methodology practiced by science professionals. This paradigm used in the development of modules is schematically depicted as:

Problem→ Model→ Method→ Implementation

Assessment

Students begin with a specific problem within a scientific discipline and then develop valid computational solutions using the techniques and software that researchers in the field would use. **Appendix F** provides an example module that was created for the NSF CCLI grant (DUE 9952806).

To emphasize an interdisciplinary, team-based approach to science problem solving. One difference between industry and traditional academia is how each values teamwork; in industry, the emphasis is on teamwork, not the individual. Because much scientific research is interdisciplinary and team-based, undergraduate education should mirror this approach. Thus, students who learn to perform as part of a research team will be more effective scientists in industry and academics. Moreover, one of the major barriers to student learning is the inability to generalize information across courses in a curriculum. In contrast, students experiencing the proposed curriculum will employ a basic set of computational skills across many disciplines. Many of the discipline-specific modules are closely tied with the core computational courses.

These team-based classroom experiences will also help to prepare students to conduct a team-based undergraduate research project as a capstone experience. The value of such capstone experiences has been well documented in a variety of sources (see, for example, Hakim, 2000).

To cultivate undergraduates' understanding of the creative nature of Computational Science. Often students believe that science and mathematics are disciplines filled with unrelated facts that require memorization. They lose sense of how necessary creativity is to the advancement of knowledge. The problems, modules, and case studies used in the proposed materials will require students to critically examine issues and to develop problem solving skills and creative solutions using a Computational Science perspective.

To improve written and oral communication related to scientific and technical projects. Cerrito (1996) emphasizes the close relationship between mathematics and writing. The current educational practice is that most writing in mathematics and science is focused toward faculty who know more about the subject than the student writer. The Boyer Commission Report states: "after college there will be little need to write up to a professor; it will be more important to write down to an audience that needs information and/or opinions, even if that audience happens to be the employer or higher authority." The proposed curriculum emphasizes comprehensive written reports as assigned projects to provide students with significant writing experiences. Local and national presentations of their work will further enhance the students' oral communication skills.

To facilitate student use of current and emerging computing technologies. In order to prepare adequately for future careers, mathematics and science majors need to become proficient in using a wide spectrum of computational resources. The use of computer technology (e.g., hand-held technology, computational software tools on PCs, workstations, and supercomputers) will be fully integrated into the curriculum. The primary theme throughout the proposed courses includes the use of visualization (e.g., from two-dimensional graphs to complex 3-D animations). Computational Science depends on various types of visualization techniques for the presentation of large data sets and the assessment of modules. The visualization techniques also serve as an excellent pedagogical tool for understanding mathematical and scientific concepts. The use of high-performance computing serves as the secondary theme. High-performance computing enables the investigation of computationally complex problems.

To increase the number of students who pursue graduate degrees in mathematics, science, and Computational Science. We share the national concern that only a small percentage of mathematics and science graduates pursue advanced degrees. Research universities continue to advance in their use of Computational Science as a new methodology in scientific discovery. The gap between predominately undergraduate institutions and research institutions is widening, yet across the country most graduate students still come from predominately undergraduate institutions. Improving the undergraduate experience in the various fields of Computational Science with the proposed materials will inspire a larger number of qualified students to pursue graduate studies in the ever-increasing computational aspects of mathematics, science, engineering, and finance offered at the graduate level (SIAM, 2001). We believe that students who experience collaborative research efforts and become familiar with a suite of sophisticated computing technologies are motivated to seek further education in more advanced formal settings. This initiative is in concert with the comments made at the 1996 Symposium on Learning and Intelligent Systems (LIS) hosted by NSF.

F. Impact: The proposed project to develop Computational Science materials will have a direct impact on mathematics, science, education, finance, and engineering majors. These disciplines constitute the core group of future scientists and engineers that will need computational skills to practice and advance their respective fields.

