

**COVER PAGE FOR TRADITIONAL AND UNDERGRADUATE ENHANCEMENT PROPOSALS
BOARD OF REGENTS SUPPORT FUND, FY 2008-09**

1. This Proposal Involves: <input checked="" type="checkbox"/> One Institution <input type="checkbox"/> More Than One Institution		2. Enhancement Subprogram: <input type="checkbox"/> TRADITIONAL ENH Program (Includes all multidisciplinary proposals) <input checked="" type="checkbox"/> UNDERGRADUATE ENH Program	
3. This Proposal Is: <input checked="" type="checkbox"/> Primarily an Equipment Request <input type="checkbox"/> Not Primarily an Equipment Request			
4. Name(s) of Submitting Institution(s) of Higher Education Dillard University Additional Institutions			
5. Address of Institution of Higher Education Computer Science Department Division of Natural Sciences and Public Health Dillard University 2601 Gentilly Blvd. New Orleans, LA 70112			
6. Title of Proposed Project		Establishing a Computing Laboratory for Multi-Discipline Instruction and Research	
7. First-Year Support Fund Money Requested \$101094	8. Second-Year Support Fund Money Requested (if applicable) \$0	9. Proposed Duration 1 Year	
10. Category In Which Proposal Is Being Submitted <input type="checkbox"/> Biological Sciences <input type="checkbox"/> Engineering B (Industrial, Materials, Mechanical, etc.) <input type="checkbox"/> Humanities <input checked="" type="checkbox"/> Computer and Information Sciences <input type="checkbox"/> Social Sciences <input type="checkbox"/> Special Multidisciplinary (See Section III.B.2.c of the RFP.) NOTE: If you check this category, you must also check at least one other eligible discipline.)		11. Taxonomy Numbers: 0499	
12. This Proposal Is a: <input checked="" type="checkbox"/> New Request <input type="checkbox"/> Request for Continuation of a Previously-Funded Support Fund Project Previous contract number:			
<small>By signing and submitting this proposal, the signators are certifying that: (1) the proposed project has not already been funded/is not currently being funded/has not been promised funding; (2) this proposal has been reviewed and approved by an Institutional Screening Committee; and (3) the institution and the proposed project are in compliance with all applicable Federal and State laws and regulations, including, but not limited to, the required certifications set forth in: (a) <u>Grants for Research and Education in Science and Engineering</u>, NSF Grant Proposals Guide (GPG), NSF 03-2, effective 10/1/02, and (b) 45CFR 620, Subpart F (Requirements for a Drug-Free Workplace).</small>			
Name (type or print)	Dept./Telephone No.	Degree/Year	Signature
Lead PI			
Campus Head or Authorized Institutional Representative	Dean		Authorized Fiscal Agent
Name/Title/email: (type or print)	Name/Title/email: (type or print)		Name/Title/email: (type or print)
Signature:	Signature:		Signature:
Date:	Telephone Number:	Date:	Telephone Number:
Date:	Telephone Number:	Date:	Telephone Number:

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PERSONNEL PAGE

Name(Last,First,MI) Zujia, Xu		Gender Male	
Race/Ethnicity Asian		Disabled? No	
Citizen of P. R. China		Residential Status: Permanent Resident	
Highest Degree Ph.D.			
Institution Dillard University			
Department Computer Science			
Position in Contract Lead Principal Investigator			
Address Computer Science Department,			
City New Orleans	State LA	Zip 70122	Phone 5048164602
		Fax 5044128274	
E-Mail Address zxu@dillard.edu		Website/URL www.dillard.edu	

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PERSONNEL PAGE

Name(Last,First,MI) Okpalaeze, Azubike				Gender Male	
Race/Ethnicity Black-Not Hispanic				Disabled? No	
Citizen of USA			Residential Status: U.S. Citizen		
Highest Degree Ph.D.					
Institution Dillard University					
Department Computer Science					
Position in Contract Faculty					
Address 2601 Gentilly Blvd.,					
City New Orleans		State LA	Zip 70112	Phone 5048164779	Fax 5048164810
E-Mail Address aokpala@Dillard.edu			Website/URL		

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Name(Last,First,MI) Aroutiounian, Svetlana				Gender Female
Race/Ethnicity White-Not Hispanic			Disabled? No	
Citizen of USA		Residential Status: U.S. Citizen		
Highest Degree Ph.D.				
Institution Dillard University				
Department Physics				
Position in Contract Faculty				
Address 2601 Gentilly Blvd.,				
City New Orleans	State LA	Zip 70112	Phone 5048164067	Fax 5048164810
E-Mail Address saroutiounian@Dillard.edu		Website/URL		

Project Summary

The goal of the proposed project is to enhance the recovery efforts of Division of Natural Sciences and Public Health at Dillard University from Hurricane Katrina, and further advance the education and research experience of underrepresented minorities in the fields of science, technology, engineering and mathematics (STEM). Through the creation of a state-of-the-art computing and modeling center, our objectives are:

1. Retain and encourage interdisciplinary undergraduate studies in Computing Sciences by training students in the development of efficient parallel codes, computer graphics, and user-friendly program interfaces to give them more business opportunities. Computing technologies and informatics are becoming an increasingly important aspect in all walks of research, be it in the physical and natural sciences, commerce, and/or engineering.
2. Promote graduate studies for bright, talented undergraduates – especially first-generation undergraduates from groups historically underrepresented in sciences.
3. Implement highly interdisciplinary projects involving parallel computations for focused and challenging scientific, physical, biological and engineering problems.
4. Build core educational and research infrastructure and foster highly-qualified teaching and research personnel for future funding acquisition.

The resources mainly consist of 15 state-of-the-art computer workstations for students and faculty members to conduct the pre and post computations, one multiple Central Processor Unit server, two laptops and applicable system and application software packages. The faculty members in computer science and physics departments are able to pursue the computing research in a variety of areas such as simulations, based on Computational Fluid Dynamic Methods, computational proteomics by Monte Carlo Model. It is expected that 2 conference and/or journal papers will be published. The project will potentially support 200 students in the division every year. The project, by the merit of its research and instructional objectives and activities, ideally responds to the criteria and goals of the enhancement program as stipulated in the guidelines.

NARRATIVE

1. THE CURRENT SITUATION

a. Institutional Description

Dillard University is a four-year historically black, co-educational, liberal arts institution in New Orleans, Louisiana that is strongly committed to the education of minority students. Dillard has as its purpose of the development of graduates who are broadly educated, culturally literate, concerned with improving the human condition, and able to meet the competitive demands of their respective professions. The university well recognizes the need for the inclusion of more African American in the science and engineering fields. The total student enrollment in 2005, before Hurricane Katrina, was about 2000 from more than 38 states, 2 U.S. possessions and 7 foreign countries. The student body is consisting of 99% black and 76% female. The majority of the students are from Louisiana, Texas, Alabama, Illinois, and Mississippi. The university offers quality and comprehensive undergraduate program, awarding degrees in Business, Liberal Arts, Natural Sciences, Nursing, and a special program in Japanese Studies.

The Division of Natural Sciences and Public Health offers degrees in Biology, Chemistry, Computer Science, Mathematics, Physics (Pre-Engineering) and Public Health. Pre-engineering 3-2 contract agreements exist between Dillard University and University of New Orleans, Auburn University, Columbia University and Georgia Institute of Technology for degrees in Mechanical, Electrical, Chemical, Civil and Computer Engineering. Pre-engineering is a dual-degree program in which Dillard University awards the Bachelor of Science Degree (Physics option) upon successful completion of a three-year curriculum in physics and the successful completion of additional two years of approved study at the engineering school of choice. The Computer Science Department has attained and maintained, over the last five years, excellence in the quality of its graduates, publications, and services. This excellence is measured not only by the quality of its product (graduates, publication, and service), but also as gauged by the relative added value.

Dillard University, with a 55-acre campus on Gentilly Boulevard, was inundated with 6 to 12 feet of water in the aftermath of Hurricane Katrina due to breaches at the London Avenue and 17th Street canals, resulting in \$400 million in damage. Three dormitory buildings were destroyed by fire as the campus sat underwater.

2. Rationale for Project

The aim of this project is the enhancement of computing technologies and sciences instruction and research with concentration on research and senior instruction in computer science and physics departments in the Division of Natural Science and Public Health at Dillard University. The rationale of this project lies on THREE keys:

1. It provides the students majoring in Physics, Math, and Computer Science with a new course – Introduction to Computing Technology and Science. The students will study the fundamental theory and application software of the numerical computations in the physics and information technologies. The knowledge that they have learned will improve high

technology and science in the state of Louisiana when they go to the industries, or help them to be admitted in competitive graduate schools.

2. The students in the Computer Science, Physics departments, and the Division of Natural Sciences and Public Health have opportunities to apply their numerical analysis, programming skills and information technologies to the multi-discipline sciences.
3. It supports the faculty in Physics, Math and Computer Science departments to pursue the computational research activities in a variety of scientific and technological areas.

