PROJECT DESCRIPTION

1. Rationale and Vision

As the 21st Century begins, computational science has emerged as a third paradigm for scientific research, joining the established approaches of analysis and laboratory experimentation. To predict the evolution of phenomena or to optimize a process, one normally must build a mathematical model to help in determining and describing the behavior of a system or process. Often the mathematical model is not fully amenable to classical analysis. Sometimes the large scale of the process or the lack of access to measured data, prohibits employing laboratory experimentation (or even observations). In such cases, with the aid of a "computational laboratory", one can apply numerical experiments that allow a sufficiently accurate understanding of the process to be able to reliably predict the behavior of the model and the process. Scientific computation is becoming ever more critical in modeling and understanding of complex and coupled phenomena.

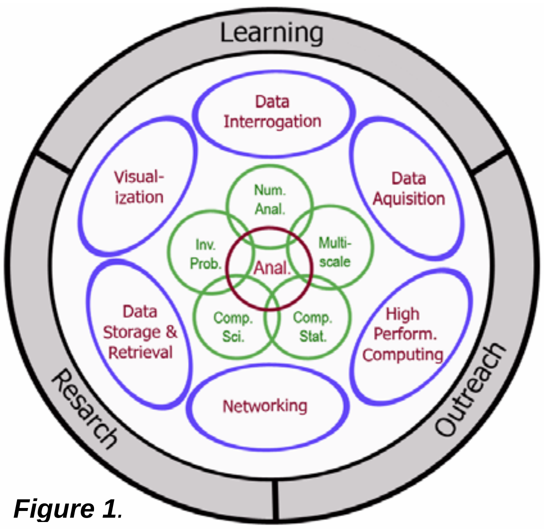

Figure 1.

To ensure that this scientific computation paradigm becomes a major strength of KAUST, Texas A&M University proposes to establish the Institute for Applied Mathematics and Computational Science (IAMCS) with a mirror institute in KAUST. We envision establishing a unique state-of-the-art, multidisciplinary computational research base with a robust infrastructure to enable large-scale scientific computation research, advanced multidisciplinary learning and education, and a large number of applications in diverse areas of science and engineering of interest to Saudi Arabia and the World (*Figure 1*). The proposed research Institute begins with a multidisciplinary core of applied mathematicians, statisticians, and computer scientists, who will be supported by state-of-the-art hardware and software infrastructure. This core research group is connected to world-renowned colleagues and research centers in diverse application areas around the world. Working together, this prominent network of people will form a unique, first-class multidisciplinary international research and education Institute. KAUST students will be connected to world-class faculty and research resources in applied mathematics and computational sciences, and will be able to expand their horizons in a cyber-enhanced learning environment. One of our main objectives is to then mirror this unique research center infrastructure and multidisciplinary educational capability in a co-located Institute within KAUST.

2. Organization and Infrastructure.

The proposed Institute for Applied Mathematics and Computational Science (IAMCS) has been formed from a combination of five interdisciplinary Centers that have provided scientific computation leadership at Texas A&M University:

- The Institute for Scientific Computation (ISC)
- The Academy for Advanced Telecommunications and Learning Technologies (AATLT)
- The Center for Statistical Bioinformatics (CSB)
- The Alliance of Bioinformatics, Computational Biology, and Systems Biology (ABCS)
- The Center for Large-Scale Scientific Simulations (CLASS)

Each of these centers is an interdisciplinary group of Texas A&M faculty from applied mathematics, statistics, computer science, and various engineering fields with research expertise in scientific computation. IAMCS will form the coordinating umbrella organization for these Centers. The Office of the Vice President for Research has established a Computational Sciences and Engineering Task Force with strong internal funding to bring these Centers together and to help build the concept of IAMCS, as proposed.

Each of the Centers has existing interdisciplinary educational programs. In addition, the ISC has substantial research infrastructure in high performance computing, data storage, networking, and visualization to support the "Library" of the Future, which enables our research, education, and outreach activities. Texas A&M has substantial additional large-scale HPC and grid computing capabilities through HiPCAT and SURAgrid. The requested computer will leverage the purchase of a large high-performance cluster to complement our large IBM cluster and grid.

Dr. Richard Ewing, Executive Director of ISC will be the Director of IAMCS. He was formerly Vice President for Research at Texas A&M and has directed several research Institutes. Dr. Ray Carroll, Director of CSB, will be Deputy Director of IAMCS. Dr. Guy Almes, chief engineer for Internet2 and former Program Director for Cyberinfrastructure at NSF will be our Leader for Infrastructure. Dr. Christine Economides, NAE and formerly of Schlumberger and Dr. Guan Qin, Research Director for ISC and formerly of Mobil and ExxonMobil will be our Leaders for Industrial Outreach. Dr. Wei Zhao, Dean of Science of Rensselaer Polytechnic Institute (RPI), Dr. Jay Walton and Dr. Andrew Skadberg will be Leaders for Education. Dr. Yalchin Efendiev will be Leader for Research. Dr. Raytcho Lazarov will be Leader for Collaboration. Ms. Christine Yang will be Leader for Administration. These Leaders and the Directors of the five interdisciplinary Centers will form an Executive Committee that will make decisions on programmatic priorities.

3. Strategy for Success

We propose to expand our existing Institute for Applied Mathematics and Computational Science, with its strong applied mathematics core, and to continue to develop hardware and software infrastructure to provide the ability to effectively interrogate large data sets to enable effective modeling and simulation in a wide variety of scientific and engineering disciplines. To achieve this, we will focus on four major deliverables:

1) A Core Applied Mathematics and Computational Science Group at Texas A&M
2) Infrastructure: The Library of the Future
3) Education: The School of the Future
4) KAUST-Texas A&M Collaboration: The Mirror

3.1 A Core Applied Mathematics and Computational Science Group at Texas A&M University

3.1.1. The core research areas

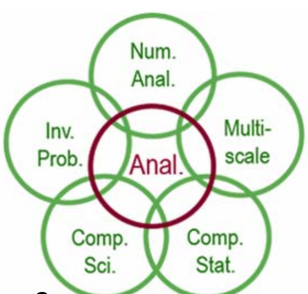

Figure 2.