As stated earlier, the potential impact at the undergraduate level is significant because the undergraduate curriculum feeds the educational pipeline in many directions. It encourages students to pursue advanced degrees in both graduate and professional schools. It produces more technologically and computationally competent in-service teachers who will excite the next generation of students. It will export technologically savvy graduates who become future policy makers or the engineers, chemists, biologists, financial analysts, geologists, physicists, and neuroscientists who will be working in critical industrial, academic, or governmental settings.

This 25-month coordinated effort for material development will avoid duplication and enrich the content of many undergraduate mathematics and science courses taught in undergraduate institutions throughout the country. The multi-institutional team from across the nation that constitutes the KUCSEC will afford a wider national impact than any one school. The appeal of the proposed curriculum and course materials lies in their ease of adoption by typical undergraduate liberal arts institutions. These institutions are in a unique position to design and successfully implement multi-disciplinary curricula because their small size fosters interdisciplinary collaboration. Large universities, where a multi-disciplinary Computational Science curriculum may be difficult to implement, could adopt one or more of the proposed modules to fit their curricular needs. Moreover, the modular aspect of the course materials facilitates developing similar courses at community colleges. Thus, an additional impact could be realized on the 30% of U.S. students who begin or end their post-secondary education in community colleges.

G. Pedagogy: This integrated curriculum is important because it emphasizes critical thinking skills, problem-solving techniques, and a team approach to undergraduate student research and technology. Modules will use inquiry-based pedagogy focused on a problem-oriented approach. Through the inquiry-based pedagogy, instructors will use problems as the context for developing theoretical concepts. Instructors will facilitate student learning by: a) presenting students with a problem to solve; b) having students work out possible solutions; c) stimulating students' thinking by asking questions; d) having students discuss their solutions; and e) having students assess their work by comparing and defending their solutions. This pedagogical strategy is endorsed in the recent Boyer Commission Report (Boyer, 1998). In addition to the inquiry-based pedagogy, modules will be structured around collaborative learning (i.e., peer instruction). Mazur (1997) developed, tested, and demonstrated the superiority of peer instruction for an introductory physics course; this methodology serves as a model for the proposed modules. The strength of this approach is that students are not passive repositories for information; they must manipulate and verbalize their understanding as they defend their position to their peers. For each course, we will develop a set of conceptual questions to serve as a resource to aid instructors in assessing students' conceptual understanding and to facilitate peer learning.

2. Budget

This budget indicates the costs incurred at each phase of the project. A description of the activities for each phase is on the following pages. This Phase II submission differs from our Phase I submission in two ways: (1) In order to accommodate the W. M. Keck Foundation's funding requirements, we have reduced the number of summer months that Keck will fund for each co-PI from 3 months to two months. Partner institutions have committed to financing, during the academic year, the work that was to be completed for the third summer month. This allows the consortium to maintain all of the members thus ensuring geographical diversity and affording the same level of national impact. (2) Material from the field of Computational Finance has been added with a co-PI from Capital University developing modules within this field.