This project will provide students a fundamental platform to learn and practice their knowledge and interests in Science, Technology, Engineering, and Mathematics (STEM) at Dillard University. The research activities play a significant role in improving the operation processes. As the power of the computers is steadily growing, it is possible to use the numerical computations to simulate complicated technology and scientific processes. The numerical simulations have a lower cost and stronger visual capacity than the traditional experiments. It is important and necessary for the students majoring in Physics (Pre-Engineering) and Computer Science to understand the principles of modern computing technologies. Their skills of currently fast updating computing technologies and science will not only definitely strengthen and refresh the traditional engineering industries but also support emerging enterprises in Louisiana.

This project will support up to 100 students in Computer Science, Math, and Physics (Pre-Engineering) as well as more than 200 students in the Division of Natural Sciences and Public Health in every academic year. It provides an excellent opportunity for our students to apply their numerical analysis abilities and programming skills to the computational science. The students also have chances to construct the server-clients system, and a Local Area Network (LAN). This will benefit the courses such as Data Communication, Operating System, and the entire division.

A fundamental computing laboratory will be established including a client-server computing system and computing science application software to support the productive instruction and research. The major hardware of the requested resources consists of twenty personal computer stations, and one Dell PowerEdge server. These computers construct the basic LAN system.

3. Impact on Existing Resources

The project will have a significant impact on instruction and research practices as well as the capabilities of the Physics/Pre-Engineering and Computer Science departments. It will enhance the teaching methodology and bring the technology into classrooms. The enhancement will affect the computing technologies and science program at Dillard University. The project will supplement the use of the existing equipment in the Physics and Computer Science digital laboratories more effectively and have a great impact on the hands-on training and interactive teaching methodology for the students.

Our current resources include a sixty Dell computers provided by other organizations to help our fast recovery process from the hurricane Katrina. These basic infrastructures support daily classroom teaching mostly for low-level computer courses such as CS 101 Computer Concepts and Applications. This project will provide the needed enhancement to instructional delivery, research support, and faculty and student development. The faculty offices and laboratories will

be completely connected, which provides electronic communications among faculty, and students through the Internet. For example, instructors will be able to assist students with programming assignments from their offices by accessing student's work done in the laboratory. Students will be able to submit assignments electronically to their teachers. The requested enhancement will result in:

1. A significant impact on the quality of teaching and therefore, a concomitant increase in learning by the students in the division of Natural Sciences and Public Health.
2. A significant research output by faculty and students of the division.
3. A significant increase of the funded research opportunities and collaborations with colleagues around the world.
4. A significant impact on the students' ability to pursue graduate school or gainfully be employed in the current fast growing computing technologies and sciences.
5. A model integration of research and education.

The instructional laboratories, Rooms 158 in the Dent Hall, will naturally host the requested resources. More than 200 students in Physics/Pre-Engineering, Computer Science departments, and the Division of Natural Sciences and Public Health will essentially utilize these resources, including selected lectures, homework assignments and undergraduate research project activities. Faculty activities that depend on the computer resources are mostly instructional and research activities. These instructional activities include daily general instructional material development, instructional delivery for entire classes in the laboratories, and software development.

2. THE ENHANCEMENT PLAN

a. Project Goals and Objectives

The project goals and objectives are list as following.

I. Retain and encourage interdisciplinary undergraduate studies in Computer Sciences by training students in the development of efficient parallel codes, computer graphics, and user-friendly program interfaces to give them more business opportunities. Computing technologies and informatics are becoming increasingly important aspects in all walks of research, be it in the physical and natural sciences, commerce, and engineering.

II. Promote graduate studies for bright, talented undergraduates – especially first-generation undergraduates from groups historically underrepresented in sciences.

III. Implement highly interdisciplinary projects involving parallel computations for focused and challenging scientific, physical, biological and engineering problems.

IV. Build core educational and research infrastructure and foster highly-qualified teaching and research personnel for future funding acquisition.

b. Work Plan of Proposed Project

The implementation plan for this project is straightforward. It consists of two parts, instruction/learning and research. First part is acquiring, installing and operating the LAN system

and application software products, then utilizing them for our instructional activities. The second part is searching the lectures on computing technologies and sciences, outlining the research topics, designing/implementing computation algorithms, testing the code, running the research programs, writing papers, bringing papers to the conferences, and finally sending the papers to the related conferences/journals. These two parts are carried out simultaneously. Before the system is installed completely, the research part will focus on searching, designing and testing. As long as the system is fully operational and applied to the instruction, the heavy computational researching programs will be loaded in the server.

Dr. Xu, the project principal investigator, Dr. Svetlana Aroutiounian an assistant professor of Physics/Pre-Engineering department, and Dr. Azubike Okpalaeze, the co-director and the chair of Computer Science department will lead the technical tasks of acquisition, installation, operation, maintenance and upgrading of the resources. Dr. Xu will open a new course, Introduction to Computing Technology and Science in fall 2009.

Dr. Xu and Dr. Aroutiounian are responsible for a variety of computing research activities. Dr. Xu has already published more than two journal papers and three conference papers on computational fluid dynamics, which were adopted modern computing technologies models. Dr. Aroutiounian's research focuses on computational biology and physics. She has published more than 10 articles and papers and received several awards related to computation scientific research. Together with the undergraduate students, they will improve the computation algorithms, expand/deepen research topics, and submit the results to the related conferences and journals.

The schedule for the instruction, learning and research can be summarized in the following table.

Time	Instruction and Learning	Research
6/1/2009 – 8/31/2009	Acquisition and installation of the hardware and software system	Literature survey; Designing numerical computational algorithms
9/1/2009 – 12/15/2009	Opening a new course “Introduction to Computing Technologies and sciences”;	Implementing the algorithms; Running the research programs; Obtaining the results; Sending paper(s) to conferences; Workshop of Advanced technologies on modern computing technologies and sciences
1/1/2010 – 5/30/2010	Serving other 27 courses in Physics/Pre-Engineering, Mathematics, Chemistry and Computer Science departments; Directing senior projects and research on computing technologies and sciences; Sending the students to the conferences	Preparing proposals for the federal research fund resources; Attending 2-3 academic conferences and communicating with computing sciences investigators nationwide; Revising the conference papers and Sending them to journals related to computing technologies and sciences

The evaluation of the project entails the gathering, assessment and reporting (to the Regents) of quantitative and qualitative pieces of information that include the following:

1. Acquisition and installation of the LAN system; this phase will include experimental learning for computer science and physics undergraduate students and faculty; the learning is to

continue through their involvement in the operation, maintenance and upgrade of the system in the future.

2. Instructional utilization – The new course, Introduction to Computing Technologies and Sciences, senior students' projects, research activities, and many natural science courses named in section b.3 will intensively utilize this system. The key outcome here is the quality of training students and the congruency of the same with the practices in graduate school and high technology sciences in Louisiana.
3. Research utilization and outcomes. Data will be collected on faculty and students' use of the system, the actual research tasks for which the system is utilized, and the outcomes that includes publications, presentations, proposals and resulting grants/contracts.

c. Evidence and Potential for Eminence

Several external funded programs support the University in producing strong students in the Natural Sciences. These include the LAMP program funded by NSF and BOR, the Math-Science Tutoring Center funded by Packard Foundation under Dillard University Leadership Enhancement in Sciences Program and the Materials and Engineering Research Program and contract funded by Wright Patterson United States Air Force Base to establish a High Energy Impact Research Laboratory for the characterization of the failure mode of composite materials. Another DOD recently funded infrastructure enhancement project for the Division of Natural Sciences and Public Health is a strong sign for the national recognition of the departments progress, which insure its bright present and future Eminence. All these successful projects are well-recognized and placed Dillard University in the scientific arena.

The Computer Science Department has attained and maintained, over the last five years, excellence in the quality of its graduates, publications, and service. This excellence is measures not only by the quality of its product (graduates, publication and service), but also as gauged by the relative added value. Section b.1 provides in brief form the strategies by which this project will afford us the resources needed to enhance the quality of the department.

Advanced courses such as Data Communications (CS370), Operating Systems (CS375), Computer Organization (CS430), Design and Analysis of Computer Algorithm (CS470), Computer Graphics (CS475), PHY 310 Mechanics-Statics/Dynamics, PHY 411/412 Scientific Research Methods I/II, and some other mathematics courses (MAT 201, 202,203, 410, 410) are designed and implemented to facilitate our students' transition to graduate school and /or high technology professions. Furthermore, Dillard University has established a faculty fellow program. Its purpose is to assist our graduates to get into graduate schools. At the present there are eight identified prospective graduates. Thus, they will also be using the resources in their work to ensure a smooth transition to graduate school.

The LAMP program is a prime example, and has been a backbone for students involved in a model mentoring and research involvement program for undergraduate students. Dr. Zujia Xu, Dr. Svetlana Aroutiounian, and Dr. Azubike Okpalaeze are deeply involved in a model mentoring and working with students, and are instrumental in executing the LAMP program. Our students take part in the local and national technical presentations. Dr. Azubike Okpalaeze took a

group of five students to the American Society for Engineering Education (ASEE), and Association of Computing Machinery (ACM) Southeast Regional Conference proceedings where technical papers were presented. This venture is to expose our students to the international conferences; to stimulate their computational interests; to facilitate networking within the computational science international community, and to gain the required experience in their research areas. It is certain that the project will help us to increase such international participation in the computational environmental sciences.