The research group at A&M has strong expertise in applied mathematics, modeling, statistics, and computer science. The research includes the main directions of modern numerical analysis, efficient solution techniques (such as multi-grid and domain decomposition methods), inverse problems with various applications in imaging and parameter estimation, multiscale analysis and simulation methods and their applications, computer science, and computational statistics, biology, and chemistry (*Figure 2*).

For the core research, our focus will be on discretization and solution techniques (J. Bramble, C. Douglas, R. Ewing, J-L. Guermond, G. Kanschat, R. Lazarov, J. Pasciak, B. Popov), multi-scale modeling and simulation techniques (Y. Efendiev, R. Ewing, J-L. Guermond, R. Lazarov, J. Walton and P. Popov), inverse problems and imaging (P. Kuchment, W. Rundell, W. Bangerth, R. DeVore and M. Pilant), computational statistics (B. Mallick, R. Carroll), and computer science (C. Douglas, N. Amato, L. Rauchwerger, B. Stroustrup and V. Sarin).

3.1.2. Impact of Core Research to Applied Science and Engineering

The proposed research center has been built on existing research centers at Texas A&M University. In the past years, these centers have built and maintained rich and active research collaborations with industry and academic research institutions. Corporate research collaborations include ExxonMobil, Sinopec, Chevron, Hewlett-Packard, Saudi Aramco, and Computer Modeling Group (CMG). International academic collaborations include Fraunhofer Institute (Germany),

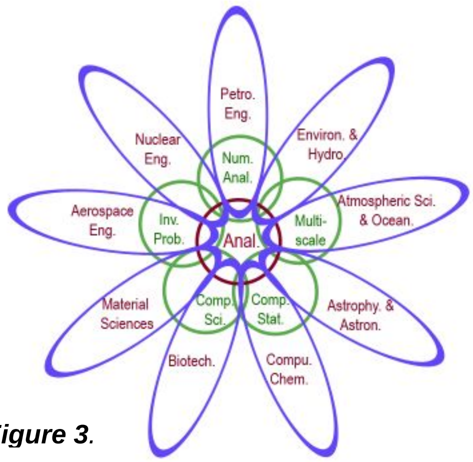

Figure 3.

University of Calgary (Canada), University of Stuttgart (Germany), University of Heidelberg (Germany), Peking University (China), University of Bergen (Norway), LNCC (Brasil), Bulgarian Academy of Sciences (Bulgaria), Bedford Institute of Oceanography (Canada), and Utrecht University (Netherlands). U.S. academic collaborations include the following universities: Kentucky, Utah, Princeton, Purdue, Penn State, Stanford, South Carolina, Texas, Rensselaer Polytechnic Institute, Montana State, Louisiana State, North Carolina, William and Mary, Florida, Miami, Caltech, and Alabama-Huntsville.

The core research will enable significant scientific computation capabilities in many application areas shown in *Figure 3*. Through working with science and engineering researchers in various disciplines, the core research will be extended to address some critical issues that are very important to Saudi Arabia and the world. The proposed research well represents the frontier research in applied mathematics and computational sciences and also the research strengths at Texas A&M University and in its collaborating institutions. To illustrate how we have begun to effectively extend the core research into the application areas which are shown in *Figure 3*, we pair scientific leaders in the core research areas with the leaders in the identified application areas to work as a multidisciplinary team. In particular, we will collaborate in the following research areas of interest to Saudi Arabia (we list team leaders and planned research topics):

- Petroleum Engineering Leaders: C. Economides , R. Ewing , M. Espedal, G. Qin
  - Large scale computer simulation for oil reservoirs
  - Numerical well testing in heterogeneous petroleum reservoirs
  - Compositional models for multi-phase flow and transport
  - Efficient linear solution methods for Large coupled systems of equations
  - Modeling of flow in fractured carbonate karst reservoirs
- Environmental Engineering/Hydrology Leaders: M. Binayak, M. Celia, R. Helmig, Y. Efendiev
  - Modeling of contaminant transport in heterogeneous aquifers
  - Geological sequestration of CO_2
  - Subsurface flows in vadoze zone and soil moisture data assimilation
  - Aquifer recharge optimization
- Atmospheric Sciences Leaders: J. North, R. Carroll, C. Douglas
  - Data assimilation in atmospheric sciences and 4D-VAR
  - Contaminant transport in atmosphere
  - Computational climate forecasting and uncertainty assessment
  - Atmosphere and ocean modeling of tropical cyclones
- Computational Chemistry Leaders: M. Hall, G. Almes, C. Douglas
  - Molecular modeling of complex chemical structures
  - Protein modeling
  - Data assimilation in atmospheric chemistry
- Material Sciences Leaders: D. Lagoudas, J. Walton, T. Cagin
  - Multiscale computational material sciences from atomistic to continuum length scales
  - Flows in high porosity media with complex microstructure such as metal foams
  - Multifunctional materials for extreme environment sensors and actuators
- Computational Biology Leaders: E. Dougherty, R. Caroll, N. Amato, J. Walton
  - Bioinformatics and biostatistics
  - Biomechanics and tissue modeling
  - Use of genomic data for cancer prediction
- Nuclear Engineering Leaders: M. Adams, R. Lazarov, G. Kanschat
  - Computational radiation transport

- Aerospace Engineering Leaders: J. Junkins, J-L. Guermond
    - Guidance, navigation, and astronautics
    - Smart Sensor Technology
    - Efficient Navier-Stokes solvers with adaptivity

We next describe some of the major research directions, projects, expected outcomes, and potential impact for research in each of the five major core research areas. We believe that we are addressing many research areas of specific interest to Saudi Arabia and KAUST, in particular.

a. Numerical analysis. Discretization and solution techniques

Motivation and impact. One of the most challenging topics in applied mathematics has been the development of analytical theory and numerical approximations of various partial differential equations (PDEs) that are used in mathematical modeling of physical and engineering problems. In the last decade substantial progress has been achieved in developing flexible, accurate, and stable methods.