3. Timetable for Implementation

PHASE I			
Timeline	**Activity**	**Course**	**Personnel**
June 2002	Meeting in San Diego to refine format of materials. Sub-groups of co-PIs within the same discipline coordinate efforts.		All Co-PIs
June/ July 2002	Material Development; Details in **Appendix B**	Details in **Appendix A**	
	Module: Vector Spaces and Subspaces	*C & A Math*	Baker
	Module: Statistical Mechanics	*Comp Chem*	Baldridge
	Module: Tools for Genomics, Proteomics	*Comp Chem* *Comp Bio*	Becktel
	Module: Gene Finding	*Comp Bio*	Daniels
	Module: Pattern Formation in Biological Systems and Stochastic Models of Cell Growth	*Comp Sci II* *Par & HP*	de Pillis & Radunskaya
	Module: Thermal Conduction	*Comp EnvGeo*	Grosfils
	Module: Modeling Temporal Aspects of Behavior	*Comp N & P*	Karkowski
	Module: Spatial Data Analysis in Environmental Science	*Comp EnvGeo*	Lahm
	Module: Volume Visualization	*Sci Vis*	Machiraju
	Module: Friction and Faulting	*Comp EnvGeo*	Reinen
	Module: Mathematics in Neurophysiology	*Comp Bio* *Comp N & P*	Romstedt
	Module: Atomic Structure of Single Electron Elements	*Comp Phys*	Shields
	Module: Simulation of Animal Behavior in Searching for Food	*C & A Math* *Comp N & P* *Comp Bio*	Shiflet & Shiflet
	Module: Image Reconstruction in Image Tomography	*Comp Sci II* *C & A Math*	Soares
	Module: Performance for Steady-state Heat Diffusion with LAPACK, Part I	*Par & HP*	Stewart
	Module: Flood Prediction	*Comp EvnGeo*	Thorbjarnarson
	Module: Artificial Neural Networks	*Comp N & P*	Torello
	Module: Elementary PDEs: From Analytic to Numerical Techniques	*C & A Math*	Vakalis
August 2002	Evaluators review developed materials Details in **Section 7** and **Appendix D**		Evaluators

PHASE II			
Timeline	**Activity**	**Course**	**Personnel**
Sep 2002 – May 2003	Class testing and dissemination of materials		All co PIs
	Material Development; Details in **Appendix B** (1/2 the module developed during this time)	Details in **Appendix A**	
	Module: Eigenvalues and Eigenvectors	*C & A Math*	Baker
	Module: Visualizing Protein Structures and Computing Structural Properties	*Comp Chem* *Comp Bio*	Becktel
	Module: Modeling Tumor-Immune Interactions	*Comp Bio* *Comp Sci II*	de Pillis & Radunskaya
	Module: Thermal Conduction, Part II	*Comp EnvGeo*	Grosfils
	Module: Modeling Scheduled Reinforcement Contingencies of Behavior	*Comp N & P*	Karkowski
	Module: Watershed Data Analysis and Visualization	*Comp EnvGeo*	Lahm
	Module: Cash Flow Analysis	*Comp Fin*	Lawson
	Module: Friction and Faulting, Part II	*Comp EnvGeo*	Reinen
	Module: Diffusion Across Cell Membranes	*Comp Bio*	Romstedt
	Module: Electrostatic Potentials Using the Laplace Equation	*Comp Phys*	Shields
	Module: Modeling Blood Cell Population	*C & A Math* *Comp Bio*	Shiflet & Shiflet
	Module: Principal Component Analysis of Satellite Imagery	*Comp Sci II*	Soares
	Module: Performance for Steady-state Heat Diffusion with LAPACK, Part III	*Par & HP*	Stewart
	Module: Modeling Aggression	*Comp N & P*	Torello
	Module: Parallel Shortest Path Algorithms on Distributed Memory Machines: A Comparative Analysis & Calculating the Electrostatic Potential in Parallel	*Par & HP*	Vakalis
May 2003	Creation of Annual Report		Vakalis & Karkowski