The following research activities will be significantly supported by the project.

- a. Direct Numerical Simulations of Flows in Ecosystems by using the Lattice Boltzmann Method. Dr. Xu is leading these efforts. A Computational Fluid Dynamic (CFD) approach called Lattice Boltzmann Method has been applied to simulate the flow across an ecosystem.

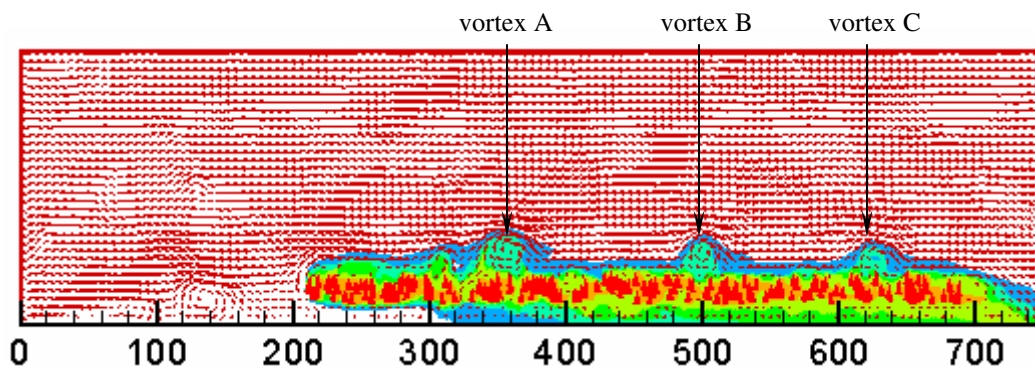


Fig. 1 Air Profile when it crosses an Ecosystem
(Including distribution of CO₂ concentration at one certain time)

This direct numerical method has the advantage that it resolves all the scales of turbulence, which usually occur in the large number of Reynolds number, allowed by the choice of the grid, uses a relatively simple sub-grid model and accounts easily for any boundary condition without the use of special theory for the boundaries or empirical wall functions. Simulation results over a two-dimensional canopy indicate that the formation and shedding of vortical structures, which are similar to the ones observed in flows over steps or pass cylinders and particles (Schlichting, 1978) and affect the flow field. CO₂ flux monitoring over such canopies must take into account these vortical structures in the averaging and reduction of data. Figure 1 is the computational result of air flows through two-dimensional canopy system, which depicts the structures of vortex over the ecosystem and the distribution of CO₂ concentration. The result of current investigation has been submitted to the Journal of Agricultural and Forest Meteorology to review.

- b. Implementing the parallel Lattice Boltzmann Simulation. The research team will be engaged into the parallel computation of Lattice Boltzmann Method (LBM). The parallel computation is a state-of-the-art numerical simulation method. It will accelerate the process of the computation by fully utilizing the Central Process Units (CPUs) so that thousands of particles can be simulated. The LBM is an ideal parallel algorithm since the values in each grid depend only on its neighbors.

- c. Dr. Svetlana Aroutiounian, an assistant professor of Physics Department at Dillard University, will lead research activities on computational Genomics and Proteomics. She is a computational biophysicist. The overall number of her publications exceeds ten papers. Her research interests include two parts:

Computational Genomics: On a coarse-grained time-scale, the protein production from a DNA can be seen as a chain of six operations (unwinding-untwisting, transcription, splicing, membrane-crossing, and translation) each of which yields a distinct intermediate structure. Motivated by the understanding that biology "wants" to become mathematicized, Dr. Aroutiounian proposed that the determination of the 3D structure of protein product from its 1D DNA sequence can be formalized by a chain of mathematical operations sequentially applied to the intermediate structure. She is also motivated by consideration that there is a high likelihood for a functionally similar proteins to be a better carriers of traces of common operations acting during protein production. She suggests that the DNA sequence serves as an initial eigen-function and the protein product is an eigen-value to be determined from a Schrödinger-like equation of sequentially applied operators:

$$\hat{Pr}(dna) = \hat{R}\hat{x}\hat{M}\hat{x}\hat{S}\hat{x}\hat{T}\hat{x}\hat{U}tw(dna)$$

$$S = \begin{vmatrix} u & g & c & a \\ a & a & u & u \\ g & u & a & c \\ c & c & g & g \end{vmatrix}.$$

Professor Aroutiounian's approach shows that the exon splicing operation appears to be a leveraging mechanism for the speciation of genes expressing to the same protein-family. The symmetry property of the \hat{S} -Matrix appears to carry the universal character of the splicing operation, indeed. The application of letter-form of the matrix operator to other families of functionally similar proteins is in a process.

The future questions will be: are the MOES of functionally similar proteins and MOES of proteins sharing similar folds pass the same evolutionary bottleneck? Shall investigators look for mathematical solutions for all the sub-nuclear and intracellular machinery operations?

Computational Proteomics:

I) *Equilibrium motion* in a protein studied by *Monte Carlo simulations* of fluctuations in a *coarse-grained rigid-polypeptide-plane model protein*. The inter-residue interactions are approximated by Go-like contact potential. The details of residue content are taken into account by introduction of the Ramachandran and hydrophobic propensities in MC simulations. The full sampling is achieved through the assessment of the convergence of conformational trajectories – a sequence of snapshots of the accepted conformations. Comparison of the recent proposed MC computational profiles with computational profiles obtained in the X-ray crystallography and NMR spectroscopy experiments shows that the protein fluctuations described on a coarse-grained level are in a qualitative agreement with the experimental data. For a small protein (~90 residues) the production run of $\sim 2 \times 10^9$ MC

moves requires about a week of simulations on Xeon 2.4 GHz processor. A fast computational system is desperately needed.

II) The free energy landscape (FEL) perspective in studies of a protein folding transitions reflects notion that since there are $\sim 10^N$ conformations available for a protein of length N to scan in search of lowest free energy state, random search is beyond biological timescale. Therefore, protein folding must follow certain pathways and evolutionary selected proteins have FEL with the kinetics of folding dominating over kinetic traps. Coarse-grained model protein is not very accurate but affords simulations close to biologically relevant size and timescale. Go-like potential secures the funnel shape of FEL. Ramachandran propensities and hydrophobic/hydrophilic contacts act as “friction” interactions signifying the bottleneck of the funnel. This combination is a good model for functional robustness of natural proteins. Boltzmann-weighted ensemble of protein conformations and histogram method are used to obtain from MC sampling of conformational space the approximate probability distribution for a protein to be in a certain conformation. Thus, the protein free energy landscape is determined as $F(\text{rmsd}) = -1/\beta \cdot \text{Ln}[\text{Hist}(\text{rmsd})]$, $\beta = k_B T$ and rmsd is root-mean-square-deviation from native conformation. The main idea is that there is a mathematical relation between the FEL of a protein and a set of key residues providing stability to folding transition.

The essential question will be “Is the set also conserved for the functional reasons?” Dr. Aroutiounian’s preliminary results might be suggestive that primary sequence (not the symmetry of the protein architecture) is the rule settler.

The Computer Science, Mathematics, Physics/Pre-Engineering, and Chemistry majors engage in meaningful research before graduation. Students will spend at least one summer doing research in industrial, federal laboratories, including NASA, Bell Laboratories, State Farm, Martin Marietta, and IBM. The publications of the faculty are at the forefront in their respective fields. The publications of the investigators that are partly listed in their vita, clearly illustrates the quality and productivity of our research endeavors. The proposed project will allow us maintain our high level of quality and productivity and of very good instruction and learning.