Research directions and state of the art. We will work in three interrelated directions: (1) discretization methods, (2) adaptivity and error control and (3) efficient solution methods. Our expertise and interests are in several fundamental directions of *numerical discretization* which include finite element, finite volume, discontinuous Galerkin, finite difference methods, domain decomposition, mortar approximations, Eulerian-Lagrangian localized adjoint methods for the advection-diffusion equation, and high-order shock capturing schemes for nonlinear conservation laws. These discretization methods require *adaptivity and error control* for robust and accurate simulation purposes. The discretization of mathematical models described in terms of PDEs results in large systems of linear equations. In general, these systems are sparse and ill-conditioned and require *efficient solution methods*.

Expected results.

- Study and develop high order, adaptive schemes for linear and nonlinear partial differential equations (R. Lazarov, G. Kanschat, J-L. Guermond).
- Study and develop computationally efficient and accurate numerical algorithms for nonlinear conservation laws (B. Popov, J-L. Guermond, Y. Efendiev, R. Ewing, P. Popov).
- Develop efficient and reliable local error estimators (or indicators) for transport, Stokes and Navier-Stokes equations and develop a grid refinement strategy that is fast and convergent (G. Kanschat, R. Lazarov, W. Bangerth).
- Develop both special-purpose methods (multi-grid and multi-level methods) and general methods based on Krylov subspace iterations (J. Pasciak, C. Douglas, R. Ewing, J. Bramble, G. Kanschat).

b. Inverse problems and imaging

Motivation and impact. Many major challenges of the contemporary applied mathematics belong to the class of the inverse problems, i.e. problems where system parameters need to be estimated from external measurements. These measurements are of either signals coming naturally from the system, or of those triggered by the observer. Such, for instance, are problems of geophysics, reservoir characterization, and medical tomography, where X-rays, ultrasound, and electromagnetic waves are used as external signals. Inverse problems are also central in industrial non-destructive testing. It is known that mathematical methods—both analytic and numerical—are crucial for inverse problems. It is well established that inverse problems are extremely challenging due to their instability with respect to measurement and hardware errors and discretization, etc. Thus, significant mathematical expertise is required for handling these issues. This expertise is readily available at A&M, where several mathematics and engineering faculty members have made major contributions to the area of inverse problems

Research directions and state of the art. It is planned to work, in particular, in the following novel directions: (1) Analytic and numerical methods for the newly developing thermoacoustic (also called photoacoustic and optoacoustic) tomography (TAT) for medical applications and related issues of diffraction tomography and geophysical imaging; (2) Analytic and numerical methods for the newly developing ultrasound modulated optical tomography (UMOT) for biomedical applications; (3) Analytic and numerical methods for the newly developing ultrasound modulated electrical impedance tomography (UEIT) for biomedical and industrial applications; (4) Analytic and numerical methods for the fluorescence optical tomography (FOT) for biomedical applications; (5) Heterogeneous subsurface characterization based on seismic, pressure and tracer data.

Expected results.

- Development of efficient analytic and numerical reconstruction methods for TAT, UOT, UEIT, and FOT (P. Kuchment, W. Bangerth, W. Rundell).
- High-resolution subsurface characterization using dynamic data information (Y. Efendiev, R. Ewing, A. Datta-Gupta).
- Optimal experimental design for inverse problems in biomedical imaging (W. Bangerth).
- Massively parallel solution of partial differential equations using adaptive finite element methods (W. Bangerth).
- Imaging compression algorithms (R. DeVore).

c. Multiscale modeling and simulation techniques

Motivation and impact. A broad range of scientific and engineering problems involve multiple scales. Traditional approaches are known to be valid for limited spatial and temporal scales. Conventional methods cannot cope with physical phenomena operating across large ranges of scales such as in the modeling of atomistic effects in materials, in the modeling of protein folding and modeling the effects of the fractures in the large-scale flow and transport processes. The tyranny of scales dominates simulation efforts not just at the atomistic or molecular levels, but wherever large disparities in spatial and temporal scales are encountered. Such disparities appear in virtually all areas of modern science and engineering, e.g., in astrophysics, atmospheric science, geosciences, nanotechnology, biology, computational fluid dynamics, and space sciences. There is a growing need to develop systematic modeling and simulation approaches for multiscale problems. These numerical simulation techniques will ultimately help to improve our understanding of wide range of physical processes.

Research directions and state of the art. The Texas A&M group's focus has been on various important areas of multiscale modeling and simulation with emphasis on applications in areas such as material science, porous media flow and transport, fracture of brittle materials, and turbulent flows. Multiscale analysis and simulation requires understanding subgrid effects and the coupling of physics at different scales. Various subgrid approaches have been developed for modeling the effects of the small scales at Texas A&M. These techniques are successfully employed in various applications such as subsurface flow and transport, and coupling atomistic and continuum scales in materials.

Expected results.

