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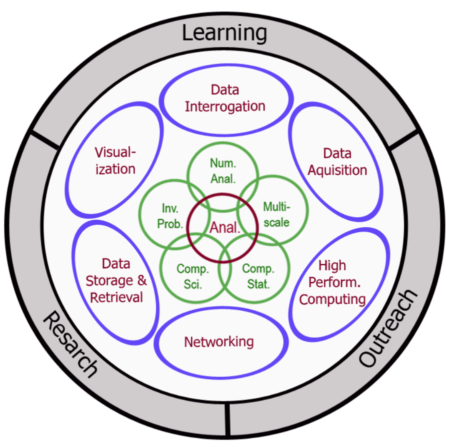
PROJECT DESCRIPTION

1. Rationale and Vision

As the 21st Century begins, Scientific Computation has emerged as a third paradigm for scientific research, joining the established approaches of Analysis and Laboratory Experimentation (see Figure 1). To predict the behavior of phenomena or to optimize a process, one normally must build some type of mathematical model to help in determining and describing the behavior. 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 complex, coupled phenomena. Figure 1: General Concept



To ensure that this Scientific Computation paradigm become a major strength of KAUST, Texas A&M University proposes the Institute for Applied Mathematics and Scientific Computation (IAMSC). We envision establishing a unique state-of-the-art, multidisciplinary Computational Laboratory and a supporting infrastructure to enable large-scale scientific computation to addressing a large number of applications in diverse areas of science and engineering of interest to Saudi Arabia and the world. This computational laboratory begins with a multidisciplinary core of applied mathematicians, statisticians, and computer scientists, which will be supported by state-of-the-art hardware and software infrastructure. This core group is strongly connected to excellent colleagues and research centers in diverse application areas and around the world. Working together, they can produce a unique multidisciplinary international research and education institute. KAUST students will be able to expand their horizons enormously in this virtual learning environment. We will then mirror this unique computational laboratory infrastructure and multidisciplinary educational capability to Saudi Arabia to assist in the development of KAUST.

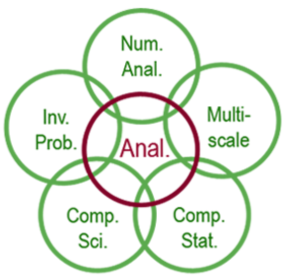
2. Strategy for Success

We propose to expand our existing Institute for Applied Mathematics and Scientific Computation 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 Math Group at Texas A&M: Center for Scientific Computation
2) Infrastructure: The Library of the Future
3) Education: The School of the Future
4) KAUST-A&M Collaboration: The Mirror

2.1 A Core Applied Mathematics Group at Texas A&M: Institute for Applied Mathematics and Scientific Computation (IAMSC)

2.1.1. The core research areas



The 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 environmental sciences, multiscale analysis and simulation methods and their applications, computational statistics and chemistry as well as computer science.

In 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 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, V. Sarin).

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 a substantial progress has been achieved in developing flexible methods, that preserve the natural properties of the physics (e.g., local mass conservation, monotonicity, and global energy conservation) and that are accurate and stable. Accurate and efficient numerical techniques are crucial for reliable predictions of physical and environmental systems.

Research directions and state-of-the-art. We will work on three different 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 method 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 practical implementation of adaptivity revolves around the paradigm “solve (the system) - estimate (the error) - refine (the mesh)”. 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*. Our team will focus on projects outlined below.

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 and their application (B. Popov, J.L. Guermond, Y. Efendiev, R. Ewing, P. Popov).

● Develop efficient and reliable local error estimators (or indicators) for convection-diffusion equations, Stokes and Navier-Stokes equations and develop grid refinement strategy that is inexpensive, 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 so called inverse problems, i.e. problems where the parameters of a system that is inaccessible (non-transparent) 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 are, for instance, problems of geophysics, reservoir characterization, and medical tomography, where external signals (X-rays, ultrasound, electromagnetic waves, etc.) are used to trigger a response that would reveal the internal structure of the patient's body. 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 also well established that inverse problems are extremely challenging in terms of their instability with respect to measurement and hardware errors, 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 have known to be valid for limited spatial and temporal scales. Conventional methods can not 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, for example, in astrophysics, atmospheric science, geological sciences, and etc. 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 TAMU 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, turbulent flows, and etc. Multiscale analysis and simulation require understand subgrid effects as well as coupling of physics at different scales. Various subgrid approaches have been developed for modeling the effects of the small scales and these techniques are successfully employed in various applications. For examples, subgrid capturing schemes in porous media are used to avoid empirical upscaling techniques. A new theory of fracture which extends continuum models to the molecular scale in the neighborhood of fracture surfaces and edges has been studied in TAMU. In this proposal, we will focus on various areas as outlined below.