Dillard University’s track record in the Natural Science is very good. Current surveys document among Dillard’s graduates 110 physicians, 40 PhD’s in physics, chemistry and biology, 42 dentists, 26 engineers, 19 pharmacists, 12 veterinarians, 9 podiatrists, 6 optometrists and numerous workers in the health professions. Alumni notables include the Chairman of the Department of Surgery at Meharry Medical School, the Executive Vice President of the Harvard University Medical School, the Chairman of Chemistry at the University of Utah and an executive at the National Research Council.

d. Impact on Curriculum and Instruction

The impact of the funding for the proposed project on our curriculum and instruction will be the increase in efficiency of computation integration in the Division of Natural Sciences and Public Health of our curriculum instruction. Computing technologies are the necessary tools in industries, laboratories, and graduate schools. Simulation, modeling, graphical representation, and laboratory report also make extensive use of computers in instruction and learning. This

project will allow us to continue the replication of this extensive utilization at the undergraduate level. The extensive research utilization of this system has instructional and learning values beyond the specific courses. The project will take into consideration the recommendation of NSF in the reform of undergraduate education. Computer-aided homework should be assigned for every new concept, with emphasis on evaluation and explanation, inquiry-based, hands-on teaching, self-confidence building through problem-solving. The utilization of the current and requested sources will have direct positive impact on the following 28 courses (12 courses in Physics department, 1 course in Chemistry department, 10 courses in Computer Science department and 5 courses in Mathematics department):

Courses	Computer Usage
Introduction to Computing Technologies and Sciences (new course)	Computational technology, Simulating Sedimentation, Drawing graphs and Making animations
Engineering Physics I (PHY 111)	Concepts and Applications of Numerical Computation
Engineering Physics II. (PHY 112)	Numerical Algorithms, Demonstration of engineering graphics, Computer Aided Design
General Physics I: Particle dynamics in solids (PHY 220); Mechanics-Static (PHY 307, PHY 308); Intermediate Classical Mechanics (PHY 309)	Compute and animate the motion, rotation and collision of solid particles
General Physics II (and Lab): Particle dynamics in fluids (PHY 222 and 222L)	Numerical simulation of the motion of the fluid under a variety of conditions, such as Couette Flow, Atmospheric Flow
Thermodynamics and Statistical Mechanical. (PHY 305)	Implementation of numerical solutions for Partial Differential Equations on heat transfer, thermodynamics
Scientific Research Method (PHY 411)	Introducing the fundamental theories and methods on numerical engineering approaches
Physics Research (PHY 409); Senior Research Thesis (PHY 412)	Designing computation algorithms; Implementing them by software or programming languages, such as Ansys, Matlab, C/C++ and Fortran
Organic Chemistry II (and Lab): (CHE 212 and 212 L)	Modeling the hydrocarbon compounds Computer Simulations
Introduction to Programming (CS160)	Parallel Programming techniques
Unix Operating System (CS230)	Linux operating system kernel
Systems Analysis and Design (CS360)	Hardware/Software development and testing
Data Communications (CS370)	Error control protocols, TCP/IP, ATM, Simulations
Operating Systems (CS375)	Synchronization, schedulers, linkers, loaders
Compiler Theory (Cs420)	Design methodology, optimization, parsing
Computer Organization (CS430)	Circuit logic design techniques
Artificial Intelligence (CD410)	Computer vision, robotics

Design and Analysis of Computer Algorithm (CS470)	Dynamic programming complexity and verification
Computer Graphics (CS475)	Raster graphics/Algorithms, Visual reality Graphical modeling, Simulations
Discrete Mathematics (CS/MAT 330)	Hamilton path, Algorithm, Digraphs
Finite Mathematics (MAT 131); Matrix Analysis (MAT 305)	Numerical Solutions for Matrix Operations by using Matlab
Differential Equations (MAT 302)	Solving differential equations by programming
Numerical Analysis (MAT 410)	Comparison a variety of computational chemical engineering algorithms

e. Impact on the Quality of Students

The proposed project will directly affect more than 300 students majoring in Physics/Pre-Engineering, Math and Computer Science. More students will be attracted to computing technologies and sciences based on the new course, the workshops and the research projects. The Division of Natural Sciences and Public Health will have great resources, the hardware, software and personnel, to well educate the students in computing science and keep them competitive either in the graduate schools or in the workforce.

As it mentioned in section b.3, the project will support 28 courses in Physics, Chemistry, Computer Science, and Mathematics departments in the Division of Natural Sciences and Public Health. The impact of this project on the quality of the students will be significant. It is an established fact that numerical computational programming requires a great deal of CPU time. The client-server prototype and the multiple CPU server will enhance the process. The department responsibility is to integrate technology, not only in the advanced courses, but also at the junior level courses to promote such productivity. Hence, the entire student body will benefit from this project, as we enhance technology integration into the junior and senior level courses. It is also to be noted that the student population related to computer major is one of the largest at Dillard University, since computer science courses are the requirements for every student. It is estimated that the number of students majoring in Mathematics, Physics/Pre-Engineering, and Computer Science-related subjects like business (Management Information systems) which we service, are about half number of the entire school students.

Students from all divisions who are pursuing projects and writing research papers will utilize the computing resources described above. The project will affect the quality of the departments by the enhancement of the effectiveness of its curriculum and instruction, and undergraduate research as a tool to motivate students for graduate education. The research activities will require knowledge of scientific facts, concepts, processes, development of skills, and applications. The objective is to improve skills through competition, collaboration and cooperation, and to make learning exciting through motivations. A number of promising participants will be selected each year to receive special scholarships, stipends and incentive awards. Quality students from local and regional high schools will be invited to have a direct experience and contact with the successful research program. The summer recruitment bridge activities will also benefit from the resources. These bridge activities have been the major recruitment tool to attract high quality students from the local and national high schools.

e. Impact on Faculty Development

The proposed project will significantly improve the quality and effectiveness of faculty teaching, learning and research. Dr. Xu will open a new course, Introduction to Computing Technologies and Sciences, which is totally based on the required hardware and software. Dr. Aroutiounian and Dr. Okpalaeze have taught a number of computer science and physics/pre-engineering courses that will be affected by the project listed in section b.3. They are going to exhaustively use the requested computer system to add more computer practices and theories for each of courses in Physics/Pre-Engineering and Computer Science departments.

Dr. Xu will simulate the hydrodynamic interactions and distribution of CO₂ concentration as the high velocity air flows across an two-dimensional ecosystem by using of computational fluid dynamic approaches. Based on the two research projects mentioned in section a.2, Dr. Xu will improve the computation algorithm, the LBM, from two-dimensional to three-dimensional cases. To fully use the four CPUs in the requested Dell PowerEdge server, Dr. Xu will design a state-of-the-art parallel LBM program to accelerate the computation process. He will also collaborate with other investigators to publish 2-3 conference papers based on the computation results. Dr. Aroutiounian will utilize the state-of-the-art computing infrastructure to continue her research on computational biology and physics areas. Her further investigations will be of great benefit from the this project.

The proposed project will allow us to retain highly talented faculty members whose research productivity will measurably increase. It will also support us to recruit high quality faculty member in Computer Science, Biology, Chemistry and Mathematics departments. One important aspect of the above positive impact on the faculty stems from the fact that enhanced computational and network infrastructure is a key factor for the success of our research projects.

f. Performance Measures

The performance of the project will be measured by activities such as the establishment of a computing technology and science laboratory, the number of courses hosted by the equipment, the number of faculty and student utilizing the infrastructure, and the regional or national conferences to the faculty and student to present their research results.

3. EQUIPMENT

a. Equipment Request

The nature, scope and intrinsic requirements of our research and instructional work led to the selection of the requested equipment. The server is Dell PowerEdge 6600 with multiple (four) CPUs which is linked to the 15 personal computers via the fast switch. The personal computers are requested to meet the pre and post computational analysis for faculty research activities and instructions. The two laptops are essentially for the presentations in the classrooms and national conferences. Network devices and accessories are included in the total acquisition. The software includes the programming language C/C++ compiler. Tecplot will be used to do the post computation work, such as drawing charts, creating fluid velocity vector graph, generating animations and etc. Matlab and Ansys are the powerful and popular software for the engineers to finish the design, computing, analysis and testing in both academic and industrial fields.

Related system and applications software product needed for research and for instruction are listed below.

Software

SoftWare	Quantity	Unit Price	Total Price
Tecplot 10 (Multi-platform for Linux)	1	\$3,200.00	\$3,200.00
Matlab (Education Version, Optimization Toolbox, Compiler, Partial Differential Equation Toolbox)	1	\$2,400.00	\$2,400.00
Fluent for Linux (including CFD package)	1	\$9,500.00	\$9,500.00
ANSI C/C++ Compiler	1	\$2,500.00	\$2,500.00
		Total	\$17,600.00

Hardware

Equipment	Quantity	Unit Price	Total Price
Personal Computer Dell Precision 690, Pentium 3.0 GHz, 1G RAM, 10/100 Ethernet, 160 GB Hard Drive, Windows XP Professional, 17" monitor	20	\$2,021.90	\$40,438.00
Server Dell PowerEdge 2900 II, 4 Intel Xeon 2.0 GHz CPUs, 375 GB Hard Drive, Red Hat Linux 2.1 Advanced Server, 2 GB RAM, 15" monitor	1	\$12,487.33	\$12,487.33
Laptop Dell Latitude E6500, Pentium 2.7 GHz, 2G RAM, 250 GB Hard Drive, Windows Vista	2	\$1,976.50	\$3,953.00
Printer HP color LaserJet 4600dn printer C9661A	1	\$2,500.00	\$2,500.00
Network Switches and Cables Dell PowerConnect 3348, 48 Port FE Stackable Managed Switch, 2 GbE Combo Ports	1	\$1,615.40	\$1,615.40
		Total	\$60,993.73

b. Equipment on Hand

The equipment on hand for the proposed project is the Departmental network. This network connects every office, classroom, and laboratory of the Division to the T1-node Internet. The remaining computers resources in the computer science department include 60 Dell basic personal computers. The equipment is located in Dent Hall rooms 162 and 167. Unfortunately, the processing power that we possess can not meet the basic standards of modern computing technologies. With the network card installed in each computer, faculty and students will be able to remotely submit and follow the progress of their computational “jobs” at any time and on any day. The computers in faculty offices have mainly been acquired other grants.

c. Equipment Housing and Maintenance

The Dell server will be housed in Dent Hall, room 158. This spacious room has the required space, electrical outlets, and other amenities (i.e. temperature control) for the proper housing of the equipment. The operation of the equipment is the responsibility of the systems administrator, whose salary is provided by the division. In addition to insuring optimum operation conditions

for the system, the system administrator will also assist faculty and students in their interfacing with the system, particularly in the beginning of the project. (This mainly means providing the up-to-date utilities for the system).