- Development and study of multiscale simulation techniques for fluid-structure interaction problems with emphasis on porous media and filters (Y. Efendiev, P. Popov).
- Development and study of multiscale hierarchical techniques for flows and transport in highly heterogeneous porous media (Y. Efendiev, R. Ewing, P. Popov, G. Qin).
- Multiscale hybrid methods for coupling atomistic and continuum scales for simulation of fracture in brittle materials (J. Walton, J. Slattery).
- Multiscale modeling of active multifunctional materials and nano-composites for next generation smart vehicle concepts (P. Popov, D.C. Lagoudas, I. Karaman).
- Development and study of lower-dimensional mathematical models of meso- and nano-structures (Y. Efendiev, P. Kuchment, D.C. Lagoudas).
- Analysis of mathematical models of photonic crystal based devises, such as waveguides, beam splitters, PC slabs, and light slowing media (P. Kuchment).
- Spectral analysis of quantum graph models of quantum wire circuits and carbon and boron nanostructures (P. Kuchment, G. Berkolaiko, S. Fulling).
- Multiresolution techniques for image analysis (R. DeVore).

d. Computational statistics and predictive science

Motivation and impact. The ultimate goal of statistical modeling is to predict biological or physical events or the behaviors of engineered systems. These processes have uncertainties due to immeasurable or unknown factors, such as incomplete knowledge of the underlying biology, physics or due to the inherent nature of all models as incomplete characterizations of nature. It is natural to ask whether specific decisions can rely on the predicted outcomes of an event and how accurate are the predictions? What level of confidence can one assign a predicted outcome based on the observations?

Bayesian methods where model parameters treated as random are often used. Posterior distributions of the parameters quantify the uncertainty based on the available information. This approach provides the predictive distribution of the unobserved quantities with uncertainty bounds. Usually the models are complex and it is impossible to obtain the posterior or predictive distributions explicitly. We need to use Markov chain Monte Carlo (MCMC) based simulation tools which will be computationally demanding and can result in gigantic increases in the complexity of data volume, storage, manipulation, and retrieval requirements. Thus, efficient simulation techniques combined with fast uncertainty quantification techniques are necessary for robust and accurate predictions.

Research directions and state of the art. At Texas A&M, we have been working on various problems related to uncertainty quantification using hierarchical Bayesian techniques, MCMC based computation and stochastic perturbation methods. For example, we use our approaches for reliable predictions based on the dynamic data obtained at different scales. Examples are carbonate reservoirs, soil moisture predictions, and pollution tracking and identification of the source(s). In carbonate reservoirs, the challenge is to identify the location and distribution of “unswept” or bypassed oil and untapped “compartments” in the reservoir so that we can design “targeted” drilling or enhanced oil recovery schemes. Sophisticated Bayesian updating techniques help us in understanding the risk and the relative worth of different data in managing the risk. Bayesian modeling in bioinformatics is another active research area at A&M. Here we want to predict the chance of cancer for new patients based on observed genomic data. Developing gene selection, cancer classification and gene clustering models using gene expression data has been actively studied at A&M. Bayesian semi-parametric modeling and MCMC based computation are the basis of these developments.

Expected results.

- Development and study of hierarchical Bayesian models for parameter estimation and uncertainty quantification (Y. Efendiev, B. Mallick, A. Datta-Gupta, B. Mohanty)
- Polynomial chaos and collocation methods for uncertainty quantification of systems described by stochastic partial differential equations (Y. Efendiev, P. Popov)
- Development of novel network models to explore gene dependencies (B.Mallick, E. Dougherty)
- Data assimilation techniques (B. Mallick, Y. Efendiev, C. Douglas)

e. Computer science, dynamic data driven simulations and visualization

Motivation and impact. One of the most challenging problems in computer science is to create a comprehensive start to finish environment to create, use, and visualize problems and simulations that can be used by both expert computer scientists and by people with little or no computer science background. Problem solving environments have been created in the last 10-20 years. Flexible systems that run on a laptop, workstation, and all the way up to a Grid based parallel supercomputer need to be developed that non-experts can learn quickly and use efficiently are crucial to computational sciences and verifying the usefulness of new applied mathematics.

Research directions and state of the art. We will work in three different directions: (1) parallel algorithms, languages, environments, and hardware core design, (2) dynamic data-driven applications, and (3) visualization. Our expertise and interests are in methods to solve problems as fast as practical, visualizing problems and results, new ways of programming and comprehensive programming environments. Several CPU vendors allow designs for specialty computational elements (or cores) that can be added to standard computer cores in a short period of time, thus possibly producing ultra fast computing for specific problems of great interest to KAUST. Dynamic applications will create network of sensor based applications, similar to how the entire Saudi pipeline system has been modeled and run since the late 1970's, for many other problems that have been modeled haphazardly for decades and will provide self correcting predictions based on updated data instead of having to be run repeatedly with new, static data sets.

Expected results.

- Parallel algorithms (C. Douglas, R. Lazarov, J. Pasciak, V. Sarin).
- Languages and problem solving environments (N. Amato, C. Johnson, L. Rauchwerger, B. Stroustrup).
- Specialty computational elements (G. Qin, C. He, C. Douglas, R. Ewing).
- Dynamic data-driven applications (C. Douglas, Y. Efendiev, R. Ewing, R. Lazarov. W. Zhao, J. Henlder).
- Visualization techniques for one or more processors, locally or on a Grid (C. Johnson).

3.1.3 Interaction with KAUST

The proposed 5 core research areas well represent the frontier research in applied mathematics and computational sciences and also the research strength at Texas A&M University and our collaborators. The proposed research will be conducted in pairing with faculties and graduate students on KAUST campus to serve the purpose of training the younger generation in Saudi Arabia and enhancing KAUST's research capabilities.

3.2 Infrastructure: The Library of the Future

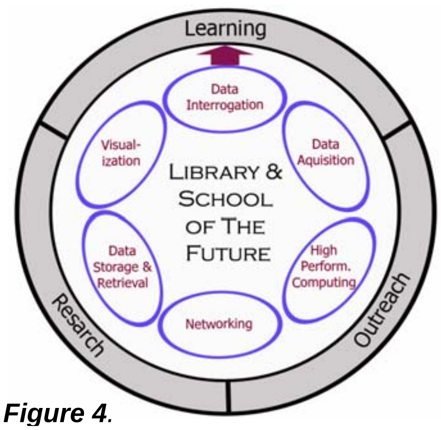

***Figure 4**.*

3.2.1. Motivation and Impact

As part of the IAMCS, we propose an infrastructure named "Library of the Future." This infrastructure integrates a set of facilities and tools to enable new knowledge generation from a wealth of digital data.