PHASE III			
Timeline	**Activity**		**Personnel**
June/ July 2003	Material Development; Details in **Appendix B**	Details in **Appendix A**	
	Module: Linear Transformations & Curve Fitting	*C & A Math*	Baker
	Module: Quantum Mechanics and Kinetics	*Comp Chem* *Comp Phys*	Baldridge
	Module: Predicting Protein Structure and Function from Sequence	*Comp Chem* *Comp Bio*	Becktel
	Module: Gene Identification	*Comp Bio*	Daniels
	Module: Optimizing Chemotherapy Protocols with Dynamic Programming and Genetic Algorithms	*Comp Bio*	de Pillis & Radunskaya
	Module: Volcanic Ballistic Trajectories	*Comp EnvGeo*	Grosfils
	Module: Extension of Groundwater Flow Modeling	*Comp EnvGeo*	Lahm
	Module: Imaging Pipeline	*Sci Vis*	Machiraju
	Module: Object-Order Projection Visualization	*Sci Vis*	Reed
	Module: The Influence of Mechanical Layering in Rock Deformation	*Comp EnvGeo*	Reinen
	Module: Gas Exchange in Living Systems	*Comp Bio*	Romstedt
	Module: Diffusion-limited Aggregation	*Comp Phys*	Shields
	Module: Tomography	*C & A Math* *Comp Sci II*	Shiflet & Shiflet
	Module: Image Reconstruction in Emission Tomography: Iterative Inversion	*Comp Sci II*	Soares
	Module: Performance for Steady-state Heat Diffusion with LAPACK, Part II	*Par & HP*	Stewart
	Module: Environmental Pollution	*Comp EvnGeo*	Thorbjarnarson
	Module: Neural Networks: Applications in the Behavioral Sciences	*Comp N & P*	Torello
	Module: Modeling Traffic Flow	*Comp Sci II*	Vakalis
August 2003	Evaluators review developed materials Details in **Section 7** and **Appendix D**		Evaluators

PHASE IV			
Timeline	**Activity**	**Course**	**Personnel**
Sep 2003 – May 2004	Class testing and dissemination of materials		All co PIs
	Material Development; Details in **Appendix B** (1/2 the module developed during this time)	Details in **Appendix A**	
	Module: Fourier Series	*C & A Math*	Baker
	Module: Visualizing Protein Structures and Computing Structural Properties	*Comp Chem* *Comp Bio*	Becktel
	Module: Using Fourier Transforms to Understand Heart Conditions	*Comp Bio*	de Pillis & Radunskaya
	Module: Volcanic Ballistic Trajectories, Part II	*Comp Geo*	Grosfils
	Module: Modeling Scheduled Reinforcement Contingencies of Behavior	*Comp N & P*	Karkowski
	Module: Watershed Data Analysis and Visualization	*Comp Env*	Lahm
	Module: Option Pricing	*Comp Fin*	Lawson
	Module: The Influence of Mechanical Layering in Rock Deformation, Part II	*Comp Geo*	Reinen
	Module: Diffusion Across Cell Membranes	*Comp Bio*	Romstedt
	Module: Electrostatic Potentials Using the Laplace Equation	*Comp Phys*	Shields
	Module: Modeling Blood Cell Population	*C & A Math* *Comp Bio*	Shiflet & Shiflet
	Module: Processing Images Corrupted by Noise and Its Relation to Signal Detection	*Comp Sci II*	Soares
	Module: Performance for Steady-state Heat Diffusion with LAPACK, Part III	*Par & HP*	Stewart
	Module: Modeling Aggression	*Comp N & P*	Torello
	Module: Diffusion in Biology & Pharmacokinetics: Analysis of Drug Distribution in Living Organisms	*Comp Sci II*	Vakalis

PHASE V		
Timeline	**Activity**	**Personnel**
June 2004	Meeting in San Diego to: • Report what was completed during the year • Conduct final evaluation (Details in **Section 7** and **Appendix D**) • Final revision of modules and updates to consortium web site	All Co-PIs and Evaluators
	Creation of Final Report	Vakalis & Karkowski

4. Biographical Sketches

The KUCSEC faculty consists of 22 co-PIs from eight institutions that are actively involved in discipline-specific Computational Science research and teaching. The KUCSEC faculty will be aided by an evaluation team, which will provide feedback about the developed materials through formative and summative evaluation. Capital University is well positioned to implement the proposed course and curriculum project because of their experiences with the NSF CCLI grant (DUE 9952806). Each team member brings a unique set of skills, knowledge and expertise, necessary to complete the project successfully. Of particular note is that two of the co-PIs, **Eric Grosfils** and **Linda Reinen**, have for the past six years contributed significantly to the success of the **Keck Geology Consortium**.