The maintenance of the equipment is the responsibility of the division, as well as the funds for the materials and supplies related to the system and for the maintenance of the system for the next subsequent years! We underscore the fact that the university's regular maintenance program will also cover our requested system. A solid source of support for the operation and upgrading of this system consists of the research grants of productive faculty members. The Information Technology department of Dillard University is fully responsible for the software update and hardware maintenance.

4. FACULTY AND STAFF EXPERTISE

The following highly experienced faculty members will utilize, administer, and maintain the requested resources. It includes the principal investigators, Dr. Zujia Xu, Dr. Svetlana Aroutiounian and Dr. Okpalaeze. All of the PIs are faculty members in the Division of Natural Science and Public Health. They will develop the undergraduate research program at the beginning of fall 2009.

The project director, Dr. Zujia Xu, is an assistant professor in computer science department at Dillard University. He earned two Bachelor degrees of science in Mechanical Engineering and Electronic Engineering in 1995, a Master of Science in Power Mechanical Engineering in 1998, a Master of Science in Computer Science and a Ph.D. degree in computational fluid dynamics from Tulane University in 2003. He has solid computer knowledge, finished one thesis and submitting two conference papers. Dr. Xu's Ph.D. dissertation focuses on the investigation of hydrodynamic interactions by using of computational fluid dynamic approach – Lattice Boltzmann Method. Dr. Xu has published two journal papers and three conference papers in the computational fluid dynamic field. He had been a visiting professor at Southcentral Regional Center (SCRC) of the National Institute of Global Environmental Change (NIGEC) in the summers of 2004 and 2005. Dr. Xu is working with investigators from NIGEC and other research centers for the projects of evaluating ecosystem by using of computational fluid dynamic models.

Dr. Svetlana Aroutiounian is an assistant professor of Physics/Pre-Engineering Department at Dillard University since 2006. Her research activities focus on computational Genomics and Proteomics. She is a computational biophysics. The overall number of her publications exceeds ten papers. She was an adjunct professor in the Department of Physics of North Carolina A&T State University. In 2005, she was a post-doctor fellow in the Department of Computational Biology of University of Pittsburg.

Dr. Okpalaeze is currently the Chairperson of the Computer Science Department. He is responsible for maintaining the department's computer infrastructure and integrating Web Technology into our curriculum, and will also be implementing High Performance Cluster Computing (HPCC). Dr. Azubike Okpalaeze, had a double BS degree in Computer Management and Data Processing, and Business Management from West Virginia State University Montgomery, West Virginia. He holds M.S. and Ph.D. degrees in Computer Science from

Southern University and Agricultural & Mechanical College at Baton Rouge, Louisiana. He has been trained for setting up parallel PC clusters using Linux and MPI through Minority Serving Institution High Performance Computing (MSI HPC) workshop on Cluster Computing. He has a formal training in systems and network administration. Dr. Okpalaeze plays an important role in advising and supervising LAMP and STP projects and program at Dillard. He has managed well over \$95,000.00 of external funds for the past five year. He received the grand of \$65,000, Enhancement of Computer Science Instruction and Research – Phase I, from the LA Board of Regent in 2003.

5. ECONOMIC AND/OR CULTURAL DEVELOPMENT AND IMPACT

a. Relationship with Industrial/Institutional Sponsors

This project will produce highly qualified computing technology engineers and other computer-related graduates such as computer scientists, mathematicians, physicists, chemists, biologists, and economists at the undergraduate levels. The division of Natural Science and Public Health and several industrial and federal laboratories will be able to establish partnerships through the success of these graduates. Many of the graduates majoring in natural sciences are employed at various laboratories and corporations such as IBM, State Farm, Shell, and etc. The project will also provide the students with opportunities to conduct internship at oil refineries such as NORCO, Shell and Chevron, governmental offices and agents such as CIA, and FBI. This will increase industrial ties and interest in the division.

Every summer several our undergraduate students do their summer research in Federal, university and industrial laboratories. The funding of this project will make it possible for us to increase the number of students sent to these laboratories. It will enable our laboratories to recruit students from other universities for summer internship. This will increase the cooperation with other universities, the Federal and industrial laboratories. The Physics/Mathematics/Computer Science Departments are prominent members of the developing Historically Black Colleges and Universities (HBCU); so the funding of the project will permit us to conduct productive research, and to recruit other doctoral colleagues and partners.

b. Promotion of Economic Development

The project which enhances the fundamental science of computing technologies and sciences will support a variety of disciplines, such as chemical engineering which is one of most important industry in the state of Louisiana. Due to the current shortage of scientists and engineers, with an acute emphasis on that of African-Americans, this project at Dillard will foster an increase in the supply of such professionals. Annual publications of the National Science Foundation, relative to the science and engineering manpower, support this contention. We are therefore obligated to step up the production of engineers and scientists to meet the obvious demand.

According to the Digital Opportunity for Louisiana's Youth: Fact Sheet, in the state of Louisiana, between 2004 and 2014, jobs in the information technology fields are expected to increase by about 30%, for an addition of over 1 million jobs nationally. There will be 27 out of every 1,000 private sector workers in Louisiana are employed by high-tech firms. In Louisiana, high-technology industry workers earn an average of \$17,495 more per year than other private sector

workers. Although high technology is becoming the most hot industrial area state wide, there are tremendous gap between our state and the nation.

- Louisiana ranks 31st in the U.S. for overall number of high-technology workers and 44th for average high-tech wage.
- 71% of households in Louisiana earning less than \$15,000 per year do not own a computer compared to 48% of all Louisiana's households and 38% of all households nationally.
- 83% of households in Louisiana earning less than \$15,000 per year do not use the Internet at home compared to 56% of all Louisiana's households and 45% of all households nationally.
- 10% of all Louisiana's households have broadband compared to 20% of all households nationally.
- Among the 50 states and the District of Columbia, Louisiana ranks 49th in percentage of households with a computer, 49th in percentage of households with Internet access, and 48th in percentage of households with broadband access

Highly qualified scientists and engineers are the backbone of economic development and diversification in the state Louisiana. Since the State is interested in integrating high technology into the traditional industries such as biology, chemical engineering, and petroleum industry, the proposed project, which trains and supports the future engineers with advanced computational technologies, is a great investment towards the promotion of economic development.

To the above economic merit of the project, one should add the fact that the current federal research funding in the Division of Natural Science and Public Health is more than 3 Millions, constitutes a direct and immediate infusion of funds into the State's economy. Dillard University, the leading recipient of BORSF support funds is now leading to further external funding of our quality instructional and research programs. This claim is partly substantiated by the very nature of the current computer-intensive research projects in the division.

6. ADDITIONAL FUNDING SOURCES

The Congress has supported Dillard University's recovery process through a number of awards. Since 2006, the university has secured over \$48M in grant/contract resources, a significant portion of which is dedicated to activities associated with Computer Science and other Natural Science disciplines. The proposed project will be sustainable when it is finished. All the machines will be continued fully utilized for undergraduate instruction and research.

Dillard University is now actively engaged in an effort with the Army Corp of Engineers to conduct GIS research in the city of New Orleans. The popular ArcGIS software package with 15 licenses has been purchased from ESRI Company. This activity will provide additional funding for the computer technology and science laboratory.

BIOGRAPHICAL SKETCH			
Provide the following information for the key personnel and consultants and collaborators. Begin with the principal investigator/program director. Photocopy this page for each person.			
Name Zujia Xu		Position Title Assistant Professor	
EDUCATION (Begin with baccalaureate or other initial professional education and include postdoctoral training.)			
INSTITUTION AND LOCATION	DEGREE	YEAR CONFERRED	FIELD OF STUDY
Shanghai Jiaotong University	B.S.	1995	Mechanical Engineering
Shanghai Jiaotong University	B.S.	1995	Electrical Engineering
Shanghai Jiaotong University	M.S.	1998	Mechanical Engineering
Tulane University	M.S.	2003	Computer Science
Tulane University	Ph.D.	2003	Engineering

RESEARCH AND PROFESSIONAL EXPERIENCE: Starting with present position, list, in reverse chronological order, previous relevant employment, experience, and honors. Key personnel includes the principal investigator and any other individuals who participate in the development or execution of the project. Key personnel typically will include all individuals with doctoral or other professional degrees, but in some projects will include individuals at the masters or baccalaureate level provided they contribute in a substantive way to the development or execution of the project. Include present membership on any Federal Government public advisory committee. List, in reverse chronological order, the titles, all authors, and complete references to pertinent publications during the past five years and to representative earlier publications pertinent to this application. DO NOT EXCEED TWO PAGES.