Effective scientific computation can only be achieved with access to large, fast, state-of-the-art computing facilities, networked at high speed to the emerging international cyber-infrastructure. Such a computing and network infrastructure will prove useful both to the proposed IAMCS and also to other KAUST Centers. This is shown, for example, by the National Center for Supercomputing Applications (NCSA), which serves as a major computational science center and also supports many U.S.-based researchers in such fields as astronomy, medical research, meteorology, and fluid dynamics.

We aim to build a strong balanced cyber-infrastructure to support the high-performance computing, networking, data storage, visualization and data interrogation, needs to the IAMCS, KAUST, and other KAUST Centers. Complementing the needed hardware facilities, we will develop new methodologies and integrate them into the facilities and tools required for knowledge creation and understanding from massive digital data across science and engineering.

3.2.2. Architecture and Features

Figure 4 shows the Library of the Future as a set of closely related infrastructure components embracing the IAMCS core focus areas. These components include:

- A high-performance computing facility with massive on-line storage
- Advanced visualization facilities
- High-speed connections to the international research network
- Highly skilled operations and advanced user support staffs
- Innovative 'Data Center' software to support the aggressive use of the infrastructure
- Strong, federated, identify, authorization, and authentication support
- Curriculum support to ensure effective infrastructure use

Key to this cyber-infrastructure is a holistic approach, stressing the integration of these components.

We recommend that KAUST create, at its main campus, a central supercomputer facility with world-class high-performance computing (at least 200 teraflops) and massive (at least 2 petabytes) online storage resources. This central facility would also require modern software to support massively parallel and data-intensive computation and secure sharing of data by researchers. We recommend that the IAMCS collaborate with KAUST and its centers to select the specific systems for this facility. We further recommend that this facility be connected to the international research network, either through the European Géant network or through the U.S. Internet2 network, at a minimum of 10 Gb/s. Of the essence is dependable network performance in support of large file transfers and collaboration support tools among KAUST and its centers.

Similarly, at the IAMCS, we propose a smaller, but compatible and interoperable high-performance computing facility with massive on-line storage. As with the central facility, the IAMCS computing facility will support massively parallel and data-intensive computation. We recommend that similar computing/storage facilities be located at other KAUST-related centers. The central facility and these smaller facilities would be connected as a grid, using modern grid software and the high-speed network connections described above. They would use coordinated scheduling, rotating around the world interactive periods for code development by students and researchers. There will be economic benefits in a group purchase and the common computing fabric will enhance interaction among KAUST and its centers.

Building on the IAMCS's existing Immersive Visualization Center, we will ensure that advanced visualization is a normative tool for our users. Advanced visualization studios, together with high-speed networking, can form the basis of effective video-conferencing and common viewing of scientific visualizations. Both will serve to facilitate the collaborations key to IAMCS/KAUST success.

Since Texas A&M is connected (via the Texas LEARN regional optical network) to the Internet2 network at 10 Gb/s, with the prospects for several parallel 10-Gb/s connections in the future, this would enable multi-Gb/s data flows between the KAUST facilities and those at the IAMCS.

The Library's computing, storage, network, and visualization facilities will be operated by highly-skilled staffs, complemented by an advanced users support team to ensure that our core science team is able to make effective use of the facilities.

The Library will include one key innovative software development, called the Data Center. This software structure, already prototyped and in use in the SCOOP hurricane science project here, supports software module reuse, separation of concerns in application development, and allows rapid reconfiguration of modules to respond to emergent demands. In its advanced support for modularity, the Data Center also facilitates collaboration on scientific software development.

The Library will deploy modern secure networking and data-sharing protocols, to ensure the integrity of research data and the appropriate limited access to it, while also maximizing dependable high-speed access to it. Key to this will be the next generation of virtual organization middleware, including federated identity, authentication, and authorization technologies such as Shibboleth and Grouper. We recommend that this be done at KAUST, at IAMCS, and at other key KAUST centers to facilitate collaboration and security.

3.2.3. Timetable and Deliverables

The Library of the Future will require many parallel efforts. All will generally begin in Year 1, but deliverables will be achieved at different times:

- By the end of Year 1, the IAMCS and KAUST will select specific architectures for the high-performance computing and on-line storage facilities. The facility at IAMCS will be acquired and deployed to serve users at the IAMCS, at KAUST, and at KAUST-related centers. The fiber-optic connection of KAUST to the international research network will be designed and deployed. Scientific computing collaborations using these networked facilities will be initiated.

- By the end of Year 2, strong federated identity, authorization, and authentication software and operations will be deployed. Video-conferencing and common viewing of scientific visualizations will become routine.
- By the end of Year 3, selected scientific computing projects will be supported via the Data Center project.
- During Year 4, the high-performance computing facility at IAMCS will be refreshed.
- By the end of Year 5, a broad set of scientific computing projects will be supported via the Data Center project.

In every phase, we will collaborate with KAUST, transfer the technology, deploy the system at KAUST, obtain feedback, and guide Library evolution in response to KAUST priorities.

3.3 The School of the Future

3.3.1. Motivation and Impact:

The IAMCS “School of the Future” will focus on providing quality, multi-disciplinary learning opportunities combining state-of-the-art technologies with hands-on experiences.

The guiding principles for the IAMCS School of the Future should address two critical challenges (1) Quality of Access, and (2) Pervasiveness of Access.