Expected results:

● Development and study of multiscale simulation techniques for fluid-structure interaction problems with emphasis on porous media, filters and etc. (Y. Efendiev, P. Popov)
● Development and study of multiscale hierarchical techniques for porous media 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 materials and nano-composites for next generation aerospace vehicles (P. Popov, D.C. Lagoudas, I. Karaman)
● Development and study of lower dimensional mathematical models of meso- and nano-structures, e.g. photonic crystals. Analysis of mathematical models of photonic

crystal based devises, such as waveguides, beam splitters, PC slabs, light slowing media, etc. (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 (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 our 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 base don the observations?

We will use Bayesian methods where model parameters are treated as random. Posterior distributions of the parameters quantify the uncertainty based on the available information. This approach will provide the predictive distribution of the unobserved quantities with uncertainty bounds. Usually the models are complex and it is not possible 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 TAMU, 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 etc. 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 understanding the risk and the relative worth of different data in managing the risk. Bayesian modeling in bioinformatics is another active research area in TAMU. 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 have been actively studied at TAMU. Bayesian semi-parametric modeling and MCMC based computation are the basis of these developments. We will focus on various areas as outlined below.

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. Daugherty)

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 on 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. Our team will focus on the projects outlined below.

Expected results:

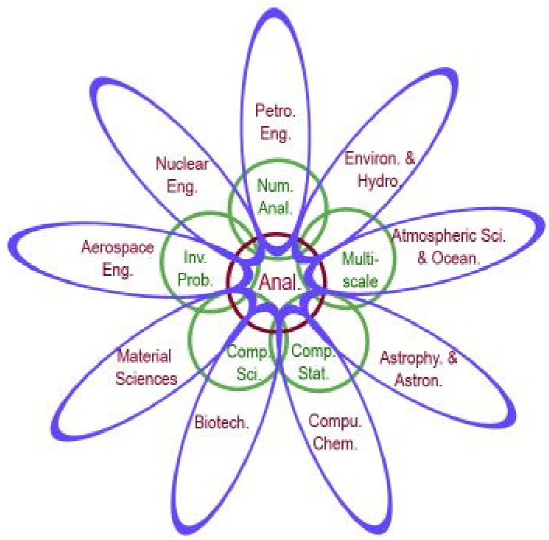
- Parallel algorithms (C. Douglas)
- Languages and environments (N. Amato, L. Rauchwerger)
- Specialty computational elements (G. Qin, C. He, C. Douglas, and R. Ewing)
- Dynamic data-driven applications (C. Douglas, Y. Efendiev, R. Ewing, R. Lazarov)
- Visualization techniques for one or more processors, locally or on a Grid (C. Johnson)

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. The proposaed research will be conducted in pairing with faculties and graduate students on KAUST campus to serve the purpose of

traning younger generation in Saudi Arabia and enhancing KAUST research capability.

2.1.2. Impact of core research to applied science and engineering

Reach out to industry and applications national, and international wide. ?



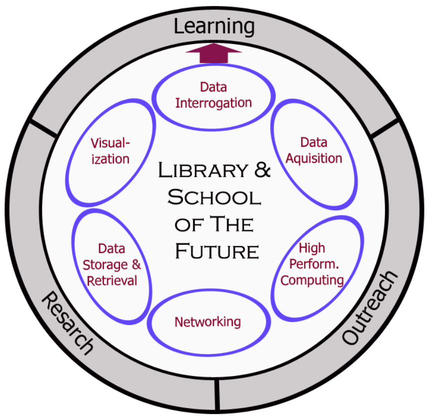
The proposed research center will be built on an existing research centers at Texas A&M University In the past years, these centers have build and maintain a rich and active research collaborations with industry and academic research institutions. Corporate research collaborations include ExxonMobil, Sinopec, Chevron, Hewlett-Packard, Saudi Aramco, Computer Modeling Group (CMG). 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), Bedford Institute of Oceanography (Canada). U.S. academic collaborations include the following universities: Kentucky, Utah, Princeton, Purdue, Penn State, Stanford, Louisiana State, North Carolina, William and Mary, Florida, Miami, Caltech, Alabama-Huntsville.