PROFESSIONAL EXPERIENCES:

- National Institute of Global Environmental Exchange (NIGEC) South-Central Center
Visiting Professor
Lattice Boltzmann Model for Eddy Covariance Method

2005.5 – 2005.8
- National Institute of Global Environmental Exchange (NIGEC) South-Central Center
Visiting Professor
Numerical modeling flows in an open ecosystem

2004.5 – 2004.8
- Computer Science Department at Dillard University
Assistant Professor
Teaching Computer Applications, Programming II, Data Structure and Analysis Algorithms

2003.9 – Present
- Mechanical Engineering of Tulane University
Research Assistant
Simulated soil erosions under various conditions; Concluded several rules for particle sedimentation and fluidization, which can be applied to refinery, waste water treatment, and food process industries; Developed animation tools, implemented by Java, to visualize multiphase flow including particles and fluid motions

1998 – 2003
- Computer Science of Tulane University
Research Assistant
Created an Artificial Intelligent tool to analyses DNA sequences; Fundamental research on Support Vector Machine (SVM)

2000 - 2002

Engineering School of Tulane University

1998 - 2003

Teaching Assistant

Taught, including classes and labs, Heat Transfer, Thermal Power Plant, Thermal Dynamics, Fluid Dynamics, Mechanical Materials, Algorithms, C/C++, Database, Data Structure

ICMF, New Orleans

2001.5

Assistant Organizer

Co-organized International Conference of Multiphase Flow (ICMF)

South Physical Institute in China

1998

Assistant Engineer

Drafted, designed and tested HVAC & Refrigeration systems

MEMBERSHIPS

Member of ASME

Member of IEEE

Member of A. I. Ch. E.

Grants

1. Principal Investigator, Louisiana Board of Regents, "Enhancement of Chemical Engineering Instruction and Research", \$56,000, 2004 – 2005
2. Principal Investigator, Louisiana Board of Regents, "Enhancement of Computational Science Instruction and Research", \$59,500, 2006 – 2007

SELECTED PUBLICATIONS

1. Xu, Z.-J., Tran-Cong, S., Feng, Z. and Michaelides, E.E., School of Engineering and Soutcentral Regional Center of NIGEC, Tulane University, "Direct Numerical Simulations of Flows in Ecosystems using the Lattice Boltzmann Method", Reviewed by Agricultural and Forest Meteorology
2. Xu, Z.-J., Tran-Cong, S., Feng, Z. and Michaelides, E.E., School of Engineering and Soutcentral Regional Center of NIGEC, Tulane University, "The full governing and closure equations for the evaluation of Net Ecosystem Exchange (NEE)", Submitted to Bound-Layer Meteorol
3. Zhang, K., Xu, Z-J, Peng, J. and Buckles, B., "Empirical Comparison of Robustness of Probability Estimation Trees on Different Evaluation Metrics", In Proceeding of 5th International Conference on Data Mining (ICDM), November 2005, New Orleans, Louisiana (Accepted Ratio 22%).
4. Xu, Z-J, Buckles, B. and Zhang, K., "DNA Sequence Classification Using Support Vector Machine", In Proceedings of SCI, Orlando, July 2004.
5. Zhang, K., Xu, Z-J and Buckles, B., "Using Multimembered Evolution Strategies For Oblique Decision Tree Induction(ESODT)", In Proceedings of SPIE, Orlando, March, 2005.
6. Xu, Z-J and Michaelides, E., E., "Sedimentation of bidisperse suspension", Fluid Dynamic Research, 2005 (In Review).
7. Xu, Z-J and Michaelides, E., E., "The effect of particle interactions on the sedimentation process", International Journal of Multiphase Flow, vol. 29, pp. 959 – 982, 2003.
8. Xu, Z-J and Michaelides, E., E., "Non-Cohesive Particles Sediment in Inclined Vessels", Journal of chemical engineering communication, vol. 192, Number 4, pp. 532 – 549, 2005.
9. Michaelides, Efstathios E. and Xu, Z-J, "Lattice Boltzmann Simulation of the Sedimentation Process with Non-Cohesive Particles ", proceedings of FLUID-PARTICLE INTERACTIONS VI, Italy, August 25-30, 2002.
10. Michaelides, E. E. and Xu, Z-J, "Particle interactions during sedimentation", 55th annual proceedings of American Physical Society, Dallas, November, 2002.
11. Xu, Z-J, Michaelides, E. E. and Nikitopoulos, D.E. "The influence of Large Scale Structures of an Axisymmetric Jet in the Evaporation of Droplets," APS-DFD annual meeting, New Orleans, November 1999.
12. Xu, Z-J and Meng, Y. "The experimental research on Cavitation in pump system", Journal of Fluid Machinery (in Chinese), 1998, January.
13. 11. Xu, Z-J, Huang, J. and Zhou, J., "The fundamental mechanism of Cavitation in pump system", Journal of Fluid Machinery (in Chinese), 1998, June.

BIOGRAPHICAL SKETCH

Provide the following information for the key personnel and consultants and collaborators. Begin with the principal investigator/program director. Photocopy this page for each person.

Name

Azubike Damian Okpalaeze

Position Title

Assistant Professor

EDUCATION (Begin with baccalaureate or other initial professional education and include postdoctoral training.)

INSTITUTION AND LOCATION

DEGREE

YEAR
CONFERRED

FIELD OF STUDY

West Virginia Institute of Technology

B.S.

1982

Computer Management and Data
Communications

West Virginia Institute of Technology

B.S.

1982

Business Management

Southern University A&M College

M.S.

1985

Computer Science

Southern University A&M College

Ph.D.

2005

Math/Science Educational

RESEARCH AND PROFESSIONAL EXPERIENCE: Starting with present position, list, in reverse chronological order, previous relevant employment, experience, and honors. Key personnel includes the principal investigator and any other individuals who participate in the development or execution of the project. Key personnel typically will include all individuals with doctoral or other professional degrees, but in some projects will include individuals at the masters or baccalaureate level provided they contribute in a substantive way to the development or execution of the project. Include present membership on any Federal Government public advisory committee. List, in reverse chronological order, the titles, all authors, and complete references to pertinent publications during the past five years and to representative earlier publications pertinent to this application. DO NOT EXCEED TWO PAGES.

PRESENT POSITION:

Presides as an Interim Chairperson and an Assistant Professor in Computer Science department with responsibilities of overseeing the functionality of the department and of instructing computer programming languages such as Cobol, LISP, Fortran, Pascal, C++. Also instructs courses in Data Communications, Artificial Intelligent, Database Management System, Systems Analysis and Design, Computer Network, Compiler Construction, Operating System and other application software packages such as Microsoft Office Manager. Builds the students level of confidence in their computer literacy, and teaches them to use the computer as a tool of instruction, communication, and problem solving.

PROFESSIONAL EXPERIENCE

DATES

AGENCY/INSTITUTION

POSITION

1996 - Present

Melton Foundation (Dillard University)
Le Mars, Iowa

Technology Specialist
Faculty Task Team

1990 – Present

Innovative Endeavors
New Orleans, Louisiana

Hardware Consultant

1993 – 1999

Delgado Community College
Technology Division,

Adjunct Professor

1992 – Summer

Bike-Tech Computer Systems
Design Division, New Orleans, Louisiana

Project Manager

ACADEMIC EXPERIENCE

DATES	AGENCY/INSTITUTION	POSITION
1989 – Present	Dillard University Computer Science Department	Assistant Professor Computer Science Department
1993 – Present	Delgado Community College Technology Division	Adjunct Professor Technology Division
1986 – 1989	Southern University Computer Science Department New Orleans, Louisiana	Assistant Professor Computer Science

PUBLICATIONS

Okpalaeze, Azubike D., Spring 1994, “The Impact of Computer Network and Data Communication Channels on Multimedia and Classroom of the Future”, (American Society of Engineering Education (ASEE/GSW))

Okpalaeze, Azubike D., Fall 1994, Co-Author, “The Implementation of Natural Language in Expert System”, Association of Computing Machinery (ACM), Southeast Regional Conference

CERTIFICATES OF ACHIEVEMENT

High Performance Computing (MSI HPC) on Cluster computing
FOCUS 101 for Data Processing Professional
FOCUS 102 for Data Processing Professional

PROFESSIONAL SERVICES

1982 – Present Association of Computing Machinery
1981 – Present Data Processing Management Association
1885 – Present Society of Advance Management

GRANTS

Principal Investigator , State Farm College Grant
Principal Investigator, UNCF/ORACLE College Initiative
Co-PI, Enhancement of Computer Science Instruction (Board of Regents)

DEPARTMENT COMMITTEES

Spring 2001 Dillard University Information Technology Committee
Spring 2000 Faculty Search Committee - Natural Science Division
1989-1999 Committee on Self-Study for the Division of Natural Science
1997-1998 Committee on Information Technology Standardization
Spring 1996 Committee on Curriculum Development and Evaluation

SERVICE ACTIVITIES

1996 – Present Faculty Task Team – Melton Foundation (Dillard University)
1989 – Present Co-Advisor – Disk Online System (DOS) Computer Science club
1994 – Present Dillard University Auxiliary – Member
1997 – Present Mentor – Summer Transition Program / Louisiana Alliance for Minority Program (STP/LAMP)

COURSES TAUGHT

Advanced Cobol Programming Language	Advanced Systems Analysis and Design
Artificial Intelligence	Compiler Construction
Computer Concepts and Application	Data Communications
Data Structures	Database Management System
Fortran Programming	Introduction to Microcomputers
Introduction to Problem Solving	Introduction to Unix and C Programming

BIOGRAPHICAL SKETCH

Provide the following information for the key personnel and consultants and collaborators. Begin with the principal investigator/program director. Photocopy this page for each person.