Several significant items must be considered in the development of a system that will coordinate courses and academic programs at different, and/or multiple, institutions are significant. Time is probably the most critical limiting factor for educators and administrators. In order to ensure success for IAMCS it will be necessary to create a platform that is efficient and that supports: (1) effective time management, (2) effective teaching and program development, and (3) seamless and easy use for all audiences including: students, faculty, research staff and administrators. Additionally, this collaboration network needs to create a productive working environment and one that promotes communication.

a. Guiding principle 1: quality of access

To achieve the highest quality education, we have been working on learning tools that assist instructors to: (1) Provide rigorous, quality and engaging educational experiences to students from around the globe, (2) Provide students and educators seamless access to the tools and resources that are state-of-the-art in applied mathematics and computational science, (3) Provide students easy access to data and computational support for manipulation, conversion and modeling of data, (4) Support efficient and effective communication and collaboration and exchange between educators, students and institutions, and (5) Push innovative and engaged learning experiences via cutting-edge learning technologies and hands-on, real world experiences in the laboratory and through collaboration with industry.

b. Guiding principle 2: pervasiveness of access

A key to success for a multi-disciplinary, multi-institutional endeavor like the School of the Future will be to coordinate and meld the relationships between the various institutions. Three fundamental aspects of business alliances that apply to higher education: (1) Successful alliances yield benefits for the partners and evolve progressively in there possibilities, (2) Successful alliances involve collaboration rather than mere exchange, (3) Successful alliances are supported by a dense web of interpersonal connections and infrastructures that enhance learning; they cannot be controlled by formal systems.

3.3.2 Architecture and Features:

Our aim for the School of the Future will be to evolve and expand existing collaboration, networking and distance learning capabilities. We are aware that there are numerous tools and systems that are available for effective distance education. We observe, however, that these tools tend to be disparate and not combined to provide a complete learning solution.

We will use existing capabilities but also improve on them, initially by using the techniques outlined below. At the outset, consider that students are "fluent" and totally adapted to an online environment. Thus, our ultimate audience is well prepared to utilize the resources and platform (Internet) that we intend to use. They should also be instrumental in our efforts to extend our impacts and capabilities. Important features to provide users include: (1) multi-mode distance learning/teaching and support capabilities supporting communication, video-conferencing and document/presentation shared mark-up, (2) virtual environments (adapting gaming environments for more immersed user experiences), (3) team and project coordination tools (e.g., calendar and course projects), (4) user feedback, and (5) student performance evaluation and testing.

A primary challenge of the IAMCS School of the Future will be to develop an effective educational management infrastructure that supports student access to courses and program degrees from collaborating institutions and joint degrees when appropriate. Additionally, adequate computational capabilities and infrastructure will be a critical element for success.

Since IAMCS will focus on applied mathematics and computational sciences, the areas of disciplinary specialization highlighted in Section 3.1 are of primary concern. Preliminarily the School of the Future will provide the following: (1) virtual classrooms, (2) virtual laboratories, (3) discussion boards, chat rooms, and other communication platforms, and (4) tools supporting distance collaboration and project management. Drawing from the experiences of several distance education programs at A&M (e.g., CLASS) and interdisciplinary degree programs (e.g., IGERT, CSCP) we will identify the appropriate avenues for creating a robust set of courses and degree programs utilizing the strengths of our partner institutions.

3.3.3 Bridging Technology to Experiential Learning:

An interesting dichotomy is taking place where technology might appear to be leading students away from the real world into "virtual worlds". This would seem to conflict with real-world learning experiences, but the reality is that hands-on experiential learning is also on the rise. Here at Texas A&M we see this as an exciting opportunity to create a synergy between these two expanding realms. There are innumerable examples across the A&M campus of students that are gaining access to new technologies that are grounded in addressing real world problems. Here we will briefly mention three.

The Immersive Visualization Center (IVC): Featuring a 25' x 8' semi-rigid, rear projected, curved screen, the IVC facilitates the 3-dimensional imaging of very large datasets from a diverse set of disciplines. Geophysics, life and physical sciences, engineering, and architecture are all able to gain a better understanding of their research by taming the complexity of their data through visualization. Researchers, students and faculty can utilize this new visualization platform for gaining novel perspectives of their work. Increased awareness of the IVC is being supported by student competitions that have showcased a vast array of projects including, but not limited to, cutting-edge geospatial research to new gaming/virtual imaging.

The Virtual Network Engineering Laboratory (VNEL): Funded by the National Science Foundation, VNEL can remotely manipulate equipment and conduct well-defined problem-solving exercises in a controlled high-fidelity environment via the Internet using Web browsers. VNEL enables instruction to be efficiently and effectively distributed across geographic regions, thereby reaching greater numbers of students than would be possible through traditional face-to-face or on-site laboratory instruction. Moreover, this interactive learning environment has already been proven to reduce costs and increase facility use among university students.

AggieSat Lab, A&M Aerospace Engineering: Established in 2005 and epitomizing collaborative learning initiatives at A&M, the AggieSat lab has arch sports rivals Texas A&M and the University of Texas working on a joint project to send two satellites into space. Cooperation is paramount since the two teams of students (each from rival schools) are responsible for launching a satellite that will dock with the other in space. Students of all experience levels (freshman through PhD) and from 18 different majors (from engineering to business to science and mathematics to liberal arts) have participated. Students are working in a lab and actually constructing the vehicles, getting hands-on experience with tools in a demanding collaborative environment.

Just these three examples highlight tremendous opportunities to expand students applied learning experiences while in school. Access to state-of-the-art technologies and real laboratories provides students with an engaging learning experience. This also creates a natural bridge to industry. In fact, the impetus for the AggieSat lab was the lab manager's experience with the US Air Forces Experimental Satellite program. He was often faced with the challenge of having to train recent graduates for two years before they had adequate applied skills to work on projects.

As highlighted in Section 3.1.2, we have significant connections to industry. The three learning and technology projects under Texas A&M to support virtual and distance learning establish a natural bridge to industry. Creating connections to industry and communities through internships, joint collaborative projects and service experiences will enhance the IAMCS ARC impact in student's lives and with the world at large.