The core research will play an important role in various application areas which are shown in Figure 2. Through working with engineering researchers in various disciplines, the core research will be extended to address some critical issues that are address some critical issues that are related to atmosphere, ocean, land subsurface, materials and bio-technologies. In particular, we will collaborate in the following research areas:

- Large scale computer simulation for oil reservoirs (R. Ewing, G. Qin, Y. Efendiev, R. Lazarov, A. Datta-Gupta, J. Douglas, Z. Chen, industry)
- Subsurface flows in vadoze zone and soil moisture data assimilation (Y. Efendiev, B. Mohanty)
- Data assimilation in atmospheric sciences and 4D-VAR (B. Mallick, Zhu)
- Computational material sciences (P. Popov, Y. Efendiev, D.C. Lagoudas)
- Computational radiation transport (G. Kanschat, M. Adams, J. Morel, J. Ragusa)
- Bioinformatics and biostatistics (B. Mallick. R. Carroll)
- Biomechanics and tissue modeling (J. Walton, J. Humpherey)
- Contaminant transport in atmosphere and subsurface (R. Lazarov, R. Ewing, Y. Efendiev, H. Zhang)
- Computational chemistry (M. Hall)
- Combination of different kinds of genomic data for cancer prediction (B. Mallick)

- Numerial well testing in heterogeneous petroleum reservoirs (C. Ehlig-Econmide, G. Qin)
- Computational chemistry (M. Hall)
- Flows in high porosity media with complex microstructure such as metal foams (O. Iliev, Y. Efendiev, P. Popov, R. Ewing)
- Geological sequestration of CO2 (G. Qin, M. Celia, R. Ewing)
- Modeling of contaminant transport in heterogeneous aquifers (R. Helmig, R. Ewing, Y. Efendiev, G. Qin)
- Compositional models for multi-phase flow and transport (M. Espedal, G. Qin. R. Ewing)
- Atmosphere and ocean modeling of tropical cyclones (G. Creager)
- Computational climate forecasting and uncertainty assessment (Ping, Saravanan, Mallick)

2.2 Infrastructure: The Library of the Future



2.2.1. Motive and Impact

As part of the IAMSC, we propose an infrastructure named "The 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 cyberinfrastructure. Such a computing and network infrastructure will prove useful both to the proposed IAMSC, 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 cyberinfrastructure to support the high-performance computational, data, networking, and visualization needs to the IAMSC, KAUST, and the 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.

2.2.2. Architecture and Features

Figure X shows the Library of the Future as a set of closely related infrastructure components embracing the IAMSC 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, and
- Curriculum support to ensure effective infrastructure use.

Key to this cyberinfrastructure 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 IAMSC 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 at least 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 IAMSC, we propose a smaller, but compatible and interoperable high-performance computing facility with massive on-line storage. As with the central facility, the IAMSC 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 IAMSC's existing Immersive Visualization Center, we will ensure that advanced visualization is a normative tool for our users.

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 IAMSC.

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 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 IAMSC, and at other key KAUST centers to facilitate collaboration and security.

2.2.3. 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 IAMSC and KAUST will select specific architectures for the high-performance computing and on-line storage facilities. The facility at IAMSC will be acquired and deployed to serve users at the IAMSC, at KAUST, and at KAUST-related centers. The 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.
- 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 IAMSC 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.

2.3 The School of the Future

2.3.1. Motive and Impact: The focus of the IAMCS School of the Future will be to provide quality multi-disciplinary, learning opportunities utilizing state-of-the-art technologies in combination 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.:

Items that need to 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 In order to achieve the highest quality educational experience, we have been working on learning tools that assist our 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 of knowledge and ideas with ease 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 IAMCS Virtual School will be to coordinate and meld the relationships between the various institutions. Rosabeth Moss Kanter (1994) identified three fundamental aspects of business alliances that apply to higher education: a) Successful alliances yield benefits for the partners and evolve progressively in there possibilities, b) Successful alliances involve collaboration (creating new value together) rather than mere exchange (getting something back for what you put in), c) Successful alliances are supported by a dense web of interpersonal connections and infrastructures that enhance learning; they cannot be controlled by formal systems.

2.3.2 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. However, our observation is that these tools tend to be disparate and not combined to provide a complete learning solution.

We intend to utilize existing capabilities but also to improve on them, initially by using the techniques outlined below. At the outset, an important realization is 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, course projects, etc.), 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 2.1 are of primary concern. Preliminarily the IAMCS Virtual School 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 TAMU (e.g. CLASS[1], CAPSO[2]) and interdisciplinary degree programs (e.g. IGERT[3], CSCP[4]) we will identify the appropriate avenues for creating a robust set of courses and degree programs utilizing the strengths of our partner institutions.

2.3.3 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 TAMU 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 NSF, VNEL can remotely manipulate equipment and conduct well-defined problem-solving exercises in a controlled high-fidelity environment via the Internet using their Web browsers. VNEL enables instruction to be efficiently and effectively distributed across geographic regions, thereby reaching greater numbers of students, including traditionally underrepresented 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, TAMU Aerospace Engineering: Established in 2005 and epitomizing collaborative learning initiatives at TAMU, 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 and 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 a rounded and 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 2.1.2, we have significant connections to industry. The three cited TAMU examples of applied learning and technology to support virtual and distance learning, establishes 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.