Name
VETLANA AROUTIOUNIAN

Position Title
Assistant Professor

EDUCATION (Begin with baccalaureate or other initial professional education and include postdoctoral training.)

INSTITUTION AND LOCATION

DEGREE

YEAR
CONFERRED

FIELD OF STUDY

Yerevan State University, Yerevan, Armenia

M.S.

1974

Physics

Wake Forest University, Winston-Salem, NC,
USA

Ph.D.

2002

Physics

RESEARCH AND PROFESSIONAL EXPERIENCE: Starting with present position, list, in reverse chronological order, previous relevant employment, experience, and honors. Key personnel includes the principal investigator and any other individuals who participate in the development or execution of the project. Key personnel typically will include all individuals with doctoral or other professional degrees, but in some projects will include individuals at the masters or baccalaureate level provided they contribute in a substantive way to the development or execution of the project. Include present membership on any Federal Government public advisory committee. List, in reverse chronological order, the titles, all authors, and complete references to pertinent publications during the past five years and to representative earlier publications pertinent to this application. DO NOT EXCEED TWO PAGES.

Research and Educational Work Experience

2006- Assistant Professor, Dpt. of Physics and pre-Engineering, Dillard University
2005-2006 Postdoc-Scholar, Dpt. of Computational Biology, University of Pittsburg
2000-2005 Adjunct Assistant Professor, Dpt. of Physics, NC A&T State University
1991-1992 Research-Scholar, CNRS/Lab. de l'Accélérateur Linéaire/IN2P3. Orsay, France
1980-1993 Staff Scientist, Div. of Physics of Cosmic Rays, YerPhI. Yerevan, Armenia
1974-1978 Staff Scientist, Div. of Theor. Phys., NSRIRM (VNIIRI), Yerevan, Armenia

Qualifications And Skills

Ph.D. Specialization

Mechanisms and kinetics of melting of sickle cell hemoglobin (HBS) aggregates. Time-resolved extinction measurements. Mathematical modeling of dissociation of HBS aggregates.

Current research - Computational biophysics/Physics:

- i) Equilibrium motions in a protein. Computational (Monte Carlo) studies using coarse-grained rigid-polypeptide-plane protein model (Go-like contact potential, Ramachandran and hydrophobic propensities). Convergence of conformational trajectories: optimal MC move and temperature. X-Ray and NMR experimental fluctuation profiles of equilibrium motions in a protein compared with that obtained in MC computations.
- ii) Free Energy Landscape computations of the protein folding/unfolding transitions: search for key residues.
- iii) Mathematical approaches in Genomics.
- iv) Renormalization Group computations. Structural phase transitions' flow diagrams.

Publications (selected)

1. M. Ytreberg, S. Aroutiounian, D. Zuckerman “Demonstrated convergence of the equilibrium ensemble of a fast united-residue protein model” (*submitted*)
2. Aroutiounian, S., On Matrix Operator of Exon Splicing, *Proceedings of 9th Annual Conference on Computational Genomics*, Baltimore, MD, October 28-31, 2006
3. S. Kh. Aroutiounian, “CO partial pressure dependence of the kinetics of melting of HbS aggregates studied in high concentration phosphate buffer” *Talk-Presentation, SESAPS Meeting*, Auburn, AL, October, 2002
4. S. Kh. Aroutiounian, J. G. Louderback, S. K. Ballas, D. B. Kim-Shapiro, Evidence for carbon monoxide binding to sickle cell polymers during melting. *Biophysical Chemistry*, **91**: 167-181, 2001
5. J. G. Louderback, S. Kh. Aroutiounian, W. C. Kerr, S. K. Ballas and D. B. Kim-Shapiro, Temperature and domain size dependence of sickle cell hemoglobin polymer melting in high concentration phosphate buffer. *Biophys. Chem.* **80**:21-30,1999
6. A.A.Chilingarian, S.Kh.Harutunyan, On the possibility of a multidimensional kinematic information analysis by means of nearest-neighbor estimations of dimensionality. *Nuclear Instruments and Methods in Physics Research*, **A281**:388-392,1989
7. S. Aroutiounian, A. Chilingarian, R. Kokoulin and A. Yerlikin “Comparison of Iron and Lead Variants of the ANI pair-Meter” (in Russian) *Prep.YerPhI-1137(14)*-89, 1989
8. S. Aroutiounian, A. Chilingarian and R. Kokoulin “On nonparametrical Methods of Suppression of Nuclear Cascade Background in measuring of Muon Spectrum with Pair-Meter” (in Russian), *Prep.YerPhI-940(91)*-86, 1986
9. S. Aroutiounian “The geometrical properties of Mahalonobis generalized distance” (in Russian), *Prep.YerPhI-337(41)*-84, 1984
10. S. Aroutiounian, E. Gazazian “Radiation from charged particles traversing a waveguide with a rectangular aperture” (in Russian), *Izv. Acad. Nauk Arm. Fiz.* **11**:234-237,1976

Presentations (recent)

1. S. Aroutiounian, On Matrix Operator of Exon Splicing. *Poster Session. Genomes, Medicine and the Environment Conference*, South Carolina, October, 2006.
2. S. Aroutiounian, M. Ytreberg, D. Zuckerman Fluctuations in a fast united-residue model. *Poster Session. 50th Annual Meeting of Biophysics Society*, Salt Lake City, UT, 2006.
3. S. Kh. Aroutiounian, S. Danagouljian “Fractal correlation dimensionalities and pattern formation – genomic application” *Talk-Presentation, 2nd Conference on Analysis and Probability on Fractals*, Cornell University, NY, May, 2005

Awards

- 2005–2006 Ruth L. Kirschstein NRSA Trainee. Award to the Department of Environmental and Occupational Health, University of Pittsburgh, School of Public Health.
- July, 2004 Genome Scholar, Short Course on “Current Topics In Genomic Research”, NHGRI / NIH, Bethesda, MD
- 1976 “Best Young Scientist of the Year”. NSRIRM (VNIIRI), Yerevan, Armenia

CURRENT AND PENDING SUPPORT

(From ALL sources, including Board of Regents Support Fund)

The following information MUST be provided for each investigator and other senior personnel. Use additional sheets as necessary.

NAME OF INVESTIGATOR: Zujia Xu, Ph.D., Azubike Okpalaeze, Ph.D., Svetlana Aroutiounian, Ph.D.

Status of Support: ___Current ___Pending ___Submission Planned in Near Future

Contract Number/Proposal Title:

Source of Support:

Award Amount (or Annual Rate): \$_____ Period Covered:_____

Location of Activity:

Person-Months or % of Effort Committed to the Project: ____Cal Yr ____Acad. ____Summer

Status of Support: ___Current ___Pending ___Submission Planned in Near Future

Contract Number/Proposal Title:

Source of Support:

Award Amount (or Annual Rate): \$_____ Period Covered:_____

Location of Activity:

Person-Months or % of Effort Committed to the Project: ____Cal Yr ____Acad. ____Summer

Status of Support: ___Current ___Pending ___Submission Planned in Near Future

Contract Number/Proposal Title:

Source of Support:

Award Amount (or Annual Rate): \$_____ Period Covered:_____

Location of Activity:

Person-Months or % of Effort Committed to the Project: ____Cal Yr ____Acad. ____Summer

Status of Support: ___Current ___Pending ___Submission Planned in Near Future

Contract Number/Proposal Title:

Source of Support:

Award Amount (or Annual Rate): \$_____ Period Covered:_____

Location of Activity:

Person-Months or % of Effort Committed to the Project: ____Cal Yr ____Acad. ____Summer

**BOARD OF REGENTS SUPPORT FUND
TRADITIONAL AND UNDERGRADUATE ENHANCEMENT, FY 2008-09**

Budget Pages

Year 1:

	Support Fund Money Requested	Institutional Match ¹	Private/Other Match ²
A. Equipment ³	\$60994	\$	\$
B. Software	\$17600	\$	\$
C. Supplies	\$	\$	\$
D. Shipping/handling	\$	\$	\$
E. Installation	\$	\$	\$
F. Personnel training	\$	\$	\$
G. Other	\$22500	\$	\$
H. Indirect costs	Not allowed	\$17657 (in kind)	\$
I. Maintenance	Strongly discouraged	\$	\$
J. Total costs (A-I)	\$101094	\$17657	\$0

Year 2(Only if the proposed duration is 2 years):

	Support Fund Money Requested	Institutional Match ¹	Private/Other Match ²
A. Equipment ³	\$	\$	\$
B. Software	\$	\$	\$
C. Supplies	\$	\$	\$
D. Shipping/handling	\$	\$	\$
E. Installation	\$	\$	\$
F. Personnel training	\$	\$	\$
G. Other	\$	\$	\$
H. Indirect costs	Not allowed	\$	\$
I. Maintenance	Strongly discouraged	\$	\$
J. Total costs (A-I)	\$0	\$0	\$0

1 Stipulate whether in-cash or in-kind. The Board strongly encourages the sharing of costs for proposed projects. Applicants and institutional officials should note, however, that the employing institution will be required to honor the commitments made in the original proposal before any awards are made. Discounts for equipment purchases are not allowable as institutional match.