3.3.4 IAMCS Graduate Degree Program (GDP)

Based on existing programs at Texas A&M (IGERT, CSCP, CLASS) we will develop a new interdisciplinary graduate degree program combining our strengths in applied mathematics, statistics, and computer science with its research focus on solving applied problems.

There are two ways that GDP will be unique from other programs. The first is its integrated multidisciplinary character. Students will have two co-advisers, one being an IAMCS mathematics, statistics, or computer science faculty member and the other can be chosen from any other IAMCS collaborating department outside the core. This will afford students a broader perspective and allow them to learn to work in a situation similar to the real world. The program will require that students do extensive coursework outside the core IAMCS disciplines.

Secondly, students will be able to draw from a pool of advisors, disciplines and research from our partnering institutions. Actual research activities will be conducted here at Texas A&M and ultimately KAUST, but may be co-directed from a leading academic or researcher from another institution in another state or country, potentially through existing Memorandum of Agreements or MOA's (e.g., with the universities of Paris 6, Kaiserslautern, and Mexico).

a. Curriculum

The IAMCS multidisciplinary program will provide a broad-based enhancement to a student's degree(s) and the learning experience he/she will need to be a leader in his/her chosen field. Since the IAMCS has such a broad base of expertise across mathematics, statistics and computational science, a unique curriculum will be developed for each student dependent on his/her particular interests and educational goals. Curriculum will consist of core IAMCS sciences courses and courses in various application areas.

b. Research

IAMCS will serve as a platform for students to participate in multidisciplinary research under the following disciplines: applied mathematics, data management, mathematical modeling, numerical methods, computer simulations and visualization. Students will be rotated between research groups to provide them exposure to a broader array of research activities. A dynamic result of these new interdisciplinary research programs will be expanded inter-collaboration between students and advisors. This added benefit provides a much more dynamic and robust exchange between students, scholars and institutions. This dynamism will also enhance recruiting and IAMCS connection to industry.

c. Recruitment and selection of students

We have found that inter-institution collaboration leads to recruitment of high caliber students. Because relationships have been pre-established, students are better prepared for graduate programs. Professors who are already collaborating know the students, including their strengths, capabilities, challenges and can provide solid recommendations. This "pre-paving" provides a smooth transition for students and allows them to begin their coursework and identify a preliminary focus for their research. Due the extended reach of our network for IAMCS, we anticipate recruiting to be a relatively routine task. This will be supported through MOA's between collaborating institutions. Additionally, we will conduct other forms of promotion via the IAMCS Web site and traditional methods for recruiting students. Students for this program will be expected to be top-tier students. Marketing and recruiting techniques will be adapted from the existing interdisciplinary programs already being offered here at Texas A&M and our collaborating institutions.

3.3.5. Timetable and Deliverables

In the first year IAMCS will provide an aggressive advertising campaign with intentions of having an entering class of approximately 10 graduate students. These all will be supported by IAMCS with scholarships named after KAUST. Below is a table with the expected number of graduate students that will be supported under the auspices of the KAUST IAMCS.

Year	***1***	***2***	***3***	***4***	***5***
Number of KAUST Graduate Students	10	12	14	14	16

In the first academic year the students will go through rigorous education and training (classes, projects, labs) in the area of applied mathematics, statistics, and computational science. This program will be combined with existing classes in the departments of mathematics, statistics and computer science and a set of new classes, depending on identified interdisciplinary research areas, (e.g., scientific computing with finite elements, parallel computing, data assimilation, stochastic methods in mathematical modeling, multi-scale and multi-physics methods) will be developed and offered.

In the second year the students will begin their research with a supervising faculty and will form a committee for their degree. For an MS degree, we expect the student to write a thesis. For a PhD degree, we expect the students to pass qualifying examinations, identify the area for research, form a committee, and file a degree plan within 2-2.5 years from the admission.

Through our collaboration and interaction with industry we expect each PhD student to have a summer internship with one of our industrial or academic partners, or in a national laboratory. We expect completion of Masters degrees in 2-2.5 years and PhD degrees in 4.5-5 years.

3.3.6. Capabilities and Preliminary Work

The participating faculty members from Texas A&M have a very strong record of training and supervising MS and PhD students. They have advised and supervised more than 150 PhD students and 300 Master students.

3.3.7. Interaction with KAUST

The interaction with KAUST will be done in the following directions:
(1) Recruitment of qualified students from KAUST for the Texas A&M MS and PhD programs
(2) Exchange of students (for one or two semesters), a practice already in place with the University of Kaiserslautern and Ulm (Germany)
(3) Joint KAUST/Texas A&M course and labs development in areas of common interest.

3.4. Mirror

The proposed research will be conducted in pairing with faculties and graduate students on KAUST campus to serve the purpose of training the younger generation in Saudi Arabia and enhancing KAUST research capabilities.

3.4.1. Motivation

The IAMCS and KAUST should work jointly so that both KAUST and Texas A&M are at the cutting edge and state of the art in research and development in applied mathematics, computational and traditional sciences, and technology. While MIT, Caltech, the Ecole Polytechnique, and Tsinghua University are widely regarded as world-class science and technology academic centers, the original model of a graduate only school at the University of Chicago in the 1890's offers a better template on which to improve. While Chicago had traditional divisions and departments, KAUST will have multidisciplinary centers that can quickly focus on new as well as traditional problems arising in science and technology. IAMCS will focus on the providing impact as follows.