Co-PIs are listed in alphabetical order with the co-authors from participating institutions followed by the co-authors from Capital University (host institution); a two page biographical sketch for each co-PI is available in **Appendix C**:

- Dr. Greg Baker: An Ohio Eminent Scholar in Scientific Computing from The Ohio State University. He will be developing modules in Linear Algebra and Numerical Analysis for the Computational and Applied Mathematics course.
- Dr. Kim Baldridge: Director, NBCR, at San Diego Supercomputer Center (SDSC) and senior research scientist at SDSC (http://www.sdsc.edu/~kimb/kimb.html). Dr. Baldridge has extensive experience in the field of Computational Chemistry.
- Dr. Chuck Daniels: A professor of Microbiology at the Ohio State University. For the last 10 years he has conducted research in the area of DNA sequencing methods to obtain complete genome sequences. He has cultivated an expertise in developing courses in the area of

Bioinformatics to analyze microbial genomes (http://www.biosc.ohio-state.edu/~genomes/mthermo/).

- Dr. Lisette de Pillis: An associate professor of Mathematics at Harvey Mudd College and recipient of the 2000 Maria Goeppert-Mayer distinguished scholar at Argonne National Laboratories (http://www.math.hmc.edu/~depillis). A proven researcher with specialties in Numerical Analysis and Parallel Computing. She will be developing modules for the Parallel and High Performance Computing courses and Computational Science II.
- Dr. Eric Grosfils: An associate professor of Geology at Pomona College and recipient of the 2001 Geological Society of America Biggs Award for Excellence in Earth Science Teaching. Dr. Grosfils is a planetary geologist with 11 years experience studying physical volcanism on Earth, Venus and Mars. In collaboration with Dr. Reinen, he has been instrumental in bringing quantitative and computational problem solving techniques into the Pomona College geology curriculum. Dr. Grosfils will develop modules for the Computational Geology and Environmental Science courses.
- Dr. Raghu Machiraju: An assistant professor of Computer Science at the Ohio State University. He has eight years of research and teaching experience in the field of computer graphics and scientific visualization (http://www.cis.ohio-state.edu/~raghu). He will be developing modules for the Scientific Visualization course.
- Dr. Linda Reinen: An associate professor of Geology at Pomona College. Dr. Reinen has 12 years experience developing numerical models of natural and experimental fault systems. In collaboration with Dr. Grosfils, she has introduced computational problem solving techniques in the Pomona College geology curriculum. She will develop courses for the Computational Geology and Environmental Science courses.

- Dr. Ami Radunskaya: An associate professor of Mathematics at Pomona College. For the last 10 years Dr. Radunskaya has conducted research in the area of dynamical systems. She has taught courses on this topic in Pomona College for the last 8 years. In conjunction with Dr. de Pillis, she will develop materials for Computational Science II.
- Dr. Angela Shiflet: A professor of Mathematics and Computer Science at Wofford College (http://cs1.wofford.edu/ecs). Dr. Shiflet has published five textbooks in computer science and mathematics. For the past 11 years she has conducted research at government scientific laboratories (LLNL, PNL, JPL). She will be developing modules suitable for the Computational Biology and Computational Psychology Courses.
- Dr. George Shiflet: A professor of Biology at Wofford College. Dr. Shiflet has written two successful proposals to NSF under the former ILI (Instrumentation and Laboratory Improvement) program and has written and administered a successful Hughes Foundation Grant in 1993-1996. To maintain currency in the area of Molecular Biology, he has been a visiting research fellow at the USC School of Medicine, the University of California Berkeley and the University of California at Los Angeles. Presently Dr. Shiflet serves as a consultant for NSF CCLI-EMD Grant 0087979, "Enhancing Computation in the Sciences." He will assist in the creation of material for Computational Biology.
- Dr. Edward Soares: An assistant professor of Mathematics at the College of the Holy Cross. Dr. Soares has 12 years experience conducting research in the field of medical imaging. His formal qualifications and research publications are in the areas of Computational and Applied Mathematics.
- Dr. Kris Stewart: A professor of Computer Science at San Diego Supercomputer Center and the director of the Educational Center on Computational Science and Engineering

(http://www.edcenter.sdsu.edu). For the last 16 years she has taught courses in supercomputing and numerical analysis. She will develop materials for Parallel and High Performance Computing.