2.3.4. IAMCS Applied Research & Collaboration (ARC) Certificate/Degree

Based on existing programs at Texas A&M (IGERT, CSCP, CLASS) we will develop a new interdisciplinary graduate degree program where core research focuses heavily on solving applied problems.

There are two ways that ARC is 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. ARC will require that students do extensive coursework outside the core AMCS disciplines.

Secondly, students participating in ARC 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, but may be co-directed from a leading academic or researcher from another institution in another state or country, potentially through existing MOA with Paris 6, Kaiserslauten, and Mexico.

a. Curriculum: The IAMCS ARC multidisciplinary program will provide a broad-based enhancement to student's degrees and the intellectual tools they will need to be leaders in their 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 some application areas.

b. Research: IAMCS will serve as a platform for students to participate in applied multidisciplinary research under the four disciplines of scientific computation: data management, mathematical modeling, numerical solutions 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 and applied research focused programs has been expanded inter-collaboration between student's and their advisors. This added benefit, beyond student collaboration, 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 the recruitment of the highest caliber students. Because relationships have been pre-established, students are better prepared for a program like the ARC Certificate. Professors who are already collaborating know the students, 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 already identified for IAMCS, we anticipate recruiting to be a relatively mundane task. This will be supported through MOA's between collaborating institutions. Additionally, we will also conduct other forms of promotion via a Web site and other traditional methods for attracting students. Students for this program will be expected to be top-tier students, so a set of qualifications will be identified. These practices likely will be adapted from our existing interdisciplinary programs already being offered here at Texas A&M.

2.3.4. Timetable and Deliverables

2.3.5. Capabilities and Preliminary Work

2.3.6. Interaction with KAUST

2.4. Mirror

2.4.1. Motive.

The IAMCS and KAUST should work to jointly make KAUST, which will improve Saudi Arabia, and Texas A&M so that both 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 top tier science and technology academic centers of the world, the original model of a graduate only school at the University of Chicago in the 1890's offers a better example of what to improve on. Whereas 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.

2.4.2. 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.
- 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 pursued.

3. Collaboration with Industry

Traditionally, corporate and academic research have different goals and carry different missions. Corporate research is focused on the business needs so that the research and development can help business competitiveness. Therefore, the corporate research is likely with clear application potential. On the other hand, academic research is focused on innovations and grand challenges that address societal needs. It also carries the educational mission to train young generation to be creative. However, corporate and academic research needs go hand-in-hand. Because industry and academic need to well understand each other to efficiently carry out their own research missions in terms of effectiveness, efficiency, professional training and education. With well balanced funding mechanism, the proposed research center will have the infrastructure and organizational structure create the synergy for industry and academic work together. The key to the success is to the effective communication between industry and academic.

The group of multi-disciplinary researchers at Texas A&M University has, beyond their excellent academic research records, long time research collaboration with industry people and a lot of them also have industry working experience. One successful example is the long time research collaborations with Upstream Strategic Research Center at Mobil Technology Company and then Exxon Mobil Upstream Research Company and Institute for Scientific Computation (ISC). Outcome of this research partnership is huge and mutually beneficial. Through this almost 10 year research partnership, ISC has the unsolicited industry funding to work on development of advanced numerical methods that enhances its research capability and graduate student training. The company efficiently leverages the university research capability to help its internal research and development. Moreover, it helps create graduate student pipelines for its workforce development.

Based on this successful experience, the proposed center will stress on the link between industry and academic to achieve their goals in an efficient manner.

4. Organization and Infrastructure.

The Institute for Applied Mathematics and Scientific Computation (IAMSC) has been formed from a combination of four interdisciplinary centers that have provided scientific computation leadership at Texas A&M University:

- the Institute for Scientific Computation (ISC) (http://isc.tamu.edu), established in 1985,
- the Center for Statistical Bioinformatics (CSB) (http://statbio.stat.tamu.edu),
- the Alliance of Bioinformatics, Computational Biology, and Systems Biology (ABCS), and
- the Center for Large-Scale Simulations (CLASS).

Each of these centers is an interdisciplinary group of A&M faculty from applied mathematics, statistics, computer science, science, or engineering with research expertise in scientific computation. IAMSC forms 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 a computational laboratory, as proposed.

Each of the centers have existing interdisciplinary educational programs described in the various web sites. 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. The university has substantial additional large-scale HPC and grid computing capabilities through HiPCaT and SURAgrid. The requested computer will leverage the purchase of a large Linux cluster to complement our existing large IBM cluster and grid.

BIOGRAPHICAL INFORMATION SUMMARY

CURRENT AND PENDING SUPPORT

BUDGET SUMMERY

BUDGET JUSTIFICATION SUMMARY