3.4.2. Expected Results and New, Common Infrastructure.

- Rapidly initiate and expand world class and university-based research in areas of applied mathematics, science, and engineering central to KAUST's mission of contributions to the Kingdom, region, and world.
- Common, new courses whose focus and content can change quickly for emerging technologies.
- Establish close working relationships between KAUST and world class research institutions, industrial partners, scientists, and engineers throughout the globe. Technology transfer to and from industry is key to usefulness in applied multidisciplinary research and demonstrating the usefulness of the new KAUST organizational approach.
- A common computing infrastructure that is Grid enabled and optimized for high-performance data-intensive scientific computation.
- Develop a common set of international conferences and smaller workshops showcasing research of interest to KAUST and IAMCS.
- Disseminate results quickly from IAMCS and KAUST to the world. Outside people will learn the needs of the Kingdom and KAUST members will be able to interact with outsiders quickly and easily. A KAUST-owned and -operating publishing house should be considered.

4. Collaboration with Industry

Traditionally, corporate and academic research have different goals and carry out different missions. Corporate research is usually considered a profit center and is focused on business and customer needs so that the research and development can contribute to the bottom line. Therefore, corporate research is rarely risky and instead has clear success potential. Academic research is focused on innovations and grand challenges that address long term societal needs and is willing to attempt risky research. It also carries the educational mission to train a younger generation to be creative. However, corporate and academic research needs go hand-in-hand. Industry and academic need to understand each other to efficiently carry out their research missions in terms of effectiveness, efficiency, professional training, and education. With a well balanced funding mechanism, the proposed IAMCS will have the infrastructure and organizational structure to create the synergy for industry and academics to work together successfully. The key to success is effective communication between both groups.

The multi-disciplinary group of researchers at Texas A&M has, besides their excellent academic research records, long time research collaboration with industry, many of whom also have industrial working experience. The multi-national corporations which are listed in Section 3.1.2, such as Exxon Mobil, Saudi Aramco, Sinopec, Hewlett-Packard (HP), and Computer Modeling Group (CMG) have supported academic research programs at a number of universities in various ways that include unsolicited research awards, consortium, infrastructure support, and faculty and student support. Texas A&M has had a long term research collaboration with several corporations that has proven mutually beneficial to both the university and industry.

Over a number of years, Exxon Mobil has invested millions of dollars in research programs at Texas A&M. Sinopac and Saudi Aramco have invested nearly a million dollars each in the past in Texas A&M. Hewlett-Packard and CMG have invested millions of dollars each into two of our key partner researcher's programs. Most of these have been *unsolicitated* funds.

One particularly successful example is the research collaborations with the Upstream Strategic Research Center at Mobil Technology Company and then Exxon Mobil Upstream Research Company and the Institute for Scientific Computation (ISC). The outcome of this research partnership has been significant and mutually beneficial. Through this decade long research partnership, ISC has had *unsolicited* industry funding to work on development of advanced numerical methods that enhances the joint research capability of both parties and has supported graduate student training. The company efficiently leverages the university's research capabilities to help its internal research and development. Moreover, it helps create graduate student pipelines for its own workforce.

Based on a series of successful industrial collaborations, the IAMCS will strengthen and expand its existing industry research collaborations by fostering interactions between faculty and corporate experts. We will continue to reach out to industry so they understand our research programs and we understand their critical issues. We anticipate a strong industry response to the proposed research center in financial support as well as in graduate student recruiting.

BIOGRAPHICAL INFORMATION SUMMARY

We have an outstanding team of scientists and engineers from Texas A&M, other U.S. Universities, and Foreign Institutions. We have worked with all of these researchers, including extensively with most. The PI has been PI on several highly-funded multi-institutional interdisciplinary grants and contracts, supported by many millions of dollars. There are joint publications involving pairs or more of most of the team members. We already have a strong existing network connecting many strong research centers and researchers from around the globe that we can tie into the developing KAUST research network.

Of our team, Economides, Junkins, and Straustrup belong to the National Academy of Engineers, DeVore is in the American Academy of Arts and Scientists, Ewing is in Academia Europea, and Espedal belongs to the Norwegian Academy. Among the on-campus team, Ewing, Carroll, Junkins, and North are Distinguished Professors and 15 of our team hold endowed chairs or professorships. We have strong groups in mathematics, computer science, statistics, science, and engineering and outstanding educators.

CURRENT AND PENDING SUPPORT

Each of the investigators and collaborators that will receive funding from IAMCS have confirmed that they are willing to spend the proposed amount of time with the Center and its research and education. The main leaders of the various aspects of the center will receive 2 months of support/year wih most of the rest 1 month/year. We will include full current and pending support information for all in our final proposal.

BUDGET JUSTIFICATION SUMMARY

Because the mission for the KAUST IAMSC is to be a "World Class Center of Excellence" in research and education, the budget emphasizes personnel costs. We budgeted for 25 faculty from Texas A&M and several consultants (6 from other U.S. institutions and 4 from abroad) to strengthen existing ties to strong research centers worldwide. We will also fund 10 graduate students, 8 postdocs, and 4 staff to support infrastructure applications, and administration. International academic collaborations include Fraunhofer Institute (Germany), University of Calgary (Canada), University of Stuttgart (Germany), University of Heidelberg (Germany), University of Bergen (Norway), LNCC (Brasil), Bulgarian Academy of Sciences (Bulgaria), Peking University (Beijing), and Utrecht University (Netherlands). U.S. academic collaborations include the following universities: Kentucky, Utah, Princeton, Purdue, Penn State, Stanford, South Carolina, Texas, Rensselaer Polytechnic Institute, Montana State, Louisiana State, North Carolina, William and Mary, Florida, Miami, Caltech, Alabama-Huntsville. Travel will occur primarily between Texas A&M and U.S. Institutions with some international travel. Travel costs will allow us to network effectively among our colleagues.

We have included conservative expenditures in years 1 and 4 to significantly leverage existing cyber-infrastructure capabilities. We hope to match the KAUST IAMCS hardware capabilities as it develops. IAMSC will also require significant software capabilities for effectively coordinating access to the Library and School of the Future. We have included realistic expenditures in years 1 through 4 for developing customized state-of-the-art educational and networking software and systems. We will increase our support to graduate students to 16 in year 4.