2 The budget page(s) must reflect and the budget justification pages must explain any external funds that are claimed in the proposal. External funds and their expenditure must be accounted for in the same manner as Support Fund money and institutional match.

3 Equipment. If applicable, itemize and describe briefly the proposed equipment and its intended use in the project. Include the name, model number, and manufacturer(s).

**BOARD OF REGENTS SUPPORT FUND
TRADITIONAL AND UNDERGRADUATE ENHANCEMENT, FY 2008-09
Budget Pages**

Composite Budget Page:

	Total Support Fund Money Requested	Total Institutional Match ¹	Total Private/Other Match ²
A. Equipment ³	\$60994	\$0	\$0
B. Software	\$17600	\$0	\$0
C. Supplies	\$0	\$0	\$0
D. Shipping/handling	\$0	\$0	\$0
E. Installation	\$0	\$0	\$0
F. Personnel training	\$0	\$0	\$0
G. Other	\$22500	\$0	\$0
H. Indirect costs	Not allowed	\$17657	\$0
I. Maintenance	Strongly discouraged	\$0	\$0
J. Total costs (A-I)	\$101094	\$17657	\$0

II. **BUDGET JUSTIFICATION: (Attach pages, as needed, to each budget page.)**

Each line item on the preceding budget page under ASupport Fund Money Requested@ must be itemized, fully explained, and justified. Each line item under AInstitutional Match@ and APrivate Sector/Other Match@ must also be itemized, explained, and justified.

Description of Proposed Equipment - If applicable, itemize and describe briefly the proposed equipment. Include the name, model number, and manufacturer(s).

Equipment. Section C.1 provides a detailed listing of the acquisitions (equipment and software) with models and prices. The vendors provided the prices as listed (i.e., quotes). The need for the 20 personal computer stations was as a result of the very nature of the computations to be carried out by each of the principal investigators and by the students who are taking the related courses annually. The personal computational stations, which will be connected to the server, will finish the pre- and post- computation work. The pre-computation includes algorithm design and analysis, writing and testing programs and submitting computation jobs. And the post-computation tasks mainly are, drawing charts, writing reports and papers, designing and generating complicate vector figures or animations that require high capacity memory (1G MB RAM). The cost for the computers is $20 \times \$2,021.90 = \$40,438$. The Dell PowerEdge multiple CPU server is a high powerful machine for intensive serial and parallel scientific computations. The cost for the server is \$12,487.33. The specifications of the personal workstations and the server are showed the in the following two tables. The two laptops will be used for the presentations for the instructions, workshops and conferences. The remaining items in the equipment category are networking devices and accessories as quoted by vendors (the lowest, responsive quotes are the ones listed). Table A.1 and A.2 are the detail specifications for the personal computers and PowerEdege server.

Software. The software products, as per the narrative, are needed research, the integration of research and education, and for extensive code development and analysis work. Tecplot 10 for Linux will be used to do the post computation work, such as drawing charts, creating fluid velocity vector graph, generating animations and etc. Matlab will be applied to the simple program design, numerical methods analysis and simple graphics. Since there are many Matlab routines available, it is a must-learned tool for the students and faculty. Ansys is one of the most powerful and popular commercial software package for the engineers in both academic and industrial fields. It can design (pre-computation), compute and draw dynamic graphs (post-computation). The C/C++ compiler allows us to implement advanced serial and parallel computation programs. These software products will ensure the congruency of our instruction with the practices in graduate schools and in high technology industries. The listed prices are the lowest responsive quotes.

Conferences and Workshops. It is estimated that three papers will be submitted to different conferences related to computing technology and science. It is necessary for the principal investigators to publicly publish the research results and communicate with the computing engineers/professors (inter) nationwide. The conference expense will cover the registration fee, transportation and accommodation for the participants including faculty and students. There will a couple of workshops. Some outstanding investigators from international computing technology research centers such as IBM will be invited to Dillard to give academic seminars on the state-of-

art computing technology models. The three conferences that Dr. Xu intends to participate are: International Conference on Computational Science, International Conference on Computer, Electrical, and Systems Science, and Engineering, and The CSITEd (Computer Science & Information Technology Education) conference.

Institutional Support. The Division of Natural Science and Public Health will support this project. Additional equipments, such as projectors, and software including Microsoft Office will be supplied by the division. The division also supports the faculty and students attending the conferences. The approximate financial aid from Dillard University is \$17,657, as listed before. The IT technical responsible for installing, upgrading and housing the equipment will be provided by Dillard University. The estimated cost from the school is 18% of request proposal cost.

Very limited personnel costs. As noted below, the computer science faculty provides most of the personnel cost for the implementation of this timely new project (during and after the BORSF funding period.) The request for one (2) months support (summer support) for Dr. Zujia Xu is needed in light of the demand on his time- for the installation and operation of the Local Access Network (LAN) system and for the integration of the high performance parallel computing into student instruction and faculty research. He will dedicate to the research tasks listed in the proposal in the two-month summer time. The major job includes conducting research projects which will result to conference papers, and instructing undergraduate students' computational environmental sciences research. We expect two students, if not more, to possibly build a relevant research proposal around the design, operations, benchmark of this system. The personal payment is only two summer months support for Dr. Xu and summer financial sponsorship for the undergraduate students.

Table A.1 Specification of personal computers

Dell Personal Computer (20), Price: \$2,021.90 each	
Catalog Number:	25 Retail RC956904
Precision 690 Series P4:	Pentium® 4 Processor at 3.0GHz with 400MHz front side bus BP224PE
Memory:	1G MB Shared DDR SDRAM at 333MHz 512M3
Keyboard:	Dell™ Quietkey® Keyboard QK
Monitor:	17 in (16.0 in v.i.s., .27dp)E773c Monitor E773
Video Card:	Integrated Intel® 3D Extreme Graphics IV
Hard Drive:	360GB ATA/100 Value Hard Drive 40V
Floppy Drive	3.5 in Floppy Drive FD
Operating System:	Microsoft® Windows® Vista
Mouse:	Dell® 2-Button Scroll Mouse SM
Network Interface:	Integrated 10/100 Ethernet IN
CD or DVD Drive:	48x CD-RW Drive with Sonic RecordNow 48CDRW
Limited Warranty	3 Year Limited Warranty plus 3 Year NBD On-Site Service

Table A.2 Specification of PowerEdge Server

Dell PowerEdge 2600 II with 4 processors, Price: \$12,487.33	
Catalog Number:	25 Retail RC956904
Base:	Intel® Xeon™ 2.0GHz/1MB Cache, Redundant Power 660201
Additional Processors:	Quad Processor Intel Xeon, 2.0GHz/1MB Cache PowerEdge 66XX
Memory:	2GB DDR SDRAM (4X512MB) 2GB4D
Keyboard:	Standard Windows Keyboard,Gray S
Monitors:	15" E551 15MON
Hard Drive:	73GB 10K RPM Ultra 320 SCSI Drive 7310320
Controller:	PERC3,DC,128MB,1-INT,1-EXT CHANNELS P3D128I
Floppy Drive:	Floppy Drive FD
Operating System:	Red Hat Linux 2.1 Advanced Server with Documentation and Media
Mouse:	Logitec Mouse L
Network Adapters:	Intel Pro 100S IN100S
Modem:	BroadCom, 56K PCI Internal Modem, V.92
CD ROM:	24X IDE CD-RW/DVD ROM Drive
Documentation:	Printed Documentation, PowerEdge 6600 66DOCS
2nd Hard Drive:	73GB 10K RPM Ultra 320 SCSI Drive 3610320
HD Configuration:	Add-in Card RAID 5, No Drives in Media Bay AR5N
Chassis Style:	Tower Chassis Orientation,P6600 TOWER
Hardware Support Services:	3Yr Same Day 4Hr Response Parts + Onsite Labor
Installation Support Services:	No Installation NOINSTL
3rd Hard Drive:	36GB 10K RPM Ultra 320 SCSI Drive 3610320