- Dr. Kathryn Thorbjarnarson: An associate professor of the department of Geological Sciences at San Diego State University. For the last 16 years she has worked as a researcher in the field of hydrogeology, using computational simulations of groundwater flow and pollutant transport methods.

Capital University co-PIs

- Dr. Wayne Becktel: An assistant professor of Chemistry. He is an expert in Protein Engineering and Bioinformatics. For the last 8 years he has conducted research in the fields of biochemistry utilizing computational techniques. He will co-develop modules for the Computational Biology and Computational Chemistry courses.
- Dr. Andrea M. Karkowski: An associate professor of Psychology. Dr. Karkowski has extensive experience in using mathematical models in research and she also teaches mathematical models of learning and behavior. Dr. Karkowski will develop materials for the Computational Neuroscience and Psychology course and she will coordinate the evaluation of materials.
- Dr. Terry Lahm: An assistant professor of Environmental Science and the director of the Environmental Science program at Capital University. Dr. Lahm is a geologist specializing in hydrogeology. He has extensive research and teaching experience in mathematical modeling of geologic, hydrologic and atmospheric processes and will be developing modules for the Computational Geology and Environmental Science courses.

- Dr. Robert Lawson: An associate professor of Economics. Dr. Lawson currently holds the George H. Moor Endowed Chair in Economics. He is also the Director of the Center for Economic Growth and Prosperity at the Buckeye Institute for Public Policy Solutions. He is an adjunct scholar for the Mackinac Institute and a Faculty Affiliate for the DeVoe Moore Policy Sciences Center at Florida State University.
- Dr. Dave Reed: An assistant professor of Computer Science. He has conducted research and specializes in the area of scientific visualization. His experience includes research projects conducted at the Advanced Computing Center for the Arts and Design at the Ohio State University. He will develop modules for the Scientific Visualization course.
- Dr. Karl Romstedt: An associate professor of Biology. Dr. Romstedt has conducted research in the area of software development for analog/digital interfaces for platelet aggregation experiments. He has extensive experience in using mathematical techniques in Biology.
- Dr. Pat Shields: An associate professor of Physics. Dr. Shields has extensive experience in mathematical physics and has conducted research on numerical techniques at the Naval Surface Weapons Center in Dahlgren, VA. He has also piloted a course in Computational Physics at Capital University.
- Dr. Michael Torello: An associate professor of Psychology and Neuroscience. He has 14 years of experience in brain imaging and volumetric reconstruction of multi-slice brain MRI. He has developed multi-modal EEG/MRI computer visualization techniques. Dr. Torello will develop materials for the Computational Neuroscience and Psychology course.
- Dr. Ignatios Vakalis: Project Director. An associate professor of Mathematics and Computer Science. Dr. Vakalis has 10 years experience in the fields of numerical analysis, parallel computing and Computational Science. In 1995 – 1997, he received an NSF ILI grant (DUE:

9551259) to create two courses in parallel computing. He also serves as the PI-PD for the NSF CCLI grant (DUE 9952806) “Computational Science Across the Curriculum”. He will oversee and coordinate all activities, related to this grant for the W. M. Keck Foundation and he will develop materials for Computational Science II, Computational and Applied Math Course, and Parallel and High Performance Computing.

5. Other Sources of Financial Support

Letters of support and financial commitment from the various institutions are available in **Appendix E**. The following table outlines the contribution from each institution.

Source		Amount
Capital University		$51,884
College of the Holy Cross		$9,969
Harvey Mudd College		$6,600
The Ohio State University		$39,742
Pomona College		$36,000
San Diego State University		$45,530
Wofford College		$18,000
	TOTAL:	**$207,725**

6. Acknowledgement of W.M. Keck and Dissemination

All developed materials will clearly identify the contributions of the W.M. Keck Foundation. Course materials will be platform independent and available in multiple versions (computer languages, computer algebra systems), thus encouraging a wide national impact. The modular approach increases their ease for adoption as either a whole course or a subset of modules depending on the hardware and software availability at the adopting institution.

Dissemination will occur in three overlapping stages. The *first stage* will begin within the granting period. All authored materials will be Web-based. A dedicated web site will be built for depositing the materials and will include a statement of the W. M. Keck Foundation’s contributions to the project. A text-based version will also be created to make the materials available for persons with special needs. All materials will be reviewed (see **Section 7**) to ensure quality and adherence with the agreed upon style of presentation. This process facilitates national and international dissemination and acts as a means to refine and sustain the project.

The *second stage* of dissemination will begin once materials have been created. This will involve presenting our model materials and organizing workshops at national academic conferences including the Project Kaleidoscope (PKAL) Summer Institute (six co-PIs are members of PKAL's Faculty 21) and disciplinary societies (e.g., Mathematical Association of America, Special Interest Group in Computer Science Education, American Chemical Society, National Institute on the Teaching of Psychology, Supercomputing National Meeting, American Geophysical Union). At each of these presentations, the W. M. Keck Foundation will be acknowledged as a major contributor to the project. The presentations and workshops at national meetings of the various mathematics and science societies will focus on the innovative materials and the aspects of the comprehensive Computational Science curriculum.

During the *third stage* of dissemination, co-PIs will author articles about the developed materials to be submitted to peer-reviewed, pedagogical journals such as *Teaching Mathematics and Its Applications*, *SIGCSE Bulletin – In Roads*, *Computing in Science and Engineering*, *Journal of Geoscience Education*, *Mathematical Geology*, and *Teaching of Psychology*. Support of the W. M. Keck Foundation will be acknowledged in each of these manuscripts.

7. Evaluation and Assessment

For all modules, two types of evaluation (formative and summative) will occur in three overlapping phase: *Phase one*: Developed materials will be reviewed by co-PIs within the same discipline or who are creating materials for the same course. *Phase two*: the Evaluation Team of national experts (described below) will review developed materials. *Phase three*: Developed and reviewed materials will be class tested. The purpose of the formative evaluation is to assess the development of the modules (*phases one* and *two*). The purpose of the summative evaluation is to determine the effectiveness of the developed modules (*phase three*).

A matrix of evaluation activities and assessment materials appears in **Appendix D**. This matrix includes the evaluation questions, methods of data collection, timing of evaluation activities, and the type of evaluation. The assessment materials provided in **Appendix D** were originally developed by professional evaluators to assess the Computational Science materials developed for Capital University's NSF CCLI grant (DUE 9952806); these assessment materials have been modified to accommodate the needs of this project.

Andrea M. Karkowski from Capital University will coordinate the evaluation and assessment efforts. Dr. Karkowski has experience with pedagogical assessment techniques through her research and she has coordinated and conducted assessment of curricular materials for two other grants. A team of national experts has agreed to assess the modules to ensure high quality. The team includes:

Individual	Position and Institution
Dr. J. Corones	President of Krell Institute
Dr. E. Frost	Computational Geologist at SDSU
Dr. C. Hadad	Computational Chemist at Ohio State University
Dr. L. Jessup	Numerical analyst/ High Performance Computing at University of Colorado
Dr. R. M. Panoff	Executive Director, Shodor Education Foundation, Inc.
Dr. C. Smith	Computational Biologist at San Diego Supercomputer Center

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